Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:10 PM UTC

PDB ID	:	2G82 / pdb_00002g82
Title	:	High Resolution Structures of Thermus aquaticus Glyceraldehyde-3-Phospha te Dehydrogenase: Role of 220's Loop Motion in Catalysis
Authors	:	Jenkins, J.L.; Buencamino, R.; Tanner, J.J.
Deposited on	:	2006-03-01
Resolution	:	1.65 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 ⓘ 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 ⓘ) were used in the production of this report:

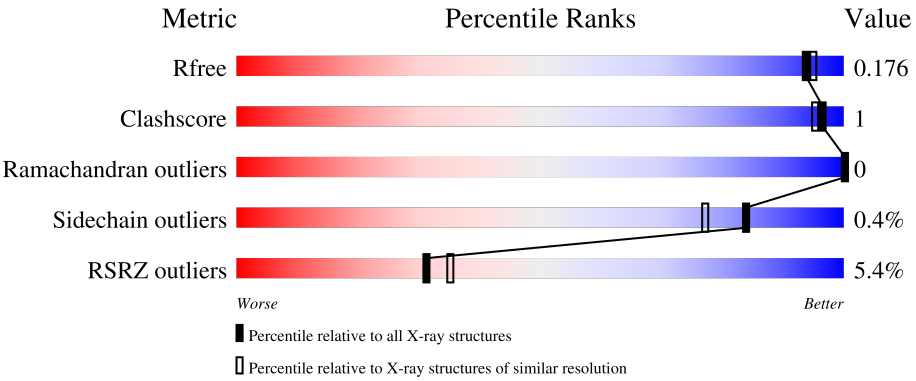
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.65 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.



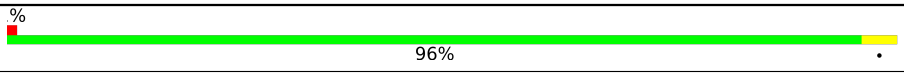
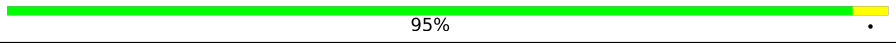
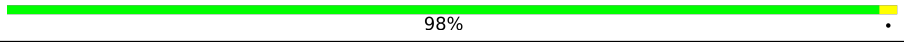
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	331	97%
1	B	331	7% 96%
1	C	331	% 98%
1	D	331	9% 96%
1	O	331	25% 96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	P	331	
1	Q	331	
1	R	331	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 22023 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.

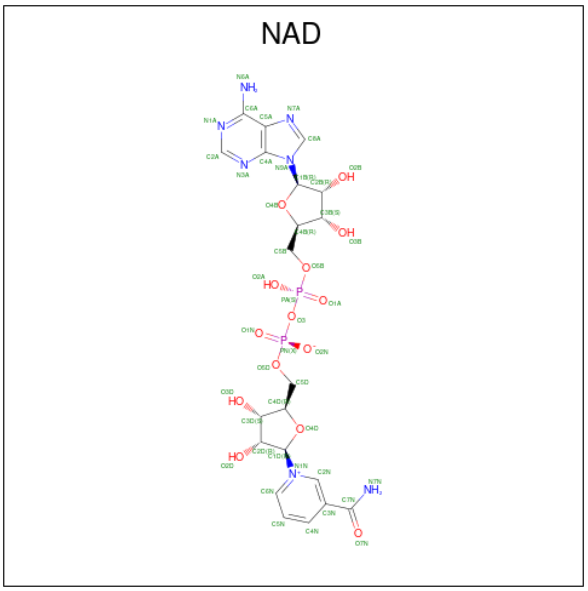
- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	330	Total	C	N	O	S	0	4	0
			2499	1582	436	474	7			
1	P	330	Total	C	N	O	S	0	4	0
			2522	1594	443	478	7			
1	Q	330	Total	C	N	O	S	0	4	0
			2515	1591	441	476	7			
1	R	330	Total	C	N	O	S	0	4	0
			2514	1591	440	476	7			
1	A	330	Total	C	N	O	S	0	4	0
			2492	1577	436	472	7			
1	B	330	Total	C	N	O	S	0	4	0
			2505	1586	436	476	7			
1	C	330	Total	C	N	O	S	0	4	0
			2511	1591	439	474	7			
1	D	330	Total	C	N	O	S	0	4	0
			2490	1579	437	467	7			

There are 8 discrepancies between the modelled and reference sequences:

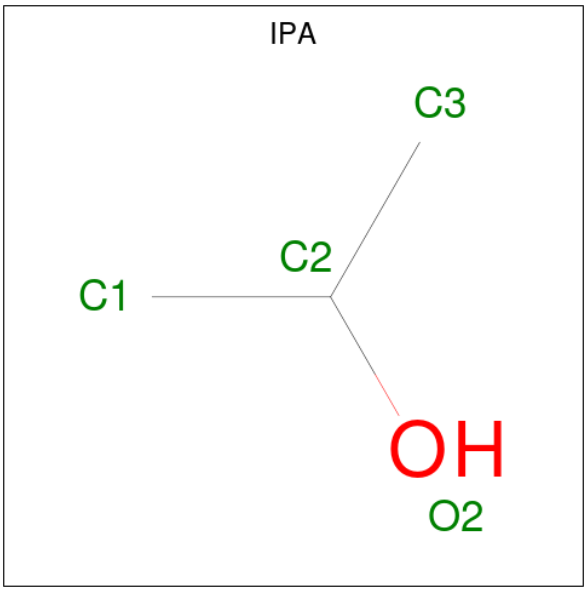
Chain	Residue	Modelled	Actual	Comment	Reference
O	149	CSD	CYS	modified residue	UNP P00361
P	149	CSD	CYS	modified residue	UNP P00361
Q	149	CSD	CYS	modified residue	UNP P00361
R	149	CSD	CYS	modified residue	UNP P00361
A	149	CSD	CYS	modified residue	UNP P00361
B	149	CSD	CYS	modified residue	UNP P00361
C	149	CSD	CYS	modified residue	UNP P00361
D	149	CSD	CYS	modified residue	UNP P00361

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



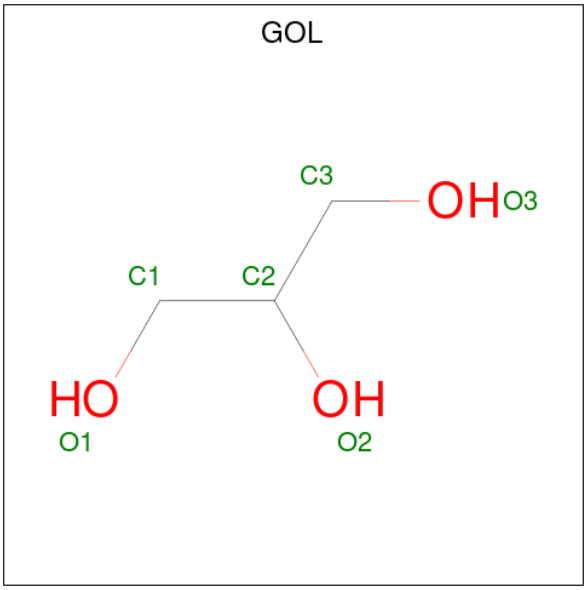
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	P	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	Q	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	R	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C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

- Molecule 3 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Q	1	Total C O 4 3 1	0	0
3	C	1	Total C O 4 3 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Q	1	Total C O 6 3 3	0	0
4	R	1	Total C O 6 3 3	0	0

Continued on next page...

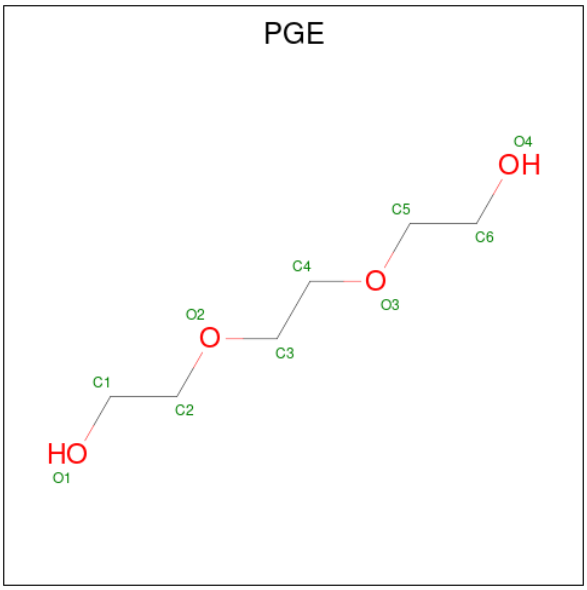
Continued from previous page...

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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Na 1 1	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 10 6 4	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	O	189	Total O 189 189	0	0
7	P	236	Total O 236 236	0	0
7	Q	240	Total O 240 240	0	0
7	R	228	Total O 228 228	0	0

Continued on next page...

Continued from previous page...

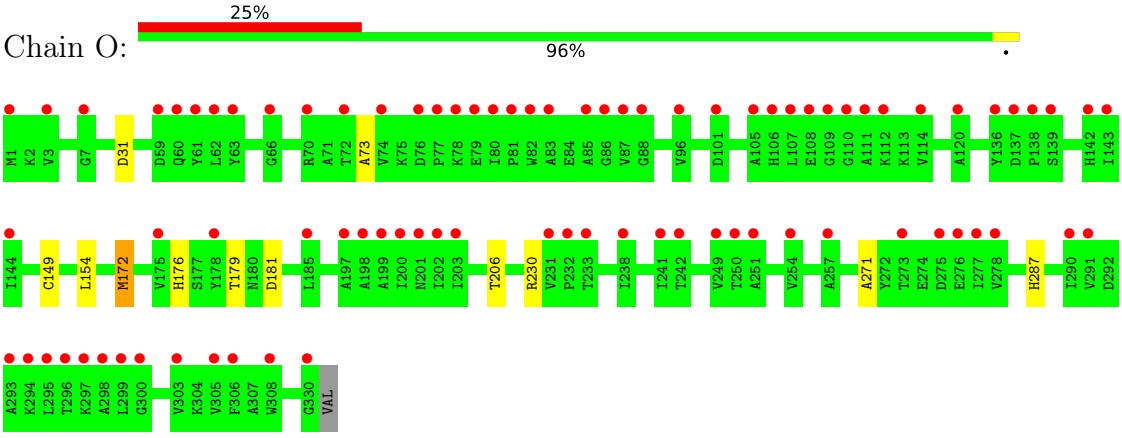
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	175	Total O 175 175	0	0
7	B	145	Total O 145 145	0	0
7	C	226	Total O 226 226	0	0
7	D	147	Total O 147 147	0	0

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.

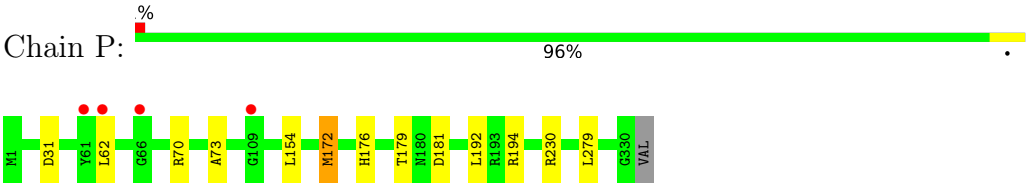
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain O:



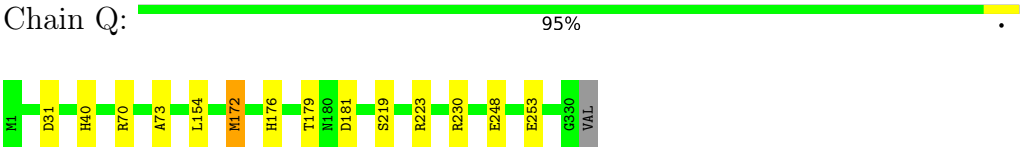
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain P:



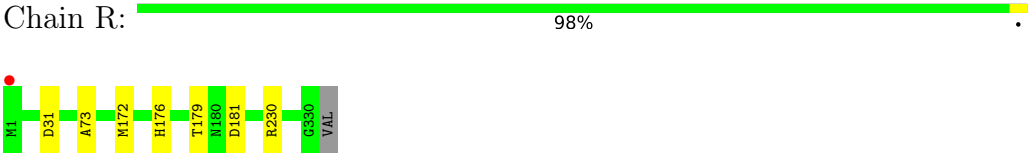
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain Q:



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain R:



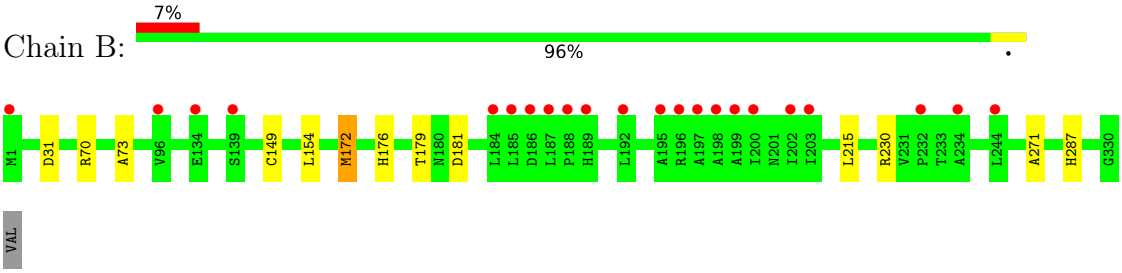
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain A:



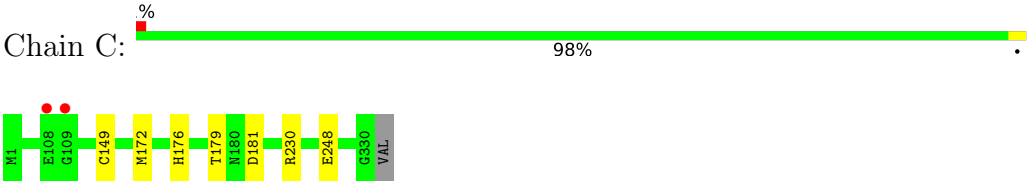
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain B:



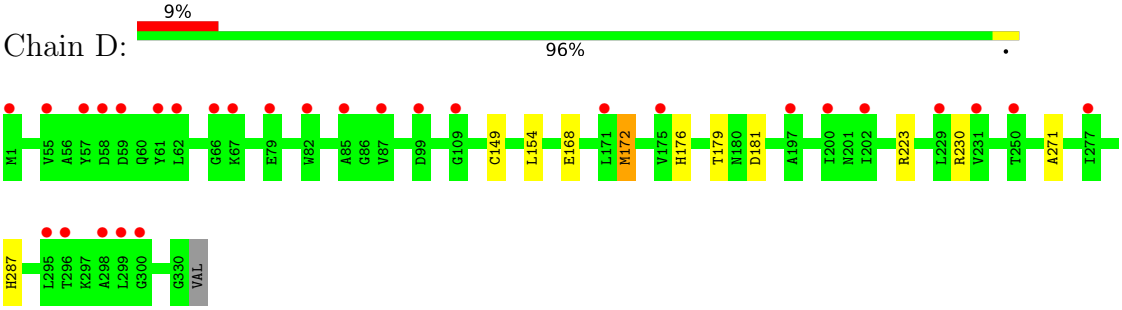
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain C:



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	141.55Å 147.40Å 147.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.94 – 1.65 65.94 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (65.94-1.65) 98.5 (65.94-1.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.158 , 0.172 0.164 , 0.176	Depositor DCC
R_{free} test set	18372 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	18.7	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 38.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k 0.003 for -l,-k,-h 0.004 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22023	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, IPA, CSD, NA, NAD, GOL

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	0.54	1/2450 (0.0%)	0.73	0/3336
1	B	0.54	1/2463 (0.0%)	0.75	0/3351
1	C	0.56	1/2469 (0.0%)	0.72	0/3357
1	D	0.57	1/2448 (0.0%)	0.72	0/3332
1	O	0.60	1/2457 (0.0%)	0.75	0/3344
1	P	0.65	1/2480 (0.0%)	0.75	0/3371
1	Q	0.63	1/2473 (0.0%)	0.73	0/3362
1	R	0.65	1/2472 (0.0%)	0.73	0/3361
All	All	0.59	8/19712 (0.0%)	0.74	0/26814

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	172	MET	SD-CE	-19.48	1.30	1.79
1	P	172	MET	SD-CE	-19.00	1.32	1.79
1	Q	172	MET	SD-CE	-16.34	1.38	1.79
1	O	172	MET	SD-CE	-14.03	1.44	1.79
1	D	172	MET	SD-CE	-11.88	1.49	1.79
1	C	172	MET	SD-CE	-11.74	1.50	1.79
1	B	172	MET	SD-CE	-9.39	1.56	1.79
1	A	172	MET	SD-CE	-9.08	1.56	1.79

There are no bond angle outliers.

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	2492	0	2471	4	0
1	B	2505	0	2489	5	0
1	C	2511	0	2504	2	0
1	D	2490	0	2473	6	0
1	O	2499	0	2481	6	0
1	P	2522	0	2520	9	0
1	Q	2515	0	2514	7	0
1	R	2514	0	2509	3	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	O	44	0	26	0	0
2	P	44	0	26	0	0
2	Q	44	0	26	0	0
2	R	44	0	26	0	0
3	C	4	0	8	0	0
3	Q	4	0	8	0	0
4	D	6	0	8	0	0
4	Q	6	0	8	0	0
4	R	6	0	8	0	0
5	C	1	0	0	0	0
6	C	10	0	14	0	0
7	A	175	0	0	0	0
7	B	145	0	0	0	0
7	C	226	0	0	0	0
7	D	147	0	0	0	0
7	O	189	0	0	1	0
7	P	236	0	0	0	0
7	Q	240	0	0	0	0
7	R	228	0	0	0	0
All	All	22023	0	20223	40	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 1.

All (40) 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:179:THR:OG1	1:O:181[C]:ASP:OD1	2.01	0.78
1:D:179:THR:OG1	1:D:181[C]:ASP:OD2	2.01	0.77
1:P:181[C]:ASP:OD1	1:P:194[C]:ARG:NH1	2.19	0.76
1:C:179:THR:OG1	1:C:181[C]:ASP:OD2	2.09	0.71
1:R:179:THR:OG1	1:R:181[C]:ASP:OD2	2.13	0.67
1:Q:179:THR:OG1	1:Q:181[C]:ASP:OD2	2.15	0.63
1:D:154:LEU:HD21	1:D:172:MET:HE3	1.79	0.63
1:B:154:LEU:HD21	1:B:172:MET:HE3	1.81	0.62
1:A:179:THR:OG1	1:A:181[C]:ASP:OD1	2.24	0.55
1:A:154:LEU:HD21	1:A:172:MET:HE3	1.89	0.55
1:P:179:THR:OG1	1:P:181[C]:ASP:OD2	2.26	0.54
1:Q:253:GLU:OE1	1:D:223:ARG:NE	2.38	0.54
1:D:176:HIS:HB3	1:D:230[B]:ARG:HD3	1.90	0.53
1:O:176:HIS:HB3	1:O:230[B]:ARG:HD3	1.91	0.52
1:R:176:HIS:HB3	1:R:230[B]:ARG:HD3	1.92	0.51
1:B:271:ALA:HB2	1:B:287:HIS:CD2	2.49	0.48
1:P:192:LEU:HB3	1:Q:40:HIS:CD2	2.50	0.47
1:A:176:HIS:HB3	1:A:230[B]:ARG:HD3	1.97	0.46
1:Q:176:HIS:HB3	1:Q:230[B]:ARG:HD3	1.96	0.46
1:C:176:HIS:HB3	1:C:230[B]:ARG:HD3	1.97	0.46
1:O:271:ALA:HB2	1:O:287:HIS:CD2	2.51	0.45
1:D:271:ALA:HB2	1:D:287:HIS:CD2	2.52	0.45
1:P:181[C]:ASP:CG	1:P:194[C]:ARG:NH1	2.74	0.45
1:B:176:HIS:HB3	1:B:230[B]:ARG:HD3	1.99	0.45
1:A:83:ALA:HB2	1:A:110:GLY:HA3	1.99	0.44
1:O:206[C]:THR:HG22	7:O:441:HOH:O	2.17	0.44
1:Q:219:SER:O	1:Q:223:ARG:HD3	2.16	0.44
1:P:154:LEU:HD21	1:P:172:MET:HE3	2.00	0.44
1:B:31:ASP:O	1:B:73:ALA:HA	2.18	0.43
1:P:181[C]:ASP:CG	1:P:194[C]:ARG:HH11	2.25	0.43
1:P:31:ASP:O	1:P:73:ALA:HA	2.19	0.43
1:B:179:THR:OG1	1:B:181[C]:ASP:OD2	2.36	0.43
1:O:31:ASP:O	1:O:73:ALA:HA	2.19	0.42
1:O:154:LEU:HD21	1:O:172:MET:HE3	2.01	0.42
1:Q:154:LEU:HD21	1:Q:172:MET:HE3	2.02	0.41
1:Q:31:ASP:O	1:Q:73:ALA:HA	2.20	0.41
1:R:31:ASP:O	1:R:73:ALA:HA	2.20	0.41
1:P:176:HIS:HB3	1:P:230[B]:ARG:HD3	2.04	0.40
1:P:279:LEU:HD23	1:P:279:LEU:C	2.47	0.40
1:D:168:GLU:O	1:D:223:ARG:HD3	2.22	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	331/331 (100%)	323 (98%)	8 (2%)	0	100	100
1	B	331/331 (100%)	318 (96%)	13 (4%)	0	100	100
1	C	331/331 (100%)	321 (97%)	10 (3%)	0	100	100
1	D	331/331 (100%)	320 (97%)	11 (3%)	0	100	100
1	O	331/331 (100%)	322 (97%)	9 (3%)	0	100	100
1	P	331/331 (100%)	322 (97%)	9 (3%)	0	100	100
1	Q	331/331 (100%)	320 (97%)	11 (3%)	0	100	100
1	R	331/331 (100%)	322 (97%)	9 (3%)	0	100	100
All	All	2648/2648 (100%)	2568 (97%)	80 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/264 (92%)	242 (100%)	1 (0%)	84	77
1	B	245/264 (93%)	243 (99%)	2 (1%)	73	60
1	C	245/264 (93%)	244 (100%)	1 (0%)	84	77
1	D	240/264 (91%)	240 (100%)	0	100	100
1	O	244/264 (92%)	244 (100%)	0	100	100
1	P	249/264 (94%)	247 (99%)	2 (1%)	73	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Q	248/264 (94%)	246 (99%)	2 (1%)	73 60
1	R	247/264 (94%)	247 (100%)	0	100 100
All	All	1961/2112 (93%)	1953 (100%)	8 (0%)	84 77

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	62	LEU
1	P	70	ARG
1	Q	70	ARG
1	Q	248	GLU
1	A	70	ARG
1	B	70	ARG
1	B	215	LEU
1	C	248	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	255	ASN
1	P	60	GLN
1	P	255	ASN
1	Q	255	ASN
1	R	255	ASN
1	A	60	GLN
1	A	255	ASN
1	B	60	GLN
1	B	255	ASN
1	C	255	ASN
1	D	255	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)

8 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	CSD	O	149	1	4,7,8	1.39	0	1,8,10	2.88	1 (100%)
1	CSD	Q	149	1	4,7,8	1.15	0	1,8,10	1.43	0
1	CSD	D	149	1	4,7,8	1.41	1 (25%)	1,8,10	1.66	0
1	CSD	C	149	1	4,7,8	1.54	1 (25%)	1,8,10	2.13	1 (100%)
1	CSD	A	149	1	4,7,8	1.31	0	1,8,10	2.28	1 (100%)
1	CSD	P	149	1	4,7,8	1.29	0	1,8,10	1.51	0
1	CSD	R	149	1	4,7,8	1.06	0	1,8,10	0.38	0
1	CSD	B	149	1	4,7,8	1.61	1 (25%)	1,8,10	2.16	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	CSD	O	149	1	-	0/2/6/8	-
1	CSD	Q	149	1	-	0/2/6/8	-
1	CSD	D	149	1	-	0/2/6/8	-
1	CSD	C	149	1	-	0/2/6/8	-
1	CSD	A	149	1	-	1/2/6/8	-
1	CSD	P	149	1	-	0/2/6/8	-
1	CSD	R	149	1	-	0/2/6/8	-
1	CSD	B	149	1	-	0/2/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	CSD	OD1-SG	-2.55	1.45	1.47
1	C	149	CSD	OD1-SG	-2.44	1.45	1.47
1	D	149	CSD	OD1-SG	-2.10	1.45	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	149	CSD	OD1-SG-CB	2.88	110.91	105.60
1	A	149	CSD	OD1-SG-CB	2.28	109.81	105.60
1	B	149	CSD	OD1-SG-CB	2.16	109.58	105.60
1	C	149	CSD	OD1-SG-CB	2.13	109.52	105.60

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	149	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	D	336	-	46,48,48	1.34	7 (15%)	64,73,73	1.57	8 (12%)
2	NAD	R	336	-	46,48,48	1.20	6 (13%)	64,73,73	1.59	12 (18%)
2	NAD	C	336	-	46,48,48	1.45	6 (13%)	64,73,73	1.63	10 (15%)
2	NAD	Q	336	-	46,48,48	1.21	5 (10%)	64,73,73	1.57	10 (15%)
2	NAD	A	336	-	46,48,48	1.26	5 (10%)	64,73,73	1.55	9 (14%)
4	GOL	Q	3503	-	5,5,5	0.39	0	5,5,5	0.48	0
6	PGE	C	1700	5	9,9,9	0.71	0	8,8,8	0.55	0
3	IPA	Q	1801	-	3,3,3	0.56	0	3,3,3	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAD	B	336	-	46,48,48	1.17	5 (10%)	64,73,73	1.61	10 (15%)
2	NAD	P	336	-	46,48,48	1.22	5 (10%)	64,73,73	1.64	10 (15%)
4	GOL	R	3502	-	5,5,5	0.42	0	5,5,5	0.38	0
2	NAD	O	336	-	46,48,48	1.35	7 (15%)	64,73,73	1.60	10 (15%)
3	IPA	C	1800	-	3,3,3	0.59	0	3,3,3	0.14	0
4	GOL	D	3504	-	5,5,5	0.36	0	5,5,5	0.36	0

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	D	336	-	-	5/30/62/62	0/5/5/5
2	NAD	R	336	-	-	4/30/62/62	0/5/5/5
2	NAD	C	336	-	-	5/30/62/62	0/5/5/5
2	NAD	Q	336	-	-	4/30/62/62	0/5/5/5
2	NAD	A	336	-	-	5/30/62/62	0/5/5/5
4	GOL	Q	3503	-	-	3/4/4/4	-
6	PGE	C	1700	5	-	4/7/7/7	-
2	NAD	B	336	-	-	4/30/62/62	0/5/5/5
2	NAD	P	336	-	-	4/30/62/62	0/5/5/5
4	GOL	R	3502	-	-	2/4/4/4	-
2	NAD	O	336	-	-	4/30/62/62	0/5/5/5
4	GOL	D	3504	-	-	2/4/4/4	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	336	NAD	C2N-N1N	6.45	1.42	1.35
2	O	336	NAD	C2N-N1N	5.44	1.41	1.35
2	D	336	NAD	C2N-N1N	5.32	1.40	1.35
2	A	336	NAD	C2N-N1N	5.04	1.40	1.35
2	P	336	NAD	C2N-N1N	4.64	1.40	1.35
2	Q	336	NAD	C2N-N1N	4.51	1.39	1.35
2	B	336	NAD	C2N-N1N	4.44	1.39	1.35
2	R	336	NAD	C2N-N1N	4.26	1.39	1.35
2	C	336	NAD	O4D-C1D	3.37	1.45	1.40
2	O	336	NAD	O4D-C1D	3.29	1.45	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	336	NAD	PA-O3	3.07	1.62	1.59
2	D	336	NAD	C5A-N7A	-3.05	1.33	1.39
2	A	336	NAD	C5A-N7A	-2.90	1.33	1.39
2	B	336	NAD	C5A-N7A	-2.88	1.33	1.39
2	C	336	NAD	C5A-N7A	-2.79	1.34	1.39
2	D	336	NAD	PN-O3	2.79	1.62	1.59
2	P	336	NAD	C5A-N7A	-2.75	1.34	1.39
2	O	336	NAD	C5A-N7A	-2.73	1.34	1.39
2	R	336	NAD	C5A-N7A	-2.72	1.34	1.39
2	A	336	NAD	O4D-C1D	2.62	1.44	1.40
2	Q	336	NAD	C4A-N9A	-2.52	1.32	1.37
2	B	336	NAD	PN-O3	2.51	1.62	1.59
2	Q	336	NAD	C6N-N1N	2.46	1.40	1.35
2	O	336	NAD	PA-O3	2.45	1.62	1.59
2	R	336	NAD	PN-O3	2.45	1.62	1.59
2	D	336	NAD	O4D-C1D	2.41	1.44	1.40
2	Q	336	NAD	O4D-C1D	2.36	1.44	1.40
2	A	336	NAD	C4A-N9A	-2.35	1.32	1.37
2	Q	336	NAD	C5A-N7A	-2.34	1.34	1.39
2	R	336	NAD	C4A-N9A	-2.32	1.32	1.37
2	R	336	NAD	O4D-C1D	2.32	1.43	1.40
2	C	336	NAD	C4A-N9A	-2.32	1.32	1.37
2	O	336	NAD	C4A-N9A	-2.25	1.33	1.37
2	B	336	NAD	C4A-N9A	-2.25	1.33	1.37
2	D	336	NAD	C6N-N1N	2.20	1.40	1.35
2	C	336	NAD	C6N-N1N	2.18	1.40	1.35
2	O	336	NAD	C6N-N1N	2.17	1.40	1.35
2	A	336	NAD	PN-O3	2.14	1.61	1.59
2	P	336	NAD	C4A-N9A	-2.11	1.33	1.37
2	C	336	NAD	PA-O3	2.10	1.61	1.59
2	R	336	NAD	C6N-N1N	2.09	1.40	1.35
2	O	336	NAD	C3N-C7N	2.06	1.53	1.50
2	P	336	NAD	C6N-N1N	2.04	1.40	1.35
2	D	336	NAD	C4A-N9A	-2.03	1.33	1.37
2	B	336	NAD	C8A-N9A	-2.01	1.34	1.37
2	D	336	NAD	C3N-C7N	2.00	1.53	1.50

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	336	NAD	C5A-C4A-N3A	-5.26	119.47	126.72
2	B	336	NAD	C5A-C4A-N3A	-5.14	119.65	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	336	NAD	C5A-C4A-N3A	-5.10	119.70	126.72
2	Q	336	NAD	C5A-C4A-N3A	-4.89	119.99	126.72
2	C	336	NAD	C5A-C4A-N3A	-4.86	120.02	126.72
2	P	336	NAD	C5A-C4A-N3A	-4.79	120.12	126.72
2	P	336	NAD	N3A-C2A-N1A	-4.77	121.36	128.58
2	C	336	NAD	N3A-C2A-N1A	-4.75	121.40	128.58
2	R	336	NAD	C5A-C4A-N3A	-4.73	120.20	126.72
2	A	336	NAD	C5A-C4A-N3A	-4.64	120.33	126.72
2	R	336	NAD	N3A-C2A-N1A	-4.62	121.59	128.58
2	B	336	NAD	N3A-C2A-N1A	-4.60	121.62	128.58
2	O	336	NAD	N3A-C2A-N1A	-4.46	121.83	128.58
2	Q	336	NAD	N3A-C2A-N1A	-4.45	121.85	128.58
2	A	336	NAD	N3A-C2A-N1A	-4.40	121.93	128.58
2	D	336	NAD	N3A-C2A-N1A	-3.97	122.58	128.58
2	P	336	NAD	N9A-C8A-N7A	-3.77	108.59	113.94
2	B	336	NAD	C2A-N3A-C4A	3.70	120.87	111.83
2	O	336	NAD	N9A-C8A-N7A	-3.62	108.80	113.94
2	O	336	NAD	C2A-N3A-C4A	3.62	120.67	111.83
2	B	336	NAD	N9A-C8A-N7A	-3.57	108.86	113.94
2	Q	336	NAD	C4A-C5A-N7A	-3.55	106.53	110.58
2	D	336	NAD	N9A-C8A-N7A	-3.51	108.95	113.94
2	P	336	NAD	C2A-N3A-C4A	3.51	120.40	111.83
2	C	336	NAD	N9A-C8A-N7A	-3.50	108.97	113.94
2	B	336	NAD	C4A-C5A-N7A	-3.50	106.58	110.58
2	R	336	NAD	N9A-C8A-N7A	-3.49	108.99	113.94
2	C	336	NAD	C2A-N3A-C4A	3.43	120.21	111.83
2	Q	336	NAD	C2A-N3A-C4A	3.42	120.19	111.83
2	R	336	NAD	C4A-C5A-N7A	-3.39	106.71	110.58
2	R	336	NAD	C2A-N3A-C4A	3.36	120.03	111.83
2	Q	336	NAD	N9A-C8A-N7A	-3.35	109.19	113.94
2	D	336	NAD	C2A-N3A-C4A	3.35	120.00	111.83
2	C	336	NAD	C4A-C5A-N7A	-3.30	106.81	110.58
2	A	336	NAD	C2A-N3A-C4A	3.28	119.83	111.83
2	O	336	NAD	C4A-C5A-N7A	-3.27	106.84	110.58
2	A	336	NAD	C4A-C5A-N7A	-3.22	106.90	110.58
2	D	336	NAD	N3A-C4A-N9A	3.22	132.64	127.17
2	B	336	NAD	C5A-N7A-C8A	3.13	108.37	103.45
2	D	336	NAD	C5A-N7A-C8A	3.13	108.37	103.45
2	O	336	NAD	N3A-C4A-N9A	3.13	132.48	127.17
2	D	336	NAD	C4A-C5A-N7A	-3.12	107.01	110.58
2	O	336	NAD	C5A-N7A-C8A	3.11	108.34	103.45
2	P	336	NAD	C5A-N7A-C8A	3.10	108.32	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	336	NAD	N9A-C8A-N7A	-3.08	109.56	113.94
2	P	336	NAD	C4A-C5A-N7A	-3.06	107.09	110.58
2	C	336	NAD	C4D-O4D-C1D	-3.05	107.14	109.92
2	P	336	NAD	N3A-C4A-N9A	3.01	132.29	127.17
2	C	336	NAD	C5A-N7A-C8A	2.99	108.16	103.45
2	R	336	NAD	C5A-N7A-C8A	2.98	108.14	103.45
2	Q	336	NAD	C5A-N7A-C8A	2.86	107.94	103.45
2	B	336	NAD	N3A-C4A-N9A	2.86	132.03	127.17
2	P	336	NAD	C4D-O4D-C1D	-2.82	107.34	109.92
2	O	336	NAD	C4D-O4D-C1D	-2.81	107.35	109.92
2	C	336	NAD	N3A-C4A-N9A	2.80	131.92	127.17
2	P	336	NAD	C2N-C3N-C4N	2.76	121.47	118.26
2	A	336	NAD	C5A-N7A-C8A	2.73	107.73	103.45
2	Q	336	NAD	C4D-O4D-C1D	-2.61	107.54	109.92
2	R	336	NAD	N3A-C4A-N9A	2.55	131.50	127.17
2	R	336	NAD	C4D-O4D-C1D	-2.55	107.59	109.92
2	P	336	NAD	C4A-N9A-C8A	2.54	108.40	105.74
2	Q	336	NAD	N3A-C4A-N9A	2.52	131.46	127.17
2	Q	336	NAD	C5A-C4A-N9A	2.52	108.55	105.81
2	A	336	NAD	C4D-O4D-C1D	-2.48	107.66	109.92
2	D	336	NAD	C4D-O4D-C1D	-2.44	107.69	109.92
2	A	336	NAD	N3A-C4A-N9A	2.43	131.31	127.17
2	A	336	NAD	C5A-C4A-N9A	2.34	108.37	105.81
2	R	336	NAD	C6N-N1N-C2N	-2.34	119.89	121.88
2	O	336	NAD	C4A-N9A-C8A	2.33	108.18	105.74
2	O	336	NAD	O2N-PN-O1N	2.32	123.25	112.44
2	B	336	NAD	C5A-C4A-N9A	2.31	108.33	105.81
2	B	336	NAD	O3-PA-O1A	-2.28	103.83	110.70
2	R	336	NAD	C5A-C4A-N9A	2.28	108.30	105.81
2	C	336	NAD	C4A-N9A-C8A	2.17	108.01	105.74
2	Q	336	NAD	C2N-C3N-C4N	2.14	120.75	118.26
2	R	336	NAD	O2A-PA-O1A	2.09	122.17	112.44
2	C	336	NAD	C5A-C4A-N9A	2.06	108.06	105.81
2	R	336	NAD	C4A-N9A-C8A	2.02	107.86	105.74
2	B	336	NAD	C4A-N9A-C8A	2.02	107.86	105.74

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	336	NAD	O4D-C1D-N1N-C2N
2	O	336	NAD	O4D-C1D-N1N-C6N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	O	336	NAD	C2D-C1D-N1N-C2N
2	O	336	NAD	C2D-C1D-N1N-C6N
2	P	336	NAD	O4D-C1D-N1N-C2N
2	P	336	NAD	O4D-C1D-N1N-C6N
2	P	336	NAD	C2D-C1D-N1N-C2N
2	P	336	NAD	C2D-C1D-N1N-C6N
2	Q	336	NAD	O4D-C1D-N1N-C2N
2	Q	336	NAD	O4D-C1D-N1N-C6N
2	Q	336	NAD	C2D-C1D-N1N-C2N
2	Q	336	NAD	C2D-C1D-N1N-C6N
2	R	336	NAD	O4D-C1D-N1N-C2N
2	R	336	NAD	O4D-C1D-N1N-C6N
2	R	336	NAD	C2D-C1D-N1N-C2N
2	R	336	NAD	C2D-C1D-N1N-C6N
2	A	336	NAD	O4D-C1D-N1N-C2N
2	A	336	NAD	O4D-C1D-N1N-C6N
2	A	336	NAD	C2D-C1D-N1N-C2N
2	A	336	NAD	C2D-C1D-N1N-C6N
2	B	336	NAD	O4D-C1D-N1N-C2N
2	B	336	NAD	O4D-C1D-N1N-C6N
2	B	336	NAD	C2D-C1D-N1N-C2N
2	B	336	NAD	C2D-C1D-N1N-C6N
2	C	336	NAD	O4D-C1D-N1N-C2N
2	C	336	NAD	O4D-C1D-N1N-C6N
2	C	336	NAD	C2D-C1D-N1N-C2N
2	C	336	NAD	C2D-C1D-N1N-C6N
2	D	336	NAD	O4D-C1D-N1N-C2N
2	D	336	NAD	O4D-C1D-N1N-C6N
2	D	336	NAD	C2D-C1D-N1N-C2N
2	D	336	NAD	C2D-C1D-N1N-C6N
4	Q	3503	GOL	C1-C2-C3-O3
4	R	3502	GOL	C1-C2-C3-O3
4	R	3502	GOL	O2-C2-C3-O3
4	D	3504	GOL	C1-C2-C3-O3
4	D	3504	GOL	O2-C2-C3-O3
4	Q	3503	GOL	O2-C2-C3-O3
6	C	1700	PGE	O1-C1-C2-O2
6	C	1700	PGE	O2-C3-C4-O3
4	Q	3503	GOL	O1-C1-C2-C3
6	C	1700	PGE	O3-C5-C6-O4
6	C	1700	PGE	C1-C2-O2-C3
2	A	336	NAD	PN-O3-PA-O2A

Continued on next page...

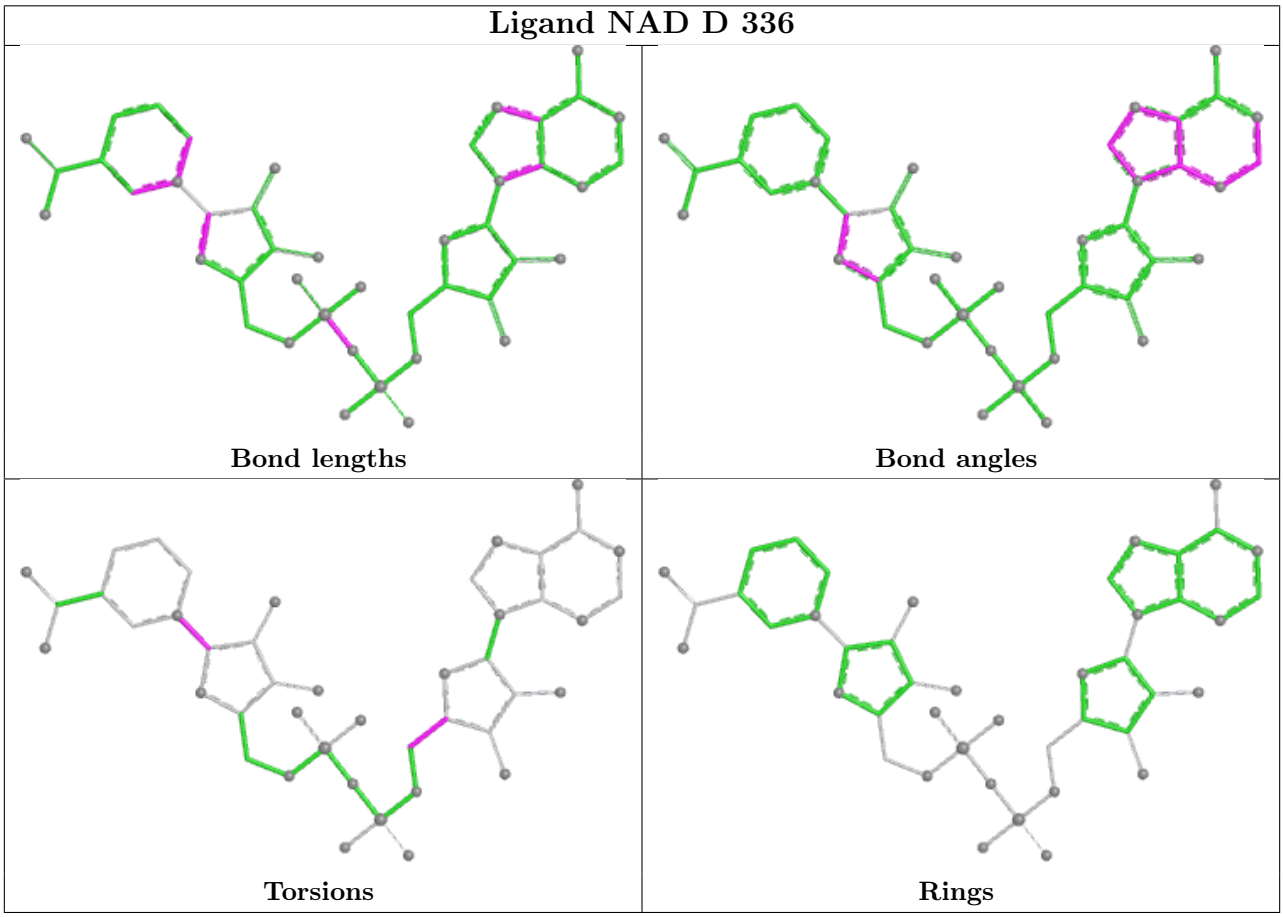
Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	336	NAD	O4B-C4B-C5B-O5B
2	C	336	NAD	PN-O3-PA-O2A

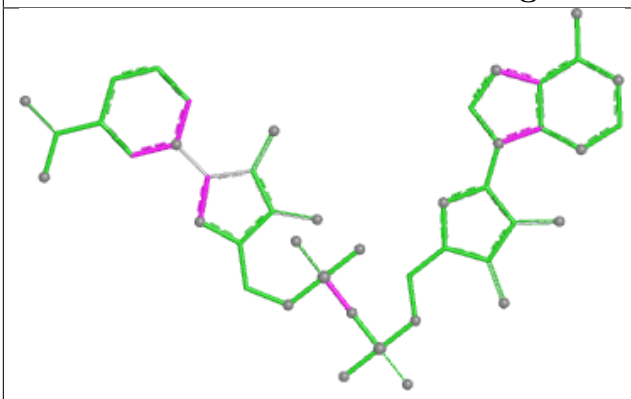
There are no ring outliers.

No monomer is involved in short contacts.

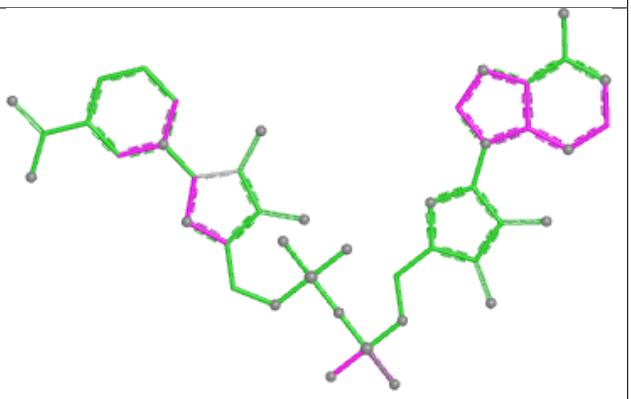
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



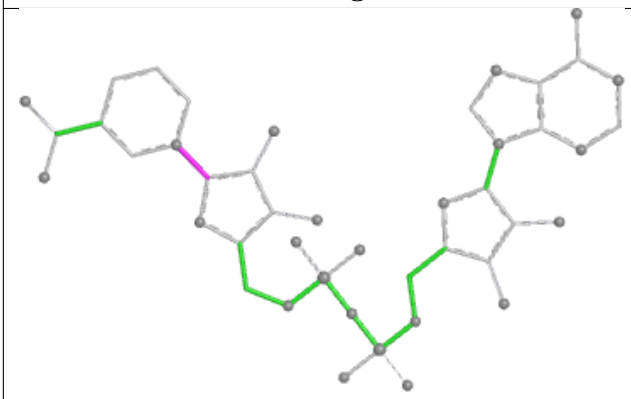
Ligand NAD R 336



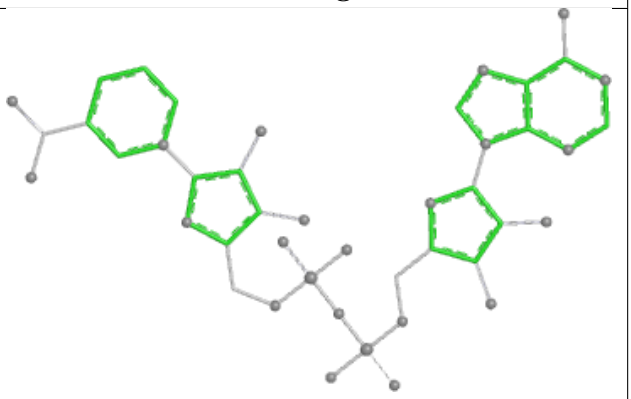
Bond lengths



Bond angles

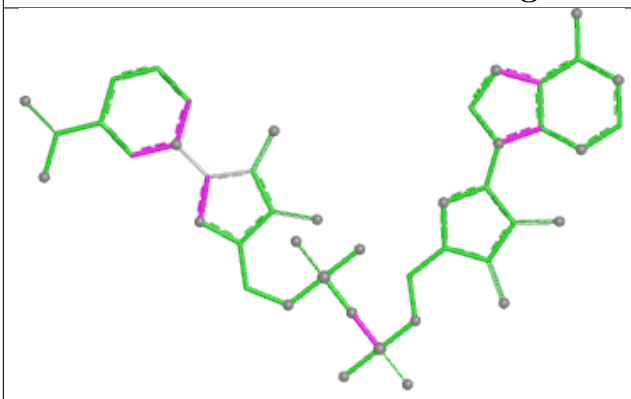


Torsions

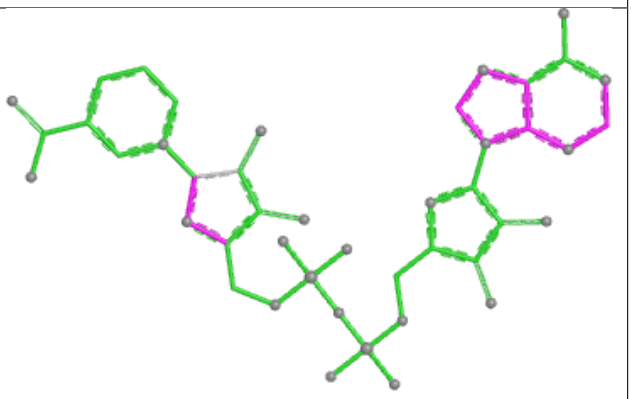


Rings

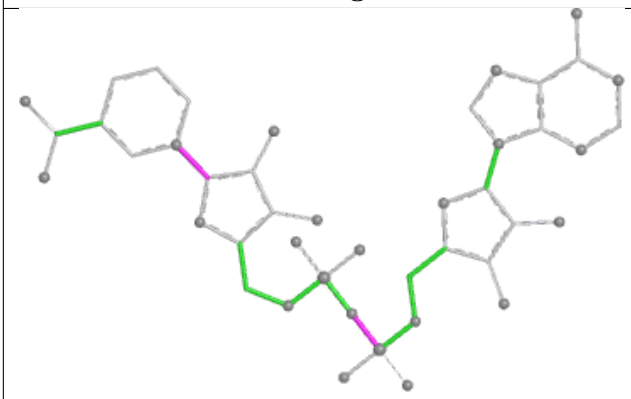
Ligand NAD C 336



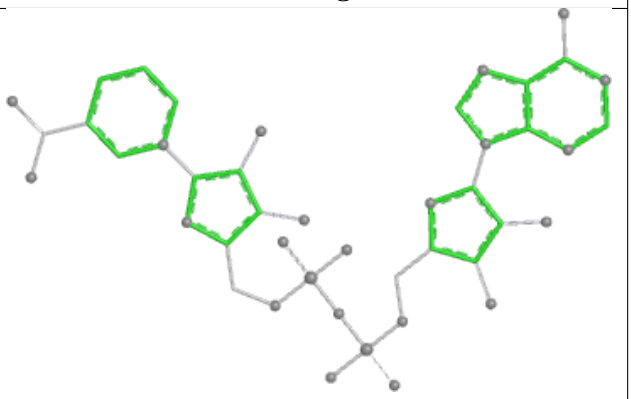
Bond lengths



Bond angles

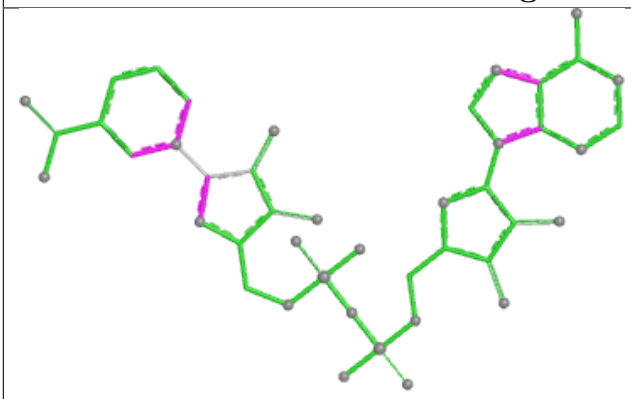


Torsions

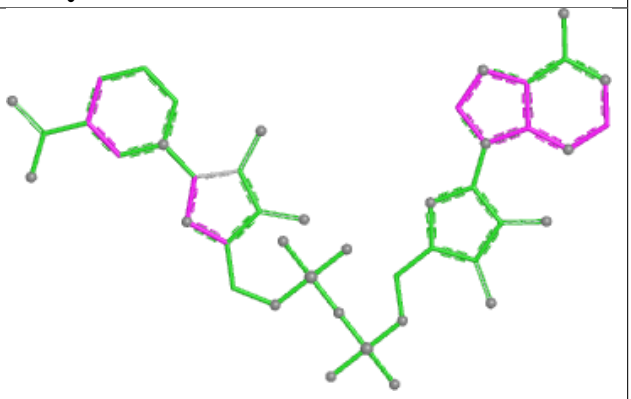


Rings

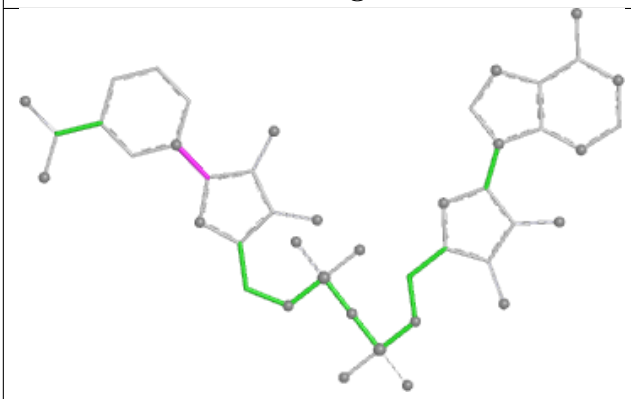
Ligand NAD Q 336



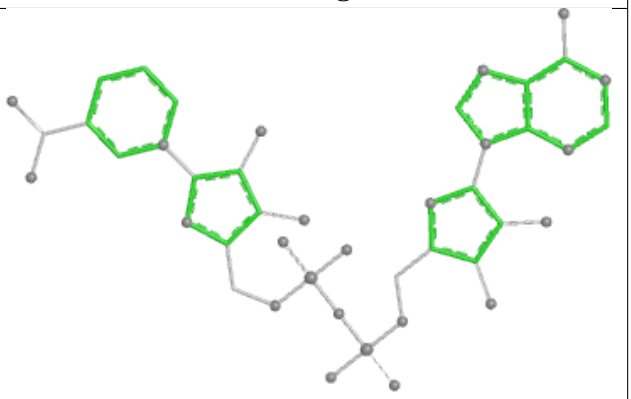
Bond lengths



Bond angles

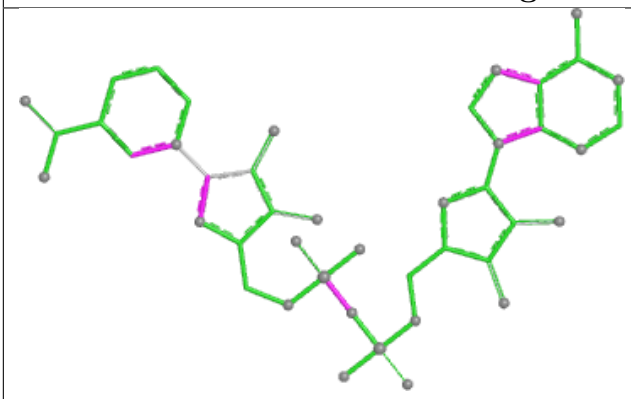


Torsions

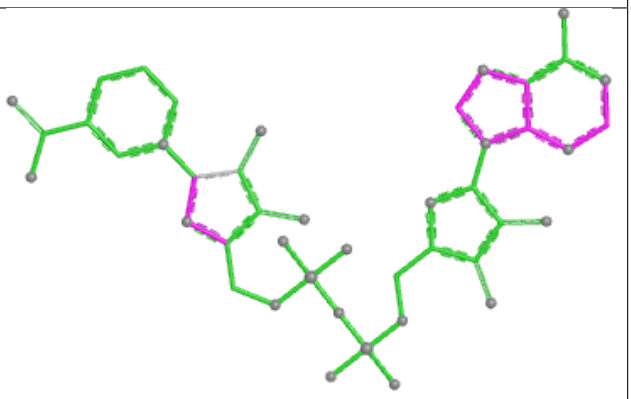


Rings

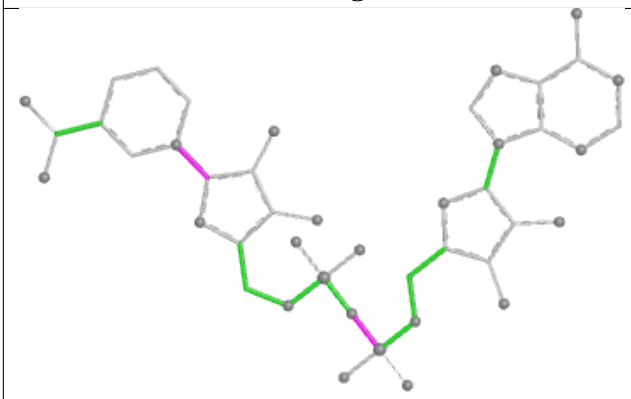
Ligand NAD A 336



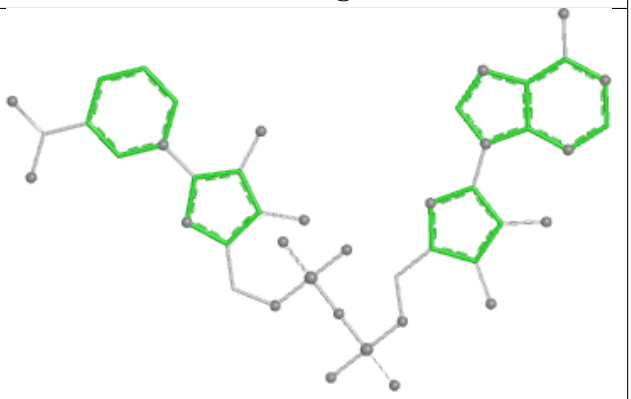
Bond lengths



Bond angles

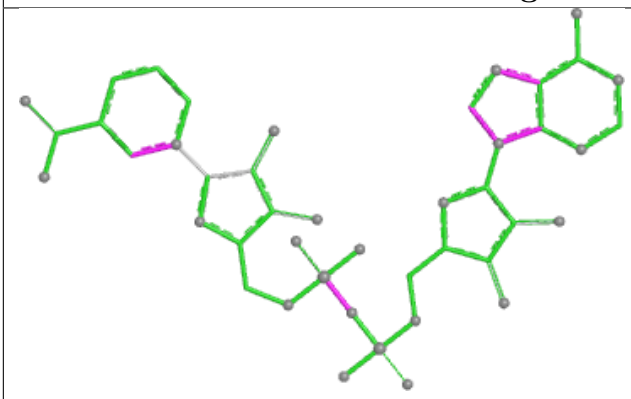


Torsions

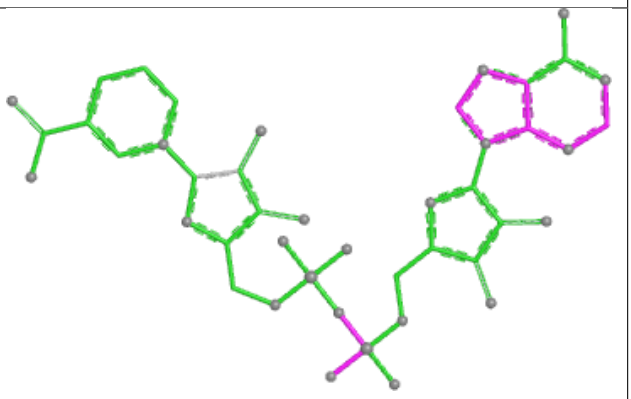


Rings

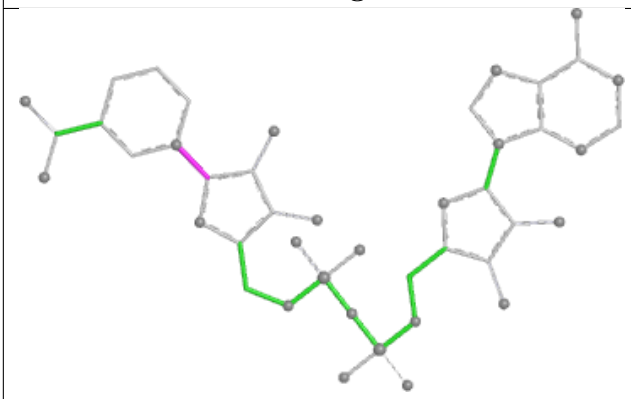
Ligand NAD B 336



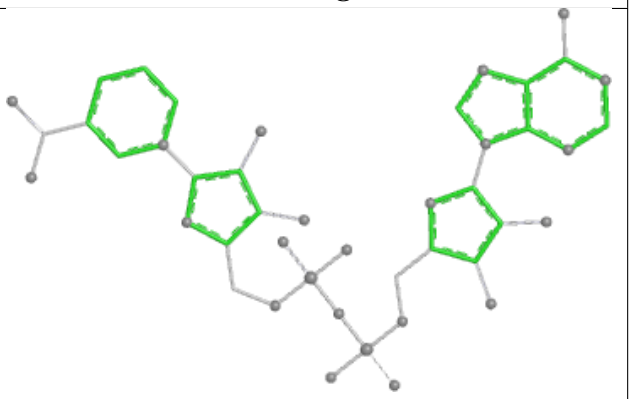
Bond lengths



Bond angles

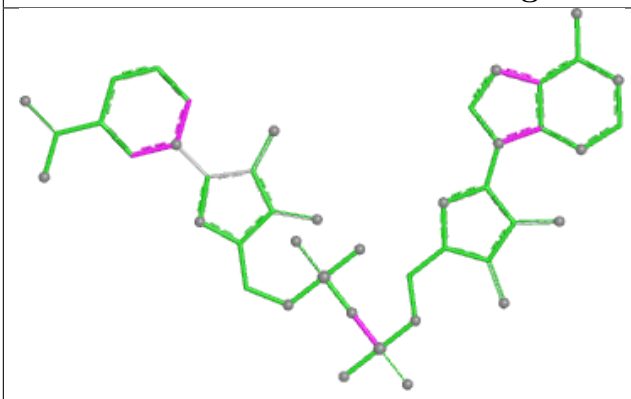


Torsions

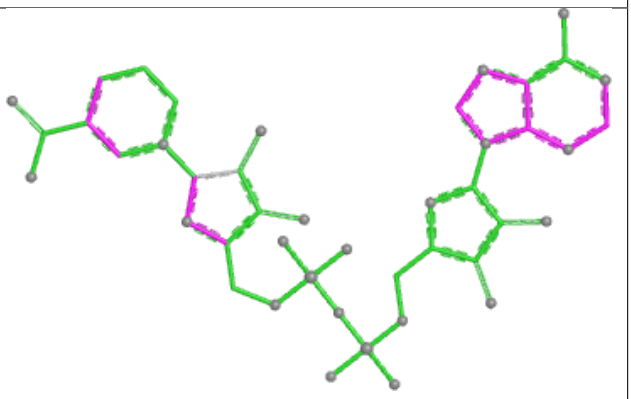


Rings

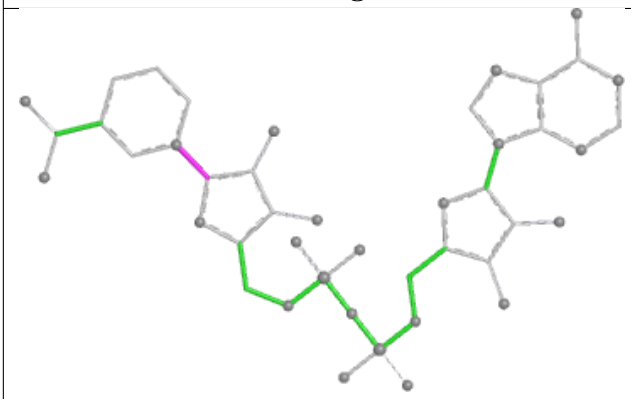
Ligand NAD P 336



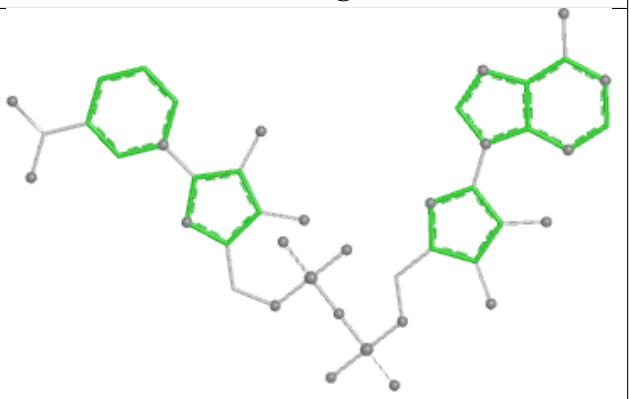
Bond lengths



Bond angles

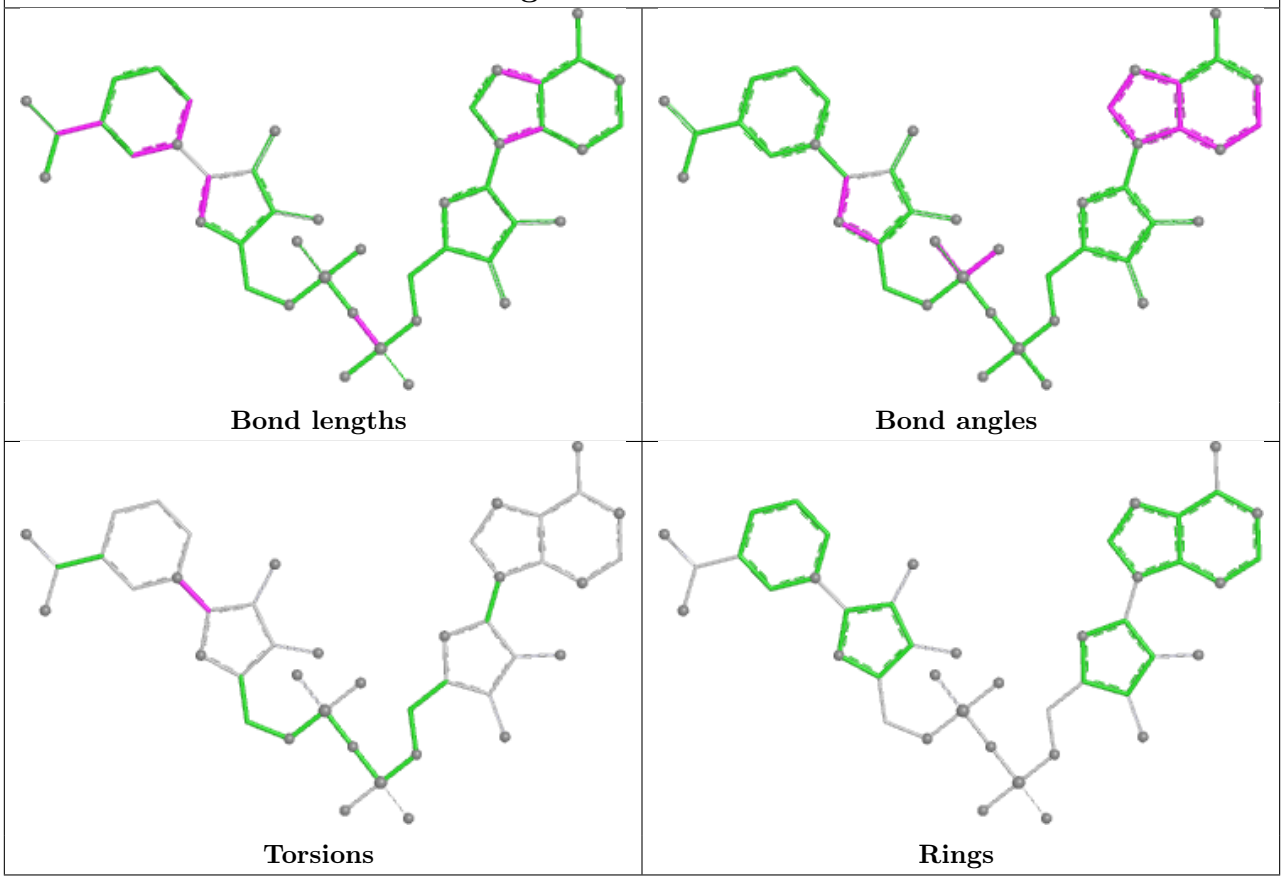


Torsions



Rings

Ligand NAD O 336



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	329/331 (99%)	0.11	1 (0%) 90 93	6, 12, 19, 22	4 (1%)
1	B	329/331 (99%)	0.70	22 (6%) 24 27	5, 12, 19, 22	4 (1%)
1	C	329/331 (99%)	0.01	2 (0%) 85 90	6, 11, 18, 24	4 (1%)
1	D	329/331 (99%)	0.77	29 (8%) 15 17	6, 12, 18, 22	4 (1%)
1	O	329/331 (99%)	1.23	84 (25%) 1 1	5, 12, 20, 24	4 (1%)
1	P	329/331 (99%)	0.26	4 (1%) 76 81	6, 11, 18, 24	4 (1%)
1	Q	329/331 (99%)	-0.22	0 100 100	6, 11, 18, 24	4 (1%)
1	R	329/331 (99%)	-0.16	1 (0%) 90 93	6, 11, 19, 24	4 (1%)
All	All	2632/2648 (99%)	0.34	143 (5%) 31 35	5, 12, 19, 24	32 (1%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	200	ILE	5.1
1	O	81	PRO	5.0
1	O	142	HIS	4.8
1	D	66	GLY	4.8
1	B	185	LEU	4.3
1	O	111	ALA	4.2
1	O	61	TYR	4.2
1	O	277	ILE	4.1
1	O	107	LEU	4.1
1	D	61	TYR	4.0
1	O	202	ILE	4.0
1	O	101	ASP	4.0
1	O	109	GLY	4.0
1	B	197	ALA	3.9
1	O	231	VAL	3.8
1	B	184	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	295	LEU	3.7
1	O	83	ALA	3.7
1	O	293	ALA	3.7
1	O	278	VAL	3.6
1	O	62	LEU	3.6
1	D	202	ILE	3.5
1	O	200	ILE	3.5
1	D	109	GLY	3.5
1	O	298	ALA	3.4
1	O	82	TRP	3.4
1	B	188	PRO	3.4
1	D	200	ILE	3.4
1	O	232	PRO	3.4
1	D	59	ASP	3.3
1	B	198	ALA	3.3
1	O	143	ILE	3.3
1	O	108	GLU	3.3
1	O	120	ALA	3.2
1	B	187	LEU	3.2
1	D	231	VAL	3.2
1	O	87	VAL	3.1
1	O	291	VAL	3.1
1	D	229	LEU	3.1
1	B	192	LEU	3.0
1	D	300	GLY	3.0
1	O	79	GLU	3.0
1	B	195	ALA	3.0
1	B	199	ALA	3.0
1	B	202	ILE	3.0
1	O	139	SER	3.0
1	O	137	ASP	2.9
1	P	62	LEU	2.9
1	O	80	ILE	2.9
1	O	85	ALA	2.9
1	O	299	LEU	2.9
1	O	203	ILE	2.9
1	D	58	ASP	2.9
1	B	234	ALA	2.8
1	B	139	SER	2.8
1	B	203	ILE	2.8
1	D	57	TYR	2.8
1	O	254	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	76	ASP	2.7
1	O	66	GLY	2.7
1	D	79	GLU	2.7
1	O	70	ARG	2.7
1	P	66	GLY	2.7
1	O	198	ALA	2.7
1	O	175	VAL	2.7
1	O	199	ALA	2.7
1	O	251	ALA	2.7
1	C	108	GLU	2.6
1	O	306	PHE	2.6
1	O	72	THR	2.6
1	O	78	LYS	2.6
1	O	330	GLY	2.6
1	O	197	ALA	2.6
1	B	186	ASP	2.6
1	D	82	TRP	2.6
1	O	88	GLY	2.6
1	D	171	LEU	2.6
1	O	114	VAL	2.6
1	P	61	TYR	2.5
1	O	249	VAL	2.5
1	O	296	THR	2.5
1	O	1	MET	2.5
1	B	196	ARG	2.5
1	D	299	LEU	2.5
1	O	273	THR	2.5
1	O	294	LYS	2.5
1	D	1	MET	2.5
1	D	298	ALA	2.5
1	O	300	GLY	2.5
1	O	77	PRO	2.4
1	O	3	VAL	2.4
1	D	62	LEU	2.4
1	D	85	ALA	2.4
1	O	233	THR	2.4
1	O	250	THR	2.4
1	O	308	TRP	2.4
1	O	7	GLY	2.3
1	O	138	PRO	2.3
1	B	232	PRO	2.3
1	O	144	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	305	VAL	2.3
1	D	55	VAL	2.3
1	O	201	ASN	2.3
1	O	59	ASP	2.3
1	D	250	THR	2.3
1	O	86	GLY	2.3
1	O	275	ASP	2.3
1	D	99	ASP	2.3
1	O	136	TYR	2.3
1	B	1	MET	2.3
1	D	197	ALA	2.2
1	O	110	GLY	2.2
1	O	238	ILE	2.2
1	D	296	THR	2.2
1	O	112	LYS	2.2
1	O	297	LYS	2.2
1	C	109	GLY	2.2
1	O	63	TYR	2.2
1	R	1	MET	2.2
1	P	109	GLY	2.2
1	B	244	LEU	2.2
1	O	241	ILE	2.2
1	O	242	THR	2.2
1	A	206[B]	THR	2.2
1	O	303	VAL	2.1
1	O	60	GLN	2.1
1	B	134	GLU	2.1
1	O	185	LEU	2.1
1	O	96	VAL	2.1
1	O	257	ALA	2.1
1	O	276	GLU	2.1
1	B	189	HIS	2.1
1	D	295	LEU	2.1
1	D	67	LYS	2.1
1	O	178	TYR	2.1
1	O	290	ILE	2.1
1	O	105	ALA	2.0
1	O	106	HIS	2.0
1	D	277	ILE	2.0
1	O	74	VAL	2.0
1	B	96	VAL	2.0
1	D	87	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	175	VAL	2.0

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, 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
1	CSD	P	149	8/9	0.94	0.09	10,11,17,20	0
1	CSD	A	149	8/9	0.95	0.10	11,11,17,18	0
1	CSD	D	149	8/9	0.95	0.08	10,11,17,18	0
1	CSD	O	149	8/9	0.96	0.08	11,12,18,19	0
1	CSD	B	149	8/9	0.96	0.07	11,12,15,18	0
1	CSD	R	149	8/9	0.96	0.09	10,11,17,19	0
1	CSD	Q	149	8/9	0.97	0.09	10,11,16,18	0
1	CSD	C	149	8/9	0.98	0.07	10,11,16,19	0

6.3 Carbohydrates (i)

There are no oligosaccharides 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
4	GOL	R	3502	6/6	0.66	0.27	49,50,50,51	0
6	PGE	C	1700	10/10	0.68	0.22	26,29,30,31	0
4	GOL	Q	3503	6/6	0.69	0.22	45,46,48,48	0
3	IPA	Q	1801	4/4	0.75	0.20	34,35,35,35	0
4	GOL	D	3504	6/6	0.77	0.20	45,46,46,47	0
3	IPA	C	1800	4/4	0.88	0.14	26,27,27,28	0
2	NAD	D	336	44/44	0.94	0.10	8,10,12,12	0
2	NAD	O	336	44/44	0.95	0.08	10,12,13,13	0
2	NAD	B	336	44/44	0.96	0.08	8,10,12,13	0

Continued on next page...

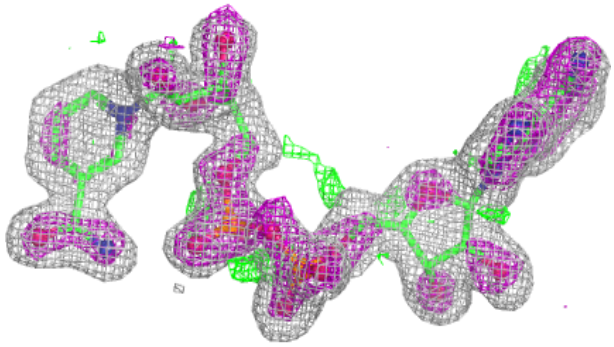
Continued from previous page...

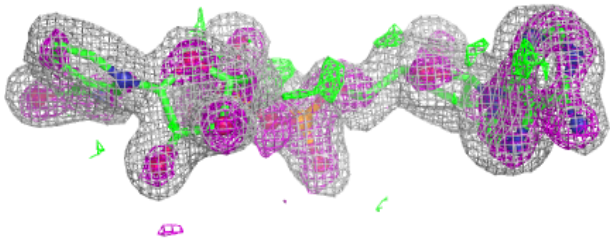
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	A	336	44/44	0.96	0.08	9,10,12,12	0
2	NAD	C	336	44/44	0.97	0.06	9,10,11,13	0
2	NAD	Q	336	44/44	0.98	0.05	8,10,11,12	0
2	NAD	R	336	44/44	0.98	0.06	8,10,11,12	0
5	NA	C	1600	1/1	0.98	0.06	19,19,19,19	0
2	NAD	P	336	44/44	0.98	0.06	8,9,11,12	0

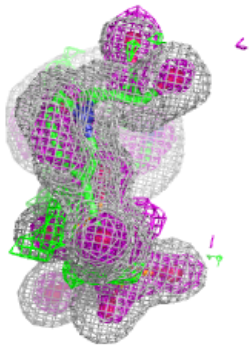
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 336:

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

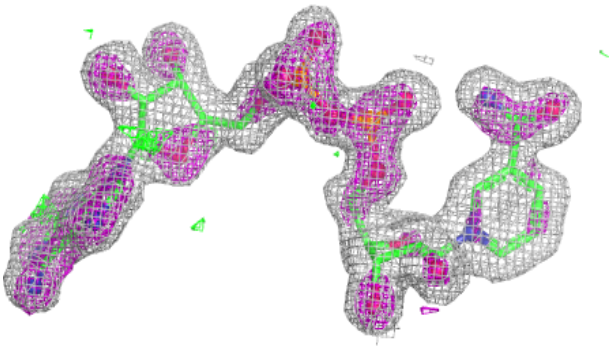


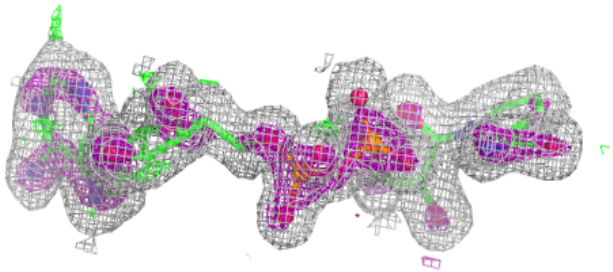


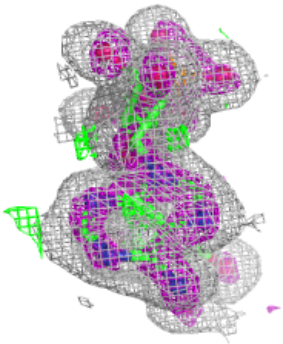


Electron density around NAD O 336:

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

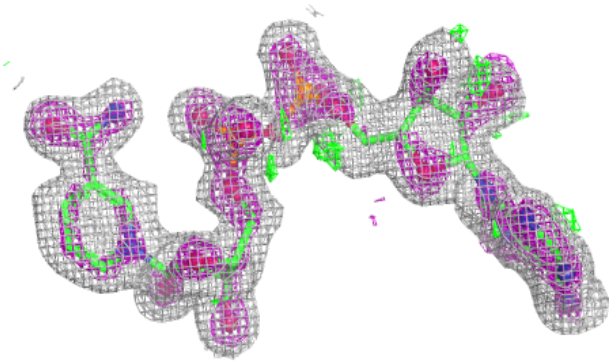


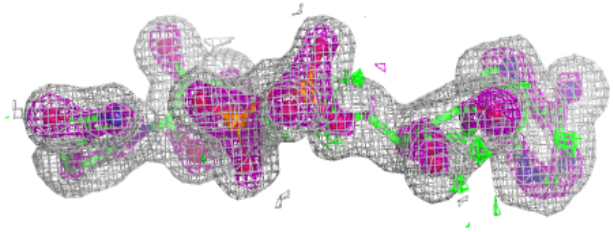


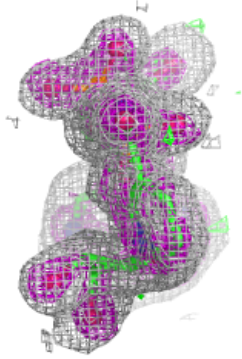


Electron density around NAD B 336:

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

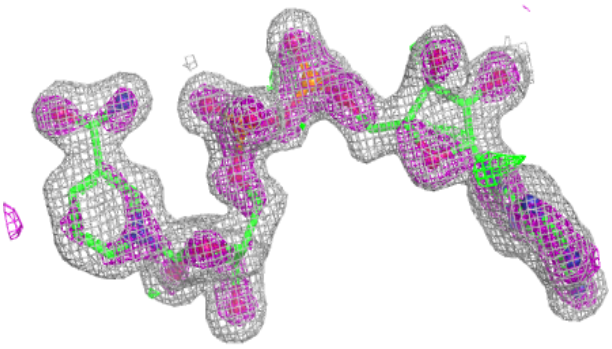


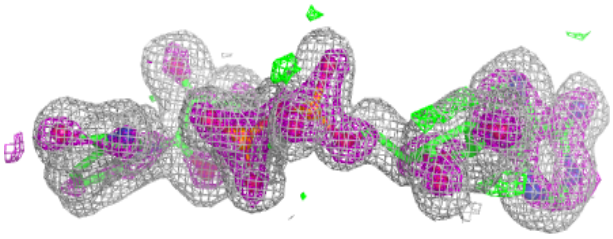


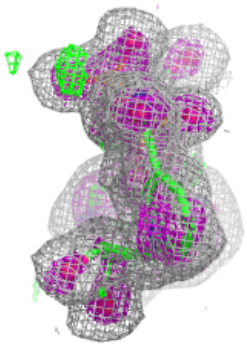


Electron density around NAD A 336:

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

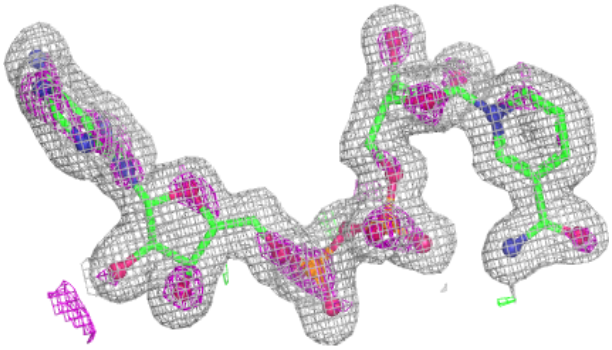


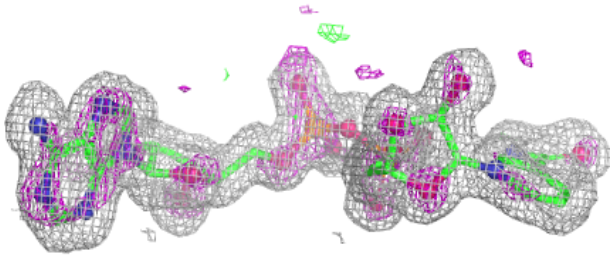


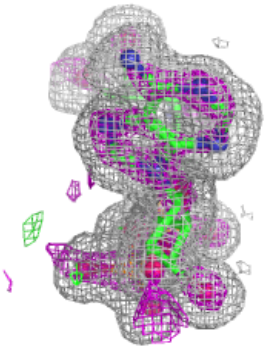


Electron density around NAD C 336:

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

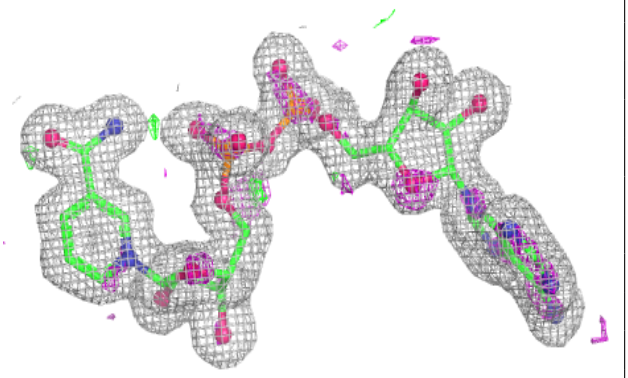


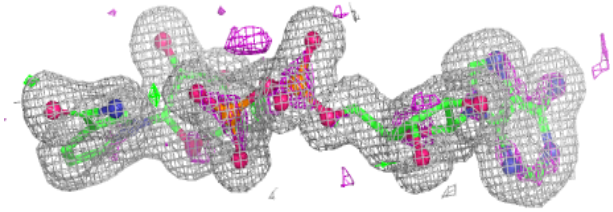


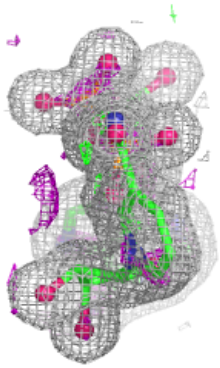


Electron density around NAD Q 336:

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

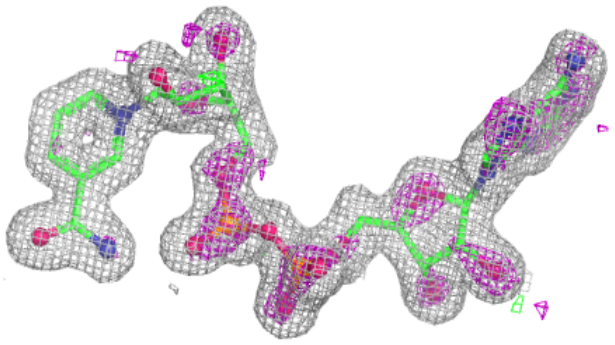


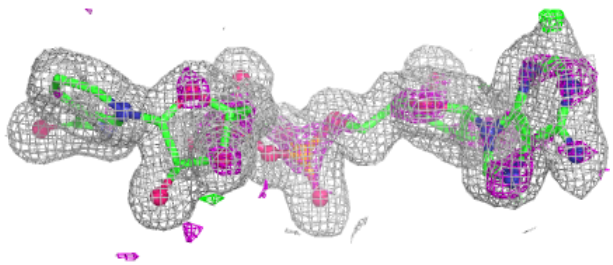


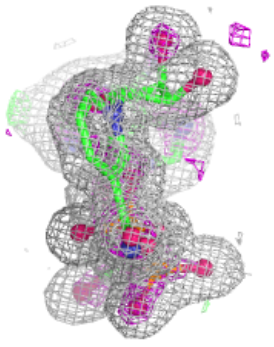


Electron density around NAD R 336:

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

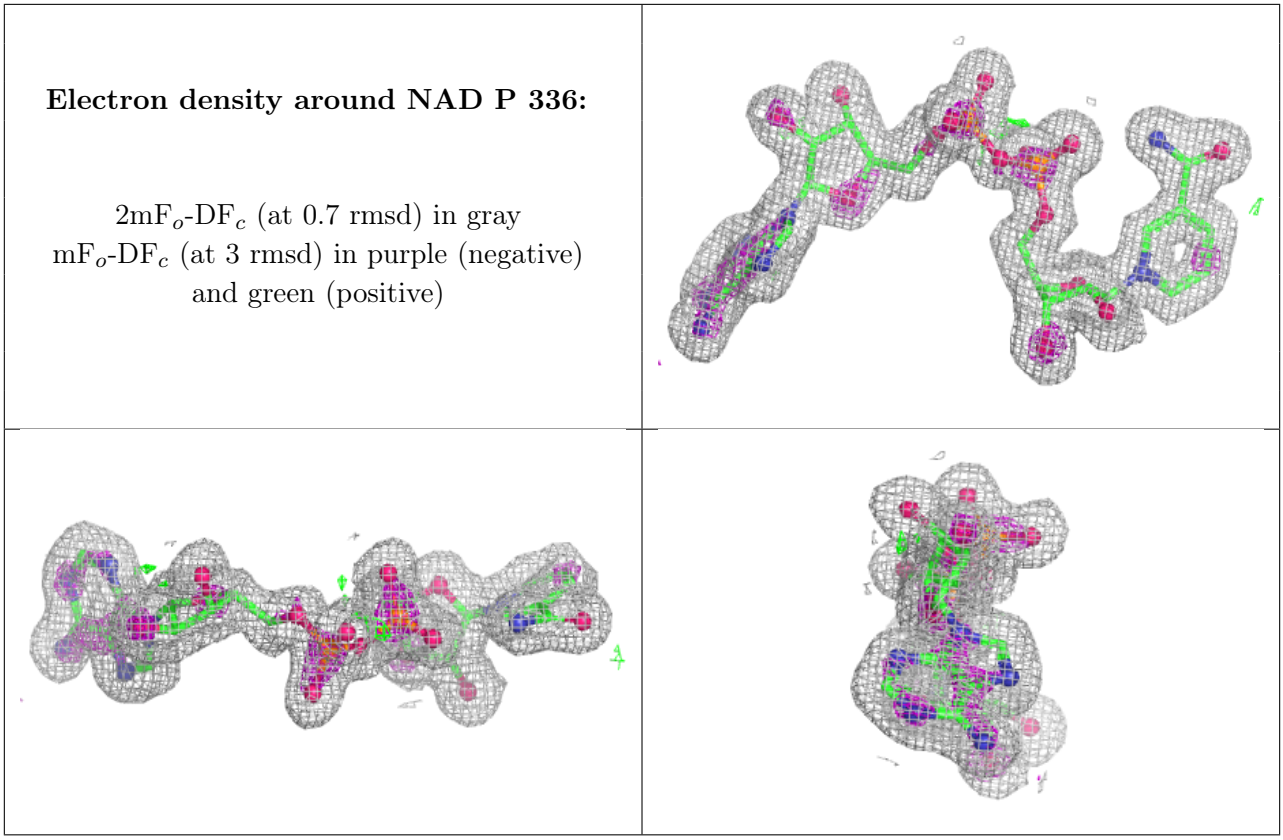






Electron density around NAD P 336:

$2mF_o$-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.