Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:23 am BST

PDB ID	:	6ITE
Title	:	Crystal structure of group A Streptococcal surface dehydrogenase (SDH)
Authors	:	Yuan, C.; Li, R.; Huang, M.D.
Deposited on	:	2018-11-21
Resolution	:	1.74 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 following versions of software and data (see references ⓘ) were used in the production of this report:

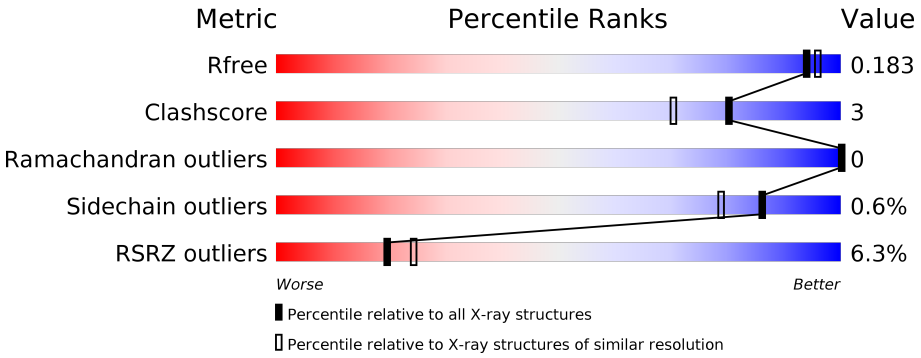
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance

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

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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

Mol	Chain	Length	Quality of chain
1	O	342	4% 95%
1	P	342	3% 94% 6%
1	Q	342	3% 93% 5%
1	R	342	14% 94%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11514 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	P	339	Total	C	N	O	S	0	1	0
			2564	1604	449	501	10			
1	Q	336	Total	C	N	O	S	0	1	0
			2534	1586	440	498	10			
1	R	336	Total	C	N	O	S	0	0	0
			2526	1582	438	496	10			
1	O	341	Total	C	N	O	S	0	1	0
			2584	1616	455	503	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-5	HIS	-	expression tag	UNP P0C0G6
P	-4	HIS	-	expression tag	UNP P0C0G6
P	-3	HIS	-	expression tag	UNP P0C0G6
P	-2	HIS	-	expression tag	UNP P0C0G6
P	-1	HIS	-	expression tag	UNP P0C0G6
P	0	HIS	-	expression tag	UNP P0C0G6
Q	-5	HIS	-	expression tag	UNP P0C0G6
Q	-4	HIS	-	expression tag	UNP P0C0G6
Q	-3	HIS	-	expression tag	UNP P0C0G6
Q	-2	HIS	-	expression tag	UNP P0C0G6
Q	-1	HIS	-	expression tag	UNP P0C0G6
Q	0	HIS	-	expression tag	UNP P0C0G6
R	-5	HIS	-	expression tag	UNP P0C0G6
R	-4	HIS	-	expression tag	UNP P0C0G6
R	-3	HIS	-	expression tag	UNP P0C0G6
R	-2	HIS	-	expression tag	UNP P0C0G6
R	-1	HIS	-	expression tag	UNP P0C0G6
R	0	HIS	-	expression tag	UNP P0C0G6
O	-5	HIS	-	expression tag	UNP P0C0G6
O	-4	HIS	-	expression tag	UNP P0C0G6
O	-3	HIS	-	expression tag	UNP P0C0G6

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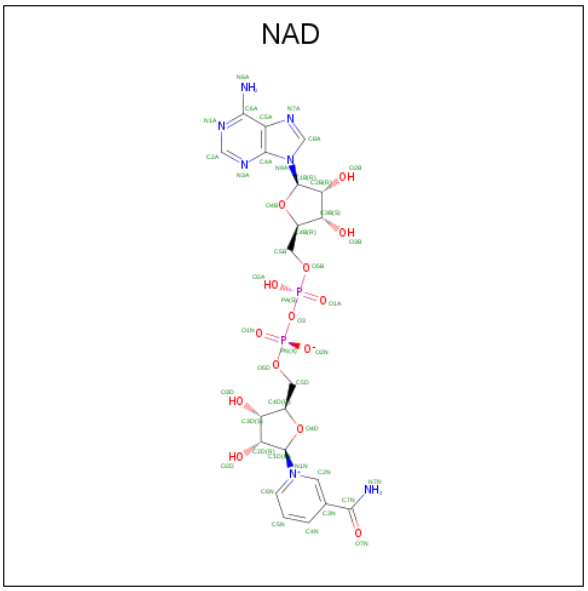
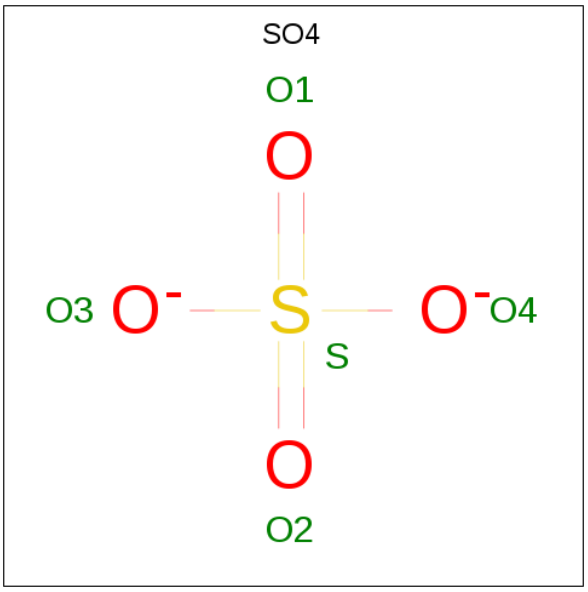
Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	HIS	-	expression tag	UNP P0C0G6
O	-1	HIS	-	expression tag	UNP P0C0G6
O	0	HIS	-	expression tag	UNP P0C0G6

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



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total O S 5 4 1	0	0
3	Q	1	Total O S 5 4 1	0	0
3	Q	1	Total O S 5 4 1	0	0
3	R	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0
3	O	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

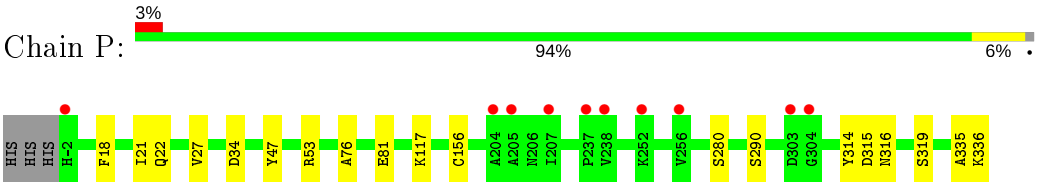
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	318	Total O 318 318	0	0
4	Q	300	Total O 300 300	0	0
4	R	221	Total O 221 221	0	0
4	O	261	Total O 261 261	0	0

3 Residue-property plots (i)

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

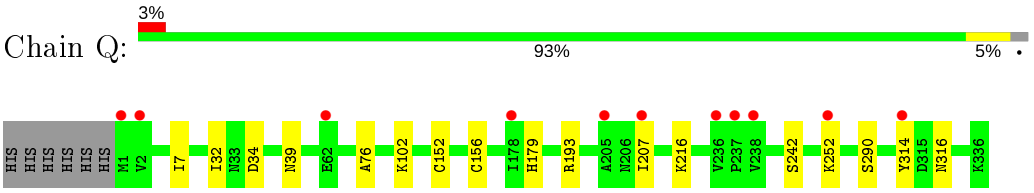
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain P:



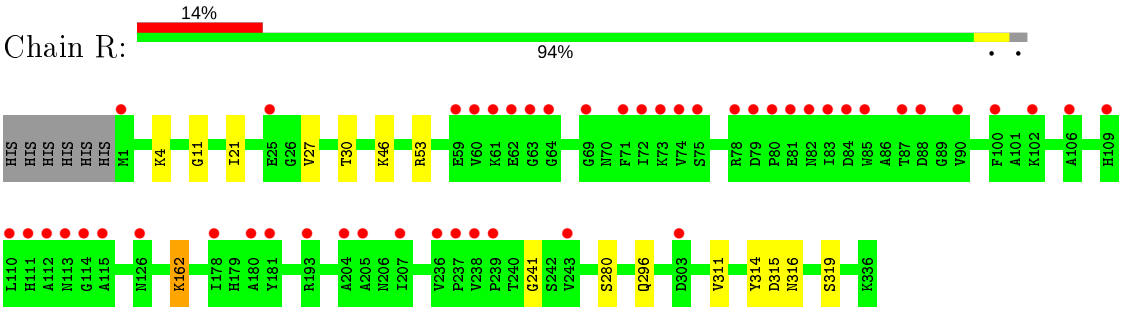
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain Q:



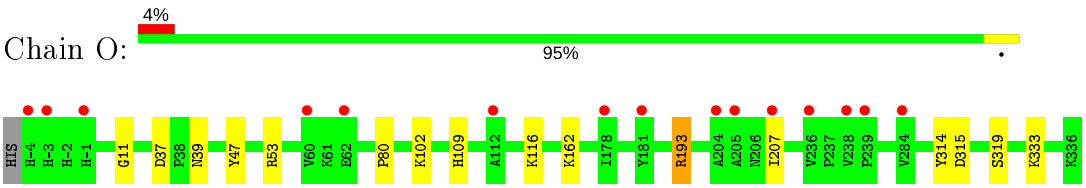
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain R:



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	135.43Å 82.78Å 148.92Å 90.00° 102.05° 90.00°	Depositor
Resolution (Å)	44.58 – 1.74 44.58 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.58-1.74) 99.7 (44.58-1.74)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 1.74Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.142 , 0.181 0.146 , 0.183	Depositor DCC
R_{free} test set	8269 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11514	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: SO4, 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	O	0.32	0/2628	0.52	0/3563
1	P	0.40	0/2606	0.55	0/3533
1	Q	0.35	0/2573	0.54	0/3488
1	R	0.31	0/2565	0.51	0/3477
All	All	0.35	0/10372	0.53	0/14061

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2584	0	2561	12	0
1	P	2564	0	2547	12	0
1	Q	2534	0	2526	18	0
1	R	2526	0	2521	15	0
2	O	44	0	25	1	0
2	P	44	0	25	1	0
2	Q	44	0	25	1	0
2	R	44	0	24	1	0
3	O	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	5	0	0	0	0
3	Q	10	0	0	0	0
3	R	5	0	0	0	0
4	O	261	0	0	3	0
4	P	318	0	0	1	0
4	Q	300	0	0	4	0
4	R	221	0	0	1	0
All	All	11514	0	10254	55	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 3.

All (55) 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:Q:152:CYS:HB2	1:Q:314:TYR:HE1	1.35	0.90
1:Q:316:ASN:HD22	2:Q:401:NAD:H72N	1.23	0.85
1:P:316:ASN:HD22	2:P:401:NAD:H72N	1.26	0.84
1:Q:179:HIS:CD2	1:Q:314:TYR:OH	2.31	0.83
1:Q:152:CYS:HB2	1:Q:314:TYR:CE1	2.16	0.80
1:O:162:LYS:HE2	4:O:733:HOH:O	1.86	0.76
1:Q:179:HIS:HD2	1:Q:314:TYR:OH	1.72	0.72
1:Q:242:SER:HB2	1:Q:314:TYR:CE2	2.26	0.69
1:P:21:ILE:HG23	1:P:27:VAL:HG23	1.77	0.67
1:Q:102:LYS:HD2	4:Q:783:HOH:O	2.01	0.60
1:Q:216:LYS:NZ	4:Q:501:HOH:O	2.35	0.60
1:R:46:LYS:HG3	1:R:53:ARG:HH21	1.67	0.59
1:O:193:ARG:H	1:O:193:ARG:NH1	2.02	0.58
1:R:296:GLN:HB2	1:R:311:VAL:CG2	2.32	0.58
1:O:102:LYS:HE2	4:O:515:HOH:O	2.05	0.56
1:P:81:GLU:HG3	4:P:589:HOH:O	2.05	0.56
1:Q:7:ILE:HB	1:Q:32:ILE:HD13	1.89	0.55
1:Q:152:CYS:CB	1:Q:314:TYR:HE1	2.14	0.53
1:O:193:ARG:H	1:O:193:ARG:HH11	1.56	0.53
1:Q:156:CYS:HA	1:Q:290:SER:HB2	1.91	0.52
1:P:117:LYS:NZ	1:P:336:LYS:HG3	2.25	0.51
1:O:315:ASP:O	1:O:319:SER:HB2	2.11	0.51
1:R:296:GLN:HB2	1:R:311:VAL:HG21	1.91	0.51
1:R:46:LYS:HG3	1:R:53:ARG:NH2	2.27	0.50
1:Q:39[B]:ASN:ND2	4:Q:504:HOH:O	2.41	0.48
1:Q:39[B]:ASN:ND2	4:Q:503:HOH:O	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:117:LYS:CE	1:P:336:LYS:HG3	2.45	0.47
1:R:296:GLN:HB2	1:R:311:VAL:HG22	1.97	0.46
1:P:117:LYS:HE3	1:P:335:ALA:HB1	1.98	0.45
1:Q:252:LYS:HA	1:Q:252:LYS:HD3	1.82	0.45
1:R:162:LYS:HE3	4:R:644:HOH:O	2.15	0.45
1:O:333:LYS:HE2	1:O:333:LYS:HB3	1.73	0.45
1:Q:207:ILE:HB	1:R:280:SER:HB3	1.98	0.45
1:P:315:ASP:O	1:P:319:SER:HB2	2.18	0.44
1:R:296:GLN:CD	1:R:311:VAL:HG21	2.37	0.44
1:R:46:LYS:HE3	1:R:53:ARG:NH2	2.32	0.44
1:P:280:SER:HB3	1:O:207:ILE:HB	2.00	0.44
1:R:11:GLY:HA3	2:R:401:NAD:O5B	2.18	0.44
1:R:315:ASP:O	1:R:319:SER:HB2	2.18	0.44
1:P:156:CYS:HA	1:P:290:SER:HB2	1.99	0.44
1:P:47:TYR:CE1	1:P:53:ARG:HD3	2.53	0.43
1:R:21:ILE:HG23	1:R:27:VAL:HG23	2.00	0.43
1:Q:242:SER:CB	1:Q:314:TYR:CE2	2.97	0.43
1:O:47:TYR:CE1	1:O:53:ARG:HD3	2.53	0.43
1:Q:34:ASP:O	1:Q:76:ALA:HA	2.19	0.43
1:O:116:LYS:NZ	4:O:511:HOH:O	2.52	0.42
1:O:37:ASP:OD1	1:O:39[B]:ASN:HB2	2.19	0.42
1:O:11:GLY:HA3	2:O:401:NAD:O5B	2.20	0.42
1:P:34:ASP:O	1:P:76:ALA:HA	2.20	0.41
1:R:241:GLY:H	1:R:316:ASN:ND2	2.17	0.41
1:R:4:LYS:HD3	1:R:30:THR:HG21	2.01	0.41
1:P:18:PHE:O	1:P:22:GLN:HG2	2.20	0.41
1:O:80:PRO:HB3	1:O:109:HIS:CE1	2.55	0.41
1:R:241:GLY:H	1:R:316:ASN:HD21	1.67	0.41
1:Q:102:LYS:HD3	1:Q:102:LYS:HA	1.95	0.41

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	340/342 (99%)	325 (96%)	15 (4%)	0	100	100
1	P	338/342 (99%)	326 (96%)	12 (4%)	0	100	100
1	Q	335/342 (98%)	323 (96%)	12 (4%)	0	100	100
1	R	334/342 (98%)	320 (96%)	14 (4%)	0	100	100
All	All	1347/1368 (98%)	1294 (96%)	53 (4%)	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	O	276/276 (100%)	274 (99%)	2 (1%)	84	75
1	P	274/276 (99%)	273 (100%)	1 (0%)	91	86
1	Q	271/276 (98%)	270 (100%)	1 (0%)	91	86
1	R	270/276 (98%)	268 (99%)	2 (1%)	84	75
All	All	1091/1104 (99%)	1085 (100%)	6 (0%)	86	83

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	314	TYR
1	Q	193	ARG
1	R	162	LYS
1	R	314	TYR
1	O	193	ARG
1	O	314	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 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	O	401	-	42,48,48	4.55	18 (42%)	50,73,73	1.66	11 (22%)
2	NAD	R	401	-	42,48,48	4.55	18 (42%)	50,73,73	1.54	8 (16%)
3	SO4	Q	402	-	4,4,4	0.12	0	6,6,6	0.13	0
2	NAD	P	401	-	42,48,48	4.23	17 (40%)	50,73,73	1.63	10 (20%)
3	SO4	O	402	-	4,4,4	0.18	0	6,6,6	0.08	0
3	SO4	Q	403	-	4,4,4	0.12	0	6,6,6	0.14	0
3	SO4	P	402	-	4,4,4	0.13	0	6,6,6	0.17	0
3	SO4	O	403	-	4,4,4	0.14	0	6,6,6	0.14	0
2	NAD	Q	401	-	42,48,48	4.33	16 (38%)	50,73,73	1.62	9 (18%)
3	SO4	R	402	-	4,4,4	0.17	0	6,6,6	0.20	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	Q	401	-	-	5/26/62/62	0/5/5/5
2	NAD	R	401	-	-	5/26/62/62	0/5/5/5
2	NAD	O	401	-	-	5/26/62/62	0/5/5/5
2	NAD	P	401	-	-	5/26/62/62	0/5/5/5

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	401	NAD	C2B-C1B	-16.30	1.29	1.53
2	O	401	NAD	C2B-C1B	-15.78	1.29	1.53
2	Q	401	NAD	C2B-C1B	-15.36	1.30	1.53
2	P	401	NAD	C2B-C1B	-15.11	1.30	1.53
2	O	401	NAD	O4B-C1B	14.94	1.61	1.41
2	R	401	NAD	O4B-C1B	14.29	1.61	1.41
2	Q	401	NAD	O4B-C1B	13.19	1.59	1.41
2	P	401	NAD	O4B-C1B	13.11	1.59	1.41
2	R	401	NAD	C2D-C3D	-9.83	1.26	1.53
2	O	401	NAD	C2D-C3D	-9.69	1.26	1.53
2	Q	401	NAD	C2D-C3D	-9.41	1.27	1.53
2	P	401	NAD	C2D-C3D	-9.13	1.28	1.53
2	Q	401	NAD	C7N-N7N	6.88	1.46	1.33
2	R	401	NAD	O4D-C1D	6.88	1.50	1.41
2	R	401	NAD	C7N-N7N	6.79	1.45	1.33
2	O	401	NAD	O4D-C1D	6.73	1.50	1.41
2	O	401	NAD	C7N-N7N	6.54	1.45	1.33
2	P	401	NAD	C7N-N7N	6.42	1.45	1.33
2	P	401	NAD	O4D-C1D	6.27	1.49	1.41
2	Q	401	NAD	O4D-C1D	6.07	1.49	1.41
2	R	401	NAD	O4B-C4B	-6.03	1.31	1.45
2	Q	401	NAD	O4B-C4B	-6.01	1.31	1.45
2	O	401	NAD	O4D-C4D	-5.70	1.32	1.45
2	R	401	NAD	O4D-C4D	-5.67	1.32	1.45
2	O	401	NAD	O4B-C4B	-5.66	1.32	1.45
2	Q	401	NAD	O4D-C4D	-5.42	1.32	1.45
2	P	401	NAD	O4B-C4B	-5.38	1.33	1.45
2	R	401	NAD	C3D-C4D	5.28	1.66	1.53
2	Q	401	NAD	C3D-C4D	5.26	1.66	1.53
2	P	401	NAD	O4D-C4D	-5.25	1.33	1.45
2	O	401	NAD	C2D-C1D	5.04	1.61	1.53
2	O	401	NAD	C3D-C4D	5.00	1.65	1.53
2	P	401	NAD	C3D-C4D	5.00	1.65	1.53
2	Q	401	NAD	C2D-C1D	4.68	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	401	NAD	C2D-C1D	4.52	1.60	1.53
2	R	401	NAD	C2D-C1D	4.49	1.60	1.53
2	P	401	NAD	C6A-N6A	3.75	1.47	1.34
2	Q	401	NAD	C6A-N6A	3.64	1.47	1.34
2	O	401	NAD	C6A-N6A	3.59	1.47	1.34
2	R	401	NAD	C6A-N6A	3.53	1.46	1.34
2	O	401	NAD	C3N-C7N	3.34	1.55	1.50
2	Q	401	NAD	O2D-C2D	3.18	1.50	1.43
2	O	401	NAD	O2D-C2D	3.10	1.50	1.43
2	O	401	NAD	C2A-N3A	3.05	1.37	1.32
2	R	401	NAD	C3N-C7N	3.03	1.55	1.50
2	P	401	NAD	O2D-C2D	3.02	1.50	1.43
2	R	401	NAD	O2D-C2D	2.98	1.50	1.43
2	Q	401	NAD	C3N-C7N	2.97	1.55	1.50
2	O	401	NAD	O2B-C2B	2.95	1.49	1.43
2	P	401	NAD	C3N-C7N	2.89	1.54	1.50
2	P	401	NAD	O2B-C2B	2.83	1.49	1.43
2	R	401	NAD	O2B-C2B	2.75	1.49	1.43
2	Q	401	NAD	O2B-C2B	2.67	1.49	1.43
2	P	401	NAD	C2A-N3A	2.64	1.36	1.32
2	Q	401	NAD	C5A-C4A	-2.57	1.34	1.40
2	R	401	NAD	C2A-N3A	2.48	1.36	1.32
2	R	401	NAD	C5A-C4A	-2.47	1.34	1.40
2	R	401	NAD	O3B-C3B	-2.43	1.37	1.43
2	P	401	NAD	C5A-C4A	-2.42	1.34	1.40
2	O	401	NAD	O3D-C3D	2.42	1.48	1.43
2	O	401	NAD	C5A-C4A	-2.37	1.34	1.40
2	R	401	NAD	O7N-C7N	-2.33	1.19	1.24
2	Q	401	NAD	C2A-N3A	2.29	1.35	1.32
2	O	401	NAD	O7N-C7N	-2.27	1.19	1.24
2	Q	401	NAD	O3D-C3D	2.24	1.48	1.43
2	O	401	NAD	O3B-C3B	-2.23	1.37	1.43
2	P	401	NAD	O3B-C3B	-2.09	1.38	1.43
2	P	401	NAD	O3D-C3D	2.07	1.47	1.43
2	R	401	NAD	O3D-C3D	2.05	1.47	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	401	NAD	N3A-C2A-N1A	-6.00	119.31	128.68
2	R	401	NAD	N3A-C2A-N1A	-5.84	119.56	128.68
2	O	401	NAD	N3A-C2A-N1A	-5.80	119.61	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	401	NAD	N3A-C2A-N1A	-5.48	120.11	128.68
2	O	401	NAD	C5A-C6A-N6A	4.04	126.50	120.35
2	P	401	NAD	O4D-C1D-C2D	-3.71	101.50	106.93
2	P	401	NAD	C5A-C6A-N6A	3.67	125.93	120.35
2	O	401	NAD	O7N-C7N-C3N	3.63	123.97	119.63
2	R	401	NAD	C5A-C6A-N6A	3.54	125.74	120.35
2	P	401	NAD	O7N-C7N-C3N	3.51	123.84	119.63
2	Q	401	NAD	C5A-C6A-N6A	3.21	125.23	120.35
2	R	401	NAD	O4D-C1D-C2D	-3.13	102.35	106.93
2	Q	401	NAD	O7N-C7N-C3N	3.06	123.29	119.63
2	O	401	NAD	C2N-C3N-C4N	2.94	121.59	118.26
2	Q	401	NAD	O4D-C1D-C2D	-2.91	102.67	106.93
2	Q	401	NAD	C3N-C7N-N7N	-2.91	114.26	117.75
2	R	401	NAD	C2N-C3N-C4N	2.86	121.50	118.26
2	Q	401	NAD	C2N-C3N-C4N	2.85	121.49	118.26
2	P	401	NAD	C3N-C7N-N7N	-2.66	114.55	117.75
2	P	401	NAD	C2N-C3N-C4N	2.61	121.22	118.26
2	O	401	NAD	N6A-C6A-N1A	-2.56	113.25	118.57
2	O	401	NAD	C3N-C7N-N7N	-2.53	114.71	117.75
2	P	401	NAD	O3D-C3D-C4D	-2.53	103.75	111.05
2	R	401	NAD	O7N-C7N-C3N	2.49	122.61	119.63
2	Q	401	NAD	C6N-N1N-C2N	-2.47	119.72	121.97
2	Q	401	NAD	O3D-C3D-C4D	-2.45	103.97	111.05
2	O	401	NAD	O3D-C3D-C4D	-2.39	104.14	111.05
2	O	401	NAD	O4D-C1D-C2D	-2.32	103.53	106.93
2	P	401	NAD	O4B-C1B-C2B	-2.21	103.69	106.93
2	P	401	NAD	C6N-N1N-C2N	-2.17	120.00	121.97
2	O	401	NAD	C3N-C2N-N1N	-2.16	118.32	120.43
2	R	401	NAD	N6A-C6A-N1A	-2.12	114.18	118.57
2	R	401	NAD	PN-O3-PA	-2.08	125.69	132.83
2	R	401	NAD	C3N-C2N-N1N	-2.07	118.40	120.43
2	O	401	NAD	C6N-N1N-C2N	-2.06	120.10	121.97
2	Q	401	NAD	O4B-C1B-C2B	-2.05	103.93	106.93
2	P	401	NAD	N6A-C6A-N1A	-2.04	114.35	118.57
2	O	401	NAD	PN-O3-PA	-2.00	125.95	132.83

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	401	NAD	O4D-C1D-N1N-C2N
2	O	401	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	O	401	NAD	C2D-C1D-N1N-C2N
2	O	401	NAD	C2D-C1D-N1N-C6N
2	R	401	NAD	O4D-C1D-N1N-C2N
2	R	401	NAD	O4D-C1D-N1N-C6N
2	R	401	NAD	C2D-C1D-N1N-C6N
2	P	401	NAD	O4D-C1D-N1N-C2N
2	P	401	NAD	O4D-C1D-N1N-C6N
2	P	401	NAD	C2D-C1D-N1N-C2N
2	P	401	NAD	C2D-C1D-N1N-C6N
2	Q	401	NAD	O4D-C1D-N1N-C2N
2	Q	401	NAD	O4D-C1D-N1N-C6N
2	Q	401	NAD	C2D-C1D-N1N-C2N
2	Q	401	NAD	C2D-C1D-N1N-C6N
2	R	401	NAD	C2D-C1D-N1N-C2N
2	R	401	NAD	O4B-C4B-C5B-O5B
2	O	401	NAD	O4B-C4B-C5B-O5B
2	P	401	NAD	O4B-C4B-C5B-O5B
2	Q	401	NAD	O4B-C4B-C5B-O5B

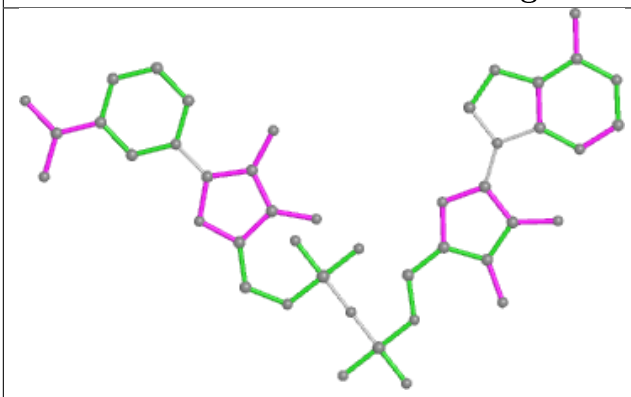
There are no ring outliers.

4 monomers are involved in 4 short contacts:

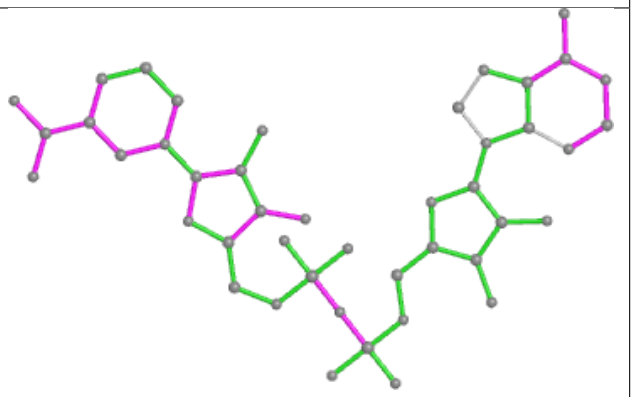
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	401	NAD	1	0
2	R	401	NAD	1	0
2	P	401	NAD	1	0
2	Q	401	NAD	1	0

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.

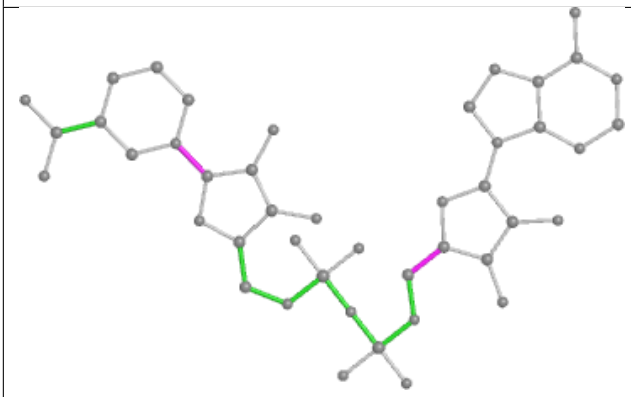
Ligand NAD O 401



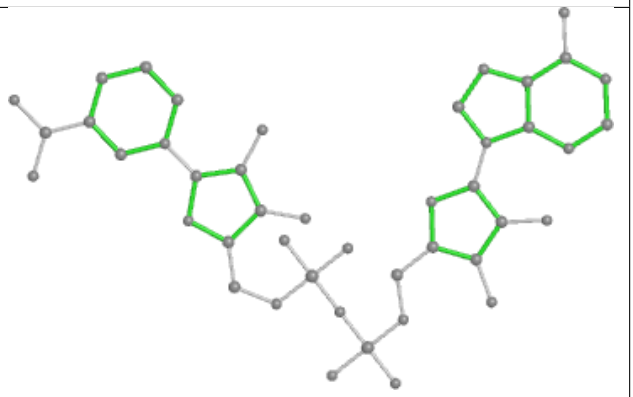
Bond lengths



Bond angles

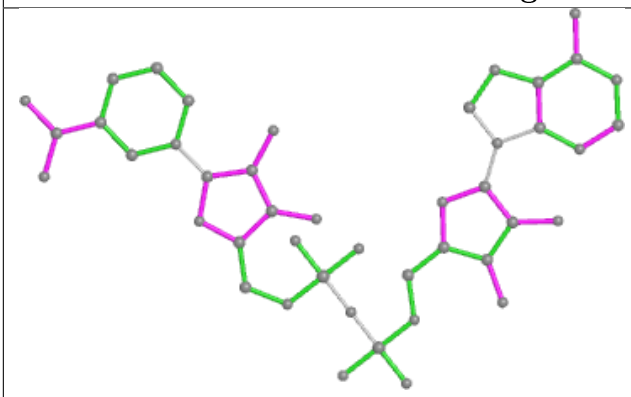


Torsions

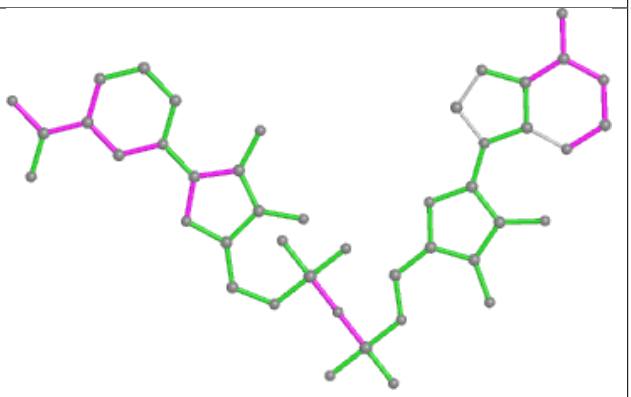


Rings

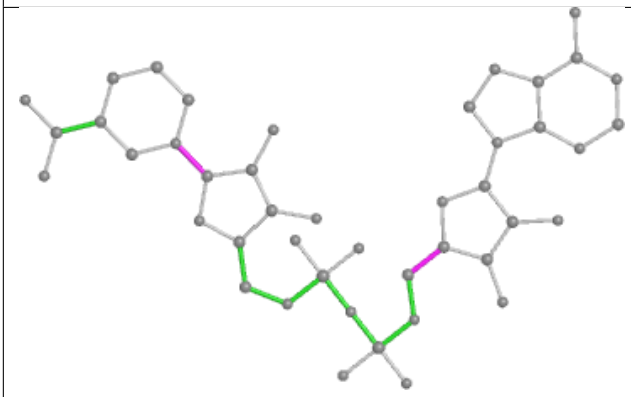
Ligand NAD R 401



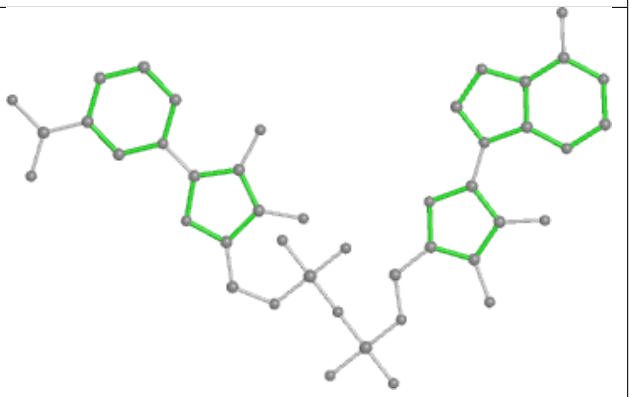
Bond lengths



Bond angles

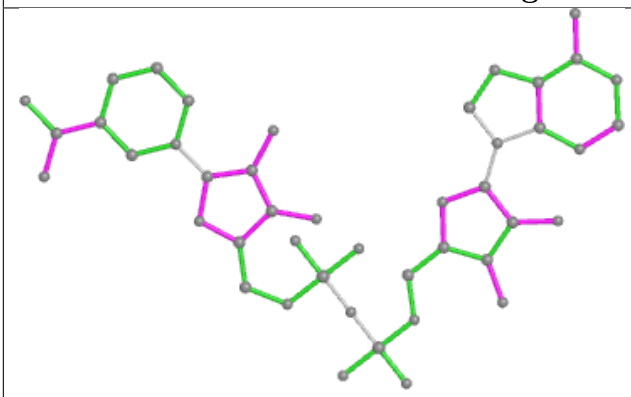


Torsions

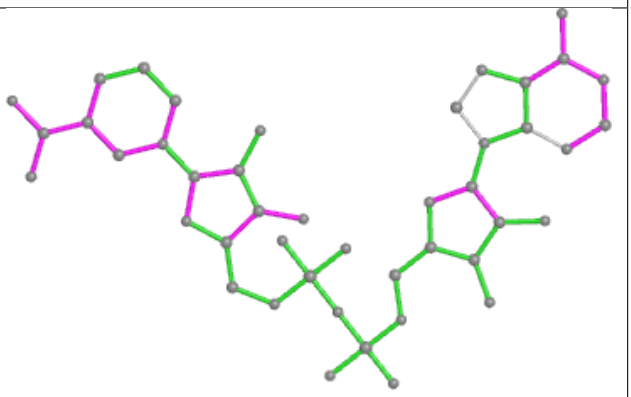


Rings

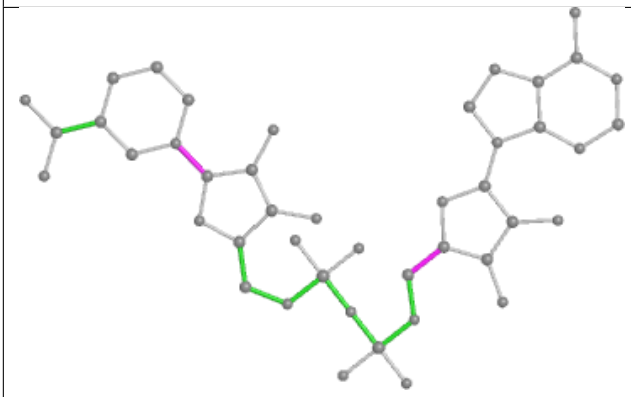
Ligand NAD P 401



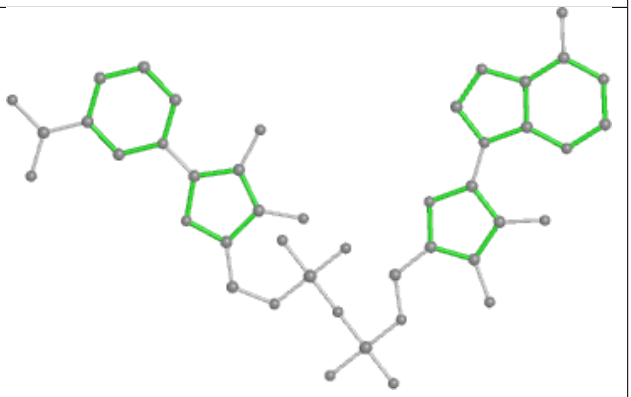
Bond lengths



Bond angles

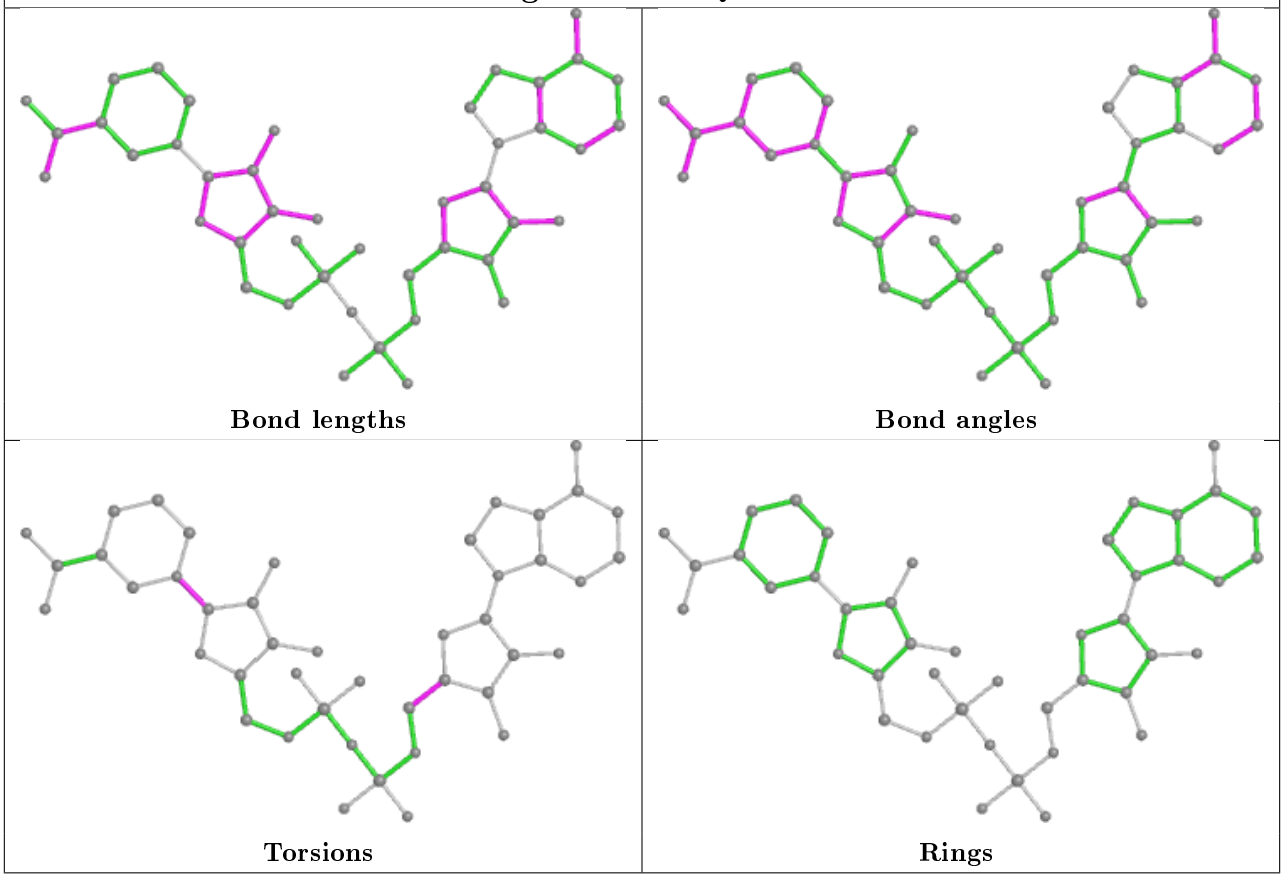


Torsions



Rings

Ligand NAD Q 401



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	O	341/342 (99%)	0.10	15 (4%) 34 39	20, 33, 52, 97	0
1	P	339/342 (99%)	-0.11	10 (2%) 51 57	16, 25, 43, 65	0
1	Q	336/342 (98%)	-0.03	11 (3%) 46 52	17, 26, 44, 75	0
1	R	336/342 (98%)	0.36	49 (14%) 2 3	19, 34, 58, 81	0
All	All	1352/1368 (98%)	0.08	85 (6%) 20 24	16, 30, 53, 97	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	-4	HIS	7.4
1	R	1	MET	4.5
1	R	71	PHE	4.2
1	R	115	ALA	3.8
1	Q	1	MET	3.7
1	Q	205	ALA	3.5
1	Q	207	ILE	3.5
1	R	236	VAL	3.4
1	R	243	VAL	3.4
1	R	87	THR	3.3
1	R	83	ILE	3.3
1	R	62	GLU	3.3
1	R	238	VAL	3.2
1	Q	178	ILE	3.2
1	R	80	PRO	3.1
1	R	61	LYS	3.1
1	Q	238	VAL	3.1
1	P	303	ASP	3.1
1	R	85	TRP	3.0
1	O	-3	HIS	3.0
1	Q	314	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	R	193	ARG	2.9
1	R	25	GLU	2.9
1	R	113	ASN	2.9
1	P	-2	HIS	2.9
1	R	81	GLU	2.9
1	P	304	GLY	2.9
1	Q	236	VAL	2.8
1	R	60	VAL	2.8
1	O	60	VAL	2.8
1	P	237	PRO	2.7
1	Q	62	GLU	2.7
1	O	181	TYR	2.7
1	R	205	ALA	2.7
1	R	73	LYS	2.6
1	R	181	TYR	2.6
1	Q	252	LYS	2.6
1	R	126	ASN	2.6
1	O	112	ALA	2.5
1	P	205	ALA	2.5
1	R	112	ALA	2.5
1	R	178	ILE	2.5
1	P	238	VAL	2.5
1	P	252	LYS	2.5
1	P	204	ALA	2.4
1	R	100	PHE	2.4
1	O	284	VAL	2.4
1	R	74	VAL	2.4
1	O	62	GLU	2.4
1	R	237	PRO	2.4
1	R	180	ALA	2.4
1	R	239	PRO	2.4
1	R	84	ASP	2.4
1	R	114	GLY	2.4
1	R	78	ARG	2.3
1	R	82	ASN	2.3
1	O	239	PRO	2.3
1	R	88	ASP	2.3
1	O	204	ALA	2.3
1	Q	237	PRO	2.3
1	R	204	ALA	2.3
1	O	205	ALA	2.3
1	R	69	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	256	VAL	2.2
1	R	207	ILE	2.2
1	O	238	VAL	2.2
1	R	111	HIS	2.2
1	R	63	GLY	2.2
1	O	236	VAL	2.1
1	R	110	LEU	2.1
1	R	303	ASP	2.1
1	R	72	ILE	2.1
1	O	178	ILE	2.1
1	R	106	ALA	2.1
1	R	102	LYS	2.1
1	R	64	GLY	2.1
1	O	207	ILE	2.1
1	R	109	HIS	2.1
1	O	-1	HIS	2.1
1	R	59	GLU	2.1
1	P	207	ILE	2.1
1	Q	2	VAL	2.1
1	R	75	SER	2.1
1	R	90	VAL	2.0
1	R	79	ASP	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	SO4	R	402	5/5	0.91	0.14	59,60,65,66	0

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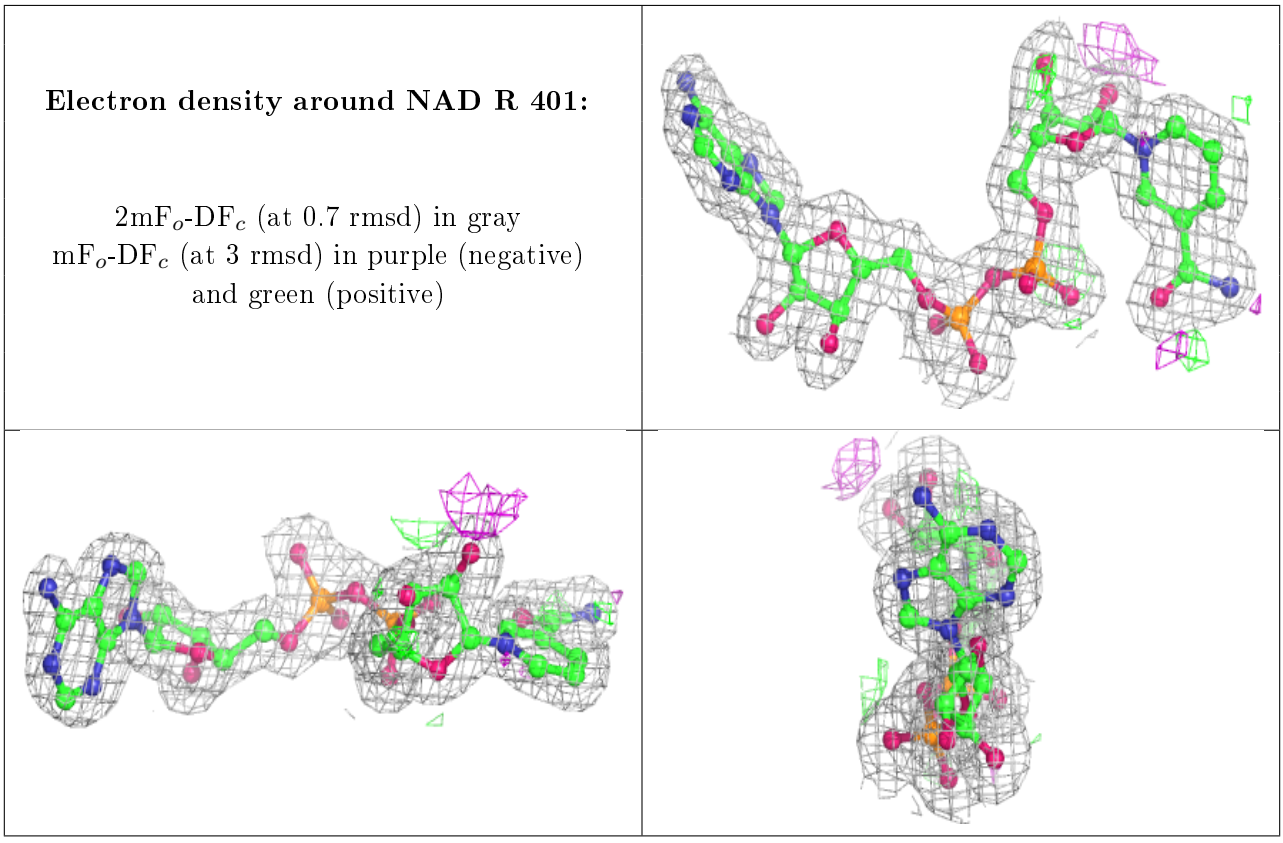
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	R	401	44/44	0.95	0.09	24,29,36,38	0
3	SO4	O	403	5/5	0.96	0.11	63,63,69,69	0
2	NAD	O	401	44/44	0.97	0.09	22,27,34,35	0
2	NAD	Q	401	44/44	0.98	0.07	17,19,22,24	0
2	NAD	P	401	44/44	0.98	0.07	15,18,20,23	0
3	SO4	P	402	5/5	0.99	0.07	30,33,34,35	0
3	SO4	Q	402	5/5	0.99	0.09	29,32,33,34	0
3	SO4	O	402	5/5	0.99	0.08	43,45,46,46	0
3	SO4	Q	403	5/5	0.99	0.09	48,49,55,56	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.

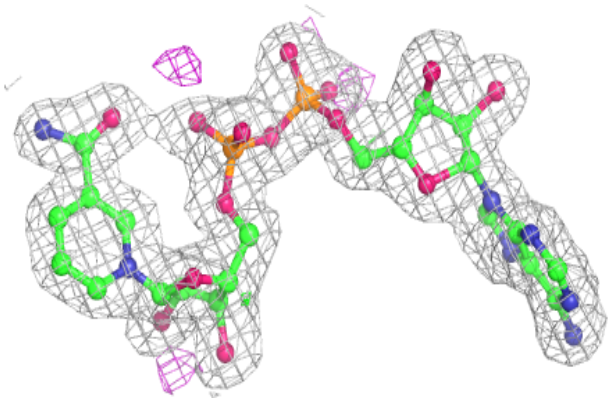
Electron density around NAD R 401:

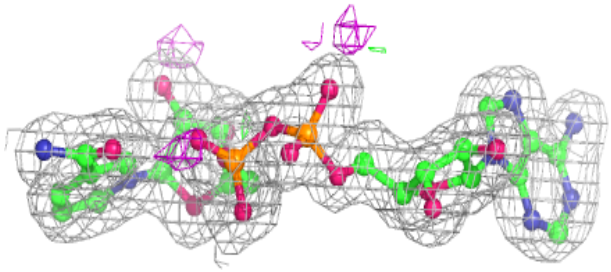
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

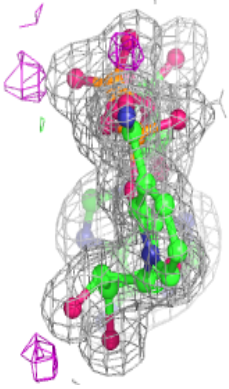


Electron density around NAD O 401:

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

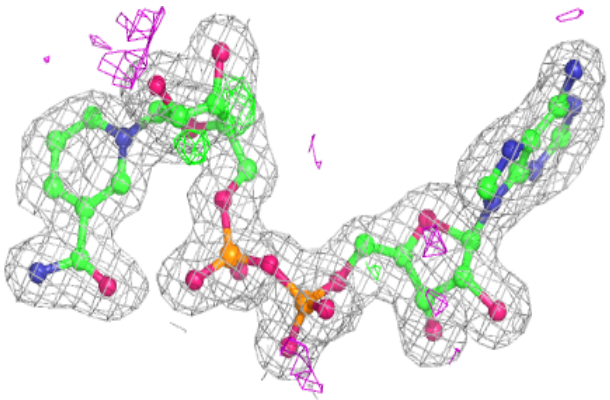


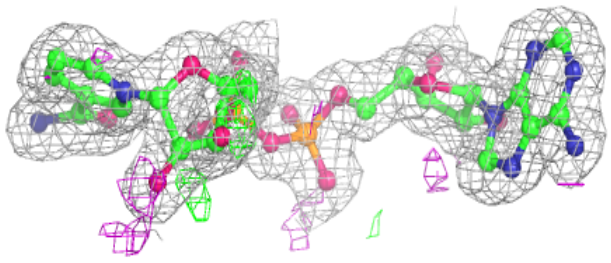


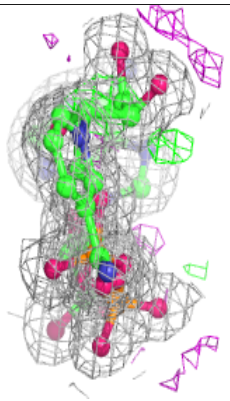


Electron density around NAD Q 401:

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

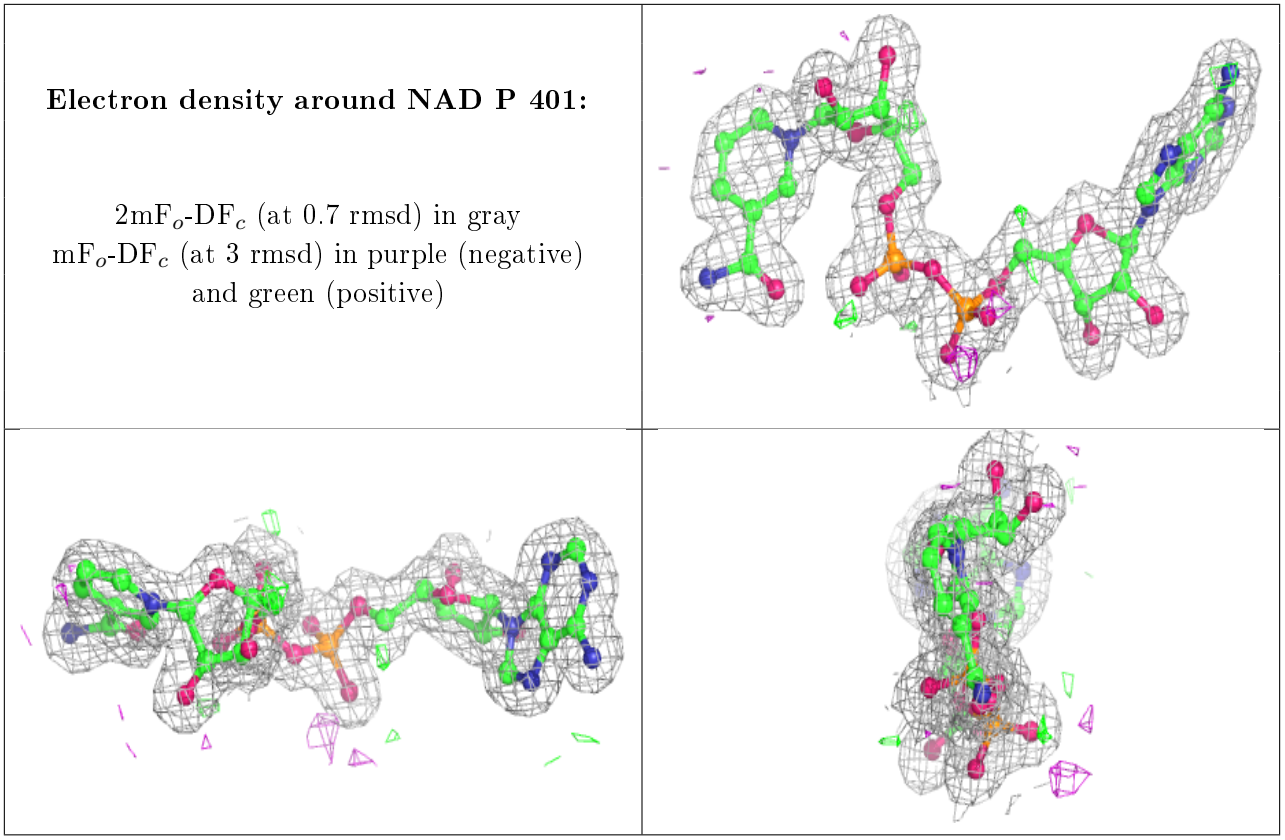






Electron density around NAD P 401:

$2mF_o$-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.