



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 29, 2025 – 02:35 PM JST

PDB ID : 9L3E / pdb\_00009l3e  
Title : Structure of GAPDH complexed with Leu-F  
Authors : Gong, L.  
Deposited on : 2024-12-18  
Resolution : 1.77 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

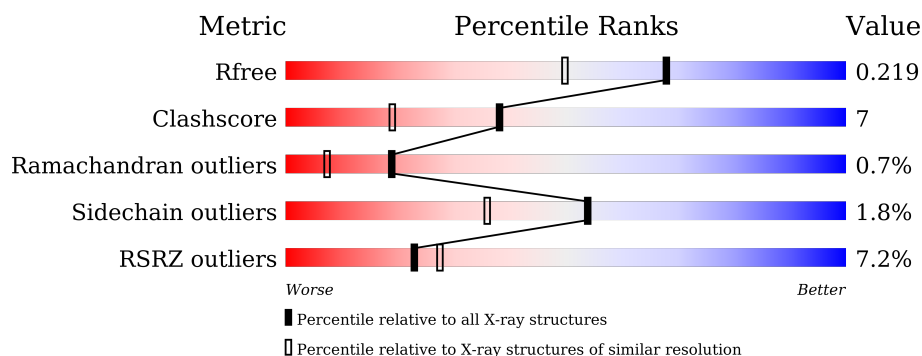
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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))
$R_{free}$	164625	1191 (1.78-1.78)
Clashscore	180529	1282 (1.78-1.78)
Ramachandran outliers	177936	1270 (1.78-1.78)
Sidechain outliers	177891	1270 (1.78-1.78)
RSRZ outliers	164620	1191 (1.78-1.78)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	336	
1	P	336	
1	Q	336	
1	R	336	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	A1L6Z	O	401	X	-	X	-
4	CL	O	404	-	-	X	-
4	CL	P	403	-	-	X	-
4	CL	Q	403	-	-	X	-
5	NAD	O	406	X	-	X	-
5	NAD	Q	404	X	-	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11395 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.

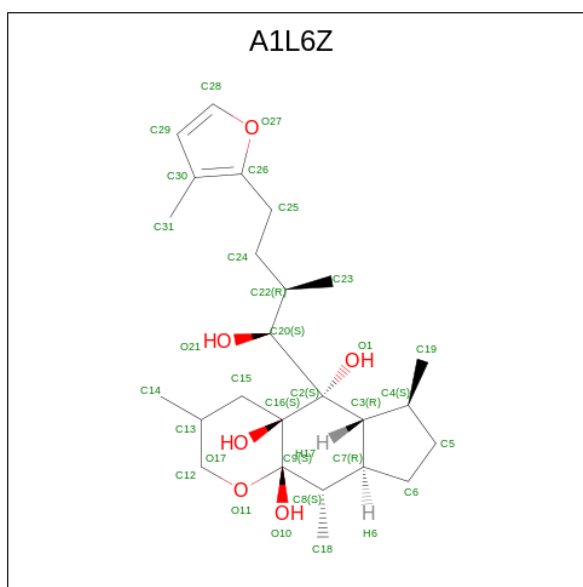
- Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	333	Total	C	N	O	S	0	4	0
			2545	1614	439	479	13			
1	P	336	Total	C	N	O	S	0	7	0
			2578	1634	444	487	13			
1	R	334	Total	C	N	O	S	0	9	0
			2576	1632	447	485	12			
1	Q	333	Total	C	N	O	S	32	5	0
			2550	1615	443	480	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	0	SER	-	expression tag	UNP P04406
P	0	SER	-	expression tag	UNP P04406
R	0	SER	-	expression tag	UNP P04406
Q	0	SER	-	expression tag	UNP P04406

- Molecule 2 is (4 {a} {S},5 {S},5 {a} {R},6 {S},8 {a} {R},9 {S},9 {a} {S})-3,6,9-trimethyl-5-[(1 {S},2 {R})-2-methyl-4-(3-methylfuran-2-yl)-1-oxidanyl-butyl]-3,4,5 {a},6,7,8,8 {a},9-octahydro-2 {H}-cyclopenta[g]chromene-4 {a},5,9 {a}-triol (CCD ID: A1L6Z) (formula: C<sub>25</sub>H<sub>40</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	O	1	Total	C O	0	0
			31	25 6		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	2	Total	Zn	0	0
			2	2		
3	P	2	Total	Zn	0	0
			2	2		
3	R	1	Total	Zn	0	0
			1	1		
3	Q	2	Total	Zn	0	0
			2	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	2	Total	Cl	0	0
			2	2		
4	P	1	Total	Cl	0	0
			1	1		
4	R	1	Total	Cl	0	0
			1	1		
4	Q	1	Total	Cl	0	0
			1	1		

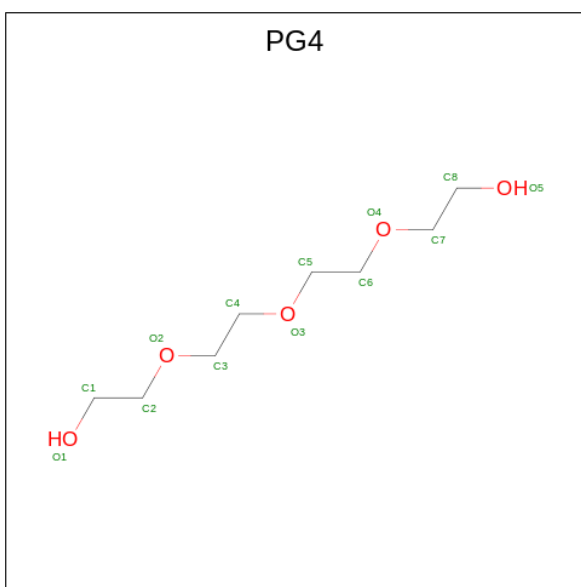
- # NAD

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	O	1	Total	C	O	0	0
			7	4	3		
6	P	1	Total	C	O	0	0
			7	4	3		
6	R	1	Total	C	O	0	0
			7	4	3		
6	R	1	Total	C	O	0	0
			7	4	3		
6	Q	1	Total	C	O	0	0
			7	4	3		
6	Q	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	P	1	Total C O 13 8 5	0	0
7	R	1	Total C O 13 8 5	0	0

- Molecule 8 is water.

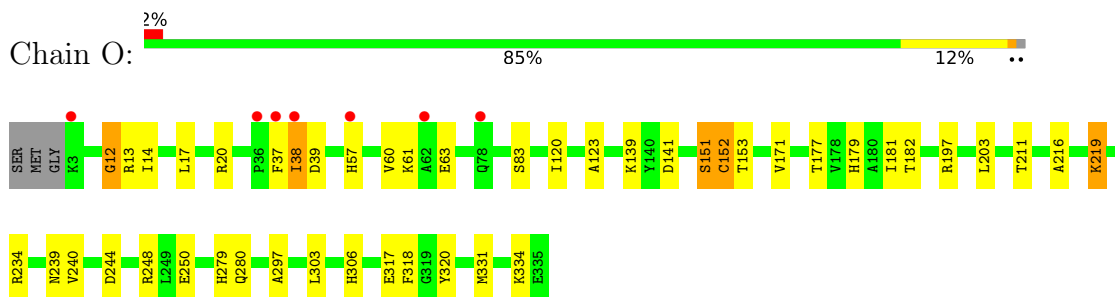
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	O	188	Total O 188 188	0	0
8	P	276	Total O 276 276	0	0
8	R	266	Total O 266 266	0	0
8	Q	129	Total O 129 129	0	0



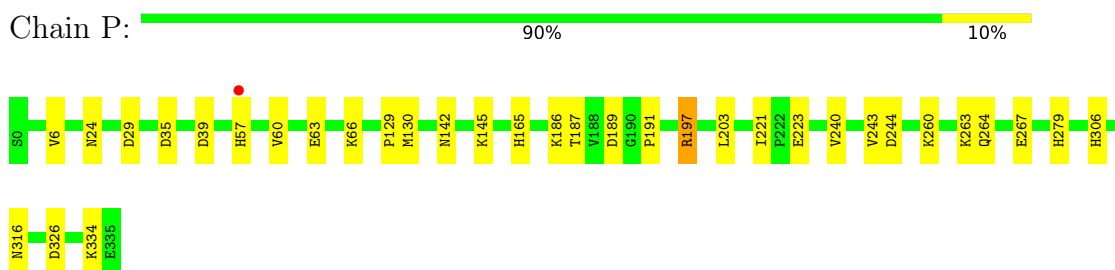
### 3 Residue-property plots [i](#)

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.

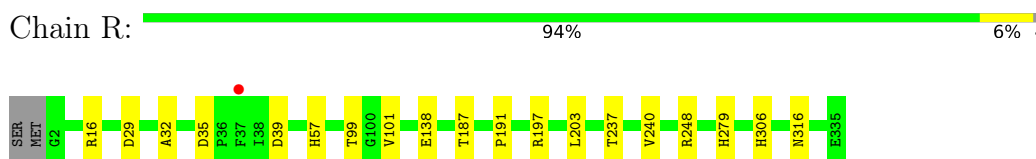
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



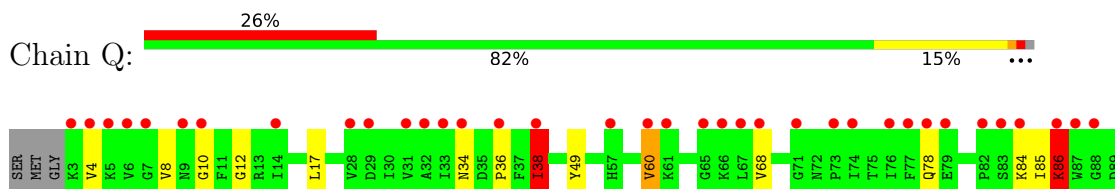
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

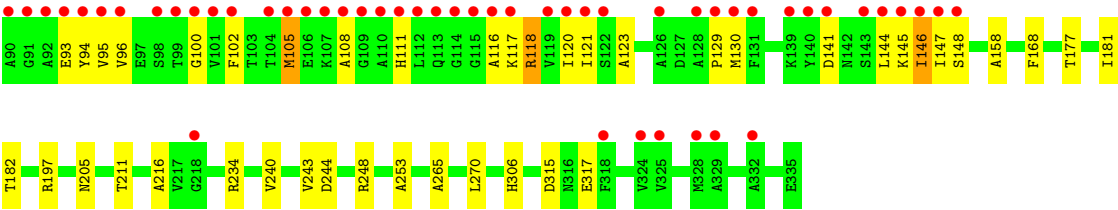


- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.26Å 133.02Å 146.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.00 – 1.77 64.00 – 1.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.00-1.77) 100.0 (64.00-1.77)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.180 , 0.211 0.189 , 0.219	Depositor DCC
$R_{free}$ test set	7744 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11395	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: PEG, ZN, NAD, CL, A1L6Z, PG4

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	1.06	6/2607 (0.2%)	1.11	7/3525 (0.2%)
1	P	1.02	2/2649 (0.1%)	1.04	5/3581 (0.1%)
1	Q	0.92	1/2615 (0.0%)	1.13	4/3536 (0.1%)
1	R	0.96	1/2653 (0.0%)	1.04	4/3588 (0.1%)
All	All	0.99	10/10524 (0.1%)	1.08	20/14230 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	4
1	P	0	1
1	Q	0	4
1	R	0	2
All	All	0	11

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	152	CYS	C-N	11.48	1.49	1.33
1	O	151	SER	C-N	10.25	1.48	1.33
1	O	303	LEU	C-O	-5.99	1.16	1.24
1	P	6	VAL	N-CA	5.99	1.53	1.46
1	P	63	GLU	CD-OE2	5.97	1.36	1.25
1	O	297	ALA	C-O	-5.92	1.17	1.24
1	Q	158	ALA	N-CA	5.67	1.51	1.46
1	O	151	SER	C-O	5.36	1.31	1.23
1	O	139	LYS	C-O	-5.17	1.17	1.24
1	R	32	ALA	N-CA	-5.05	1.40	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	138	GLU	CB-CG-CD	9.14	128.15	112.60
1	O	244	ASP	CA-CB-CG	7.45	120.05	112.60
1	O	12	GLY	CA-C-O	-7.16	114.74	122.76
1	O	39	ASP	CA-CB-CG	6.97	119.57	112.60
1	O	151	SER	O-C-N	-6.94	112.77	122.76
1	Q	244	ASP	CA-CB-CG	6.84	119.44	112.60
1	O	13	ARG	N-CA-CB	6.82	120.14	110.12
1	O	13	ARG	CB-CA-C	-6.42	100.13	110.79
1	Q	36	PRO	CA-C-N	-6.24	110.51	122.61
1	Q	36	PRO	C-N-CA	-6.24	110.51	122.61
1	R	39	ASP	CA-CB-CG	6.16	118.76	112.60
1	P	39	ASP	CA-CB-CG	5.77	118.37	112.60
1	R	29[A]	ASP	CA-CB-CG	5.57	118.17	112.60
1	R	29[B]	ASP	CA-CB-CG	5.57	118.17	112.60
1	P	244	ASP	CA-CB-CG	5.43	118.03	112.60
1	P	189	ASP	CA-CB-CG	5.36	117.96	112.60
1	P	326	ASP	CA-CB-CG	5.34	117.94	112.60
1	Q	36	PRO	N-CA-C	-5.22	106.73	113.57
1	O	152	CYS	N-CA-C	-5.07	105.46	111.69
1	P	29	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	151	SER	Mainchain
1	O	197	ARG	Sidechain
1	O	20	ARG	Sidechain
1	O	248	ARG	Sidechain
1	P	197	ARG	Sidechain
1	Q	118	ARG	Sidechain
1	Q	197	ARG	Sidechain
1	Q	205	ASN	Peptide
1	Q	78	GLN	Peptide
1	R	16	ARG	Sidechain
1	R	197	ARG	Sidechain

## 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	2545	0	2562	57	0
1	P	2578	0	2604	24	0
1	Q	2550	0	2566	37	0
1	R	2576	0	2601	11	0
2	O	31	0	0	29	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
3	Q	2	0	0	0	0
3	R	1	0	0	0	0
4	O	2	0	0	3	0
4	P	1	0	0	2	0
4	Q	1	0	0	2	0
4	R	1	0	0	1	0
5	O	44	0	24	25	0
5	P	44	0	25	4	0
5	Q	44	0	25	5	0
5	R	44	0	25	4	0
6	O	7	0	10	0	0
6	P	7	0	10	2	0
6	Q	14	0	20	1	0
6	R	14	0	20	0	0
7	P	13	0	18	4	0
7	R	13	0	18	1	0
8	O	188	0	0	5	0
8	P	276	0	0	8	0
8	Q	129	0	0	7	0
8	R	266	0	0	3	0
All	All	11395	0	10528	142	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 (142) 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:306:HIS:CD2	8:O:584:HOH:O	1.89	1.23
1:Q:306:HIS:NE2	4:Q:403:CL:CL	2.12	1.18
1:O:179:HIS:HE1	2:O:401:A1L6Z:C19	1.62	1.12
1:O:152:CYS:HB3	2:O:401:A1L6Z:O17	1.44	1.11
1:O:179:HIS:CE1	2:O:401:A1L6Z:C19	2.36	1.08
1:P:306:HIS:CD2	8:P:689:HOH:O	2.08	1.04
1:O:57:HIS:NE2	4:O:404:CL:CL	2.28	1.03
1:O:57:HIS:CE1	4:O:404:CL:CL	2.48	1.03
2:O:401:A1L6Z:C19	2:O:401:A1L6Z:O21	2.09	1.00
1:O:306:HIS:NE2	4:O:405:CL:CL	2.32	0.97
1:Q:100:GLY:HA3	5:Q:404:NAD:H1D	1.46	0.96
1:O:306:HIS:HD2	8:O:584:HOH:O	1.35	0.95
2:O:401:A1L6Z:C12	5:O:406:NAD:H3D	1.96	0.95
2:O:401:A1L6Z:O11	5:O:406:NAD:H3D	1.66	0.94
1:P:57:HIS:NE2	4:P:403:CL:CL	2.40	0.92
1:O:152:CYS:CB	2:O:401:A1L6Z:O17	2.19	0.90
1:R:57:HIS:NE2	4:R:402:CL:CL	2.43	0.89
1:O:234:ARG:HH21	2:O:401:A1L6Z:C25	1.90	0.84
7:R:404:PG4:H61	8:R:655:HOH:O	1.76	0.83
1:O:153:THR:OG1	2:O:401:A1L6Z:C28	2.26	0.83
1:O:14:ILE:HG13	5:O:406:NAD:C5D	2.09	0.83
1:Q:105:MET:HB2	8:Q:501:HOH:O	1.82	0.78
1:O:123:ALA:HB1	5:O:406:NAD:H2N	1.65	0.78
1:O:14:ILE:CG1	5:O:406:NAD:C5D	2.61	0.78
1:O:14:ILE:HG13	5:O:406:NAD:H52N	1.67	0.75
1:O:14:ILE:CD1	2:O:401:A1L6Z:C18	2.65	0.74
1:P:57:HIS:CE1	4:P:403:CL:CL	2.78	0.74
1:O:14:ILE:HG12	5:O:406:NAD:O2N	1.88	0.73
1:Q:105:MET:CB	8:Q:501:HOH:O	2.36	0.72
1:R:279:HIS:CE1	8:R:517:HOH:O	2.43	0.71
1:O:14:ILE:CG1	5:O:406:NAD:H51N	2.20	0.71
1:Q:306:HIS:CE1	4:Q:403:CL:CL	2.81	0.69
1:P:130:MET:H	7:P:406:PG4:H41	1.57	0.69
1:O:12:GLY:HA3	5:O:406:NAD:O5B	1.92	0.69
1:Q:100:GLY:HA3	5:Q:404:NAD:C1D	2.21	0.69
1:O:14:ILE:HG13	5:O:406:NAD:H51N	1.73	0.67
1:O:123:ALA:HB2	5:O:406:NAD:HO2N	1.60	0.67
7:P:406:PG4:H21	8:P:639:HOH:O	1.94	0.67
1:O:37:PHE:O	1:O:38:ILE:HD13	1.94	0.67
1:O:123:ALA:CB	5:O:406:NAD:O2D	2.43	0.67
1:Q:121:ILE:HD12	1:Q:147:ILE:O	1.95	0.67
1:O:12:GLY:HA3	5:O:406:NAD:H4B	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:401:A1L6Z:C14	5:O:406:NAD:O2D	2.45	0.65
1:O:320:TYR:CD2	2:O:401:A1L6Z:O10	2.52	0.63
1:O:83:SER:O	8:O:501:HOH:O	2.15	0.63
1:P:129:PRO:HA	7:P:406:PG4:H41	1.81	0.63
1:O:14:ILE:CG1	5:O:406:NAD:H52N	2.25	0.62
7:P:406:PG4:H42	8:P:639:HOH:O	2.00	0.62
1:O:37:PHE:C	1:O:38:ILE:HD13	2.25	0.62
1:O:123:ALA:HB2	5:O:406:NAD:O2D	1.99	0.61
2:O:401:A1L6Z:C12	5:O:406:NAD:C3D	2.76	0.61
1:O:14:ILE:HG12	5:O:406:NAD:PN	2.43	0.58
1:Q:129:PRO:HA	6:Q:405:PEG:H22	1.84	0.58
1:O:14:ILE:HD11	2:O:401:A1L6Z:C18	2.35	0.57
1:O:179:HIS:NE2	2:O:401:A1L6Z:O21	2.38	0.57
1:O:14:ILE:HG12	5:O:406:NAD:C5D	2.35	0.57
1:P:142[A]:ASN:ND2	1:P:334:LYS:O	2.38	0.56
1:P:203:LEU:HD22	1:Q:181:ILE:HD13	1.87	0.56
1:Q:12:GLY:HA3	5:Q:404:NAD:H4B	1.86	0.56
1:Q:100:GLY:CA	5:Q:404:NAD:H1D	2.29	0.55
1:O:203[B]:LEU:HD21	1:R:203:LEU:HB2	1.89	0.54
1:O:153:THR:HG1	2:O:401:A1L6Z:C28	2.19	0.54
1:O:61:LYS:HE2	1:O:63:GLU:OE1	2.07	0.54
1:P:35:ASP:OD2	5:P:404:NAD:H1B	2.06	0.54
1:O:181:ILE:HD12	1:R:187:THR:HB	1.89	0.54
1:Q:4:VAL:HG21	1:Q:94:TYR:CD2	2.43	0.54
1:Q:102:PHE:O	1:Q:108:ALA:HB2	2.08	0.54
1:R:35:ASP:OD2	5:R:403:NAD:H1B	2.08	0.54
1:Q:17:LEU:HD13	1:Q:317:GLU:HB3	1.90	0.54
2:O:401:A1L6Z:C12	5:O:406:NAD:O2D	2.55	0.53
1:O:216:ALA:HA	1:O:219:LYS:HD3	1.91	0.53
1:P:145[B]:LYS:HG2	8:P:664:HOH:O	2.10	0.52
1:O:171:VAL:HG22	1:O:250[A]:GLU:HG2	1.92	0.51
1:P:279:HIS:CE1	6:P:405:PEG:O2	2.64	0.51
1:P:142[A]:ASN:OD1	1:P:334:LYS:O	2.28	0.51
1:Q:141:ASP:O	1:Q:144:LEU:HD12	2.10	0.51
1:Q:182:THR:OG1	1:Q:234[A]:ARG:NH1	2.43	0.51
1:Q:123:ALA:O	1:Q:148:SER:OG	2.27	0.51
1:O:12:GLY:CA	5:O:406:NAD:H4B	2.41	0.51
1:O:123:ALA:CB	5:O:406:NAD:H2N	2.38	0.50
1:Q:17:LEU:CD1	1:Q:317:GLU:HB3	2.42	0.50
1:R:237[B]:THR:HG21	8:R:548:HOH:O	2.12	0.50
1:Q:111:HIS:HB3	8:Q:544:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:187:THR:HB	1:Q:181:ILE:HD12	1.94	0.49
1:P:165:HIS:CD2	1:P:223[A]:GLU:HG3	2.48	0.49
1:Q:177:THR:HG21	8:Q:586:HOH:O	2.13	0.49
1:O:234:ARG:NH2	2:O:401:A1L6Z:C25	2.69	0.49
2:O:401:A1L6Z:C5	8:O:538:HOH:O	2.61	0.49
1:Q:4:VAL:HG21	1:Q:94:TYR:CE2	2.47	0.49
2:O:401:A1L6Z:C31	8:O:671:HOH:O	2.61	0.48
2:O:401:A1L6Z:C23	2:O:401:A1L6Z:C26	2.89	0.48
1:P:279:HIS:NE2	6:P:405:PEG:O2	2.47	0.48
1:P:221:ILE:HG22	1:P:223[A]:GLU:HG2	1.95	0.48
1:O:280:GLN:HE21	1:P:197:ARG:HE	1.60	0.48
1:P:145[A]:LYS:NZ	8:P:506:HOH:O	2.46	0.47
1:O:177:THR:HG21	2:O:401:A1L6Z:C28	2.44	0.47
1:Q:248:ARG:HA	1:Q:306:HIS:O	2.14	0.47
1:R:316:ASN:HD22	5:R:403:NAD:H72N	1.62	0.47
1:O:279:HIS:ND1	1:Q:49:TYR:OH	2.48	0.47
1:O:182:THR:CG2	2:O:401:A1L6Z:C19	2.92	0.46
1:O:38:ILE:HD11	1:R:191:PRO:HB3	1.98	0.46
1:P:186:LYS:NZ	1:P:191:PRO:O	2.49	0.46
5:R:403:NAD:O5D	5:R:403:NAD:H2D	2.16	0.46
5:P:404:NAD:O5D	5:P:404:NAD:H2D	2.16	0.45
1:Q:95:VAL:HG11	8:Q:544:HOH:O	2.16	0.45
1:Q:130:MET:HE1	1:Q:216:ALA:HB1	1.99	0.45
5:Q:404:NAD:O2D	5:Q:404:NAD:H52N	2.16	0.45
1:P:24:ASN:ND2	8:P:510:HOH:O	2.48	0.45
1:Q:8:VAL:HG12	1:Q:10:GLY:O	2.17	0.44
1:O:120:ILE:HD11	1:O:331:MET:HE1	1.98	0.44
1:Q:111:HIS:O	1:Q:116:ALA:HB3	2.18	0.44
1:O:239:ASN:OD1	1:O:317:GLU:HG3	2.18	0.44
1:Q:315:ASP:OD1	1:Q:315:ASP:C	2.61	0.44
1:O:211:THR:OG1	2:O:401:A1L6Z:C31	2.66	0.44
1:Q:265:ALA:HB1	1:Q:270:LEU:HD12	2.01	0.43
5:R:403:NAD:H2D	5:R:403:NAD:H2N	1.77	0.43
1:Q:60:VAL:HA	1:Q:68:VAL:O	2.19	0.43
1:O:182:THR:HG22	2:O:401:A1L6Z:C19	2.48	0.43
1:P:66:LYS:HE2	8:P:740:HOH:O	2.18	0.43
1:Q:168:PHE:CD1	1:Q:253:ALA:HB2	2.54	0.43
1:O:211:THR:OG1	2:O:401:A1L6Z:C29	2.67	0.43
1:Q:211:THR:HG23	8:Q:596:HOH:O	2.19	0.42
1:P:316:ASN:HD22	5:P:404:NAD:H72N	1.67	0.42
1:P:142[A]:ASN:CG	1:P:334:LYS:O	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:401:A1L6Z:C13	5:O:406:NAD:H3D	2.49	0.42
1:Q:38:ILE:O	1:Q:38:ILE:HG22	2.19	0.42
1:Q:86:LYS:HE3	1:Q:86:LYS:HB3	1.96	0.41
1:O:12:GLY:HA3	5:O:406:NAD:C4B	2.48	0.41
1:Q:96:VAL:HA	1:Q:120:ILE:O	2.19	0.41
1:P:306:HIS:HD2	8:P:689:HOH:O	1.71	0.41
1:O:14:ILE:N	5:O:406:NAD:O2N	2.45	0.41
1:P:263:LYS:NZ	1:P:267:GLU:OE1	2.53	0.41
1:R:203:LEU:O	1:R:203:LEU:HD12	2.21	0.41
1:Q:94:TYR:CE1	1:Q:118:ARG:HD2	2.56	0.41
1:O:17:LEU:CD1	1:O:317:GLU:HB3	2.50	0.41
1:R:99:THR:OG1	1:R:101:VAL:HG22	2.20	0.41
1:O:334[B]:LYS:HA	1:O:334[B]:LYS:HD2	1.89	0.40
5:P:404:NAD:H2D	5:P:404:NAD:H2N	1.79	0.40
1:R:248[B]:ARG:HA	1:R:306:HIS:O	2.21	0.40
1:O:152:CYS:SG	2:O:401:A1L6Z:O17	2.79	0.40
2:O:401:A1L6Z:C24	2:O:401:A1L6Z:O1	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	335/336 (100%)	322 (96%)	12 (4%)	1 (0%)	37	23
1	P	341/336 (102%)	329 (96%)	11 (3%)	1 (0%)	37	23
1	Q	335/336 (100%)	309 (92%)	20 (6%)	6 (2%)	7	1
1	R	341/336 (102%)	325 (95%)	15 (4%)	1 (0%)	37	23
All	All	1352/1344 (101%)	1285 (95%)	58 (4%)	9 (1%)	19	7

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	240	VAL
1	P	240	VAL
1	R	240	VAL
1	Q	38	ILE
1	Q	117	LYS
1	Q	146	ILE
1	Q	240	VAL
1	Q	86	LYS
1	Q	93	GLU

### 5.3.2 Protein sidechains ⓘ

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	274/272 (101%)	269 (98%)	5 (2%)	54	36
1	P	279/272 (103%)	275 (99%)	4 (1%)	62	47
1	Q	275/272 (101%)	265 (96%)	10 (4%)	30	10
1	R	279/272 (103%)	279 (100%)	0	100	100
All	All	1107/1088 (102%)	1088 (98%)	19 (2%)	54	38

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	38	ILE
1	O	60	VAL
1	O	141	ASP
1	O	219	LYS
1	O	318	PHE
1	P	60	VAL
1	P	243	VAL
1	P	260	LYS
1	P	264	GLN
1	Q	34	ASN
1	Q	38	ILE
1	Q	60	VAL
1	Q	84	LYS

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Mol	Chain	Res	Type
1	Q	85	ILE
1	Q	86	LYS
1	Q	105	MET
1	Q	145	LYS
1	Q	146	ILE
1	Q	243	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	72	ASN
1	O	280	GLN
1	P	306	HIS
1	P	322	ASN
1	R	72	ASN
1	R	204	GLN
1	R	322	ASN
1	Q	72	ASN
1	Q	78	GLN
1	Q	167	ASN
1	Q	239	ASN
1	Q	264	GLN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 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	A1L6Z	O	401	1	25,34,34	3.34	7 (28%)	31,55,55	4.40	19 (61%)
6	PEG	R	405	-	6,6,6	0.70	0	5,5,5	0.71	0
6	PEG	O	407	-	6,6,6	0.46	0	5,5,5	0.20	0
7	PG4	R	404	-	12,12,12	0.66	0	11,11,11	1.06	1 (9%)
6	PEG	R	406	-	6,6,6	0.49	0	5,5,5	0.51	0
5	NAD	Q	404	-	42,48,48	4.12	17 (40%)	50,73,73	1.16	3 (6%)
6	PEG	P	405	-	6,6,6	0.48	0	5,5,5	0.77	0
7	PG4	P	406	-	12,12,12	0.76	0	11,11,11	0.68	0
6	PEG	Q	405	-	6,6,6	0.42	0	5,5,5	0.64	0
5	NAD	P	404	-	42,48,48	4.12	17 (40%)	50,73,73	1.19	4 (8%)
5	NAD	R	403	-	42,48,48	4.13	17 (40%)	50,73,73	1.19	4 (8%)
5	NAD	O	406	-	42,48,48	4.04	22 (52%)	50,73,73	2.42	20 (40%)
6	PEG	Q	406	-	6,6,6	0.58	0	5,5,5	0.64	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	A1L6Z	O	401	1	1/1/10/10	5/11/73/73	0/4/4/4
6	PEG	R	405	-	-	1/4/4/4	-
6	PEG	O	407	-	-	2/4/4/4	-
7	PG4	R	404	-	-	5/10/10/10	-
6	PEG	R	406	-	-	3/4/4/4	-
5	NAD	Q	404	-	2/2/11/11	17/26/62/62	0/5/5/5
6	PEG	P	405	-	-	2/4/4/4	-
7	PG4	P	406	-	-	6/10/10/10	-
6	PEG	Q	405	-	-	4/4/4/4	-
5	NAD	P	404	-	-	11/26/62/62	0/5/5/5
5	NAD	R	403	-	-	10/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAD	O	406	-	3/3/11/11	10/26/62/62	0/5/5/5
6	PEG	Q	406	-	-	2/4/4/4	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	401	A1L6Z	C15-C13	-14.25	1.27	1.53
5	O	406	NAD	C2D-C3D	-10.95	1.23	1.53
5	Q	404	NAD	C2B-C3B	-10.54	1.24	1.53
5	P	404	NAD	C2B-C3B	-10.52	1.24	1.53
5	R	403	NAD	C2B-C3B	-10.51	1.24	1.53
5	O	406	NAD	C2B-C3B	-10.37	1.25	1.53
5	R	403	NAD	C2D-C3D	-9.85	1.26	1.53
5	P	404	NAD	C2D-C3D	-9.85	1.26	1.53
5	Q	404	NAD	C2D-C3D	-9.84	1.26	1.53
5	R	403	NAD	O4B-C1B	-9.82	1.27	1.41
5	P	404	NAD	O4B-C1B	-9.77	1.27	1.41
5	Q	404	NAD	O4B-C1B	-9.76	1.27	1.41
5	Q	404	NAD	C2D-C1D	9.74	1.68	1.53
5	R	403	NAD	C2D-C1D	9.69	1.68	1.53
5	P	404	NAD	C2D-C1D	9.67	1.68	1.53
5	O	406	NAD	C2D-C1D	9.12	1.67	1.53
5	O	406	NAD	O4D-C1D	-8.67	1.29	1.41
5	R	403	NAD	O4D-C1D	-8.24	1.29	1.41
5	P	404	NAD	O4D-C1D	-8.15	1.29	1.41
5	O	406	NAD	O4B-C1B	-8.15	1.29	1.41
5	Q	404	NAD	O4D-C1D	-8.11	1.29	1.41
5	R	403	NAD	C2B-C1B	7.78	1.65	1.53
5	Q	404	NAD	C2B-C1B	7.77	1.65	1.53
5	P	404	NAD	C2B-C1B	7.71	1.65	1.53
5	O	406	NAD	C2B-C1B	7.53	1.65	1.53
5	Q	404	NAD	C7N-N7N	6.19	1.44	1.33
5	P	404	NAD	C7N-N7N	6.15	1.44	1.33
5	R	403	NAD	C7N-N7N	6.14	1.44	1.33
5	Q	404	NAD	O4D-C4D	4.51	1.55	1.45
5	P	404	NAD	O4D-C4D	4.50	1.55	1.45
5	R	403	NAD	O4D-C4D	4.48	1.55	1.45
5	Q	404	NAD	C5D-C4D	-4.39	1.37	1.51
5	P	404	NAD	C5D-C4D	-4.37	1.38	1.51
5	R	403	NAD	C5D-C4D	-4.35	1.38	1.51
5	O	406	NAD	C7N-N7N	4.20	1.41	1.33
2	O	401	A1L6Z	C7-C8	-4.12	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	404	NAD	O3B-C3B	4.01	1.52	1.43
5	P	404	NAD	O3B-C3B	4.00	1.52	1.43
5	R	403	NAD	O3B-C3B	4.00	1.52	1.43
5	O	406	NAD	O3B-C3B	3.79	1.51	1.43
2	O	401	A1L6Z	C2-C16	-3.79	1.52	1.57
5	O	406	NAD	O7N-C7N	-3.73	1.17	1.24
5	P	404	NAD	O7N-C7N	-3.66	1.17	1.24
5	R	403	NAD	O7N-C7N	-3.66	1.17	1.24
5	Q	404	NAD	O7N-C7N	-3.62	1.17	1.24
5	O	406	NAD	O4D-C4D	3.53	1.52	1.45
5	P	404	NAD	O4B-C4B	3.45	1.52	1.45
5	R	403	NAD	O4B-C4B	3.44	1.52	1.45
5	Q	404	NAD	O4B-C4B	3.42	1.52	1.45
5	O	406	NAD	C5D-C4D	-3.39	1.41	1.51
5	O	406	NAD	C3N-C7N	3.24	1.55	1.50
5	Q	404	NAD	O3D-C3D	3.09	1.50	1.43
5	Q	404	NAD	C5B-C4B	-3.07	1.42	1.51
5	R	403	NAD	O3D-C3D	3.07	1.50	1.43
5	R	403	NAD	C5B-C4B	-3.06	1.42	1.51
5	P	404	NAD	O3D-C3D	3.04	1.50	1.43
5	P	404	NAD	C5B-C4B	-3.04	1.42	1.51
5	O	406	NAD	C5B-C4B	-3.03	1.42	1.51
5	O	406	NAD	PN-O5D	3.00	1.71	1.59
2	O	401	A1L6Z	C4-C3	-2.91	1.48	1.54
5	O	406	NAD	C4A-N3A	-2.81	1.31	1.35
5	O	406	NAD	C2N-N1N	-2.74	1.31	1.35
5	O	406	NAD	C3D-C4D	2.73	1.60	1.53
5	R	403	NAD	C3D-C4D	2.71	1.59	1.53
5	P	404	NAD	C3D-C4D	2.70	1.59	1.53
2	O	401	A1L6Z	O11-C12	2.67	1.47	1.43
5	Q	404	NAD	C3D-C4D	2.65	1.59	1.53
5	Q	404	NAD	C6A-N6A	2.59	1.43	1.34
5	P	404	NAD	C6A-N6A	2.58	1.43	1.34
5	R	403	NAD	C6A-N6A	2.57	1.43	1.34
5	O	406	NAD	O2B-C2B	2.55	1.49	1.43
5	P	404	NAD	O2B-C2B	2.54	1.49	1.43
5	Q	404	NAD	O2B-C2B	2.51	1.48	1.43
5	R	403	NAD	O2B-C2B	2.50	1.48	1.43
5	O	406	NAD	C3B-C4B	2.39	1.59	1.53
5	O	406	NAD	C6A-N6A	2.35	1.42	1.34
5	O	406	NAD	O4B-C4B	2.34	1.50	1.45
2	O	401	A1L6Z	C19-C4	-2.34	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	401	A1L6Z	C2-C3	-2.29	1.52	1.54
5	O	406	NAD	PA-O5B	2.19	1.68	1.59

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	401	A1L6Z	C3-C7-C8	-12.06	90.74	110.36
2	O	401	A1L6Z	C14-C13-C12	10.65	129.93	111.18
2	O	401	A1L6Z	C12-O11-C9	-9.30	103.49	114.05
2	O	401	A1L6Z	C18-C8-C9	8.95	129.05	113.85
5	O	406	NAD	N3A-C2A-N1A	-7.05	117.66	128.68
5	O	406	NAD	C3N-C7N-N7N	5.30	124.11	117.75
5	O	406	NAD	O3D-C3D-C4D	5.26	126.26	111.05
5	O	406	NAD	C3D-C2D-C1D	4.83	108.25	100.98
5	R	403	NAD	N3A-C2A-N1A	-4.63	121.44	128.68
5	P	404	NAD	N3A-C2A-N1A	-4.62	121.46	128.68
5	Q	404	NAD	N3A-C2A-N1A	-4.60	121.50	128.68
2	O	401	A1L6Z	C31-C30-C29	-4.33	118.85	125.59
2	O	401	A1L6Z	C31-C30-C26	4.31	133.07	124.94
5	O	406	NAD	C6N-N1N-C2N	-4.25	118.10	121.97
2	O	401	A1L6Z	O11-C9-C16	4.20	112.64	108.66
5	O	406	NAD	C3N-C2N-N1N	4.18	124.51	120.43
2	O	401	A1L6Z	C15-C13-C12	4.18	114.27	108.54
5	O	406	NAD	O7N-C7N-N7N	-4.09	116.77	122.58
2	O	401	A1L6Z	C6-C7-C3	4.02	111.98	102.32
2	O	401	A1L6Z	O21-C20-C2	-3.85	99.52	106.86
5	O	406	NAD	O4D-C4D-C3D	-3.36	98.46	105.11
5	O	406	NAD	C3B-C2B-C1B	3.20	105.80	100.98
5	O	406	NAD	O4D-C4D-C5D	3.13	119.68	109.37
2	O	401	A1L6Z	C14-C13-C15	3.11	115.12	110.72
2	O	401	A1L6Z	O21-C20-C22	-2.96	103.55	109.80
2	O	401	A1L6Z	O10-C9-O11	-2.88	100.85	107.23
2	O	401	A1L6Z	C15-C16-C2	-2.74	107.42	112.81
5	O	406	NAD	C2B-C3B-C4B	2.73	107.95	102.64
5	O	406	NAD	O4D-C1D-C2D	-2.69	103.00	106.93
5	P	404	NAD	PN-O3-PA	-2.66	123.69	132.83
5	R	403	NAD	PN-O3-PA	-2.65	123.74	132.83
5	Q	404	NAD	PN-O3-PA	-2.63	123.79	132.83
5	O	406	NAD	O3D-C3D-C2D	-2.61	103.39	111.82
5	O	406	NAD	C5N-C4N-C3N	-2.50	117.39	120.34
5	O	406	NAD	O5D-PN-O1N	-2.45	99.48	109.07
2	O	401	A1L6Z	C23-C22-C24	2.38	114.09	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	401	A1L6Z	C19-C4-C5	-2.32	106.09	113.56
5	P	404	NAD	C3D-C2D-C1D	2.31	104.45	100.98
7	R	404	PG4	O3-C5-C6	-2.30	100.02	110.39
5	R	403	NAD	C3D-C2D-C1D	2.28	104.41	100.98
5	P	404	NAD	C3B-C2B-C1B	2.25	104.37	100.98
2	O	401	A1L6Z	C24-C22-C20	2.25	115.11	111.34
5	R	403	NAD	C3B-C2B-C1B	2.23	104.33	100.98
5	Q	404	NAD	C3B-C2B-C1B	2.20	104.30	100.98
2	O	401	A1L6Z	C18-C8-C7	-2.18	109.27	112.41
2	O	401	A1L6Z	C9-C8-C7	-2.14	104.29	109.86
5	O	406	NAD	PN-O5D-C5D	2.13	134.18	121.68
5	O	406	NAD	O5D-C5D-C4D	2.12	116.29	108.99
5	O	406	NAD	C2A-N1A-C6A	2.12	122.37	118.75
5	O	406	NAD	O2N-PN-O5D	2.05	117.27	107.75
5	O	406	NAD	O2N-PN-O1N	2.03	122.30	112.24

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	O	401	A1L6Z	C13
5	O	406	NAD	C1D
5	O	406	NAD	C4D
5	O	406	NAD	C2D
5	Q	404	NAD	C1D
5	Q	404	NAD	C4D

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	401	A1L6Z	C3-C2-C20-C22
2	O	401	A1L6Z	O1-C2-C20-O21
2	O	401	A1L6Z	C3-C2-C20-O21
5	O	406	NAD	C5B-O5B-PA-O2A
5	O	406	NAD	O4B-C4B-C5B-O5B
5	O	406	NAD	C5D-O5D-PN-O3
5	O	406	NAD	O4D-C1D-N1N-C2N
5	P	404	NAD	C5B-O5B-PA-O1A
5	P	404	NAD	C5B-O5B-PA-O2A
5	P	404	NAD	O4B-C4B-C5B-O5B
5	P	404	NAD	C3B-C4B-C5B-O5B
5	P	404	NAD	O4D-C1D-N1N-C2N
5	P	404	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
5	P	404	NAD	C2D-C1D-N1N-C2N
5	P	404	NAD	C2D-C1D-N1N-C6N
5	R	403	NAD	C5B-O5B-PA-O2A
5	R	403	NAD	O4B-C4B-C5B-O5B
5	R	403	NAD	C3B-C4B-C5B-O5B
5	R	403	NAD	O4D-C1D-N1N-C2N
5	R	403	NAD	O4D-C1D-N1N-C6N
5	R	403	NAD	C2D-C1D-N1N-C2N
5	R	403	NAD	C2D-C1D-N1N-C6N
5	Q	404	NAD	C5B-O5B-PA-O1A
5	Q	404	NAD	C5B-O5B-PA-O2A
5	Q	404	NAD	C5B-O5B-PA-O3
5	Q	404	NAD	O4B-C4B-C5B-O5B
5	Q	404	NAD	C3B-C4B-C5B-O5B
5	Q	404	NAD	C5D-O5D-PN-O3
5	Q	404	NAD	C5D-O5D-PN-O1N
5	Q	404	NAD	C5D-O5D-PN-O2N
5	Q	404	NAD	C2D-C1D-N1N-C2N
5	Q	404	NAD	C2D-C1D-N1N-C6N
5	Q	404	NAD	C2N-C3N-C7N-O7N
5	Q	404	NAD	C2N-C3N-C7N-N7N
5	Q	404	NAD	C4N-C3N-C7N-O7N
5	Q	404	NAD	C4N-C3N-C7N-N7N
2	O	401	A1L6Z	C22-C24-C25-C26
7	R	404	PG4	O3-C5-C6-O4
6	O	407	PEG	O2-C3-C4-O4
5	O	406	NAD	C3B-C4B-C5B-O5B
6	Q	405	PEG	O1-C1-C2-O2
7	R	404	PG4	O4-C7-C8-O5
7	P	406	PG4	O3-C5-C6-O4
6	R	406	PEG	O2-C3-C4-O4
6	R	405	PEG	O1-C1-C2-O2
7	R	404	PG4	C8-C7-O4-C6
6	P	405	PEG	C1-C2-O2-C3
6	R	406	PEG	C1-C2-O2-C3
6	Q	406	PEG	O2-C3-C4-O4
6	Q	405	PEG	C4-C3-O2-C2
5	Q	404	NAD	C4D-C5D-O5D-PN
7	P	406	PG4	C3-C4-O3-C5
6	Q	406	PEG	C4-C3-O2-C2
5	O	406	NAD	C5B-O5B-PA-O3
5	O	406	NAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	O	406	NAD	C5D-O5D-PN-O1N
5	R	403	NAD	C5B-O5B-PA-O1A
7	P	406	PG4	C4-C3-O2-C2
2	O	401	A1L6Z	C24-C25-C26-C30
7	P	406	PG4	C5-C6-O4-C7
6	R	406	PEG	O1-C1-C2-O2
7	P	406	PG4	O2-C3-C4-O3
7	P	406	PG4	O1-C1-C2-O2
5	P	404	NAD	PA-O3-PN-O2N
7	R	404	PG4	C6-C5-O3-C4
6	O	407	PEG	C1-C2-O2-C3
6	Q	405	PEG	C1-C2-O2-C3
5	O	406	NAD	O4D-C4D-C5D-O5D
5	O	406	NAD	C3D-C4D-C5D-O5D
5	P	404	NAD	C5B-O5B-PA-O3
5	R	403	NAD	C5B-O5B-PA-O3
6	P	405	PEG	O2-C3-C4-O4
7	R	404	PG4	O1-C1-C2-O2
5	Q	404	NAD	O4D-C4D-C5D-O5D
5	P	404	NAD	PA-O3-PN-O1N
5	R	403	NAD	PA-O3-PN-O1N
6	Q	405	PEG	O2-C3-C4-O4
5	Q	404	NAD	C4B-C5B-O5B-PA

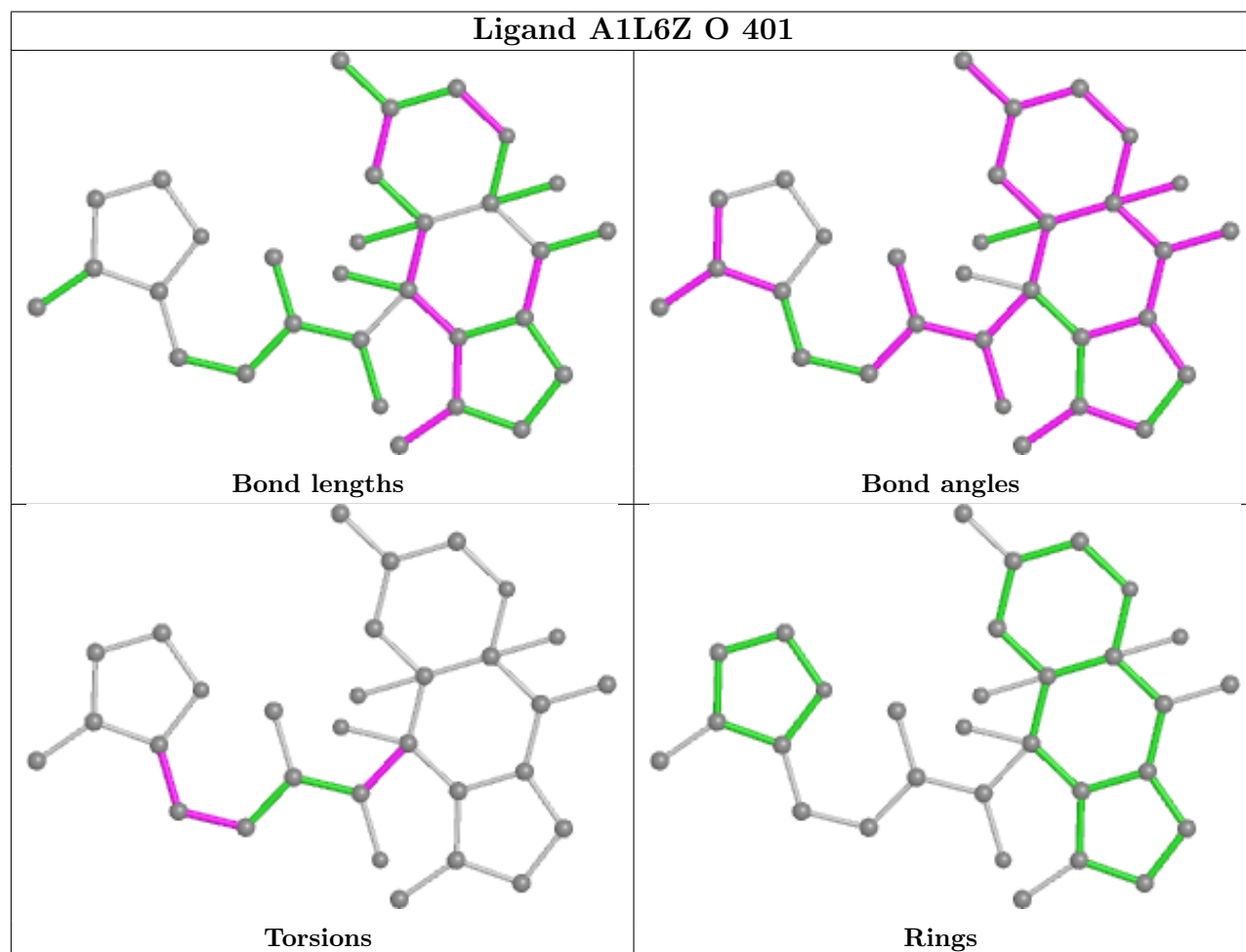
There are no ring outliers.

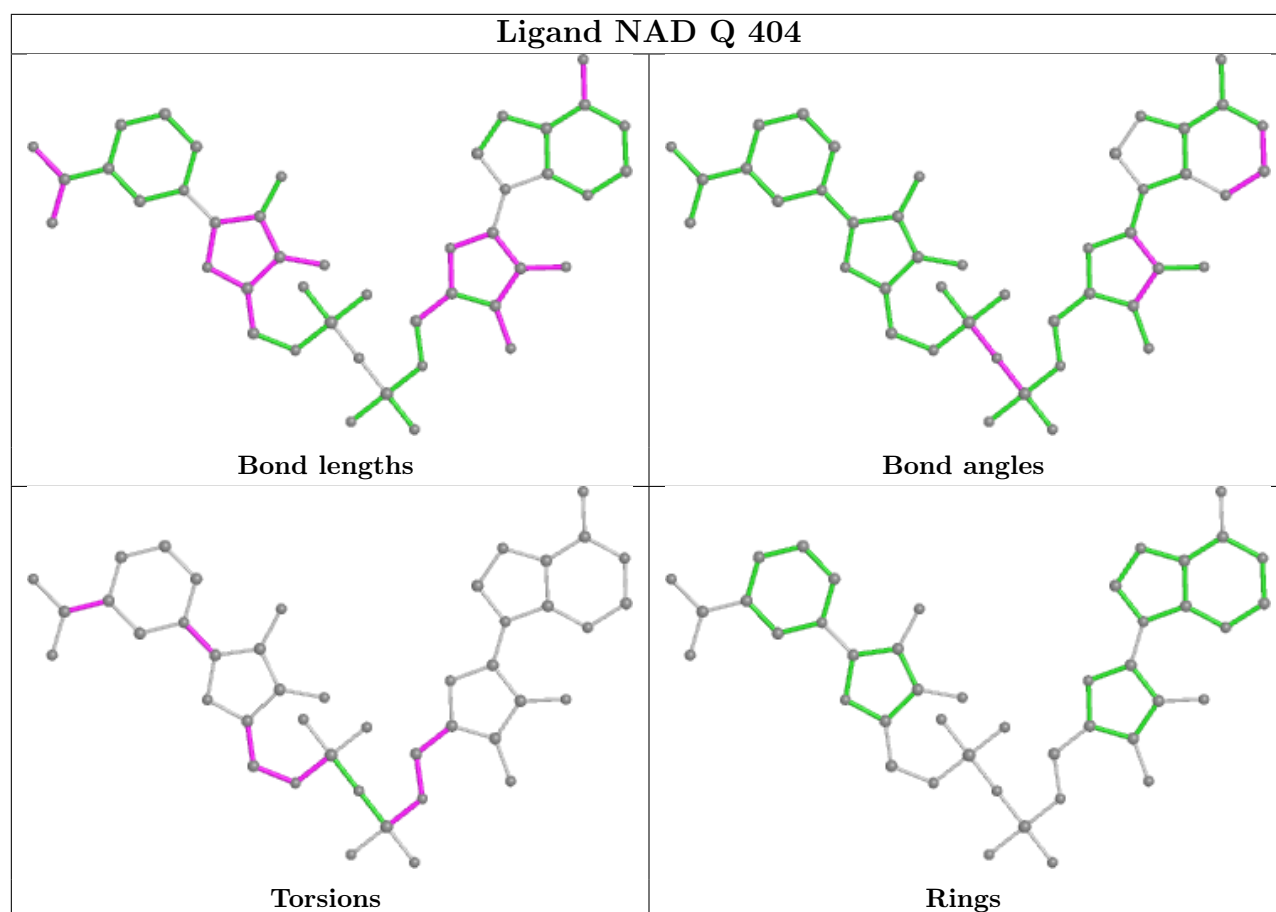
9 monomers are involved in 69 short contacts:

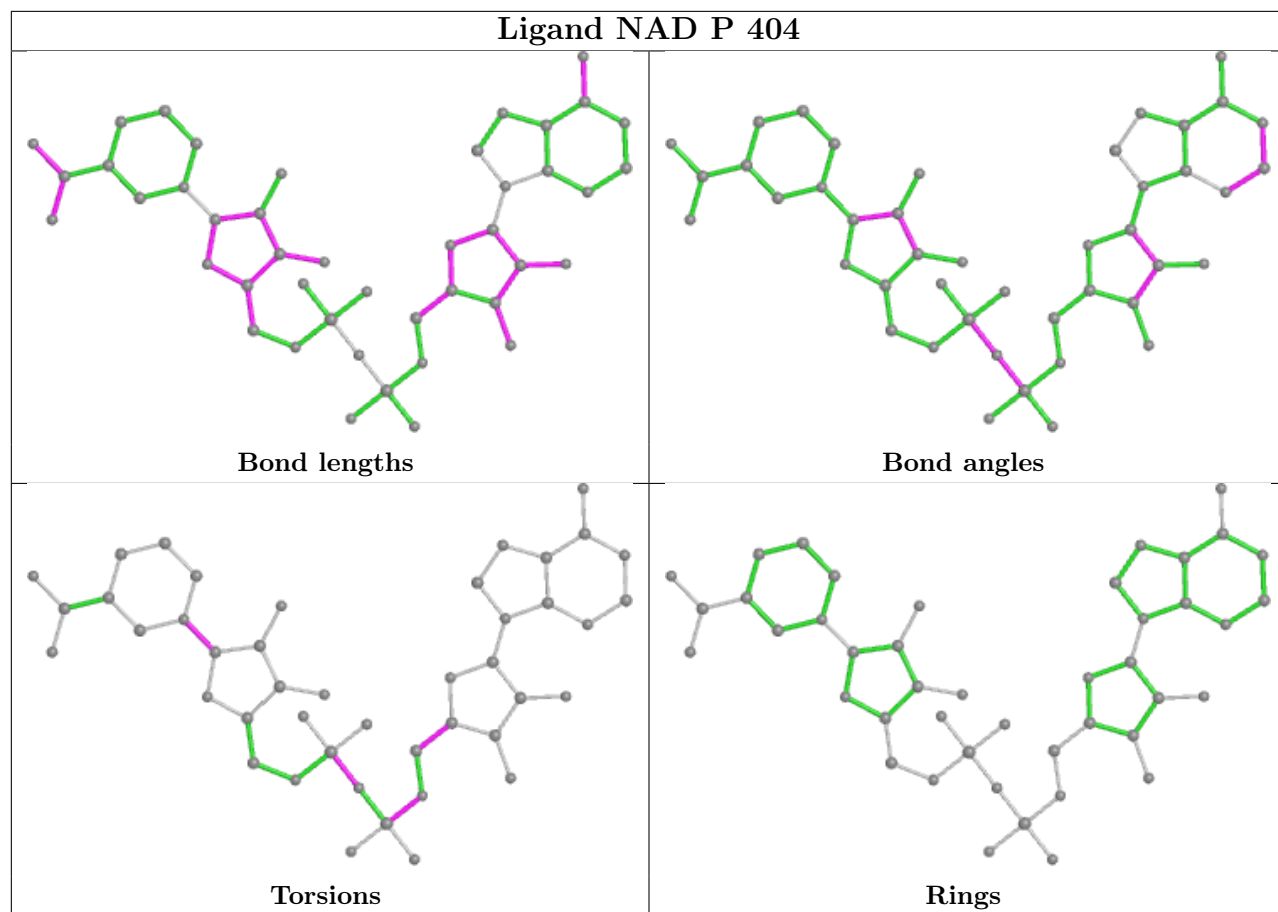
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	401	A1L6Z	29	0
7	R	404	PG4	1	0
5	Q	404	NAD	5	0
6	P	405	PEG	2	0
7	P	406	PG4	4	0
6	Q	405	PEG	1	0
5	P	404	NAD	4	0
5	R	403	NAD	4	0
5	O	406	NAD	25	0

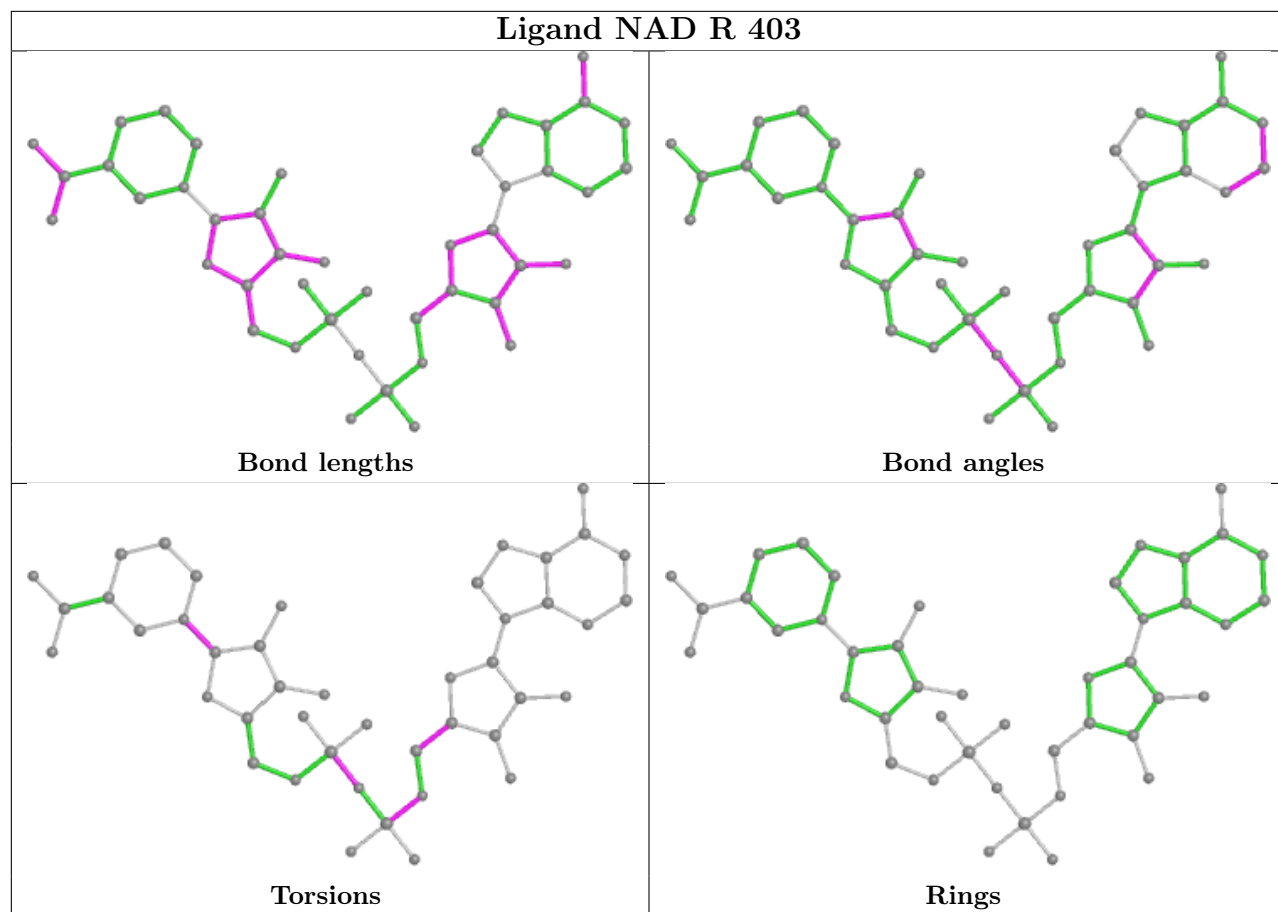
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

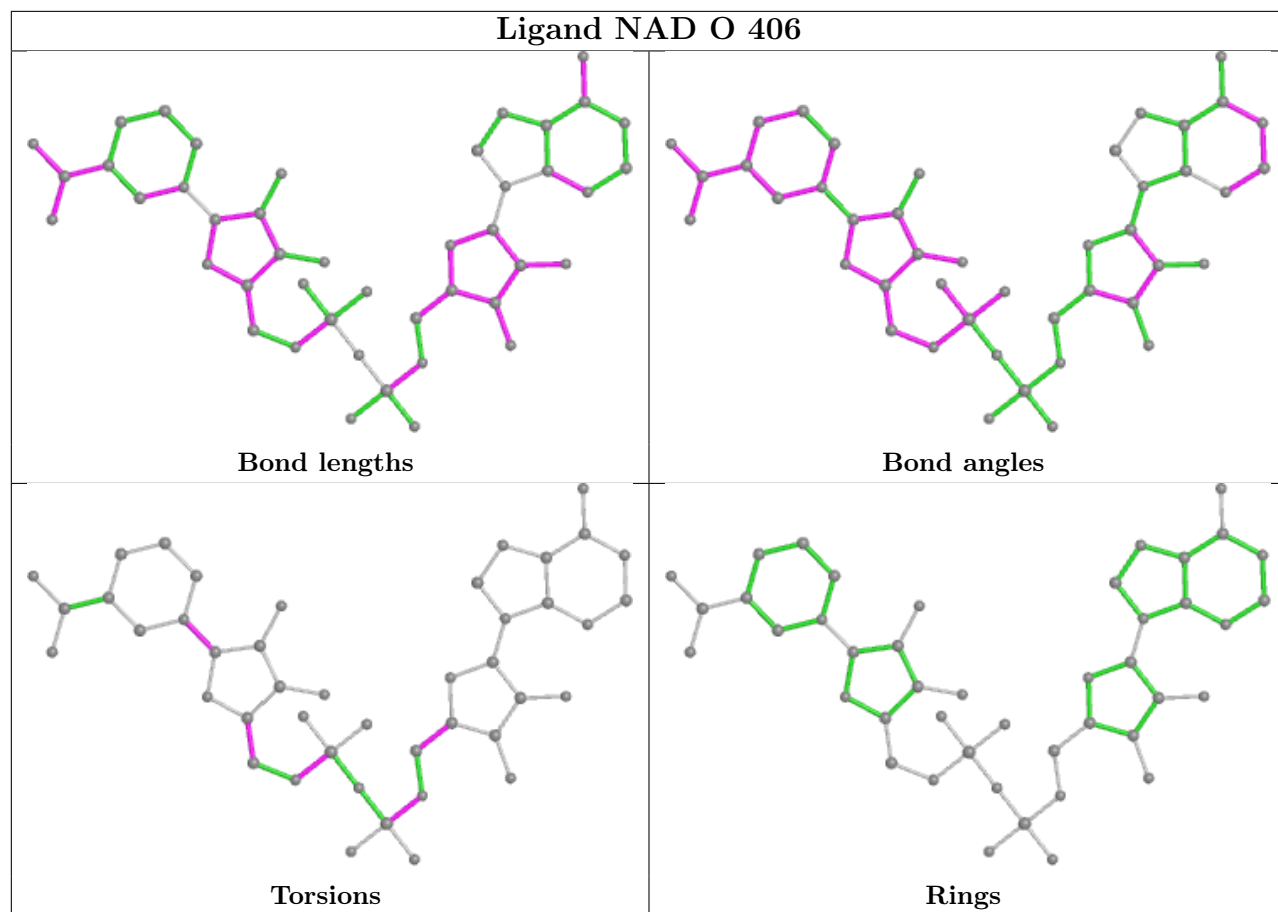
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.











## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	O	333/336 (99%)	0.09	7 (2%) 63 70	14, 29, 48, 70	5 (1%)
1	P	336/336 (100%)	-0.16	1 (0%) 90 93	13, 25, 40, 56	7 (2%)
1	Q	331/336 (98%)	1.20	87 (26%) 2 2	12, 40, 83, 105	14 (4%)
1	R	334/336 (99%)	-0.21	1 (0%) 90 93	13, 25, 37, 58	9 (2%)
All	All	1334/1344 (99%)	0.23	96 (7%) 23 27	12, 28, 65, 105	35 (2%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	146	ILE	8.2
1	Q	92	ALA	7.4
1	Q	119	VAL	6.7
1	Q	87	TRP	6.6
1	Q	112	LEU	6.4
1	Q	120	ILE	5.1
1	Q	144	LEU	4.9
1	Q	109	GLY	4.7
1	Q	145	LYS	4.6
1	Q	38	ILE	4.6
1	Q	114	GLY	4.6
1	Q	121	ILE	4.5
1	Q	36	PRO	4.4
1	Q	104	THR	4.2
1	Q	95	VAL	4.2
1	Q	106	GLU	4.1
1	Q	147	ILE	4.1
1	Q	94	TYR	4.0
1	Q	116	ALA	3.9
1	Q	90	ALA	3.8
1	Q	131	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	Q	100	GLY	3.7
1	Q	102	PHE	3.7
1	Q	82	PRO	3.6
1	Q	126	ALA	3.6
1	Q	111	HIS	3.5
1	Q	86	LYS	3.5
1	Q	6	VAL	3.4
1	Q	83	SER	3.4
1	O	37	PHE	3.3
1	Q	140	TYR	3.3
1	Q	4	VAL	3.3
1	Q	76	ILE	3.2
1	Q	93	GLU	3.2
1	Q	332	ALA	3.2
1	Q	129	PRO	3.2
1	Q	91	GLY	3.2
1	Q	329	ALA	3.1
1	Q	10	GLY	3.1
1	Q	101	VAL	3.1
1	Q	32	ALA	3.0
1	Q	88	GLY	3.0
1	Q	31	VAL	3.0
1	Q	84	LYS	2.9
1	Q	108	ALA	2.9
1	Q	105	MET	2.9
1	Q	74	ILE	2.8
1	Q	77	PHE	2.8
1	Q	79	GLU	2.8
1	O	38	ILE	2.7
1	Q	96	VAL	2.7
1	O	62	ALA	2.7
1	O	57	HIS	2.7
1	Q	28	VAL	2.7
1	Q	67	LEU	2.6
1	Q	99	THR	2.6
1	Q	110	ALA	2.6
1	Q	9	ASN	2.6
1	P	57	HIS	2.6
1	Q	33	ILE	2.5
1	Q	117	LYS	2.5
1	Q	73	PRO	2.5
1	Q	128	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	Q	143	SER	2.4
1	Q	107	LYS	2.4
1	Q	7	GLY	2.4
1	Q	78	GLN	2.4
1	Q	218	GLY	2.4
1	Q	34	ASN	2.4
1	Q	324	VAL	2.4
1	O	78	GLN	2.3
1	Q	3[A]	LYS	2.3
1	Q	61	LYS	2.3
1	Q	68	VAL	2.3
1	Q	113	GLN	2.3
1	Q	98[A]	SER	2.3
1	Q	139	LYS	2.2
1	Q	14	ILE	2.2
1	Q	5	LYS	2.2
1	Q	29	ASP	2.2
1	Q	141	ASP	2.2
1	R	37	PHE	2.2
1	Q	71	GLY	2.2
1	Q	115	GLY	2.2
1	Q	122	SER	2.2
1	Q	130	MET	2.2
1	Q	60	VAL	2.2
1	Q	57	HIS	2.1
1	Q	328	MET	2.1
1	Q	318	PHE	2.1
1	Q	66	LYS	2.1
1	Q	148	SER	2.1
1	O	36	PRO	2.1
1	O	3	LYS	2.0
1	Q	325	VAL	2.0
1	Q	65	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

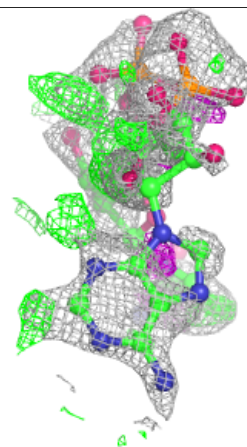
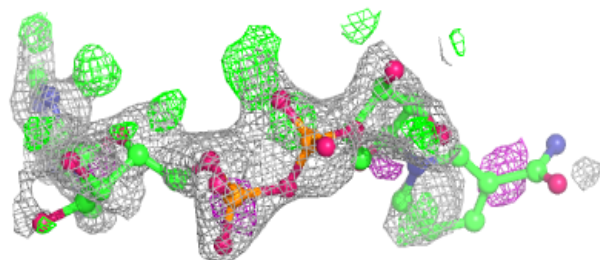
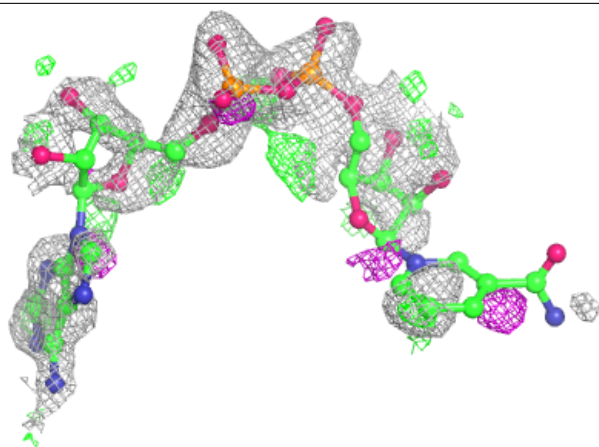
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAD	Q	404	44/44	0.62	0.25	47,69,89,93	44
2	A1L6Z	O	401	31/31	0.73	0.28	19,45,61,64	31
6	PEG	P	405	7/7	0.75	0.18	65,71,72,73	0
6	PEG	R	405	7/7	0.82	0.17	51,54,64,65	0
6	PEG	Q	406	7/7	0.82	0.18	59,61,63,64	0
3	ZN	O	402	1/1	0.83	0.10	100,100,100,100	0
5	NAD	O	406	44/44	0.83	0.22	18,33,42,44	44
6	PEG	Q	405	7/7	0.84	0.17	56,59,65,66	0
5	NAD	P	404	44/44	0.85	0.13	25,29,32,36	0
6	PEG	R	406	7/7	0.87	0.14	52,53,60,66	0
5	NAD	R	403	44/44	0.87	0.12	21,25,28,29	44
3	ZN	P	401	1/1	0.87	0.11	93,93,93,93	0
6	PEG	O	407	7/7	0.89	0.13	57,60,72,78	0
4	CL	O	405	1/1	0.90	0.14	62,62,62,62	0
7	PG4	P	406	13/13	0.90	0.12	28,37,51,57	0
4	CL	Q	403	1/1	0.91	0.10	57,57,57,57	0
7	PG4	R	404	13/13	0.91	0.12	31,41,56,56	0
3	ZN	Q	401	1/1	0.93	0.08	83,83,83,83	0
3	ZN	Q	402	1/1	0.93	0.07	76,76,76,76	0
4	CL	P	403	1/1	0.94	0.09	42,42,42,42	0
4	CL	R	402	1/1	0.96	0.07	36,36,36,36	0
4	CL	O	404	1/1	0.97	0.07	46,46,46,46	0
3	ZN	O	403	1/1	0.98	0.04	42,42,42,42	0
3	ZN	R	401	1/1	0.99	0.03	27,27,27,27	0
3	ZN	P	402	1/1	0.99	0.02	28,28,28,28	0

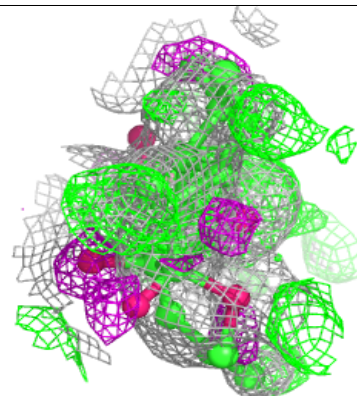
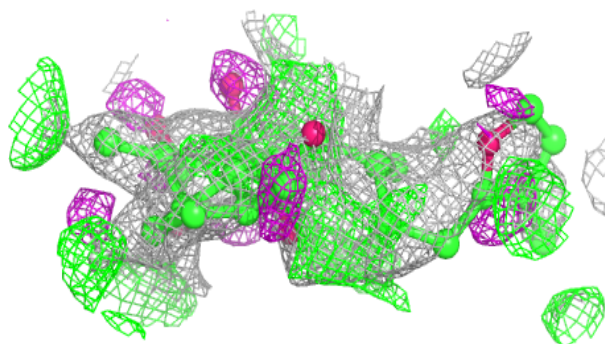
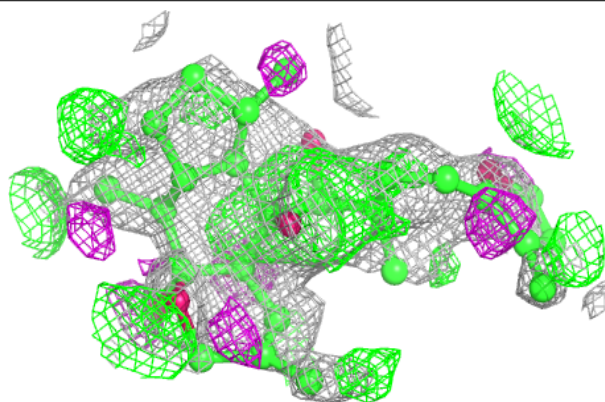
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAD Q 404:**

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

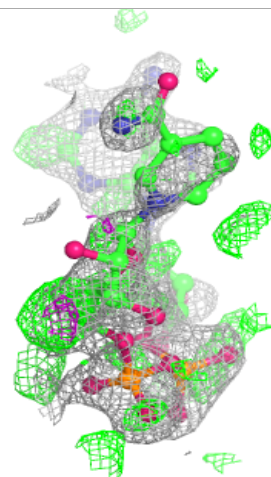
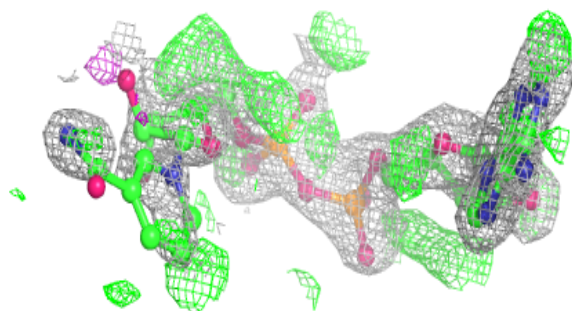
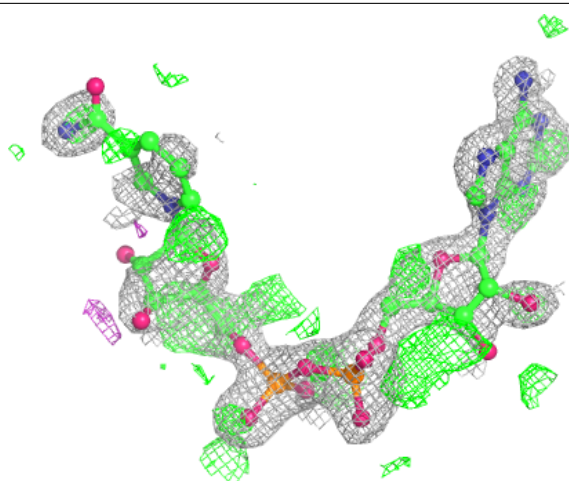
**Electron density around A1L6Z O 401:**

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



**Electron density around NAD O 406:**

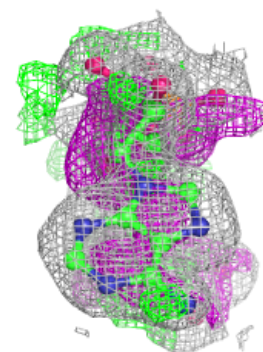
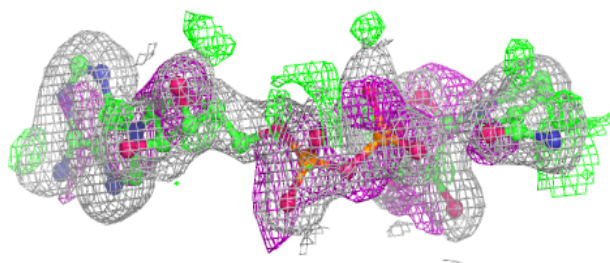
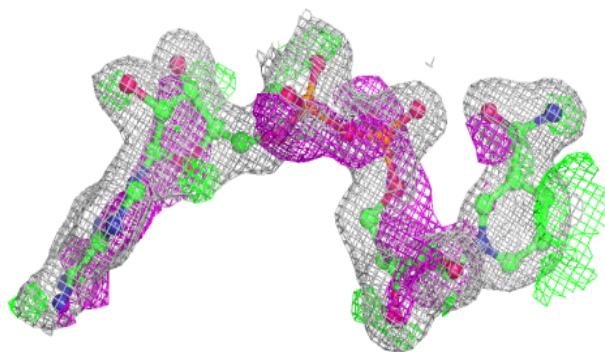
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



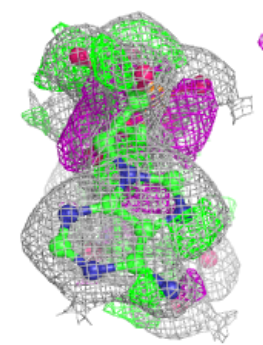
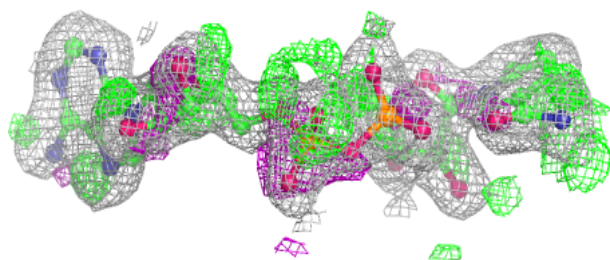
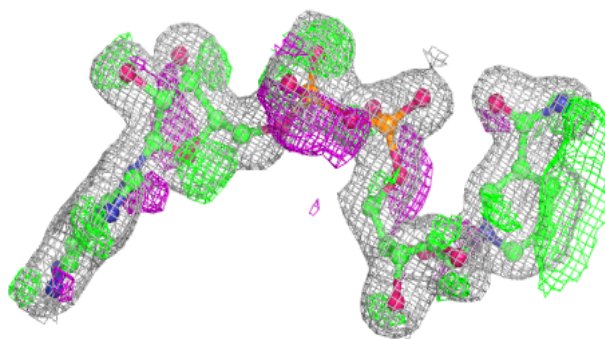


**Electron density around NAD P 404:**

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

**Electron density around NAD R 403:**

$2mF_o-DF_c$  (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.