



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:43 PM UTC

PDB ID : 2B4T / pdb_00002b4t
Title : Crystal structure of glyceraldehyde-3-phosphate dehydrogenase from Plasmodium falciparum at 2.25 Angstrom resolution reveals intriguing extra electron density in the active site
Authors : Robien, M.A.; Bosch, J.; Hol, W.G.J.; Structural Genomics of Pathogenic Protozoa Consortium (SGPP)
Deposited on : 2005-09-26
Resolution : 2.50 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](#) ①) were used in the production of this report:

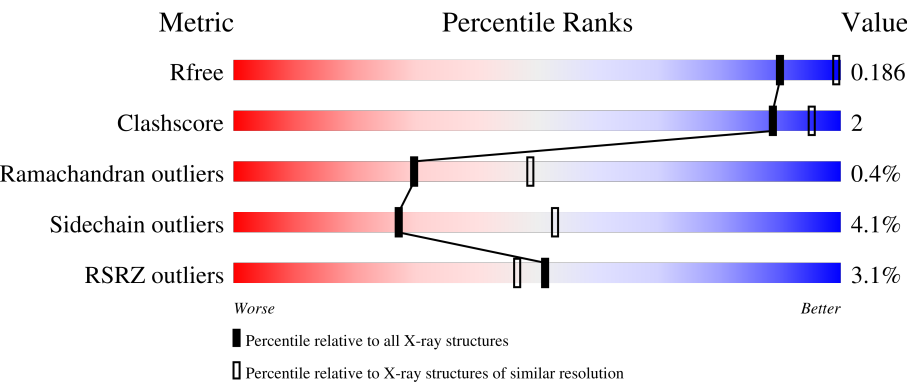
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	345	% 87%7% . .
1	P	345	4% 85%9% . .
1	Q	345	6% 87%8% . .
1	R	345	% 85%9% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10631 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	56	0	0
			2546	1624	437	472	13			
1	P	333	Total	C	N	O	S	73	0	0
			2546	1624	437	472	13			
1	Q	333	Total	C	N	O	S	57	0	0
			2546	1624	437	472	13			
1	R	333	Total	C	N	O	S	46	0	0
			2546	1624	437	472	13			

There are 44 discrepancies between the modelled and reference sequences:

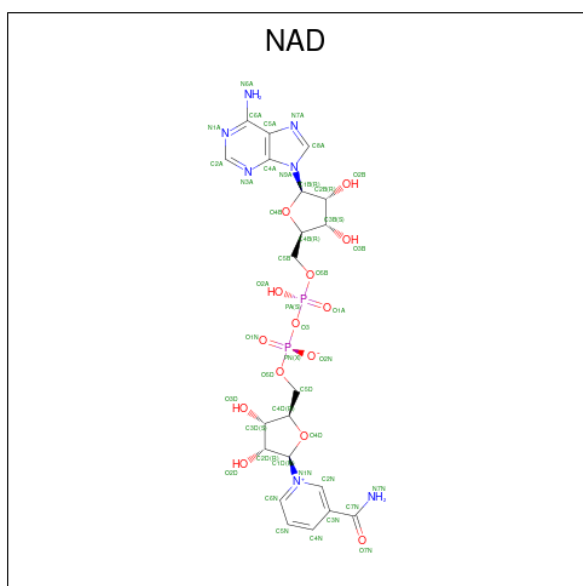
Chain	Residue	Modelled	Actual	Comment	Reference
O	-7	MET	-	cloning artifact	UNP Q8T6B1
O	-6	ALA	-	cloning artifact	UNP Q8T6B1
O	-5	HIS	-	expression tag	UNP Q8T6B1
O	-4	HIS	-	expression tag	UNP Q8T6B1
O	-3	HIS	-	expression tag	UNP Q8T6B1
O	-2	HIS	-	expression tag	UNP Q8T6B1
O	-1	HIS	-	expression tag	UNP Q8T6B1
O	0	HIS	-	expression tag	UNP Q8T6B1
O	3	ALA	VAL	engineered mutation	UNP Q8T6B1
O	336	THR	ASN	engineered mutation	UNP Q8T6B1
O	337	SER	ASN	engineered mutation	UNP Q8T6B1
P	-7	MET	-	cloning artifact	UNP Q8T6B1
P	-6	ALA	-	cloning artifact	UNP Q8T6B1
P	-5	HIS	-	expression tag	UNP Q8T6B1
P	-4	HIS	-	expression tag	UNP Q8T6B1
P	-3	HIS	-	expression tag	UNP Q8T6B1
P	-2	HIS	-	expression tag	UNP Q8T6B1
P	-1	HIS	-	expression tag	UNP Q8T6B1
P	0	HIS	-	expression tag	UNP Q8T6B1
P	3	ALA	VAL	engineered mutation	UNP Q8T6B1
P	336	THR	ASN	engineered mutation	UNP Q8T6B1

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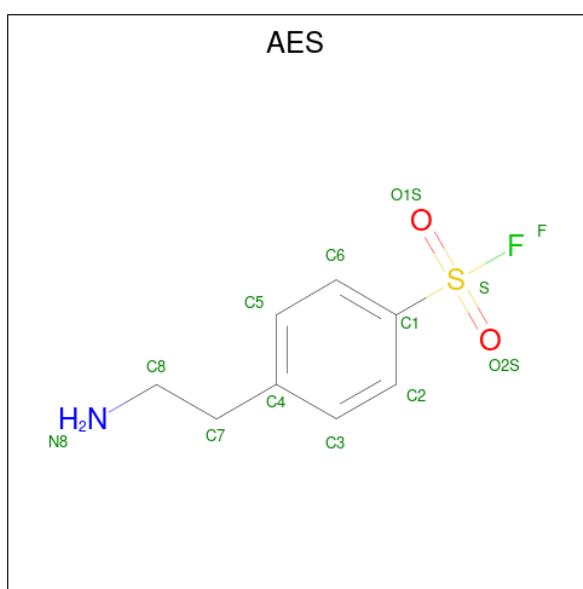
Chain	Residue	Modelled	Actual	Comment	Reference
P	337	SER	ASN	engineered mutation	UNP Q8T6B1
Q	-7	MET	-	cloning artifact	UNP Q8T6B1
Q	-6	ALA	-	cloning artifact	UNP Q8T6B1
Q	-5	HIS	-	expression tag	UNP Q8T6B1
Q	-4	HIS	-	expression tag	UNP Q8T6B1
Q	-3	HIS	-	expression tag	UNP Q8T6B1
Q	-2	HIS	-	expression tag	UNP Q8T6B1
Q	-1	HIS	-	expression tag	UNP Q8T6B1
Q	0	HIS	-	expression tag	UNP Q8T6B1
Q	3	ALA	VAL	engineered mutation	UNP Q8T6B1
Q	336	THR	ASN	engineered mutation	UNP Q8T6B1
Q	337	SER	ASN	engineered mutation	UNP Q8T6B1
R	-7	MET	-	cloning artifact	UNP Q8T6B1
R	-6	ALA	-	cloning artifact	UNP Q8T6B1
R	-5	HIS	-	expression tag	UNP Q8T6B1
R	-4	HIS	-	expression tag	UNP Q8T6B1
R	-3	HIS	-	expression tag	UNP Q8T6B1
R	-2	HIS	-	expression tag	UNP Q8T6B1
R	-1	HIS	-	expression tag	UNP Q8T6B1
R	0	HIS	-	expression tag	UNP Q8T6B1
R	3	ALA	VAL	engineered mutation	UNP Q8T6B1
R	336	THR	ASN	engineered mutation	UNP Q8T6B1
R	337	SER	ASN	engineered mutation	UNP Q8T6B1

- 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		

- Molecule 3 is 4-(2-AMINOETHYL)BENZENESULFONYL FLUORIDE (CCD ID: AES) (formula: C₈H₁₀FNO₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	O	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0
3	P	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0
3	R	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	O	65	Total 65 O 65	0	0
4	P	63	Total 63 O 63	0	0

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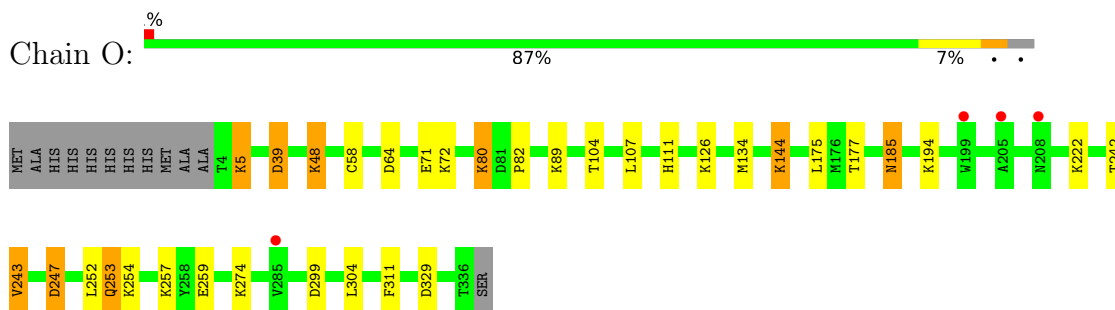
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	49	Total	O	0	0
			49	49		
4	R	55	Total	O	0	0
			55	55		

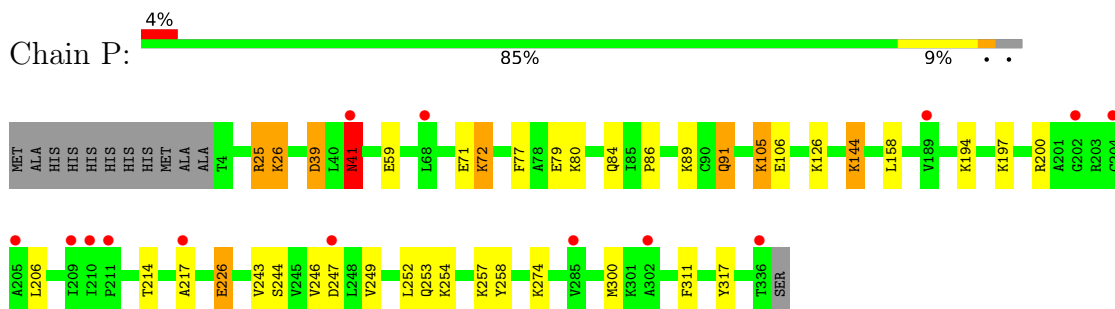
3 Residue-property plots

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.

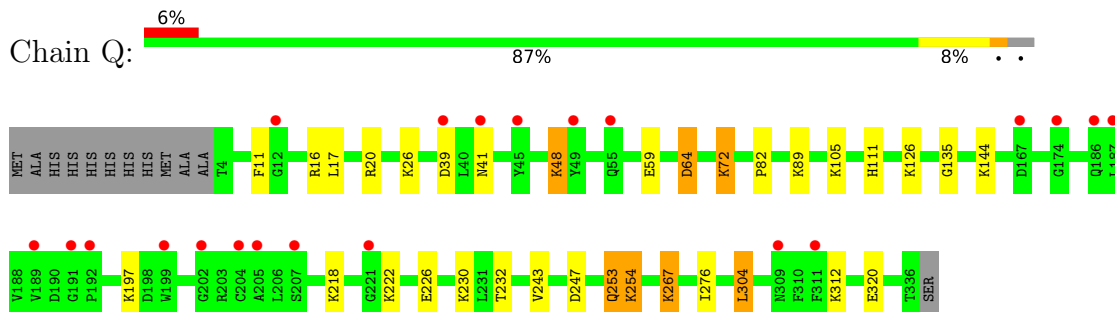
- Molecule 1: glyceraldehyde-3-phosphate dehydrogenase



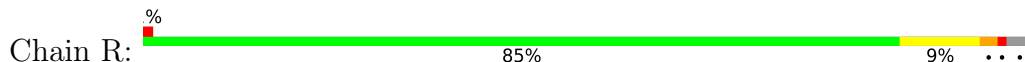
- Molecule 1: glyceraldehyde-3-phosphate dehydrogenase

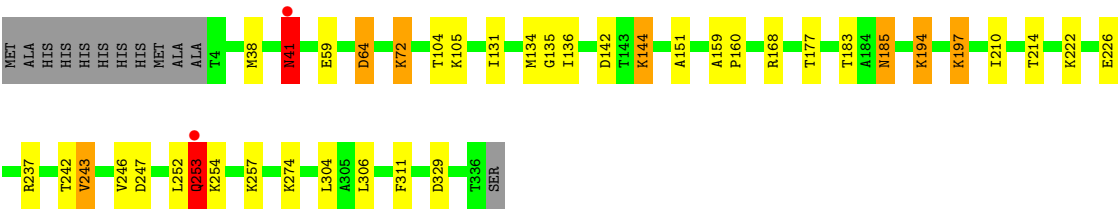


- Molecule 1: glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: glyceraldehyde-3-phosphate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.69Å 106.06Å 91.06Å 90.00° 107.24° 90.00°	Depositor
Resolution (Å)	43.48 – 2.50 43.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (43.48-2.50) 97.7 (43.48-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.174 , 0.217 0.186 , 0.186	Depositor DCC
R_{free} test set	2115 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10631	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, AES

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	1.78	17/2598 (0.7%)	1.70	20/3521 (0.6%)
1	P	1.38	14/2598 (0.5%)	1.37	32/3521 (0.9%)
1	Q	1.39	12/2598 (0.5%)	1.45	27/3521 (0.8%)
1	R	1.90	13/2598 (0.5%)	1.44	24/3521 (0.7%)
All	All	1.63	56/10392 (0.5%)	1.50	103/14084 (0.7%)

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	P	0	1
1	Q	0	1
1	R	0	2
All	All	0	4

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	253	GLN	CG-CD	72.14	3.32	1.52
1	O	71	GLU	CA-CB	-55.88	0.79	1.52
1	Q	254	LYS	CB-CG	-36.98	0.41	1.52
1	O	64	ASP	CA-CB	35.97	2.07	1.53
1	P	25	ARG	CG-CD	-32.84	0.54	1.52
1	Q	230	LYS	CD-CE	-30.65	0.60	1.52
1	P	59	GLU	CB-CG	-29.96	0.62	1.52
1	R	105	LYS	CD-CE	28.84	2.38	1.52
1	O	144	LYS	CA-CB	27.91	2.03	1.53
1	R	194	LYS	CB-CG	24.82	2.27	1.52
1	O	48	LYS	CD-CE	-24.50	0.79	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	72	LYS	CG-CD	-23.02	0.83	1.52
1	Q	72	LYS	CG-CD	-21.79	0.87	1.52
1	R	144	LYS	CB-CG	21.59	2.17	1.52
1	R	72	LYS	CG-CD	-21.47	0.88	1.52
1	P	105	LYS	CB-CG	-20.30	0.91	1.52
1	P	71	GLU	CG-CD	-18.16	1.06	1.52
1	P	41	ASN	CB-CG	18.15	1.97	1.52
1	R	41	ASN	CB-CG	-17.37	1.08	1.52
1	O	5	LYS	CB-CG	-17.25	1.00	1.52
1	Q	267	LYS	CB-CG	-17.16	1.00	1.52
1	R	254	LYS	CB-CG	16.58	2.02	1.52
1	Q	41	ASN	CB-CG	-15.69	1.12	1.52
1	Q	64	ASP	CA-CB	-15.01	1.30	1.53
1	Q	39	ASP	CB-CG	-14.98	1.14	1.52
1	O	126	LYS	CG-CD	-14.24	1.09	1.52
1	Q	26	LYS	CB-CG	-14.14	1.10	1.52
1	Q	144	LYS	CB-CG	-13.62	1.11	1.52
1	R	144	LYS	CG-CD	-13.59	1.11	1.52
1	O	194	LYS	CG-CD	-13.21	1.12	1.52
1	O	72	LYS	CG-CD	12.98	1.91	1.52
1	O	89	LYS	CD-CE	12.43	1.89	1.52
1	O	274	LYS	CG-CD	-12.39	1.15	1.52
1	P	194	LYS	CG-CD	-11.62	1.17	1.52
1	O	194	LYS	CB-CG	-11.59	1.17	1.52
1	P	126	LYS	CG-CD	-10.82	1.20	1.52
1	O	254	LYS	CD-CE	-10.62	1.20	1.52
1	O	257	LYS	CG-CD	-10.46	1.21	1.52
1	P	26	LYS	CB-CG	-9.99	1.22	1.52
1	P	226	GLU	CG-CD	-9.97	1.27	1.52
1	O	39	ASP	CB-CG	-9.80	1.27	1.52
1	R	59	GLU	CB-CG	9.14	1.79	1.52
1	R	257	LYS	CG-CD	8.62	1.78	1.52
1	O	253	GLN	CG-CD	-8.28	1.31	1.52
1	P	126	LYS	CD-CE	8.09	1.76	1.52
1	Q	197	LYS	CB-CG	-8.07	1.28	1.52
1	R	64	ASP	CA-CB	-7.75	1.40	1.53
1	R	197	LYS	CB-CG	-7.57	1.29	1.52
1	P	89	LYS	CB-CG	7.00	1.73	1.52
1	O	80	LYS	CB-CG	-6.79	1.32	1.52
1	P	274	LYS	CG-CD	-6.78	1.32	1.52
1	Q	253	GLN	CG-CD	6.56	1.68	1.52
1	Q	144	LYS	CD-CE	6.49	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	257	LYS	CG-CD	-5.49	1.35	1.52
1	O	259	GLU	CG-CD	-5.03	1.39	1.52
1	R	254	LYS	CD-CE	5.01	1.67	1.52

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	41	ASN	CA-CB-CG	45.20	157.80	112.60
1	O	71	GLU	CB-CA-C	-42.34	56.89	111.50
1	O	64	ASP	CA-CB-CG	-41.17	71.42	112.60
1	P	41	ASN	CA-CB-CG	-35.15	77.45	112.60
1	O	64	ASP	CB-CA-C	-31.12	62.34	111.51
1	R	253	GLN	CB-CG-CD	-29.41	62.60	112.60
1	O	71	GLU	CA-CB-CG	-28.55	57.01	114.10
1	R	41	ASN	CA-CB-CG	28.34	140.94	112.60
1	O	80	LYS	CA-CB-CG	25.73	165.56	114.10
1	O	247	ASP	CA-CB-CG	24.80	137.40	112.60
1	P	25	ARG	CB-CG-CD	24.05	166.62	111.30
1	R	253	GLN	CG-CD-NE2	23.53	151.69	116.40
1	R	253	GLN	CG-CD-OE1	-21.42	77.96	120.80
1	Q	72	LYS	CB-CG-CD	21.28	160.24	111.30
1	P	226	GLU	CB-CG-CD	20.57	147.57	112.60
1	R	64	ASP	CA-CB-CG	20.08	132.68	112.60
1	Q	39	ASP	CA-CB-CG	18.62	131.22	112.60
1	P	72	LYS	CB-CG-CD	18.50	153.86	111.30
1	Q	41	ASN	CB-CG-ND2	17.62	142.83	116.40
1	R	41	ASN	CB-CG-ND2	-16.42	91.77	116.40
1	P	106	GLU	CB-CG-CD	15.86	139.56	112.60
1	Q	72	LYS	CG-CD-CE	15.62	147.22	111.30
1	O	48	LYS	CD-CE-NZ	15.36	161.06	111.90
1	Q	253	GLN	CB-CG-CD	-14.91	87.25	112.60
1	R	197	LYS	CA-CB-CG	14.87	143.83	114.10
1	R	144	LYS	CA-CB-CG	-14.69	84.73	114.10
1	R	257	LYS	CB-CG-CD	-14.62	77.67	111.30
1	R	254	LYS	CA-CB-CG	14.60	143.29	114.10
1	Q	64	ASP	CA-CB-CG	14.46	127.06	112.60
1	O	253	GLN	CB-CG-CD	14.38	137.04	112.60
1	R	105	LYS	CG-CD-CE	-14.36	78.27	111.30
1	O	72	LYS	CG-CD-CE	14.09	143.70	111.30
1	R	64	ASP	CB-CA-C	13.57	131.61	111.80
1	R	72	LYS	CG-CD-CE	13.56	142.49	111.30
1	Q	41	ASN	CB-CG-OD1	-13.20	94.41	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	71	GLU	CA-CB-CG	11.85	137.81	114.10
1	O	194	LYS	CB-CG-CD	11.83	138.51	111.30
1	O	64	ASP	N-CA-CB	11.72	130.11	112.30
1	Q	222	LYS	CG-CD-CE	-11.68	84.44	111.30
1	R	257	LYS	CG-CD-CE	-11.60	84.63	111.30
1	Q	254	LYS	CB-CG-CD	-11.56	84.71	111.30
1	Q	197	LYS	CA-CB-CG	-11.50	91.11	114.10
1	O	259	GLU	CB-CG-CD	11.43	132.04	112.60
1	O	39	ASP	CB-CG-OD1	-11.13	92.79	118.40
1	O	257	LYS	CB-CG-CD	11.11	136.85	111.30
1	P	91	GLN	N-CA-CB	-10.99	95.91	111.62
1	R	197	LYS	CB-CG-CD	10.83	136.22	111.30
1	P	72	LYS	CG-CD-CE	10.83	136.20	111.30
1	Q	64	ASP	CB-CA-C	10.73	128.46	111.51
1	O	39	ASP	CB-CG-OD2	10.67	142.94	118.40
1	Q	254	LYS	CA-CB-CG	-10.66	92.77	114.10
1	O	39	ASP	CA-CB-CG	10.30	122.90	112.60
1	P	194	LYS	CB-CG-CD	10.23	134.84	111.30
1	Q	197	LYS	CB-CG-CD	-9.97	88.36	111.30
1	R	274	LYS	CB-CG-CD	9.87	134.00	111.30
1	P	253	GLN	CB-CG-CD	9.82	129.29	112.60
1	Q	105	LYS	CA-CB-CG	-9.79	94.52	114.10
1	O	126	LYS	CG-CD-CE	-9.43	89.60	111.30
1	Q	26	LYS	CB-CG-CD	9.38	132.88	111.30
1	P	91	GLN	CB-CA-C	9.32	125.94	111.95
1	O	126	LYS	CB-CG-CD	-9.29	89.92	111.30
1	Q	267	LYS	CB-CG-CD	-9.20	90.14	111.30
1	Q	126	LYS	CG-CD-CE	8.97	131.93	111.30
1	P	274	LYS	CB-CG-CD	-8.83	90.98	111.30
1	R	254	LYS	CB-CG-CD	8.71	131.33	111.30
1	P	254	LYS	CB-CG-CD	8.66	131.23	111.30
1	P	226	GLU	CG-CD-OE1	-8.54	98.77	118.40
1	P	274	LYS	CG-CD-CE	-8.40	91.97	111.30
1	Q	105	LYS	CB-CG-CD	-8.37	92.05	111.30
1	R	274	LYS	CG-CD-CE	8.10	129.92	111.30
1	P	126	LYS	CB-CG-CD	8.06	129.83	111.30
1	P	26	LYS	CB-CG-CD	8.04	129.78	111.30
1	R	41	ASN	CB-CG-OD1	7.69	136.18	120.80
1	P	41	ASN	CB-CG-OD1	-7.56	105.68	120.80
1	P	144	LYS	CD-CE-NZ	-7.30	88.55	111.90
1	Q	48	LYS	CG-CD-CE	7.15	127.74	111.30
1	Q	253	GLN	CG-CD-NE2	-7.12	105.72	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	226	GLU	CG-CD-OE2	6.98	134.46	118.40
1	P	105	LYS	CA-CB-CG	6.74	127.58	114.10
1	P	39	ASP	CA-CB-CG	-6.72	105.88	112.60
1	P	39	ASP	CB-CG-OD1	6.64	133.69	118.40
1	P	126	LYS	CG-CD-CE	-6.34	96.72	111.30
1	P	71	GLU	CG-CD-OE2	6.33	132.96	118.40
1	P	39	ASP	CB-CG-OD2	-6.19	104.17	118.40
1	R	105	LYS	CD-CE-NZ	6.18	131.69	111.90
1	P	194	LYS	CG-CD-CE	6.14	125.43	111.30
1	P	71	GLU	CG-CD-OE1	-6.02	104.55	118.40
1	O	254	LYS	CG-CD-CE	-5.99	97.52	111.30
1	P	106	GLU	CG-CD-OE2	5.99	132.18	118.40
1	Q	126	LYS	CB-CG-CD	5.94	124.97	111.30
1	P	106	GLU	CG-CD-OE1	-5.87	104.91	118.40
1	Q	39	ASP	CB-CG-OD1	-5.79	105.08	118.40
1	O	144	LYS	CB-CA-C	-5.79	98.37	110.17
1	Q	39	ASP	CB-CG-OD2	5.63	131.36	118.40
1	R	64	ASP	N-CA-CB	-5.57	103.55	111.84
1	Q	218	LYS	CG-CD-CE	-5.51	98.62	111.30
1	Q	64	ASP	N-CA-CB	-5.38	104.12	112.30
1	Q	267	LYS	CA-CB-CG	-5.37	103.37	114.10
1	P	253	GLN	CG-CD-NE2	5.24	124.25	116.40
1	R	144	LYS	CG-CD-CE	5.22	123.31	111.30
1	P	253	GLN	CG-CD-OE1	-5.12	110.57	120.80
1	R	254	LYS	CG-CD-CE	-5.04	99.70	111.30
1	R	194	LYS	CB-CG-CD	-5.00	99.79	111.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	41	ASN	Sidechain
1	Q	253	GLN	Sidechain
1	R	253	GLN	Sidechain
1	R	41	ASN	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	2546	0	2573	10	1
1	P	2546	0	2573	12	1
1	Q	2546	0	2573	9	0
1	R	2546	0	2573	13	1
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	O	13	0	10	0	0
3	P	13	0	10	0	0
3	R	13	0	10	0	0
4	O	65	0	0	1	1
4	P	63	0	0	0	0
4	Q	49	0	0	2	0
4	R	55	0	0	1	0
All	All	10631	0	10426	39	2

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 2.

All (39) 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:177:THR:OG1	1:P:247:ASP:OD2	2.08	0.71
1:Q:312:LYS:NZ	1:R:177:THR:OG1	2.27	0.67
1:R:185:ASN:HD22	1:R:185:ASN:H	1.49	0.58
1:P:206:LEU:HD22	4:Q:842:HOH:O	2.04	0.58
1:R:183:THR:OG1	1:R:185:ASN:ND2	2.37	0.57
1:P:79:GLU:HG2	1:P:84:GLN:HB2	1.90	0.53
1:P:252:LEU:HD12	1:P:311:PHE:CE1	2.44	0.53
1:O:185:ASN:H	1:O:185:ASN:HD22	1.57	0.52
1:O:104:THR:HG22	1:O:107:LEU:HD12	1.92	0.50
1:O:39:ASP:HB2	4:O:654:HOH:O	2.13	0.48
1:Q:20:ARG:HB2	4:Q:824:HOH:O	2.12	0.48
1:R:159:ALA:HB3	1:R:160:PRO:HD3	1.95	0.48
1:O:242:THR:HG23	1:O:243:VAL:HG23	1.96	0.47
1:Q:11:PHE:CE2	1:Q:16:ARG:HG2	2.50	0.47
1:R:131:ILE:CG2	1:R:151:ALA:HB2	2.45	0.46
1:Q:82:PRO:HB3	1:Q:111:HIS:CE1	2.51	0.46
1:R:134:MET:HE2	1:R:329:ASP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:135:GLY:HA3	1:Q:276:ILE:HD13	1.99	0.44
1:R:242:THR:HG23	1:R:243:VAL:HG23	1.99	0.44
1:Q:17:LEU:CD1	1:Q:320:GLU:HB3	2.48	0.44
1:R:142:ASP:HB3	4:R:943:HOH:O	2.16	0.44
1:O:134:MET:HE2	1:O:329:ASP:HB3	2.00	0.44
1:O:82:PRO:HB3	1:O:111:HIS:CE1	2.52	0.44
1:P:247:ASP:OD1	1:P:247:ASP:C	2.61	0.44
1:O:175:LEU:HD12	1:P:249:VAL:HG13	2.00	0.43
1:P:206:LEU:N	1:P:206:LEU:HD12	2.33	0.43
1:P:244:SER:HB2	1:P:317:TYR:CZ	2.53	0.43
1:R:247:ASP:OD1	1:R:247:ASP:C	2.60	0.43
1:R:135:GLY:C	1:R:136:ILE:HD12	2.44	0.43
1:O:252:LEU:HD12	1:O:311:PHE:CE1	2.54	0.42
1:P:158:LEU:HD23	1:P:217:ALA:HA	2.00	0.42
1:Q:17:LEU:HD13	1:Q:320:GLU:HB3	2.01	0.42
1:R:210:ILE:HB	1:R:237:ARG:HB2	2.03	0.41
1:P:77:PHE:CZ	1:P:86:PRO:HG2	2.55	0.41
1:R:252:LEU:HD12	1:R:311:PHE:CE1	2.56	0.41
1:Q:304:LEU:HD23	1:Q:312:LYS:HB3	2.04	0.40
1:P:258:TYR:OH	1:P:300:MET:O	2.33	0.40
1:Q:232:THR:HG22	1:R:306:LEU:HD13	2.03	0.40
1:O:299:ASP:OD2	1:P:200:ARG:NH2	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:144:LYS:CE	4:O:662:HOH:O[2_545]	1.52	0.68
1:O:253:GLN:NE2	1:R:253:GLN:CG[1_554]	1.95	0.25

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	331/345 (96%)	313 (95%)	17 (5%)	1 (0%)	36	55
1	P	331/345 (96%)	311 (94%)	19 (6%)	1 (0%)	36	55
1	Q	331/345 (96%)	310 (94%)	20 (6%)	1 (0%)	36	55
1	R	331/345 (96%)	311 (94%)	18 (5%)	2 (1%)	21	38
All	All	1324/1380 (96%)	1245 (94%)	74 (6%)	5 (0%)	30	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	243	VAL
1	R	243	VAL
1	Q	243	VAL
1	O	243	VAL
1	R	38	MET

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	277/286 (97%)	268 (97%)	9 (3%)	34	62
1	P	277/286 (97%)	265 (96%)	12 (4%)	26	51
1	Q	277/286 (97%)	267 (96%)	10 (4%)	31	58
1	R	277/286 (97%)	263 (95%)	14 (5%)	21	43
All	All	1108/1144 (97%)	1063 (96%)	45 (4%)	27	53

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	5	LYS
1	O	48	LYS
1	O	58	CYS
1	O	80	LYS
1	O	144	LYS
1	O	185	ASN

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Mol	Chain	Res	Type
1	O	222	LYS
1	O	247	ASP
1	O	304	LEU
1	P	25	ARG
1	P	26	LYS
1	P	39	ASP
1	P	41	ASN
1	P	72	LYS
1	P	80	LYS
1	P	91	GLN
1	P	105	LYS
1	P	197	LYS
1	P	214	THR
1	P	226	GLU
1	P	246	VAL
1	Q	48	LYS
1	Q	59	GLU
1	Q	64	ASP
1	Q	72	LYS
1	Q	89	LYS
1	Q	226	GLU
1	Q	247	ASP
1	Q	254	LYS
1	Q	267	LYS
1	Q	304	LEU
1	R	41	ASN
1	R	64	ASP
1	R	72	LYS
1	R	104	THR
1	R	144	LYS
1	R	168	ARG
1	R	185	ASN
1	R	194	LYS
1	R	197	LYS
1	R	214	THR
1	R	222	LYS
1	R	226	GLU
1	R	246	VAL
1	R	304	LEU

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	42	HIS
1	O	55	GLN
1	O	138	HIS
1	O	185	ASN
1	P	84	GLN
1	P	138	HIS
1	Q	139	HIS
1	Q	140	GLN
1	Q	333	HIS
1	R	140	GLN
1	R	185	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
3	AES	P	602	-	12,13,13	0.51	0	17,18,18	1.40	2 (11%)
2	NAD	P	701	-	46,48,48	1.64	5 (10%)	64,73,73	1.60	9 (14%)
3	AES	R	603	-	12,13,13	0.55	0	17,18,18	1.41	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	O	501	-	46,48,48	1.73	5 (10%)	64,73,73	1.58	8 (12%)
3	AES	O	601	-	12,13,13	0.48	0	17,18,18	1.44	3 (17%)
2	NAD	Q	801	-	46,48,48	1.87	6 (13%)	64,73,73	1.54	8 (12%)
2	NAD	R	901	-	46,48,48	1.70	5 (10%)	64,73,73	1.60	9 (14%)

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
3	AES	P	602	-	-	5/9/9/9	0/1/1/1
2	NAD	P	701	-	-	7/30/62/62	0/5/5/5
3	AES	R	603	-	-	6/9/9/9	0/1/1/1
2	NAD	O	501	-	-	8/30/62/62	0/5/5/5
3	AES	O	601	-	-	7/9/9/9	0/1/1/1
2	NAD	Q	801	-	-	10/30/62/62	0/5/5/5
2	NAD	R	901	-	-	3/30/62/62	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	801	NAD	O7N-C7N	9.64	1.42	1.24
2	O	501	NAD	O7N-C7N	9.10	1.41	1.24
2	R	901	NAD	O7N-C7N	9.05	1.41	1.24
2	P	701	NAD	O7N-C7N	8.62	1.40	1.24
2	Q	801	NAD	C2A-N1A	3.27	1.39	1.33
2	Q	801	NAD	C2N-N1N	3.07	1.38	1.35
2	R	901	NAD	C2A-N1A	2.89	1.39	1.33
2	O	501	NAD	C2N-N1N	2.77	1.38	1.35
2	O	501	NAD	C2A-N3A	2.76	1.38	1.33
2	O	501	NAD	C2A-N1A	2.73	1.38	1.33
2	P	701	NAD	C2A-N1A	2.73	1.38	1.33
2	R	901	NAD	C2A-N3A	2.71	1.38	1.33
2	Q	801	NAD	C2A-N3A	2.71	1.38	1.33
2	P	701	NAD	C2A-N3A	2.66	1.38	1.33
2	Q	801	NAD	PN-O3	2.60	1.62	1.59
2	R	901	NAD	C2N-N1N	2.32	1.37	1.35
2	R	901	NAD	C8A-N7A	2.18	1.35	1.31
2	O	501	NAD	C8A-N7A	2.18	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	801	NAD	C8A-N7A	2.16	1.35	1.31
2	P	701	NAD	C2N-N1N	2.07	1.37	1.35
2	P	701	NAD	C8A-N7A	2.01	1.35	1.31

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	901	NAD	N3A-C2A-N1A	-5.71	119.94	128.58
2	Q	801	NAD	N3A-C2A-N1A	-5.52	120.23	128.58
2	O	501	NAD	N3A-C2A-N1A	-5.33	120.52	128.58
2	P	701	NAD	N3A-C2A-N1A	-5.18	120.74	128.58
2	R	901	NAD	C5A-C4A-N3A	-4.79	120.12	126.72
2	O	501	NAD	C5A-C4A-N3A	-4.58	120.41	126.72
2	P	701	NAD	N9A-C8A-N7A	-4.57	107.46	113.94
2	P	701	NAD	C5A-C4A-N3A	-4.33	120.75	126.72
2	Q	801	NAD	C5A-C4A-N3A	-4.31	120.78	126.72
2	P	701	NAD	C5A-N7A-C8A	4.20	110.05	103.45
2	Q	801	NAD	N9A-C8A-N7A	-4.08	108.14	113.94
3	R	603	AES	O2S-S-C1	-3.98	104.88	110.92
2	O	501	NAD	N9A-C8A-N7A	-3.94	108.35	113.94
2	R	901	NAD	C5A-N7A-C8A	3.84	109.49	103.45
2	R	901	NAD	N9A-C8A-N7A	-3.82	108.52	113.94
2	O	501	NAD	C5A-N7A-C8A	3.81	109.43	103.45
2	R	901	NAD	C2A-N3A-C4A	3.70	120.88	111.83
2	Q	801	NAD	C5A-N7A-C8A	3.70	109.26	103.45
3	P	602	AES	O2S-S-C1	-3.64	105.41	110.92
3	O	601	AES	O1S-S-C1	-3.47	105.66	110.92
2	O	501	NAD	C2A-N3A-C4A	3.38	120.08	111.83
2	R	901	NAD	C4A-C5A-N7A	-3.34	106.76	110.58
2	Q	801	NAD	C2A-N3A-C4A	3.31	119.91	111.83
2	P	701	NAD	C2A-N3A-C4A	3.24	119.74	111.83
2	P	701	NAD	C4A-C5A-N7A	-3.20	106.92	110.58
2	O	501	NAD	C4A-C5A-N7A	-3.07	107.07	110.58
2	Q	801	NAD	N3A-C4A-N9A	3.04	132.34	127.17
3	O	601	AES	O2S-S-C1	-2.98	106.40	110.92
3	P	602	AES	C2-C1-S	2.84	121.26	119.25
2	O	501	NAD	N3A-C4A-N9A	2.79	131.91	127.17
3	R	603	AES	O1S-S-C1	-2.71	106.81	110.92
2	R	901	NAD	N3A-C4A-N9A	2.68	131.73	127.17
2	P	701	NAD	N3A-C4A-N9A	2.67	131.71	127.17
2	Q	801	NAD	C4A-C5A-N7A	-2.53	107.69	110.58
3	O	601	AES	C2-C1-S	2.40	120.95	119.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	701	NAD	O4B-C1B-N9A	2.20	112.31	108.09
2	Q	801	NAD	C4A-N9A-C8A	2.18	108.02	105.74
2	P	701	NAD	C4A-N9A-C8A	2.18	108.02	105.74
2	R	901	NAD	C5A-C4A-N9A	2.15	108.15	105.81
2	R	901	NAD	C2N-C3N-C4N	2.12	120.73	118.26
2	O	501	NAD	C6A-C5A-C4A	2.05	119.98	117.18

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	501	NAD	O4D-C1D-N1N-C2N
2	O	501	NAD	O4D-C1D-N1N-C6N
2	O	501	NAD	C2D-C1D-N1N-C2N
2	O	501	NAD	C2D-C1D-N1N-C6N
2	P	701	NAD	O4D-C1D-N1N-C2N
2	P	701	NAD	O4D-C1D-N1N-C6N
2	P	701	NAD	C2D-C1D-N1N-C2N
2	P	701	NAD	C2D-C1D-N1N-C6N
2	Q	801	NAD	C5B-O5B-PA-O1A
2	Q	801	NAD	O4D-C1D-N1N-C2N
2	Q	801	NAD	O4D-C1D-N1N-C6N
2	R	901	NAD	O4D-C1D-N1N-C2N
2	R	901	NAD	O4D-C1D-N1N-C6N
3	O	601	AES	C2-C1-S-F
3	O	601	AES	C2-C1-S-O1S
3	O	601	AES	C6-C1-S-F
3	O	601	AES	C6-C1-S-O1S
3	O	601	AES	C4-C7-C8-N8
3	P	602	AES	C2-C1-S-F
3	P	602	AES	C2-C1-S-O1S
3	P	602	AES	C6-C1-S-F
3	P	602	AES	C6-C1-S-O1S
3	P	602	AES	C4-C7-C8-N8
3	R	603	AES	C2-C1-S-F
3	R	603	AES	C2-C1-S-O1S
3	R	603	AES	C6-C1-S-F
3	R	603	AES	C6-C1-S-O1S
2	Q	801	NAD	O4B-C4B-C5B-O5B
2	Q	801	NAD	C3B-C4B-C5B-O5B
3	O	601	AES	C2-C1-S-O2S
2	P	701	NAD	C2B-C1B-N9A-C8A

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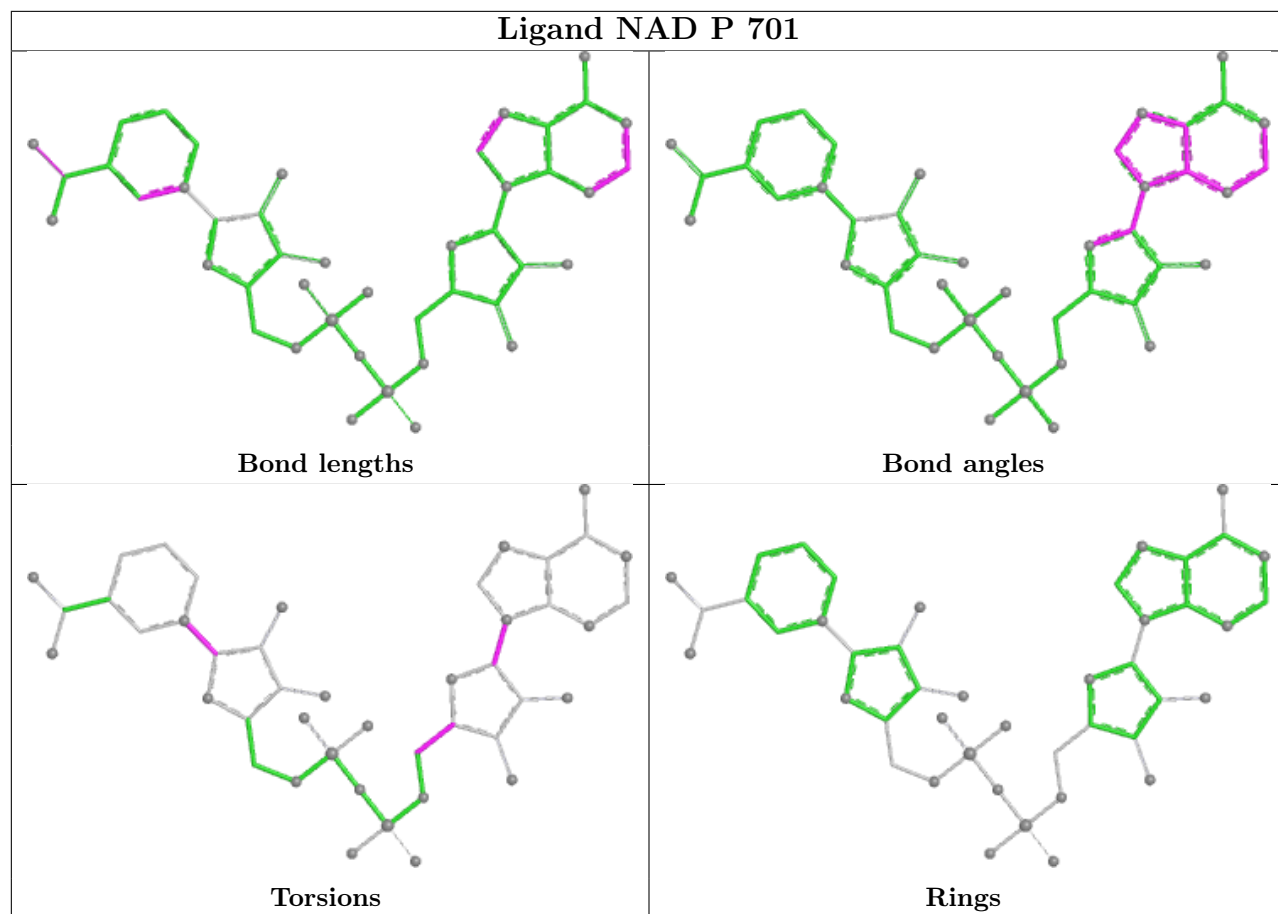
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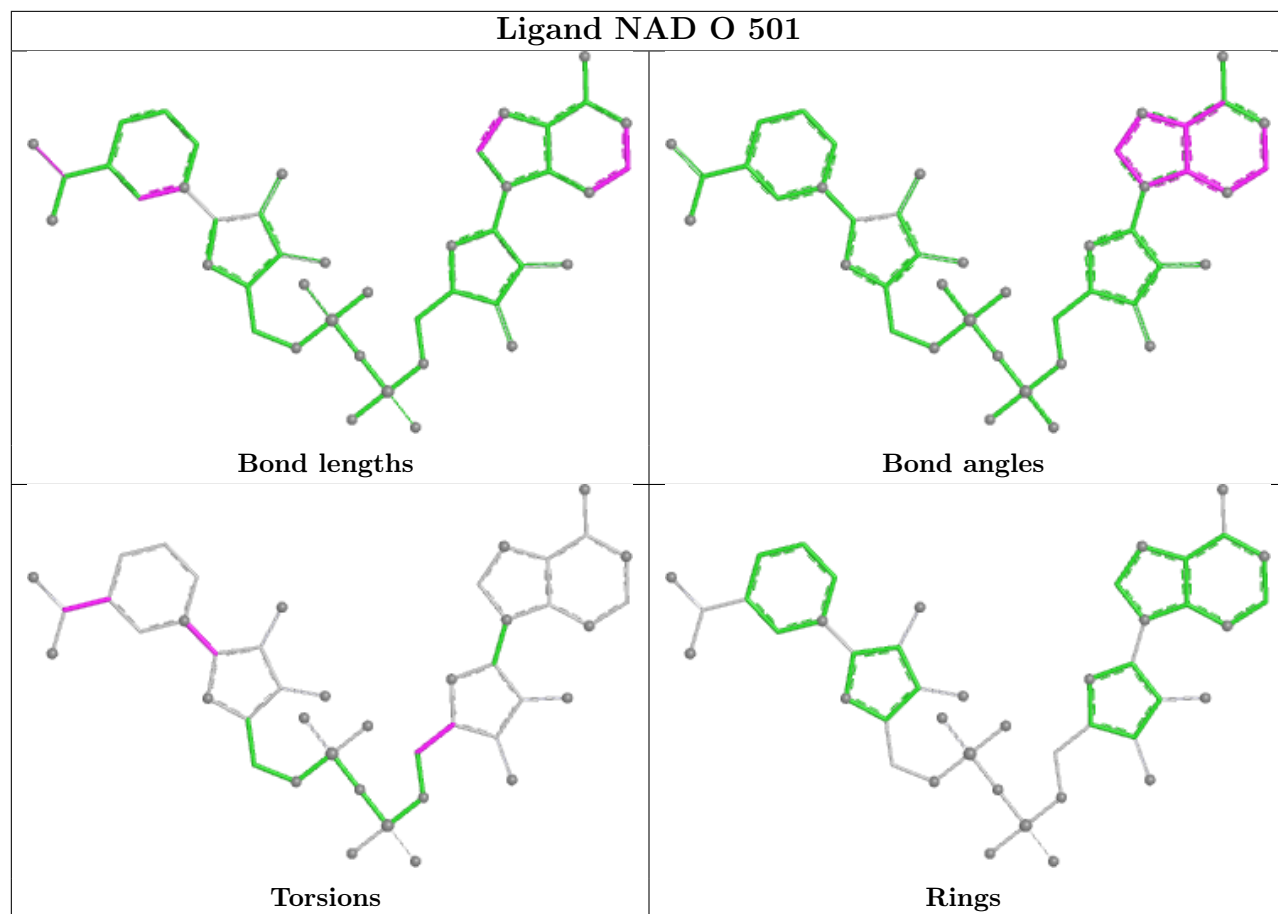
Mol	Chain	Res	Type	Atoms
2	Q	801	NAD	C5B-O5B-PA-O2A
2	Q	801	NAD	C5B-O5B-PA-O3
3	O	601	AES	C6-C1-S-O2S
3	R	603	AES	C2-C1-S-O2S
2	O	501	NAD	C4N-C3N-C7N-N7N
2	Q	801	NAD	C2D-C1D-N1N-C6N
2	P	701	NAD	O4B-C4B-C5B-O5B
2	R	901	NAD	O4B-C4B-C5B-O5B
2	O	501	NAD	C4N-C3N-C7N-O7N
3	R	603	AES	C6-C1-S-O2S
2	P	701	NAD	O4B-C1B-N9A-C8A
2	Q	801	NAD	PA-O3-PN-O1N
2	O	501	NAD	O4B-C4B-C5B-O5B
2	O	501	NAD	C2N-C3N-C7N-N7N
2	Q	801	NAD	PA-O3-PN-O2N

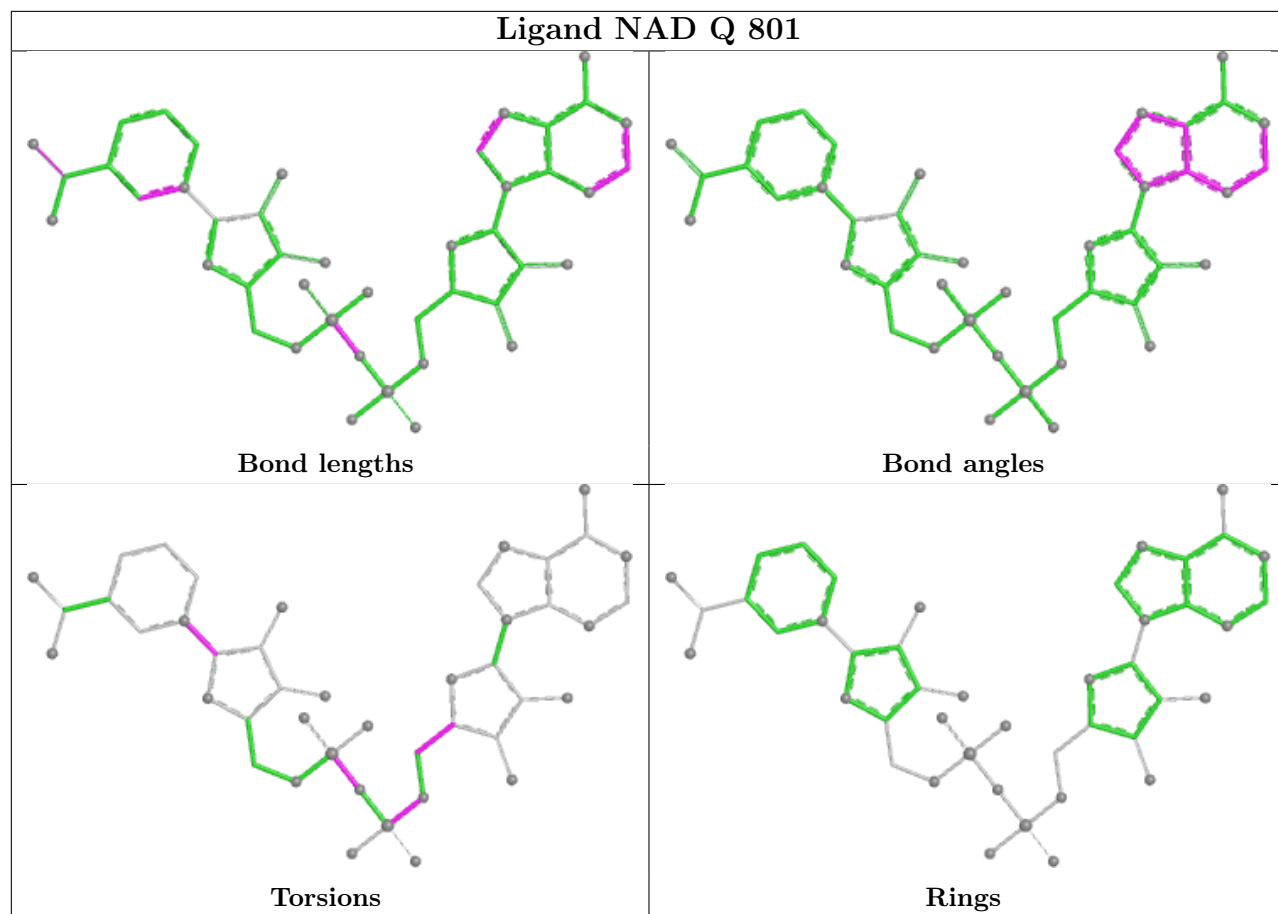
There are no ring outliers.

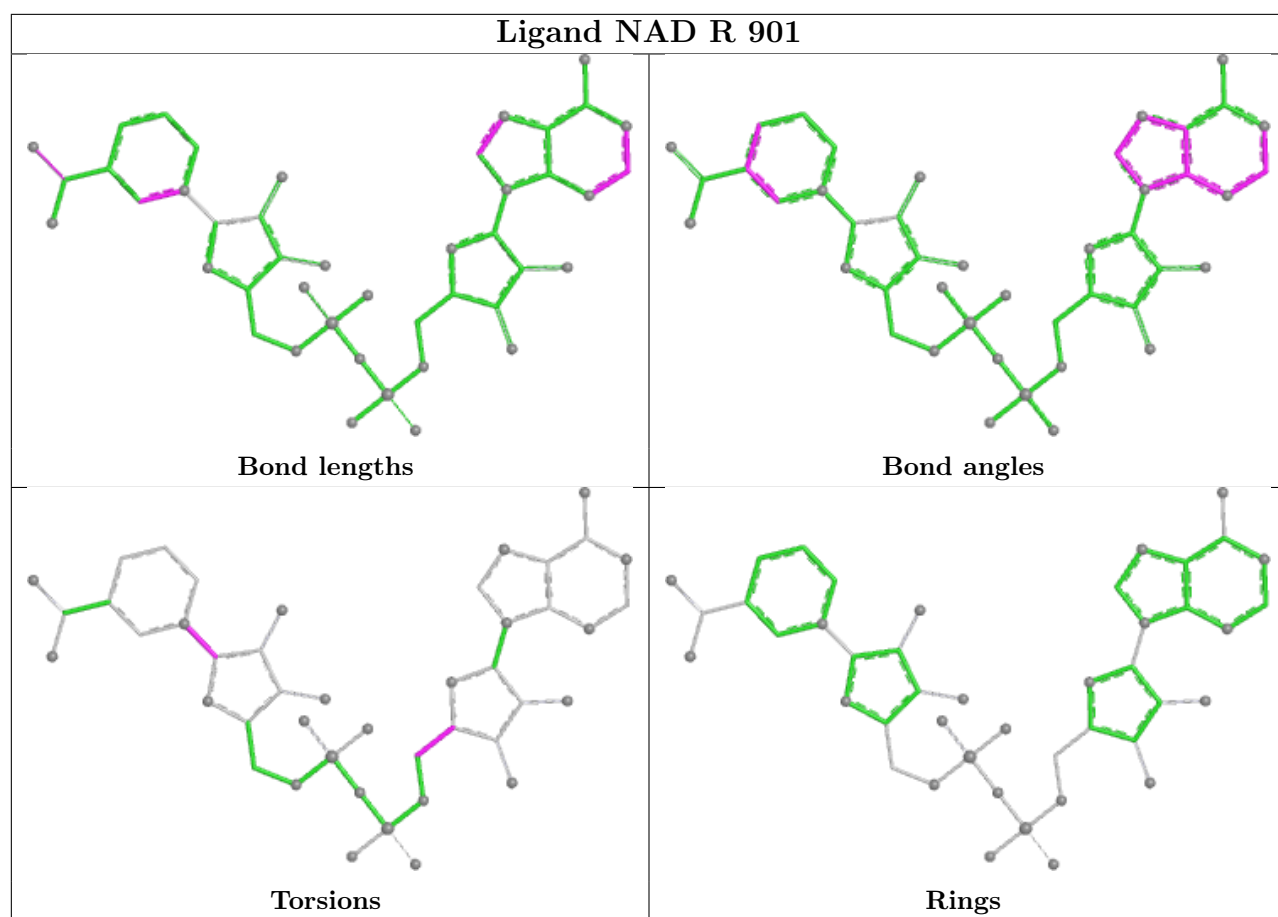
No monomer is involved in short contacts.

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 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	O	333/345 (96%)	0.55	4 (1%) 76 73	23, 52, 59, 63	17 (5%)
1	P	333/345 (96%)	0.63	14 (4%) 40 36	25, 52, 62, 68	21 (6%)
1	Q	333/345 (96%)	0.76	21 (6%) 26 23	27, 53, 62, 67	17 (5%)
1	R	333/345 (96%)	0.40	2 (0%) 85 83	28, 52, 59, 67	14 (4%)
All	All	1332/1380 (96%)	0.58	41 (3%) 51 47	23, 52, 61, 68	69 (5%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	41	ASN	3.5
1	Q	191	GLY	3.4
1	O	205	ALA	3.1
1	Q	205	ALA	3.0
1	Q	167	ASP	3.0
1	P	41	ASN	2.8
1	Q	309	ASN	2.8
1	O	285	VAL	2.8
1	Q	202	GLY	2.6
1	P	285	VAL	2.6
1	Q	192	PRO	2.5
1	P	211	PRO	2.5
1	O	199	TRP	2.5
1	Q	12	GLY	2.5
1	Q	39	ASP	2.4
1	Q	207	SER	2.4
1	P	204	CYS	2.4
1	Q	55	GLN	2.4
1	Q	174	GLY	2.3
1	P	202	GLY	2.3
1	R	41	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	336	THR	2.2
1	Q	199	TRP	2.2
1	P	205	ALA	2.2
1	P	68	LEU	2.2
1	Q	187	LEU	2.2
1	Q	189	VAL	2.2
1	P	217	ALA	2.2
1	Q	45	TYR	2.2
1	P	189	VAL	2.1
1	P	210	ILE	2.1
1	P	302	ALA	2.1
1	P	209	ILE	2.1
1	P	247	ASP	2.1
1	Q	186	GLN	2.1
1	R	253	GLN	2.0
1	Q	204	CYS	2.0
1	Q	311	PHE	2.0
1	O	208	ASN	2.0
1	Q	221	GLY	2.0
1	Q	49	TYR	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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AES	O	601	13/13	0.85	0.15	56,73,83,85	0
2	NAD	Q	801	44/44	0.88	0.13	55,66,74,75	0
3	AES	R	603	13/13	0.88	0.14	60,68,76,79	0

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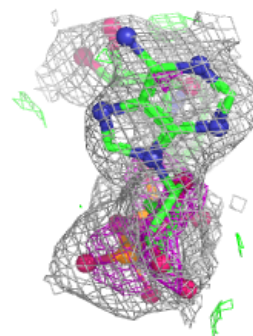
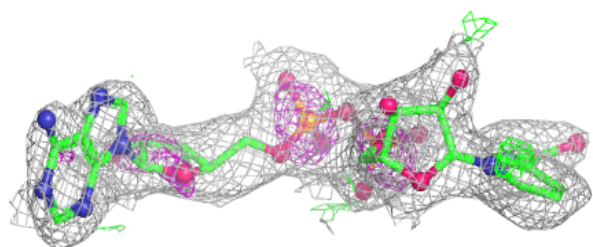
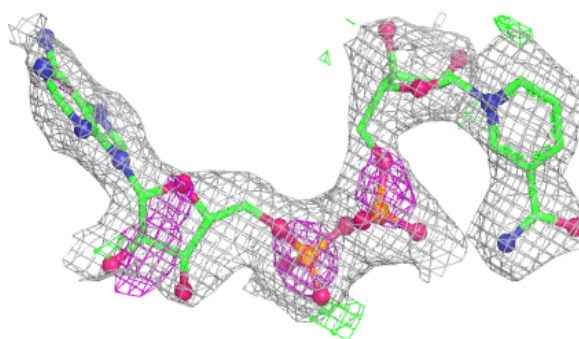
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AES	P	602	13/13	0.90	0.13	66,68,75,76	0
2	NAD	O	501	44/44	0.94	0.10	41,52,62,64	0
2	NAD	P	701	44/44	0.94	0.10	42,50,53,55	0
2	NAD	R	901	44/44	0.95	0.09	44,50,54,54	0

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.

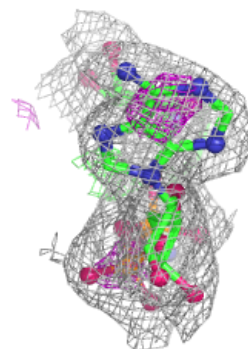
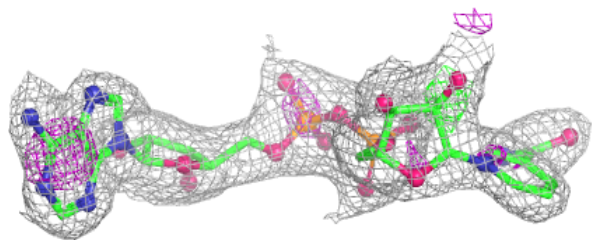
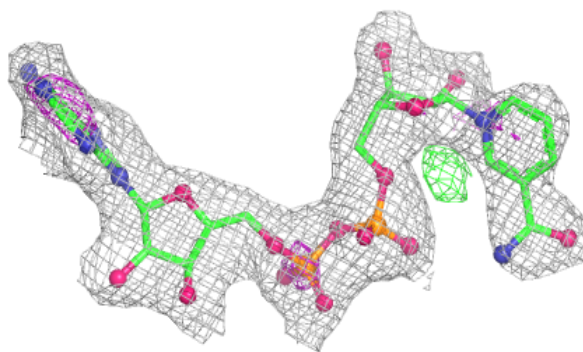
Electron density around NAD Q 801:

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

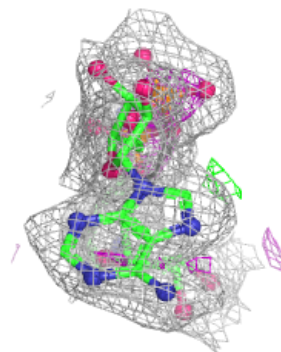
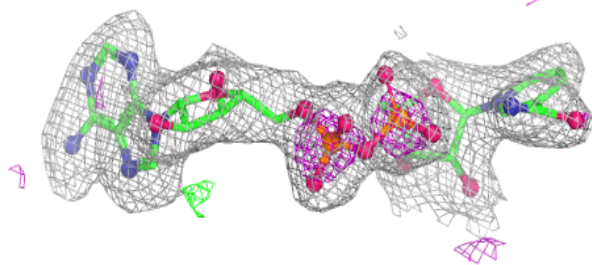
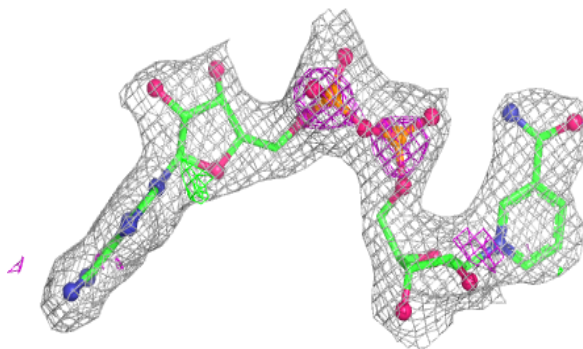


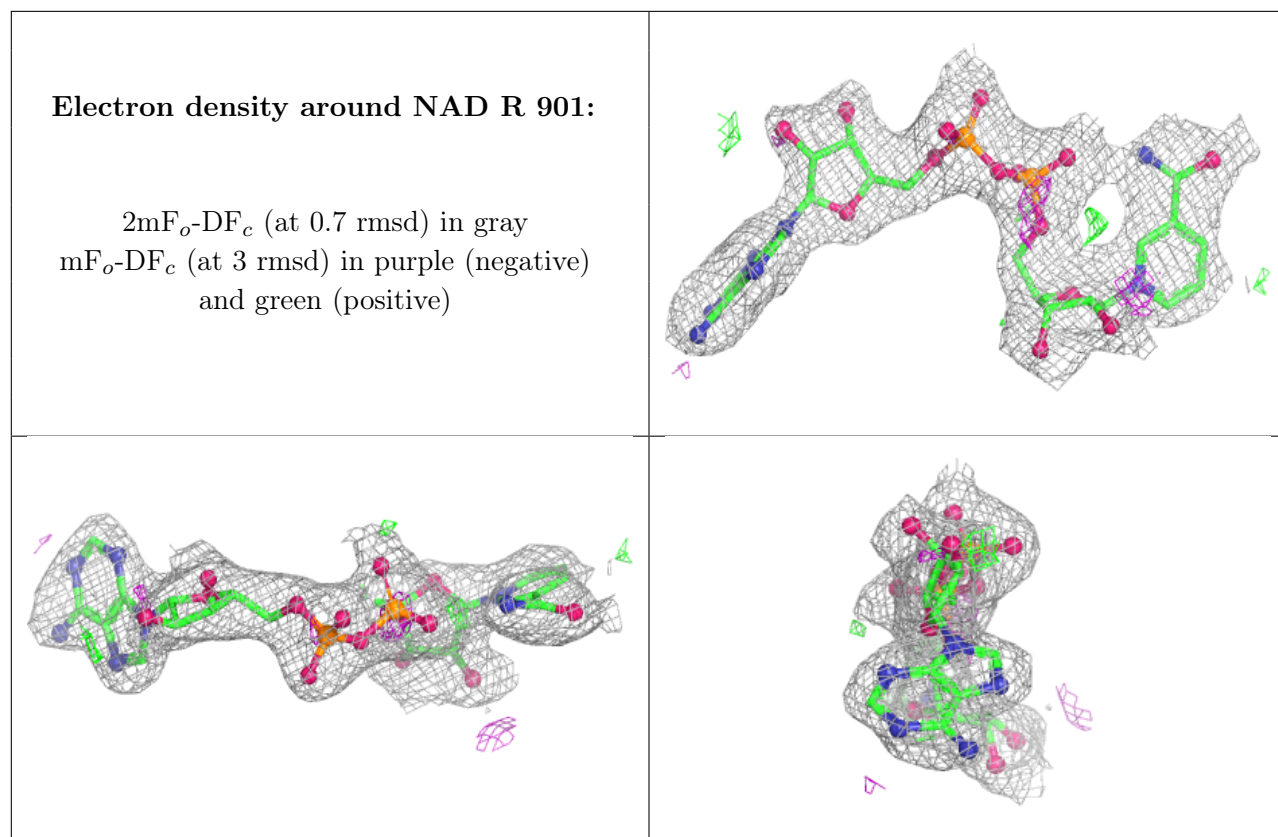
Electron density around NAD O 501:

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

**Electron density around NAD P 701:**

$2mF_o-DF_c$ (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.