



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:13 am GMT

PDB ID : 2NAD  
Title : HIGH RESOLUTION STRUCTURES OF HOLO AND APO FORMATE DE-HYDROGENASE  
Authors : Lamzin, V.S.; Dauter, Z.; Popov, V.O.; Harutyunyan, E.H.; Wilson, K.S.  
Deposited on : 1994-07-06  
Resolution : 2.05 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

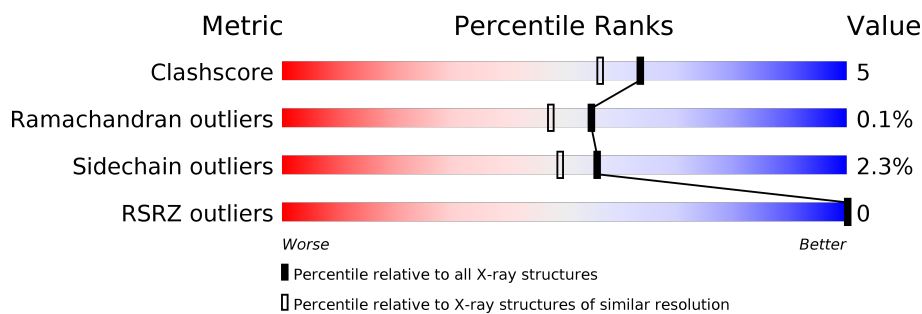
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.05 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))
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	A	393	 78% 19% ..
1	B	393	 76% 18% . .

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AZI	A	395	-	-	-	X
2	AZI	B	395	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	396	-	-	-	X

## 2 Entry composition [i](#)

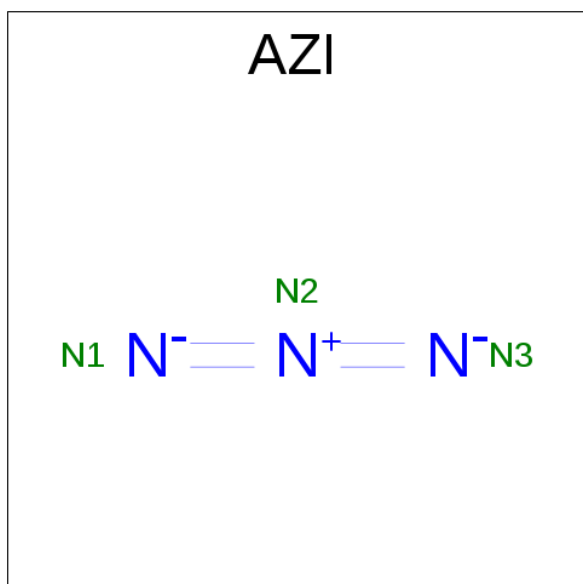
There are 5 unique types of molecules in this entry. The entry contains 6943 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NAD-DEPENDENT FORMATE DEHYDROGENASE.

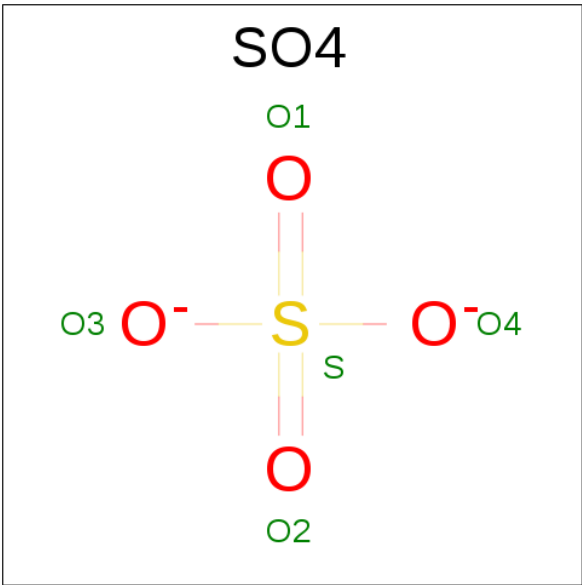
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3030	1913	533	570	14			
1	B	383	Total	C	N	O	S	0	0	0
			2983	1888	524	557	14			

- Molecule 2 is AZIDE ION (three-letter code: AZI) (formula: N<sub>3</sub>).



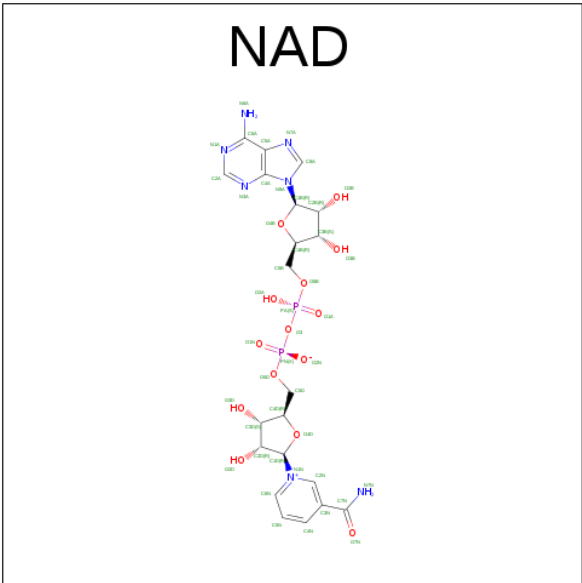
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	N	0	0
			3	3		
2	B	1	Total	N	0	0
			3	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

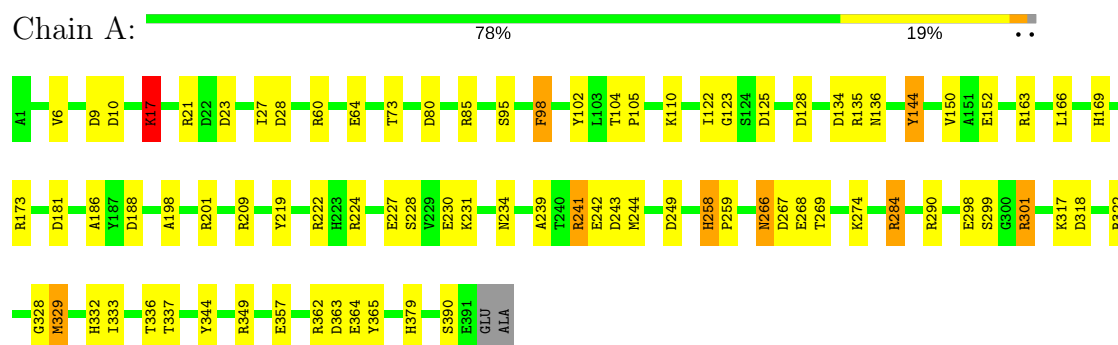
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	418	Total 418	O 418	0	0
5	B	413	Total 413	O 413	0	0

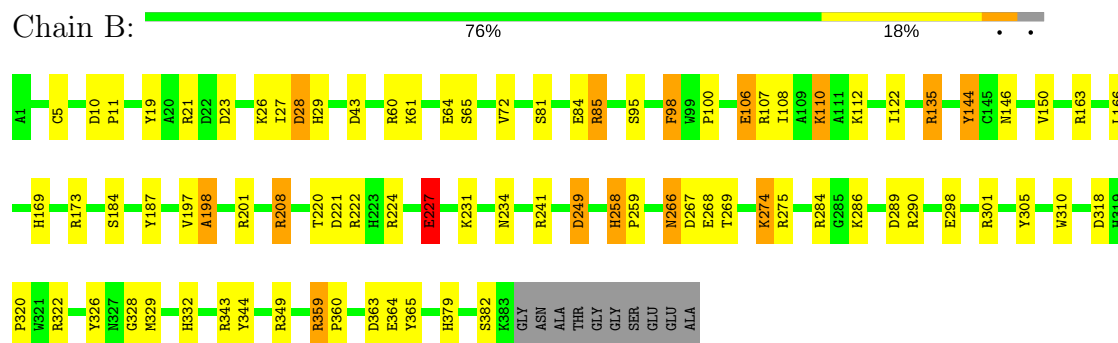
### 3 Residue-property plots

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: NAD-DEPENDENT FORMATE DEHYDROGENASE



#### • Molecule 1: NAD-DEPENDENT FORMATE DEHYDROGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.97Å 113.29Å 63.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.05 10.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.05) 96.2 (10.00-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	14.46 (at 2.04Å)	Xtriage
Refinement program	ARP/WARP, PROLSQ	Depositor
R, $R_{free}$	0.114 , (Not available) 0.124 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	13.8	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 87.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6943	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, 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	A	0.86	0/3106	1.89	69/4233 (1.6%)
1	B	0.86	0/3059	1.92	76/4170 (1.8%)
All	All	0.86	0/6165	1.90	145/8403 (1.7%)

There are no bond length outliers.

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	ARG	NE-CZ-NH2	-18.23	111.19	120.30
1	A	301	ARG	CD-NE-CZ	18.09	148.92	123.60
1	B	23	ASP	CB-CG-OD1	17.20	133.78	118.30
1	B	135	ARG	CD-NE-CZ	16.00	146.01	123.60
1	A	201	ARG	NE-CZ-NH1	15.90	128.25	120.30
1	B	208	ARG	CD-NE-CZ	15.53	145.35	123.60
1	A	21	ARG	NE-CZ-NH2	-12.82	113.89	120.30
1	B	173	ARG	NE-CZ-NH1	12.80	126.70	120.30
1	B	107	ARG	NE-CZ-NH2	12.63	126.61	120.30
1	B	60	ARG	NE-CZ-NH1	11.99	126.29	120.30
1	B	106	GLU	OE1-CD-OE2	-11.71	109.25	123.30
1	A	23	ASP	CB-CA-C	-11.43	87.53	110.40
1	A	349	ARG	NE-CZ-NH2	-11.09	114.75	120.30
1	A	318	ASP	CB-CG-OD1	10.91	128.12	118.30
1	B	274	LYS	CA-CB-CG	10.64	136.82	113.40
1	B	359	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	B	284	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	B	349	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	A	267	ASP	CB-CG-OD2	-10.10	109.21	118.30
1	B	21	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	A	274	LYS	CA-CB-CG	9.58	134.47	113.40
1	A	224	ARG	NE-CZ-NH2	9.57	125.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ARG	NE-CZ-NH1	-9.39	115.60	120.30
1	A	222	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	B	318	ASP	CB-CG-OD1	9.27	126.64	118.30
1	A	128	ASP	CB-CG-OD1	9.21	126.58	118.30
1	A	301	ARG	NE-CZ-NH2	9.18	124.89	120.30
1	A	201	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	B	322	ARG	NE-CZ-NH1	-8.84	115.88	120.30
1	A	23	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	B	359	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	A	219	TYR	CB-CG-CD2	-8.23	116.06	121.00
1	B	284	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	B	249	ASP	CB-CG-OD2	8.19	125.67	118.30
1	A	9	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	B	326	TYR	CB-CG-CD1	-8.03	116.18	121.00
1	B	344	TYR	CA-CB-CG	7.92	128.45	113.40
1	A	243	ASP	CB-CG-OD2	7.91	125.42	118.30
1	B	173	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	A	298	GLU	OE1-CD-OE2	-7.80	113.94	123.30
1	B	23	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	B	241	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	B	60	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	B	95	SER	N-CA-CB	7.61	121.92	110.50
1	A	163	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	290	ARG	CD-NE-CZ	7.55	134.17	123.60
1	B	221	ASP	CB-CG-OD1	7.50	125.05	118.30
1	B	163	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	43	ASP	CB-CG-OD2	7.48	125.03	118.30
1	A	344	TYR	CA-CB-CG	7.46	127.58	113.40
1	B	21	ARG	NH1-CZ-NH2	7.41	127.55	119.40
1	B	275	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	A	284	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	B	364	GLU	OE1-CD-OE2	7.36	132.14	123.30
1	B	224	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	A	329	MET	CA-CB-CG	7.29	125.70	113.30
1	A	80	ASP	CB-CG-OD2	-7.13	111.89	118.30
1	A	322	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	B	201	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	B	382	SER	CB-CA-C	7.05	123.50	110.10
1	B	267	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	A	298	GLU	CG-CD-OE1	7.01	132.33	118.30
1	A	209	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	344	TYR	CB-CG-CD2	7.00	125.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	GLU	OE1-CD-OE2	-6.91	115.01	123.30
1	B	349	ARG	CD-NE-CZ	-6.90	113.94	123.60
1	A	241	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	A	242	GLU	OE1-CD-OE2	6.81	131.47	123.30
1	A	258	HIS	CB-CA-C	6.79	123.98	110.40
1	B	21	ARG	NE-CZ-NH1	-6.75	116.93	120.30
1	B	64	GLU	OE1-CD-OE2	6.67	131.30	123.30
1	B	227	GLU	CB-CG-CD	6.65	132.16	114.20
1	A	95	SER	N-CA-CB	6.63	120.45	110.50
1	A	222	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	144	TYR	CB-CG-CD1	6.57	124.94	121.00
1	B	98	PHE	CB-CG-CD2	6.52	125.36	120.80
1	A	364	GLU	OE1-CD-OE2	6.51	131.11	123.30
1	B	249	ASP	CB-CG-OD1	-6.47	112.47	118.30
1	B	135	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	28	ASP	CB-CG-OD2	6.44	124.10	118.30
1	B	298	GLU	CG-CD-OE2	6.41	131.11	118.30
1	B	65	SER	CB-CA-C	-6.38	97.97	110.10
1	B	365	TYR	CB-CG-CD1	6.35	124.81	121.00
1	A	322	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	B	349	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	289	ASP	CB-CG-OD1	6.24	123.91	118.30
1	B	135	ARG	CG-CD-NE	6.24	124.89	111.80
1	A	298	GLU	CA-CB-CG	6.20	127.03	113.40
1	A	173	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	B	363	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	B	301	ARG	NH1-CZ-NH2	6.16	126.18	119.40
1	A	60	ARG	CD-NE-CZ	6.02	132.03	123.60
1	A	230	GLU	OE1-CD-OE2	-5.99	116.11	123.30
1	A	365	TYR	CG-CD2-CE2	5.98	126.08	121.30
1	A	80	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	23	ASP	OD1-CG-OD2	5.96	134.62	123.30
1	A	188	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	310	TRP	CA-CB-CG	5.92	124.95	113.70
1	B	110	LYS	CB-CA-C	-5.89	98.62	110.40
1	A	349	ARG	NH1-CZ-NH2	5.88	125.87	119.40
1	A	17	LYS	CB-CA-C	5.88	122.16	110.40
1	B	65	SER	CA-CB-OG	-5.84	95.42	111.20
1	A	144	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	B	258	HIS	CB-CA-C	5.80	122.01	110.40
1	A	110	LYS	CB-CA-C	-5.72	98.95	110.40
1	B	19	TYR	CB-CG-CD1	5.72	124.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	SER	CA-C-N	5.69	127.58	116.20
1	B	60	ARG	CD-NE-CZ	5.68	131.55	123.60
1	A	64	GLU	OE1-CD-OE2	5.65	130.08	123.30
1	B	343	ARG	O-C-N	-5.65	113.66	122.70
1	B	198	ALA	N-CA-CB	5.61	117.96	110.10
1	B	187	TYR	CD1-CE1-CZ	5.61	124.85	119.80
1	B	106	GLU	CG-CD-OE1	5.59	129.49	118.30
1	B	98	PHE	CG-CD1-CE1	5.56	126.92	120.80
1	A	186	ALA	CB-CA-C	-5.55	101.77	110.10
1	A	173	ARG	CA-CB-CG	5.53	125.57	113.40
1	B	298	GLU	OE1-CD-OE2	-5.51	116.69	123.30
1	B	220	THR	N-CA-CB	5.50	120.76	110.30
1	A	28	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	243	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	134	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	125	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	198	ALA	N-CA-CB	5.47	117.76	110.10
1	A	244	MET	O-C-N	-5.46	113.97	122.70
1	B	227	GLU	CG-CD-OE1	5.42	129.15	118.30
1	B	144	TYR	CB-CG-CD1	5.42	124.25	121.00
1	B	85	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	362	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	181	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	B	197	VAL	C-N-CA	5.31	134.99	121.70
1	B	85	ARG	CD-NE-CZ	5.31	131.03	123.60
1	A	10	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	249	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	B	184	SER	CB-CA-C	5.24	120.06	110.10
1	A	28	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	222	ARG	CD-NE-CZ	5.19	130.86	123.60
1	A	219	TYR	CB-CG-CD1	5.17	124.10	121.00
1	B	305	TYR	CB-CG-CD1	5.16	124.09	121.00
1	A	152	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	A	27	ILE	CG1-CB-CG2	-5.10	100.18	111.40
1	B	110	LYS	CD-CE-NZ	5.09	123.41	111.70
1	B	310	TRP	N-CA-CB	-5.08	101.45	110.60
1	A	98	PHE	CB-CG-CD1	-5.05	117.26	120.80
1	B	100	PRO	O-C-N	5.05	130.78	122.70
1	A	337	THR	O-C-N	-5.01	114.68	122.70

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	A	3030	0	2971	29	0
1	B	2983	0	2933	31	0
2	A	3	0	0	1	0
2	B	3	0	0	0	0
3	A	5	0	0	0	0
4	A	44	0	25	4	0
4	B	44	0	26	3	0
5	A	418	0	0	9	2
5	B	413	0	0	7	2
All	All	6943	0	5955	59	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 5.

All (59) 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:A:17:LYS:HD3	1:A:17:LYS:H	1.48	0.79
1:B:234:ASN:HB3	5:B:746:HOH:O	1.92	0.69
1:A:104:THR:HB	1:A:105:PRO:HD2	1.80	0.64
1:A:135:ARG:NH1	5:A:559:HOH:O	2.28	0.62
1:B:290:ARG:CZ	5:B:765:HOH:O	2.48	0.62
1:A:329:MET:O	1:B:169:HIS:HD2	1.84	0.61
1:B:379:HIS:HE1	5:B:436:HOH:O	1.84	0.61
1:A:266:ASN:HD22	1:A:268:GLU:H	1.50	0.60
1:A:169:HIS:HD2	1:B:329:MET:O	1.84	0.59
1:A:135:ARG:NH1	5:A:658:HOH:O	2.36	0.58
1:A:379:HIS:HE1	5:A:499:HOH:O	1.86	0.57
1:B:166:LEU:HD12	1:B:328:GLY:HA2	1.88	0.56
1:B:108:ILE:O	1:B:135:ARG:NH1	2.39	0.56
1:A:357:GLU:OE2	5:A:582:HOH:O	2.18	0.54
1:B:84:GLU:OE2	1:B:110:LYS:HE2	2.08	0.54
1:B:150:VAL:HG21	4:B:394:NAD:C4N	2.38	0.53
1:B:135:ARG:NH1	5:B:754:HOH:O	2.42	0.53
1:B:266:ASN:HD22	1:B:268:GLU:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ARG:CD	5:A:628:HOH:O	2.57	0.52
1:A:150:VAL:HG21	4:A:394:NAD:C4N	2.40	0.52
1:A:266:ASN:HD22	1:A:268:GLU:N	2.08	0.51
1:A:332:HIS:HE2	4:A:394:NAD:C7N	2.23	0.51
1:A:227:GLU:HG3	1:A:228:SER:N	2.26	0.50
1:A:266:ASN:ND2	1:A:269:THR:H	2.10	0.49
1:A:241:ARG:HD3	5:A:578:HOH:O	2.12	0.49
1:A:17:LYS:HD3	1:A:17:LYS:N	2.24	0.49
1:A:123:GLY:HA3	1:A:284:ARG:NH2	2.28	0.48
1:B:135:ARG:HD3	5:B:759:HOH:O	2.13	0.48
1:A:122:ILE:HG22	4:A:394:NAD:H3D	1.94	0.48
1:B:332:HIS:HE2	4:B:394:NAD:C7N	2.27	0.48
1:B:208:ARG:NE	5:B:692:HOH:O	2.39	0.47
1:B:266:ASN:ND2	1:B:269:THR:H	2.13	0.47
1:B:81:SER:O	1:B:85:ARG:HG3	2.16	0.46
1:B:106:GLU:O	1:B:110:LYS:HG3	2.16	0.46
2:A:395:AZI:N1	4:A:394:NAD:C3N	2.79	0.46
1:B:227:GLU:O	1:B:231:LYS:HG2	2.16	0.46
1:A:85:ARG:HG3	5:A:628:HOH:O	2.15	0.45
1:B:122:ILE:HG22	4:B:394:NAD:H3D	1.98	0.45
1:B:10:ASP:HB3	1:B:11:PRO:HD2	1.99	0.45
1:A:166:LEU:HD12	1:A:328:GLY:HA2	1.99	0.44
1:B:258:HIS:HB2	1:B:259:PRO:CD	2.47	0.44
1:B:359:ARG:HB3	1:B:360:PRO:HD2	1.99	0.44
1:A:6:VAL:HA	1:A:73:THR:O	2.18	0.43
1:B:122:ILE:HD12	1:B:146:ASN:OD1	2.17	0.43
1:A:102:TYR:CG	1:A:390:SER:HB2	2.53	0.43
1:A:258:HIS:HB2	1:A:259:PRO:CD	2.49	0.43
1:B:112:LYS:HA	1:B:135:ARG:HH22	1.83	0.43
1:A:258:HIS:HB2	1:A:259:PRO:HD2	2.00	0.42
1:A:317:LYS:HD3	1:A:317:LYS:C	2.38	0.42
1:B:266:ASN:HD22	1:B:268:GLU:N	2.15	0.42
1:A:333:ILE:HA	1:A:336:THR:HG22	2.01	0.42
1:B:266:ASN:C	1:B:266:ASN:HD22	2.23	0.41
1:B:5:CYS:O	1:B:72:VAL:HA	2.21	0.41
1:A:136:ASN:HB2	5:A:644:HOH:O	2.20	0.41
1:A:239:ALA:HB3	5:A:610:HOH:O	2.20	0.41
1:B:286:LYS:CE	5:B:675:HOH:O	2.68	0.41
1:B:28:ASP:OD2	1:B:29:HIS:HD2	2.04	0.41
1:B:290:ARG:HD2	1:B:320:PRO:HD2	2.03	0.41
1:B:249:ASP:OD1	1:B:274:LYS:HE2	2.21	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)
5:A:798:HOH:O	5:B:607:HOH:O[3_655]	2.00	0.20
5:A:613:HOH:O	5:B:577:HOH:O[3_655]	2.04	0.16

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/393 (99%)	378 (97%)	11 (3%)	0	100	100
1	B	381/393 (97%)	367 (96%)	13 (3%)	1 (0%)	44	35
All	All	770/786 (98%)	745 (97%)	24 (3%)	1 (0%)	55	47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	198	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	322/323 (100%)	314 (98%)	8 (2%)	53	46
1	B	318/323 (98%)	311 (98%)	7 (2%)	57	51
All	All	640/646 (99%)	625 (98%)	15 (2%)	56	49

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	98	PHE
1	A	144	TYR
1	A	231	LYS
1	A	234	ASN
1	A	266	ASN
1	A	301	ARG
1	A	363	ASP
1	B	26	LYS
1	B	27	ILE
1	B	61	LYS
1	B	98	PHE
1	B	144	TYR
1	B	227	GLU
1	B	266	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
1	A	234	ASN
1	A	266	ASN
1	A	379	HIS
1	B	29	HIS
1	B	169	HIS
1	B	266	ASN
1	B	379	HIS

### 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

5 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$
4	NAD	A	394	-	41,48,48	2.11	13 (31%)	43,73,73	3.91	17 (39%)
2	AZI	A	395	-	0,2,2	0.00	-	0,1,1	0.00	-
3	SO4	A	396	-	4,4,4	0.62	0	6,6,6	0.65	0
4	NAD	B	394	-	41,48,48	2.00	12 (29%)	43,73,73	3.19	16 (37%)
2	AZI	B	395	-	0,2,2	0.00	-	0,1,1	0.00	-

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
4	NAD	A	394	-	-	0/22/62/62	0/5/5/5
2	AZI	A	395	-	-	0/0/0/0	0/0/0/0
3	SO4	A	396	-	-	0/0/0/0	0/0/0/0
4	NAD	B	394	-	-	0/22/62/62	0/5/5/5
2	AZI	B	395	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	394	NAD	O2B-C2B	-3.34	1.35	1.43
4	A	394	NAD	O4B-C1B	-2.96	1.37	1.41
4	B	394	NAD	O2B-C2B	-2.23	1.37	1.43
4	B	394	NAD	O2D-C2D	-2.17	1.38	1.43
4	A	394	NAD	O2D-C2D	-2.11	1.38	1.43
4	B	394	NAD	O3B-C3B	2.08	1.47	1.43
4	A	394	NAD	O7N-C7N	2.11	1.28	1.24
4	B	394	NAD	O4B-C4B	2.20	1.50	1.45
4	B	394	NAD	C7N-N7N	2.33	1.37	1.33
4	B	394	NAD	C5N-C4N	2.37	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	394	NAD	C3D-C4D	2.43	1.59	1.53
4	A	394	NAD	C3B-C4B	2.44	1.59	1.53
4	B	394	NAD	C4A-N3A	2.48	1.39	1.35
4	A	394	NAD	C4A-N3A	2.51	1.39	1.35
4	A	394	NAD	C7N-N7N	2.93	1.38	1.33
4	A	394	NAD	C4N-C3N	3.09	1.44	1.39
4	B	394	NAD	C4N-C3N	3.14	1.44	1.39
4	B	394	NAD	C2D-C1D	3.21	1.58	1.53
4	A	394	NAD	O4D-C4D	3.29	1.52	1.45
4	A	394	NAD	C2D-C1D	3.30	1.58	1.53
4	B	394	NAD	O4D-C4D	3.98	1.54	1.45
4	B	394	NAD	C3N-C7N	4.61	1.57	1.50
4	A	394	NAD	C2A-N3A	5.59	1.41	1.32
4	A	394	NAD	C3N-C7N	5.83	1.59	1.50
4	B	394	NAD	C2A-N3A	6.33	1.42	1.32

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	394	NAD	O7N-C7N-C3N	-13.05	104.36	119.62
4	A	394	NAD	C3N-C2N-N1N	-8.54	111.83	120.43
4	A	394	NAD	C5N-C4N-C3N	-8.06	110.87	120.35
4	B	394	NAD	C3N-C2N-N1N	-7.98	112.39	120.43
4	B	394	NAD	O7N-C7N-C3N	-7.46	110.90	119.62
4	B	394	NAD	N3A-C2A-N1A	-6.86	122.88	128.86
4	A	394	NAD	N3A-C2A-N1A	-6.46	123.23	128.86
4	B	394	NAD	C5N-C4N-C3N	-6.30	112.94	120.35
4	B	394	NAD	C4B-O4B-C1B	-4.99	104.46	109.77
4	A	394	NAD	O4D-C4D-C3D	-3.54	98.14	105.17
4	A	394	NAD	C4B-O4B-C1B	-3.50	106.04	109.77
4	A	394	NAD	O3D-C3D-C4D	-3.38	101.20	111.09
4	B	394	NAD	O4D-C4D-C3D	-3.30	98.60	105.17
4	A	394	NAD	C4N-C3N-C7N	-3.10	112.84	121.07
4	A	394	NAD	C5A-C6A-N1A	-2.98	110.67	119.70
4	B	394	NAD	C5A-C6A-N1A	-2.98	110.69	119.70
4	A	394	NAD	O3B-C3B-C4B	-2.72	103.14	111.09
4	B	394	NAD	C4N-C3N-C7N	-2.62	114.11	121.07
4	B	394	NAD	O4B-C4B-C5B	-2.40	101.29	109.40
4	B	394	NAD	O3D-C3D-C4D	-2.38	104.15	111.09
4	A	394	NAD	O2N-PN-O1N	2.12	123.26	112.28
4	A	394	NAD	C6N-C5N-C4N	2.25	122.83	119.44
4	B	394	NAD	C3N-C7N-N7N	2.49	120.61	117.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	394	NAD	C2B-C3B-C4B	2.67	107.82	102.62
4	B	394	NAD	C5A-C6A-N6A	3.19	126.98	120.47
4	B	394	NAD	O7N-C7N-N7N	3.56	127.65	122.58
4	A	394	NAD	N6A-C6A-N1A	3.60	125.91	118.77
4	A	394	NAD	C3N-C7N-N7N	4.16	122.52	117.77
4	A	394	NAD	C2A-N1A-C6A	5.06	127.62	118.77
4	B	394	NAD	C2A-N1A-C6A	5.22	127.90	118.77
4	A	394	NAD	O7N-C7N-N7N	6.77	132.22	122.58
4	B	394	NAD	C2N-C3N-C4N	8.49	127.95	118.26
4	A	394	NAD	C2N-C3N-C4N	10.14	129.83	118.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	394	NAD	4	0
2	A	395	AZI	1	0
4	B	394	NAD	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	391/393 (99%)	-0.87	0 100 100	4, 11, 34, 62	0
1	B	383/393 (97%)	-0.96	0 100 100	2, 10, 30, 53	0
All	All	774/786 (98%)	-0.91	0 100 100	2, 10, 34, 62	0

There are no RSRZ outliers to report.

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	AZI	A	395	3/3	0.94	0.14	6.11	10,10,24,26	0
3	SO4	A	396	5/5	0.97	0.13	4.07	48,50,52,53	0
2	AZI	B	395	3/3	0.99	0.08	2.57	7,7,17,21	0
4	NAD	A	394	44/44	0.98	0.08	0.21	10,14,22,24	0
4	NAD	B	394	44/44	0.99	0.06	-0.02	4,6,14,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.