



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:11 AM EDT

PDB ID : 2NAD / pdb_00002nad
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

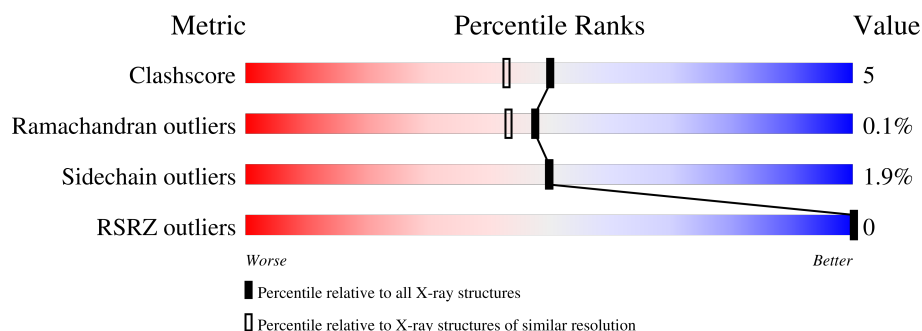
1 Overall quality at a glance

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	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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 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	A	393	
1	B	393	

2 Entry composition [i](#)

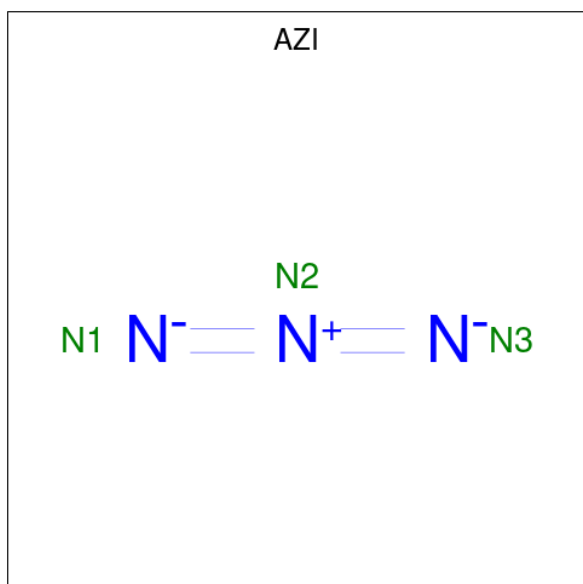
There are 5 unique types of molecules in this entry. The entry contains 6943 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

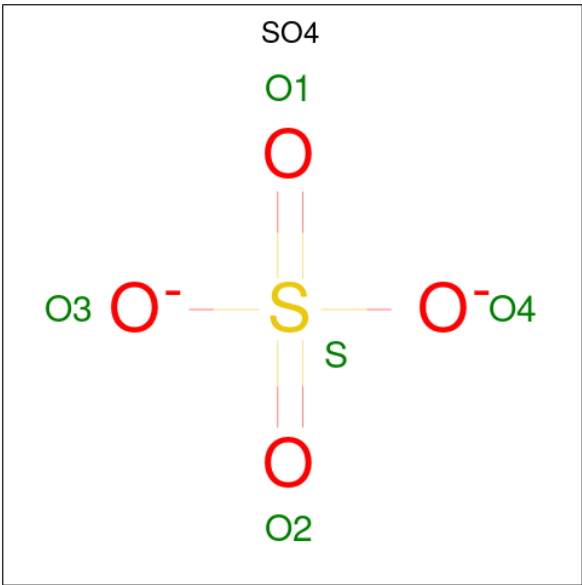
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3030	1913	533	570	14			
1	B	383	Total	C	N	O	S	0	0	0
			2983	1888	524	557	14			

- Molecule 2 is AZIDE ION (CCD ID: AZI) (formula: N₃).



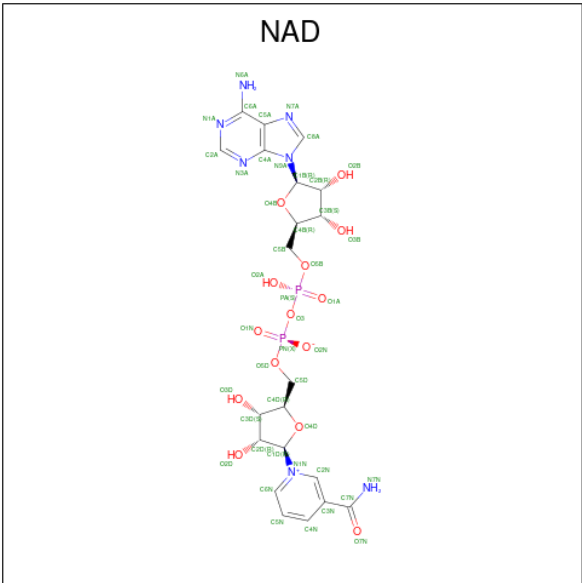
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	N	0	0
			3	3		
2	B	1	Total	N	0	0
			3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 5 is water.

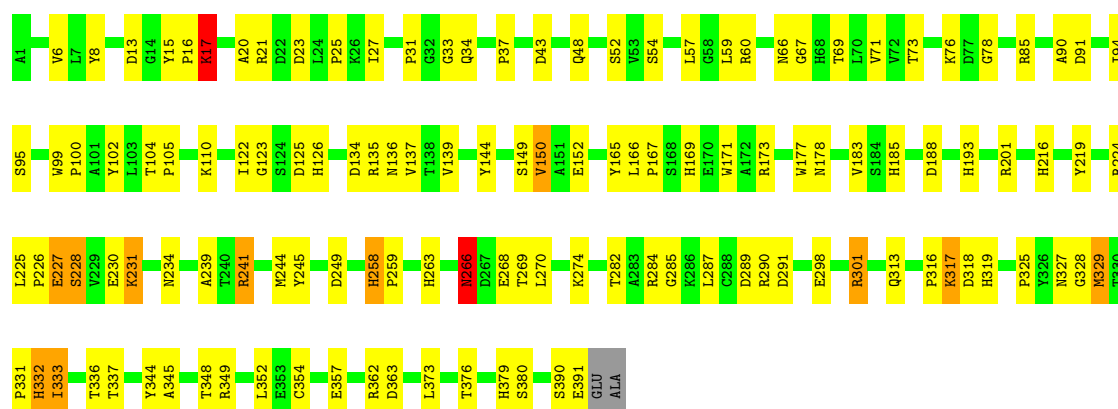
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	418	Total 418	O 418	0	0
5	B	413	Total 413	O 413	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

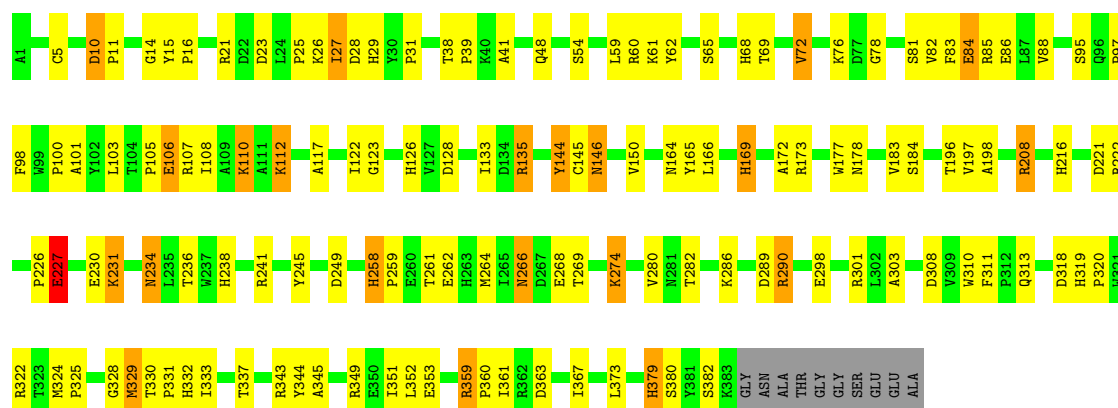
• Molecule 1: NAD-DEPENDENT FORMATE DEHYDROGENASE

Chain A: 



• Molecule 1: NAD-DEPENDENT FORMATE DEHYDROGENASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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) 95.4 (10.00-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.46 (at 2.04Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.114 , (Not available) 0.124 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 87.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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, AZI, SO4

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	1.15	0/3106	2.26	153/4233 (3.6%)
1	B	1.15	0/3059	2.22	147/4170 (3.5%)
All	All	1.15	0/6165	2.24	300/8403 (3.6%)

There are no bond length outliers.

All (300) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ARG	CD-NE-CZ	17.52	148.92	124.40
1	B	135	ARG	CD-NE-CZ	15.43	146.01	124.40
1	B	208	ARG	CD-NE-CZ	14.96	145.35	124.40
1	B	227	GLU	CB-CG-CD	11.51	132.16	112.60
1	B	274	LYS	CA-CB-CG	11.36	136.82	114.10
1	A	258	HIS	CB-CA-C	10.84	123.98	110.76
1	A	23	ASP	CB-CA-C	-10.38	87.53	110.67
1	A	274	LYS	CA-CB-CG	10.18	134.47	114.10
1	B	31	PRO	CA-C-O	9.81	131.73	121.23
1	A	258	HIS	N-CA-C	-9.26	99.83	108.07
1	A	333	ILE	N-CA-C	9.08	122.42	113.53
1	B	301	ARG	NE-CZ-NH2	-8.90	111.19	119.20
1	A	318	ASP	CA-CB-CG	8.81	121.41	112.60
1	B	164	ASN	OD1-CG-ND2	8.75	131.35	122.60
1	A	362	ARG	CA-C-O	8.64	130.38	120.96
1	B	367	ILE	N-CA-C	-8.43	104.96	111.62
1	A	245	TYR	CA-C-O	8.43	126.39	118.63
1	B	107	ARG	NE-CZ-NH2	8.24	126.61	119.20
1	B	344	TYR	CA-CB-CG	8.08	128.45	113.90
1	A	17	LYS	N-CA-C	-8.06	103.58	113.41
1	B	222	ARG	N-CA-C	-8.02	102.62	111.36
1	B	169	HIS	CA-CB-CG	-7.96	105.84	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	LEU	N-CA-C	-7.93	102.86	112.54
1	B	197	VAL	N-CA-CB	7.93	120.70	111.66
1	B	65	SER	CA-CB-OG	-7.84	95.42	111.10
1	A	344	TYR	CA-CB-CG	7.60	127.58	113.90
1	B	172	ALA	CA-C-O	7.59	128.52	120.70
1	B	98	PHE	CA-CB-CG	-7.57	106.23	113.80
1	A	69	THR	CA-C-N	7.54	133.82	123.11
1	A	69	THR	C-N-CA	7.54	133.82	123.11
1	A	66	ASN	CA-CB-CG	-7.49	105.11	112.60
1	B	349	ARG	CD-NE-CZ	-7.47	113.94	124.40
1	A	60	ARG	N-CA-C	7.46	119.05	111.07
1	B	318	ASP	CA-CB-CG	7.45	120.05	112.60
1	B	343	ARG	O-C-N	-7.44	113.66	122.15
1	A	327	ASN	OD1-CG-ND2	-7.44	115.16	122.60
1	A	230	GLU	CA-C-O	7.42	128.42	120.55
1	A	17	LYS	CB-CA-C	7.38	122.16	109.24
1	B	337	THR	N-CA-C	-7.34	100.85	110.53
1	B	112	LYS	CA-C-O	-7.25	110.46	119.38
1	B	221	ASP	CA-CB-CG	7.22	119.82	112.60
1	A	99	TRP	O-C-N	-7.19	115.94	121.19
1	A	13	ASP	CA-CB-CG	7.16	119.76	112.60
1	B	76	LYS	N-CA-C	7.16	124.07	114.12
1	A	226	PRO	CB-CA-C	-7.13	102.26	111.46
1	A	337	THR	O-C-N	-7.11	114.68	122.79
1	B	230	GLU	CA-C-N	7.06	130.31	120.29
1	B	230	GLU	C-N-CA	7.06	130.31	120.29
1	B	197	VAL	CA-C-N	7.04	134.99	121.54
1	B	197	VAL	C-N-CA	7.04	134.99	121.54
1	A	225	LEU	CA-C-N	7.00	126.97	119.76
1	A	225	LEU	C-N-CA	7.00	126.97	119.76
1	A	290	ARG	CD-NE-CZ	6.98	134.17	124.40
1	A	329	MET	CA-C-O	6.91	129.10	121.56
1	B	60	ARG	N-CA-C	6.89	118.44	111.07
1	B	324	MET	CA-C-N	6.84	126.80	119.76
1	B	324	MET	C-N-CA	6.84	126.80	119.76
1	A	266	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	A	249	ASP	CA-CB-CG	-6.83	105.77	112.60
1	A	290	ARG	N-CA-C	6.82	118.37	111.07
1	B	216	HIS	CA-C-O	-6.80	113.08	120.36
1	A	66	ASN	CB-CG-ND2	6.79	126.58	116.40
1	B	126	HIS	CA-CB-CG	-6.78	107.02	113.80
1	B	23	ASP	CA-C-O	-6.76	114.22	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	NE-CZ-NH1	6.75	128.25	121.50
1	B	238	HIS	O-C-N	-6.75	115.42	123.31
1	A	59	LEU	N-CA-C	6.74	121.67	113.38
1	A	193	HIS	O-C-N	-6.73	115.67	123.27
1	A	69	THR	O-C-N	-6.72	115.56	123.22
1	A	48	GLN	CG-CD-NE2	-6.71	106.34	116.40
1	B	23	ASP	CB-CG-OD1	6.69	133.78	118.40
1	B	146	ASN	OD1-CG-ND2	6.63	129.23	122.60
1	A	331	PRO	O-C-N	-6.61	114.78	122.71
1	A	150	VAL	CA-C-N	6.61	129.13	120.28
1	A	150	VAL	C-N-CA	6.61	129.13	120.28
1	A	285	GLY	N-CA-C	6.57	120.61	112.73
1	A	224	ARG	NE-CZ-NH2	6.54	125.08	119.20
1	A	78	GLY	CA-C-N	6.53	126.23	119.64
1	A	78	GLY	C-N-CA	6.53	126.23	119.64
1	B	216	HIS	O-C-N	6.51	130.65	123.22
1	B	216	HIS	CA-CB-CG	-6.51	107.29	113.80
1	A	67	GLY	N-CA-C	6.50	124.43	115.27
1	B	62	TYR	O-C-N	-6.49	115.38	122.07
1	A	317	LYS	CA-C-O	6.47	127.41	120.10
1	A	298	GLU	CA-CB-CG	6.47	127.03	114.10
1	B	329	MET	N-CA-C	6.44	119.58	110.50
1	A	373	LEU	CA-C-O	-6.38	114.18	121.19
1	B	382	SER	CB-CA-C	6.37	123.50	109.94
1	B	101	ALA	CA-C-O	6.37	127.54	120.92
1	A	100	PRO	N-CA-C	6.36	120.92	110.55
1	A	244	MET	O-C-N	-6.36	113.97	122.23
1	B	21	ARG	NH1-CZ-NH2	6.34	127.55	119.30
1	A	301	ARG	NE-CZ-NH2	6.32	124.89	119.20
1	A	126	HIS	CA-C-N	6.32	131.03	123.19
1	A	126	HIS	C-N-CA	6.32	131.03	123.19
1	A	316	PRO	CA-C-O	6.32	128.50	121.43
1	A	178	ASN	N-CA-CB	-6.31	102.36	111.70
1	B	289	ASP	N-CA-C	-6.29	100.35	109.59
1	B	310	TRP	N-CA-CB	-6.28	101.45	111.62
1	A	285	GLY	CA-C-O	6.28	127.21	120.75
1	A	332	HIS	CA-C-N	6.27	129.24	121.71
1	A	332	HIS	C-N-CA	6.27	129.24	121.71
1	B	313	GLN	OE1-CD-NE2	-6.27	116.33	122.60
1	A	183	VAL	N-CA-C	6.27	120.01	112.80
1	A	234	ASN	CA-CB-CG	6.26	118.86	112.60
1	B	86	GLU	CA-C-O	6.25	127.06	119.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	PRO	CA-C-N	6.25	128.94	120.38
1	B	226	PRO	C-N-CA	6.25	128.94	120.38
1	B	14	GLY	N-CA-C	6.24	122.05	112.81
1	A	228	SER	O-C-N	6.24	129.94	122.27
1	B	78	GLY	CA-C-N	6.24	125.80	119.19
1	B	78	GLY	C-N-CA	6.24	125.80	119.19
1	A	91	ASP	CA-C-O	6.22	127.15	120.24
1	A	289	ASP	N-CA-C	-6.21	99.75	109.25
1	B	21	ARG	CA-C-O	6.15	127.97	121.33
1	B	95	SER	N-CA-CB	6.14	121.92	111.66
1	B	165	TYR	N-CA-C	6.11	117.61	111.07
1	B	359	ARG	CA-C-O	6.10	126.91	120.63
1	B	72	VAL	O-C-N	-6.10	116.78	123.18
1	A	231	LYS	CA-C-O	6.09	126.97	120.70
1	A	298	GLU	CG-CD-OE1	6.05	132.33	118.40
1	B	88	VAL	N-CA-C	6.05	117.52	110.62
1	A	27	ILE	CB-CG1-CD1	-6.04	101.12	113.80
1	B	380	SER	N-CA-C	6.04	121.57	113.72
1	A	31	PRO	N-CA-CB	6.03	108.69	103.27
1	B	258	HIS	CB-CA-C	6.01	122.01	110.17
1	B	103	LEU	CA-C-O	6.00	128.91	122.13
1	B	68	HIS	CA-CB-CG	-6.00	107.80	113.80
1	B	184	SER	CA-CB-OG	-5.99	99.11	111.10
1	B	15	TYR	CB-CA-C	5.99	119.03	109.62
1	A	125	ASP	CA-CB-CG	-5.98	106.62	112.60
1	A	352	LEU	CA-C-O	-5.97	114.55	120.70
1	B	310	TRP	CA-CB-CG	5.97	124.95	113.60
1	A	99	TRP	CA-C-N	5.96	126.87	120.13
1	A	99	TRP	C-N-CA	5.96	126.87	120.13
1	B	117	ALA	O-C-N	-5.94	116.26	123.27
1	B	325	PRO	N-CA-CB	5.93	108.59	103.31
1	B	331	PRO	N-CA-C	-5.92	102.87	111.33
1	A	21	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	B	222	ARG	NE-CZ-NH1	-5.90	115.60	121.50
1	A	258	HIS	CA-C-O	5.88	125.91	120.56
1	A	317	LYS	O-C-N	-5.87	115.35	122.22
1	B	105	PRO	O-C-N	-5.87	115.49	122.24
1	B	103	LEU	O-C-N	-5.87	115.92	122.55
1	A	8	TYR	O-C-N	-5.86	116.17	122.85
1	B	280	VAL	O-C-N	-5.86	116.93	123.26
1	B	135	ARG	CG-CD-NE	5.86	124.89	112.00
1	A	71	VAL	N-CA-CB	5.85	119.04	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	SER	CB-CA-C	-5.85	97.97	110.32
1	B	351	ILE	O-C-N	-5.85	116.18	121.91
1	B	330	THR	CA-C-N	5.85	126.66	120.11
1	B	330	THR	C-N-CA	5.85	126.66	120.11
1	B	48	GLN	O-C-N	5.83	129.50	122.85
1	B	308	ASP	CA-CB-CG	5.83	118.43	112.60
1	B	183	VAL	N-CA-C	5.83	118.60	112.83
1	B	144	TYR	O-C-N	-5.82	116.03	121.56
1	A	25	PRO	CB-CA-C	-5.82	103.78	111.23
1	A	329	MET	CA-CB-CG	5.80	125.70	114.10
1	B	133	ILE	N-CA-C	-5.80	105.08	110.53
1	A	152	GLU	CB-CG-CD	5.79	122.44	112.60
1	A	270	LEU	CA-C-O	5.79	126.50	119.38
1	A	263	HIS	CA-CB-CG	-5.78	108.02	113.80
1	B	97	PRO	CA-C-N	5.77	129.83	120.60
1	B	97	PRO	C-N-CA	5.77	129.83	120.60
1	B	144	TYR	N-CA-CB	-5.76	107.60	114.17
1	A	76	LYS	N-CA-C	5.75	121.20	113.72
1	B	196	THR	CA-CB-OG1	-5.75	100.98	109.60
1	A	345	ALA	N-CA-C	-5.75	105.10	111.36
1	A	173	ARG	CA-CB-CG	5.74	125.57	114.10
1	B	100	PRO	O-C-N	5.71	130.78	122.78
1	B	82	VAL	CB-CA-C	-5.70	104.44	112.14
1	B	333	ILE	N-CA-C	5.69	121.18	109.34
1	A	48	GLN	O-C-N	5.69	129.33	122.85
1	B	106	GLU	OE1-CD-OE2	-5.69	109.25	122.90
1	B	236	THR	CA-CB-OG1	-5.68	101.08	109.60
1	A	171	TRP	N-CA-CB	5.67	118.23	110.01
1	A	43	ASP	CA-C-O	-5.67	114.14	121.17
1	B	373	LEU	N-CA-C	-5.67	103.00	110.43
1	B	352	LEU	CA-C-O	-5.66	114.55	120.55
1	A	327	ASN	CB-CG-ND2	5.66	124.89	116.40
1	A	228	SER	CA-C-O	-5.65	113.47	119.97
1	B	345	ALA	N-CA-C	-5.64	105.21	111.36
1	B	14	GLY	CA-C-O	-5.63	117.39	122.57
1	A	16	PRO	N-CA-CB	5.63	108.32	103.31
1	B	333	ILE	CB-CA-C	-5.63	102.06	111.29
1	B	322	ARG	NE-CZ-NH1	-5.62	115.88	121.50
1	B	311	PHE	CA-CB-CG	-5.62	108.18	113.80
1	A	15	TYR	CA-C-O	5.62	125.42	119.80
1	A	188	ASP	N-CA-CB	5.61	119.56	110.41
1	B	10	ASP	CA-C-N	5.60	125.61	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	ASP	C-N-CA	5.60	125.61	119.89
1	A	149	SER	O-C-N	-5.60	116.27	122.09
1	B	110	LYS	CB-CA-C	-5.59	98.62	110.31
1	A	227	GLU	CB-CG-CD	5.59	122.10	112.60
1	B	27	ILE	CB-CA-C	5.59	118.94	110.62
1	A	241	ARG	O-C-N	-5.57	115.42	122.27
1	A	282	THR	N-CA-C	-5.55	105.82	112.59
1	A	165	TYR	N-CA-C	5.54	117.00	111.07
1	B	117	ALA	N-CA-C	-5.54	99.48	108.52
1	A	134	ASP	N-CA-C	5.54	117.31	111.28
1	B	25	PRO	O-C-N	-5.53	116.22	122.91
1	B	298	GLU	CG-CD-OE2	5.53	131.11	118.40
1	B	76	LYS	N-CA-CB	-5.50	103.29	110.88
1	A	216	HIS	CA-CB-CG	-5.50	108.30	113.80
1	A	319	HIS	CA-C-N	5.49	125.32	119.28
1	A	319	HIS	C-N-CA	5.49	125.32	119.28
1	A	354	CYS	CA-C-N	5.48	127.57	120.44
1	A	354	CYS	C-N-CA	5.48	127.57	120.44
1	A	333	ILE	CB-CG1-CD1	5.47	125.30	113.80
1	B	123	GLY	O-C-N	5.47	129.82	122.70
1	A	34	GLN	O-C-N	-5.47	116.14	122.87
1	B	59	LEU	N-CA-C	5.46	120.10	113.38
1	A	391	GLU	CA-C-O	5.46	130.07	120.80
1	A	60	ARG	CD-NE-CZ	5.45	132.03	124.40
1	B	31	PRO	O-C-N	-5.43	116.76	123.01
1	A	291	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	353	GLU	O-C-N	-5.42	116.49	122.07
1	B	59	LEU	N-CA-CB	-5.41	102.46	110.53
1	A	230	GLU	O-C-N	-5.40	116.40	122.12
1	B	262	GLU	O-C-N	-5.40	116.25	122.95
1	A	57	LEU	CA-C-O	5.38	126.66	120.32
1	A	20	ALA	N-CA-C	5.38	119.10	112.54
1	A	316	PRO	CA-C-N	5.37	128.01	120.28
1	A	316	PRO	C-N-CA	5.37	128.01	120.28
1	B	363	ASP	CA-CB-CG	-5.37	107.23	112.60
1	A	16	PRO	CA-C-O	5.36	127.45	121.34
1	A	354	CYS	CA-C-O	5.36	126.44	120.82
1	B	54	SER	CA-C-O	-5.36	112.79	119.38
1	B	145	CYS	N-CA-C	5.35	118.60	111.75
1	A	313	GLN	O-C-N	5.34	126.51	121.38
1	A	219	TYR	CA-C-O	5.34	126.94	121.23
1	B	245	TYR	N-CA-C	5.34	120.19	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	ALA	CA-C-O	5.33	125.53	119.18
1	B	69	THR	CA-CB-OG1	-5.31	101.63	109.60
1	B	241	ARG	CB-CA-C	5.31	119.88	110.85
1	A	193	HIS	CA-CB-CG	-5.31	108.49	113.80
1	A	149	SER	CA-C-O	5.31	126.58	120.90
1	A	331	PRO	N-CA-C	-5.31	103.74	111.33
1	B	178	ASN	N-CA-CB	-5.31	103.64	111.71
1	B	289	ASP	O-C-N	-5.29	116.29	122.96
1	B	234	ASN	CA-CB-CG	5.29	117.89	112.60
1	B	301	ARG	NH1-CZ-NH2	5.29	126.18	119.30
1	A	27	ILE	CA-CB-CG2	5.29	119.49	110.50
1	A	110	LYS	CB-CA-C	-5.28	98.95	109.99
1	B	290	ARG	N-CA-C	5.28	117.46	111.02
1	A	185	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
1	B	84	GLU	CA-CB-CG	-5.28	103.55	114.10
1	A	348	THR	CA-CB-OG1	-5.26	101.70	109.60
1	A	95	SER	N-CA-CB	5.26	120.45	111.66
1	B	230	GLU	O-C-N	-5.26	116.54	122.12
1	A	52	SER	CA-C-N	5.25	127.94	120.53
1	A	52	SER	C-N-CA	5.25	127.94	120.53
1	B	282	THR	N-CA-C	-5.25	106.19	112.59
1	A	167	PRO	N-CA-C	-5.23	106.26	113.53
1	B	48	GLN	CA-C-O	-5.23	115.64	121.81
1	A	177	TRP	N-CA-C	-5.22	99.69	110.80
1	A	226	PRO	N-CA-CB	5.22	107.95	103.31
1	B	319	HIS	CA-C-N	5.22	125.02	119.28
1	B	319	HIS	C-N-CA	5.22	125.02	119.28
1	B	83	PHE	O-C-N	-5.21	116.70	122.07
1	A	90	ALA	CA-C-N	5.21	129.48	120.58
1	A	90	ALA	C-N-CA	5.21	129.48	120.58
1	B	173	ARG	NE-CZ-NH1	5.20	126.70	121.50
1	B	231	LYS	CA-C-N	5.20	127.25	120.28
1	B	231	LYS	C-N-CA	5.20	127.25	120.28
1	A	249	ASP	CA-C-O	5.20	125.92	119.79
1	A	34	GLN	CA-C-O	5.19	126.90	121.19
1	A	94	ILE	N-CA-CB	5.19	118.58	111.41
1	A	325	PRO	N-CA-CB	5.19	107.87	103.35
1	B	361	ILE	CA-C-O	-5.19	114.93	120.85
1	A	137	VAL	O-C-N	-5.15	117.47	122.93
1	A	33	GLY	CA-C-O	-5.14	114.08	119.27
1	B	177	TRP	N-CA-C	-5.14	99.85	110.80
1	A	376	THR	CA-C-N	5.14	125.68	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	THR	C-N-CA	5.14	125.68	119.98
1	B	379	HIS	CA-C-O	5.14	125.99	120.70
1	B	16	PRO	N-CA-CB	5.13	107.87	103.31
1	B	38	THR	N-CA-C	5.13	117.99	109.79
1	B	86	GLU	O-C-N	-5.12	115.39	122.46
1	A	333	ILE	CB-CA-C	-5.12	105.63	110.65
1	B	60	ARG	CD-NE-CZ	5.11	131.55	124.40
1	A	17	LYS	CA-CB-CG	5.10	124.31	114.10
1	B	128	ASP	CA-CB-CG	-5.10	107.50	112.60
1	A	319	HIS	N-CA-C	-5.09	103.18	109.64
1	B	245	TYR	CA-C-N	5.08	124.87	119.28
1	B	245	TYR	C-N-CA	5.08	124.87	119.28
1	A	193	HIS	CA-C-N	5.08	129.79	123.14
1	A	193	HIS	C-N-CA	5.08	129.79	123.14
1	A	249	ASP	O-C-N	-5.06	115.54	122.33
1	A	54	SER	CA-C-N	5.06	126.72	120.34
1	A	54	SER	C-N-CA	5.06	126.72	120.34
1	A	185	HIS	O-C-N	-5.06	115.41	122.19
1	A	349	ARG	NH1-CZ-NH2	5.06	125.87	119.30
1	A	37	PRO	CA-C-O	5.05	127.09	121.43
1	A	37	PRO	O-C-N	-5.04	116.58	122.99
1	B	41	ALA	CA-C-O	-5.04	116.03	121.38
1	A	380	SER	N-CA-C	5.04	119.58	113.38
1	B	241	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	A	139	VAL	N-CA-CB	5.02	118.17	111.64
1	B	39	PRO	N-CA-C	-5.01	103.90	111.41

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	30	0
1	B	2983	0	2933	35	0
2	A	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	8	2
All	All	6943	0	5955	64	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 (64) 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:B:261:THR:HB	1:B:264:MET:HE3	1.77	0.66
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:317:LYS:HD3	1:A:317:LYS:C	2.38	0.47
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:286:LYS:NZ	5:B:675:HOH:O	2.48	0.46
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
1:B:266:ASN:HD22	1:B:266:ASN:C	2.23	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:B:261:THR:CB	1:B:264:MET:HE3	2.47	0.43
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:266:ASN:HD22	1:A:266:ASN:C	2.27	0.43
1:A:258:HIS:HB2	1:A:259:PRO:HD2	2.00	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:5:CYS:O	1:B:72:VAL:HA	2.21	0.41
1:B:266:ASN:ND2	1:B:266:ASN:C	2.79	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%)	36	30
All	All	770/786 (98%)	745 (97%)	24 (3%)	1 (0%)	48	43

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%)	316 (98%)	6 (2%)	50	50
1	B	318/323 (98%)	312 (98%)	6 (2%)	50	50
All	All	640/646 (99%)	628 (98%)	12 (2%)	50	50

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	144	TYR
1	A	231	LYS
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	144	TYR
1	B	227	GLU
1	B	266	ASN

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

Mol	Chain	Res	Type
1	A	34	GLN
1	A	169	HIS
1	A	263	HIS
1	A	266	ASN
1	A	379	HIS
1	B	29	HIS
1	B	34	GLN
1	B	130	GLN
1	B	169	HIS
1	B	266	ASN
1	B	379	HIS

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

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
3	SO4	A	396	-	4,4,4	0.61	0	6,6,6	0.57	0
2	AZI	A	395	-	2,2,2	2.80	1 (50%)	0,1,1	-	-
4	NAD	B	394	-	46,48,48	2.25	14 (30%)	64,73,73	2.54	23 (35%)
2	AZI	B	395	-	2,2,2	2.10	1 (50%)	0,1,1	-	-
4	NAD	A	394	-	46,48,48	2.44	18 (39%)	64,73,73	3.14	23 (35%)

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	-	-	5/30/62/62	0/5/5/5
4	NAD	B	394	-	-	2/30/62/62	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	394	NAD	PN-O3	7.32	1.67	1.59
4	B	394	NAD	C2N-N1N	6.69	1.42	1.35
4	A	394	NAD	C3N-C7N	6.04	1.59	1.50
4	B	394	NAD	PN-O3	5.70	1.65	1.59
4	A	394	NAD	C2N-N1N	5.48	1.41	1.35
4	B	394	NAD	C2A-N3A	4.93	1.42	1.33
4	B	394	NAD	C3N-C7N	4.76	1.57	1.50
4	A	394	NAD	C2A-N3A	4.24	1.41	1.33
4	B	394	NAD	O4D-C4D	4.06	1.54	1.45
4	A	394	NAD	PA-O3	-3.92	1.55	1.59
2	A	395	AZI	N3-N2	-3.88	1.15	1.23
4	A	394	NAD	O4D-C4D	3.35	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	394	NAD	C4N-C3N	3.35	1.44	1.39
4	A	394	NAD	C4N-C3N	3.30	1.44	1.39
4	A	394	NAD	C7N-N7N	3.12	1.38	1.33
4	A	394	NAD	O2B-C2B	-3.11	1.35	1.43
4	A	394	NAD	C5A-N7A	-2.97	1.33	1.39
4	B	394	NAD	C5N-C4N	2.64	1.43	1.38
2	B	395	AZI	N3-N2	-2.64	1.17	1.23
4	A	394	NAD	C4A-N3A	2.59	1.39	1.34
4	B	394	NAD	C5A-C6A	2.58	1.48	1.41
4	B	394	NAD	C4A-N3A	2.56	1.39	1.34
4	A	394	NAD	C3B-C4B	2.52	1.59	1.53
4	A	394	NAD	C3D-C4D	2.52	1.59	1.53
4	B	394	NAD	C7N-N7N	2.49	1.37	1.33
4	A	394	NAD	C5A-C6A	2.48	1.47	1.41
4	A	394	NAD	O7N-C7N	2.37	1.28	1.24
4	B	394	NAD	O4B-C4B	2.25	1.50	1.45
4	A	394	NAD	O4B-C1B	-2.09	1.37	1.42
4	B	394	NAD	C5A-N7A	-2.09	1.35	1.39
4	B	394	NAD	O2B-C2B	-2.07	1.37	1.43
4	A	394	NAD	PA-O2A	-2.06	1.45	1.55
4	B	394	NAD	O2D-C2D	-2.02	1.38	1.43
4	A	394	NAD	C5N-C4N	2.01	1.42	1.38

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	394	NAD	O7N-C7N-C3N	-12.46	104.36	119.60
4	A	394	NAD	C2N-C3N-C4N	9.95	129.83	118.26
4	A	394	NAD	C5N-C4N-C3N	-9.66	110.87	120.36
4	B	394	NAD	C2N-C3N-C4N	8.33	127.95	118.26
4	B	394	NAD	C5N-C4N-C3N	-7.55	112.94	120.36
4	B	394	NAD	O7N-C7N-C3N	-7.11	110.90	119.60
4	A	394	NAD	O7N-C7N-N7N	6.64	132.22	122.62
4	B	394	NAD	C2A-N1A-C6A	5.58	127.90	118.73
4	A	394	NAD	C2A-N1A-C6A	5.41	127.62	118.73
4	B	394	NAD	C6N-N1N-C2N	4.17	125.42	121.88
4	A	394	NAD	C3N-C7N-N7N	3.88	122.52	117.74
4	A	394	NAD	C4A-N9A-C8A	-3.86	101.69	105.74
4	A	394	NAD	C6N-N1N-C2N	3.82	125.12	121.88
4	B	394	NAD	N3A-C2A-N1A	-3.77	122.88	128.58
4	B	394	NAD	C6A-C5A-C4A	3.56	122.03	117.18
4	A	394	NAD	O4D-C4D-C3D	-3.53	98.14	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	394	NAD	N3A-C2A-N1A	-3.53	123.23	128.58
4	B	394	NAD	O7N-C7N-N7N	3.49	127.65	122.62
4	A	394	NAD	O3D-C3D-C4D	-3.44	101.20	111.08
4	A	394	NAD	N6A-C6A-N1A	3.38	125.91	118.38
4	A	394	NAD	C6A-C5A-C4A	3.31	121.70	117.18
4	B	394	NAD	O4D-C4D-C3D	-3.30	98.60	105.15
4	A	394	NAD	C4N-C3N-C7N	-3.02	112.84	121.06
4	B	394	NAD	C3B-C2B-C1B	-2.93	95.92	101.46
4	B	394	NAD	C4A-N9A-C8A	-2.84	102.75	105.74
4	A	394	NAD	O3B-C3B-C4B	-2.77	103.14	111.08
4	B	394	NAD	C2B-C3B-C4B	2.70	107.82	102.61
4	A	394	NAD	C5A-C6A-N1A	-2.70	110.67	117.51
4	B	394	NAD	C5A-C6A-N1A	-2.69	110.69	117.51
4	A	394	NAD	C5A-C4A-N3A	-2.63	123.10	126.72
4	B	394	NAD	C4N-C3N-C7N	-2.55	114.11	121.06
4	B	394	NAD	O4B-C4B-C5B	-2.51	101.29	109.33
4	B	394	NAD	O3D-C3D-C4D	-2.41	104.15	111.08
4	B	394	NAD	O3-PN-O1N	-2.37	103.58	110.70
4	A	394	NAD	C3B-C2B-C1B	-2.36	96.99	101.46
4	A	394	NAD	C6N-C5N-C4N	2.35	122.83	119.45
4	A	394	NAD	O3-PN-O1N	-2.34	103.66	110.70
4	B	394	NAD	C3N-C7N-N7N	2.33	120.61	117.74
4	A	394	NAD	O2N-PN-O1N	2.33	123.26	112.44
4	B	394	NAD	C1B-N9A-C8A	2.27	132.14	127.09
4	B	394	NAD	C4B-O4B-C1B	-2.27	104.46	109.47
4	A	394	NAD	O3-PA-O1A	-2.22	104.03	110.70
4	B	394	NAD	C5A-C4A-N9A	2.21	108.22	105.81
4	B	394	NAD	C5A-C4A-N3A	-2.15	123.76	126.72
4	A	394	NAD	O2A-PA-O1A	2.14	122.39	112.44
4	B	394	NAD	O2N-PN-O1N	2.05	121.96	112.44

There are no chirality outliers.

All (7) torsion outliers are listed below:

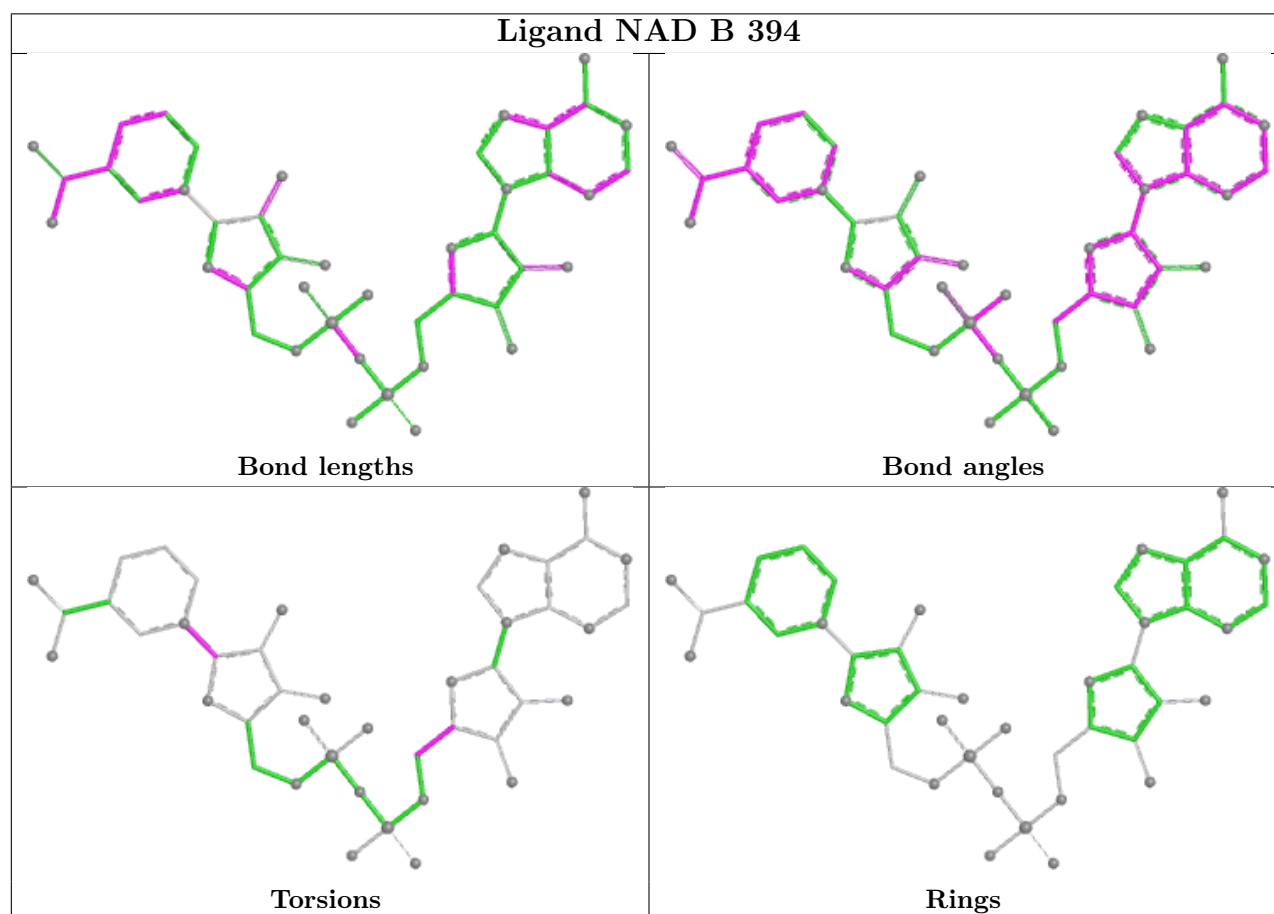
Mol	Chain	Res	Type	Atoms
4	A	394	NAD	C5B-O5B-PA-O1A
4	A	394	NAD	O4D-C1D-N1N-C6N
4	B	394	NAD	O4D-C1D-N1N-C6N
4	A	394	NAD	C3B-C4B-C5B-O5B
4	A	394	NAD	O4D-C1D-N1N-C2N
4	A	394	NAD	O4B-C4B-C5B-O5B
4	B	394	NAD	O4B-C4B-C5B-O5B

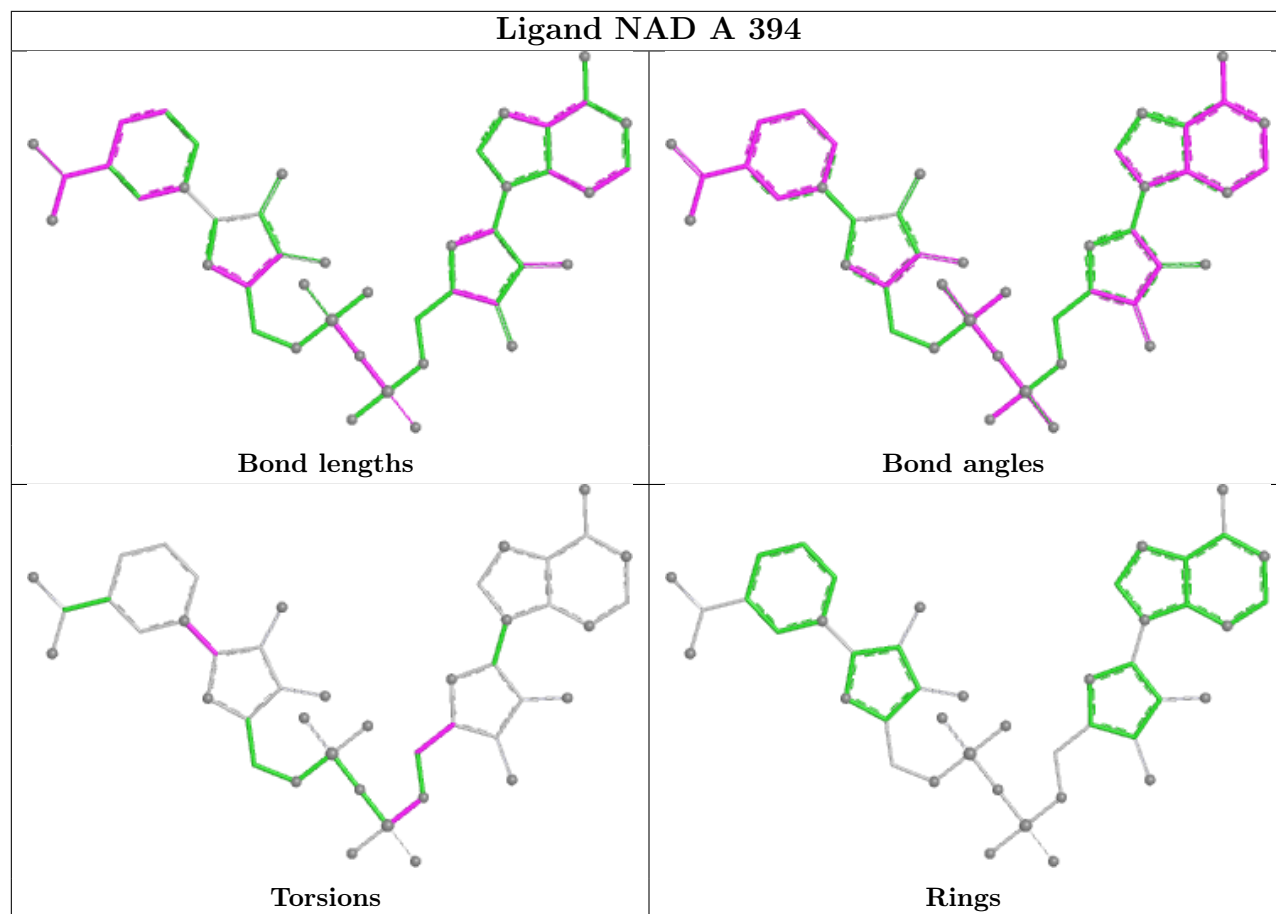
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	395	AZI	1	0
4	B	394	NAD	3	0
4	A	394	NAD	4	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 [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, 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	A	391/393 (99%)	-0.86	0 100 100	4, 11, 34, 62	0
1	B	383/393 (97%)	-0.95	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 oligosaccharides in this entry.

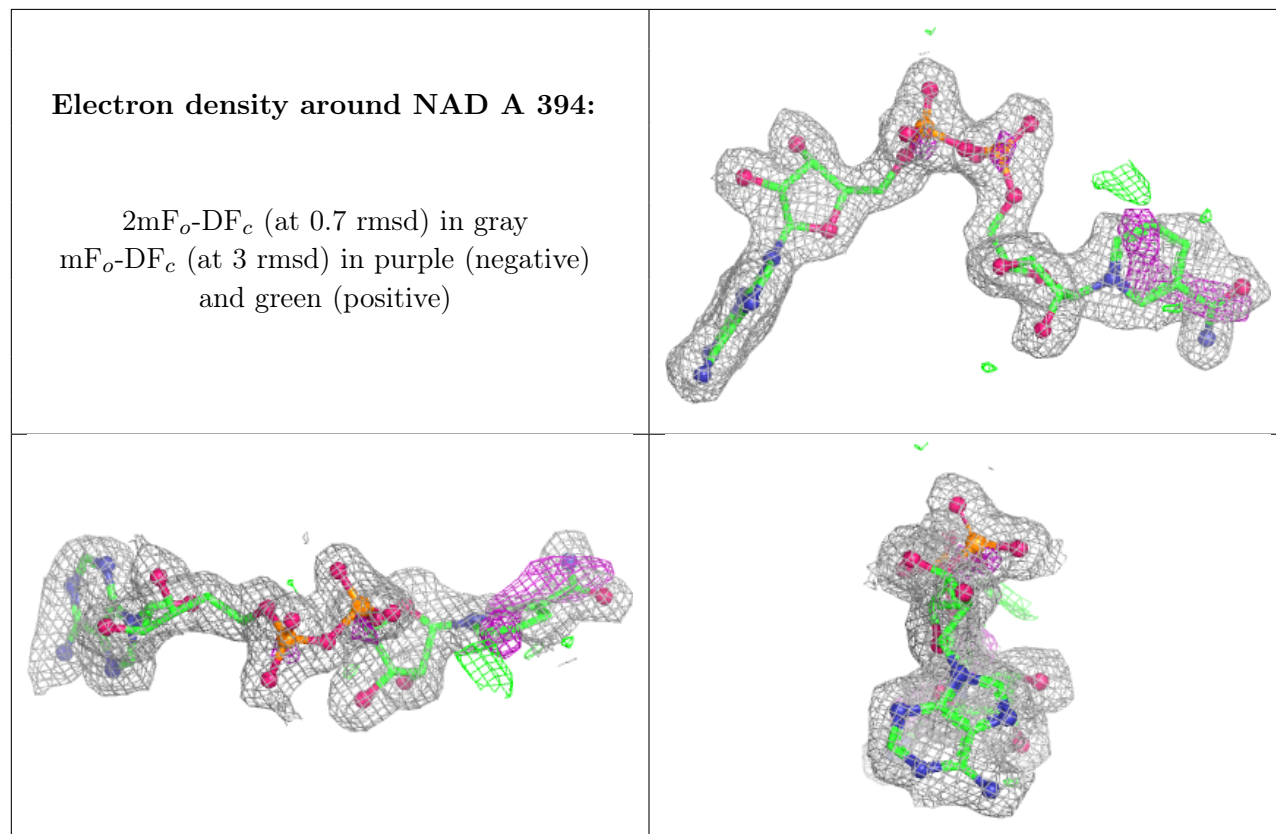
6.4 Ligands [i](#)

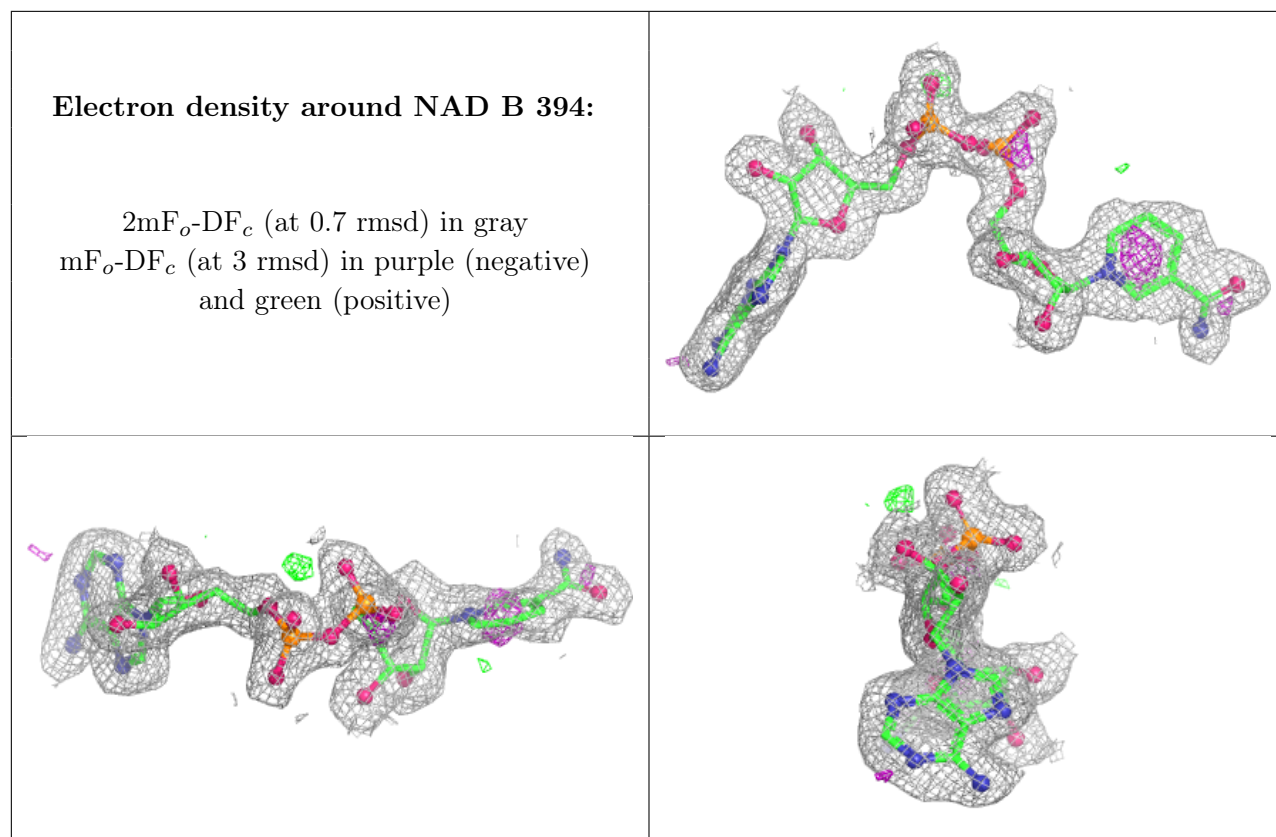
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AZI	A	395	3/3	0.95	0.08	10,10,24,26	0
3	SO4	A	396	5/5	0.95	0.10	48,50,52,53	0
2	AZI	B	395	3/3	0.97	0.07	7,7,17,21	0
4	NAD	A	394	44/44	0.97	0.05	10,14,22,24	0
4	NAD	B	394	44/44	0.98	0.04	4,6,14,16	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.