



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:06 PM UTC

PDB ID : 1EZ4 / pdb_00001ez4
Title : CRYSTAL STRUCTURE OF NON-ALLOSTERIC L-LACTATE DEHYDROGENASE FROM LACTOBACILLUS PENTOSUS AT 2.3 ANGSTROM RESOLUTION
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Deposited on : 2000-05-10
Resolution : 2.30 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

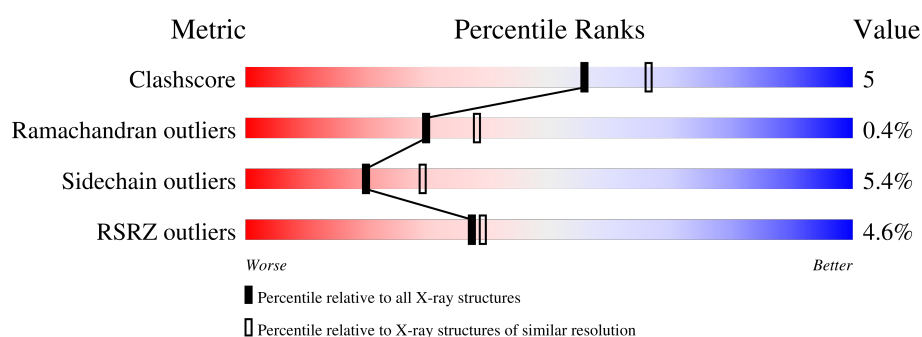
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	318	5% 77% 16% ...
1	B	318	3% 78% 17% ..
1	C	318	5% 75% 16% ...
1	D	318	4% 77% 18% ..

2 Entry composition [i](#)

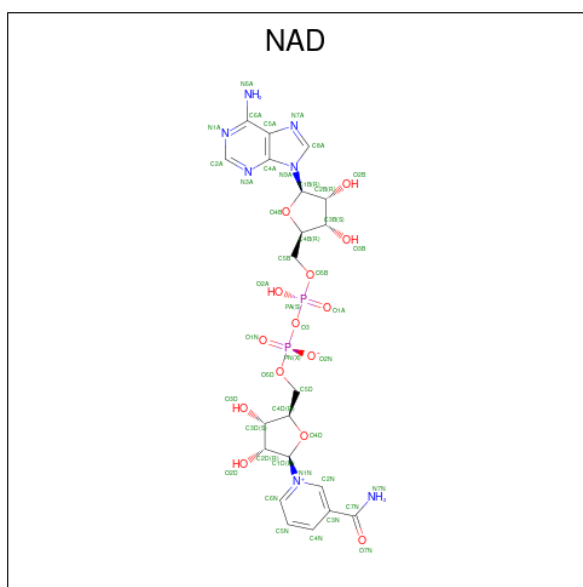
There are 3 unique types of molecules in this entry. The entry contains 10353 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2304	1455	384	458	7			
1	B	318	Total	C	N	O	S	0	0	0
			2392	1508	401	476	7			
1	C	307	Total	C	N	O	S	0	0	0
			2304	1455	384	458	7			
1	D	318	Total	C	N	O	S	0	0	0
			2392	1508	401	476	7			

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



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

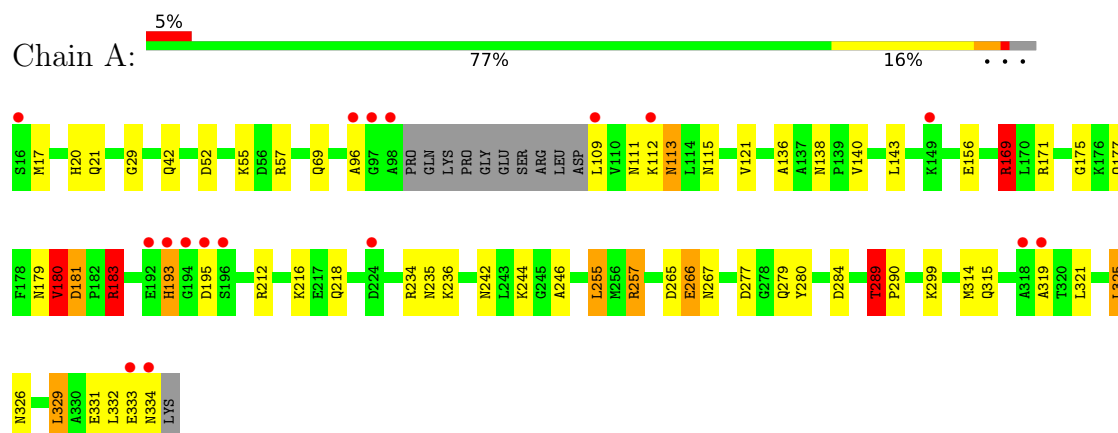
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	184	Total	O	0	0
			184	184		
3	B	219	Total	O	0	0
			219	219		
3	C	189	Total	O	0	0
			189	189		
3	D	193	Total	O	0	0
			193	193		

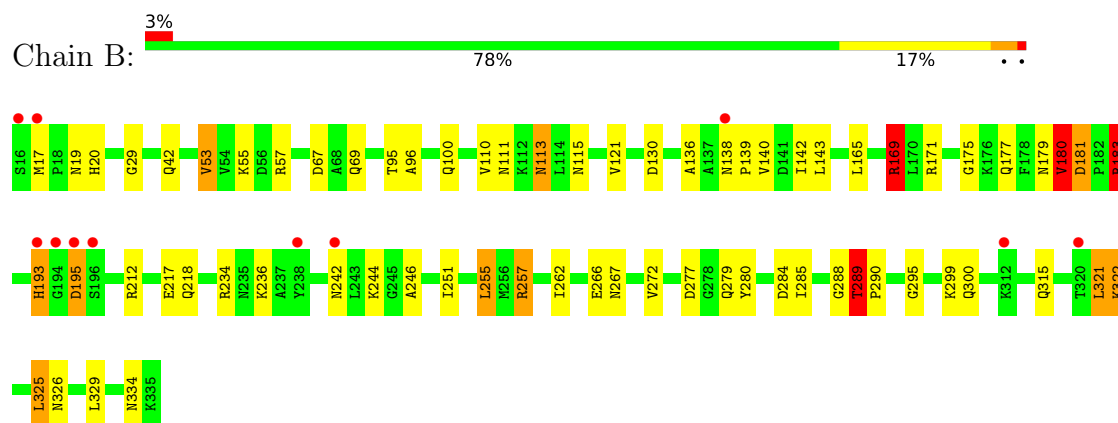
3 Residue-property plots [i](#)

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

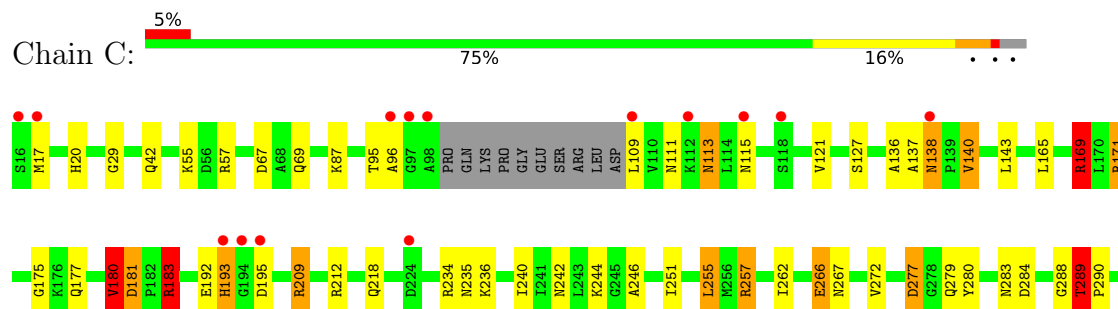
• Molecule 1: LACTATE DEHYDROGENASE

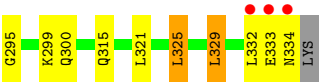


• Molecule 1: LACTATE DEHYDROGENASE

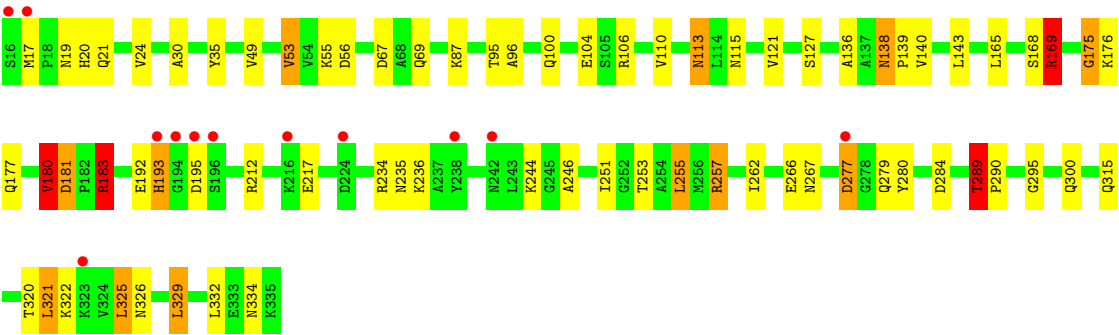
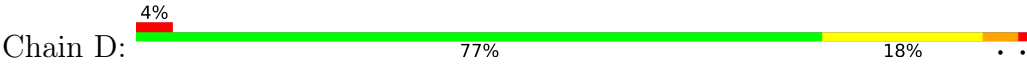


• Molecule 1: LACTATE DEHYDROGENASE





● Molecule 1: LACTATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.35Å 145.54Å 111.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 2.30 80.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (80.00-2.30) 99.6 (80.00-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.205 , 0.241 0.202 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10353	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.71% 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

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	0.96	2/2337 (0.1%)	1.83	53/3162 (1.7%)
1	B	1.01	2/2428 (0.1%)	1.84	54/3284 (1.6%)
1	C	0.98	2/2337 (0.1%)	1.80	58/3162 (1.8%)
1	D	1.00	3/2428 (0.1%)	1.82	58/3284 (1.8%)
All	All	0.99	9/9530 (0.1%)	1.82	223/12892 (1.7%)

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	A	0	1
1	B	0	2
1	C	0	3
1	D	0	1
All	All	0	7

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	20	HIS	CD2-NE2	-6.87	1.30	1.37
1	A	20	HIS	CD2-NE2	-6.68	1.30	1.37
1	B	20	HIS	CD2-NE2	-6.62	1.30	1.37
1	C	20	HIS	CD2-NE2	-6.48	1.30	1.37
1	B	193	HIS	CD2-NE2	-6.36	1.30	1.37
1	D	193	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	193	HIS	CD2-NE2	-5.99	1.31	1.37
1	C	193	HIS	CD2-NE2	-5.95	1.31	1.37
1	D	20	HIS	CG-ND1	-5.74	1.31	1.38

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	ASN	OD1-CG-ND2	-13.51	109.09	122.60
1	B	113	ASN	OD1-CG-ND2	-12.35	110.25	122.60
1	C	183	ARG	NE-CZ-NH2	12.06	130.06	119.20
1	A	113	ASN	OD1-CG-ND2	-12.01	110.59	122.60
1	B	169	ARG	NE-CZ-NH2	11.55	129.60	119.20
1	B	53	VAL	N-CA-CB	-10.70	97.10	110.47
1	B	100	GLN	OE1-CD-NE2	-10.23	112.37	122.60
1	C	169	ARG	NE-CZ-NH2	10.19	128.37	119.20
1	B	111	ASN	OD1-CG-ND2	-10.13	112.47	122.60
1	A	115	ASN	CA-CB-CG	-10.12	102.48	112.60
1	C	113	ASN	OD1-CG-ND2	-10.03	112.57	122.60
1	A	183	ARG	NE-CZ-NH2	10.01	128.21	119.20
1	B	257	ARG	NE-CZ-NH1	-9.95	111.55	121.50
1	B	138	ASN	OD1-CG-ND2	-9.81	112.79	122.60
1	D	279	GLN	OE1-CD-NE2	-9.62	112.98	122.60
1	C	257	ARG	NE-CZ-NH1	-9.56	111.94	121.50
1	A	138	ASN	OD1-CG-ND2	-9.48	113.12	122.60
1	D	177	GLN	OE1-CD-NE2	-9.46	113.14	122.60
1	A	257	ARG	NE-CZ-NH2	9.40	127.66	119.20
1	D	257	ARG	NE-CZ-NH1	-9.34	112.16	121.50
1	A	180	VAL	CB-CA-C	-9.30	95.81	110.69
1	C	267	ASN	OD1-CG-ND2	-9.11	113.49	122.60
1	A	257	ARG	NE-CZ-NH1	-9.10	112.40	121.50
1	B	115	ASN	CA-CB-CG	-8.99	103.61	112.60
1	B	169	ARG	NE-CZ-NH1	-8.92	112.58	121.50
1	B	180	VAL	CB-CA-C	-8.90	97.11	110.82
1	C	115	ASN	CA-CB-CG	-8.88	103.72	112.60
1	C	180	VAL	CB-CA-C	-8.85	96.88	110.50
1	B	177	GLN	OE1-CD-NE2	-8.84	113.76	122.60
1	B	289	THR	CB-CA-C	-8.79	95.75	109.55
1	D	140	VAL	N-CA-C	8.71	119.50	110.62
1	D	169	ARG	NE-CZ-NH2	8.70	127.03	119.20
1	C	138	ASN	OD1-CG-ND2	-8.64	113.96	122.60
1	D	53	VAL	N-CA-CB	-8.59	98.85	110.54
1	D	180	VAL	CB-CA-C	-8.48	97.76	110.82
1	A	267	ASN	OD1-CG-ND2	-8.47	114.13	122.60
1	D	138	ASN	N-CA-C	8.37	122.45	110.24
1	C	181	ASP	CA-CB-CG	8.34	120.94	112.60
1	A	177	GLN	OE1-CD-NE2	-8.32	114.28	122.60
1	D	289	THR	CB-CA-C	-8.26	96.58	109.55
1	B	57	ARG	NE-CZ-NH2	8.24	126.62	119.20
1	B	257	ARG	NE-CZ-NH2	8.21	126.59	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	ASN	CA-CB-CG	-8.19	104.41	112.60
1	C	140	VAL	N-CA-C	8.17	118.95	110.62
1	C	57	ARG	CB-CG-CD	-8.12	92.62	111.30
1	A	169	ARG	NE-CZ-NH2	8.08	126.48	119.20
1	B	42	GLN	OE1-CD-NE2	-8.08	114.52	122.60
1	B	334	ASN	OD1-CG-ND2	-8.08	114.52	122.60
1	A	289	THR	CB-CA-C	-8.03	96.95	109.55
1	D	326	ASN	CA-CB-CG	-8.01	104.59	112.60
1	C	334	ASN	OD1-CG-ND2	-7.94	114.66	122.60
1	D	326	ASN	OD1-CG-ND2	-7.86	114.74	122.60
1	D	315	GLN	OE1-CD-NE2	-7.83	114.77	122.60
1	B	138	ASN	CB-CG-ND2	7.82	128.13	116.40
1	D	334	ASN	OD1-CG-ND2	-7.76	114.84	122.60
1	D	115	ASN	CA-CB-CG	-7.75	104.86	112.60
1	C	257	ARG	NE-CZ-NH2	7.74	126.16	119.20
1	A	315	GLN	OE1-CD-NE2	-7.71	114.89	122.60
1	C	289	THR	CB-CA-C	-7.68	96.23	108.91
1	A	284	ASP	N-CA-C	7.67	122.25	111.52
1	B	100	GLN	CG-CD-NE2	7.66	127.89	116.40
1	B	181	ASP	CA-CB-CG	7.57	120.17	112.60
1	C	96	ALA	N-CA-C	7.56	121.19	110.23
1	B	315	GLN	OE1-CD-NE2	-7.50	115.11	122.60
1	D	181	ASP	CA-CB-CG	7.45	120.05	112.60
1	D	138	ASN	CB-CG-ND2	7.45	127.57	116.40
1	D	266	GLU	N-CA-C	7.44	122.12	112.89
1	B	279	GLN	OE1-CD-NE2	-7.41	115.19	122.60
1	D	267	ASN	OD1-CG-ND2	-7.38	115.22	122.60
1	B	138	ASN	N-CA-C	7.32	120.92	110.24
1	B	140	VAL	N-CA-C	7.30	118.09	110.72
1	B	267	ASN	OD1-CG-ND2	-7.28	115.32	122.60
1	A	212	ARG	NE-CZ-NH2	7.28	125.75	119.20
1	A	55	LYS	N-CA-C	7.25	120.10	111.33
1	C	138	ASN	N-CA-C	7.24	120.81	110.24
1	D	183	ARG	NE-CZ-NH2	7.24	125.71	119.20
1	A	138	ASN	CB-CG-ND2	7.21	127.22	116.40
1	D	113	ASN	CB-CG-ND2	7.13	127.09	116.40
1	A	334	ASN	OD1-CG-ND2	-7.13	115.47	122.60
1	A	113	ASN	CB-CG-ND2	7.05	126.98	116.40
1	A	96	ALA	N-CA-C	7.03	120.42	110.23
1	B	326	ASN	OD1-CG-ND2	-7.00	115.60	122.60
1	C	138	ASN	CB-CG-ND2	6.97	126.85	116.40
1	D	138	ASN	OD1-CG-ND2	-6.95	115.65	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	ARG	NE-CZ-NH2	6.95	125.45	119.20
1	D	257	ARG	NE-CZ-NH2	6.92	125.42	119.20
1	C	171	ARG	NE-CZ-NH2	6.89	125.40	119.20
1	B	69	GLN	CB-CG-CD	-6.78	101.07	112.60
1	A	140	VAL	N-CA-C	6.78	117.53	110.62
1	D	212	ARG	NE-CZ-NH2	6.76	125.28	119.20
1	A	266	GLU	N-CA-C	6.75	121.25	112.89
1	B	113	ASN	CB-CG-ND2	6.74	126.52	116.40
1	C	315	GLN	OE1-CD-NE2	-6.73	115.87	122.60
1	C	279	GLN	OE1-CD-NE2	-6.72	115.88	122.60
1	B	179	ASN	OD1-CG-ND2	-6.72	115.88	122.60
1	C	20	HIS	CB-CG-CD2	-6.71	122.48	131.20
1	A	138	ASN	N-CA-C	6.70	120.02	110.24
1	A	113	ASN	CA-CB-CG	-6.67	105.93	112.60
1	C	242	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	B	57	ARG	NE-CZ-NH1	-6.66	114.84	121.50
1	D	53	VAL	CB-CA-C	6.65	121.11	112.14
1	C	183	ARG	NE-CZ-NH1	-6.62	114.88	121.50
1	A	17	MET	O-C-N	-6.59	113.74	121.32
1	B	326	ASN	CA-CB-CG	-6.57	106.03	112.60
1	C	113	ASN	CB-CG-ND2	6.54	126.20	116.40
1	D	169	ARG	NE-CZ-NH1	-6.53	114.97	121.50
1	A	235	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	A	52	ASP	O-C-N	-6.44	115.69	123.10
1	C	177	GLN	OE1-CD-NE2	-6.41	116.19	122.60
1	A	179	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	B	53	VAL	CB-CA-C	6.39	120.42	112.04
1	A	181	ASP	CA-CB-CG	6.33	118.93	112.60
1	D	113	ASN	CA-CB-CG	-6.32	106.28	112.60
1	A	57	ARG	CB-CG-CD	-6.28	96.87	111.30
1	C	115	ASN	OD1-CG-ND2	-6.28	116.33	122.60
1	B	17	MET	O-C-N	-6.26	114.12	121.32
1	D	289	THR	O-C-N	-6.23	117.49	121.85
1	C	138	ASN	CA-CB-CG	-6.19	106.41	112.60
1	A	265	ASP	CA-CB-CG	6.18	118.78	112.60
1	D	69	GLN	OE1-CD-NE2	-6.17	116.43	122.60
1	A	121	VAL	N-CA-C	6.16	116.90	110.62
1	C	235	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	B	55	LYS	O-C-N	-6.13	115.62	122.12
1	A	20	HIS	CB-CG-CD2	-6.11	123.26	131.20
1	D	138	ASN	CA-CB-CG	-6.10	106.50	112.60
1	B	266	GLU	N-CA-C	6.07	120.42	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	56	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	326	ASN	CA-CB-CG	-6.06	106.54	112.60
1	C	289	THR	O-C-N	-6.04	117.59	121.88
1	C	169	ARG	NE-CZ-NH1	-6.03	115.47	121.50
1	D	193	HIS	CB-CG-CD2	-6.03	123.37	131.20
1	C	266	GLU	N-CA-C	6.02	120.36	112.89
1	C	111	ASN	CA-C-O	-6.01	114.05	120.42
1	A	218	GLN	OE1-CD-NE2	-6.01	116.59	122.60
1	A	319	ALA	O-C-N	-5.99	115.77	122.12
1	D	284	ASP	N-CA-C	5.98	119.68	111.54
1	C	55	LYS	N-CA-C	5.98	118.59	111.71
1	C	283	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	C	218	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	B	57	ARG	CG-CD-NE	-5.96	98.89	112.00
1	B	289	THR	O-C-N	-5.96	117.68	121.85
1	A	279	GLN	OE1-CD-NE2	-5.95	116.66	122.60
1	C	277	ASP	CA-CB-CG	-5.89	106.70	112.60
1	D	279	GLN	CG-CD-NE2	5.89	125.24	116.40
1	D	300	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	C	193	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	B	177	GLN	CG-CD-NE2	5.87	125.20	116.40
1	A	171	ARG	NE-CZ-NH2	5.85	124.47	119.20
1	D	55	LYS	N-CA-C	5.85	118.16	111.02
1	B	300	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	A	69	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	C	69	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	C	212	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	B	19	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	B	121	VAL	N-CA-C	5.80	115.99	110.42
1	C	180	VAL	N-CA-CB	5.79	120.93	111.44
1	D	121	VAL	N-CA-C	5.77	116.50	110.62
1	A	69	GLN	CB-CG-CD	-5.76	102.81	112.60
1	C	17	MET	O-C-N	-5.72	114.74	121.32
1	D	17	MET	O-C-N	-5.71	114.75	121.32
1	C	209	ARG	CG-CD-NE	-5.71	99.44	112.00
1	A	21	GLN	OE1-CD-NE2	-5.70	116.90	122.60
1	B	130	ASP	CA-CB-CG	5.69	118.29	112.60
1	D	183	ARG	NE-CZ-NH1	-5.69	115.81	121.50
1	B	171	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	D	322	LYS	CB-CG-CD	-5.63	98.36	111.30
1	A	42	GLN	OE1-CD-NE2	-5.61	116.99	122.60
1	A	326	ASN	CB-CG-ND2	5.60	124.81	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	ARG	CG-CD-NE	-5.60	99.68	112.00
1	B	284	ASP	N-CA-C	5.59	119.14	111.54
1	B	96	ALA	N-CA-C	5.59	118.43	110.10
1	B	138	ASN	CA-CB-CG	-5.54	107.06	112.60
1	C	284	ASP	N-CA-CB	-5.53	103.60	111.84
1	C	69	GLN	CB-CG-CD	-5.52	103.21	112.60
1	A	29	GLY	O-C-N	-5.51	117.91	122.92
1	D	96	ALA	N-CA-C	5.50	118.15	109.96
1	D	69	GLN	CB-CG-CD	-5.49	103.27	112.60
1	C	171	ARG	CB-CG-CD	5.48	123.90	111.30
1	A	69	GLN	N-CA-C	5.47	117.24	111.28
1	C	192	GLU	O-C-N	5.45	129.42	123.04
1	A	111	ASN	CA-C-N	-5.45	112.55	120.29
1	A	111	ASN	C-N-CA	-5.45	112.55	120.29
1	B	321	LEU	CD1-CG-CD2	-5.42	98.88	110.80
1	A	193	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	D	19	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	C	284	ASP	N-CA-C	5.38	118.86	111.54
1	C	111	ASN	CA-CB-CG	-5.37	107.23	112.60
1	D	334	ASN	CB-CG-ND2	5.34	124.42	116.40
1	D	19	ASN	CA-CB-CG	-5.33	107.27	112.60
1	B	218	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	C	121	VAL	N-CA-C	5.31	116.03	110.62
1	A	289	THR	O-C-N	-5.29	118.14	121.85
1	D	277	ASP	CA-CB-CG	-5.28	107.32	112.60
1	C	29	GLY	O-C-N	-5.28	118.11	122.92
1	D	315	GLN	CG-CD-NE2	5.28	124.32	116.40
1	D	177	GLN	CG-CD-NE2	5.26	124.29	116.40
1	B	193	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	C	42	GLN	CG-CD-NE2	5.24	124.26	116.40
1	C	300	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	A	326	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	A	257	ARG	CG-CD-NE	-5.23	100.49	112.00
1	D	30	ALA	N-CA-C	5.23	116.98	111.28
1	D	235	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	C	69	GLN	N-CA-C	5.22	116.97	111.28
1	B	242	ASN	N-CA-C	5.16	117.64	111.71
1	D	168	SER	CB-CA-C	-5.13	102.27	110.79
1	C	257	ARG	CG-CD-NE	-5.13	100.72	112.00
1	D	20	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	D	253	THR	CA-CB-OG1	-5.11	101.93	109.60
1	A	169	ARG	NE-CZ-NH1	-5.10	116.40	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	55	LYS	O-C-N	-5.08	116.64	122.08
1	C	137	ALA	N-CA-C	5.08	117.67	110.10
1	B	29	GLY	O-C-N	-5.08	118.30	122.92
1	B	212	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	B	42	GLN	CG-CD-NE2	5.07	124.00	116.40
1	D	104	GLU	N-CA-C	5.06	117.76	110.28
1	C	240	ILE	N-CA-C	-5.05	105.78	110.53
1	D	21	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	D	175	GLY	CA-C-O	5.05	125.95	120.75
1	C	334	ASN	CB-CG-ND2	5.04	123.95	116.40
1	B	193	HIS	CA-CB-CG	5.02	118.82	113.80
1	A	267	ASN	CB-CG-ND2	5.02	123.93	116.40
1	A	242	ASN	CB-CA-C	-5.01	101.36	110.63

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	257	ARG	Sidechain
1	B	257	ARG	Sidechain
1	B	289	THR	Peptide
1	C	209	ARG	Sidechain
1	C	257	ARG	Sidechain
1	C	289	THR	Peptide
1	D	289	THR	Peptide

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	2304	0	2309	20	0
1	B	2392	0	2400	21	0
1	C	2304	0	2309	24	0
1	D	2392	0	2400	25	0
2	A	44	0	26	1	0
2	B	44	0	26	4	0
2	C	44	0	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	44	0	26	2	0
3	A	184	0	0	1	0
3	B	219	0	0	2	0
3	C	189	0	0	2	0
3	D	193	0	0	0	0
All	All	10353	0	9522	89	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (89) 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:169:ARG:HD2	1:A:236:LYS:HD3	1.62	0.81
1:C:169:ARG:HD2	1:C:236:LYS:HD3	1.63	0.79
1:D:169:ARG:HD2	1:D:236:LYS:HD3	1.68	0.73
1:C:136:ALA:O	2:C:1354:NAD:H2N	1.91	0.70
1:B:169:ARG:HD2	1:B:236:LYS:HD3	1.75	0.67
1:C:95:THR:O	2:C:1354:NAD:H4D	1.97	0.64
1:A:325:LEU:HD22	1:A:329:LEU:HD22	1.81	0.61
1:B:136:ALA:O	2:B:1353:NAD:H2N	2.01	0.59
1:C:325:LEU:HD22	1:C:329:LEU:HD22	1.82	0.59
1:A:136:ALA:HB2	1:A:255:LEU:HD11	1.85	0.59
1:D:95:THR:O	2:D:1355:NAD:H4D	2.03	0.59
1:B:169:ARG:CD	1:B:236:LYS:HD3	2.34	0.57
1:B:95:THR:O	2:B:1353:NAD:H4D	2.05	0.57
1:D:244:LYS:HE3	1:D:246:ALA:O	2.04	0.57
1:D:136:ALA:HB2	1:D:255:LEU:HD11	1.85	0.57
1:A:109:LEU:HA	1:A:112:LYS:HG2	1.89	0.55
1:C:169:ARG:CD	1:C:236:LYS:HD3	2.35	0.55
1:D:192:GLU:HG3	1:D:321:LEU:HD22	1.89	0.55
1:B:244:LYS:HE3	1:B:246:ALA:O	2.07	0.54
1:C:67:ASP:OD2	1:D:169:ARG:HD3	2.08	0.54
1:D:110:VAL:HG22	1:D:139:PRO:HG3	1.90	0.54
1:D:325:LEU:HD22	1:D:329:LEU:HD22	1.89	0.53
1:B:136:ALA:HB2	1:B:255:LEU:HD11	1.90	0.53
2:C:1354:NAD:H52A	2:C:1354:NAD:H52N	1.92	0.52
1:A:169:ARG:HD3	1:B:67:ASP:OD2	2.10	0.52
3:C:1498:HOH:O	1:D:176:LYS:HE2	2.10	0.51
1:A:136:ALA:O	2:A:1352:NAD:H2N	2.11	0.51
1:B:142:ILE:HG23	1:B:325:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ASN:HB2	2:D:1355:NAD:O2D	2.11	0.50
1:A:289:THR:HG22	1:A:290:PRO:HD2	1.94	0.49
1:C:280:TYR:CE2	1:C:289:THR:HG23	2.48	0.49
1:B:195:ASP:HA	1:B:234:ARG:HD2	1.93	0.49
1:D:169:ARG:CD	1:D:236:LYS:HD3	2.40	0.49
1:C:136:ALA:HB2	1:C:255:LEU:HD11	1.93	0.49
1:C:169:ARG:HD3	1:D:67:ASP:OD2	2.12	0.49
1:C:175:GLY:HA2	1:C:180:VAL:HG23	1.96	0.48
1:A:175:GLY:HA2	1:A:180:VAL:HG23	1.96	0.48
1:A:280:TYR:CE2	1:A:289:THR:HG23	2.48	0.48
1:D:280:TYR:CE2	1:D:289:THR:HG23	2.49	0.47
1:B:165:LEU:HD22	1:B:251:ILE:HB	1.96	0.47
1:C:280:TYR:HE2	1:C:289:THR:HG23	1.80	0.47
1:C:138:ASN:HD22	1:C:140:VAL:H	1.63	0.47
1:C:244:LYS:HE3	1:C:246:ALA:O	2.15	0.47
1:C:165:LEU:HD22	1:C:251:ILE:HB	1.96	0.47
1:B:285:ILE:HG21	1:B:322:LYS:HG2	1.97	0.46
1:A:195:ASP:HA	1:A:234:ARG:HD2	1.98	0.46
1:A:244:LYS:HE3	1:A:246:ALA:O	2.15	0.45
1:A:113:ASN:HB3	1:A:143:LEU:HD11	1.97	0.45
1:A:181:ASP:HB2	1:C:266:GLU:O	2.16	0.45
1:D:35:TYR:CD1	1:D:255:LEU:HB3	2.51	0.45
1:B:110:VAL:HG22	1:B:139:PRO:HG3	1.99	0.45
1:D:280:TYR:HE2	1:D:289:THR:HG23	1.82	0.45
1:D:113:ASN:HB3	1:D:143:LEU:HD11	1.99	0.44
1:B:113:ASN:HB3	1:B:143:LEU:HD11	2.00	0.44
1:B:289:THR:HG22	1:B:290:PRO:HD2	1.99	0.44
2:C:1354:NAD:H5N	3:C:1528:HOH:O	2.18	0.44
1:B:280:TYR:CE2	1:B:289:THR:HG23	2.52	0.44
1:D:175:GLY:HA2	1:D:180:VAL:HG23	2.00	0.43
1:D:289:THR:HG22	1:D:290:PRO:HD2	2.00	0.43
1:C:262:ILE:O	1:C:295:GLY:HA2	2.18	0.43
1:A:181:ASP:OD1	1:A:183:ARG:HD3	2.19	0.43
1:A:280:TYR:HE2	1:A:289:THR:HG23	1.83	0.43
1:B:285:ILE:CG2	1:B:322:LYS:HG2	2.48	0.43
1:C:181:ASP:OD1	1:C:183:ARG:HD3	2.18	0.43
1:D:181:ASP:OD1	1:D:183:ARG:HD3	2.19	0.43
1:B:181:ASP:OD1	1:B:183:ARG:HD3	2.19	0.42
1:D:262:ILE:O	1:D:295:GLY:HA2	2.19	0.42
1:B:272:VAL:O	1:B:288:GLY:HA2	2.20	0.42
2:B:1353:NAD:H2A	3:B:1457:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:VAL:O	1:C:288:GLY:HA2	2.19	0.42
1:A:299:LYS:HA	1:A:299:LYS:HD2	1.96	0.42
1:A:266:GLU:O	1:C:181:ASP:HB2	2.20	0.42
1:C:289:THR:HG22	1:C:290:PRO:HD2	2.01	0.42
1:C:195:ASP:HA	1:C:234:ARG:HD2	2.02	0.42
1:B:262:ILE:O	1:B:295:GLY:HA2	2.20	0.41
1:C:113:ASN:HB3	1:C:143:LEU:HD11	2.00	0.41
1:A:280:TYR:CG	1:A:314:MET:HE2	2.56	0.41
1:B:175:GLY:HA2	1:B:180:VAL:HG23	2.01	0.41
2:B:1353:NAD:H5N	3:B:1544:HOH:O	2.20	0.41
1:A:156:GLU:HB3	3:A:1438:HOH:O	2.20	0.41
1:C:87:LYS:HG3	1:C:127:SER:O	2.21	0.41
1:B:299:LYS:HA	1:B:299:LYS:HD2	1.86	0.41
1:C:299:LYS:HA	1:C:299:LYS:HD2	1.92	0.41
1:D:165:LEU:HD22	1:D:251:ILE:HB	2.03	0.40
1:D:24:VAL:HG22	1:D:49:VAL:HB	2.02	0.40
1:D:234:ARG:HH21	1:D:234:ARG:HD3	1.77	0.40
1:A:109:LEU:HA	1:A:112:LYS:HE2	2.02	0.40
1:D:195:ASP:HA	1:D:234:ARG:HD2	2.03	0.40
1:D:87:LYS:HG3	1:D:127:SER:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	303/318 (95%)	288 (95%)	14 (5%)	1 (0%)	36	46
1	B	316/318 (99%)	300 (95%)	14 (4%)	2 (1%)	21	27
1	C	303/318 (95%)	291 (96%)	11 (4%)	1 (0%)	36	46
1	D	316/318 (99%)	299 (95%)	16 (5%)	1 (0%)	36	46
All	All	1238/1272 (97%)	1178 (95%)	55 (4%)	5 (0%)	30	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	HIS
1	B	193	HIS
1	C	193	HIS
1	D	193	HIS
1	B	195	ASP

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	A	245/255 (96%)	232 (95%)	13 (5%)	20	30
1	B	255/255 (100%)	243 (95%)	12 (5%)	23	35
1	C	245/255 (96%)	232 (95%)	13 (5%)	20	30
1	D	255/255 (100%)	239 (94%)	16 (6%)	16	23
All	All	1000/1020 (98%)	946 (95%)	54 (5%)	20	29

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ARG
1	A	180	VAL
1	A	183	ARG
1	A	216	LYS
1	A	255	LEU
1	A	277	ASP
1	A	289	THR
1	A	321	LEU
1	A	325	LEU
1	A	329	LEU
1	A	331	GLU
1	A	332	LEU
1	A	333	GLU
1	B	53	VAL
1	B	169	ARG

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Mol	Chain	Res	Type
1	B	180	VAL
1	B	183	ARG
1	B	217	GLU
1	B	255	LEU
1	B	277	ASP
1	B	289	THR
1	B	321	LEU
1	B	322	LYS
1	B	325	LEU
1	B	329	LEU
1	C	109	LEU
1	C	169	ARG
1	C	171	ARG
1	C	180	VAL
1	C	183	ARG
1	C	255	LEU
1	C	277	ASP
1	C	289	THR
1	C	321	LEU
1	C	325	LEU
1	C	329	LEU
1	C	332	LEU
1	C	333	GLU
1	D	53	VAL
1	D	100	GLN
1	D	106	ARG
1	D	169	ARG
1	D	180	VAL
1	D	183	ARG
1	D	217	GLU
1	D	255	LEU
1	D	257	ARG
1	D	277	ASP
1	D	289	THR
1	D	320	THR
1	D	321	LEU
1	D	325	LEU
1	D	329	LEU
1	D	332	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	B	19	ASN
1	B	21	GLN
1	B	41	GLN
1	B	138	ASN
1	B	334	ASN
1	C	21	GLN
1	D	21	GLN
1	D	138	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	B	1353	-	46,48,48	1.53	6 (13%)	64,73,73	1.92	16 (25%)
2	NAD	C	1354	-	46,48,48	1.48	5 (10%)	64,73,73	2.11	15 (23%)
2	NAD	D	1355	-	46,48,48	1.50	6 (13%)	64,73,73	1.90	18 (28%)
2	NAD	A	1352	-	46,48,48	1.46	6 (13%)	64,73,73	2.11	19 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	1353	-	-	5/30/62/62	0/5/5/5
2	NAD	C	1354	-	-	11/30/62/62	0/5/5/5
2	NAD	D	1355	-	-	5/30/62/62	0/5/5/5
2	NAD	A	1352	-	-	8/30/62/62	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1353	NAD	C2N-N1N	6.58	1.42	1.35
2	D	1355	NAD	C2N-N1N	5.77	1.41	1.35
2	C	1354	NAD	C2N-N1N	5.66	1.41	1.35
2	A	1352	NAD	C2N-N1N	5.47	1.41	1.35
2	C	1354	NAD	C3N-C7N	3.71	1.56	1.50
2	D	1355	NAD	O4D-C1D	3.71	1.45	1.40
2	D	1355	NAD	C6N-N1N	3.36	1.43	1.35
2	C	1354	NAD	O4D-C1D	3.34	1.45	1.40
2	B	1353	NAD	O4D-C1D	3.27	1.45	1.40
2	D	1355	NAD	C3N-C7N	3.14	1.55	1.50
2	A	1352	NAD	O4D-C1D	3.12	1.45	1.40
2	B	1353	NAD	C3N-C7N	3.02	1.55	1.50
2	A	1352	NAD	C3N-C7N	3.02	1.55	1.50
2	A	1352	NAD	C6N-N1N	2.99	1.42	1.35
2	A	1352	NAD	C5A-N7A	-2.98	1.33	1.39
2	B	1353	NAD	C6N-N1N	2.95	1.42	1.35
2	C	1354	NAD	C5A-N7A	-2.93	1.33	1.39
2	C	1354	NAD	C6N-N1N	2.88	1.41	1.35
2	B	1353	NAD	C5A-N7A	-2.72	1.34	1.39
2	D	1355	NAD	C5A-N7A	-2.62	1.34	1.39
2	B	1353	NAD	C4A-N9A	-2.43	1.32	1.37
2	A	1352	NAD	PA-O3	2.08	1.61	1.59
2	D	1355	NAD	C4A-N9A	-2.02	1.33	1.37

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1352	NAD	C4D-O4D-C1D	-6.81	103.68	109.92
2	C	1354	NAD	C5A-C4A-N3A	-6.13	118.28	126.72
2	C	1354	NAD	N3A-C4A-N9A	6.07	137.49	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1352	NAD	N3A-C4A-N9A	5.81	137.05	127.17
2	D	1355	NAD	C5A-C4A-N3A	-5.58	119.04	126.72
2	D	1355	NAD	C6N-N1N-C2N	-5.55	117.16	121.88
2	A	1352	NAD	C5A-C4A-N3A	-5.39	119.30	126.72
2	C	1354	NAD	N3A-C2A-N1A	-5.31	120.54	128.58
2	B	1353	NAD	C6N-N1N-C2N	-5.15	117.49	121.88
2	B	1353	NAD	C5A-C4A-N3A	-5.11	119.68	126.72
2	C	1354	NAD	C6N-N1N-C2N	-4.74	117.85	121.88
2	B	1353	NAD	N3A-C2A-N1A	-4.70	121.47	128.58
2	A	1352	NAD	N3A-C2A-N1A	-4.68	121.50	128.58
2	D	1355	NAD	N3A-C4A-N9A	4.67	135.11	127.17
2	C	1354	NAD	C4D-O4D-C1D	-4.61	105.70	109.92
2	B	1353	NAD	N3A-C4A-N9A	4.31	134.50	127.17
2	D	1355	NAD	N3A-C2A-N1A	-4.10	122.38	128.58
2	C	1354	NAD	C2A-N3A-C4A	4.07	121.77	111.83
2	B	1353	NAD	C4D-O4D-C1D	-3.93	106.33	109.92
2	D	1355	NAD	O4B-C1B-N9A	3.53	114.87	108.09
2	A	1352	NAD	C6N-N1N-C2N	-3.49	118.91	121.88
2	A	1352	NAD	C4A-N9A-C8A	3.47	109.39	105.74
2	B	1353	NAD	O4B-C1B-N9A	3.45	114.71	108.09
2	B	1353	NAD	C6A-C5A-N7A	-3.43	125.47	132.09
2	D	1355	NAD	C4D-O4D-C1D	-3.40	106.81	109.92
2	A	1352	NAD	C2A-N3A-C4A	3.21	119.68	111.83
2	C	1354	NAD	O7N-C7N-C3N	3.15	123.45	119.60
2	D	1355	NAD	C2A-N3A-C4A	3.10	119.39	111.83
2	D	1355	NAD	C6A-C5A-N7A	-3.09	126.13	132.09
2	A	1352	NAD	O4D-C4D-C3D	3.06	111.23	105.15
2	C	1354	NAD	O4B-C1B-N9A	3.05	113.94	108.09
2	B	1353	NAD	C2A-N3A-C4A	3.00	119.15	111.83
2	A	1352	NAD	C6A-C5A-N7A	-2.99	126.32	132.09
2	B	1353	NAD	C4A-N9A-C8A	2.94	108.83	105.74
2	C	1354	NAD	C4A-N9A-C8A	2.82	108.70	105.74
2	B	1353	NAD	C4B-O4B-C1B	-2.82	103.25	109.47
2	B	1353	NAD	O3D-C3D-C2D	2.79	120.75	111.82
2	D	1355	NAD	C6A-C5A-C4A	2.75	120.94	117.18
2	A	1352	NAD	C4B-O4B-C1B	-2.74	103.42	109.47
2	A	1352	NAD	C6A-C5A-C4A	2.71	120.88	117.18
2	A	1352	NAD	O4B-C1B-N9A	2.66	113.20	108.09
2	C	1354	NAD	O4D-C4D-C3D	2.55	110.22	105.15
2	A	1352	NAD	C2N-N1N-C1D	-2.55	113.50	119.13
2	A	1352	NAD	N9A-C8A-N7A	-2.52	110.36	113.94
2	D	1355	NAD	O2B-C2B-C3B	2.52	119.89	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1353	NAD	C6A-C5A-C4A	2.48	120.56	117.18
2	C	1354	NAD	N9A-C8A-N7A	-2.45	110.46	113.94
2	D	1355	NAD	C4A-N9A-C8A	2.42	108.28	105.74
2	A	1352	NAD	O2B-C2B-C3B	2.42	119.57	111.82
2	D	1355	NAD	O7N-C7N-C3N	2.38	122.50	119.60
2	D	1355	NAD	O4D-C4D-C3D	2.37	109.85	105.15
2	B	1353	NAD	C2A-N1A-C6A	2.28	122.48	118.73
2	B	1353	NAD	N9A-C8A-N7A	-2.28	110.71	113.94
2	B	1353	NAD	O4D-C4D-C3D	2.27	109.66	105.15
2	D	1355	NAD	C4B-O4B-C1B	-2.25	104.50	109.47
2	D	1355	NAD	C6N-N1N-C1D	2.22	124.09	119.73
2	C	1354	NAD	C3B-C2B-C1B	-2.22	97.26	101.46
2	B	1353	NAD	O2B-C2B-C3B	2.15	118.72	111.82
2	C	1354	NAD	C6A-C5A-N7A	-2.12	127.99	132.09
2	C	1354	NAD	O3D-C3D-C4D	2.12	117.17	111.08
2	A	1352	NAD	O3B-C3B-C2B	2.10	118.55	111.82
2	C	1354	NAD	O2N-PN-O3	2.08	112.90	107.27
2	A	1352	NAD	C2A-N1A-C6A	2.07	122.14	118.73
2	D	1355	NAD	O3B-C3B-C2B	2.07	118.46	111.82
2	D	1355	NAD	O7N-C7N-N7N	-2.07	119.63	122.62
2	A	1352	NAD	C5A-C4A-N9A	-2.04	103.59	105.81
2	A	1352	NAD	C5D-C4D-C3D	-2.03	107.89	115.21
2	D	1355	NAD	O3D-C3D-C4D	2.02	116.88	111.08

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1352	NAD	PN-O3-PA-O5B
2	A	1352	NAD	O4D-C1D-N1N-C2N
2	A	1352	NAD	C2D-C1D-N1N-C2N
2	B	1353	NAD	O4D-C1D-N1N-C2N
2	B	1353	NAD	O4D-C1D-N1N-C6N
2	B	1353	NAD	C2D-C1D-N1N-C2N
2	B	1353	NAD	C2D-C1D-N1N-C6N
2	C	1354	NAD	C5B-O5B-PA-O1A
2	C	1354	NAD	C5B-O5B-PA-O2A
2	C	1354	NAD	C5B-O5B-PA-O3
2	C	1354	NAD	O4D-C1D-N1N-C2N
2	C	1354	NAD	O4D-C1D-N1N-C6N
2	C	1354	NAD	C2D-C1D-N1N-C2N
2	C	1354	NAD	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	D	1355	NAD	O4D-C1D-N1N-C2N
2	D	1355	NAD	O4D-C1D-N1N-C6N
2	D	1355	NAD	C2D-C1D-N1N-C2N
2	D	1355	NAD	C2D-C1D-N1N-C6N
2	C	1354	NAD	PA-O3-PN-O1N
2	C	1354	NAD	PN-O3-PA-O5B
2	B	1353	NAD	O4B-C4B-C5B-O5B
2	A	1352	NAD	PA-O3-PN-O2N
2	C	1354	NAD	PA-O3-PN-O2N
2	A	1352	NAD	C2D-C1D-N1N-C6N
2	A	1352	NAD	O4D-C1D-N1N-C6N
2	A	1352	NAD	C4B-C5B-O5B-PA
2	C	1354	NAD	O4B-C4B-C5B-O5B
2	D	1355	NAD	O4B-C4B-C5B-O5B
2	A	1352	NAD	C2B-C1B-N9A-C8A

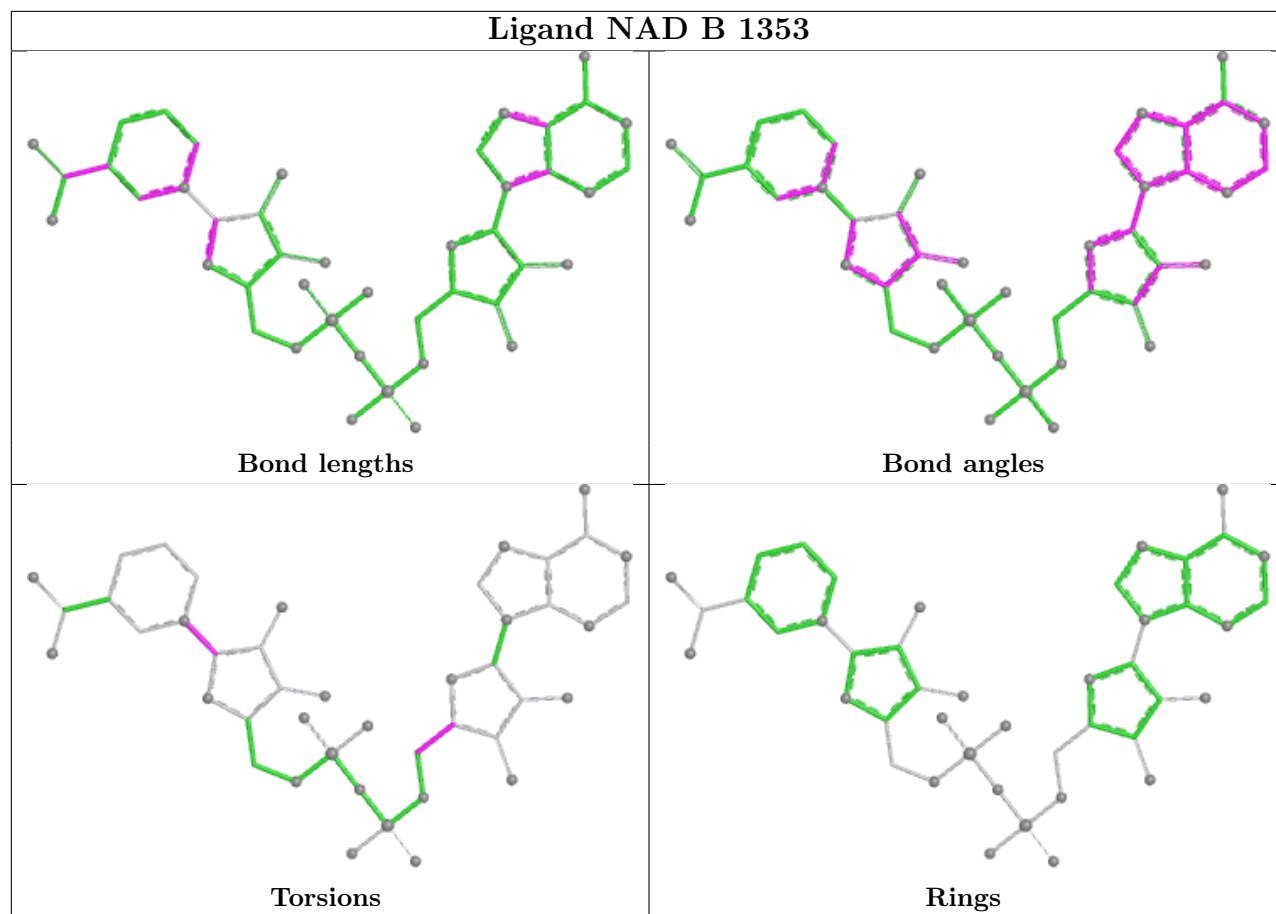
There are no ring outliers.

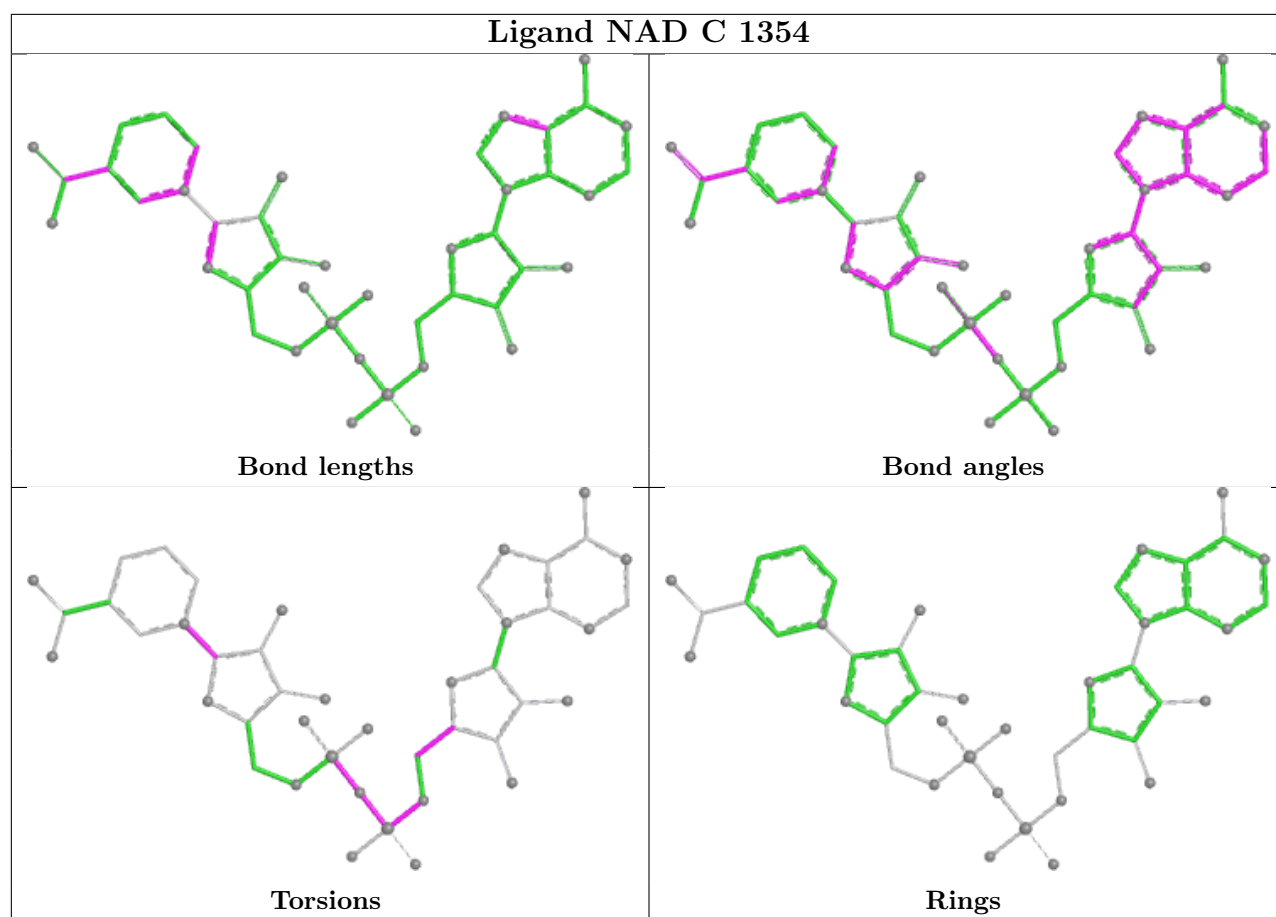
4 monomers are involved in 11 short contacts:

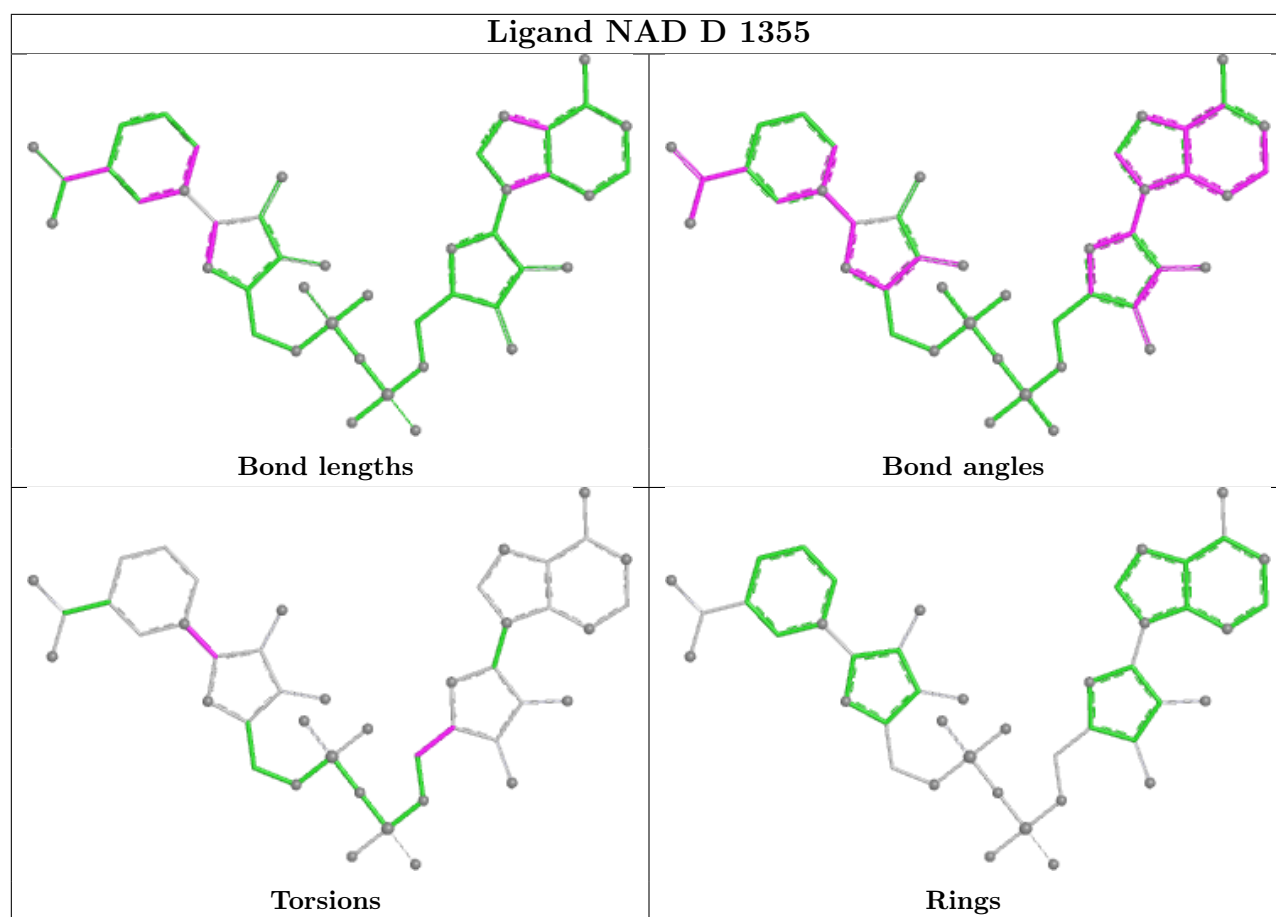
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1353	NAD	4	0
2	C	1354	NAD	4	0
2	D	1355	NAD	2	0
2	A	1352	NAD	1	0

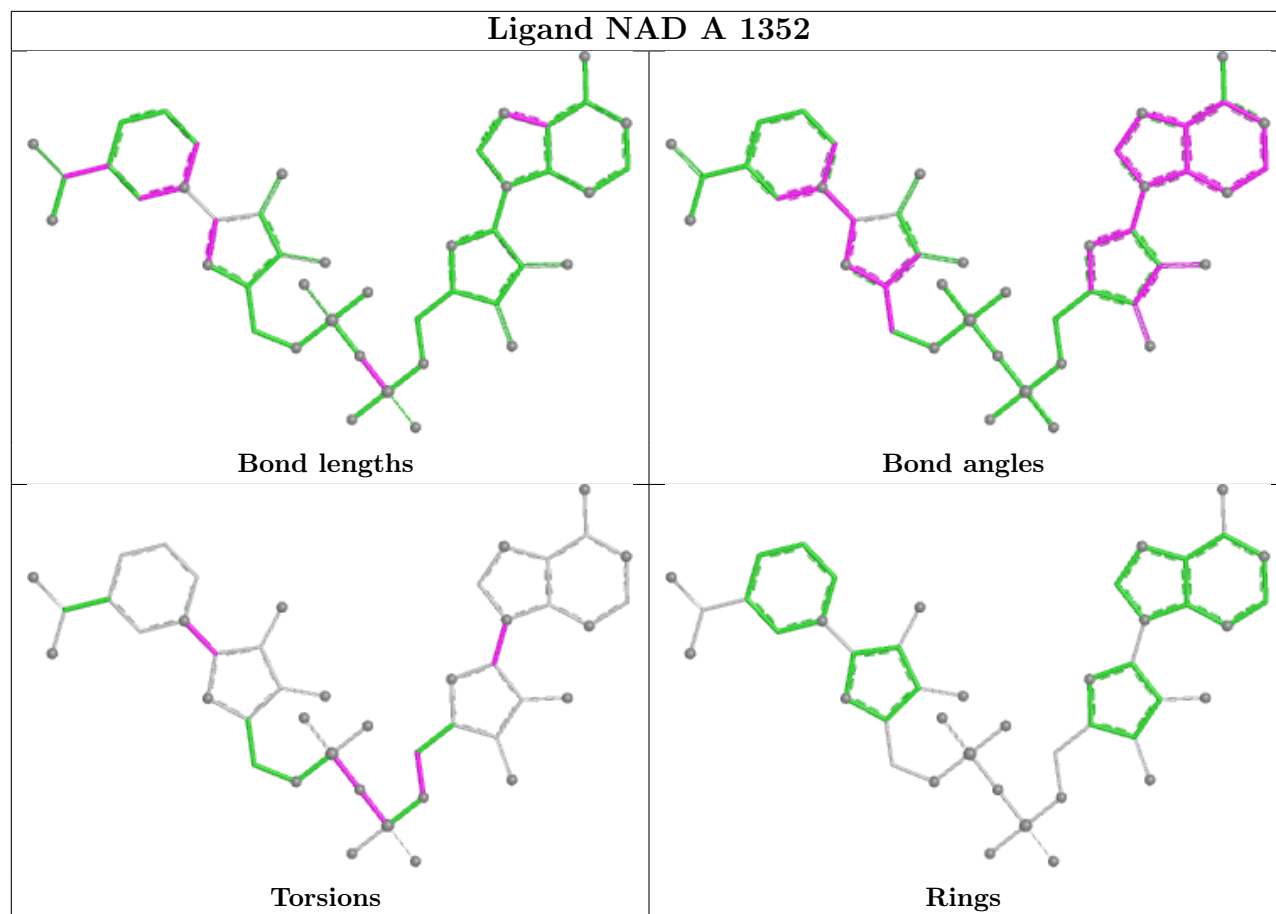
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand NAD B 1353









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	A	307/318 (96%)	-0.02	17 (5%) 30 32	8, 18, 40, 78	0
1	B	318/318 (100%)	-0.10	11 (3%) 47 49	9, 19, 44, 68	0
1	C	307/318 (96%)	-0.05	17 (5%) 30 32	8, 18, 43, 87	0
1	D	318/318 (100%)	-0.11	12 (3%) 44 46	8, 20, 42, 66	0
All	All	1250/1272 (98%)	-0.07	57 (4%) 37 39	8, 19, 43, 87	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	HIS	10.8
1	C	193	HIS	8.9
1	A	98	ALA	8.8
1	C	98	ALA	7.6
1	C	334	ASN	6.1
1	D	193	HIS	6.0
1	A	334	ASN	5.3
1	C	112	LYS	5.1
1	B	16	SER	5.0
1	B	193	HIS	5.0
1	A	194	GLY	4.9
1	C	194	GLY	4.6
1	A	16	SER	4.6
1	D	16	SER	4.6
1	B	194	GLY	4.5
1	C	333	GLU	4.5
1	C	96	ALA	4.3
1	B	195	ASP	4.3
1	D	194	GLY	4.2
1	C	195	ASP	4.1
1	C	97	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	192	GLU	3.9
1	A	97	GLY	3.9
1	B	242	ASN	3.9
1	C	109	LEU	3.7
1	A	333	GLU	3.5
1	A	195	ASP	3.4
1	D	242	ASN	3.3
1	C	332	LEU	3.3
1	A	149	LYS	3.1
1	C	138	ASN	3.1
1	A	196	SER	3.0
1	A	224	ASP	3.0
1	B	238	TYR	3.0
1	A	109	LEU	2.9
1	C	16	SER	2.9
1	D	195	ASP	2.9
1	C	115	ASN	2.9
1	A	96	ALA	2.9
1	D	238	TYR	2.8
1	A	318	ALA	2.8
1	C	17	MET	2.8
1	D	17	MET	2.7
1	D	196	SER	2.6
1	C	118	SER	2.6
1	B	138	ASN	2.5
1	A	112	LYS	2.5
1	B	196	SER	2.4
1	D	277	ASP	2.3
1	A	319	ALA	2.3
1	D	216	LYS	2.3
1	B	17	MET	2.2
1	B	320	THR	2.2
1	D	224	ASP	2.1
1	B	312	LYS	2.1
1	C	224	ASP	2.1
1	D	323	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

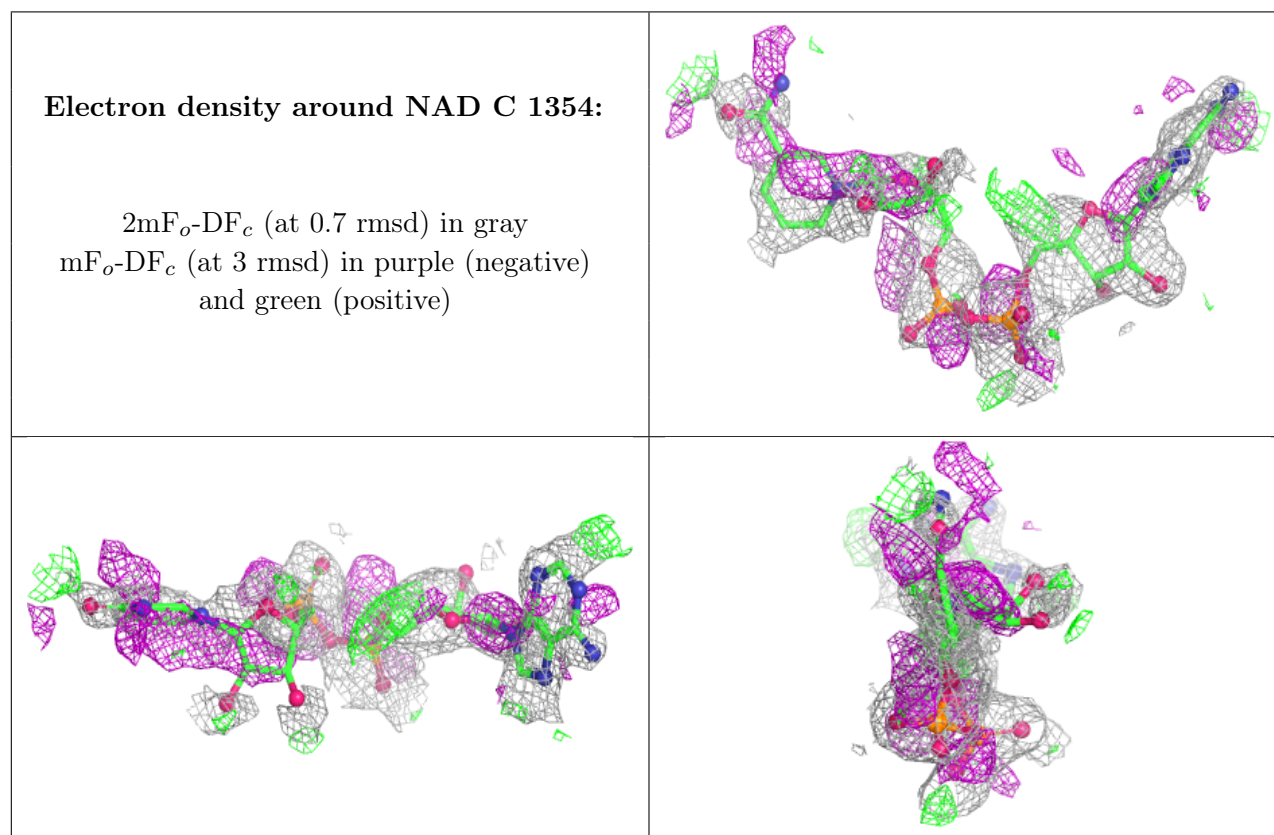
There are no oligosaccharides in this entry.

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.

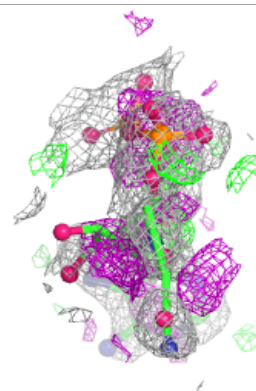
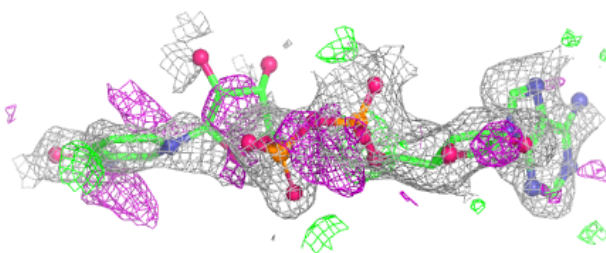
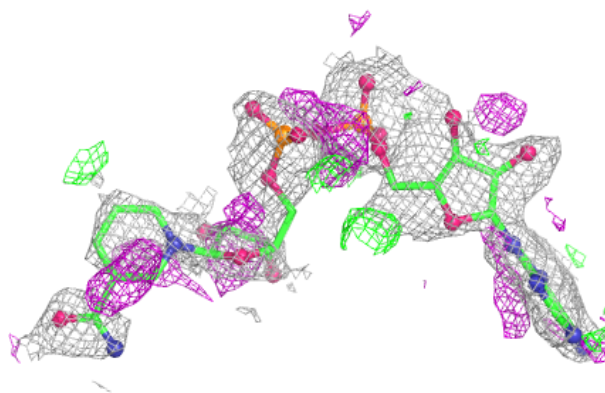
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	C	1354	44/44	0.65	0.30	66,77,86,89	0
2	NAD	A	1352	44/44	0.69	0.26	62,70,82,84	0
2	NAD	D	1355	44/44	0.69	0.28	53,74,85,86	0
2	NAD	B	1353	44/44	0.75	0.24	51,69,79,83	0

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.

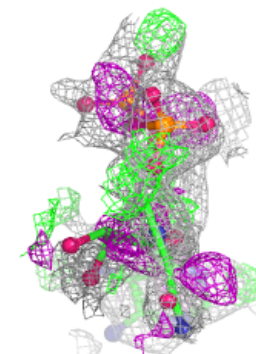
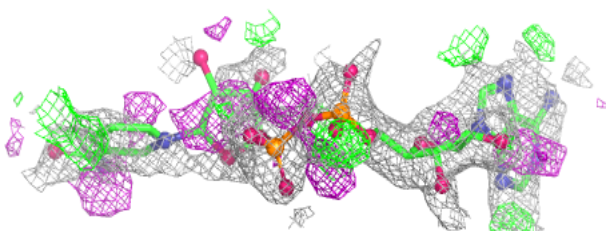
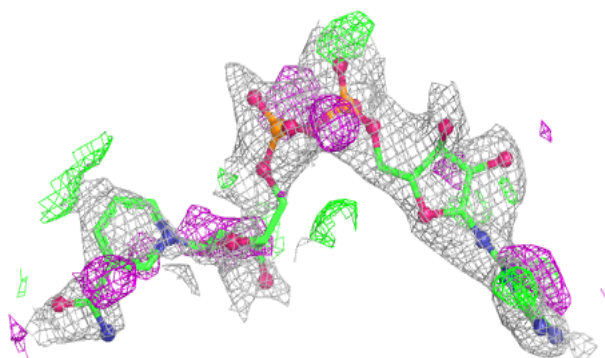


Electron density around NAD A 1352:

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

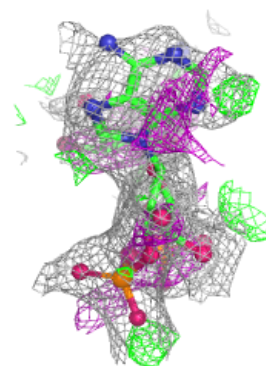
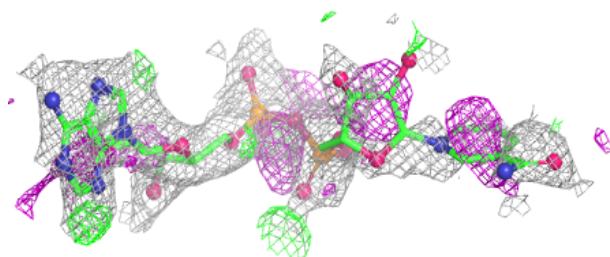
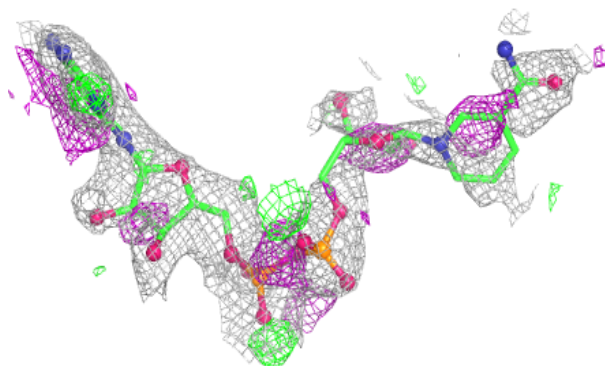
**Electron density around NAD D 1355:**

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



Electron density around NAD B 1353:

$2mF_o-DF_c$ (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.