



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:02 AM UTC

PDB ID : 1LLD / pdb_00001lld
Title : MOLECULAR BASIS OF ALLOSTERIC ACTIVATION OF BACTERIAL
L-LACTATE DEHYDROGENASE
Authors : Iwata, S.; Ohta, T.
Deposited on : 1992-06-08
Resolution : 2.00 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

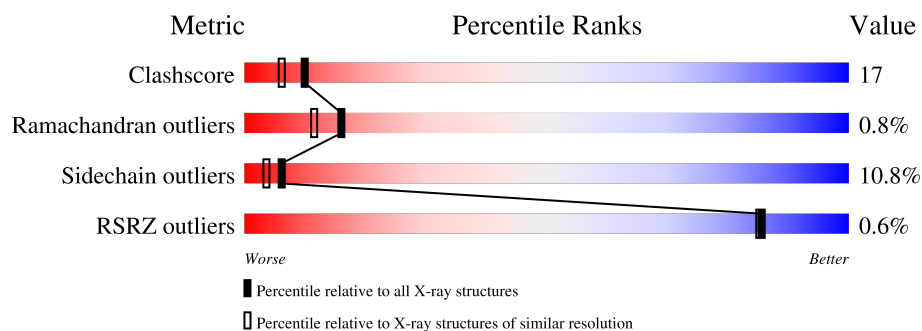
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	319	
1	B	319	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5010 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.

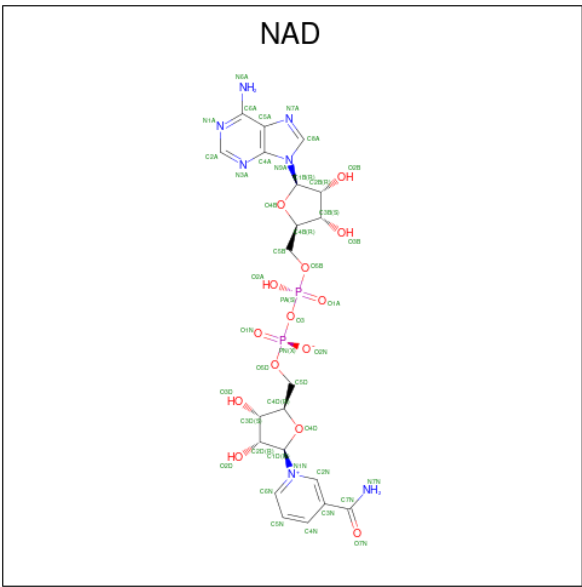
- Molecule 1 is a protein called L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2350	1474	409	457	10			
1	B	313	Total	C	N	O	S	0	0	0
			2350	1474	409	457	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	SER	CYS	conflict	UNP P19869
B	199	SER	CYS	conflict	UNP P19869

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

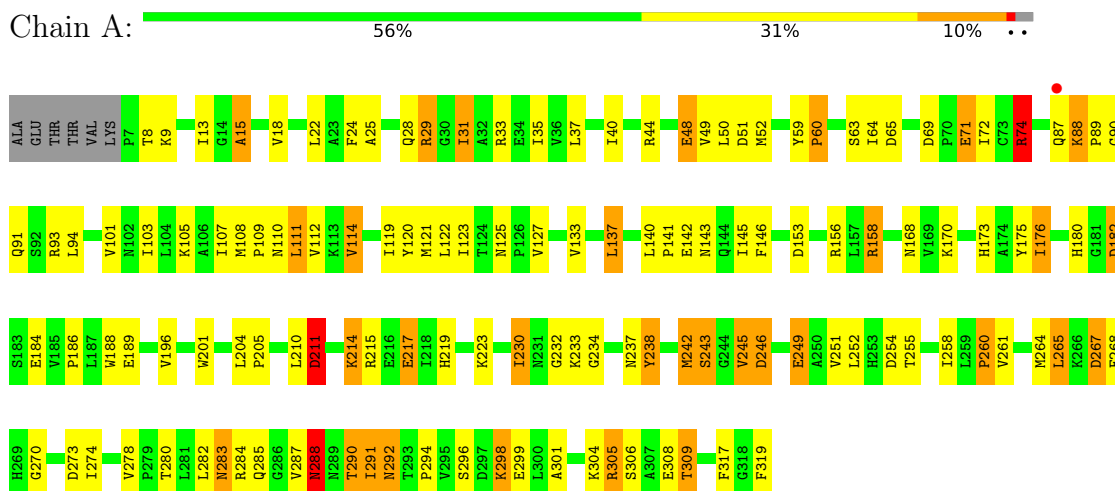
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total	O	0	0
			112	112		
3	B	110	Total	O	0	0
			110	110		

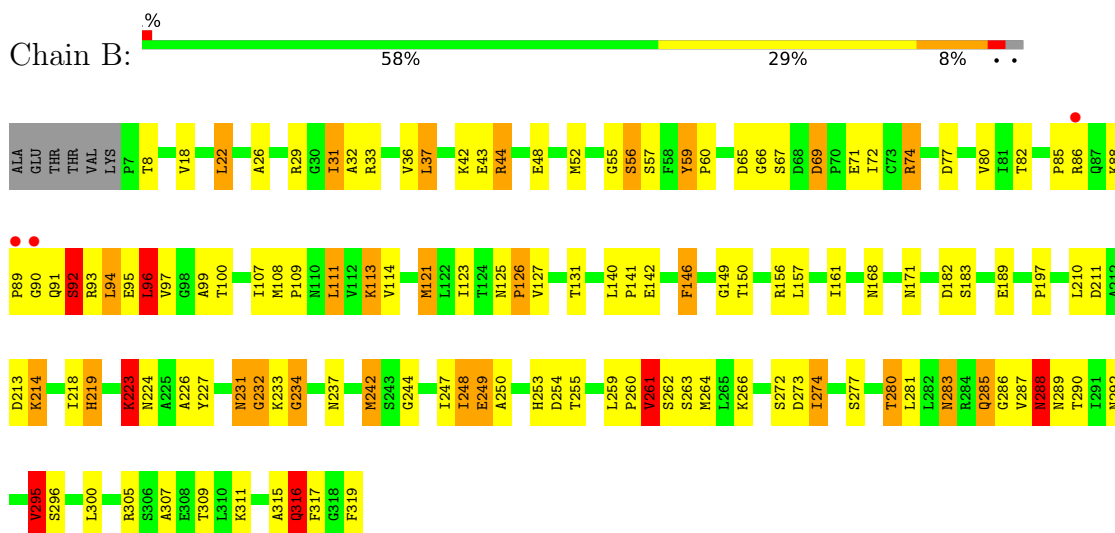
3 Residue-property plots

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: L-LACTATE DEHYDROGENASE



• Molecule 1: L-LACTATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.80Å 131.40Å 63.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 78.5 (10.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.00Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.179 , (Not available) 0.169 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5010	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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	1.26	1/2390 (0.0%)	2.11	93/3248 (2.9%)
1	B	1.25	5/2390 (0.2%)	2.04	66/3248 (2.0%)
All	All	1.25	6/4780 (0.1%)	2.07	159/6496 (2.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	ASP	CA-CB	6.09	1.63	1.53
1	B	247	ILE	CA-CB	5.97	1.62	1.54
1	B	286	GLY	N-CA	5.71	1.51	1.45
1	B	161	ILE	N-CA	5.47	1.53	1.46
1	B	248	ILE	CA-CB	5.37	1.61	1.54
1	B	232	GLY	N-CA	5.08	1.50	1.44

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	VAL	O-C-N	11.26	128.79	121.69
1	A	211	ASP	CA-CB-CG	-10.96	101.64	112.60
1	A	210	LEU	CA-C-N	10.24	139.61	120.97
1	A	210	LEU	C-N-CA	10.24	139.61	120.97
1	A	93	ARG	CD-NE-CZ	10.22	138.71	124.40
1	A	44	ARG	CD-NE-CZ	-9.00	111.80	124.40
1	A	255	THR	N-CA-C	8.84	123.85	112.89
1	B	113	LYS	CA-C-N	8.57	134.27	120.55
1	B	113	LYS	C-N-CA	8.57	134.27	120.55
1	A	88	LYS	O-C-N	8.15	128.25	121.32
1	A	35	ILE	CA-C-O	-8.00	111.89	120.36
1	A	44	ARG	NE-CZ-NH1	-7.79	113.71	121.50
1	B	259	LEU	O-C-N	7.75	127.60	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ASN	OD1-CG-ND2	7.75	130.35	122.60
1	B	69	ASP	CB-CA-C	7.64	119.73	109.42
1	A	304	LYS	CA-C-N	7.61	130.81	120.54
1	A	304	LYS	C-N-CA	7.61	130.81	120.54
1	B	127	VAL	N-CA-C	7.50	118.23	110.36
1	A	308	GLU	CA-CB-CG	7.50	129.09	114.10
1	A	317	PHE	CA-CB-CG	-7.44	106.36	113.80
1	A	211	ASP	N-CA-CB	-7.39	99.80	110.36
1	B	249	GLU	CB-CG-CD	7.18	124.80	112.60
1	A	299	GLU	CB-CG-CD	7.16	124.77	112.60
1	A	137	LEU	N-CA-CB	-7.15	99.64	110.01
1	A	158	ARG	CD-NE-CZ	7.12	134.37	124.40
1	B	263	SER	CA-C-O	-7.10	113.67	121.33
1	B	197	PRO	CB-CA-C	7.06	120.53	111.56
1	A	24	PHE	CA-CB-CG	-7.04	106.76	113.80
1	B	146	PHE	CA-C-N	7.02	127.03	122.18
1	B	146	PHE	C-N-CA	7.02	127.03	122.18
1	A	251	VAL	N-CA-C	7.02	117.63	110.82
1	B	263	SER	O-C-N	6.98	131.20	123.25
1	B	182	ASP	CA-CB-CG	6.93	119.53	112.60
1	B	171	ASN	CA-CB-CG	-6.92	105.68	112.60
1	B	261	VAL	N-CA-CB	-6.89	99.61	112.36
1	A	28	GLN	CA-C-O	-6.82	113.33	120.55
1	A	291	ILE	CB-CA-C	6.67	121.62	111.68
1	B	156	ARG	CD-NE-CZ	6.67	133.73	124.40
1	A	51	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	319	PHE	CA-CB-CG	-6.60	107.20	113.80
1	B	96	LEU	CB-CA-C	6.60	121.33	110.90
1	A	153	ASP	CA-C-O	-6.58	113.57	120.55
1	B	55	GLY	CA-C-N	6.56	129.37	120.38
1	B	55	GLY	C-N-CA	6.56	129.37	120.38
1	B	255	THR	N-CA-C	6.52	120.44	112.23
1	B	295	VAL	N-CA-CB	-6.50	101.04	111.58
1	B	123	ILE	N-CA-C	-6.49	107.17	113.53
1	A	142	GLU	O-C-N	6.42	129.73	122.22
1	B	260	PRO	CA-C-N	6.40	131.78	122.69
1	B	260	PRO	C-N-CA	6.40	131.78	122.69
1	A	243	SER	CA-C-N	6.40	127.04	119.94
1	A	243	SER	C-N-CA	6.40	127.04	119.94
1	A	141	PRO	CA-C-N	6.40	129.49	120.28
1	A	141	PRO	C-N-CA	6.40	129.49	120.28
1	A	18	VAL	CA-C-N	6.39	127.04	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	VAL	C-N-CA	6.39	127.04	119.94
1	B	289	ASN	O-C-N	6.38	130.00	122.34
1	A	267	ASP	CA-CB-CG	-6.38	106.22	112.60
1	A	254	ASP	N-CA-CB	-6.37	102.27	111.70
1	B	223	LYS	CG-CD-CE	6.31	125.81	111.30
1	B	249	GLU	CA-CB-CG	6.30	126.71	114.10
1	A	290	THR	CA-CB-OG1	-6.25	100.23	109.60
1	B	231	ASN	CA-C-N	-6.23	116.92	122.47
1	B	231	ASN	C-N-CA	-6.23	116.92	122.47
1	A	278	VAL	CA-C-O	-6.21	114.38	121.59
1	B	261	VAL	CA-CB-CG1	6.18	120.90	110.40
1	A	298	LYS	CA-CB-CG	6.17	126.44	114.10
1	A	243	SER	N-CA-C	-6.06	103.84	111.11
1	B	295	VAL	CB-CA-C	6.04	119.81	110.28
1	A	87	GLN	CB-CA-C	6.03	120.55	109.46
1	A	127	VAL	N-CA-C	6.02	116.76	110.62
1	B	219	HIS	CA-CB-CG	-6.01	107.79	113.80
1	A	44	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	A	201	TRP	CA-C-N	5.99	131.17	121.83
1	A	201	TRP	C-N-CA	5.99	131.17	121.83
1	A	246	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	35	ILE	O-C-N	5.94	129.62	123.20
1	B	22	LEU	CB-CA-C	5.94	120.20	110.88
1	B	255	THR	CA-CB-OG1	-5.94	100.69	109.60
1	B	69	ASP	CA-CB-CG	5.92	118.52	112.60
1	B	288	ASN	OD1-CG-ND2	5.89	128.49	122.60
1	B	224	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	142	GLU	CB-CA-C	-5.86	99.78	110.63
1	A	15	ALA	CA-C-N	5.80	128.94	122.55
1	A	15	ALA	C-N-CA	5.80	128.94	122.55
1	A	44	ARG	O-C-N	5.80	128.35	122.09
1	B	131	THR	CA-C-O	5.79	126.91	120.82
1	B	274	ILE	CA-C-O	-5.69	115.76	121.45
1	B	223	LYS	CB-CG-CD	5.68	124.37	111.30
1	A	142	GLU	N-CA-C	5.66	118.22	111.71
1	A	125	ASN	CA-CB-CG	5.66	118.26	112.60
1	A	146	PHE	CA-C-O	-5.66	115.39	121.38
1	A	184	GLU	CA-C-O	-5.63	114.95	121.15
1	B	213	ASP	O-C-N	5.63	127.87	122.07
1	B	210	LEU	N-CA-C	-5.63	101.78	109.71
1	A	255	THR	CA-CB-OG1	-5.62	101.17	109.60
1	A	94	LEU	N-CA-CB	-5.62	101.57	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	SER	N-CA-C	5.61	118.12	111.33
1	A	91	GLN	N-CA-C	-5.61	100.10	109.24
1	A	44	ARG	CA-C-O	-5.60	114.93	120.70
1	A	301	ALA	CA-C-N	5.58	127.69	120.44
1	A	301	ALA	C-N-CA	5.58	127.69	120.44
1	A	60	PRO	N-CA-C	5.56	121.07	113.84
1	A	65	ASP	CA-CB-CG	-5.56	107.04	112.60
1	A	196	VAL	O-C-N	5.56	125.80	121.46
1	B	273	ASP	N-CA-C	5.54	119.22	111.74
1	A	288	ASN	CB-CA-C	5.51	118.64	111.42
1	B	244	GLY	CA-C-O	5.49	126.93	121.00
1	B	224	ASN	N-CA-CB	5.48	117.96	110.01
1	B	168	ASN	CA-CB-CG	-5.48	107.12	112.60
1	B	168	ASN	OD1-CG-ND2	5.46	128.06	122.60
1	A	143	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	A	121	MET	CA-CB-CG	-5.43	103.23	114.10
1	B	261	VAL	CB-CA-C	5.42	119.46	110.30
1	A	49	VAL	CA-C-O	-5.40	115.44	121.17
1	B	127	VAL	CB-CA-C	5.40	118.80	111.88
1	A	245	VAL	CA-C-N	5.40	127.78	120.38
1	A	245	VAL	C-N-CA	5.40	127.78	120.38
1	B	305	ARG	CA-CB-CG	5.40	124.90	114.10
1	B	59	TYR	CA-C-N	5.39	126.58	119.84
1	B	59	TYR	C-N-CA	5.39	126.58	119.84
1	A	74	ARG	CA-CB-CG	5.39	124.88	114.10
1	A	176	ILE	CA-C-O	-5.38	114.78	120.53
1	A	214	LYS	N-CA-C	-5.37	105.34	111.14
1	A	94	LEU	CB-CA-C	5.36	120.97	110.67
1	A	182	ASP	CA-C-O	-5.34	114.06	120.10
1	B	226	ALA	O-C-N	5.34	127.64	122.09
1	B	150	THR	CA-CB-OG1	-5.34	101.59	109.60
1	A	264	MET	CA-C-N	5.32	129.03	121.42
1	A	264	MET	C-N-CA	5.32	129.03	121.42
1	A	119	ILE	CA-C-O	-5.31	114.28	121.02
1	B	69	ASP	CA-C-N	5.30	124.96	119.56
1	B	69	ASP	C-N-CA	5.30	124.96	119.56
1	A	156	ARG	CD-NE-CZ	5.27	131.78	124.40
1	B	233	LYS	N-CA-C	-5.25	106.58	112.87
1	B	111	LEU	N-CA-CB	-5.24	102.47	110.07
1	A	273	ASP	N-CA-C	5.23	118.61	111.39
1	A	196	VAL	N-CA-C	5.23	113.62	107.77
1	A	306	SER	CA-C-O	-5.22	115.02	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	ALA	CA-C-O	-5.22	115.32	120.90
1	B	67	SER	O-C-N	5.20	128.78	122.75
1	A	238	TYR	N-CA-C	5.19	116.63	111.07
1	A	184	GLU	CB-CA-C	-5.18	101.36	109.70
1	B	224	ASN	O-C-N	5.18	127.41	122.07
1	A	294	PRO	CA-C-O	-5.17	115.55	121.86
1	A	184	GLU	CG-CD-OE2	-5.15	106.55	118.40
1	A	29	ARG	NE-CZ-NH1	5.13	126.63	121.50
1	B	280	THR	CA-C-O	-5.11	115.13	121.11
1	A	260	PRO	CB-CA-C	5.10	116.15	111.87
1	A	69	ASP	CA-C-N	5.08	125.36	119.47
1	A	69	ASP	C-N-CA	5.08	125.36	119.47
1	A	123	ILE	CA-C-O	5.07	124.20	118.98
1	A	48	GLU	CA-C-O	5.07	125.79	120.42
1	B	149	GLY	N-CA-C	5.05	120.53	111.34
1	A	254	ASP	CA-C-O	-5.03	116.00	121.84
1	B	99	ALA	CA-C-N	5.02	127.27	120.44
1	B	99	ALA	C-N-CA	5.02	127.27	120.44
1	A	119	ILE	N-CA-C	-5.02	101.24	108.87
1	B	126	PRO	N-CD-CG	-5.01	97.79	103.80

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	2350	0	2367	82	0
1	B	2350	0	2367	85	0
2	A	44	0	26	0	0
2	B	44	0	26	3	0
3	A	112	0	0	4	0
3	B	110	0	0	2	0
All	All	5010	0	4786	167	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 17.

All (167) 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:88:LYS:CG	1:A:89:PRO:HD2	1.69	1.23
1:B:92:SER:OG	1:B:95:GLU:HG3	1.46	1.15
1:B:88:LYS:HB3	1:B:89:PRO:CD	1.76	1.15
1:A:88:LYS:HG2	1:A:89:PRO:CD	1.79	1.12
1:B:88:LYS:HB3	1:B:89:PRO:HD2	1.09	1.06
1:A:71:GLU:OE2	1:A:74:ARG:HD2	1.67	0.95
1:A:305:ARG:NH1	1:A:309:THR:HG23	1.82	0.95
1:B:88:LYS:CB	1:B:89:PRO:HD2	2.00	0.90
1:A:242:MET:HA	1:A:242:MET:HE2	1.54	0.88
1:B:272:SER:O	1:B:311:LYS:NZ	2.05	0.88
1:B:94:LEU:HD11	1:B:316:GLN:OE1	1.75	0.86
1:B:283:ASN:ND2	1:B:285:GLN:HG2	1.92	0.84
1:A:189:GLU:HG3	1:A:296:SER:HB3	1.58	0.84
1:B:283:ASN:HD21	1:B:285:GLN:HG2	1.45	0.82
1:B:26:ALA:HB1	1:B:31:ILE:HD11	1.63	0.80
1:B:189:GLU:HG3	1:B:296:SER:HB3	1.64	0.79
1:A:282:LEU:CD2	1:A:287:VAL:HG12	2.12	0.79
1:A:88:LYS:HG2	1:A:89:PRO:HD2	0.83	0.77
1:B:71:GLU:OE2	1:B:74:ARG:NH1	2.19	0.76
1:A:29:ARG:HB3	1:A:31:ILE:HD11	1.66	0.76
1:A:305:ARG:HH12	1:A:309:THR:HG23	1.50	0.73
1:A:29:ARG:HB3	1:A:31:ILE:CD1	2.18	0.73
1:A:8:THR:HG23	1:A:33:ARG:H	1.53	0.73
1:A:71:GLU:OE2	1:A:74:ARG:NH1	2.18	0.72
1:B:242:MET:HA	1:B:242:MET:HE2	1.73	0.70
1:B:29:ARG:HD3	3:B:428:HOH:O	1.92	0.69
1:A:282:LEU:HD21	1:A:287:VAL:HG12	1.74	0.68
1:A:29:ARG:NH2	1:A:249:GLU:OE1	2.27	0.68
1:A:288:ASN:HD22	1:A:290:THR:H	1.40	0.66
1:A:282:LEU:HD23	1:A:287:VAL:HG12	1.77	0.66
1:A:288:ASN:HD22	1:A:288:ASN:C	2.03	0.66
1:A:133:VAL:O	1:A:137:LEU:HB2	1.96	0.65
1:A:283:ASN:C	1:A:283:ASN:HD22	2.03	0.65
1:A:15:ALA:HB1	1:A:48:GLU:OE1	1.97	0.65
1:B:92:SER:OG	1:B:95:GLU:CG	2.37	0.63
1:B:44:ARG:NE	1:B:48:GLU:OE2	2.30	0.63
1:B:88:LYS:CB	1:B:89:PRO:CD	2.55	0.63
1:A:182:ASP:O	1:A:223:LYS:HE3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:C	1:B:22:LEU:HD23	2.23	0.62
1:A:29:ARG:CB	1:A:31:ILE:HD11	2.30	0.62
1:A:232:GLY:C	1:A:234:GLY:H	2.07	0.61
1:A:211:ASP:HB3	1:A:214:LYS:H	1.65	0.61
1:A:267:ASP:OD1	1:A:270:GLY:N	2.35	0.60
1:A:288:ASN:ND2	1:A:290:THR:H	2.00	0.59
1:A:175:TYR:HD1	1:A:260:PRO:HG3	1.68	0.59
1:A:284:ARG:O	1:A:284:ARG:HG3	2.02	0.59
1:B:232:GLY:C	1:B:234:GLY:H	2.08	0.58
1:A:13:ILE:HG13	1:A:111:LEU:HD21	1.84	0.58
1:A:283:ASN:HD22	1:A:285:GLN:H	1.51	0.58
1:B:288:ASN:C	1:B:288:ASN:HD22	2.11	0.58
1:A:71:GLU:OE2	1:A:74:ARG:CD	2.49	0.58
1:A:242:MET:HA	1:A:242:MET:CE	2.31	0.57
1:A:37:LEU:HD11	1:A:52:MET:HE1	1.85	0.57
1:B:92:SER:HG	1:B:95:GLU:HG3	1.65	0.57
1:B:66:GLY:HA2	1:B:72:ILE:HD13	1.87	0.56
1:B:85:PRO:HG3	1:B:100:THR:OG1	2.06	0.56
1:B:232:GLY:C	1:B:234:GLY:N	2.60	0.56
1:B:108:MET:N	1:B:109:PRO:HD2	2.22	0.55
1:A:173:HIS:HB3	3:A:347:HOH:O	2.07	0.55
1:A:74:ARG:HA	1:A:114:VAL:HG13	1.89	0.54
1:B:283:ASN:C	1:B:283:ASN:HD22	2.13	0.54
1:A:232:GLY:C	1:A:234:GLY:N	2.66	0.54
1:B:86:ARG:NH1	2:B:320:NAD:O1A	2.42	0.53
1:B:261:VAL:O	1:B:277:SER:HA	2.09	0.53
1:B:280:THR:HG21	1:B:287:VAL:HB	1.89	0.53
1:A:285:GLN:NE2	3:A:405:HOH:O	2.42	0.53
1:A:168:ASN:OD1	1:A:170:LYS:HD3	2.09	0.52
1:B:57:SER:O	1:B:60:PRO:HD3	2.10	0.52
1:B:82:THR:O	2:B:320:NAD:C5D	2.58	0.52
1:A:158:ARG:HD2	3:A:322:HOH:O	2.08	0.52
1:B:319:PHE:CD1	1:B:319:PHE:N	2.78	0.51
1:B:8:THR:HA	1:B:77:ASP:OD2	2.11	0.51
1:A:305:ARG:O	1:A:309:THR:OG1	2.28	0.51
1:B:26:ALA:CB	1:B:31:ILE:HD11	2.39	0.50
1:B:315:ALA:C	1:B:317:PHE:N	2.68	0.50
1:B:26:ALA:O	1:B:31:ILE:HD13	2.11	0.50
1:B:307:ALA:O	1:B:311:LYS:HG3	2.12	0.50
1:B:280:THR:CG2	1:B:287:VAL:HB	2.41	0.50
1:A:283:ASN:ND2	1:A:285:GLN:H	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:MET:HG3	1:B:146:PHE:CE2	2.46	0.49
1:A:219:HIS:CE1	1:A:223:LYS:HD2	2.47	0.49
1:B:91:GLN:C	1:B:92:SER:O	2.53	0.49
1:B:242:MET:HA	1:B:242:MET:CE	2.41	0.49
1:B:283:ASN:ND2	1:B:285:GLN:H	2.11	0.49
1:B:80:VAL:HG21	1:B:248:ILE:HD11	1.94	0.49
1:B:44:ARG:NH2	1:B:48:GLU:OE2	2.46	0.48
1:A:280:THR:CG2	1:A:287:VAL:HB	2.44	0.48
1:B:37:LEU:O	1:B:66:GLY:HA2	2.13	0.48
1:A:214:LYS:O	1:A:217:GLU:HB3	2.14	0.48
1:B:315:ALA:O	1:B:317:PHE:N	2.46	0.48
1:B:214:LYS:HA	1:B:214:LYS:HD3	1.75	0.47
1:B:29:ARG:HH21	1:B:249:GLU:HG3	1.78	0.47
1:B:74:ARG:HA	1:B:114:VAL:HG13	1.97	0.47
1:A:107:ILE:HG22	1:A:111:LEU:HD22	1.96	0.47
1:B:59:TYR:N	1:B:60:PRO:CD	2.78	0.47
1:A:29:ARG:HB3	1:A:31:ILE:HD13	1.96	0.46
1:A:9:LYS:NZ	1:A:74:ARG:O	2.43	0.46
1:B:227:TYR:CE1	1:B:231:ASN:ND2	2.83	0.46
1:A:71:GLU:CD	1:A:74:ARG:HD2	2.40	0.46
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.72	0.46
1:A:25:ALA:HB3	1:A:245:VAL:HG21	1.98	0.46
1:B:91:GLN:O	1:B:92:SER:O	2.34	0.46
1:A:305:ARG:HD3	1:A:305:ARG:HA	1.34	0.46
1:B:8:THR:HG23	1:B:32:ALA:HA	1.97	0.46
1:A:101:VAL:O	1:A:105:LYS:HG3	2.15	0.46
1:A:88:LYS:CG	1:A:89:PRO:CD	2.63	0.45
1:A:258:ILE:HA	1:A:280:THR:O	2.16	0.45
1:B:315:ALA:C	1:B:317:PHE:H	2.23	0.45
1:B:44:ARG:HE	1:B:48:GLU:CD	2.22	0.45
1:B:183:SER:HB2	3:B:395:HOH:O	2.16	0.45
1:A:243:SER:O	1:A:246:ASP:HB3	2.17	0.45
1:B:26:ALA:HA	1:B:31:ILE:CD1	2.47	0.45
1:B:36:VAL:HA	1:B:65:ASP:O	2.16	0.45
1:A:8:THR:HG23	1:A:33:ARG:N	2.28	0.45
1:A:267:ASP:OD1	1:A:270:GLY:CA	2.65	0.45
1:A:288:ASN:C	1:A:288:ASN:ND2	2.75	0.45
1:A:274:ILE:HD12	1:A:274:ILE:HA	1.72	0.44
1:B:82:THR:O	2:B:320:NAD:H52N	2.17	0.44
1:B:211:ASP:OD1	1:B:211:ASP:C	2.61	0.44
1:B:253:HIS:O	1:B:254:ASP:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:MET:HB2	1:B:264:MET:HE2	1.83	0.44
1:A:188:TRP:CZ2	1:A:215:ARG:HB3	2.52	0.44
1:A:267:ASP:OD1	1:A:270:GLY:HA2	2.17	0.44
1:A:267:ASP:CG	1:A:267:ASP:O	2.58	0.43
1:B:37:LEU:HD11	1:B:52:MET:HE1	1.99	0.43
1:B:125:ASN:ND2	1:B:126:PRO:HA	2.33	0.43
1:B:142:GLU:CD	1:B:142:GLU:H	2.26	0.43
1:A:292:ASN:HD22	1:A:292:ASN:HA	1.59	0.43
1:B:26:ALA:HB1	1:B:31:ILE:CD1	2.40	0.43
1:B:274:ILE:HA	1:B:274:ILE:HD12	1.60	0.43
1:B:157:LEU:HD12	1:B:218:ILE:HG22	1.99	0.43
1:B:146:PHE:HB2	1:B:262:SER:O	2.19	0.43
1:A:176:ILE:HA	1:A:186:PRO:HA	2.01	0.43
1:B:189:GLU:HG3	1:B:296:SER:CB	2.41	0.43
1:A:108:MET:HB2	1:A:109:PRO:HD3	1.99	0.43
1:B:69:ASP:O	1:B:72:ILE:HG22	2.18	0.43
1:A:265:LEU:HA	1:A:265:LEU:HD12	1.77	0.43
1:B:242:MET:HE2	1:B:242:MET:CA	2.41	0.43
1:B:89:PRO:O	1:B:90:GLY:C	2.62	0.42
1:B:93:ARG:O	1:B:97:VAL:HG23	2.18	0.42
1:B:93:ARG:O	1:B:93:ARG:HG2	2.19	0.42
1:A:265:LEU:HG	1:A:268:PHE:HB3	2.01	0.42
1:A:105:LYS:HD3	3:A:411:HOH:O	2.20	0.42
1:A:176:ILE:HD13	1:A:176:ILE:HG21	1.74	0.42
1:B:295:VAL:HG13	1:B:300:LEU:HB2	2.00	0.42
1:B:219:HIS:CE1	1:B:223:LYS:HD3	2.55	0.42
1:A:180:HIS:HE1	1:A:230:ILE:HD11	1.85	0.42
1:A:280:THR:HG21	1:A:287:VAL:HB	2.00	0.41
1:A:25:ALA:CB	1:A:245:VAL:HG21	2.50	0.41
1:B:283:ASN:HD22	1:B:285:GLN:H	1.68	0.41
1:B:44:ARG:CZ	1:B:48:GLU:OE2	2.67	0.41
1:A:89:PRO:O	1:A:90:GLY:C	2.62	0.41
1:A:204:LEU:HB3	1:A:205:PRO:HD2	2.02	0.41
1:B:288:ASN:HD22	1:B:290:THR:H	1.69	0.41
1:A:103:ILE:HD13	1:A:103:ILE:HG21	1.78	0.41
1:A:238:TYR:O	1:A:242:MET:HG2	2.20	0.41
1:A:107:ILE:CG2	1:A:111:LEU:HD22	2.50	0.41
1:B:37:LEU:O	1:B:66:GLY:CA	2.68	0.41
1:B:96:LEU:HD21	1:B:126:PRO:HG3	2.03	0.41
1:B:94:LEU:CD1	1:B:316:GLN:OE1	2.56	0.41
1:B:113:LYS:HB3	1:B:113:LYS:HE2	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LYS:HA	1:A:214:LYS:HD3	1.73	0.40
1:B:140:LEU:HA	1:B:141:PRO:HD3	1.91	0.40
1:B:18:VAL:HG22	1:B:237:ASN:HB3	2.02	0.40
1:A:59:TYR:N	1:A:60:PRO:HD3	2.36	0.40
1:A:120:TYR:O	1:A:145:ILE:HA	2.22	0.40
1:A:189:GLU:CG	1:A:296:SER:HB3	2.41	0.40

There are no symmetry-related clashes.

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	311/319 (98%)	298 (96%)	12 (4%)	1 (0%)	36	35
1	B	311/319 (98%)	298 (96%)	9 (3%)	4 (1%)	9	5
All	All	622/638 (98%)	596 (96%)	21 (3%)	5 (1%)	16	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	SER
1	B	234	GLY
1	A	292	ASN
1	B	316	GLN
1	B	292	ASN

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	254/259 (98%)	225 (89%)	29 (11%)	5	3
1	B	254/259 (98%)	228 (90%)	26 (10%)	7	4
All	All	508/518 (98%)	453 (89%)	55 (11%)	6	3

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	31	ILE
1	A	40	ILE
1	A	50	LEU
1	A	63	SER
1	A	64	ILE
1	A	71	GLU
1	A	72	ILE
1	A	74	ARG
1	A	111	LEU
1	A	112	VAL
1	A	114	VAL
1	A	122	LEU
1	A	140	LEU
1	A	211	ASP
1	A	217	GLU
1	A	230	ILE
1	A	233	LYS
1	A	237	ASN
1	A	242	MET
1	A	249	GLU
1	A	261	VAL
1	A	265	LEU
1	A	283	ASN
1	A	288	ASN
1	A	291	ILE
1	A	298	LYS
1	A	305	ARG
1	A	309	THR
1	B	31	ILE
1	B	33	ARG
1	B	37	LEU
1	B	42	LYS

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Mol	Chain	Res	Type
1	B	43	GLU
1	B	44	ARG
1	B	56	SER
1	B	74	ARG
1	B	92	SER
1	B	94	LEU
1	B	96	LEU
1	B	107	ILE
1	B	111	LEU
1	B	121	MET
1	B	214	LYS
1	B	223	LYS
1	B	242	MET
1	B	261	VAL
1	B	266	LYS
1	B	281	LEU
1	B	283	ASN
1	B	285	GLN
1	B	288	ASN
1	B	295	VAL
1	B	309	THR
1	B	316	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	102	ASN
1	A	125	ASN
1	A	164	GLN
1	A	173	HIS
1	A	231	ASN
1	A	256	ASN
1	A	283	ASN
1	A	288	ASN
1	A	292	ASN
1	B	28	GLN
1	B	87	GLN
1	B	102	ASN
1	B	117	ASN
1	B	125	ASN
1	B	163	GLN

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Mol	Chain	Res	Type
1	B	171	ASN
1	B	173	HIS
1	B	219	HIS
1	B	220	GLN
1	B	224	ASN
1	B	237	ASN
1	B	253	HIS
1	B	256	ASN
1	B	283	ASN
1	B	288	ASN
1	B	292	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	A	320	-	46,48,48	1.37	6 (13%)	64,73,73	2.43	14 (21%)
2	NAD	B	320	-	46,48,48	1.45	7 (15%)	64,73,73	2.53	13 (20%)

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	A	320	-	-	6/30/62/62	0/5/5/5
2	NAD	B	320	-	-	5/30/62/62	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	320	NAD	O4D-C1D	-4.27	1.35	1.40
2	A	320	NAD	O4B-C1B	-4.19	1.32	1.42
2	B	320	NAD	O4D-C1D	-4.00	1.35	1.40
2	B	320	NAD	O4B-C1B	-3.91	1.33	1.42
2	B	320	NAD	C2N-N1N	3.29	1.38	1.35
2	A	320	NAD	PA-O3	-3.16	1.56	1.59
2	B	320	NAD	C3N-C7N	3.11	1.55	1.50
2	B	320	NAD	PN-O3	2.67	1.62	1.59
2	A	320	NAD	C3N-C7N	2.50	1.54	1.50
2	B	320	NAD	C2A-N1A	2.37	1.38	1.33
2	B	320	NAD	C4N-C3N	2.11	1.42	1.39
2	A	320	NAD	C2A-N3A	-2.10	1.30	1.33
2	A	320	NAD	C4N-C3N	2.06	1.42	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	320	NAD	C3N-C7N-N7N	-10.00	105.41	117.74
2	A	320	NAD	C5N-C4N-C3N	-8.77	111.74	120.36
2	B	320	NAD	C5N-C4N-C3N	-8.66	111.86	120.36
2	A	320	NAD	C3N-C7N-N7N	-8.46	107.32	117.74
2	A	320	NAD	C6N-C5N-C4N	5.90	127.96	119.45
2	A	320	NAD	C4N-C3N-C7N	-5.65	105.69	121.06
2	B	320	NAD	O7N-C7N-N7N	5.51	130.57	122.62
2	B	320	NAD	C6N-C5N-C4N	5.36	127.17	119.45
2	A	320	NAD	C5N-C6N-N1N	-5.29	113.17	120.38
2	B	320	NAD	C2N-C3N-C4N	5.24	124.35	118.26
2	A	320	NAD	C2N-C3N-C4N	5.04	124.12	118.26
2	B	320	NAD	C4N-C3N-C7N	-4.77	108.06	121.06
2	A	320	NAD	C6N-N1N-C2N	4.63	125.82	121.88
2	B	320	NAD	C5N-C6N-N1N	-4.15	114.73	120.38
2	B	320	NAD	C2N-N1N-C1D	-4.14	110.00	119.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	320	NAD	O4B-C1B-C2B	-4.10	97.84	106.62
2	A	320	NAD	C2N-C3N-C7N	3.71	130.16	119.46
2	A	320	NAD	O7N-C7N-C3N	3.64	124.05	119.60
2	B	320	NAD	C6N-N1N-C2N	3.47	124.83	121.88
2	A	320	NAD	O4B-C1B-C2B	-3.21	99.75	106.62
2	A	320	NAD	O4B-C1B-N9A	3.16	114.16	108.09
2	B	320	NAD	C2N-C3N-C7N	2.81	127.58	119.46
2	B	320	NAD	C6N-N1N-C1D	2.77	125.16	119.73
2	B	320	NAD	O7N-C7N-C3N	2.36	122.48	119.60
2	A	320	NAD	O7N-C7N-N7N	2.35	126.00	122.62
2	A	320	NAD	C2N-N1N-C1D	-2.10	114.49	119.13
2	A	320	NAD	O3B-C3B-C4B	2.03	116.90	111.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	320	NAD	O4D-C1D-N1N-C6N
2	A	320	NAD	C2D-C1D-N1N-C6N
2	B	320	NAD	O4D-C1D-N1N-C2N
2	B	320	NAD	O4D-C1D-N1N-C6N
2	B	320	NAD	C2D-C1D-N1N-C2N
2	B	320	NAD	C2D-C1D-N1N-C6N
2	A	320	NAD	C2D-C1D-N1N-C2N
2	A	320	NAD	O4D-C1D-N1N-C2N
2	A	320	NAD	PN-O3-PA-O1A
2	A	320	NAD	PN-O3-PA-O2A
2	B	320	NAD	O4B-C4B-C5B-O5B

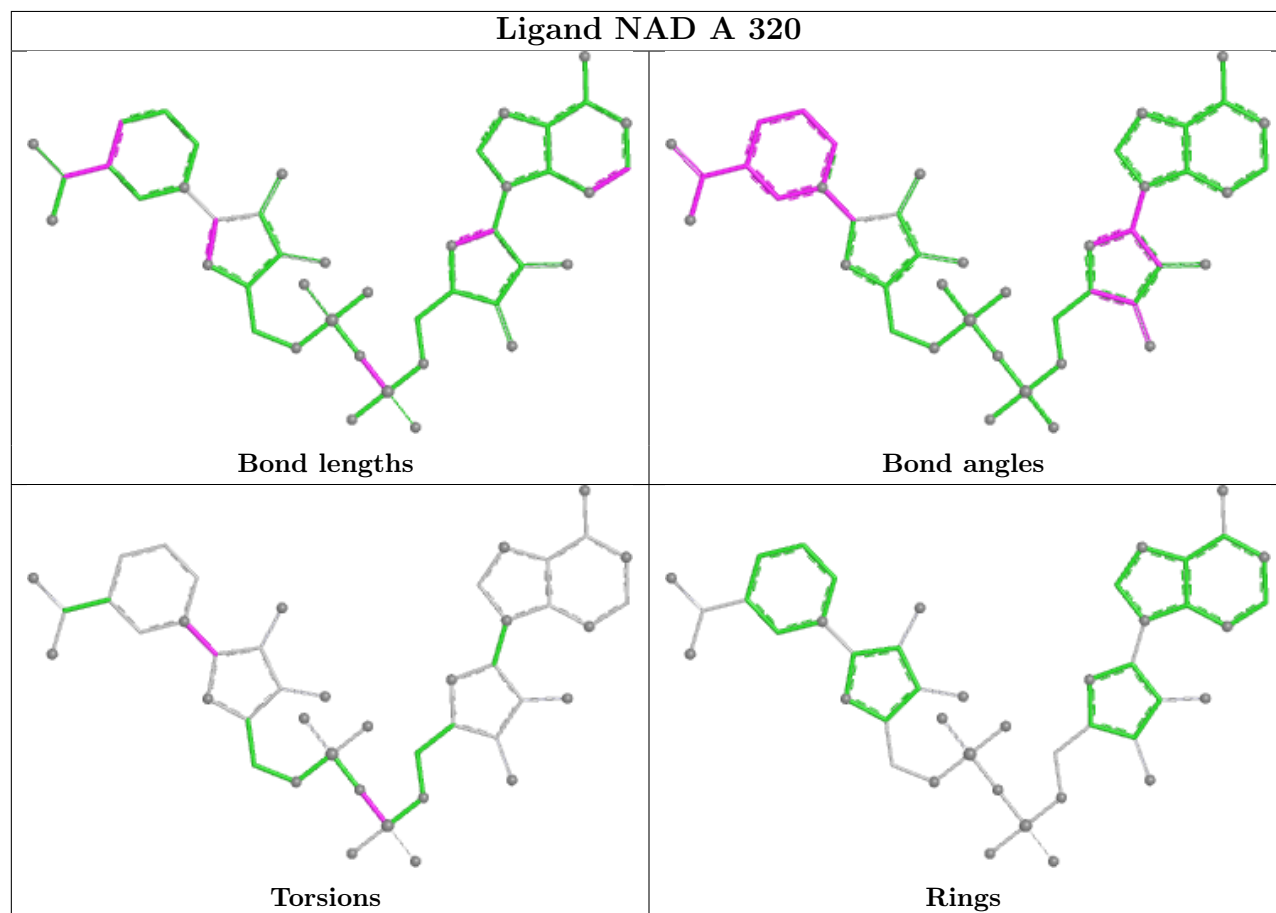
There are no ring outliers.

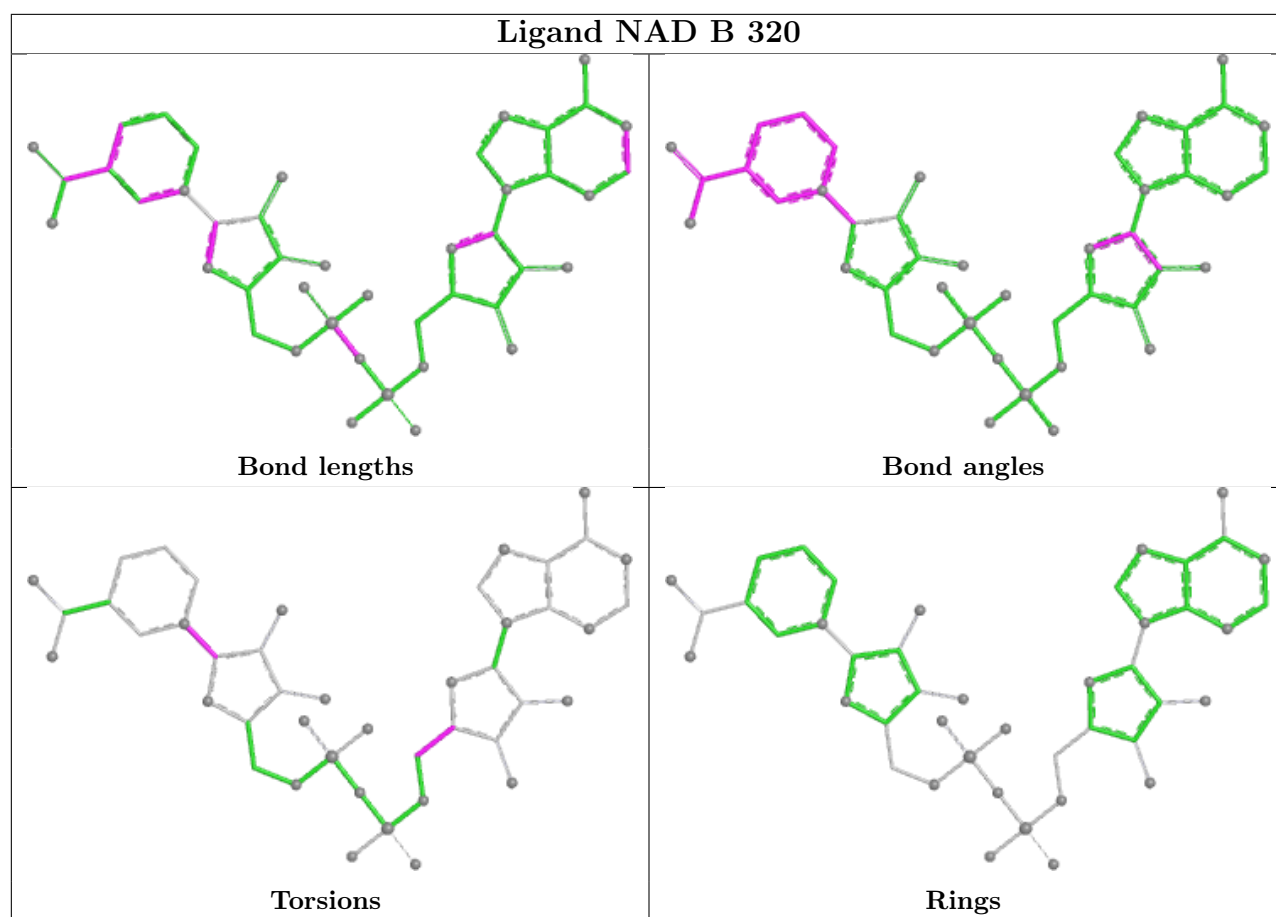
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	320	NAD	3	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	313/319 (98%)	-0.94	1 (0%) 90 89	9, 23, 44, 66	0
1	B	313/319 (98%)	-0.82	3 (0%) 79 79	8, 25, 51, 67	0
All	All	626/638 (98%)	-0.88	4 (0%) 85 85	8, 24, 48, 67	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	GLY	5.3
1	B	89	PRO	4.6
1	A	87	GLN	2.3
1	B	86	ARG	2.2

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.

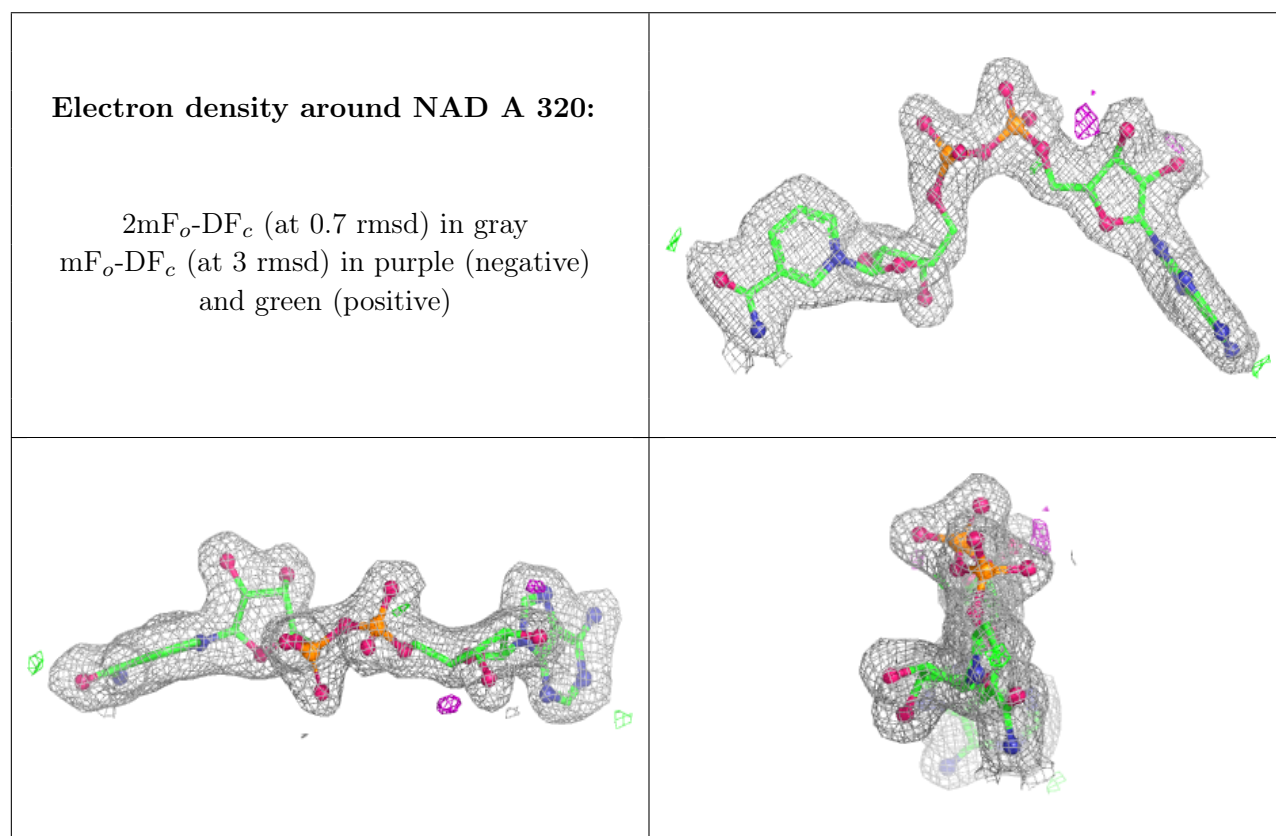
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	A	320	44/44	0.98	0.04	13,20,28,31	0

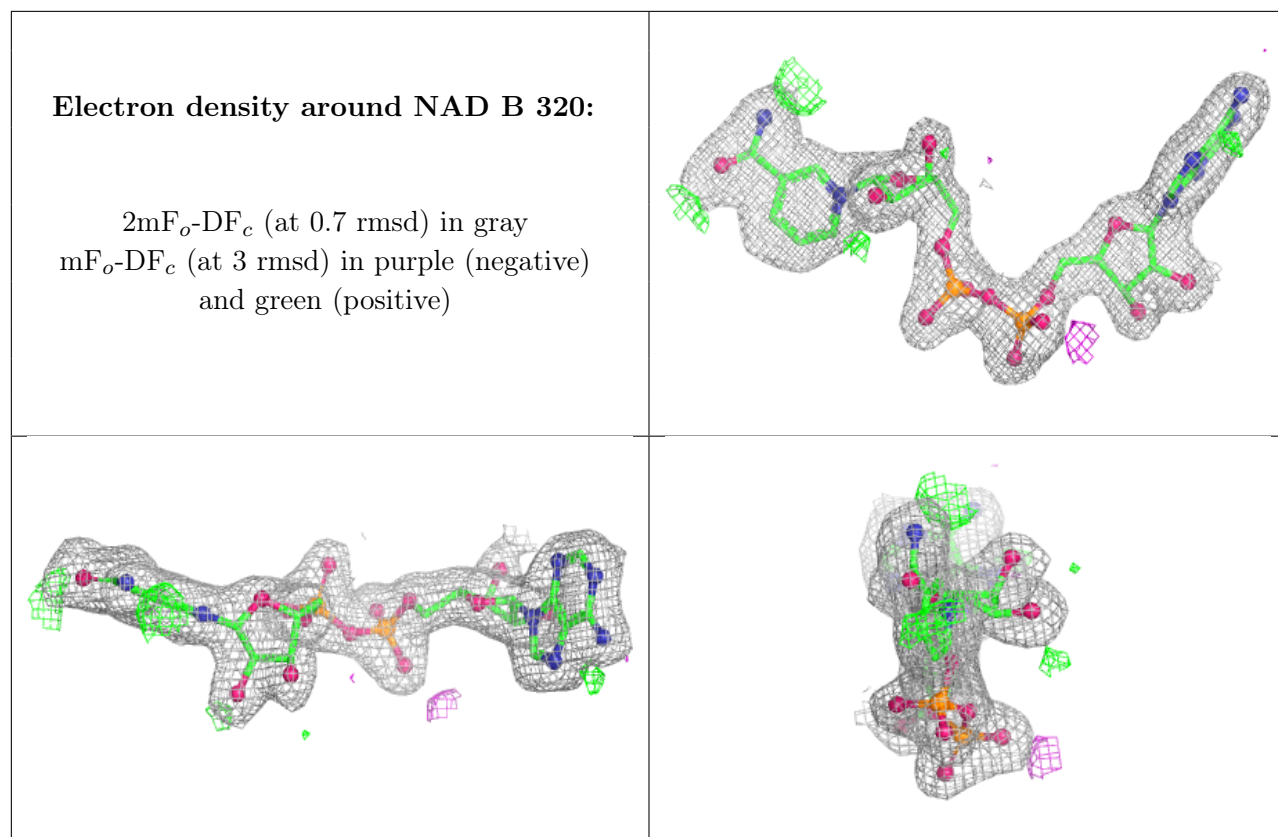
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	B	320	44/44	0.98	0.04	12,24,28,31	0

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 ⓘ

There are no such residues in this entry.