



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:22 PM UTC

PDB ID : 5MDH / pdb_00005mdh
Title : CRYSTAL STRUCTURE OF TERNARY COMPLEX OF PORCINE CYTOPLASMIC MALATE DEHYDROGENASE ALPHA-KETOMALONATE AND TNAD AT 2.4 ANGSTROMS RESOLUTION
Authors : Chapman, A.D.M.; Cortes, A.; Dafforn, T.R.; Clarke, A.R.; Brady, R.L.
Deposited on : 1998-10-08
Resolution : 2.40 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

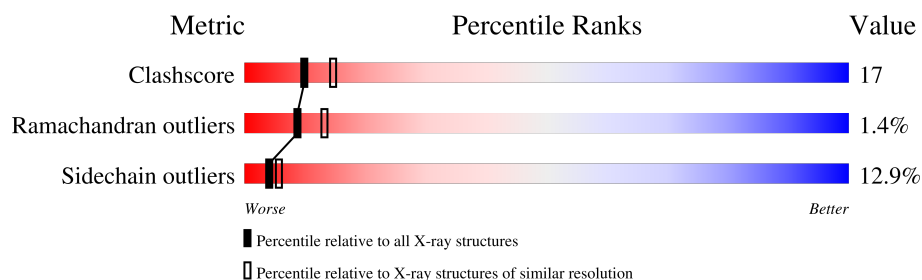
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	333	
1	B	333	

2 Entry composition [i](#)

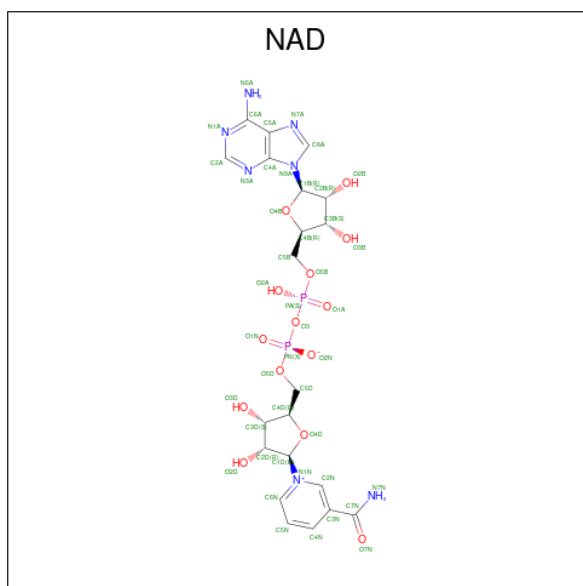
There are 4 unique types of molecules in this entry. The entry contains 5558 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MALATE DEHYDROGENASE.

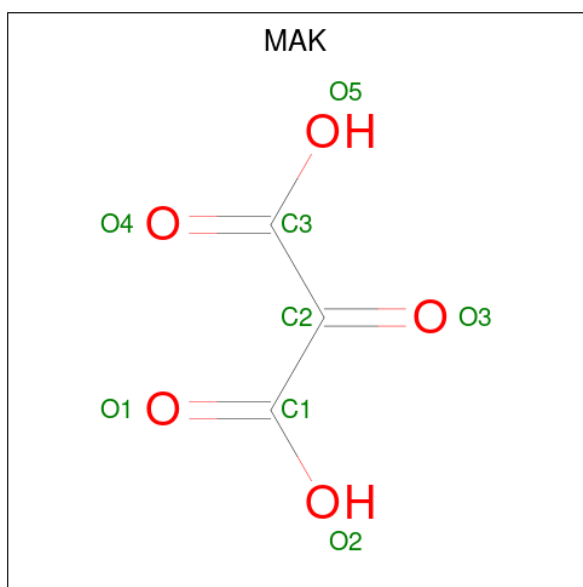
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2550	1623	427	487	13			
1	B	333	Total	C	N	O	S	121	0	0
			2550	1623	427	487	13			

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



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

- Molecule 3 is ALPHA-KETOMALONIC ACID (CCD ID: MAK) (formula: $C_3H_2O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	3	5		
3	B	1	Total	C	O	0	0
			8	3	5		

- Molecule 4 is water.

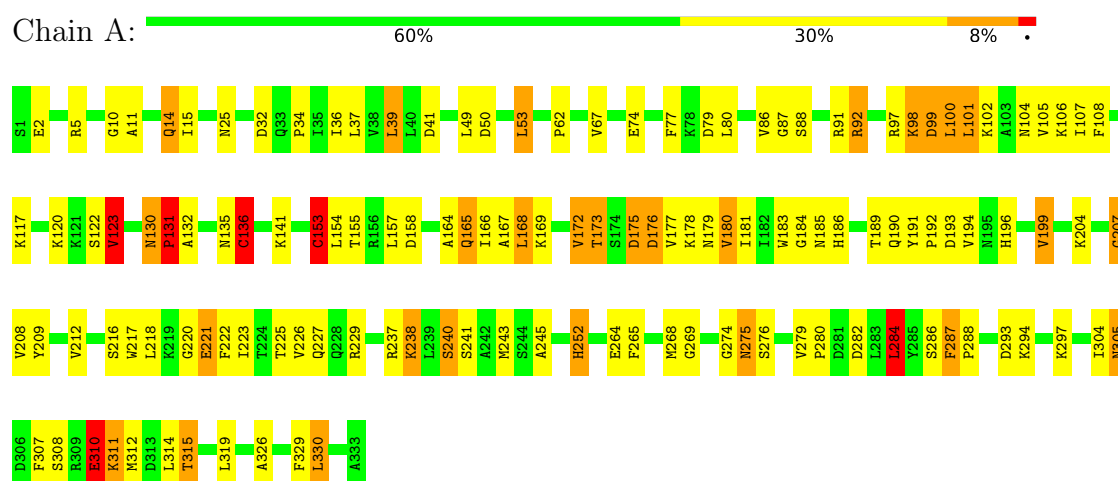
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	189	Total	O	0	0
			189	189		
4	B	165	Total	O	0	0
			165	165		

3 Residue-property plots [i](#)

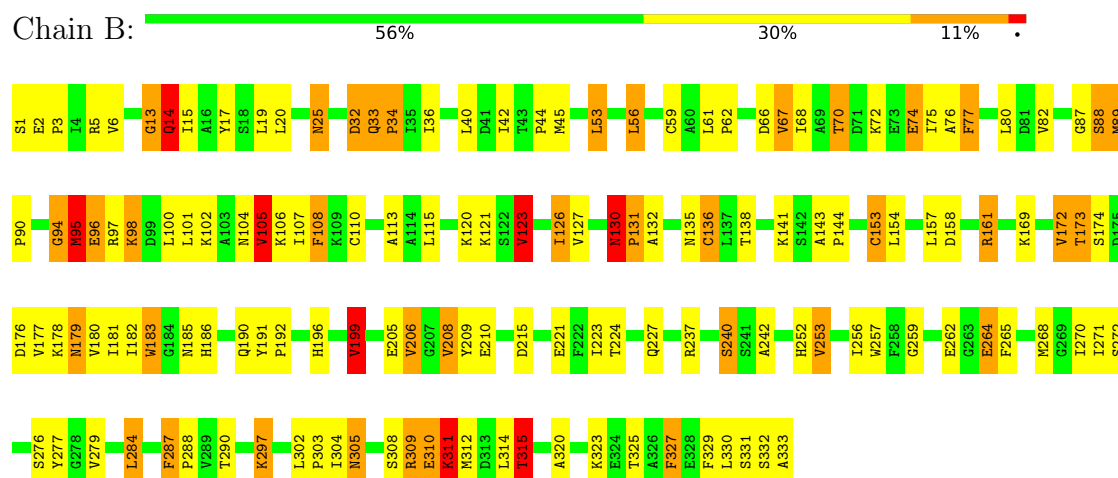
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: MALATE DEHYDROGENASE



• Molecule 1: MALATE DEHYDROGENASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.70Å 144.43Å 59.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40	Depositor
% Data completeness (in resolution range)	84.3 (15.00-2.40)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5558	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAK, 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	0.72	0/2592	1.87	63/3503 (1.8%)
1	B	1.42	4/2592 (0.2%)	2.15	74/3503 (2.1%)
All	All	1.13	4/5184 (0.1%)	2.02	137/7006 (2.0%)

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	2
1	B	0	7
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	GLU	C-N	-50.57	0.66	1.33
1	B	104	ASN	C-N	35.32	1.79	1.33
1	B	94	GLY	C-N	-8.39	1.22	1.33
1	B	90	PRO	C-N	-5.58	1.25	1.33

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	GLU	O-C-N	-45.63	63.88	123.19
1	B	94	GLY	O-C-N	-20.96	96.32	122.32
1	A	130	ASN	CA-C-O	-18.28	100.76	120.87
1	B	104	ASN	CA-C-N	-16.55	96.03	121.02
1	B	104	ASN	C-N-CA	-16.55	96.03	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	MET	CA-C-N	-14.47	100.10	122.81
1	B	95	MET	C-N-CA	-14.47	100.10	122.81
1	B	98	LYS	CG-CD-CE	-13.62	79.97	111.30
1	B	95	MET	O-C-N	-13.17	105.07	122.59
1	B	89	MET	O-C-N	-12.65	105.39	121.70
1	B	130	ASN	CA-C-O	-11.16	105.20	121.27
1	A	99	ASP	N-CA-CB	10.94	126.58	110.06
1	B	131	PRO	CA-N-CD	-10.86	96.80	112.00
1	B	96	GLU	CA-C-O	10.66	133.15	121.11
1	B	96	GLU	CA-C-N	10.54	143.07	122.61
1	B	96	GLU	C-N-CA	10.54	143.07	122.61
1	B	180	VAL	N-CA-C	-9.53	99.66	110.05
1	B	13	GLY	N-CA-C	9.14	134.85	113.18
1	B	130	ASN	CA-C-N	9.11	131.23	119.84
1	B	130	ASN	C-N-CA	9.11	131.23	119.84
1	A	92	ARG	CD-NE-CZ	9.11	137.15	124.40
1	A	97	ARG	CD-NE-CZ	9.05	137.07	124.40
1	A	176	ASP	CA-CB-CG	9.03	121.63	112.60
1	A	123	VAL	CB-CA-C	-8.99	96.67	111.51
1	A	98	LYS	CA-C-O	-8.82	111.11	120.63
1	A	99	ASP	N-CA-C	-8.81	96.28	110.20
1	B	123	VAL	CB-CA-C	-8.58	97.36	111.51
1	A	5	ARG	CA-C-O	8.57	129.46	120.54
1	B	131	PRO	N-CA-CB	8.35	112.01	103.25
1	A	123	VAL	CA-C-O	-8.20	111.68	121.28
1	B	89	MET	CA-C-N	7.87	128.31	120.52
1	B	89	MET	C-N-CA	7.87	128.31	120.52
1	B	199	VAL	CB-CA-C	-7.84	98.43	110.50
1	A	175	ASP	CA-CB-CG	7.73	120.33	112.60
1	A	92	ARG	NE-CZ-NH1	7.52	129.02	121.50
1	A	41	ASP	CA-CB-CG	-7.49	105.11	112.60
1	A	275	ASN	CA-CB-CG	7.47	120.07	112.60
1	A	154	LEU	N-CA-C	7.31	120.01	108.67
1	B	33	GLN	CA-C-O	7.29	125.49	119.36
1	B	320	ALA	CA-C-N	7.29	129.91	120.44
1	B	320	ALA	C-N-CA	7.29	129.91	120.44
1	A	14	GLN	N-CA-C	7.25	118.83	111.07
1	B	309	ARG	CD-NE-CZ	7.20	134.49	124.40
1	B	136	CYS	CA-CB-SG	7.18	130.91	114.40
1	B	90	PRO	N-CA-C	7.03	121.61	111.13
1	A	284	LEU	CA-C-O	7.03	129.75	121.11
1	B	161	ARG	CD-NE-CZ	-6.78	114.90	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	CYS	CA-CB-SG	6.78	129.99	114.40
1	A	131	PRO	CA-N-CD	-6.76	102.54	112.00
1	A	180	VAL	N-CA-C	-6.74	100.25	109.55
1	B	182	ILE	N-CA-CB	6.71	120.12	111.67
1	B	253	VAL	CA-C-O	-6.67	113.78	120.85
1	A	5	ARG	CB-CA-C	6.52	121.22	110.78
1	A	238	LYS	CA-C-N	6.48	133.31	121.85
1	A	238	LYS	C-N-CA	6.48	133.31	121.85
1	B	256	ILE	N-CA-CB	6.47	118.12	110.55
1	A	252	HIS	CA-CB-CG	6.42	120.22	113.80
1	B	104	ASN	O-C-N	6.39	128.78	122.19
1	A	284	LEU	CB-CA-C	6.38	122.26	111.41
1	B	205	GLU	CA-C-O	-6.38	113.47	120.81
1	B	290	THR	N-CA-C	-6.33	99.60	109.72
1	A	241	SER	CA-C-O	-6.25	114.75	121.56
1	B	13	GLY	O-C-N	-6.21	114.62	122.70
1	B	25	ASN	CB-CA-C	-6.21	97.71	110.38
1	B	242	ALA	N-CA-C	6.20	118.12	111.36
1	B	108	PHE	CA-CB-CG	-6.19	107.61	113.80
1	A	130	ASN	CA-CB-CG	-6.14	106.46	112.60
1	A	130	ASN	CA-C-N	6.14	127.51	119.84
1	A	130	ASN	C-N-CA	6.14	127.51	119.84
1	B	209	TYR	CA-C-N	6.12	128.48	120.28
1	B	209	TYR	C-N-CA	6.12	128.48	120.28
1	B	287	PHE	CA-CB-CG	6.08	119.88	113.80
1	B	199	VAL	N-CA-CB	6.04	121.35	111.44
1	A	107	ILE	CB-CA-C	-6.00	104.04	112.14
1	A	184	GLY	N-CA-C	5.97	121.09	110.95
1	A	108	PHE	CA-CB-CG	-5.95	107.85	113.80
1	A	36	ILE	N-CA-CB	5.93	118.83	111.41
1	B	215	ASP	CA-CB-CG	5.88	118.48	112.60
1	B	315	THR	N-CA-CB	5.88	118.86	110.16
1	A	123	VAL	O-C-N	5.86	129.02	122.75
1	B	206	VAL	N-CA-C	5.81	121.42	109.34
1	B	169	LYS	O-C-N	5.77	128.01	122.07
1	A	310	GLU	O-C-N	-5.76	116.06	122.86
1	A	183	TRP	CA-CB-CG	5.74	124.50	113.60
1	B	161	ARG	CA-C-N	5.73	127.89	120.44
1	B	161	ARG	C-N-CA	5.73	127.89	120.44
1	A	53	LEU	N-CA-CB	5.71	118.52	110.12
1	A	193	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	25	ASN	CA-CB-CG	5.64	118.24	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	LEU	N-CA-C	5.63	117.47	108.41
1	B	70	THR	CB-CA-C	-5.62	98.36	110.45
1	B	259	GLY	CA-C-O	5.61	126.83	122.29
1	A	98	LYS	CA-CB-CG	5.57	125.23	114.10
1	A	225	THR	CA-CB-OG1	-5.54	101.29	109.60
1	B	257	TRP	CA-C-O	-5.53	115.01	120.82
1	B	208	VAL	CA-C-O	-5.52	114.50	120.47
1	A	97	ARG	CA-C-N	5.52	127.94	120.38
1	A	97	ARG	C-N-CA	5.52	127.94	120.38
1	A	153	CYS	N-CA-CB	5.52	121.16	111.55
1	A	225	THR	O-C-N	5.51	127.76	122.03
1	B	172	VAL	N-CA-CB	-5.50	102.15	111.23
1	B	20	LEU	N-CA-C	5.49	117.27	111.28
1	B	5	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	A	130	ASN	N-CA-C	5.47	118.08	110.20
1	B	272	SER	N-CA-C	5.45	119.78	113.18
1	B	126	ILE	CA-C-O	-5.42	114.72	120.53
1	B	264	GLU	N-CA-C	5.42	118.24	109.40
1	A	74	GLU	CB-CA-C	-5.42	102.13	110.81
1	B	105	VAL	CA-C-O	5.39	125.46	119.42
1	A	207	GLY	N-CA-C	-5.37	105.21	112.14
1	B	34	PRO	CB-CA-C	5.34	118.31	111.21
1	B	67	VAL	N-CA-CB	5.33	119.30	111.52
1	A	183	TRP	CA-C-N	5.31	126.42	120.42
1	A	183	TRP	C-N-CA	5.31	126.42	120.42
1	A	50	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	229	ARG	CD-NE-CZ	5.27	131.78	124.40
1	B	20	LEU	CA-C-O	-5.21	115.03	120.55
1	B	179	ASN	N-CA-C	5.21	118.77	111.74
1	A	135	ASN	CA-C-N	5.21	128.03	120.79
1	A	135	ASN	C-N-CA	5.21	128.03	120.79
1	A	310	GLU	N-CA-C	-5.20	103.17	110.50
1	B	183	TRP	CA-CB-CG	5.20	123.48	113.60
1	B	311	LYS	N-CA-C	-5.18	99.77	110.80
1	A	287	PHE	CA-CB-CG	5.17	118.97	113.80
1	B	77	PHE	N-CA-C	5.17	119.31	113.15
1	A	196	HIS	CA-CB-CG	-5.15	108.65	113.80
1	B	279	VAL	CA-C-O	5.14	122.53	119.19
1	A	307	PHE	CA-C-O	-5.14	115.08	120.63
1	B	90	PRO	CA-C-N	5.09	132.90	123.32
1	B	90	PRO	C-N-CA	5.09	132.90	123.32
1	A	79	ASP	CA-CB-CG	5.08	117.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ILE	N-CA-CB	5.08	117.07	110.57
1	B	327	PHE	N-CA-C	5.08	117.71	111.82
1	A	123	VAL	N-CA-CB	5.03	118.23	110.14
1	B	19	LEU	N-CA-C	5.03	119.54	113.41
1	A	186	HIS	CA-CB-CG	-5.01	108.79	113.80
1	A	165	GLN	CA-C-O	-5.01	115.11	120.42

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	ASN	Peptide,Mainchain
1	B	130	ASN	Peptide,Mainchain
1	B	89	MET	Mainchain
1	B	94	GLY	Mainchain
1	B	95	MET	Peptide,Mainchain
1	B	96	GLU	Mainchain

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	2550	0	2615	87	0
1	B	2550	0	2610	94	0
2	A	44	0	26	3	0
2	B	44	0	26	4	0
3	A	8	0	2	1	0
3	B	8	0	1	2	0
4	A	189	0	0	10	0
4	B	165	0	0	12	0
All	All	5558	0	5280	179	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 (179) 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:B:136:CYS:SG	4:B:499:HOH:O	2.07	1.12
1:A:14:GLN:HE22	1:A:237:ARG:NH2	1.56	1.03
1:B:304:ILE:HD12	1:B:312:MET:HE1	1.42	1.01
1:A:153:CYS:SG	4:A:521:HOH:O	2.21	0.98
1:B:153:CYS:SG	4:B:500:HOH:O	2.21	0.97
1:A:14:GLN:HE22	1:A:237:ARG:HH22	0.92	0.92
1:A:14:GLN:NE2	1:A:237:ARG:HH22	1.67	0.90
1:A:304:ILE:HD12	1:A:312:MET:HE1	1.52	0.89
1:A:167:ALA:HA	1:A:172:VAL:HG12	1.53	0.89
1:B:14:GLN:HG2	1:B:240:SER:HB2	1.57	0.87
1:B:310:GLU:O	1:B:311:LYS:HB2	1.76	0.85
1:B:77:PHE:HA	1:B:80:LEU:HD11	1.59	0.85
1:A:185:ASN:H	1:A:315:THR:HG21	1.46	0.80
1:B:186:HIS:HE1	3:B:335:MAK:O5	1.64	0.80
1:A:243:MET:HE1	1:B:56:LEU:HD13	1.64	0.78
1:A:305:ASN:ND2	1:A:308:SER:H	1.81	0.78
1:B:158:ASP:HB3	1:B:190:GLN:HE22	1.48	0.78
1:A:153:CYS:SG	1:A:284:LEU:HD22	2.23	0.78
1:B:153:CYS:SG	1:B:284:LEU:HD22	2.26	0.76
1:B:126:ILE:HD12	1:B:252:HIS:CE1	2.21	0.76
1:A:237:ARG:O	1:A:238:LYS:HB2	1.88	0.74
1:A:132:ALA:O	1:A:136:CYS:HB2	1.87	0.74
1:A:308:SER:HB3	1:A:312:MET:HE3	1.71	0.73
1:A:15:ILE:HD12	2:A:334:NAD:H51N	1.71	0.72
1:A:243:MET:HE3	1:B:59:CYS:SG	2.31	0.69
1:A:305:ASN:HD22	1:A:308:SER:H	1.40	0.69
1:A:310:GLU:O	1:A:311:LYS:HB2	1.92	0.68
1:A:185:ASN:H	1:A:315:THR:CG2	2.08	0.66
1:B:186:HIS:CE1	3:B:335:MAK:O5	2.48	0.66
1:B:323:LYS:HG2	1:B:327:PHE:CE2	2.31	0.66
1:B:120:LYS:O	1:B:123:VAL:HG22	1.95	0.65
1:A:99:ASP:OD1	1:A:100:LEU:N	2.30	0.64
1:B:223:ILE:O	1:B:227:GLN:HG3	1.97	0.64
1:B:14:GLN:HE21	1:B:240:SER:H	1.43	0.64
1:A:14:GLN:NE2	1:A:237:ARG:NH2	2.36	0.63
1:B:130:ASN:HD22	1:B:132:ALA:H	1.46	0.63
1:A:155:THR:HG21	1:A:286:SER:HB2	1.82	0.62
1:A:153:CYS:SG	1:A:284:LEU:CD2	2.87	0.62
1:B:308:SER:HB3	1:B:312:MET:HE3	1.80	0.62
1:A:310:GLU:O	1:A:311:LYS:CB	2.47	0.62
1:A:157:LEU:HD22	1:A:245:ALA:HA	1.80	0.61
1:B:181:ILE:HG12	1:B:288:PRO:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:CYS:SG	1:B:284:LEU:HD22	2.41	0.60
1:B:183:TRP:CE2	1:B:312:MET:HE2	2.37	0.59
1:B:77:PHE:HA	1:B:80:LEU:CD1	2.31	0.59
1:B:130:ASN:HD21	1:B:186:HIS:HD2	1.50	0.59
1:B:331:SER:HB3	4:B:495:HOH:O	2.02	0.59
1:B:179:ASN:HD21	1:B:264:GLU:HA	1.68	0.58
1:A:101:LEU:HD11	1:A:326:ALA:HB2	1.86	0.57
1:B:332:SER:O	1:B:333:ALA:HB3	2.03	0.57
1:A:173:THR:HB	1:A:176:ASP:OD2	2.05	0.56
1:B:153:CYS:SG	1:B:284:LEU:CD2	2.93	0.56
1:A:269:GLY:HA2	1:A:286:SER:HA	1.86	0.56
1:B:77:PHE:CD1	1:B:115:LEU:HG	2.40	0.56
1:A:179:ASN:HD21	1:A:264:GLU:HA	1.70	0.56
1:A:158:ASP:HB3	1:A:190:GLN:NE2	2.21	0.55
1:B:40:LEU:HD13	1:B:76:ALA:HB2	1.87	0.55
1:B:179:ASN:ND2	1:B:265:PHE:H	2.05	0.54
1:A:164:ALA:O	1:A:168:LEU:HD12	2.07	0.54
1:B:132:ALA:O	1:B:136:CYS:HB2	2.06	0.54
1:B:87:GLY:O	1:B:88:SER:HB3	2.06	0.53
1:A:101:LEU:HD22	1:A:131:PRO:HG3	1.91	0.53
1:A:310:GLU:OE2	1:A:314:LEU:HD11	2.09	0.53
1:A:53:LEU:HD22	1:A:67:VAL:HG11	1.90	0.52
1:B:305:ASN:ND2	1:B:308:SER:H	2.08	0.52
1:A:207:GLY:HA3	4:A:468:HOH:O	2.10	0.52
1:A:240:SER:HB2	4:A:412:HOH:O	2.09	0.52
1:B:323:LYS:HE2	1:B:327:PHE:HE2	1.75	0.52
1:A:179:ASN:ND2	1:A:265:PHE:H	2.08	0.52
1:B:177:VAL:HG22	1:B:199:VAL:HG13	1.92	0.52
2:B:334:NAD:H2B	4:B:421:HOH:O	2.09	0.52
1:B:45:MET:HE2	4:B:451:HOH:O	2.10	0.51
1:B:196:HIS:HE1	4:B:366:HOH:O	1.93	0.51
1:A:11:ALA:HB1	1:A:39:LEU:HG	1.92	0.51
1:A:217:TRP:CE3	1:A:218:LEU:HD23	2.46	0.51
1:A:153:CYS:CB	4:A:521:HOH:O	2.54	0.51
1:B:36:ILE:HG23	1:B:66:ASP:HB3	1.93	0.51
1:B:287:PHE:HB3	1:B:288:PRO:HD2	1.93	0.51
1:B:126:ILE:HD12	1:B:252:HIS:HE1	1.73	0.50
1:A:181:ILE:HG12	1:A:288:PRO:HB3	1.92	0.50
1:A:120:LYS:O	1:A:123:VAL:HG22	2.12	0.50
1:B:305:ASN:C	1:B:305:ASN:HD22	2.19	0.50
1:B:53:LEU:HD13	1:B:67:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:THR:HG23	4:B:363:HOH:O	2.10	0.49
1:B:206:VAL:O	1:B:210:GLU:OE1	2.30	0.49
1:A:100:LEU:O	1:A:104:ASN:HB2	2.12	0.49
1:A:217:TRP:NE1	1:A:221:GLU:OE1	2.44	0.49
1:B:126:ILE:HG13	1:B:253:VAL:HG22	1.95	0.48
1:A:243:MET:CE	1:B:56:LEU:HD13	2.40	0.48
1:B:183:TRP:NE1	1:B:312:MET:HE2	2.28	0.48
1:A:172:VAL:HG22	1:A:176:ASP:OD2	2.13	0.48
1:B:185:ASN:H	1:B:315:THR:HG21	1.78	0.48
1:A:99:ASP:O	1:A:100:LEU:CB	2.62	0.47
1:B:17:TYR:HB2	4:B:493:HOH:O	2.14	0.47
1:A:141:LYS:NZ	1:A:282:ASP:OD1	2.47	0.47
1:B:6:VAL:HG22	1:B:82:VAL:HB	1.96	0.47
1:A:177:VAL:HG22	1:A:199:VAL:HG12	1.95	0.47
1:A:158:ASP:HB3	1:A:190:GLN:HE22	1.80	0.47
1:A:208:VAL:O	1:A:212:VAL:HG23	2.14	0.47
1:A:153:CYS:HB2	4:A:521:HOH:O	2.14	0.47
1:A:102:LYS:HD3	1:A:329:PHE:CD1	2.50	0.47
1:A:10:GLY:HA2	2:A:334:NAD:H1B	1.96	0.46
1:B:191:TYR:CD1	1:B:311:LYS:HG2	2.50	0.46
1:B:173:THR:HB	1:B:176:ASP:OD2	2.16	0.46
1:A:179:ASN:HD21	1:A:265:PHE:H	1.61	0.46
1:A:189:THR:OG1	1:A:315:THR:HG23	2.16	0.46
1:A:319:LEU:HD22	4:A:385:HOH:O	2.16	0.46
1:B:61:LEU:HA	1:B:62:PRO:HD2	1.85	0.46
1:B:210:GLU:HB2	4:B:349:HOH:O	2.15	0.46
1:B:153:CYS:CB	4:B:500:HOH:O	2.61	0.46
1:B:179:ASN:HD21	1:B:265:PHE:H	1.63	0.46
1:B:74:GLU:H	1:B:74:GLU:HG3	1.63	0.45
1:A:243:MET:HE1	1:B:56:LEU:CD1	2.42	0.45
1:A:293:ASP:O	1:A:294:LYS:HB2	2.16	0.45
1:B:141:LYS:HE3	1:B:327:PHE:CZ	2.52	0.45
1:B:157:LEU:O	1:B:161:ARG:HG3	2.17	0.45
1:A:173:THR:HG22	1:A:175:ASP:N	2.32	0.45
1:B:329:PHE:O	1:B:332:SER:HB2	2.17	0.45
1:A:136:CYS:SG	1:A:284:LEU:HD22	2.58	0.44
1:A:287:PHE:HB3	1:A:288:PRO:HD2	1.99	0.44
1:A:252:HIS:NE2	1:A:268:MET:HE3	2.31	0.44
1:A:32:ASP:O	1:A:34:PRO:HD3	2.17	0.44
1:A:190:GLN:NE2	1:A:226:VAL:HG12	2.32	0.44
1:B:70:THR:HB	1:B:72:LYS:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LYS:HB2	1:B:75:ILE:HG12	2.00	0.44
1:A:190:GLN:HG2	1:A:227:GLN:HG2	1.98	0.44
1:A:77:PHE:HA	1:A:80:LEU:HD11	1.99	0.44
1:B:15:ILE:HD12	2:B:334:NAD:H51N	1.99	0.44
1:B:70:THR:HG21	1:B:75:ILE:HB	1.99	0.44
1:B:15:ILE:HD11	2:B:334:NAD:C6N	2.48	0.43
1:B:179:ASN:HB3	1:B:265:PHE:CZ	2.53	0.43
1:B:332:SER:O	1:B:333:ALA:CB	2.66	0.43
1:A:86:VAL:O	1:A:87:GLY:C	2.59	0.43
1:A:217:TRP:HE3	1:A:218:LEU:HD23	1.83	0.43
1:B:127:VAL:HB	1:B:153:CYS:HB3	2.00	0.43
1:B:224:THR:HA	1:B:227:GLN:HE21	1.83	0.43
1:A:209:TYR:HD1	4:A:376:HOH:O	2.02	0.43
1:A:274:GLY:O	1:A:275:ASN:C	2.60	0.43
2:A:334:NAD:C4N	3:A:335:MAK:C3	2.96	0.43
1:B:110:CYS:O	1:B:113:ALA:HB3	2.19	0.43
1:B:53:LEU:HD13	1:B:67:VAL:CG1	2.49	0.43
1:B:105:VAL:HG22	1:B:138:THR:OG1	2.18	0.42
1:B:206:VAL:HG22	1:B:210:GLU:CD	2.44	0.42
1:A:62:PRO:HD2	4:A:351:HOH:O	2.18	0.42
1:A:155:THR:HG21	1:A:286:SER:CB	2.49	0.42
1:B:42:ILE:HG13	1:B:44:PRO:HD2	2.00	0.42
1:B:143:ALA:N	1:B:144:PRO:HD3	2.33	0.42
1:B:277:TYR:O	1:B:309:ARG:NH2	2.46	0.42
1:A:237:ARG:NH1	4:A:362:HOH:O	2.52	0.42
1:B:136:CYS:SG	1:B:284:LEU:CD2	3.07	0.42
1:B:70:THR:HG21	1:B:75:ILE:CB	2.49	0.42
1:A:212:VAL:HG21	1:A:218:LEU:HD21	2.01	0.42
1:A:305:ASN:HD22	1:A:305:ASN:C	2.27	0.42
1:B:191:TYR:HA	1:B:192:PRO:HD3	1.88	0.42
1:A:209:TYR:CD2	1:A:218:LEU:HD12	2.55	0.42
1:A:311:LYS:H	1:A:314:LEU:HG	1.84	0.42
1:B:32:ASP:O	1:B:34:PRO:HD3	2.20	0.42
1:B:33:GLN:HA	1:B:34:PRO:HD3	1.91	0.42
1:B:53:LEU:CD1	1:B:67:VAL:HB	2.49	0.42
1:B:108:PHE:CD2	1:B:135:ASN:HB3	2.55	0.42
1:B:237:ARG:HH11	1:B:237:ARG:HD3	1.70	0.41
1:B:108:PHE:CG	1:B:135:ASN:HB3	2.55	0.41
1:B:2:GLU:HB3	1:B:3:PRO:HD2	2.02	0.41
1:B:13:GLY:O	2:B:334:NAD:O2N	2.38	0.41
1:A:91:ARG:N	1:A:100:LEU:HD11	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LYS:HZ1	1:A:217:TRP:CD1	2.39	0.41
1:A:180:VAL:HG12	1:A:194:VAL:HG12	2.02	0.41
1:A:240:SER:HB3	4:A:479:HOH:O	2.21	0.41
1:A:329:PHE:CD2	1:A:330:LEU:HD13	2.55	0.41
1:B:153:CYS:HB2	4:B:500:HOH:O	2.21	0.41
1:B:297:LYS:HG2	4:B:371:HOH:O	2.21	0.41
1:A:216:SER:O	1:A:220:GLY:N	2.54	0.41
1:B:127:VAL:HG21	1:B:136:CYS:HA	2.02	0.41
1:A:191:TYR:HA	1:A:192:PRO:HD3	1.88	0.40
1:A:329:PHE:HD2	1:A:330:LEU:HD13	1.86	0.40
1:A:279:VAL:O	1:A:280:PRO:C	2.64	0.40
1:B:302:LEU:HA	1:B:303:PRO:HD3	1.93	0.40
1:B:53:LEU:O	1:B:53:LEU:HD12	2.22	0.40
1:A:165:GLN:HB2	1:A:222:PHE:HE1	1.85	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	331/333 (99%)	310 (94%)	18 (5%)	3 (1%)	14	22
1	B	331/333 (99%)	305 (92%)	20 (6%)	6 (2%)	6	9
All	All	662/666 (99%)	615 (93%)	38 (6%)	9 (1%)	9	13

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	LYS
1	B	95	MET
1	B	311	LYS
1	A	100	LEU

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Mol	Chain	Res	Type
1	B	100	LEU
1	B	88	SER
1	B	131	PRO
1	B	14	GLN
1	A	131	PRO

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	280/280 (100%)	249 (89%)	31 (11%)	6	9
1	B	280/280 (100%)	239 (85%)	41 (15%)	3	4
All	All	560/560 (100%)	488 (87%)	72 (13%)	4	6

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	37	LEU
1	A	39	LEU
1	A	49	LEU
1	A	88	SER
1	A	92	ARG
1	A	98	LYS
1	A	101	LEU
1	A	105	VAL
1	A	106	LYS
1	A	117	LYS
1	A	122	SER
1	A	123	VAL
1	A	136	CYS
1	A	153	CYS
1	A	168	LEU
1	A	172	VAL
1	A	173	THR

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Mol	Chain	Res	Type
1	A	178	LYS
1	A	199	VAL
1	A	204	LYS
1	A	221	GLU
1	A	223	ILE
1	A	240	SER
1	A	276	SER
1	A	284	LEU
1	A	297	LYS
1	A	305	ASN
1	A	310	GLU
1	A	315	THR
1	A	330	LEU
1	B	1	SER
1	B	14	GLN
1	B	25	ASN
1	B	32	ASP
1	B	53	LEU
1	B	56	LEU
1	B	68	ILE
1	B	74	GLU
1	B	95	MET
1	B	97	ARG
1	B	98	LYS
1	B	101	LEU
1	B	102	LYS
1	B	105	VAL
1	B	106	LYS
1	B	107	ILE
1	B	121	LYS
1	B	123	VAL
1	B	153	CYS
1	B	172	VAL
1	B	173	THR
1	B	174	SER
1	B	178	LYS
1	B	199	VAL
1	B	208	VAL
1	B	221	GLU
1	B	240	SER
1	B	262	GLU
1	B	268	MET

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Mol	Chain	Res	Type
1	B	270	ILE
1	B	271	ILE
1	B	276	SER
1	B	284	LEU
1	B	297	LYS
1	B	305	ASN
1	B	310	GLU
1	B	311	LYS
1	B	314	LEU
1	B	315	THR
1	B	325	THR
1	B	330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	135	ASN
1	A	150	ASN
1	A	179	ASN
1	A	190	GLN
1	A	305	ASN
1	B	14	GLN
1	B	25	ASN
1	B	130	ASN
1	B	135	ASN
1	B	150	ASN
1	B	179	ASN
1	B	190	GLN
1	B	227	GLN
1	B	252	HIS
1	B	305	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 [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	334	-	46,48,48	1.24	7 (15%)	64,73,73	1.90	11 (17%)
3	MAK	B	335	-	7,7,7	1.69	2 (28%)	9,9,9	0.58	0
2	NAD	A	334	-	46,48,48	1.06	4 (8%)	64,73,73	1.88	10 (15%)
3	MAK	A	335	-	7,7,7	1.70	2 (28%)	9,9,9	0.59	0

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	334	-	-	5/30/62/62	0/5/5/5
3	MAK	B	335	-	-	0/8/8/8	-
2	NAD	A	334	-	-	13/30/62/62	0/5/5/5
3	MAK	A	335	-	-	0/8/8/8	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	334	NAD	C3N-C7N	3.87	1.56	1.50
2	B	334	NAD	C3N-C7N	3.83	1.56	1.50
2	A	334	NAD	C6N-N1N	2.82	1.41	1.35
2	B	334	NAD	PN-O3	2.72	1.62	1.59
2	B	334	NAD	C6N-N1N	2.66	1.41	1.35
3	B	335	MAK	O5-C3	2.64	1.37	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	335	MAK	O5-C3	2.63	1.37	1.30
3	A	335	MAK	O2-C1	2.63	1.37	1.30
3	B	335	MAK	O2-C1	2.59	1.37	1.30
2	B	334	NAD	C4N-C3N	2.30	1.42	1.39
2	B	334	NAD	O4D-C1D	2.29	1.43	1.40
2	B	334	NAD	C2A-N3A	-2.27	1.29	1.33
2	A	334	NAD	C2A-N3A	-2.16	1.30	1.33
2	B	334	NAD	C2A-N1A	2.07	1.37	1.33
2	A	334	NAD	C2A-N1A	2.03	1.37	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	334	NAD	C5N-C4N-C3N	-8.35	112.16	120.36
2	A	334	NAD	C5N-C4N-C3N	-7.42	113.07	120.36
2	A	334	NAD	C6N-C5N-C4N	5.94	128.00	119.45
2	B	334	NAD	C6N-C5N-C4N	5.69	127.65	119.45
2	A	334	NAD	C5N-C6N-N1N	-4.96	113.62	120.38
2	B	334	NAD	C2N-C3N-C4N	4.61	123.62	118.26
2	A	334	NAD	C4N-C3N-C7N	-4.26	109.45	121.06
2	B	334	NAD	C5N-C6N-N1N	-4.00	114.92	120.38
2	A	334	NAD	C2N-C3N-C4N	3.92	122.82	118.26
2	A	334	NAD	C4D-O4D-C1D	-3.86	106.39	109.92
2	B	334	NAD	O7N-C7N-N7N	3.64	127.88	122.62
2	B	334	NAD	C4N-C3N-C7N	-3.63	111.18	121.06
2	A	334	NAD	O7N-C7N-C3N	-3.05	115.86	119.60
2	B	334	NAD	O2A-PA-O3	2.96	115.28	107.27
2	A	334	NAD	C2N-C3N-C7N	2.86	127.73	119.46
2	A	334	NAD	O7N-C7N-N7N	2.60	126.38	122.62
2	B	334	NAD	C4B-O4B-C1B	-2.60	103.73	109.47
2	B	334	NAD	C3N-C7N-N7N	-2.52	114.64	117.74
2	B	334	NAD	O3D-C3D-C4D	-2.23	104.67	111.08
2	B	334	NAD	O4B-C1B-C2B	-2.20	101.90	106.62
2	A	334	NAD	O4B-C1B-C2B	-2.06	102.20	106.62

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	334	NAD	PN-O3-PA-O5B
2	A	334	NAD	C5D-O5D-PN-O3
2	A	334	NAD	C5D-O5D-PN-O1N

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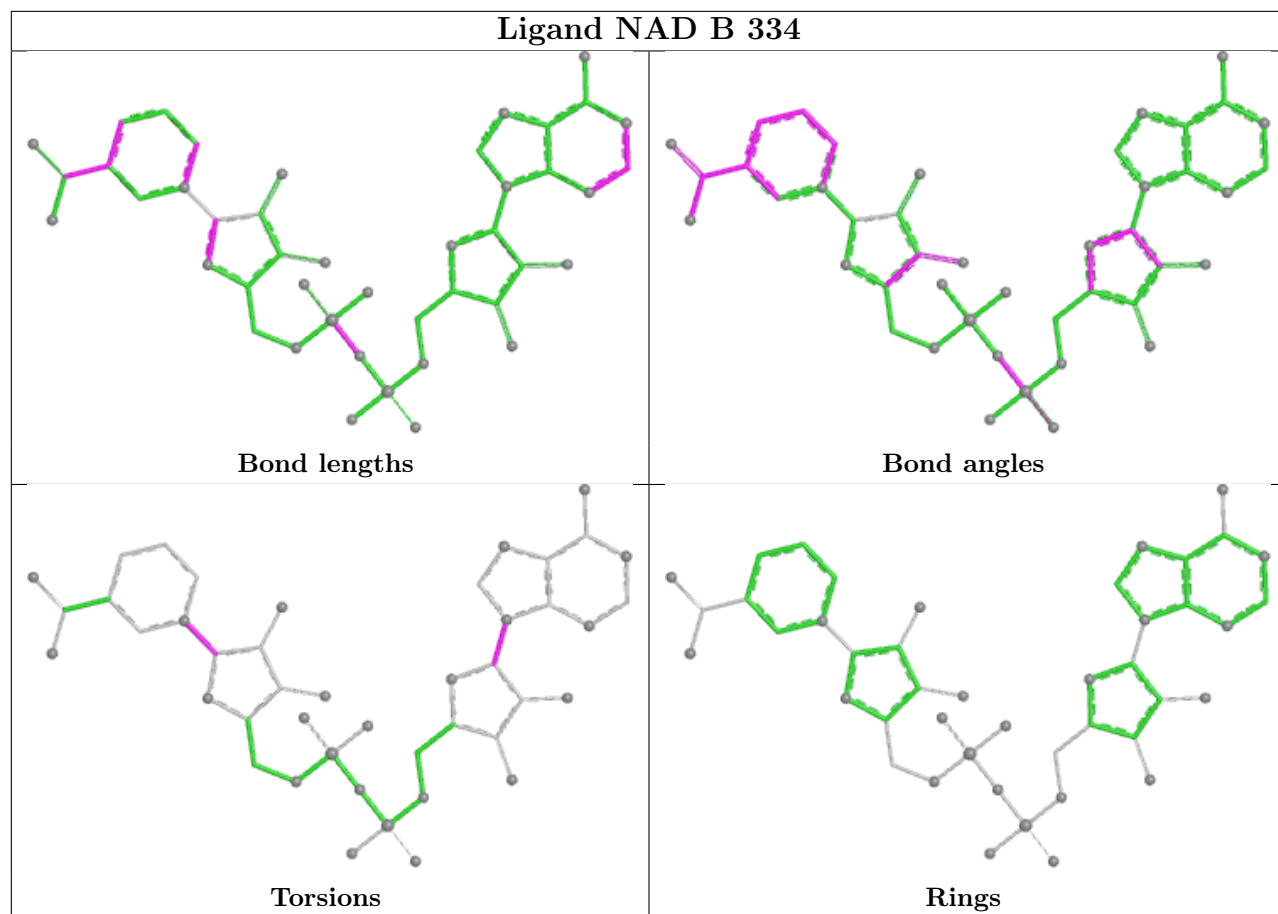
Mol	Chain	Res	Type	Atoms
2	A	334	NAD	O4D-C1D-N1N-C2N
2	A	334	NAD	O4D-C1D-N1N-C6N
2	A	334	NAD	C2D-C1D-N1N-C2N
2	A	334	NAD	C2D-C1D-N1N-C6N
2	B	334	NAD	O4D-C1D-N1N-C2N
2	B	334	NAD	O4D-C1D-N1N-C6N
2	B	334	NAD	C2D-C1D-N1N-C2N
2	B	334	NAD	C2D-C1D-N1N-C6N
2	A	334	NAD	O4D-C4D-C5D-O5D
2	A	334	NAD	C3D-C4D-C5D-O5D
2	A	334	NAD	C5B-O5B-PA-O1A
2	A	334	NAD	PN-O3-PA-O1A
2	A	334	NAD	C4D-C5D-O5D-PN
2	B	334	NAD	C2B-C1B-N9A-C8A
2	A	334	NAD	PN-O3-PA-O2A

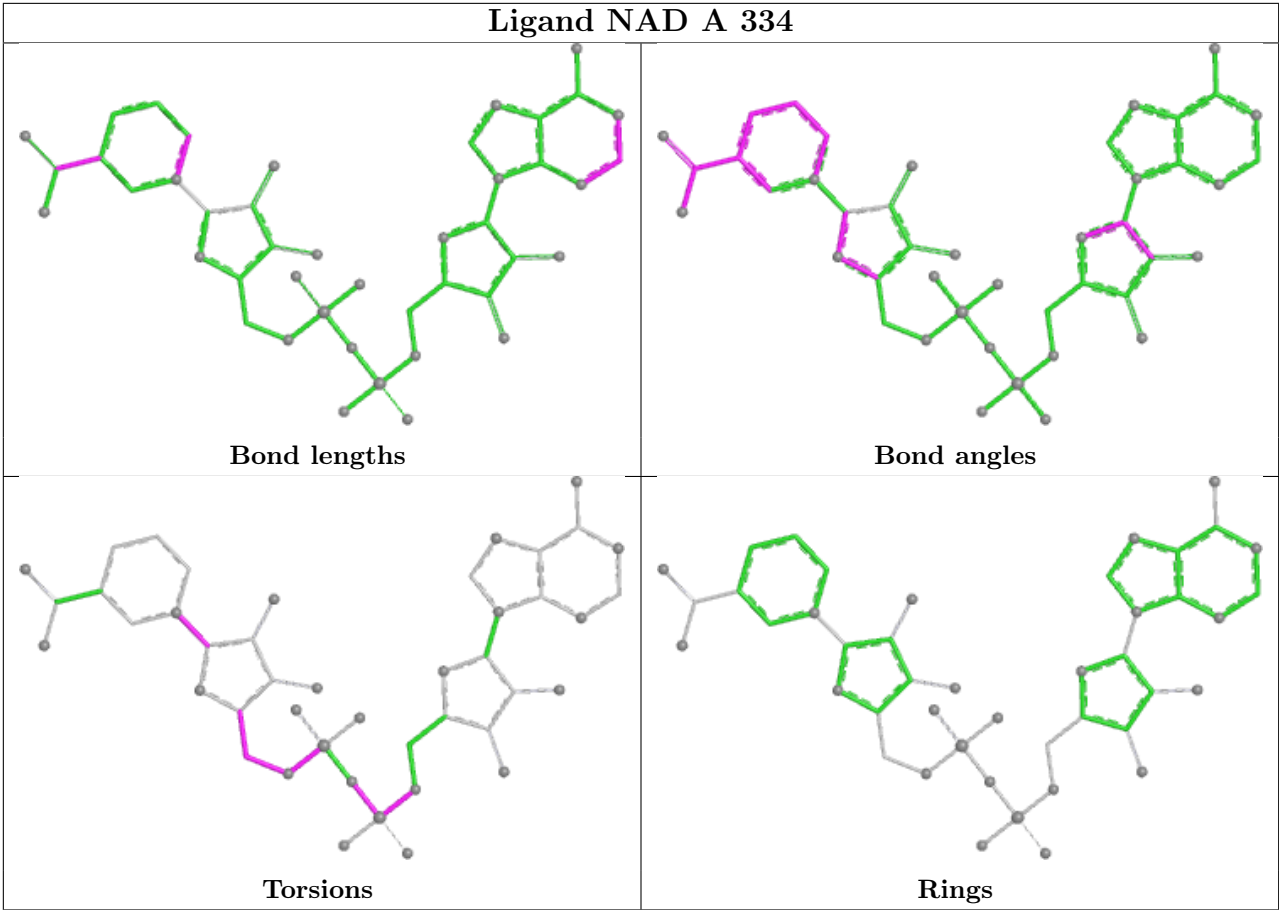
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	334	NAD	4	0
3	B	335	MAK	2	0
2	A	334	NAD	3	0
3	A	335	MAK	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.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	104:ASN	C	105:VAL	N	1.79
1	B	96:GLU	C	97:ARG	N	0.66

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.