



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:49 PM UTC

PDB ID : 1GYP / pdb_00001gyp
Title : CRYSTAL STRUCTURE OF GLYCOSOMAL GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE FROM LEISHMANIA MEXICANA: IMPLICATIONS FOR STRUCTURE-BASED DRUG DESIGN AND A NEW POSITION FOR THE INORGANIC PHOSPHATE BINDING SITE
Authors : Kim, H.; Feil, I.K.; Verlinde, C.L.M.J.; Petra, P.H.; Hol, W.G.J.
Deposited on : 1995-08-01
Resolution : 2.80 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

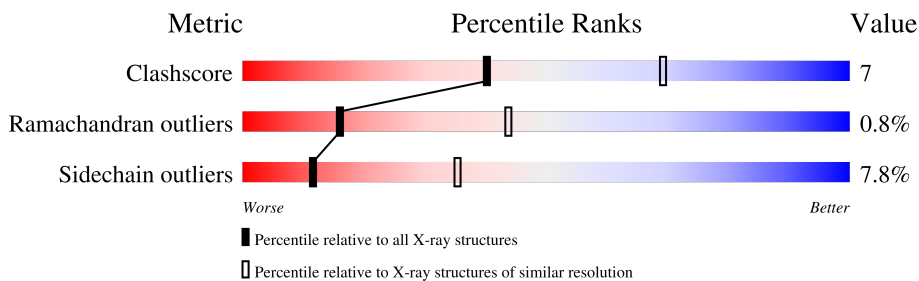
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	358	
1	B	358	
1	C	358	
1	D	358	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11080 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 GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2716	1712	474	517	13			
1	B	358	Total	C	N	O	S	0	0	0
			2716	1712	474	517	13			
1	C	358	Total	C	N	O	S	0	0	0
			2716	1712	474	517	13			
1	D	358	Total	C	N	O	S	0	0	0
			2716	1712	474	517	13			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



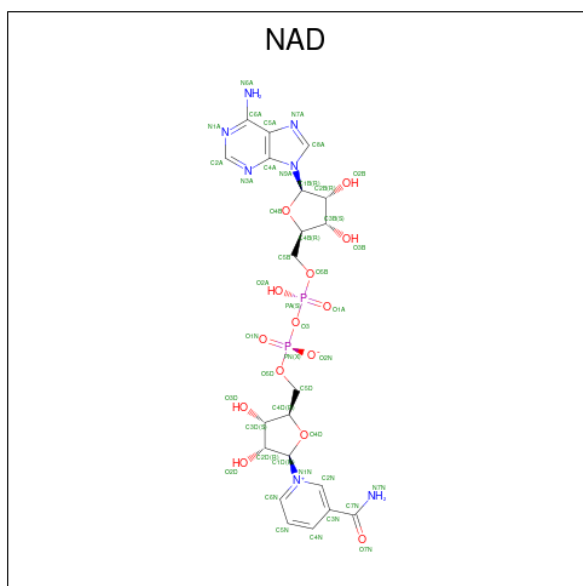
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	C	1	Total 5	O 4	P 1	0	0
2	C	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



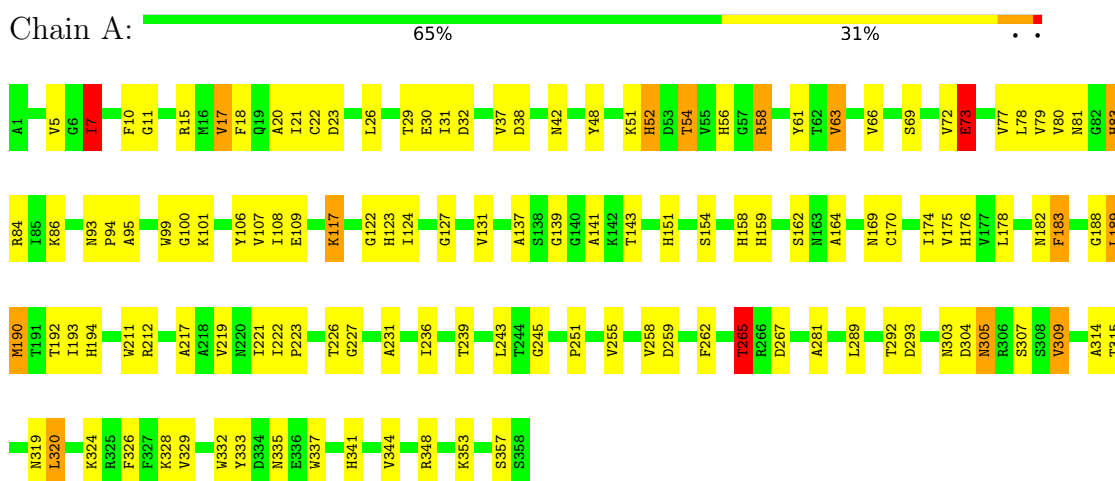
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

3 Residue-property plots

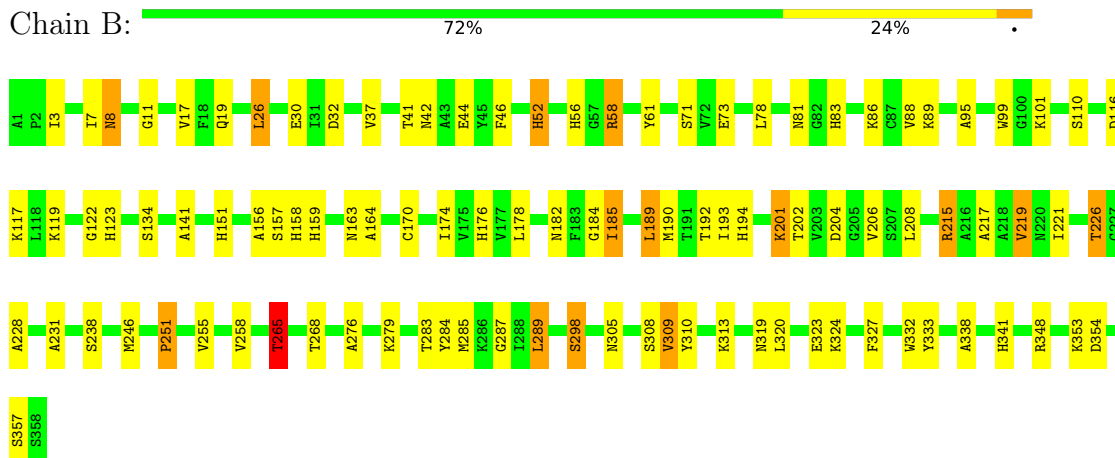
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

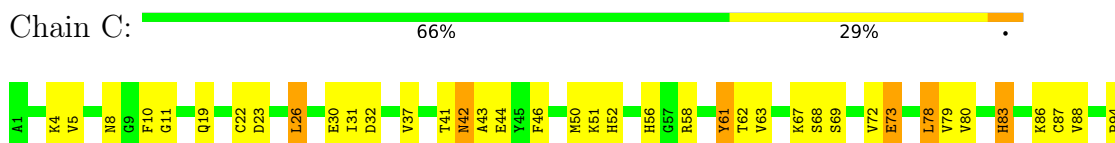
• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



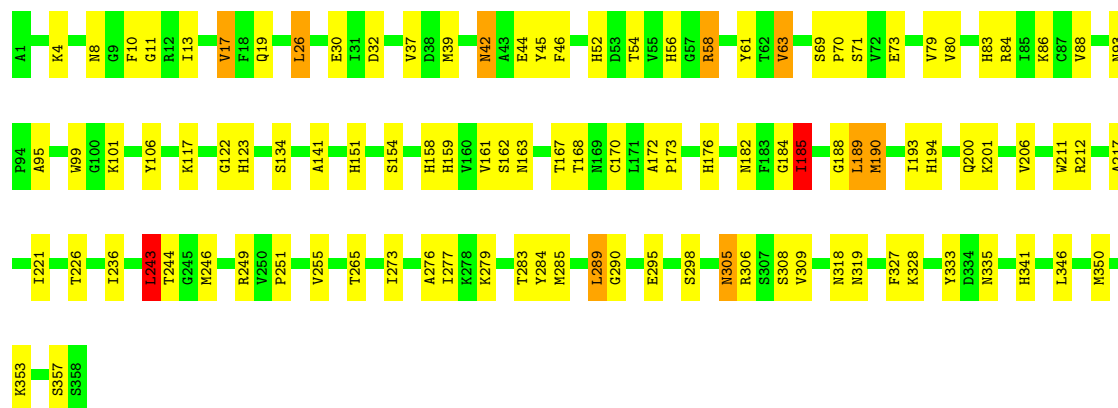
• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE





• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

Chain D: 71% 26% ..



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 21	Depositor
Cell constants a, b, c, α , β , γ	99.00Å 126.50Å 138.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11080	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: PO4, 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	1.00	14/2768 (0.5%)	1.79	60/3752 (1.6%)
1	B	1.07	17/2768 (0.6%)	1.76	49/3752 (1.3%)
1	C	0.99	15/2768 (0.5%)	1.75	59/3752 (1.6%)
1	D	1.03	13/2768 (0.5%)	1.71	41/3752 (1.1%)
All	All	1.02	59/11072 (0.5%)	1.75	209/15008 (1.4%)

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	C	0	1

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	185	ILE	CA-CB	8.17	1.65	1.54
1	B	309	VAL	CA-CB	7.95	1.62	1.53
1	B	341	HIS	CD2-NE2	-7.51	1.29	1.37
1	B	159	HIS	CD2-NE2	-7.42	1.29	1.37
1	B	123	HIS	CD2-NE2	-7.16	1.29	1.37
1	A	309	VAL	CA-CB	6.88	1.62	1.53
1	C	52	HIS	CD2-NE2	-6.87	1.30	1.37
1	A	176	HIS	CD2-NE2	-6.66	1.30	1.37
1	D	52	HIS	CD2-NE2	-6.65	1.30	1.37
1	B	151	HIS	CD2-NE2	-6.65	1.30	1.37
1	C	176	HIS	CD2-NE2	-6.65	1.30	1.37
1	C	185	ILE	CA-CB	6.57	1.62	1.54
1	A	52	HIS	CD2-NE2	-6.50	1.30	1.37
1	D	159	HIS	CD2-NE2	-6.38	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	158	HIS	CD2-NE2	-6.34	1.30	1.37
1	C	159	HIS	CD2-NE2	-6.33	1.30	1.37
1	D	176	HIS	CD2-NE2	-6.33	1.30	1.37
1	D	341	HIS	CD2-NE2	-6.32	1.30	1.37
1	D	123	HIS	CD2-NE2	-6.26	1.30	1.37
1	C	123	HIS	CD2-NE2	-6.25	1.30	1.37
1	D	83	HIS	CD2-NE2	-6.22	1.31	1.37
1	D	151	HIS	CD2-NE2	-6.19	1.31	1.37
1	B	176	HIS	CD2-NE2	-6.16	1.31	1.37
1	C	194	HIS	CD2-NE2	-6.11	1.31	1.37
1	D	56	HIS	CD2-NE2	-6.10	1.31	1.37
1	A	83	HIS	CD2-NE2	-6.10	1.31	1.37
1	A	159	HIS	CD2-NE2	-6.10	1.31	1.37
1	C	151	HIS	CD2-NE2	-6.06	1.31	1.37
1	B	151	HIS	CG-ND1	-6.04	1.31	1.38
1	B	56	HIS	CD2-NE2	-6.02	1.31	1.37
1	B	56	HIS	CG-ND1	-5.93	1.31	1.38
1	A	123	HIS	CD2-NE2	-5.90	1.31	1.37
1	B	52	HIS	CG-ND1	-5.89	1.31	1.38
1	B	52	HIS	CD2-NE2	-5.88	1.31	1.37
1	C	56	HIS	CD2-NE2	-5.87	1.31	1.37
1	B	341	HIS	CG-ND1	-5.87	1.31	1.38
1	C	83	HIS	CD2-NE2	-5.85	1.31	1.37
1	C	158	HIS	CD2-NE2	-5.82	1.31	1.37
1	B	194	HIS	CG-ND1	-5.80	1.31	1.38
1	B	158	HIS	CD2-NE2	-5.79	1.31	1.37
1	B	83	HIS	CD2-NE2	-5.79	1.31	1.37
1	D	194	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	56	HIS	CG-ND1	-5.73	1.31	1.38
1	A	341	HIS	CD2-NE2	-5.72	1.31	1.37
1	D	158	HIS	CD2-NE2	-5.70	1.31	1.37
1	B	194	HIS	CD2-NE2	-5.62	1.31	1.37
1	C	194	HIS	CG-ND1	-5.58	1.32	1.38
1	C	341	HIS	CD2-NE2	-5.57	1.31	1.37
1	A	52	HIS	CG-ND1	-5.56	1.32	1.38
1	A	151	HIS	CD2-NE2	-5.45	1.31	1.37
1	D	151	HIS	CG-ND1	-5.45	1.32	1.38
1	C	341	HIS	CG-ND1	-5.42	1.32	1.38
1	C	52	HIS	CG-ND1	-5.34	1.32	1.38
1	D	52	HIS	CG-ND1	-5.22	1.32	1.38
1	A	194	HIS	CG-ND1	-5.12	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	176	HIS	CG-ND1	-5.10	1.32	1.38
1	D	185	ILE	CA-CB	5.05	1.60	1.54
1	A	194	HIS	CD2-NE2	-5.02	1.32	1.37

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ASN	N-CA-C	10.17	125.08	112.47
1	B	284	TYR	N-CA-C	8.95	123.99	112.89
1	C	284	TYR	N-CA-C	8.87	123.20	112.38
1	B	217	ALA	N-CA-C	8.55	120.67	111.36
1	D	284	TYR	N-CA-C	8.42	123.36	113.18
1	C	182	ASN	N-CA-C	8.38	123.18	113.38
1	D	32	ASP	CA-CB-CG	8.37	120.97	112.60
1	A	217	ALA	N-CA-C	8.12	120.13	111.28
1	B	26	LEU	N-CA-C	7.98	122.12	112.38
1	B	32	ASP	CA-CB-CG	7.91	120.50	112.60
1	A	221	ILE	N-CA-C	-7.84	95.83	107.51
1	B	283	THR	CA-C-O	-7.58	114.30	119.68
1	D	182	ASN	N-CA-C	7.56	121.81	112.58
1	C	23	ASP	CA-CB-CG	7.51	120.11	112.60
1	B	185	ILE	CA-C-O	7.45	126.85	120.22
1	C	193	ILE	N-CA-C	-7.42	96.87	108.23
1	B	8	ASN	CA-CB-CG	7.42	120.02	112.60
1	D	217	ALA	N-CA-C	7.38	121.53	112.23
1	B	219	VAL	N-CA-CB	-7.34	99.11	111.23
1	A	193	ILE	N-CA-C	-7.29	96.36	107.73
1	A	304	ASP	CA-CB-CG	7.27	119.87	112.60
1	A	259	ASP	CA-CB-CG	7.14	119.75	112.60
1	D	42	ASN	OD1-CG-ND2	-6.97	115.62	122.60
1	B	156	ALA	N-CA-C	6.89	118.80	111.28
1	B	231	ALA	N-CA-C	6.85	120.52	111.75
1	D	327	PHE	N-CA-C	6.84	120.56	109.40
1	D	163	ASN	CA-CB-CG	6.83	119.43	112.60
1	A	305	ASN	N-CA-C	6.82	120.57	112.93
1	C	231	ALA	N-CA-C	6.82	119.55	111.71
1	C	303	ASN	OD1-CG-ND2	-6.79	115.81	122.60
1	B	338	ALA	CA-C-O	-6.75	113.95	120.90
1	A	337	TRP	N-CA-C	6.72	118.40	111.14
1	D	193	ILE	N-CA-C	-6.71	98.61	108.54
1	C	217	ALA	N-CA-C	6.71	120.69	112.23
1	C	335	ASN	CB-CG-ND2	6.62	126.33	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ASP	CA-CB-CG	6.62	119.22	112.60
1	C	252	THR	CA-C-N	6.61	126.20	119.19
1	C	252	THR	C-N-CA	6.61	126.20	119.19
1	A	81	ASN	CA-CB-CG	6.60	119.20	112.60
1	C	320	LEU	CA-C-N	6.59	126.09	119.24
1	C	320	LEU	C-N-CA	6.59	126.09	119.24
1	D	221	ILE	N-CA-C	-6.59	99.09	108.58
1	A	217	ALA	O-C-N	6.54	129.05	122.12
1	D	17	VAL	N-CA-C	-6.51	104.41	110.53
1	C	219	VAL	N-CA-CB	-6.51	100.49	111.23
1	A	99	TRP	CG-CD2-CE3	6.49	140.39	133.90
1	B	221	ILE	N-CA-C	-6.43	98.61	107.99
1	D	318	ASN	N-CA-C	6.42	119.78	112.97
1	C	341	HIS	CA-C-O	-6.38	114.13	120.70
1	C	99	TRP	CG-CD2-CE3	6.37	140.27	133.90
1	A	183	PHE	N-CA-C	-6.32	104.31	111.14
1	B	208	LEU	N-CA-C	6.27	119.09	111.82
1	D	99	TRP	N-CA-C	6.24	118.60	111.11
1	A	192	THR	CA-CB-OG1	-6.22	100.27	109.60
1	D	159	HIS	CB-CG-CD2	-6.20	123.14	131.20
1	B	265	THR	CA-CB-OG1	-6.19	100.32	109.60
1	B	332	TRP	CG-CD2-CE3	6.14	140.04	133.90
1	B	182	ASN	N-CA-C	6.12	120.05	112.58
1	C	154	SER	CA-C-N	6.11	125.79	119.56
1	C	154	SER	C-N-CA	6.11	125.79	119.56
1	D	8	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	A	42	ASN	OD1-CG-ND2	-6.06	116.54	122.60
1	B	354	ASP	CA-CB-CG	6.05	118.65	112.60
1	C	302	ILE	O-C-N	6.05	129.62	122.66
1	B	251	PRO	N-CA-C	6.05	124.93	112.47
1	D	93	ASN	CA-C-N	6.05	127.40	119.84
1	D	93	ASN	C-N-CA	6.05	127.40	119.84
1	B	313	LYS	CA-CB-CG	-5.99	102.12	114.10
1	C	32	ASP	CA-CB-CG	5.99	118.59	112.60
1	C	68	SER	N-CA-C	5.98	117.80	111.28
1	C	163	ASN	CB-CG-ND2	5.95	125.33	116.40
1	A	176	HIS	CB-CG-CD2	-5.93	123.49	131.20
1	B	159	HIS	CB-CG-CD2	-5.89	123.54	131.20
1	A	10	PHE	N-CA-CB	-5.88	103.35	110.53
1	A	222	ILE	CA-C-O	-5.88	114.78	119.25
1	D	357	SER	CA-C-N	5.87	132.26	121.70
1	D	357	SER	C-N-CA	5.87	132.26	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	301	PHE	CA-CB-CG	-5.87	107.93	113.80
1	C	123	HIS	CA-CB-CG	-5.86	107.94	113.80
1	A	29	THR	N-CA-C	5.85	119.60	112.23
1	B	310	TYR	N-CA-C	5.82	118.92	110.42
1	C	8	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	C	357	SER	CA-C-N	5.79	132.12	121.70
1	C	357	SER	C-N-CA	5.79	132.12	121.70
1	B	287	GLY	CA-C-N	5.78	128.64	122.97
1	B	287	GLY	C-N-CA	5.78	128.64	122.97
1	A	341	HIS	CA-CB-CG	-5.76	108.04	113.80
1	D	26	LEU	N-CA-C	5.76	120.30	113.28
1	A	265	THR	CA-CB-OG1	-5.75	100.97	109.60
1	A	194	HIS	CA-CB-CG	5.71	119.52	113.80
1	A	51	LYS	CB-CG-CD	-5.68	98.22	111.30
1	B	123	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	A	293	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	305	ASN	CA-CB-CG	5.68	118.28	112.60
1	C	341	HIS	N-CA-C	-5.65	105.03	111.14
1	A	22	CYS	N-CA-C	5.65	117.12	111.07
1	B	338	ALA	N-CA-C	-5.65	104.76	111.03
1	D	58	ARG	N-CA-C	-5.65	102.93	109.93
1	D	123	HIS	CB-CG-CD2	-5.65	123.86	131.20
1	C	41	THR	N-CA-C	-5.64	107.03	114.31
1	D	194	HIS	CB-CG-CD2	-5.64	123.86	131.20
1	B	159	HIS	CA-CB-CG	-5.62	108.18	113.80
1	A	222	ILE	N-CA-CB	-5.62	104.68	111.31
1	A	7	ILE	CA-CB-CG2	-5.61	100.96	110.50
1	B	81	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	303	ASN	N-CA-C	5.59	120.05	113.23
1	A	31	ILE	CA-C-O	5.57	126.50	120.43
1	C	161	VAL	N-CA-CB	-5.56	105.43	112.60
1	D	251	PRO	N-CA-C	5.56	123.48	113.70
1	D	283	THR	CA-C-O	-5.55	116.17	119.55
1	B	193	ILE	N-CA-C	-5.54	100.34	108.54
1	A	251	PRO	N-CA-C	5.54	123.88	112.47
1	C	163	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	A	320	LEU	CA-C-N	5.52	125.18	119.05
1	A	320	LEU	C-N-CA	5.52	125.18	119.05
1	C	215	ARG	NE-CZ-NH1	5.52	127.02	121.50
1	D	305	ASN	N-CA-C	5.52	119.64	113.02
1	D	319	ASN	CA-CB-CG	-5.50	107.10	112.60
1	C	236	ILE	CA-C-N	5.50	125.17	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	236	ILE	C-N-CA	5.50	125.17	119.56
1	A	123	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	D	39	MET	N-CA-C	5.49	117.97	111.33
1	D	8	ASN	CB-CG-ND2	5.47	124.61	116.40
1	B	192	THR	CA-CB-OG1	-5.47	101.40	109.60
1	A	48	TYR	N-CA-C	-5.47	105.40	111.36
1	C	351	ALA	N-CA-C	5.46	117.99	111.71
1	C	133	ILE	N-CA-CB	5.46	117.23	111.00
1	C	337	TRP	N-CA-C	5.45	117.03	111.14
1	B	348	ARG	CA-CB-CG	-5.45	103.20	114.10
1	C	159	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	B	313	LYS	CA-C-O	-5.44	115.10	120.70
1	C	316	LEU	N-CA-C	5.43	117.28	111.36
1	D	99	TRP	CG-CD2-CE3	5.42	139.32	133.90
1	C	137	ALA	N-CA-C	5.42	118.29	109.24
1	B	357	SER	CA-C-N	5.41	131.44	121.70
1	B	357	SER	C-N-CA	5.41	131.44	121.70
1	B	332	TRP	CE2-CD2-CG	-5.41	100.71	107.20
1	C	172	ALA	CA-C-N	5.39	124.85	119.24
1	C	172	ALA	C-N-CA	5.39	124.85	119.24
1	C	311	ASP	CA-CB-CG	5.39	117.99	112.60
1	D	201	LYS	N-CA-C	5.39	118.19	109.40
1	A	357	SER	CA-C-N	5.39	131.41	121.70
1	A	357	SER	C-N-CA	5.39	131.41	121.70
1	C	133	ILE	CB-CA-C	-5.39	104.44	110.96
1	A	281	ALA	N-CA-C	5.38	118.06	111.82
1	A	226	THR	CA-CB-OG1	-5.36	101.55	109.60
1	D	168	THR	N-CA-C	-5.36	105.36	111.14
1	A	99	TRP	CB-CG-CD1	-5.35	118.87	126.90
1	B	332	TRP	CB-CG-CD1	-5.35	118.87	126.90
1	D	236	ILE	CA-C-N	5.35	125.02	119.56
1	D	236	ILE	C-N-CA	5.35	125.02	119.56
1	D	176	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	C	192	THR	CA-CB-OG1	-5.34	101.59	109.60
1	C	123	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	C	69	SER	O-C-N	-5.32	117.22	121.80
1	B	163	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	B	163	ASN	CB-CG-ND2	5.32	124.37	116.40
1	B	99	TRP	CE2-CD2-CG	-5.31	100.83	107.20
1	C	61	TYR	N-CA-C	5.31	117.38	110.43
1	B	17	VAL	N-CA-C	-5.30	105.33	110.42
1	C	318	ASN	OD1-CG-ND2	-5.30	117.30	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	332	TRP	CE2-CD2-CG	-5.30	100.84	107.20
1	A	73	GLU	N-CA-C	5.30	117.14	111.36
1	C	176	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	C	318	ASN	N-CA-C	5.28	119.03	112.59
1	A	21	ILE	CA-C-O	-5.27	115.65	121.29
1	A	99	TRP	CE2-CD2-CG	-5.26	100.88	107.20
1	A	231	ALA	N-CA-C	5.26	118.48	111.75
1	B	159	HIS	N-CA-C	5.26	119.69	113.12
1	A	154	SER	CA-C-N	5.24	125.55	119.47
1	A	154	SER	C-N-CA	5.24	125.55	119.47
1	A	332	TRP	CE2-CD2-CG	-5.24	100.92	107.20
1	A	236	ILE	CA-C-N	5.22	124.89	119.56
1	A	236	ILE	C-N-CA	5.22	124.89	119.56
1	C	159	HIS	CA-CB-CG	-5.22	108.58	113.80
1	A	17	VAL	N-CA-C	-5.21	105.46	110.72
1	C	341	HIS	CA-CB-CG	-5.21	108.59	113.80
1	A	93	ASN	CA-C-N	5.19	126.33	119.84
1	A	93	ASN	C-N-CA	5.19	126.33	119.84
1	C	99	TRP	CB-CG-CD1	-5.19	119.12	126.90
1	A	211	TRP	CG-CD2-CE3	5.18	139.08	133.90
1	B	226	THR	N-CA-CB	-5.18	102.56	110.85
1	B	323	GLU	N-CA-C	5.17	117.93	110.28
1	D	99	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	D	243	LEU	N-CA-CB	-5.16	101.66	111.00
1	B	110	SER	N-CA-C	5.14	117.04	110.61
1	A	32	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	219	VAL	CB-CA-C	5.11	119.66	111.29
1	D	206	VAL	N-CA-C	5.10	116.09	108.54
1	B	3	ILE	N-CA-C	-5.09	101.25	108.58
1	C	22	CYS	N-CA-C	5.08	116.89	111.36
1	D	158	HIS	N-CA-C	5.08	116.58	108.41
1	B	202	THR	O-C-N	5.05	127.91	122.15
1	D	154	SER	CA-C-N	5.05	124.84	119.28
1	D	154	SER	C-N-CA	5.05	124.84	119.28
1	A	223	PRO	N-CA-CB	5.04	107.80	103.31
1	B	327	PHE	N-CA-C	5.04	117.81	109.85
1	A	56	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	A	159	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	A	292	THR	O-C-N	5.03	129.42	123.33
1	C	99	TRP	CE2-CD2-CG	-5.02	101.17	107.20
1	C	326	PHE	CA-CB-CG	5.02	118.82	113.80
1	C	42	ASN	OD1-CG-ND2	-5.02	117.58	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	313	LYS	CA-CB-CG	-5.02	104.06	114.10
1	D	211	TRP	CG-CD2-CE3	5.02	138.92	133.90
1	A	124	ILE	N-CA-C	5.01	115.78	110.72
1	A	326	PHE	N-CA-C	5.01	116.77	108.20
1	B	320	LEU	CA-C-N	5.01	124.80	119.28
1	B	320	LEU	C-N-CA	5.01	124.80	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	215	ARG	Sidechain

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	2716	0	2736	43	0
1	B	2716	0	2736	31	0
1	C	2716	0	2736	47	0
1	D	2716	0	2736	35	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
3	A	44	0	26	2	0
3	B	44	0	26	2	0
3	C	44	0	26	3	0
3	D	44	0	26	2	0
All	All	11080	0	11048	146	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 7.

All (146) 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:C:190:MET:HE2	1:C:226:THR:HG21	1.61	0.82
1:B:116:ASP:HB3	1:B:119:LYS:HG3	1.72	0.70
1:D:190:MET:HE2	1:D:226:THR:HG21	1.73	0.69
1:A:63:VAL:HG13	1:A:80:VAL:HG22	1.77	0.66
1:A:190:MET:HG3	1:A:245:GLY:HA3	1.76	0.66
1:A:5:VAL:HG12	1:A:106:TYR:HB2	1.77	0.65
1:D:117:LYS:HB2	1:D:141:ALA:HB2	1.79	0.64
1:A:169:ASN:O	1:A:307:SER:HB3	1.99	0.63
1:D:37:VAL:HG22	1:D:88:VAL:HB	1.79	0.63
1:A:7:ILE:HD13	1:A:108:ILE:HD12	1.79	0.62
1:D:200:GLN:OE1	1:D:249:ARG:HD2	2.00	0.61
1:C:290:GLY:HA3	1:C:306:ARG:NH1	2.15	0.61
1:B:184:GLY:HA3	1:B:265:THR:HB	1.83	0.60
1:C:204:ASP:OD1	1:C:215:ARG:HD2	2.00	0.60
1:B:41:THR:HG23	1:B:89:LYS:HE2	1.83	0.60
1:C:5:VAL:HG12	1:C:106:TYR:HB2	1.84	0.60
1:A:315:THR:HG23	1:A:328:LYS:O	2.02	0.58
1:C:10:PHE:CD2	1:C:46:PHE:HD2	2.21	0.57
1:D:190:MET:CE	1:D:226:THR:HG21	2.35	0.57
1:C:37:VAL:HG22	1:C:88:VAL:HB	1.88	0.56
1:D:188:GLY:O	1:D:243:LEU:HA	2.05	0.56
1:A:267:ASP:HB3	1:A:324:LYS:HD2	1.86	0.56
1:A:183:PHE:O	1:A:265:THR:HB	2.06	0.56
1:B:134:SER:O	3:B:361:NAD:H1D	2.05	0.56
1:A:66:VAL:HG23	1:A:77:VAL:HB	1.88	0.55
1:C:95:ALA:HA	1:C:122:GLY:O	2.07	0.55
1:A:258:VAL:HG23	1:A:333:TYR:CE1	2.42	0.54
1:B:42:ASN:HD21	1:B:44:GLU:HB2	1.73	0.54
1:B:19:GLN:HG3	1:B:61:TYR:HE2	1.72	0.54
1:C:11:GLY:HA3	3:C:361:NAD:O5B	2.08	0.54
1:C:267:ASP:HB3	1:C:324:LYS:HD2	1.90	0.53
1:A:38:ASP:OD1	3:A:361:NAD:H1B	2.09	0.53
1:C:258:VAL:HG23	1:C:333:TYR:HE1	1.74	0.53
1:D:79:VAL:HG22	1:D:84:ARG:HG2	1.89	0.53
1:C:43:ALA:HB1	1:C:78:LEU:HD13	1.91	0.52
1:B:190:MET:HE3	1:B:226:THR:HG21	1.91	0.52
1:A:61:TYR:HE1	1:A:63:VAL:HG22	1.75	0.52
1:A:258:VAL:HG23	1:A:333:TYR:HE1	1.75	0.52
1:A:95:ALA:HA	1:A:122:GLY:O	2.10	0.52
1:B:190:MET:HE1	1:B:228:ALA:HB3	1.92	0.51
1:A:61:TYR:CE1	1:A:63:VAL:HG22	2.45	0.51
1:C:37:VAL:HG12	3:C:361:NAD:H2A	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:SER:O	1:A:72:VAL:HG22	2.10	0.51
1:B:204:ASP:OD2	1:B:215:ARG:HD2	2.11	0.51
1:B:258:VAL:HG23	1:B:333:TYR:HE1	1.76	0.51
1:A:117:LYS:HG2	1:A:139:GLY:O	2.10	0.50
1:B:258:VAL:HG23	1:B:333:TYR:CE1	2.45	0.50
1:A:328:LYS:HB2	1:D:189:LEU:HD23	1.92	0.50
1:A:18:PHE:CZ	1:A:80:VAL:HG21	2.46	0.50
1:A:262:PHE:HE1	1:A:329:VAL:HG23	1.77	0.50
1:A:175:VAL:HG11	1:A:239:THR:HG21	1.94	0.49
1:C:108:ILE:HD11	1:C:347:VAL:HG21	1.95	0.49
1:A:107:VAL:HB	1:A:131:VAL:HG22	1.95	0.48
1:D:11:GLY:HA3	3:D:361:NAD:O5B	2.13	0.48
1:C:19:GLN:HG3	1:C:61:TYR:CE2	2.49	0.48
1:A:212:ARG:HG2	1:D:295:GLU:HB3	1.96	0.47
1:D:170:CYS:HA	1:D:308:SER:HB2	1.96	0.47
1:D:134:SER:O	3:D:361:NAD:H1D	2.15	0.47
1:C:62:THR:O	1:C:80:VAL:HA	2.14	0.47
1:B:8:ASN:HA	1:B:37:VAL:HB	1.96	0.47
1:B:95:ALA:HA	1:B:122:GLY:O	2.14	0.47
1:C:43:ALA:HA	1:C:46:PHE:HD1	1.79	0.47
1:A:79:VAL:HG22	1:A:84:ARG:HG2	1.97	0.47
1:C:26:LEU:HB3	1:C:31:ILE:HB	1.96	0.47
1:C:73:GLU:H	1:C:73:GLU:CD	2.23	0.47
1:B:276:ALA:HA	1:B:279:LYS:HE2	1.97	0.47
1:B:117:LYS:HB2	1:B:141:ALA:HB2	1.97	0.46
1:B:19:GLN:HG3	1:B:61:TYR:CE2	2.50	0.46
1:A:52:HIS:HD2	1:A:58:ARG:NH1	2.13	0.46
1:B:268:THR:O	1:B:324:LYS:HA	2.15	0.46
1:C:134:SER:O	3:C:361:NAD:H1D	2.16	0.46
1:D:10:PHE:HD2	1:D:46:PHE:HD2	1.64	0.46
1:C:211:TRP:CE2	1:D:45:TYR:HD1	2.33	0.46
1:C:78:LEU:HD22	1:C:87:CYS:SG	2.55	0.46
1:D:10:PHE:CD2	1:D:46:PHE:HD2	2.34	0.46
1:C:42:ASN:HD21	1:C:44:GLU:HB2	1.79	0.46
1:C:79:VAL:HA	1:C:83:HIS:O	2.15	0.46
1:A:188:GLY:O	1:A:243:LEU:HA	2.16	0.46
1:A:17:VAL:HG11	1:A:108:ILE:HD13	1.98	0.45
1:D:276:ALA:HA	1:D:279:LYS:HE2	1.98	0.45
1:D:290:GLY:HA3	1:D:306:ARG:NH1	2.32	0.45
1:B:42:ASN:ND2	1:B:44:GLU:HB2	2.32	0.45
1:B:285:MET:HB3	1:B:289:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD23	1:D:328:LYS:HB2	1.98	0.45
1:A:320:LEU:HG	1:D:244:THR:HG22	1.99	0.45
1:C:188:GLY:O	1:C:243:LEU:HA	2.17	0.45
1:C:19:GLN:HG3	1:C:61:TYR:HE2	1.82	0.45
1:A:52:HIS:HD2	1:A:58:ARG:HH11	1.65	0.44
1:D:273:ILE:O	1:D:277:ILE:HG13	2.18	0.44
1:A:227:GLY:N	2:A:359:PO4:O2	2.51	0.44
1:C:151:HIS:HA	1:C:349:TYR:OH	2.17	0.44
1:A:11:GLY:O	1:A:15:ARG:HG3	2.18	0.44
1:B:298:SER:HB3	1:C:221:ILE:H	1.83	0.44
1:C:258:VAL:HG23	1:C:333:TYR:CE1	2.53	0.43
1:D:19:GLN:HG3	1:D:61:TYR:HE2	1.82	0.43
1:A:37:VAL:HG12	3:A:361:NAD:H2A	1.99	0.43
1:C:171:LEU:HD22	1:C:190:MET:SD	2.57	0.43
1:D:42:ASN:HD21	1:D:44:GLU:HB2	1.83	0.43
1:A:54:THR:HB	1:B:204:ASP:OD1	2.18	0.43
1:C:193:ILE:HD12	1:C:193:ILE:N	2.33	0.43
1:B:246:MET:HE3	1:B:246:MET:HB2	1.90	0.43
1:C:183:PHE:O	1:C:265:THR:HB	2.19	0.43
1:C:170:CYS:SG	1:C:333:TYR:CD1	3.09	0.43
1:C:200:GLN:HB3	1:C:217:ALA:HB2	2.00	0.43
1:D:13:ILE:O	1:D:17:VAL:HG23	2.19	0.42
1:A:170:CYS:SG	1:A:333:TYR:CD1	3.12	0.42
1:B:42:ASN:O	1:B:46:PHE:HD1	2.02	0.42
1:C:276:ALA:HA	1:C:279:LYS:HE2	2.01	0.42
1:D:346:LEU:O	1:D:350:MET:HG3	2.18	0.42
1:D:246:MET:HE3	1:D:246:MET:HB2	1.88	0.42
1:B:37:VAL:HG22	1:B:88:VAL:HB	2.02	0.42
1:B:174:ILE:O	1:B:178:LEU:HG	2.20	0.42
1:A:174:ILE:O	1:A:178:LEU:HG	2.20	0.42
1:B:42:ASN:ND2	1:B:44:GLU:H	2.18	0.42
1:C:5:VAL:HA	1:C:106:TYR:O	2.19	0.42
1:C:271:GLN:O	1:C:275:LYS:HG3	2.20	0.42
1:C:156:ALA:O	1:C:159:HIS:HE1	2.03	0.41
1:D:63:VAL:HG13	1:D:80:VAL:HG22	2.02	0.41
1:A:73:GLU:CD	1:A:73:GLU:H	2.28	0.41
1:B:170:CYS:HA	1:B:308:SER:HB2	2.01	0.41
1:A:79:VAL:HA	1:A:83:HIS:O	2.19	0.41
1:D:285:MET:HB3	1:D:289:LEU:HB2	2.02	0.41
1:A:314:ALA:HB2	1:D:212:ARG:NH2	2.36	0.41
1:D:95:ALA:HA	1:D:122:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:HIS:HD2	1:B:58:ARG:NH1	2.18	0.41
1:C:215:ARG:O	1:C:216:ALA:C	2.63	0.41
1:D:161:VAL:HG21	1:D:350:MET:SD	2.61	0.41
1:A:100:GLY:H	1:A:127:GLY:HA3	1.85	0.41
1:A:143:THR:HA	1:A:162:SER:O	2.21	0.41
1:C:46:PHE:O	1:C:50:MET:SD	2.79	0.41
1:C:67:LYS:HB3	1:C:72:VAL:CG2	2.51	0.41
1:D:185:ILE:HD11	1:D:243:LEU:HB2	2.02	0.41
1:A:137:ALA:HB3	1:A:141:ALA:HB3	2.03	0.40
1:C:10:PHE:CD2	1:C:46:PHE:CD2	3.07	0.40
1:D:172:ALA:HB3	1:D:173:PRO:HD3	2.03	0.40
1:C:42:ASN:ND2	1:C:44:GLU:HB2	2.37	0.40
1:C:106:TYR:OH	1:C:351:ALA:HA	2.20	0.40
1:C:215:ARG:NH1	1:D:54:THR:OG1	2.53	0.40
1:D:106:TYR:CD1	1:D:106:TYR:N	2.89	0.40
1:B:11:GLY:HA3	3:B:361:NAD:O5B	2.22	0.40
1:A:20:ALA:HB3	1:A:344:VAL:HG21	2.04	0.40
1:B:189:LEU:HD22	1:C:326:PHE:HD1	1.86	0.40
1:B:201:LYS:HE3	1:B:206:VAL:O	2.22	0.40
1:C:167:THR:HB	2:C:359:PO4:O4	2.22	0.40
1:C:246:MET:HE3	1:C:246:MET:HB2	1.92	0.40
1:D:170:CYS:SG	1:D:333:TYR:CD1	3.15	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	356/358 (99%)	326 (92%)	26 (7%)	4 (1%)	11	36
1	B	356/358 (99%)	333 (94%)	20 (6%)	3 (1%)	16	44
1	C	356/358 (99%)	330 (93%)	25 (7%)	1 (0%)	36	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	356/358 (99%)	332 (93%)	21 (6%)	3 (1%)	16	44
All	All	1424/1432 (99%)	1321 (93%)	92 (6%)	11 (1%)	16	44

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	VAL
1	B	255	VAL
1	C	255	VAL
1	D	70	PRO
1	D	184	GLY
1	D	255	VAL
1	A	117	LYS
1	A	164	ALA
1	B	164	ALA
1	A	219	VAL
1	B	251	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	294/294 (100%)	272 (92%)	22 (8%)	12	37
1	B	294/294 (100%)	271 (92%)	23 (8%)	11	35
1	C	294/294 (100%)	270 (92%)	24 (8%)	10	33
1	D	294/294 (100%)	271 (92%)	23 (8%)	11	35
All	All	1176/1176 (100%)	1084 (92%)	92 (8%)	11	35

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	26	LEU
1	A	30	GLU

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Mol	Chain	Res	Type
1	A	54	THR
1	A	58	ARG
1	A	63	VAL
1	A	73	GLU
1	A	78	LEU
1	A	86	LYS
1	A	94	PRO
1	A	101	LYS
1	A	109	GLU
1	A	189	LEU
1	A	190	MET
1	A	265	THR
1	A	289	LEU
1	A	305	ASN
1	A	309	VAL
1	A	319	ASN
1	A	335	ASN
1	A	348	ARG
1	A	353	LYS
1	B	7	ILE
1	B	26	LEU
1	B	30	GLU
1	B	58	ARG
1	B	71	SER
1	B	73	GLU
1	B	78	LEU
1	B	86	LYS
1	B	101	LYS
1	B	157	SER
1	B	185	ILE
1	B	189	LEU
1	B	201	LYS
1	B	215	ARG
1	B	219	VAL
1	B	238	SER
1	B	265	THR
1	B	289	LEU
1	B	298	SER
1	B	305	ASN
1	B	309	VAL
1	B	319	ASN
1	B	353	LYS

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Mol	Chain	Res	Type
1	C	4	LYS
1	C	26	LEU
1	C	30	GLU
1	C	51	LYS
1	C	58	ARG
1	C	63	VAL
1	C	73	GLU
1	C	78	LEU
1	C	86	LYS
1	C	94	PRO
1	C	101	LYS
1	C	166	CYS
1	C	173	PRO
1	C	177	VAL
1	C	185	ILE
1	C	189	LEU
1	C	190	MET
1	C	202	THR
1	C	219	VAL
1	C	265	THR
1	C	289	LEU
1	C	309	VAL
1	C	343	VAL
1	C	353	LYS
1	D	4	LYS
1	D	26	LEU
1	D	30	GLU
1	D	58	ARG
1	D	63	VAL
1	D	69	SER
1	D	71	SER
1	D	73	GLU
1	D	86	LYS
1	D	101	LYS
1	D	162	SER
1	D	167	THR
1	D	185	ILE
1	D	189	LEU
1	D	190	MET
1	D	243	LEU
1	D	265	THR
1	D	289	LEU

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Mol	Chain	Res	Type
1	D	298	SER
1	D	305	ASN
1	D	309	VAL
1	D	335	ASN
1	D	353	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	42	ASN
1	A	52	HIS
1	A	91	GLN
1	A	159	HIS
1	A	305	ASN
1	A	318	ASN
1	B	42	ASN
1	B	49	GLN
1	B	52	HIS
1	B	151	HIS
1	B	159	HIS
1	B	305	ASN
1	B	341	HIS
1	C	42	ASN
1	C	52	HIS
1	C	151	HIS
1	C	159	HIS
1	C	341	HIS
1	D	8	ASN
1	D	24	GLN
1	D	42	ASN
1	D	159	HIS
1	D	305	ASN
1	D	341	HIS

5.3.3 RNA ⓘ

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](#)

12 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	PO4	A	360	-	4,4,4	1.15	0	6,6,6	0.54	0
3	NAD	D	361	-	46,48,48	1.31	4 (8%)	64,73,73	1.78	11 (17%)
3	NAD	C	361	-	46,48,48	1.49	8 (17%)	64,73,73	1.73	9 (14%)
2	PO4	A	359	-	4,4,4	0.89	0	6,6,6	0.69	0
3	NAD	A	361	-	46,48,48	1.36	5 (10%)	64,73,73	1.74	12 (18%)
2	PO4	B	359	-	4,4,4	0.84	0	6,6,6	1.06	0
2	PO4	C	359	-	4,4,4	1.06	0	6,6,6	1.02	0
2	PO4	D	359	-	4,4,4	1.32	1 (25%)	6,6,6	0.65	0
2	PO4	B	360	-	4,4,4	1.09	0	6,6,6	0.59	0
3	NAD	B	361	-	46,48,48	1.22	4 (8%)	64,73,73	1.81	8 (12%)
2	PO4	D	360	-	4,4,4	0.92	0	6,6,6	0.42	0
2	PO4	C	360	-	4,4,4	1.21	0	6,6,6	0.65	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
3	NAD	D	361	-	-	5/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	C	361	-	-	4/30/62/62	0/5/5/5
3	NAD	B	361	-	-	10/30/62/62	0/5/5/5
3	NAD	A	361	-	-	9/30/62/62	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	361	NAD	C2N-N1N	6.40	1.42	1.35
3	C	361	NAD	C2N-N1N	6.37	1.42	1.35
3	D	361	NAD	C2N-N1N	5.85	1.41	1.35
3	B	361	NAD	C2N-N1N	5.03	1.40	1.35
3	B	361	NAD	C5A-N7A	-3.47	1.32	1.39
3	D	361	NAD	C5A-N7A	-3.41	1.32	1.39
3	A	361	NAD	C5A-N7A	-3.11	1.33	1.39
3	C	361	NAD	C5A-N7A	-2.96	1.33	1.39
3	A	361	NAD	O4D-C1D	2.91	1.44	1.40
3	C	361	NAD	PN-O3	2.89	1.62	1.59
3	C	361	NAD	PA-O3	2.85	1.62	1.59
2	D	359	PO4	P-O1	2.55	1.56	1.50
3	C	361	NAD	O4D-C1D	2.48	1.44	1.40
3	D	361	NAD	C6N-N1N	2.45	1.40	1.35
3	C	361	NAD	C6N-N1N	2.44	1.40	1.35
3	A	361	NAD	C6N-N1N	2.36	1.40	1.35
3	B	361	NAD	O4D-C1D	2.28	1.43	1.40
3	C	361	NAD	C4A-N9A	-2.27	1.33	1.37
3	C	361	NAD	C3N-C7N	2.27	1.54	1.50
3	A	361	NAD	C4A-N9A	-2.23	1.33	1.37
3	B	361	NAD	C6N-N1N	2.18	1.40	1.35
3	D	361	NAD	C4A-N9A	-2.01	1.33	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	361	NAD	C5A-C4A-N3A	-6.77	117.40	126.72
3	B	361	NAD	C5A-C4A-N3A	-6.69	117.50	126.72
3	B	361	NAD	N3A-C4A-N9A	6.45	138.14	127.17
3	C	361	NAD	C5A-C4A-N3A	-6.38	117.93	126.72
3	D	361	NAD	N3A-C4A-N9A	6.13	137.59	127.17
3	C	361	NAD	N3A-C4A-N9A	5.98	137.33	127.17
3	A	361	NAD	N3A-C4A-N9A	5.76	136.96	127.17
3	A	361	NAD	C5A-C4A-N3A	-5.53	119.10	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	361	NAD	N3A-C2A-N1A	-4.44	121.86	128.58
3	A	361	NAD	N3A-C2A-N1A	-4.31	122.05	128.58
3	C	361	NAD	C6A-C5A-C4A	4.17	122.87	117.18
3	B	361	NAD	N3A-C2A-N1A	-4.17	122.27	128.58
3	C	361	NAD	N3A-C2A-N1A	-4.10	122.37	128.58
3	B	361	NAD	C6A-C5A-C4A	3.91	122.52	117.18
3	D	361	NAD	C6A-C5A-C4A	3.79	122.35	117.18
3	D	361	NAD	C2A-N3A-C4A	3.70	120.87	111.83
3	B	361	NAD	C6A-C5A-N7A	-3.65	125.05	132.09
3	A	361	NAD	C4A-N9A-C8A	3.62	109.54	105.74
3	C	361	NAD	C6A-C5A-N7A	-3.51	125.33	132.09
3	B	361	NAD	C2A-N3A-C4A	3.48	120.33	111.83
3	C	361	NAD	C2A-N3A-C4A	3.21	119.66	111.83
3	A	361	NAD	C6A-C5A-C4A	3.21	121.56	117.18
3	B	361	NAD	C4D-O4D-C1D	-3.18	107.01	109.92
3	D	361	NAD	C6A-C5A-N7A	-3.18	125.96	132.09
3	A	361	NAD	C2A-N3A-C4A	3.14	119.51	111.83
3	A	361	NAD	C6A-C5A-N7A	-2.91	126.49	132.09
3	A	361	NAD	N9A-C8A-N7A	-2.82	109.93	113.94
3	C	361	NAD	C4A-N9A-C8A	2.67	108.54	105.74
3	A	361	NAD	O2A-PA-O3	2.54	114.12	107.27
3	B	361	NAD	C4A-N9A-C8A	2.34	108.19	105.74
3	D	361	NAD	C4A-N9A-C8A	2.30	108.16	105.74
3	D	361	NAD	N9A-C8A-N7A	-2.27	110.72	113.94
3	C	361	NAD	O2A-PA-O3	2.23	113.31	107.27
3	C	361	NAD	N9A-C8A-N7A	-2.15	110.88	113.94
3	D	361	NAD	O2N-PN-O1N	2.15	122.43	112.44
3	A	361	NAD	C2N-N1N-C1D	2.12	123.82	119.13
3	D	361	NAD	C6N-N1N-C2N	-2.07	120.12	121.88
3	A	361	NAD	C4A-N9A-C1B	-2.03	121.89	126.63
3	D	361	NAD	C2B-C1B-N9A	2.03	118.34	113.30
3	A	361	NAD	C6N-N1N-C2N	-2.02	120.16	121.88

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	361	NAD	C5B-O5B-PA-O1A
3	A	361	NAD	O4D-C1D-N1N-C2N
3	A	361	NAD	O4D-C1D-N1N-C6N
3	B	361	NAD	C5B-O5B-PA-O1A
3	B	361	NAD	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
3	B	361	NAD	O4D-C1D-N1N-C2N
3	C	361	NAD	O4D-C1D-N1N-C2N
3	D	361	NAD	O4D-C1D-N1N-C2N
3	D	361	NAD	C2D-C1D-N1N-C2N
3	B	361	NAD	PN-O3-PA-O5B
3	A	361	NAD	C2B-C1B-N9A-C8A
3	B	361	NAD	C2B-C1B-N9A-C8A
3	C	361	NAD	C2B-C1B-N9A-C8A
3	A	361	NAD	C5B-O5B-PA-O2A
3	A	361	NAD	C2D-C1D-N1N-C2N
3	B	361	NAD	O4D-C1D-N1N-C6N
3	C	361	NAD	O4D-C1D-N1N-C6N
3	D	361	NAD	O4D-C1D-N1N-C6N
3	B	361	NAD	O4B-C1B-N9A-C8A
3	C	361	NAD	O4B-C1B-N9A-C8A
3	D	361	NAD	O4B-C4B-C5B-O5B
3	A	361	NAD	O4B-C1B-N9A-C8A
3	A	361	NAD	PA-O3-PN-O1N
3	B	361	NAD	PA-O3-PN-O1N
3	B	361	NAD	PA-O3-PN-O2N
3	D	361	NAD	PA-O3-PN-O1N
3	A	361	NAD	O4B-C4B-C5B-O5B
3	B	361	NAD	O4B-C4B-C5B-O5B

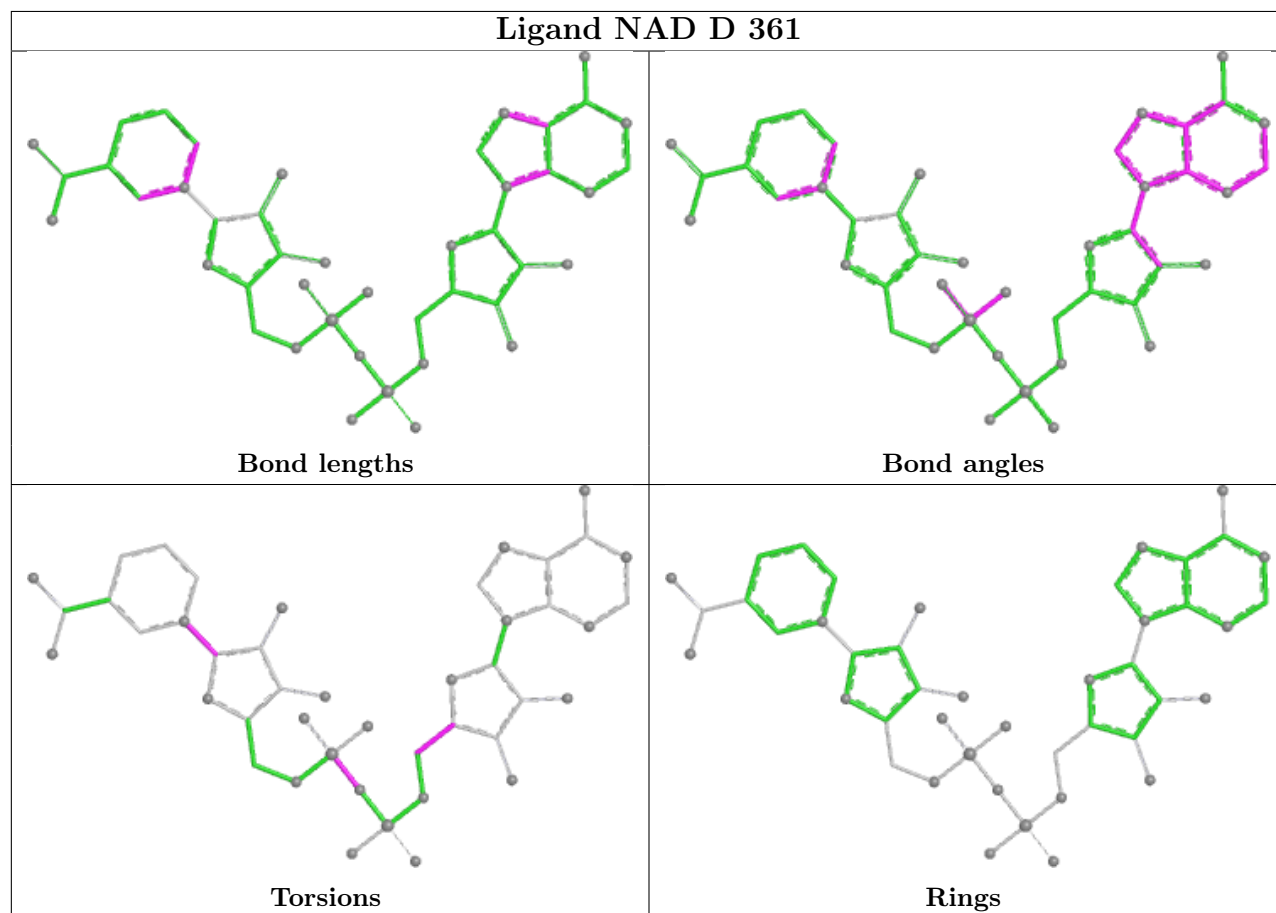
There are no ring outliers.

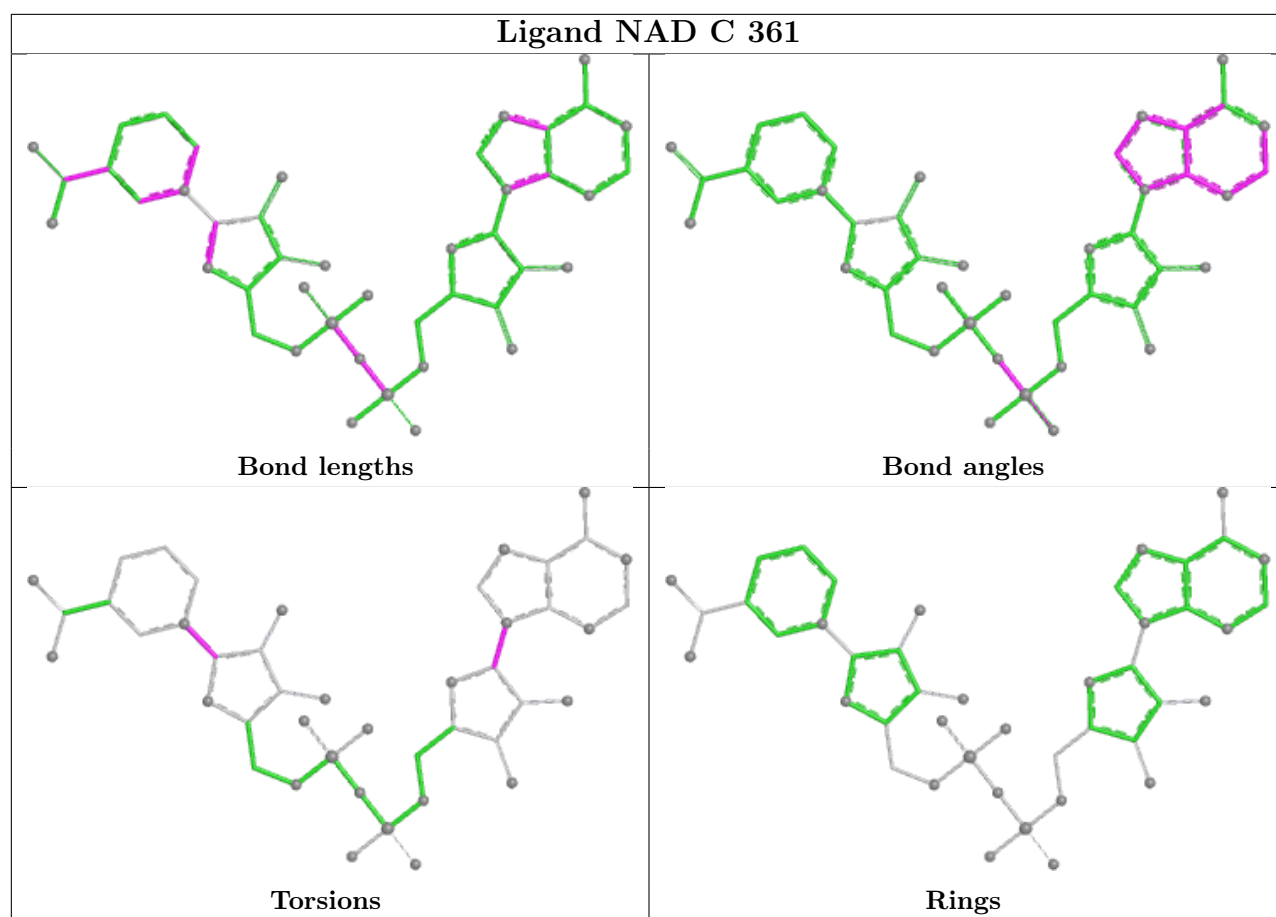
6 monomers are involved in 11 short contacts:

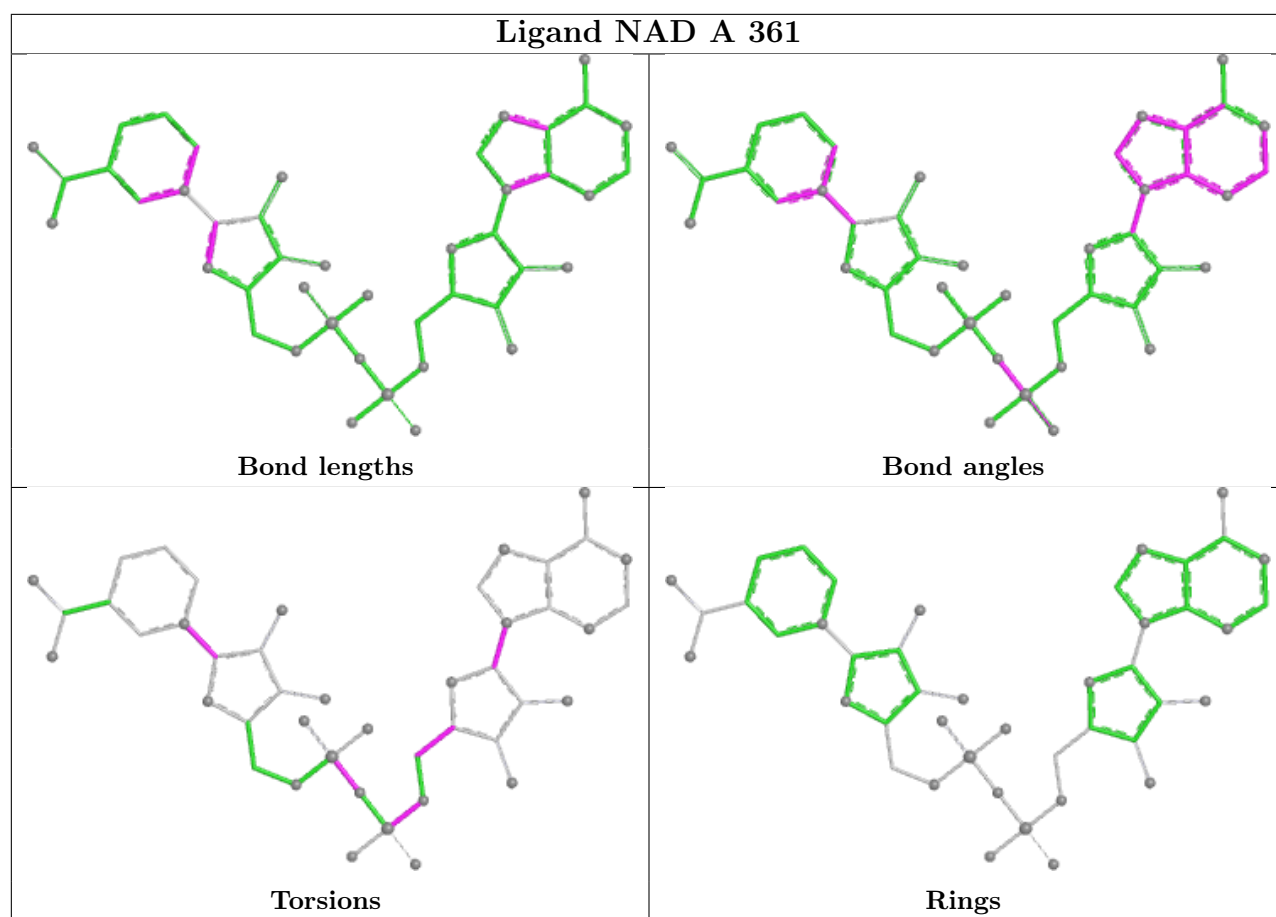
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	361	NAD	2	0
3	C	361	NAD	3	0
2	A	359	PO4	1	0
3	A	361	NAD	2	0
2	C	359	PO4	1	0
3	B	361	NAD	2	0

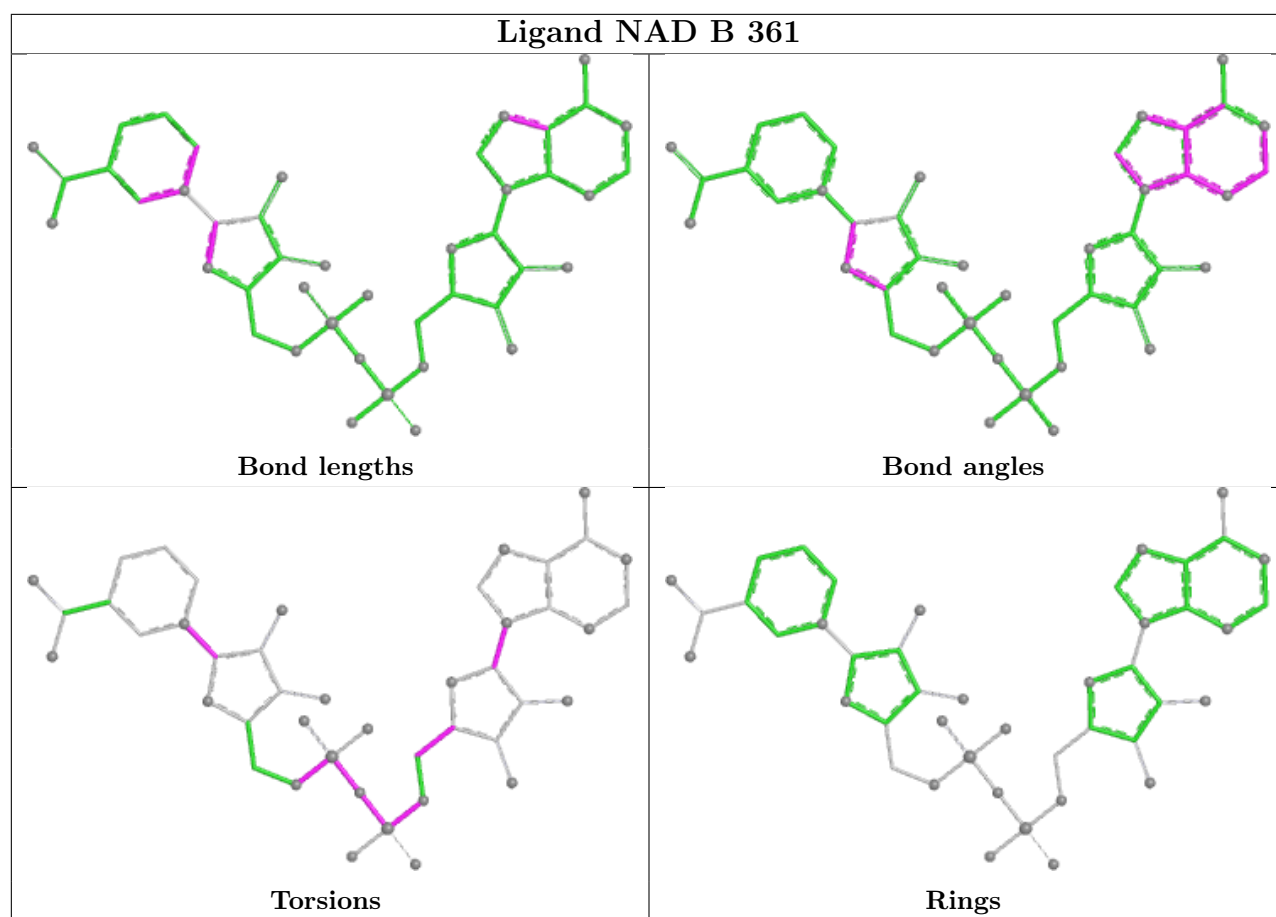
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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.