



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:50 am BST

PDB ID : 1GYP
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

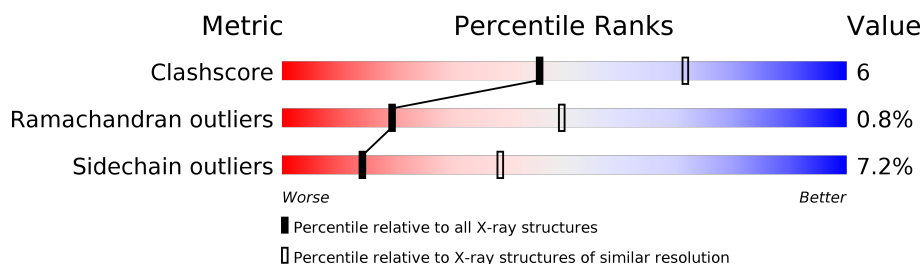
1 Overall quality at a glance

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 on 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 (three-letter code: PO4) (formula: O₄P).



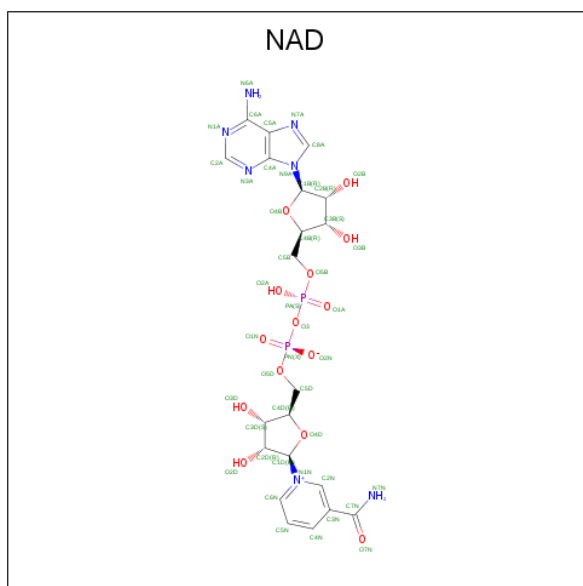
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



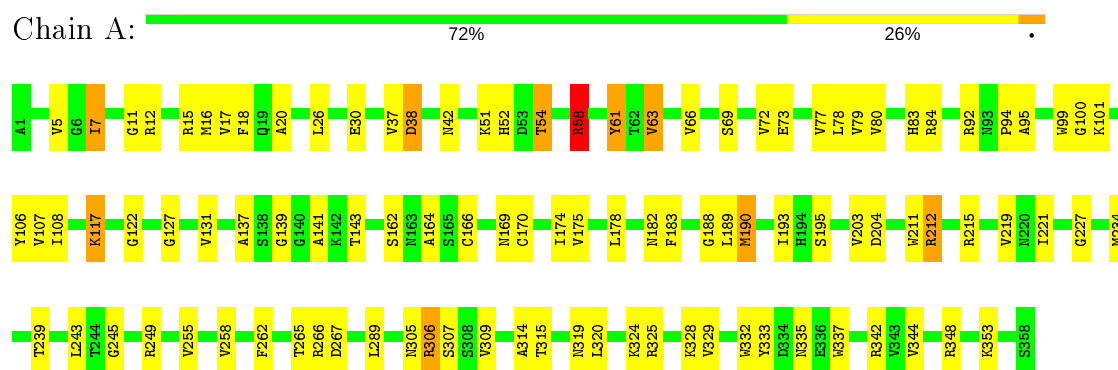
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

3 Residue-property plots

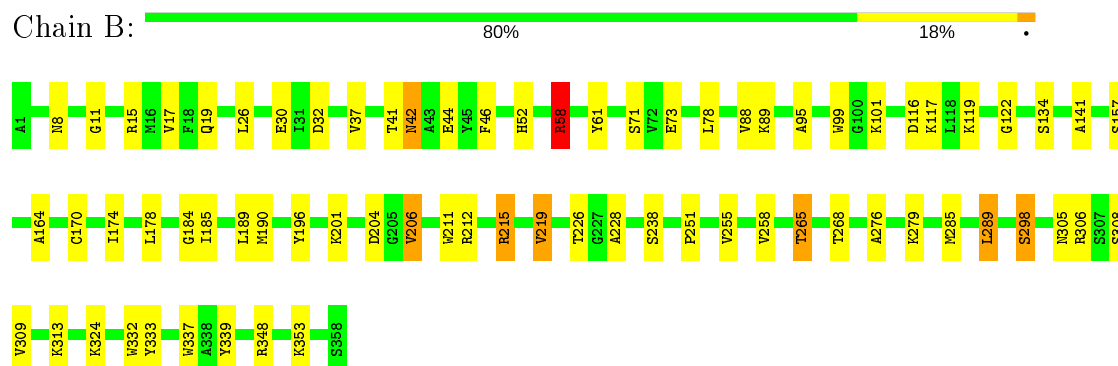
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

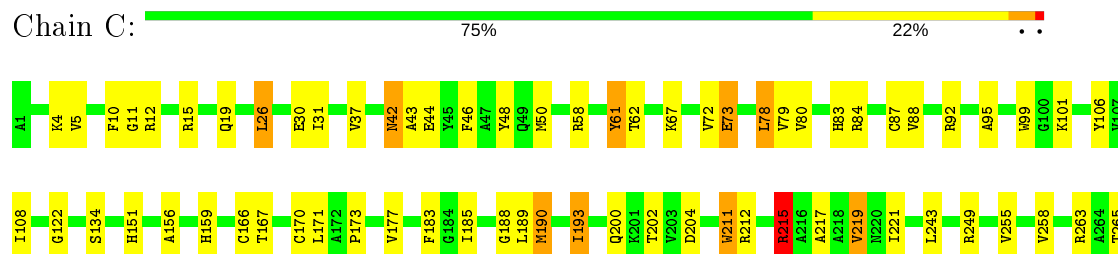
• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



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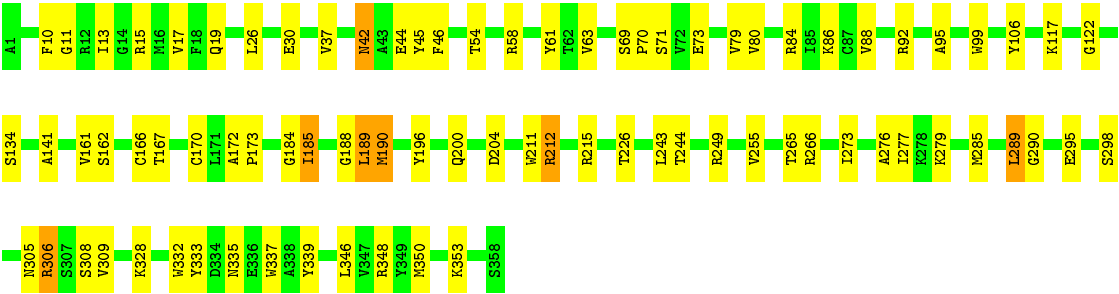


• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE





● Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE 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 21	Depositor
Cell constants a, b, c, α , β , γ	99.00 Å 126.50 Å 138.90 Å 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	0.75	0/2768	1.48	34/3752 (0.9%)
1	B	0.79	0/2768	1.44	26/3752 (0.7%)
1	C	0.75	0/2768	1.47	35/3752 (0.9%)
1	D	0.77	0/2768	1.43	24/3752 (0.6%)
All	All	0.76	0/11072	1.46	119/15008 (0.8%)

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

There are no bond length outliers.

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	ARG	NE-CZ-NH1	13.44	127.02	120.30
1	A	215	ARG	NE-CZ-NH1	12.01	126.30	120.30
1	C	215	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	C	332	TRP	CD1-CG-CD2	9.66	114.03	106.30
1	D	332	TRP	CD1-CG-CD2	9.46	113.87	106.30
1	B	332	TRP	CD1-CG-CD2	9.30	113.74	106.30
1	B	99	TRP	CD1-CG-CD2	8.93	113.44	106.30
1	D	99	TRP	CD1-CG-CD2	8.88	113.41	106.30
1	A	337	TRP	CD1-CG-CD2	8.78	113.32	106.30
1	D	215	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	D	337	TRP	CD1-CG-CD2	8.53	113.12	106.30
1	A	332	TRP	CD1-CG-CD2	8.48	113.08	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	TRP	CE2-CD2-CG	-8.24	100.71	107.30
1	A	99	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	B	99	TRP	CE2-CD2-CG	-8.09	100.83	107.30
1	C	332	TRP	CE2-CD2-CG	-8.08	100.84	107.30
1	A	99	TRP	CE2-CD2-CG	-8.02	100.88	107.30
1	B	337	TRP	CD1-CG-CD2	8.02	112.72	106.30
1	A	332	TRP	CE2-CD2-CG	-7.98	100.92	107.30
1	D	99	TRP	CE2-CD2-CG	-7.87	101.00	107.30
1	C	99	TRP	CD1-CG-CD2	7.87	112.59	106.30
1	C	337	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	C	15	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	C	99	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	C	211	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	A	337	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	D	337	TRP	CE2-CD2-CG	-7.61	101.22	107.30
1	B	348	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	D	332	TRP	CE2-CD2-CG	-7.53	101.27	107.30
1	D	215	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	C	337	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	D	211	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	B	337	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	A	99	TRP	CG-CD2-CE3	7.21	140.39	133.90
1	D	348	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	D	211	TRP	CD1-CG-CD2	7.12	112.00	106.30
1	C	99	TRP	CG-CD2-CE3	7.08	140.27	133.90
1	B	15	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	C	211	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	B	211	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	B	332	TRP	CG-CD2-CE3	6.82	140.04	133.90
1	A	58	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	A	211	TRP	CE2-CD2-CG	-6.77	101.89	107.30
1	C	306	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	12	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	D	15	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	D	15	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	C	249	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	C	249	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	B	211	TRP	CD1-CG-CD2	6.42	111.43	106.30
1	C	332	TRP	CG-CD1-NE1	-6.40	103.70	110.10
1	A	325	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	99	TRP	CB-CG-CD1	-6.25	118.87	127.00
1	B	332	TRP	CB-CG-CD1	-6.25	118.87	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	339	TYR	CB-CG-CD1	-6.25	117.25	121.00
1	D	332	TRP	CG-CD1-NE1	-6.24	103.86	110.10
1	A	342	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	332	TRP	CG-CD1-NE1	-6.15	103.95	110.10
1	D	348	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	C	263	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	D	266	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	C	99	TRP	CB-CG-CD1	-6.06	119.12	127.00
1	A	16	MET	CG-SD-CE	6.03	109.85	100.20
1	D	99	TRP	CG-CD2-CE3	6.03	139.32	133.90
1	C	15	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	211	TRP	CD1-CG-CD2	5.98	111.08	106.30
1	A	266	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	C	348	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	206	VAL	CG1-CB-CG2	-5.86	101.53	110.90
1	B	212	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	58	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	D	266	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	D	92	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	234	MET	CA-CB-CG	5.76	123.09	113.30
1	A	211	TRP	CG-CD2-CE3	5.75	139.08	133.90
1	A	215	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	58	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	212	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	166	CYS	CA-CB-SG	5.67	124.20	114.00
1	C	348	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	B	58	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	219	VAL	N-CA-CB	-5.63	99.11	111.50
1	A	221	ILE	N-CA-C	-5.62	95.83	111.00
1	D	211	TRP	CG-CD2-CE3	5.57	138.92	133.90
1	C	325	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	306	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	99	TRP	CG-CD2-CE3	5.53	138.88	133.90
1	B	339	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	D	99	TRP	CG-CD1-NE1	-5.52	104.58	110.10
1	A	249	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	99	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	A	92	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	D	196	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	A	203	VAL	CG1-CB-CG2	-5.43	102.21	110.90
1	A	193	ILE	N-CA-C	-5.42	96.36	111.00
1	C	306	ARG	NE-CZ-NH2	-5.41	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	D	99	TRP	CB-CG-CD1	-5.34	120.06	127.00
1	B	17	VAL	CG1-CB-CG2	-5.31	102.40	110.90
1	C	99	TRP	CG-CD1-NE1	-5.31	104.79	110.10
1	A	332	TRP	CG-CD2-CE3	5.30	138.67	133.90
1	C	48	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	A	212	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	215	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	193	ILE	N-CA-C	-5.23	96.87	111.00
1	B	196	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	A	182	ASN	N-CA-C	5.21	125.08	111.00
1	B	32	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	51	LYS	CB-CG-CD	-5.14	98.22	111.60
1	B	15	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	302	ILE	CA-C-N	-5.14	105.90	117.20
1	B	313	LYS	CA-CB-CG	-5.13	102.12	113.40
1	C	12	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	C	339	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	C	61	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	C	84	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	C	332	TRP	CG-CD2-CE3	5.01	138.41	133.90
1	A	61	TYR	CB-CG-CD2	-5.01	118.00	121.00
1	C	219	VAL	N-CA-CB	-5.00	100.49	111.50

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	42	0
1	B	2716	0	2736	30	0
1	C	2716	0	2736	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	141	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 6.

All (141) 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:116:ASP:HB3	1:B:119:LYS:HG3	1.72	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:262:PHE:HE1	1:A:329:VAL:HG23	1.77	0.50
1:A:18:PHE:CZ	1:A:80:VAL:HG21	2.46	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:190:MET:HE2	1:D:226:THR:HG21	1.93	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:95:ALA:HA	1:B:122:GLY:O	2.14	0.47
1:B:8:ASN:HA	1:B:37:VAL:HB	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:285:MET:HB3	1:B:289:LEU:HB2	1.98	0.45
1:B:42:ASN:ND2	1:B:44:GLU:HB2	2.32	0.45
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:190:MET:HE3	1:B:226:THR:HG21	1.99	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:190:MET:HE2	1:B:228:ALA:HB3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:GLU:H	1:C:73:GLU:CD	2.23	0.42
1:B:174:ILE:O	1:B:178:LEU:HG	2.20	0.42
1:B:37:VAL:HG22	1:B:88:VAL:HB	2.02	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:271:GLN:O	1:C:275:LYS:HG3	2.20	0.42
1:C:5:VAL:HA	1:C:106:TYR:O	2.19	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: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
1:B:52:HIS:HD2	1:B:58:ARG:NH1	2.18	0.41
1:D:167:THR:HG1	2:D:359:PO4:P	2.43	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:106:TYR:OH	1:C:351:ALA:HA	2.20	0.40
1:C:42:ASN:ND2	1:C:44:GLU:HB2	2.37	0.40
1:D:106:TYR:N	1:D:106:TYR:CD1	2.89	0.40
1:C:215:ARG:NH1	1:D:54:THR:OG1	2.53	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: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:B:189:LEU:HD22	1:C:326:PHE:HD1	1.86	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%)	14	41
1	B	356/358 (99%)	333 (94%)	20 (6%)	3 (1%)	19	49
1	C	356/358 (99%)	330 (93%)	25 (7%)	1 (0%)	41	72
1	D	356/358 (99%)	332 (93%)	21 (6%)	3 (1%)	19	49
All	All	1424/1432 (99%)	1321 (93%)	92 (6%)	11 (1%)	19	49

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 [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	294/294 (100%)	271 (92%)	23 (8%)	12	35
1	B	294/294 (100%)	275 (94%)	19 (6%)	17	44
1	C	294/294 (100%)	274 (93%)	20 (7%)	16	42
1	D	294/294 (100%)	271 (92%)	23 (8%)	12	35
All	All	1176/1176 (100%)	1091 (93%)	85 (7%)	14	38

All (85) 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
1	A	38	ASP
1	A	42	ASN
1	A	54	THR
1	A	58	ARG
1	A	63	VAL
1	A	73	GLU
1	A	78	LEU
1	A	94	PRO
1	A	101	LYS
1	A	190	MET
1	A	195	SER
1	A	204	ASP
1	A	289	LEU
1	A	305	ASN
1	A	306	ARG
1	A	309	VAL
1	A	319	ASN
1	A	335	ASN
1	A	348	ARG
1	A	353	LYS
1	B	26	LEU
1	B	30	GLU
1	B	42	ASN
1	B	58	ARG
1	B	71	SER
1	B	73	GLU
1	B	78	LEU
1	B	101	LYS
1	B	157	SER
1	B	185	ILE

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Mol	Chain	Res	Type
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	306	ARG
1	B	309	VAL
1	B	353	LYS
1	C	4	LYS
1	C	26	LEU
1	C	30	GLU
1	C	42	ASN
1	C	58	ARG
1	C	73	GLU
1	C	78	LEU
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	289	LEU
1	C	306	ARG
1	C	309	VAL
1	C	353	LYS
1	D	26	LEU
1	D	30	GLU
1	D	42	ASN
1	D	58	ARG
1	D	69	SER
1	D	71	SER
1	D	73	GLU
1	D	86	LYS
1	D	162	SER
1	D	166	CYS
1	D	185	ILE
1	D	189	LEU
1	D	190	MET

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Mol	Chain	Res	Type
1	D	204	ASP
1	D	212	ARG
1	D	265	THR
1	D	289	LEU
1	D	298	SER
1	D	305	ASN
1	D	306	ARG
1	D	309	VAL
1	D	335	ASN
1	D	353	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	42	ASN
1	A	52	HIS
1	A	159	HIS
1	A	305	ASN
1	B	8	ASN
1	B	42	ASN
1	B	52	HIS
1	B	151	HIS
1	B	305	ASN
1	C	8	ASN
1	C	42	ASN
1	C	52	HIS
1	C	81	ASN
1	C	159	HIS
1	D	8	ASN
1	D	42	ASN
1	D	81	ASN
1	D	305	ASN

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 carbohydrates 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$
3	NAD	D	361	-	42,48,48	1.21	3 (7%)	50,73,73	1.17	5 (10%)
2	PO4	D	360	-	4,4,4	0.87	0	6,6,6	0.39	0
3	NAD	B	361	-	42,48,48	1.12	2 (4%)	50,73,73	1.21	3 (6%)
2	PO4	B	360	-	4,4,4	1.05	0	6,6,6	0.56	0
2	PO4	B	359	-	4,4,4	0.79	0	6,6,6	1.02	0
2	PO4	C	359	-	4,4,4	1.00	0	6,6,6	0.98	0
2	PO4	A	359	-	4,4,4	0.83	0	6,6,6	0.66	0
2	PO4	C	360	-	4,4,4	1.16	0	6,6,6	0.62	0
3	NAD	C	361	-	42,48,48	1.27	4 (9%)	50,73,73	1.17	3 (6%)
2	PO4	A	360	-	4,4,4	1.10	0	6,6,6	0.51	0
3	NAD	A	361	-	42,48,48	1.31	5 (11%)	50,73,73	1.22	4 (8%)
2	PO4	D	359	-	4,4,4	1.26	1 (25%)	6,6,6	0.61	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	C	361	-	-	2/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	D	361	-	-	3/26/62/62	0/5/5/5
3	NAD	A	361	-	-	7/26/62/62	0/5/5/5
3	NAD	B	361	-	-	7/26/62/62	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	361	NAD	C2N-N1N	5.79	1.42	1.35
3	C	361	NAD	C2N-N1N	5.76	1.42	1.35
3	D	361	NAD	C2N-N1N	5.30	1.41	1.35
3	B	361	NAD	C2N-N1N	4.56	1.40	1.35
3	A	361	NAD	O4D-C1D	2.60	1.44	1.41
2	D	359	PO4	P-O1	2.43	1.56	1.50
3	C	361	NAD	C3N-C7N	2.26	1.54	1.50
3	D	361	NAD	C6N-N1N	2.25	1.40	1.35
3	C	361	NAD	C6N-N1N	2.24	1.40	1.35
3	A	361	NAD	O4B-C1B	2.24	1.44	1.41
3	D	361	NAD	O4B-C1B	2.23	1.44	1.41
3	C	361	NAD	O4D-C1D	2.20	1.44	1.41
3	A	361	NAD	C2B-C1B	-2.19	1.50	1.53
3	A	361	NAD	C6N-N1N	2.16	1.40	1.35
3	B	361	NAD	O4D-C1D	2.01	1.43	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	361	NAD	N3A-C2A-N1A	-4.37	121.86	128.68
3	A	361	NAD	N3A-C2A-N1A	-4.24	122.05	128.68
3	B	361	NAD	N3A-C2A-N1A	-4.10	122.27	128.68
3	C	361	NAD	N3A-C2A-N1A	-4.03	122.37	128.68
3	B	361	NAD	C4A-C5A-N7A	2.91	112.43	109.40
3	A	361	NAD	C1B-N9A-C4A	-2.70	121.89	126.64
3	A	361	NAD	C4A-C5A-N7A	2.45	111.95	109.40
3	C	361	NAD	C4A-C5A-N7A	2.31	111.80	109.40
3	B	361	NAD	O4D-C1D-C2D	-2.23	103.67	106.93
3	D	361	NAD	C4A-C5A-N7A	2.20	111.69	109.40
3	C	361	NAD	C5A-C6A-N1A	-2.14	115.50	120.35
3	A	361	NAD	C2N-N1N-C1D	2.10	123.82	119.14
3	D	361	NAD	O2N-PN-O1N	2.06	122.43	112.24
3	D	361	NAD	C6N-N1N-C2N	-2.04	120.12	121.97
3	D	361	NAD	O4B-C1B-C2B	-2.00	104.00	106.93

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	361	NAD	O4D-C1D-N1N-C2N
3	D	361	NAD	C2D-C1D-N1N-C2N
3	C	361	NAD	O4D-C1D-N1N-C2N
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	C5D-O5D-PN-O2N
3	B	361	NAD	O4D-C1D-N1N-C2N
3	B	361	NAD	PN-O3-PA-O5B
3	B	361	NAD	C5D-O5D-PN-O3
3	A	361	NAD	C5B-O5B-PA-O2A
3	B	361	NAD	C5B-O5B-PA-O1A
3	D	361	NAD	O4B-C4B-C5B-O5B
3	A	361	NAD	O4B-C4B-C5B-O5B
3	B	361	NAD	O4B-C4B-C5B-O5B
3	A	361	NAD	C5B-O5B-PA-O3
3	A	361	NAD	C2D-C1D-N1N-C2N
3	B	361	NAD	C5D-O5D-PN-O1N
3	C	361	NAD	O4B-C4B-C5B-O5B

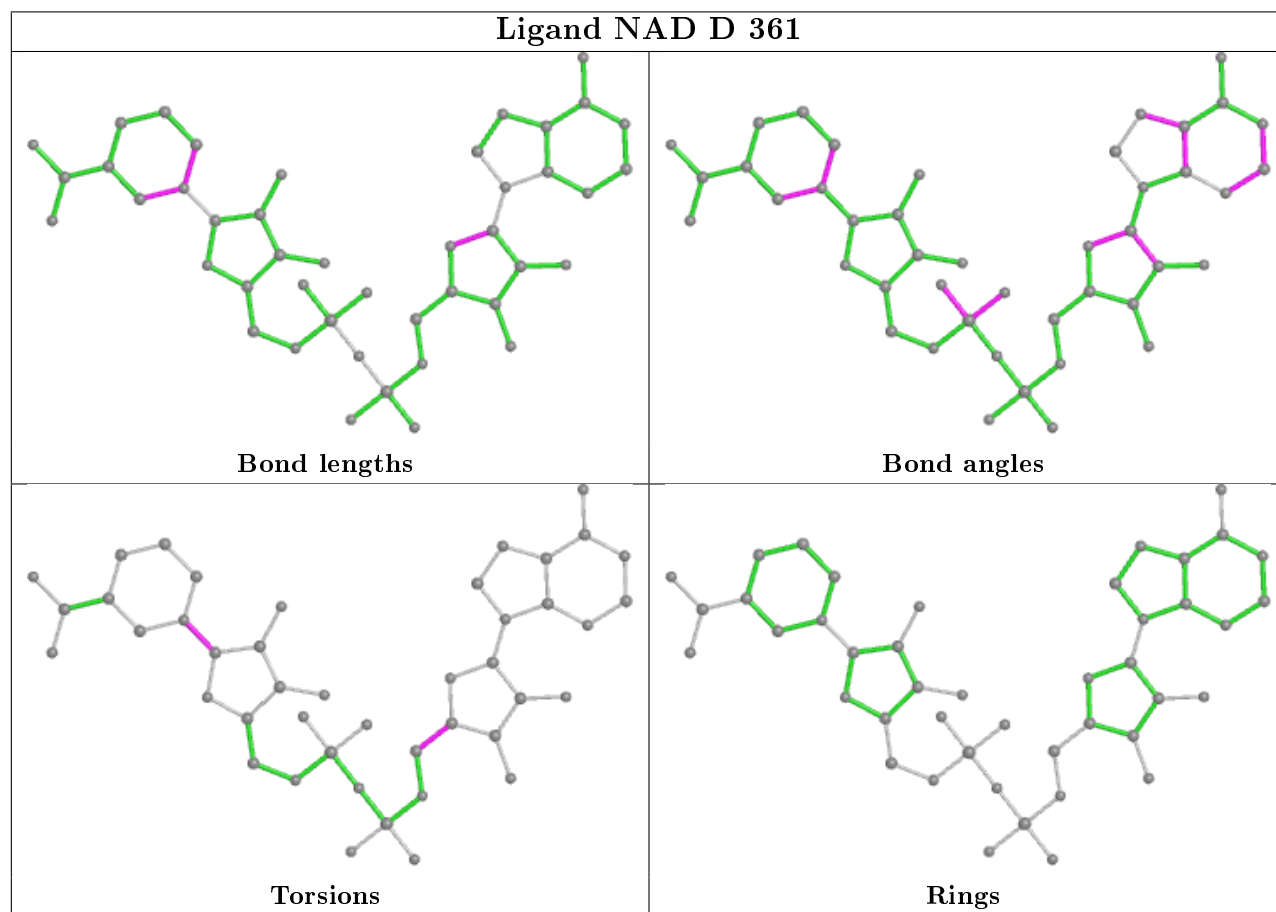
There are no ring outliers.

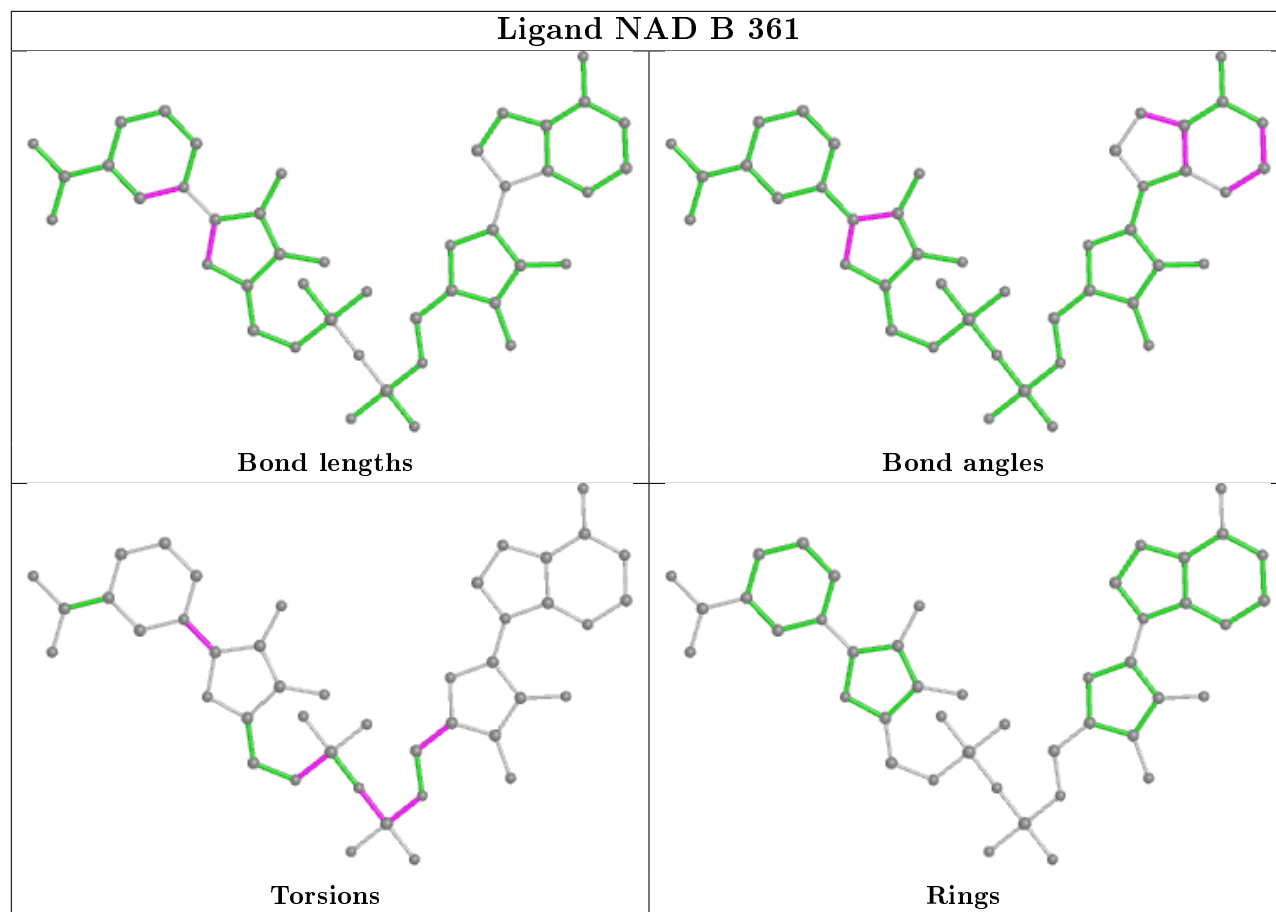
7 monomers are involved in 12 short contacts:

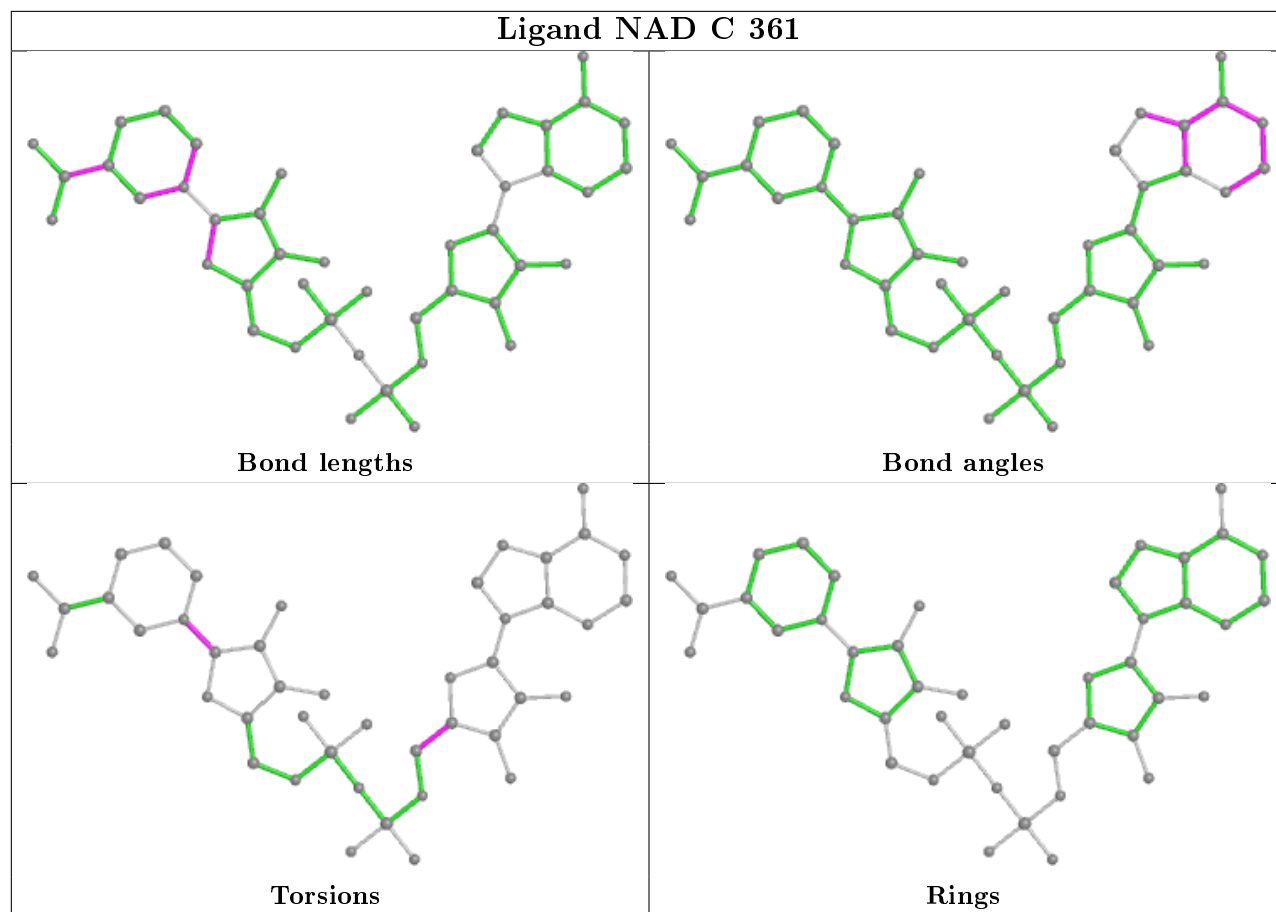
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	361	NAD	2	0
3	B	361	NAD	2	0
2	C	359	PO4	1	0
2	A	359	PO4	1	0
3	C	361	NAD	3	0
3	A	361	NAD	2	0
2	D	359	PO4	1	0

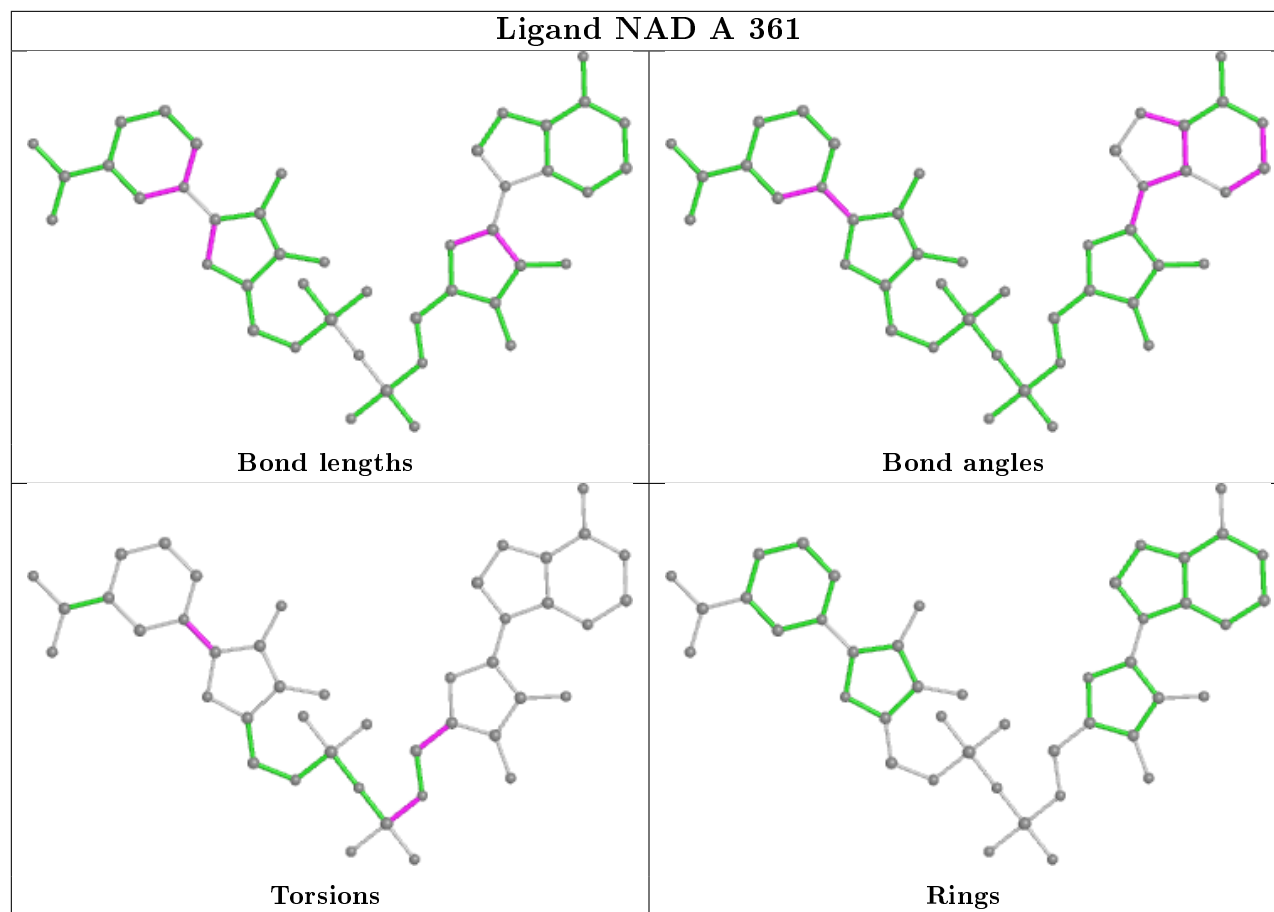
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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