



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 11:53 PM UTC

PDB ID : 1A7K / pdb_00001a7k
Title : GLYCOSOMAL GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE IN A MONOCLINIC CRYSTAL FORM
Authors : Kim, H.; Hol, W.G.J.
Deposited on : 1998-03-16
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

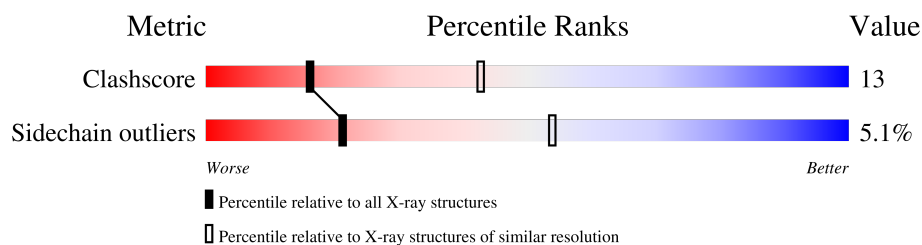
1 Overall quality at a glance

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)
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	360	69% 28% ..
1	B	360	59% 37% ..
1	C	360	71% 26% ..
1	D	360	66% 31% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	361	-	-	X	-

2 Entry composition [i](#)

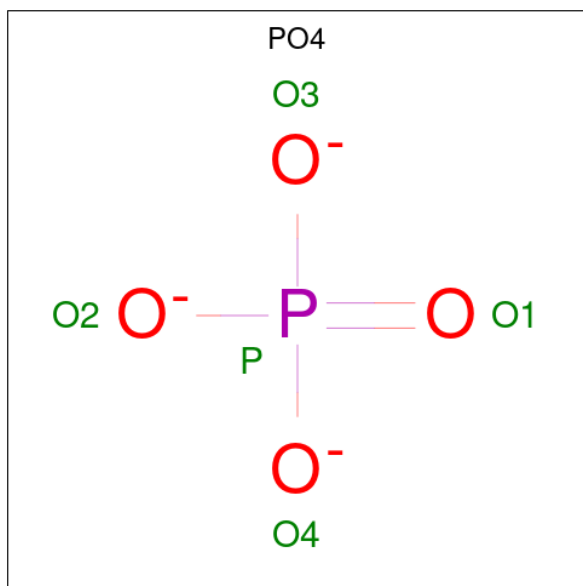
There are 3 unique types of molecules in this entry. The entry contains 11076 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			2715	1712	474	516	13			
1	B	358	Total	C	N	O	S	0	0	0
			2715	1712	474	516	13			
1	C	358	Total	C	N	O	S	0	0	0
			2715	1712	474	516	13			
1	D	358	Total	C	N	O	S	0	0	0
			2715	1712	474	516	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		

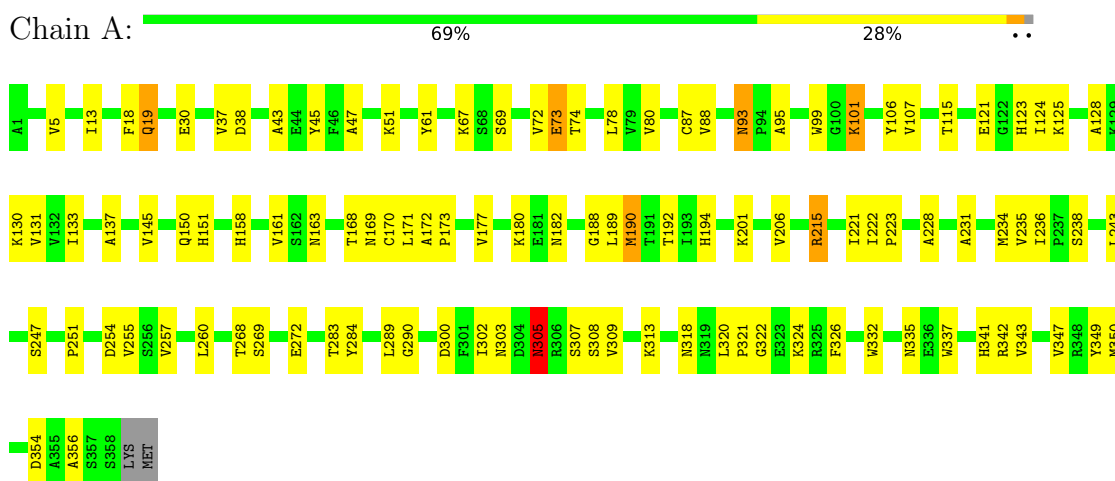
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3 Residue-property plots

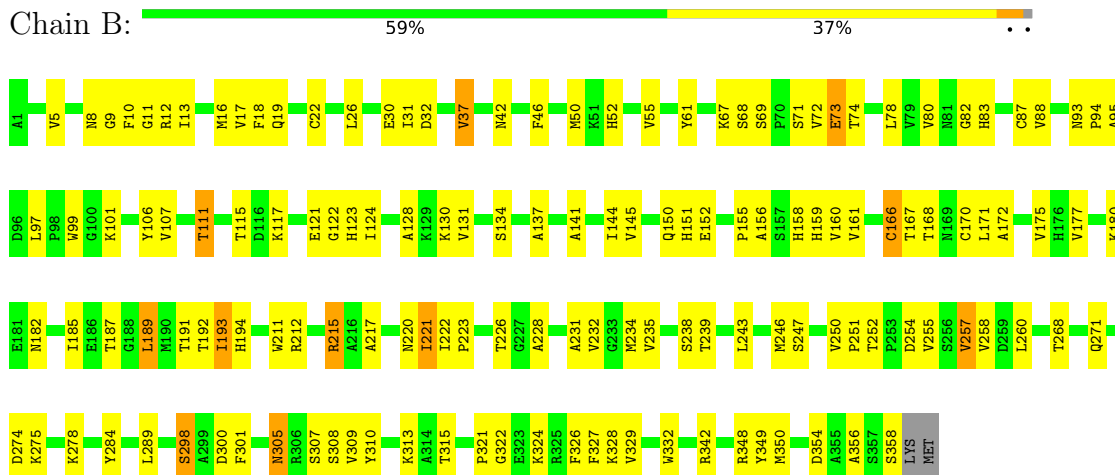
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

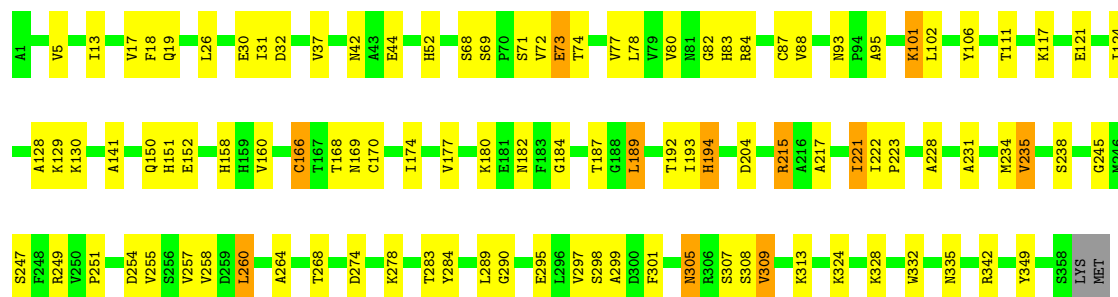


• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



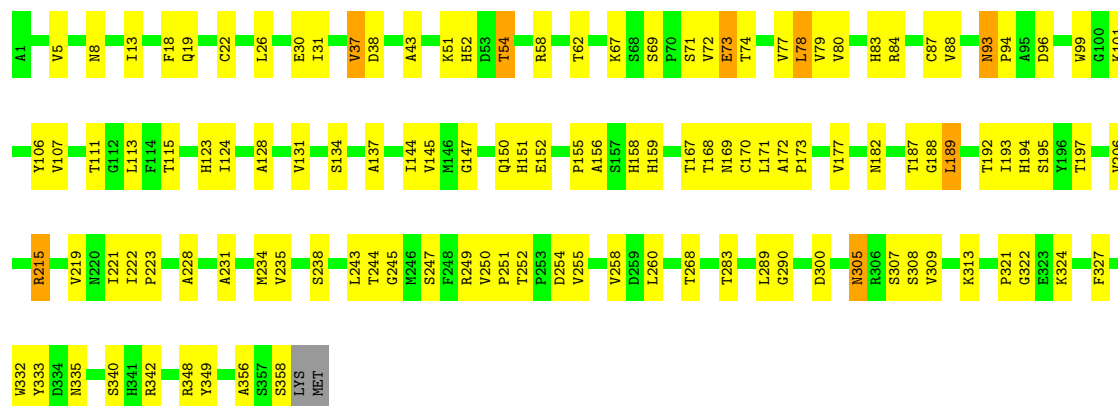
• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE





● Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

Chain D: 66% 31% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.90Å 81.00Å 131.90Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	81.0 (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.217 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11076	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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	0.67	1/2767 (0.0%)	1.07	17/3752 (0.5%)
1	B	0.63	0/2767	1.04	15/3752 (0.4%)
1	C	0.65	0/2767	1.07	14/3752 (0.4%)
1	D	0.64	1/2767 (0.0%)	1.05	17/3752 (0.5%)
All	All	0.65	2/11068 (0.0%)	1.06	63/15008 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	250	VAL	CA-CB	-5.66	1.50	1.55
1	A	222	ILE	CA-C	-5.53	1.48	1.53

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	221	ILE	N-CA-C	-7.97	95.63	107.51
1	A	222	ILE	N-CA-C	7.78	115.25	107.55
1	C	221	ILE	N-CA-C	-7.61	96.11	107.37
1	C	335	ASN	N-CA-C	7.44	121.45	112.38
1	B	221	ILE	N-CA-C	-7.26	96.69	107.51
1	A	320	LEU	CA-C-N	7.08	126.33	118.97
1	A	320	LEU	C-N-CA	7.08	126.33	118.97
1	C	194	HIS	N-CA-C	6.89	120.69	109.59
1	C	305	ASN	N-CA-C	6.86	121.35	113.19
1	C	158	HIS	N-CA-C	6.64	118.97	108.67
1	A	158	HIS	N-CA-C	6.61	118.67	109.15
1	C	235	VAL	N-CA-C	-6.53	106.61	111.90
1	D	356	ALA	N-CA-C	-6.50	103.81	111.03
1	C	217	ALA	N-CA-C	6.30	118.67	111.11
1	B	305	ASN	N-CA-C	6.24	120.50	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	158	HIS	N-CA-C	6.19	118.06	109.15
1	A	305	ASN	N-CA-C	6.18	120.68	113.20
1	D	305	ASN	N-CA-C	6.06	120.40	113.19
1	B	158	HIS	N-CA-C	6.03	117.83	109.15
1	B	55	VAL	N-CA-C	6.02	119.51	111.44
1	A	356	ALA	N-CA-C	-6.00	104.38	111.03
1	D	37	VAL	N-CA-C	6.00	116.50	108.11
1	C	111	THR	N-CA-C	-5.99	105.81	113.23
1	B	222	ILE	N-CA-C	5.99	113.47	107.55
1	A	283	THR	N-CA-C	5.90	117.50	108.12
1	A	335	ASN	N-CA-C	5.86	119.52	112.38
1	D	111	THR	N-CA-C	-5.74	106.12	113.23
1	B	37	VAL	N-CA-C	5.73	116.14	108.11
1	B	111	THR	N-CA-C	-5.66	106.21	113.23
1	A	221	ILE	N-CA-C	-5.65	98.30	106.88
1	D	93	ASN	CA-C-N	5.61	125.27	119.05
1	D	93	ASN	C-N-CA	5.61	125.27	119.05
1	A	318	ASN	N-CA-C	5.56	119.25	111.30
1	B	194	HIS	N-CA-C	5.56	118.55	109.59
1	B	193	ILE	N-CA-C	-5.52	99.65	107.98
1	D	182	ASN	N-CA-C	5.49	119.26	112.24
1	D	335	ASN	N-CA-C	5.48	119.46	112.34
1	A	182	ASN	N-CA-C	5.44	119.21	112.24
1	D	222	ILE	N-CA-C	5.40	113.38	107.60
1	C	222	ILE	N-CA-C	5.27	113.24	107.60
1	B	356	ALA	N-CA-C	-5.27	105.18	111.03
1	D	283	THR	N-CA-C	5.23	116.46	108.30
1	D	206	VAL	N-CA-C	5.20	116.07	108.58
1	B	250	VAL	CA-C-N	5.20	126.34	119.84
1	B	250	VAL	C-N-CA	5.20	126.34	119.84
1	C	283	THR	N-CA-C	5.18	116.36	108.12
1	A	236	ILE	CA-C-N	5.18	124.98	119.28
1	A	236	ILE	C-N-CA	5.18	124.98	119.28
1	B	327	PHE	N-CA-C	5.15	117.23	109.41
1	D	197	THR	N-CA-C	5.14	116.48	109.18
1	C	260	LEU	N-CA-C	5.14	117.94	109.76
1	A	93	ASN	CA-C-N	5.13	125.17	119.32
1	A	93	ASN	C-N-CA	5.13	125.17	119.32
1	D	245	GLY	N-CA-C	5.13	119.08	110.56
1	C	223	PRO	N-CA-C	-5.13	103.14	111.19
1	C	245	GLY	N-CA-C	5.12	118.06	110.42
1	D	327	PHE	N-CA-C	5.12	117.64	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	HIS	N-CA-C	5.11	117.82	109.59
1	C	182	ASN	N-CA-C	5.09	118.75	112.24
1	B	217	ALA	N-CA-C	5.06	117.20	111.02
1	A	222	ILE	CB-CA-C	-5.04	105.09	111.04
1	B	182	ASN	N-CA-C	5.04	118.69	112.24
1	D	54	THR	N-CA-C	5.00	117.38	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2715	0	2736	69	0
1	B	2715	0	2736	102	0
1	C	2715	0	2736	67	0
1	D	2715	0	2736	75	0
2	A	10	0	0	0	0
2	B	10	0	0	2	0
2	C	10	0	0	2	0
2	D	10	0	0	1	0
3	A	44	0	26	2	0
3	B	44	0	26	5	0
3	C	44	0	26	1	0
3	D	44	0	26	3	0
All	All	11076	0	11048	290	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 13.

All (290) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HG22	1:A:88:VAL:HB	1.58	0.83
1:B:166:CYS:SG	3:B:363:NAD:H4N	2.20	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:THR:O	1:B:324:LYS:HA	1.82	0.80
1:D:268:THR:O	1:D:324:LYS:HA	1.88	0.73
1:C:268:THR:O	1:C:324:LYS:HA	1.89	0.73
1:B:251:PRO:HB2	1:C:251:PRO:HB2	1.71	0.71
1:B:298:SER:HB3	1:C:221:ILE:H	1.55	0.70
1:A:268:THR:O	1:A:324:LYS:HA	1.91	0.70
1:A:192:THR:HG23	1:A:247:SER:HB2	1.73	0.70
1:B:22:CYS:SG	1:B:80:VAL:HG11	2.32	0.68
1:C:13:ILE:O	1:C:17:VAL:HG23	1.92	0.68
1:C:168:THR:OG1	1:C:228:ALA:HA	1.92	0.68
1:D:156:ALA:O	1:D:159:HIS:HE1	1.78	0.66
1:B:168:THR:OG1	1:B:228:ALA:HA	1.96	0.66
1:C:78:LEU:CD2	1:C:87:CYS:SG	2.84	0.66
1:D:18:PHE:CZ	1:D:80:VAL:HG21	2.31	0.66
1:B:166:CYS:SG	3:B:363:NAD:C4N	2.85	0.65
1:A:5:VAL:HG12	1:A:106:TYR:HB2	1.79	0.65
1:D:18:PHE:HZ	1:D:80:VAL:HG21	1.62	0.65
1:D:192:THR:HG23	1:D:247:SER:HB2	1.79	0.64
1:D:188:GLY:O	1:D:243:LEU:HD12	1.98	0.64
1:C:231:ALA:HA	1:C:234:MET:HE3	1.80	0.63
1:D:5:VAL:HG12	1:D:106:TYR:HB2	1.80	0.62
1:B:73:GLU:HG2	1:B:74:THR:HG23	1.79	0.62
1:C:170:CYS:HA	1:C:308:SER:HB2	1.82	0.61
1:C:194:HIS:HB3	1:C:249:ARG:HD3	1.81	0.61
1:C:313:LYS:HA	1:C:313:LYS:HE2	1.81	0.61
1:A:337:TRP:O	1:A:341:HIS:HD2	1.83	0.61
1:A:251:PRO:HB2	1:D:251:PRO:HB2	1.81	0.61
1:B:12:ARG:O	1:B:16:MET:HG2	2.01	0.61
1:B:313:LYS:HE2	1:B:313:LYS:HA	1.83	0.60
1:A:321:PRO:HG2	1:A:322:GLY:H	1.65	0.60
1:A:168:THR:OG1	1:A:228:ALA:HA	2.01	0.59
1:A:19:GLN:HG2	1:A:61:TYR:HE2	1.67	0.59
1:A:188:GLY:O	1:A:243:LEU:HD12	2.02	0.59
1:D:321:PRO:HG2	1:D:322:GLY:H	1.67	0.59
1:A:67:LYS:HB2	1:A:72:VAL:HG23	1.85	0.59
1:B:212:ARG:HG2	1:C:295:GLU:HB3	1.84	0.59
1:B:13:ILE:O	1:B:17:VAL:HG23	2.03	0.59
1:D:69:SER:O	1:D:72:VAL:HG22	2.03	0.59
1:D:151:HIS:HA	1:D:349:TYR:OH	2.02	0.59
1:B:161:VAL:HG21	1:B:350:MET:SD	2.42	0.59
1:D:43:ALA:HB1	1:D:78:LEU:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:CYS:HA	1:A:308:SER:HB2	1.83	0.58
1:B:134:SER:O	3:B:363:NAD:H1D	2.04	0.58
1:D:37:VAL:HG22	1:D:88:VAL:HB	1.86	0.58
1:C:73:GLU:HG2	1:C:74:THR:HG23	1.85	0.58
1:B:5:VAL:HG12	1:B:106:TYR:HB2	1.86	0.57
1:B:144:ILE:CG2	1:B:150:GLN:HA	2.34	0.57
1:A:69:SER:O	1:A:72:VAL:HG22	2.03	0.57
1:B:124:ILE:HA	1:B:128:ALA:O	2.04	0.57
1:B:167:THR:HB	2:B:361:PO4:O4	2.04	0.57
1:B:223:PRO:HG2	1:C:332:TRP:HZ2	1.68	0.57
1:D:231:ALA:HA	1:D:234:MET:HE3	1.85	0.57
1:A:43:ALA:HB1	1:A:78:LEU:HD13	1.86	0.56
1:B:175:VAL:HG11	1:B:239:THR:HG21	1.87	0.56
1:C:69:SER:O	1:C:72:VAL:HG22	2.05	0.56
1:D:168:THR:OG1	1:D:228:ALA:HA	2.06	0.56
1:B:99:TRP:HA	1:B:99:TRP:CE3	2.40	0.56
1:C:78:LEU:HD22	1:C:87:CYS:SG	2.46	0.56
1:C:5:VAL:HG12	1:C:106:TYR:HB2	1.86	0.56
1:A:188:GLY:C	1:A:243:LEU:HD12	2.31	0.55
1:B:151:HIS:HA	1:B:349:TYR:OH	2.06	0.55
1:B:231:ALA:HA	1:B:234:MET:HE3	1.88	0.55
1:D:195:SER:HB3	1:D:252:THR:O	2.06	0.55
1:B:170:CYS:SG	1:B:258:VAL:CG2	2.94	0.55
1:C:174:ILE:HD13	1:C:289:LEU:HD11	1.89	0.55
1:D:78:LEU:HD22	1:D:87:CYS:SG	2.46	0.55
1:D:258:VAL:HG23	1:D:333:TYR:HE1	1.71	0.55
1:B:123:HIS:HB2	1:B:131:VAL:HG21	1.88	0.54
1:C:151:HIS:CE1	1:C:152:GLU:HG3	2.43	0.54
1:B:180:LYS:HD3	1:B:284:TYR:CE2	2.43	0.54
1:B:170:CYS:SG	1:B:258:VAL:HG21	2.48	0.54
1:C:192:THR:HG23	1:C:247:SER:HB2	1.90	0.54
1:C:101:LYS:HD3	1:C:101:LYS:C	2.33	0.53
1:B:170:CYS:HA	1:B:308:SER:HB2	1.90	0.53
1:D:107:VAL:HB	1:D:131:VAL:HG22	1.91	0.53
1:B:18:PHE:CZ	1:B:80:VAL:HG21	2.44	0.53
1:B:141:ALA:HB1	1:B:160:VAL:O	2.09	0.53
1:B:156:ALA:O	1:B:159:HIS:HE1	1.91	0.53
1:B:307:SER:OG	1:B:342:ARG:HD2	2.08	0.53
1:D:258:VAL:HG23	1:D:333:TYR:CE1	2.43	0.53
1:B:37:VAL:HG22	1:B:88:VAL:HB	1.90	0.53
1:B:192:THR:HG23	1:B:247:SER:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:PHE:CE2	1:B:332:TRP:CG	2.96	0.53
1:D:124:ILE:HA	1:D:128:ALA:O	2.09	0.53
1:D:170:CYS:HA	1:D:308:SER:HB2	1.90	0.52
1:B:150:GLN:N	1:B:150:GLN:OE1	2.42	0.52
1:B:226:THR:HG1	2:B:361:PO4:P	2.33	0.52
1:D:67:LYS:HB2	1:D:72:VAL:HG23	1.91	0.52
1:B:99:TRP:HA	1:B:99:TRP:HE3	1.75	0.52
1:B:69:SER:O	1:B:72:VAL:HG22	2.09	0.52
1:B:171:LEU:HD11	1:B:260:LEU:HD22	1.92	0.52
1:B:42:ASN:O	1:B:46:PHE:HD1	1.93	0.52
1:D:8:ASN:HD22	1:D:37:VAL:HB	1.75	0.52
1:B:221:ILE:HB	1:C:298:SER:HB3	1.91	0.51
1:B:95:ALA:HA	1:B:122:GLY:O	2.11	0.51
1:B:78:LEU:CD2	1:B:87:CYS:SG	2.98	0.51
1:C:37:VAL:HG22	1:C:88:VAL:HB	1.92	0.51
1:B:289:LEU:C	1:B:289:LEU:HD23	2.36	0.51
1:A:78:LEU:HD22	1:A:87:CYS:SG	2.50	0.51
1:B:11:GLY:HA3	3:B:363:NAD:O5B	2.11	0.51
1:C:307:SER:OG	1:C:342:ARG:HD2	2.11	0.51
1:D:151:HIS:CE1	1:D:152:GLU:HG3	2.45	0.51
1:A:67:LYS:HB2	1:A:72:VAL:CG2	2.41	0.51
1:B:221:ILE:HD13	1:C:193:ILE:HG22	1.93	0.50
1:A:223:PRO:HG2	1:D:332:TRP:HZ2	1.77	0.50
1:D:123:HIS:HB2	1:D:131:VAL:HG21	1.94	0.50
1:A:18:PHE:CZ	1:A:80:VAL:HG21	2.47	0.50
1:A:124:ILE:HA	1:A:128:ALA:O	2.11	0.50
1:B:215:ARG:HG3	1:C:297:VAL:HG11	1.94	0.50
1:D:254:ASP:O	1:D:255:VAL:HB	2.12	0.49
1:A:101:LYS:O	1:A:101:LYS:HE2	2.12	0.49
1:D:115:THR:O	1:D:137:ALA:HA	2.12	0.49
1:A:313:LYS:HE2	1:A:313:LYS:HA	1.93	0.49
1:A:307:SER:OG	1:A:342:ARG:HD2	2.12	0.49
1:C:151:HIS:HA	1:C:349:TYR:OH	2.12	0.49
1:C:166:CYS:SG	2:C:361:PO4:O3	2.68	0.49
1:C:169:ASN:O	1:C:307:SER:HB3	2.13	0.49
1:C:289:LEU:HD23	1:C:290:GLY:N	2.28	0.49
1:B:144:ILE:HG21	1:B:150:GLN:HA	1.95	0.48
1:B:189:LEU:HD23	1:C:328:LYS:HB2	1.94	0.48
1:C:93:ASN:OD1	1:C:95:ALA:HB3	2.13	0.48
1:C:78:LEU:HD21	1:C:87:CYS:SG	2.53	0.48
1:C:170:CYS:SG	1:C:258:VAL:HG21	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:LYS:HD3	1:C:284:TYR:CE2	2.49	0.48
1:D:172:ALA:HB3	1:D:173:PRO:HD3	1.95	0.48
1:A:332:TRP:HZ2	1:D:223:PRO:HG2	1.78	0.48
1:B:8:ASN:HD22	1:B:37:VAL:HB	1.78	0.48
1:B:97:LEU:HD13	1:B:99:TRP:CZ2	2.49	0.48
1:C:301:PHE:CZ	1:C:332:TRP:CD1	3.02	0.48
1:B:82:GLY:O	1:B:83:HIS:HB2	2.14	0.47
1:B:191:THR:HA	1:B:246:MET:O	2.14	0.47
1:B:328:LYS:HB2	1:C:189:LEU:HD23	1.97	0.47
1:C:170:CYS:SG	1:C:258:VAL:CG2	3.02	0.47
1:A:115:THR:O	1:A:137:ALA:HA	2.14	0.47
1:B:52:HIS:HB3	1:D:300:ASP:OD1	2.14	0.47
1:D:219:VAL:HG12	1:D:219:VAL:O	2.12	0.47
1:A:231:ALA:O	1:A:235:VAL:HG23	2.15	0.47
1:A:289:LEU:HD23	1:A:290:GLY:N	2.30	0.47
1:B:67:LYS:HB2	1:B:72:VAL:HG23	1.96	0.47
1:C:18:PHE:CZ	1:C:80:VAL:HG21	2.49	0.47
2:C:362:PO4:O4	3:C:363:NAD:O2D	2.32	0.47
1:D:169:ASN:O	1:D:307:SER:HB3	2.15	0.47
1:A:47:ALA:O	1:A:51:LYS:HG3	2.15	0.47
1:A:215:ARG:NH2	1:D:300:ASP:OD2	2.48	0.47
1:C:231:ALA:O	1:C:235:VAL:HG23	2.15	0.47
1:A:321:PRO:HG2	1:A:322:GLY:N	2.30	0.46
1:C:290:GLY:O	1:C:309:VAL:HA	2.14	0.46
1:D:134:SER:O	3:D:363:NAD:H1D	2.16	0.46
1:D:99:TRP:CE3	1:D:99:TRP:HA	2.51	0.46
1:A:171:LEU:HD11	1:A:260:LEU:HD22	1.96	0.46
1:A:268:THR:OG1	1:A:269:SER:N	2.48	0.46
1:B:115:THR:O	1:B:137:ALA:HA	2.15	0.46
1:C:141:ALA:HB1	1:C:160:VAL:O	2.16	0.46
1:D:189:LEU:HD12	1:D:244:THR:HG22	1.97	0.46
1:D:219:VAL:O	1:D:219:VAL:CG1	2.64	0.46
1:C:73:GLU:HG2	1:C:74:THR:N	2.31	0.46
1:D:170:CYS:SG	1:D:258:VAL:HG21	2.56	0.46
1:D:194:HIS:HB3	1:D:249:ARG:HD3	1.98	0.46
1:B:151:HIS:CE1	1:B:152:GLU:HG3	2.51	0.46
1:A:107:VAL:HB	1:A:131:VAL:HG22	1.98	0.46
1:D:26:LEU:HD23	1:D:348:ARG:HD2	1.98	0.46
1:C:124:ILE:HA	1:C:128:ALA:O	2.16	0.45
1:D:193:ILE:HD12	1:D:193:ILE:N	2.31	0.45
1:D:313:LYS:HE2	1:D:313:LYS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:HG2	1:A:74:THR:HG23	1.98	0.45
1:B:326:PHE:HE1	1:C:189:LEU:HB2	1.81	0.45
1:D:22:CYS:SG	1:D:80:VAL:HG11	2.56	0.45
1:D:77:VAL:HG21	1:D:84:ARG:NH2	2.30	0.45
1:D:155:PRO:HB3	1:D:358:SER:O	2.16	0.45
1:B:78:LEU:HD22	1:B:87:CYS:SG	2.56	0.45
1:C:42:ASN:ND2	1:C:44:GLU:HB2	2.31	0.45
1:A:130:LYS:HE3	1:A:354:ASP:OD2	2.16	0.45
1:C:260:LEU:O	1:C:328:LYS:HA	2.17	0.45
1:A:231:ALA:HA	1:A:234:MET:HE3	1.97	0.45
1:A:300:ASP:OD2	1:D:215:ARG:NH2	2.49	0.45
1:A:326:PHE:HE2	1:D:189:LEU:HB2	1.80	0.45
1:B:301:PHE:CE2	1:B:332:TRP:CD2	3.05	0.45
1:D:93:ASN:HB3	1:D:96:ASP:OD2	2.17	0.45
1:D:171:LEU:HD11	1:D:260:LEU:HD22	1.99	0.45
1:B:9:GLY:CA	1:B:111:THR:HG22	2.46	0.45
1:B:10:PHE:CD2	1:B:46:PHE:CD2	3.05	0.45
1:B:69:SER:C	1:B:71:SER:H	2.25	0.45
1:B:145:VAL:HG23	1:B:235:VAL:HG21	1.98	0.45
1:D:289:LEU:HD23	1:D:290:GLY:O	2.16	0.45
1:A:99:TRP:HA	1:A:99:TRP:CE3	2.52	0.45
1:D:289:LEU:HD23	1:D:290:GLY:N	2.32	0.45
1:A:73:GLU:HG2	1:A:74:THR:N	2.32	0.44
1:C:101:LYS:C	1:C:101:LYS:CD	2.90	0.44
1:D:145:VAL:HB	1:D:235:VAL:HG11	1.99	0.44
1:A:18:PHE:HZ	1:A:80:VAL:HG21	1.82	0.44
1:B:170:CYS:SG	1:B:258:VAL:HG23	2.57	0.44
1:C:117:LYS:O	1:C:121:GLU:HG3	2.16	0.44
1:B:301:PHE:CZ	1:B:332:TRP:CD1	3.06	0.44
1:D:69:SER:C	1:D:71:SER:H	2.26	0.44
1:A:13:ILE:HB	3:A:363:NAD:H51N	1.99	0.44
1:C:101:LYS:HD3	1:C:102:LEU:N	2.32	0.44
1:C:193:ILE:N	1:C:193:ILE:HD12	2.32	0.44
1:B:232:VAL:HG21	1:B:243:LEU:HD23	1.99	0.44
1:C:254:ASP:O	1:C:255:VAL:HB	2.18	0.44
1:D:167:THR:HB	2:D:361:PO4:O4	2.18	0.44
1:A:37:VAL:HG12	3:A:363:NAD:H2A	1.99	0.43
1:A:343:VAL:O	1:A:347:VAL:HG23	2.18	0.43
1:B:26:LEU:HD23	1:B:348:ARG:HD2	2.00	0.43
1:B:271:GLN:O	1:B:275:LYS:HG3	2.18	0.43
1:A:254:ASP:O	1:A:255:VAL:HB	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:SER:OG	1:D:342:ARG:HD2	2.18	0.43
1:B:10:PHE:HD2	1:B:46:PHE:CD2	2.36	0.43
1:B:107:VAL:HB	1:B:131:VAL:HG22	2.00	0.43
1:B:223:PRO:CG	1:C:332:TRP:HZ2	2.31	0.43
1:A:151:HIS:HA	1:A:349:TYR:OH	2.19	0.43
1:B:254:ASP:O	1:B:255:VAL:HB	2.17	0.43
1:D:31:ILE:HD11	1:D:348:ARG:CG	2.49	0.43
1:D:62:THR:O	1:D:80:VAL:HA	2.18	0.43
1:A:201:LYS:HE3	1:A:206:VAL:O	2.19	0.43
1:B:117:LYS:O	1:B:121:GLU:HG3	2.19	0.43
1:C:18:PHE:HZ	1:C:80:VAL:HG21	1.84	0.43
1:C:31:ILE:HG22	1:C:32:ASP:N	2.33	0.43
1:A:169:ASN:O	1:A:307:SER:HB3	2.19	0.43
1:B:342:ARG:HE	1:B:342:ARG:HA	1.84	0.43
1:A:300:ASP:OD1	1:C:52:HIS:HB3	2.19	0.42
1:B:124:ILE:HG23	1:B:128:ALA:O	2.19	0.42
1:B:145:VAL:HG11	1:B:172:ALA:HB3	2.01	0.42
1:C:42:ASN:ND2	1:C:44:GLU:H	2.16	0.42
1:A:150:GLN:OE1	1:A:150:GLN:N	2.51	0.42
1:B:73:GLU:HG2	1:B:74:THR:N	2.33	0.42
1:B:67:LYS:HB2	1:B:72:VAL:CG2	2.49	0.42
1:A:300:ASP:OD1	1:D:215:ARG:NH2	2.50	0.42
1:A:188:GLY:O	1:A:243:LEU:HA	2.20	0.42
1:C:257:VAL:HB	1:C:332:TRP:CE3	2.54	0.42
1:B:31:ILE:HG22	1:B:32:ASP:N	2.34	0.42
1:D:79:VAL:HA	1:D:83:HIS:O	2.20	0.42
1:B:13:ILE:HG13	3:B:363:NAD:C2N	2.50	0.42
1:C:77:VAL:HG21	1:C:84:ARG:NH2	2.35	0.42
1:D:144:ILE:CG2	1:D:150:GLN:HA	2.50	0.42
1:B:300:ASP:OD1	1:D:52:HIS:HB3	2.20	0.42
1:B:310:TYR:HE1	1:B:329:VAL:HG13	1.84	0.42
1:C:184:GLY:O	1:C:264:ALA:HA	2.20	0.42
1:A:93:ASN:OD1	1:A:95:ALA:HB3	2.19	0.42
1:A:305:ASN:C	1:A:305:ASN:HD22	2.27	0.42
1:B:193:ILE:HG22	1:C:221:ILE:HD13	2.01	0.42
1:B:274:ASP:O	1:B:278:LYS:HG3	2.20	0.42
1:D:189:LEU:CD1	1:D:244:THR:HG22	2.49	0.42
1:A:192:THR:HG23	1:A:247:SER:CB	2.48	0.41
1:B:130:LYS:HE3	1:B:354:ASP:OD2	2.20	0.41
1:B:260:LEU:O	1:B:328:LYS:HA	2.20	0.41
1:A:123:HIS:HB2	1:A:131:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:MET:HB3	1:B:61:TYR:OH	2.20	0.41
1:B:321:PRO:HG2	1:B:322:GLY:H	1.85	0.41
1:B:342:ARG:HA	1:B:342:ARG:NE	2.35	0.41
1:D:189:LEU:HD12	1:D:189:LEU:HA	1.89	0.41
1:A:180:LYS:HD3	1:A:284:TYR:CE2	2.55	0.41
1:A:302:ILE:O	1:A:303:ASN:HB2	2.19	0.41
1:D:73:GLU:HG2	1:D:74:THR:N	2.35	0.41
1:D:31:ILE:HD11	1:D:348:ARG:HG3	2.01	0.41
1:B:220:ASN:OD1	1:C:299:ALA:HB2	2.20	0.41
1:B:106:TYR:CD2	1:B:130:LYS:HB2	2.55	0.41
1:C:82:GLY:O	1:C:83:HIS:HB2	2.21	0.41
1:A:172:ALA:HB3	1:A:173:PRO:HD3	2.02	0.41
1:C:204:ASP:OD2	1:C:215:ARG:NH1	2.53	0.41
1:D:51:LYS:O	1:D:58:ARG:HG2	2.21	0.41
1:D:73:GLU:HG2	1:D:74:THR:HG23	2.02	0.41
1:D:93:ASN:HA	1:D:94:PRO:HD3	1.91	0.41
1:D:113:LEU:CD1	3:D:363:NAD:N7A	2.84	0.41
1:A:171:LEU:HD22	1:A:190:MET:HE2	2.03	0.41
1:A:161:VAL:HG21	1:A:350:MET:SD	2.60	0.41
1:B:99:TRP:CD1	1:B:107:VAL:HG21	2.56	0.41
1:B:257:VAL:HB	1:B:332:TRP:CE3	2.56	0.41
1:C:150:GLN:HG2	1:C:151:HIS:N	2.35	0.41
1:D:188:GLY:C	1:D:243:LEU:HD12	2.45	0.41
1:B:155:PRO:HB3	1:B:358:SER:O	2.21	0.41
1:A:145:VAL:HB	1:A:235:VAL:HG11	2.03	0.40
1:B:18:PHE:HZ	1:B:80:VAL:HG21	1.83	0.40
1:C:129:LYS:HG2	1:C:130:LYS:HG2	2.02	0.40
1:C:274:ASP:O	1:C:278:LYS:HG3	2.21	0.40
1:A:78:LEU:CD2	1:A:87:CYS:SG	3.09	0.40
1:A:133:ILE:HD12	1:A:137:ALA:CB	2.51	0.40
1:A:163:ASN:O	1:A:163:ASN:CG	2.64	0.40
1:B:93:ASN:HA	1:B:94:PRO:HD3	1.88	0.40
1:C:69:SER:C	1:C:71:SER:H	2.29	0.40
1:D:13:ILE:HG13	3:D:363:NAD:C2N	2.51	0.40
1:D:147:GLY:H	1:D:150:GLN:NE2	2.20	0.40
1:A:45:TYR:HD1	1:B:211:TRP:CE2	2.39	0.40
1:A:121:GLU:O	1:A:125:LYS:HE2	2.21	0.40
1:A:145:VAL:HG11	1:A:172:ALA:HB3	2.04	0.40
1:B:315:THR:HG23	1:B:328:LYS:O	2.22	0.40
1:A:337:TRP:O	1:A:341:HIS:CD2	2.71	0.40
1:B:144:ILE:HG23	1:B:150:GLN:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:HIS:HA	1:D:349:TYR:HH	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	294/296 (99%)	280 (95%)	14 (5%)	23	56
1	B	294/296 (99%)	277 (94%)	17 (6%)	18	49
1	C	294/296 (99%)	280 (95%)	14 (5%)	23	56
1	D	294/296 (99%)	279 (95%)	15 (5%)	21	54
All	All	1176/1184 (99%)	1116 (95%)	60 (5%)	21	54

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	30	GLU
1	A	38	ASP
1	A	73	GLU
1	A	101	LYS
1	A	177	VAL
1	A	189	LEU
1	A	190	MET
1	A	215	ARG
1	A	238	SER

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Mol	Chain	Res	Type
1	A	257	VAL
1	A	272	GLU
1	A	305	ASN
1	A	309	VAL
1	B	19	GLN
1	B	30	GLU
1	B	68	SER
1	B	73	GLU
1	B	101	LYS
1	B	166	CYS
1	B	177	VAL
1	B	185	ILE
1	B	187	THR
1	B	189	LEU
1	B	215	ARG
1	B	238	SER
1	B	252	THR
1	B	257	VAL
1	B	298	SER
1	B	305	ASN
1	B	309	VAL
1	C	19	GLN
1	C	26	LEU
1	C	30	GLU
1	C	68	SER
1	C	73	GLU
1	C	101	LYS
1	C	166	CYS
1	C	177	VAL
1	C	187	THR
1	C	189	LEU
1	C	215	ARG
1	C	238	SER
1	C	305	ASN
1	C	309	VAL
1	D	19	GLN
1	D	30	GLU
1	D	38	ASP
1	D	54	THR
1	D	73	GLU
1	D	78	LEU
1	D	101	LYS

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Mol	Chain	Res	Type
1	D	177	VAL
1	D	187	THR
1	D	189	LEU
1	D	215	ARG
1	D	238	SER
1	D	305	ASN
1	D	309	VAL
1	D	340	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	19	GLN
1	A	24	GLN
1	A	42	ASN
1	A	81	ASN
1	A	305	ASN
1	A	341	HIS
1	B	8	ASN
1	B	42	ASN
1	B	49	GLN
1	B	52	HIS
1	B	81	ASN
1	B	159	HIS
1	B	176	HIS
1	B	305	ASN
1	B	341	HIS
1	C	8	ASN
1	C	19	GLN
1	C	24	GLN
1	C	42	ASN
1	C	49	GLN
1	C	81	ASN
1	C	163	ASN
1	C	169	ASN
1	C	176	HIS
1	C	305	ASN
1	C	341	HIS
1	D	8	ASN
1	D	19	GLN
1	D	24	GLN

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Mol	Chain	Res	Type
1	D	42	ASN
1	D	49	GLN
1	D	52	HIS
1	D	81	ASN
1	D	159	HIS
1	D	305	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D	362	-	4,4,4	1.21	0	6,6,6	0.94	0
3	NAD	B	363	-	46,48,48	1.25	5 (10%)	64,73,73	2.78	24 (37%)
3	NAD	D	363	-	46,48,48	1.62	7 (15%)	64,73,73	2.06	20 (31%)
2	PO4	D	361	-	4,4,4	0.65	0	6,6,6	1.10	0
3	NAD	C	363	-	46,48,48	1.67	6 (13%)	64,73,73	1.84	16 (25%)
2	PO4	C	361	-	4,4,4	1.07	0	6,6,6	0.67	0
2	PO4	B	362	-	4,4,4	1.26	0	6,6,6	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	B	361	-	4,4,4	0.80	0	6,6,6	0.98	1 (16%)
2	PO4	A	362	-	4,4,4	1.43	0	6,6,6	0.76	0
3	NAD	A	363	-	46,48,48	1.27	6 (13%)	64,73,73	2.01	16 (25%)
2	PO4	C	362	-	4,4,4	1.39	0	6,6,6	0.74	0
2	PO4	A	361	-	4,4,4	1.52	1 (25%)	6,6,6	1.19	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	363	-	-	20/30/62/62	0/5/5/5
3	NAD	B	363	-	-	10/30/62/62	0/5/5/5
3	NAD	A	363	-	-	19/30/62/62	0/5/5/5
3	NAD	D	363	-	-	11/30/62/62	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	363	NAD	C2N-N1N	8.44	1.44	1.35
3	D	363	NAD	C2N-N1N	6.43	1.42	1.35
3	A	363	NAD	C2N-N1N	4.95	1.40	1.35
3	B	363	NAD	C2N-N1N	4.57	1.40	1.35
3	D	363	NAD	PA-O3	4.30	1.64	1.59
3	C	363	NAD	C5A-N7A	-3.40	1.32	1.39
3	D	363	NAD	PN-O3	3.19	1.62	1.59
3	B	363	NAD	C5A-N7A	-3.18	1.33	1.39
3	A	363	NAD	C4A-N9A	-2.92	1.31	1.37
3	D	363	NAD	O4D-C1D	2.86	1.44	1.40
3	D	363	NAD	C5A-N7A	-2.82	1.33	1.39
3	A	363	NAD	C5A-N7A	-2.68	1.34	1.39
3	C	363	NAD	C4A-N9A	-2.60	1.32	1.37
3	C	363	NAD	O4D-C1D	2.52	1.44	1.40
3	B	363	NAD	C4A-N9A	-2.47	1.32	1.37
3	C	363	NAD	C6N-N1N	2.43	1.40	1.35
3	C	363	NAD	C3N-C7N	2.38	1.54	1.50
3	D	363	NAD	C3N-C7N	2.36	1.54	1.50
3	A	363	NAD	PA-O3	2.28	1.62	1.59
3	A	363	NAD	C6N-N1N	2.26	1.40	1.35
3	D	363	NAD	C4A-N9A	-2.25	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	363	NAD	C2B-C1B	-2.16	1.46	1.53
2	A	361	PO4	P-O4	-2.14	1.48	1.54
3	B	363	NAD	O4D-C1D	2.05	1.43	1.40
3	B	363	NAD	C6N-N1N	2.00	1.39	1.35

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	363	NAD	C4D-O4D-C1D	-14.39	96.75	109.92
3	D	363	NAD	N3A-C4A-N9A	5.80	137.03	127.17
3	A	363	NAD	N3A-C4A-N9A	5.71	136.88	127.17
3	A	363	NAD	C5A-C4A-N3A	-5.70	118.87	126.72
3	C	363	NAD	C5A-C4A-N3A	-5.66	118.93	126.72
3	D	363	NAD	C4A-N9A-C8A	5.57	111.58	105.74
3	B	363	NAD	N3A-C4A-N9A	5.16	135.94	127.17
3	A	363	NAD	C4A-N9A-C8A	5.00	110.98	105.74
3	D	363	NAD	C5A-C4A-N3A	-4.97	119.88	126.72
3	C	363	NAD	N3A-C4A-N9A	4.96	135.60	127.17
3	B	363	NAD	C5A-C4A-N3A	-4.83	120.07	126.72
3	D	363	NAD	N3A-C2A-N1A	-4.80	121.31	128.58
3	B	363	NAD	C6A-C5A-C4A	4.48	123.29	117.18
3	B	363	NAD	C6A-C5A-N7A	-4.44	123.53	132.09
3	D	363	NAD	N9A-C8A-N7A	-4.31	107.82	113.94
3	B	363	NAD	O4B-C1B-N9A	-4.10	100.22	108.09
3	C	363	NAD	C6A-C5A-C4A	4.08	122.75	117.18
3	A	363	NAD	N9A-C8A-N7A	-3.89	108.41	113.94
3	C	363	NAD	C6A-C5A-N7A	-3.82	124.73	132.09
3	B	363	NAD	N3A-C2A-N1A	-3.81	122.82	128.58
3	A	363	NAD	N3A-C2A-N1A	-3.79	122.84	128.58
3	A	363	NAD	O2A-PA-O3	3.71	117.29	107.27
3	B	363	NAD	O3-PA-O1A	-3.59	99.92	110.70
3	D	363	NAD	C6A-C5A-C4A	3.46	121.90	117.18
3	C	363	NAD	C2B-C1B-N9A	3.43	121.83	113.30
3	B	363	NAD	O7N-C7N-N7N	3.42	127.56	122.62
3	A	363	NAD	C6A-C5A-C4A	3.34	121.74	117.18
3	B	363	NAD	C5N-C4N-C3N	-3.33	117.09	120.36
3	C	363	NAD	O2N-PN-O1N	3.32	127.88	112.44
3	A	363	NAD	O5D-C5D-C4D	-3.30	97.75	108.99
3	C	363	NAD	C4D-O4D-C1D	-3.16	107.03	109.92
3	C	363	NAD	C6N-N1N-C1D	-3.14	113.57	119.73
3	B	363	NAD	O2N-PN-O1N	3.13	126.99	112.44
3	A	363	NAD	C2A-N3A-C4A	3.12	119.45	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	363	NAD	C4A-N9A-C1B	-3.07	119.45	126.63
3	D	363	NAD	C6N-N1N-C1D	-3.01	113.83	119.73
3	B	363	NAD	C2A-N1A-C6A	3.00	123.65	118.73
3	D	363	NAD	C6A-C5A-N7A	-2.99	126.32	132.09
3	C	363	NAD	N3A-C2A-N1A	-2.96	124.11	128.58
3	B	363	NAD	O7N-C7N-C3N	-2.92	116.03	119.60
3	D	363	NAD	C2A-N3A-C4A	2.91	118.93	111.83
3	D	363	NAD	C3B-C2B-C1B	-2.88	96.02	101.46
3	B	363	NAD	C4A-N9A-C8A	2.80	108.68	105.74
3	D	363	NAD	C2A-N1A-C6A	2.78	123.30	118.73
3	B	363	NAD	O5B-C5B-C4B	-2.63	100.03	108.99
3	C	363	NAD	O4B-C1B-C2B	-2.53	101.20	106.62
3	D	363	NAD	C5A-C4A-N9A	-2.50	103.09	105.81
3	C	363	NAD	C2A-N3A-C4A	2.46	117.84	111.83
3	D	363	NAD	C2N-N1N-C1D	2.45	124.55	119.13
3	A	363	NAD	C6A-C5A-N7A	-2.43	127.41	132.09
3	A	363	NAD	O2N-PN-O1N	2.42	123.72	112.44
3	A	363	NAD	C4D-O4D-C1D	2.40	112.12	109.92
3	A	363	NAD	O3-PA-O1A	-2.35	103.63	110.70
3	B	363	NAD	O3D-C3D-C2D	-2.35	104.28	111.82
3	D	363	NAD	O3D-C3D-C4D	-2.30	104.49	111.08
3	B	363	NAD	N6A-C6A-N1A	2.28	123.46	118.38
3	A	363	NAD	O7N-C7N-C3N	-2.27	116.82	119.60
3	B	363	NAD	C4A-C5A-N7A	2.27	113.17	110.58
3	B	363	NAD	O4D-C4D-C3D	2.24	109.60	105.15
3	C	363	NAD	C2N-N1N-C1D	2.23	124.06	119.13
3	B	363	NAD	C4B-O4B-C1B	-2.23	104.55	109.47
3	D	363	NAD	O2N-PN-O1N	2.21	122.72	112.44
3	D	363	NAD	C2N-C3N-C7N	2.18	125.75	119.46
3	B	363	NAD	C2A-N3A-C4A	2.16	117.11	111.83
3	C	363	NAD	O4B-C4B-C5B	-2.16	102.41	109.33
3	B	363	NAD	C2N-C3N-C4N	2.16	120.77	118.26
3	B	363	NAD	C6N-C5N-C4N	2.14	122.54	119.45
3	D	363	NAD	PN-O5D-C5D	-2.12	109.19	121.35
3	D	363	NAD	N6A-C6A-N1A	2.10	123.06	118.38
3	A	363	NAD	O7N-C7N-N7N	2.10	125.66	122.62
3	A	363	NAD	C4A-N9A-C1B	-2.10	121.72	126.63
3	C	363	NAD	O2B-C2B-C3B	-2.07	105.19	111.82
3	C	363	NAD	C2N-C3N-C7N	2.05	125.39	119.46
3	D	363	NAD	O2D-C2D-C3D	2.04	118.34	111.82
2	B	361	PO4	O4-P-O1	-2.03	103.75	110.95
3	B	363	NAD	O2A-PA-O1A	2.01	121.81	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	363	NAD	C5N-C4N-C3N	2.00	122.34	120.36

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	363	NAD	C5B-O5B-PA-O1A
3	A	363	NAD	C5D-O5D-PN-O2N
3	A	363	NAD	O4D-C1D-N1N-C2N
3	A	363	NAD	O4D-C1D-N1N-C6N
3	A	363	NAD	C2D-C1D-N1N-C2N
3	A	363	NAD	C2D-C1D-N1N-C6N
3	B	363	NAD	C5B-O5B-PA-O1A
3	B	363	NAD	PN-O3-PA-O5B
3	B	363	NAD	C5D-O5D-PN-O2N
3	B	363	NAD	O4D-C1D-N1N-C2N
3	C	363	NAD	C5B-O5B-PA-O1A
3	C	363	NAD	C5B-O5B-PA-O3
3	C	363	NAD	C5D-O5D-PN-O3
3	C	363	NAD	C5D-O5D-PN-O1N
3	C	363	NAD	C5D-O5D-PN-O2N
3	C	363	NAD	O4D-C1D-N1N-C2N
3	C	363	NAD	O4D-C1D-N1N-C6N
3	C	363	NAD	C2D-C1D-N1N-C2N
3	C	363	NAD	C2D-C1D-N1N-C6N
3	D	363	NAD	C5B-O5B-PA-O1A
3	D	363	NAD	C5B-O5B-PA-O3
3	D	363	NAD	O4D-C1D-N1N-C2N
3	D	363	NAD	C2D-C1D-N1N-C2N
3	C	363	NAD	O4D-C4D-C5D-O5D
3	C	363	NAD	C3D-C4D-C5D-O5D
3	D	363	NAD	O4B-C4B-C5B-O5B
3	A	363	NAD	C2N-C3N-C7N-O7N
3	D	363	NAD	C3B-C4B-C5B-O5B
3	A	363	NAD	O4B-C4B-C5B-O5B
3	A	363	NAD	C3B-C4B-C5B-O5B
3	A	363	NAD	C4N-C3N-C7N-O7N
3	A	363	NAD	C4N-C3N-C7N-N7N
3	A	363	NAD	C2N-C3N-C7N-N7N
3	C	363	NAD	C2B-C1B-N9A-C8A
3	D	363	NAD	C2B-C1B-N9A-C8A
3	C	363	NAD	PA-O3-PN-O2N

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Mol	Chain	Res	Type	Atoms
3	C	363	NAD	C3B-C4B-C5B-O5B
3	A	363	NAD	C5B-O5B-PA-O2A
3	A	363	NAD	C5B-O5B-PA-O3
3	A	363	NAD	C5D-O5D-PN-O3
3	B	363	NAD	C5D-O5D-PN-O3
3	C	363	NAD	C5B-O5B-PA-O2A
3	D	363	NAD	C5B-O5B-PA-O2A
3	C	363	NAD	PA-O3-PN-O1N
3	A	363	NAD	C3D-C4D-C5D-O5D
3	D	363	NAD	C4B-C5B-O5B-PA
3	D	363	NAD	O4D-C1D-N1N-C6N
3	C	363	NAD	C4B-C5B-O5B-PA
3	C	363	NAD	O4B-C4B-C5B-O5B
3	C	363	NAD	C2B-C1B-N9A-C4A
3	C	363	NAD	O4B-C1B-N9A-C8A
3	B	363	NAD	C4B-C5B-O5B-PA
3	D	363	NAD	O4B-C1B-N9A-C8A
3	B	363	NAD	C2B-C1B-N9A-C8A
3	A	363	NAD	PA-O3-PN-O2N
3	B	363	NAD	PA-O3-PN-O1N
3	B	363	NAD	PA-O3-PN-O2N
3	B	363	NAD	O4B-C4B-C5B-O5B
3	A	363	NAD	C2B-C1B-N9A-C8A
3	A	363	NAD	PA-O3-PN-O1N

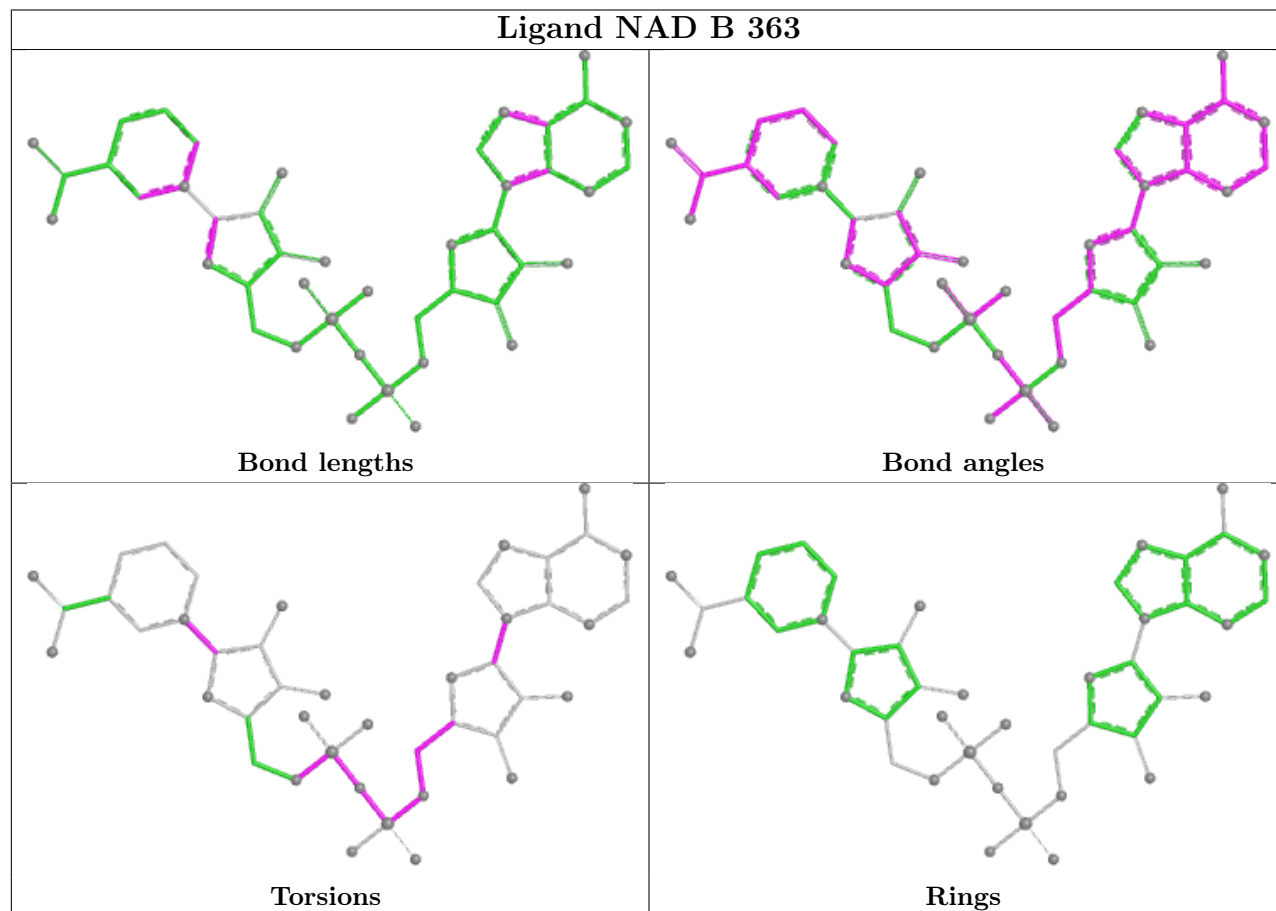
There are no ring outliers.

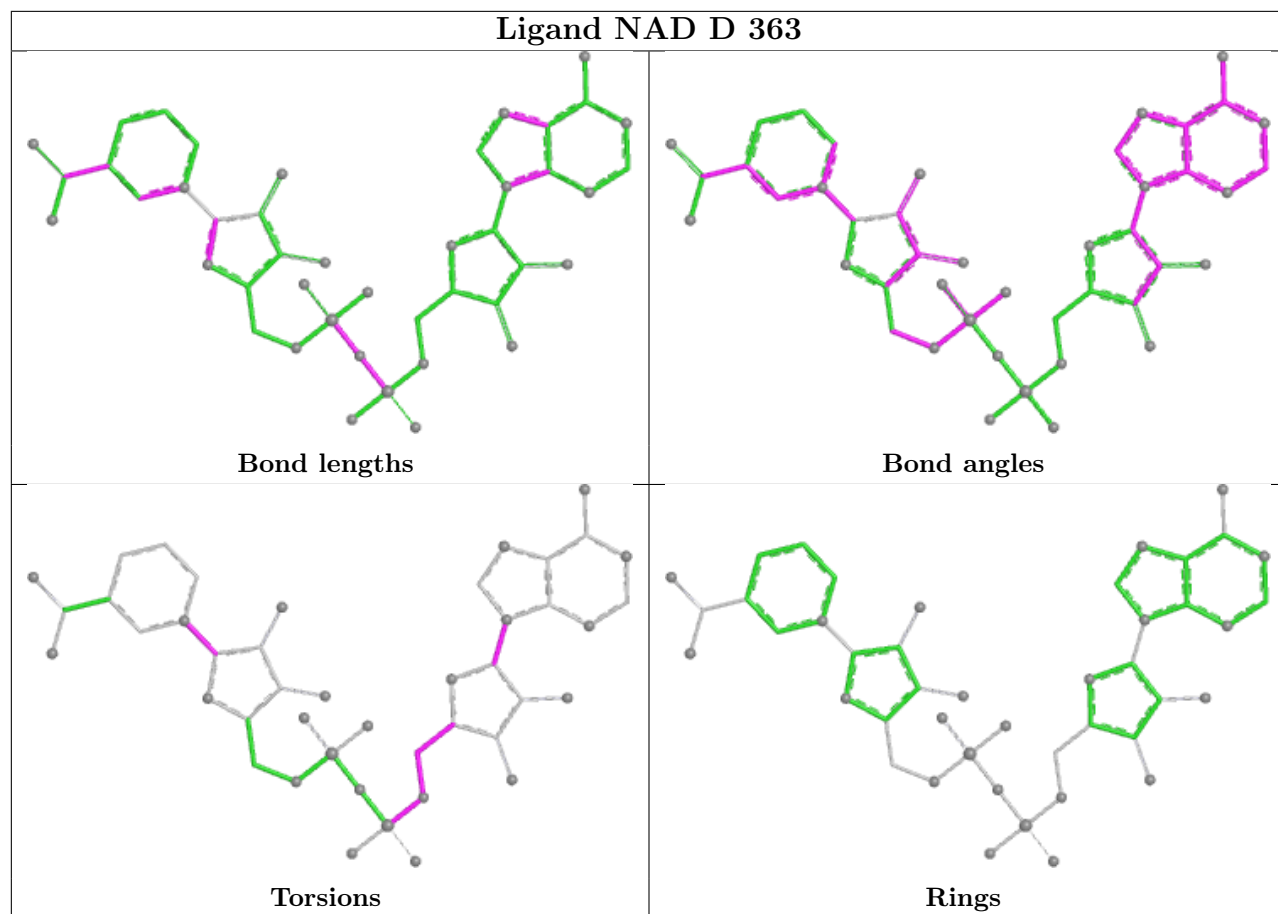
8 monomers are involved in 15 short contacts:

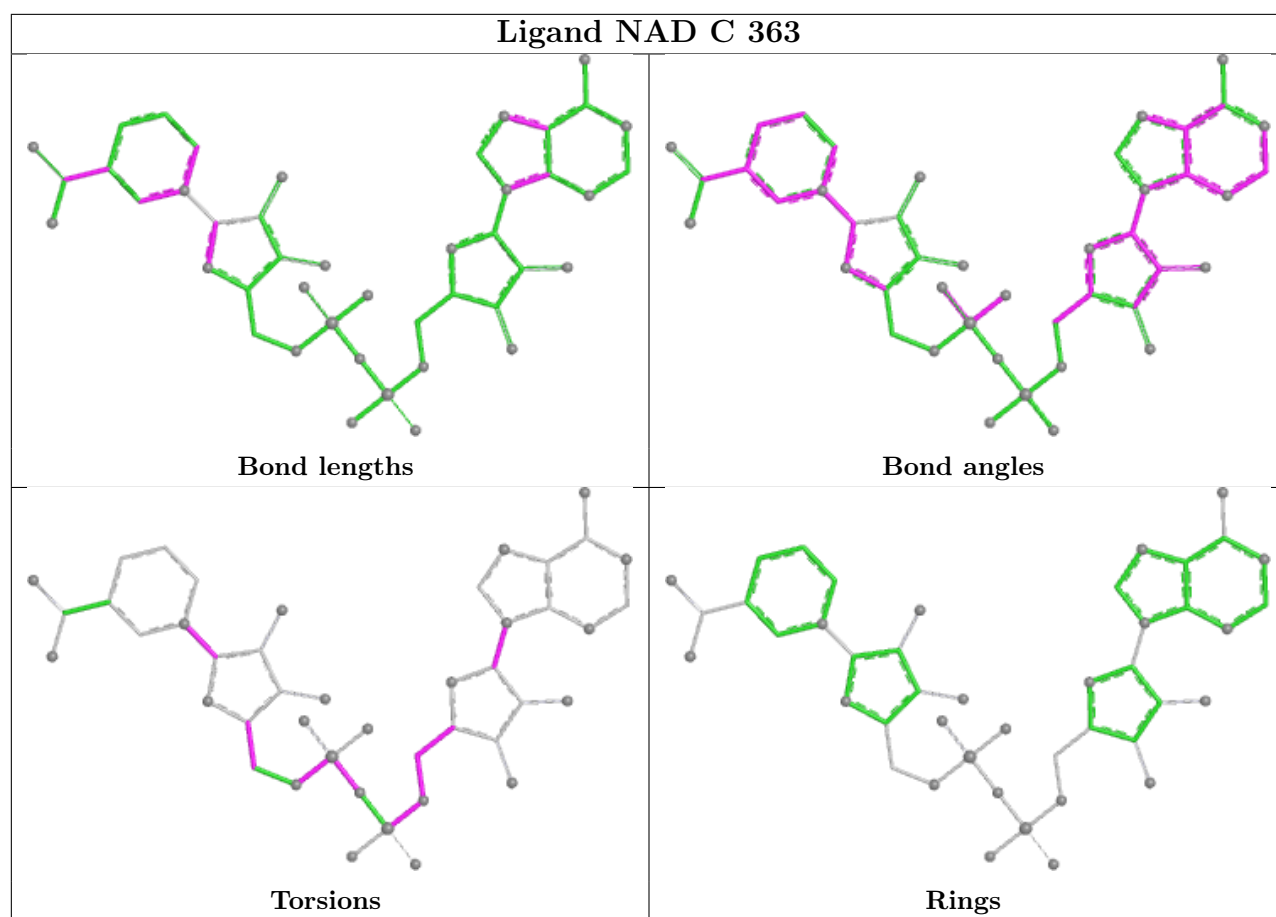
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	363	NAD	5	0
3	D	363	NAD	3	0
2	D	361	PO4	1	0
3	C	363	NAD	1	0
2	C	361	PO4	1	0
2	B	361	PO4	2	0
3	A	363	NAD	2	0
2	C	362	PO4	1	0

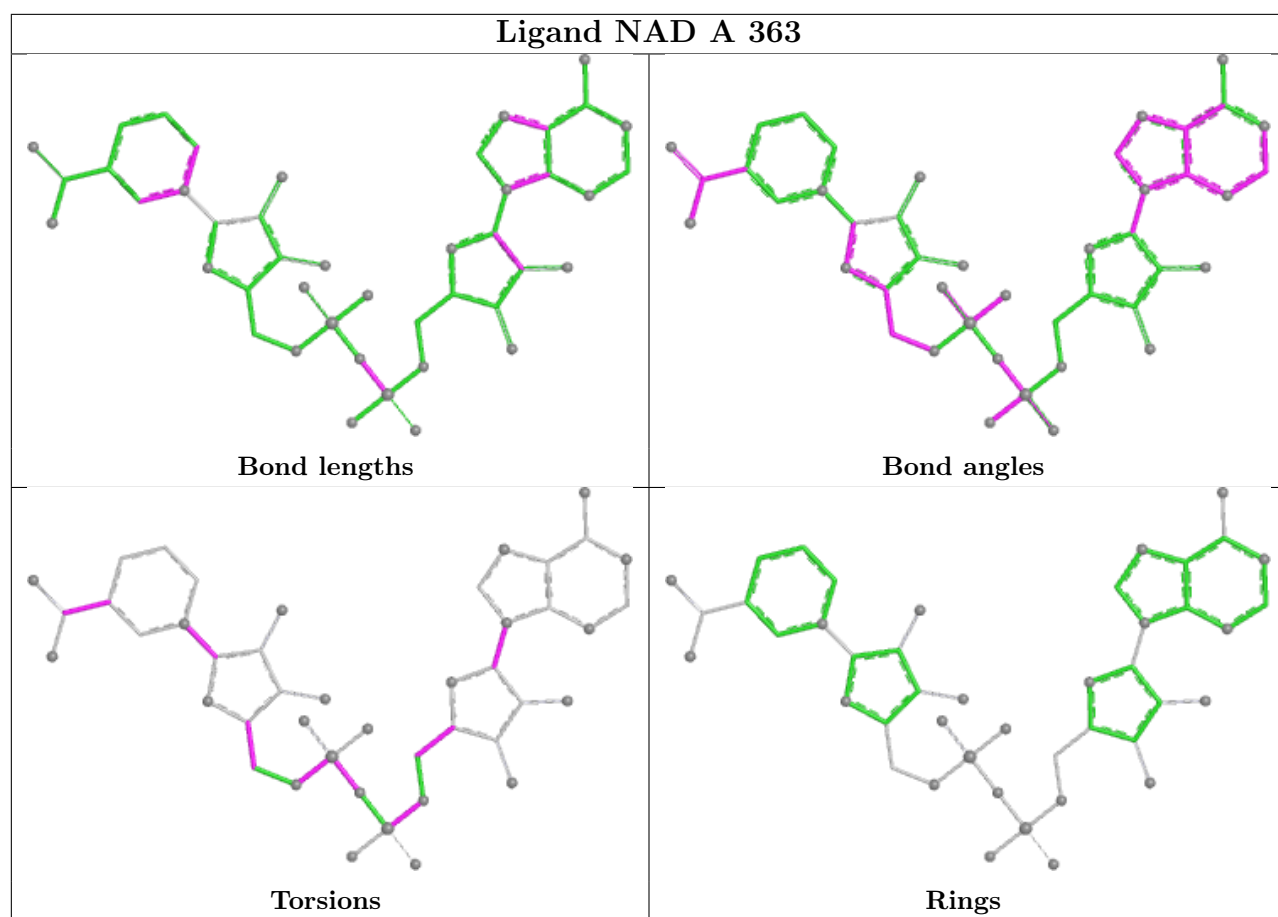
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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