Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:07 am BST

PDB ID	:	1BXK
Title	:	DTDP-GLUCOSE 4,6-DEHYDRATASE FROM E. COLI
Authors	:	Thoden, J.B.; Hegeman, A.D.; Frey, P.A.; Holden, H.M.
Deposited on	:	1998-10-05
Resolution	:	1.90 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:

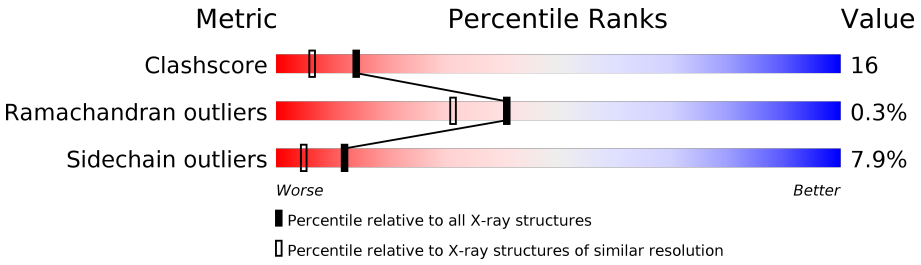
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	355	58% 28% 10%
1	B	355	60% 29% 7%

2 Entry composition

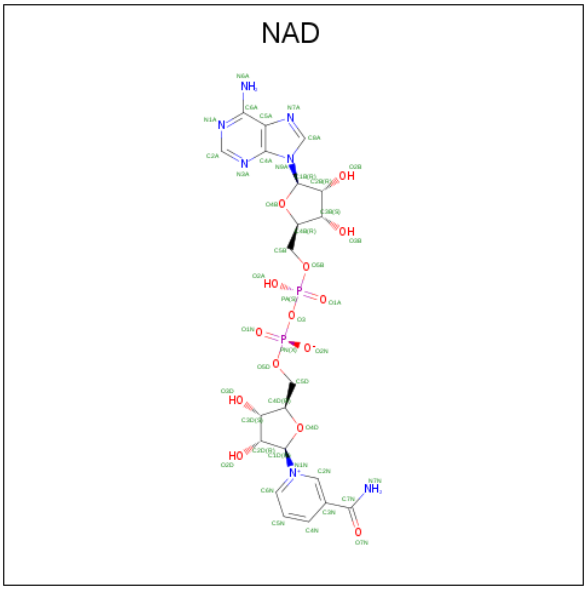
There are 3 unique types of molecules in this entry. The entry contains 5856 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (DTDP-GLUCOSE 4,6-DEHYDRATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	2	0
			2699	1713	459	516	11			
1	B	344	Total	C	N	O	S	0	0	0
			2710	1722	462	515	11			

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	196	Total O 196 196	0	0
3	B	163	Total O 163 163	0	0

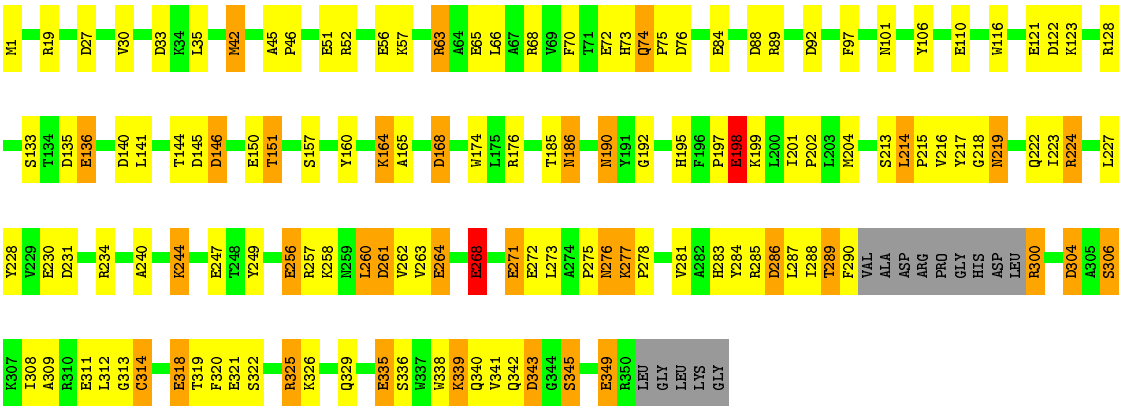
3 Residue-property plots (i)

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.

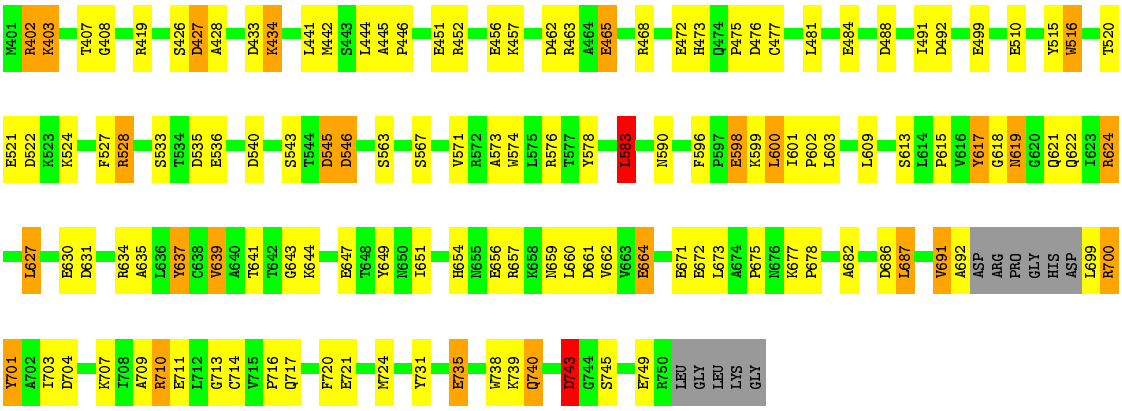
- Molecule 1: PROTEIN (DTDP-GLUCOSE 4,6-DEHYDRATASE)

Chain A:



- Molecule 1: PROTEIN (DTDP-GLUCOSE 4,6-DEHYDRATASE)

Chain B:



4 Data and refinement statistics (i)

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	68.40Å 109.20Å 128.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90	Depositor
% Data completeness (in resolution range)	96.3 (30.00-1.90)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5856	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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: 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	1.05	19/2773 (0.7%)	1.54	54/3771 (1.4%)
1	B	2.50	22/2776 (0.8%)	1.48	41/3777 (1.1%)
All	All	1.92	41/5549 (0.7%)	1.51	95/7548 (1.3%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	691	VAL	CB-CG2	102.89	3.69	1.52
1	B	691	VAL	CB-CG1	59.97	2.78	1.52
1	B	457	LYS	CE-NZ	-11.86	1.19	1.49
1	B	451	GLU	CD-OE1	10.12	1.36	1.25
1	B	672	GLU	CD-OE1	8.56	1.35	1.25
1	A	268	GLU	CD-OE2	8.55	1.35	1.25
1	A	335	GLU	CD-OE1	8.15	1.34	1.25
1	A	51	GLU	CD-OE1	7.69	1.34	1.25
1	B	510	GLU	CD-OE2	7.59	1.34	1.25
1	B	521	GLU	CD-OE1	7.51	1.33	1.25
1	B	536	GLU	CD-OE1	7.39	1.33	1.25
1	B	456	GLU	CD-OE2	7.36	1.33	1.25
1	B	630	GLU	CD-OE1	7.29	1.33	1.25
1	B	598	GLU	CD-OE1	7.25	1.33	1.25
1	A	264	GLU	CD-OE1	7.13	1.33	1.25
1	A	121	GLU	CD-OE2	7.03	1.33	1.25
1	B	735	GLU	CD-OE1	6.90	1.33	1.25
1	A	150	GLU	CD-OE1	6.80	1.33	1.25
1	A	311	GLU	CD-OE2	6.64	1.32	1.25
1	A	84	GLU	CD-OE1	6.63	1.32	1.25
1	A	321	GLU	CD-OE1	6.56	1.32	1.25
1	B	664	GLU	CD-OE1	6.51	1.32	1.25
1	A	198[A]	GLU	CD-OE1	6.50	1.32	1.25
1	A	198[B]	GLU	CD-OE1	6.50	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	671	GLU	CD-OE1	6.32	1.32	1.25
1	A	272	GLU	CD-OE1	6.27	1.32	1.25
1	B	499	GLU	CD-OE2	-6.13	1.19	1.25
1	B	711	GLU	CD-OE2	6.10	1.32	1.25
1	A	230	GLU	CD-OE1	6.04	1.32	1.25
1	A	349	GLU	CD-OE1	6.00	1.32	1.25
1	B	472	GLU	CD-OE1	5.99	1.32	1.25
1	B	656	GLU	CD-OE1	5.91	1.32	1.25
1	A	65	GLU	CD-OE2	5.85	1.32	1.25
1	B	484	GLU	CD-OE1	5.82	1.32	1.25
1	A	256	GLU	CD-OE1	5.69	1.31	1.25
1	A	110	GLU	CD-OE2	-5.46	1.19	1.25
1	B	465	GLU	CD-OE1	5.44	1.31	1.25
1	A	136	GLU	CD-OE1	5.35	1.31	1.25
1	A	56	GLU	CD-OE2	5.27	1.31	1.25
1	B	510	GLU	CD-OE1	-5.27	1.19	1.25
1	B	721	GLU	CD-OE1	5.15	1.31	1.25

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	ARG	NE-CZ-NH2	-13.91	113.34	120.30
1	A	52	ARG	NE-CZ-NH2	-11.64	114.48	120.30
1	B	743	ASP	CB-CG-OD1	-11.55	107.91	118.30
1	B	691	VAL	CA-CB-CG1	10.70	126.94	110.90
1	B	476	ASP	CB-CG-OD2	-10.54	108.81	118.30
1	A	88	ASP	CB-CG-OD1	9.92	127.23	118.30
1	A	135	ASP	CB-CG-OD2	-9.45	109.80	118.30
1	B	528	ARG	CD-NE-CZ	-8.95	111.06	123.60
1	A	89	ARG	NE-CZ-NH1	-8.51	116.04	120.30
1	B	661	ASP	CB-CG-OD1	-8.46	110.69	118.30
1	A	140	ASP	CB-CG-OD1	-8.36	110.78	118.30
1	A	261	ASP	CB-CG-OD1	-8.35	110.78	118.30
1	A	92	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	A	186	ASN	N-CA-CB	8.19	125.34	110.60
1	A	92	ASP	CB-CG-OD1	8.01	125.51	118.30
1	B	402	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	B	540	ASP	CB-CG-OD1	-7.98	111.12	118.30
1	A	176	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	231	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	343	ASP	CB-CG-OD1	-7.83	111.25	118.30
1	B	463	ARG	NE-CZ-NH2	7.82	124.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	535	ASP	CB-CG-OD1	7.76	125.28	118.30
1	B	546	ASP	CB-CG-OD1	-7.72	111.36	118.30
1	A	160	TYR	CB-CG-CD1	-7.62	116.43	121.00
1	B	427	ASP	CB-CG-OD2	7.57	125.11	118.30
1	B	476	ASP	CB-CG-OD1	7.52	125.06	118.30
1	A	74	GLN	CB-CA-C	-7.46	95.47	110.40
1	A	343	ASP	CB-CA-C	-7.33	95.75	110.40
1	A	325	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	19	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	68	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	76	ASP	CB-CG-OD1	-6.88	112.10	118.30
1	A	88	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	B	583	LEU	N-CA-CB	6.82	124.04	110.40
1	B	631	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	A	231	ASP	CB-CG-OD1	6.73	124.36	118.30
1	A	63	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	B	576	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	106	TYR	CB-CG-CD1	6.56	124.94	121.00
1	A	76	ASP	CB-CG-OD2	6.44	124.09	118.30
1	A	168	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	462	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	B	527	PHE	CB-CG-CD2	-6.35	116.36	120.80
1	A	304	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	B	700	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	A	106	TYR	CB-CG-CD2	-6.19	117.28	121.00
1	A	42	MET	CG-SD-CE	6.19	110.10	100.20
1	A	122	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	B	535	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	A	145	ASP	CB-CG-OD1	-6.13	112.79	118.30
1	A	135	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	639	VAL	CA-CB-CG2	-6.11	101.73	110.90
1	A	146	ASP	CB-CG-OD1	-6.05	112.85	118.30
1	B	573	ALA	CB-CA-C	6.01	119.11	110.10
1	A	240	ALA	N-CA-CB	5.99	118.49	110.10
1	A	304	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	151	THR	N-CA-CB	-5.87	99.14	110.30
1	A	140	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	743	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	545	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	217	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	B	714	CYS	N-CA-CB	5.68	120.83	110.60
1	B	545	ASP	CB-CG-OD1	-5.66	113.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	PHE	CB-CG-CD1	-5.65	116.84	120.80
1	B	700	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	B	662	VAL	CG1-CB-CG2	-5.62	101.91	110.90
1	A	145	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	185	THR	N-CA-CB	5.50	120.74	110.30
1	A	261	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	27	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	30	VAL	N-CA-CB	5.40	123.37	111.50
1	B	477	CYS	N-CA-CB	-5.39	100.90	110.60
1	A	271	GLU	CG-CD-OE2	-5.36	107.58	118.30
1	A	75	PRO	CA-N-CD	5.35	119.19	111.70
1	B	731	TYR	CA-CB-CG	-5.32	103.29	113.40
1	B	522	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	520	THR	CA-CB-CG2	-5.30	104.98	112.40
1	B	492	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	128	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	73	HIS	N-CA-CB	-5.24	101.17	110.60
1	B	710	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	300	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	578	TYR	CB-CG-CD2	-5.19	117.88	121.00
1	A	160	TYR	CB-CG-CD2	5.18	124.11	121.00
1	B	701	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	B	492	ASP	CB-CG-OD1	-5.16	113.66	118.30
1	A	318	GLU	CG-CD-OE1	-5.15	107.99	118.30
1	A	116	TRP	N-CA-CB	-5.14	101.35	110.60
1	B	649	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	122	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	687	LEU	CB-CG-CD2	-5.06	102.39	111.00
1	B	427	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	B	637	TYR	CB-CG-CD2	5.04	124.02	121.00
1	A	249	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	B	516	TRP	N-CA-CB	-5.03	101.55	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2699	0	2604	84	0
1	B	2710	0	2623	84	0
2	A	44	0	26	0	0
2	B	44	0	26	1	0
3	A	196	0	0	4	0
3	B	163	0	0	4	0
All	All	5856	0	5279	168	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 16.

All (168) 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:619:ASN:HB2	1:B:621:GLN:CG	1.87	1.03
1:B:619:ASN:HB2	1:B:621:GLN:HG2	1.40	1.03
1:B:617:TYR:CD2	1:B:691:VAL:HG13	2.00	0.96
1:B:442:MET:CE	1:B:740:GLN:HE21	1.86	0.88
1:A:45:ALA:HB3	1:A:46:PRO:HD3	1.57	0.86
1:A:234:ARG:NH2	3:A:570:HOH:O	2.11	0.84
1:A:213:SER:O	1:A:215:PRO:HD3	1.80	0.82
1:B:442:MET:HE3	1:B:740:GLN:HE21	1.45	0.81
1:A:256:GLU:OE2	1:A:300:ARG:NH1	2.15	0.80
1:A:146:ASP:O	1:A:300:ARG:NH2	2.14	0.79
1:B:618:GLY:H	1:B:692:ALA:HA	1.49	0.78
1:B:617:TYR:CE2	1:B:691:VAL:HG13	2.19	0.77
1:A:285:ARG:O	1:A:288:ILE:HG13	1.84	0.76
1:A:258:LYS:O	1:A:261:ASP:HB2	1.84	0.76
1:A:219:ASN:N	1:A:219:ASN:ND2	2.32	0.75
1:B:709:ALA:O	1:B:713:GLY:HA2	1.86	0.74
1:B:619:ASN:HB2	1:B:621:GLN:HG3	1.70	0.73
1:A:260:LEU:O	1:A:263:VAL:HG12	1.88	0.73
1:A:263:VAL:HG13	1:A:264:GLU:N	2.04	0.72
1:A:308:ILE:HG12	1:A:314:CYS:SG	2.30	0.71
1:B:707:LYS:NZ	3:B:349:HOH:O	2.22	0.71
1:B:624:ARG:NH1	1:B:701:TYR:CD1	2.60	0.70
1:B:644:LYS:HD3	1:B:647:GLU:HG2	1.74	0.69
1:A:222:GLN:OE1	1:A:224:ARG:NH1	2.26	0.69
1:A:271:GLU:HG2	1:A:284:TYR:HD2	1.56	0.69
1:A:263:VAL:CG1	1:A:264:GLU:N	2.56	0.68
1:B:465:GLU:HA	1:B:465:GLU:OE1	1.93	0.67
1:A:335:GLU:O	1:A:339:LYS:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:SER:O	1:B:615:PRO:HD3	1.96	0.65
1:B:664:GLU:HA	1:B:664:GLU:OE1	1.96	0.65
1:A:319:THR:H	1:A:322:SER:HB3	1.62	0.64
1:B:735:GLU:HA	1:B:738:TRP:NE1	2.12	0.64
1:B:596:PHE:HB3	1:B:598:GLU:OE2	1.98	0.64
1:B:445:ALA:N	1:B:446:PRO:HD2	2.14	0.63
1:A:199:LYS:HB2	1:A:202:PRO:HG2	1.81	0.63
1:A:278:PRO:HG2	1:A:281:VAL:HG21	1.80	0.62
1:B:444:LEU:C	1:B:446:PRO:HD2	2.20	0.62
1:A:276:ASN:N	1:A:276:ASN:HD22	1.97	0.61
1:B:691:VAL:CG1	1:B:691:VAL:CB	2.78	0.61
1:B:442:MET:HE1	1:B:740:GLN:HE21	1.62	0.61
1:A:325:ARG:O	1:A:329:GLN:HG3	2.01	0.60
1:A:219:ASN:N	1:A:219:ASN:HD22	1.98	0.60
1:B:599:LYS:O	1:B:603:LEU:HB2	2.02	0.60
1:A:133:SER:HB3	1:A:186:ASN:ND2	2.16	0.59
1:B:545:ASP:N	1:B:545:ASP:OD1	2.35	0.59
1:B:677:LYS:HB3	1:B:678:PRO:HD2	1.85	0.59
1:A:308:ILE:CG1	1:A:314:CYS:SG	2.91	0.58
1:A:304:ASP:OD1	1:A:306:SER:OG	2.23	0.57
1:B:644:LYS:HD3	1:B:647:GLU:CG	2.35	0.57
1:A:275:PRO:O	1:A:277:LYS:HD2	2.04	0.57
1:B:488:ASP:HB3	3:B:314:HOH:O	2.05	0.57
1:B:583:LEU:N	1:B:583:LEU:HD12	2.21	0.56
1:B:634:ARG:NH1	3:B:264:HOH:O	2.35	0.56
1:A:144:THR:O	1:A:144:THR:HG22	2.05	0.56
1:A:45:ALA:HB3	1:A:46:PRO:CD	2.33	0.56
1:A:218:GLY:C	1:A:219:ASN:HD22	2.09	0.55
1:B:543:SER:HB3	1:B:546:ASP:CG	2.27	0.55
1:B:533:SER:O	2:B:780:NAD:H6N	2.07	0.55
1:B:543:SER:OG	1:B:545:ASP:OD1	2.08	0.55
1:B:743:ASP:HB3	1:B:745:SER:H	1.72	0.55
1:A:190:ASN:HA	1:A:227:LEU:O	2.07	0.54
1:A:216:VAL:CG2	1:A:288:ILE:HG23	2.37	0.54
1:A:276:ASN:ND2	1:A:276:ASN:N	2.55	0.54
1:A:45:ALA:N	1:A:46:PRO:HD2	2.23	0.54
1:B:516:TRP:O	1:B:524:LYS:HD2	2.08	0.53
1:A:318:GLU:OE1	1:A:322:SER:OG	2.25	0.53
1:A:57:LYS:NZ	3:A:460:HOH:O	2.41	0.53
1:B:442:MET:HE1	1:B:740:GLN:NE2	2.22	0.53
1:B:618:GLY:H	1:B:692:ALA:CA	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PRO:HA	1:A:289:THR:HG23	1.91	0.52
1:A:273:LEU:C	1:A:275:PRO:HD3	2.28	0.52
1:A:336:SER:O	1:A:340:GLN:HG3	2.10	0.52
1:B:428:ALA:HA	1:B:452:ARG:HB3	1.91	0.52
1:A:284:TYR:O	1:A:287:LEU:HB2	2.09	0.52
1:A:33:ASP:O	1:A:57:LYS:HA	2.10	0.51
1:B:622:GLN:HG3	1:B:699:LEU:O	2.11	0.51
1:B:682:ALA:HB3	1:B:686:ASP:OD2	2.10	0.51
1:B:590:ASN:HA	1:B:627:LEU:O	2.10	0.51
1:B:699:LEU:HB3	1:B:701:TYR:CE1	2.46	0.51
1:B:709:ALA:O	1:B:713:GLY:CA	2.58	0.51
1:A:228:TYR:CD2	1:A:318:GLU:HG3	2.46	0.51
1:B:654:HIS:CD2	1:B:716:PRO:HD2	2.45	0.51
1:B:735:GLU:HG3	1:B:738:TRP:CZ2	2.46	0.51
1:A:312:LEU:HB2	1:A:314:CYS:SG	2.51	0.50
1:A:338:TRP:O	1:A:342:GLN:HG3	2.10	0.50
1:B:445:ALA:N	1:B:446:PRO:CD	2.75	0.50
1:A:45:ALA:N	1:A:46:PRO:CD	2.74	0.50
1:A:63:ARG:NH1	1:A:63:ARG:HG2	2.26	0.49
1:A:262:VAL:HG22	1:A:320:PHE:HZ	1.77	0.49
1:A:343:ASP:CB	1:A:345:SER:OG	2.60	0.49
1:B:619:ASN:CB	1:B:621:GLN:HG2	2.29	0.49
1:B:624:ARG:NH1	1:B:701:TYR:HD1	2.06	0.49
1:A:190:ASN:HD22	1:A:190:ASN:N	2.10	0.49
1:A:192:GLY:O	1:A:195:HIS:HB2	2.12	0.49
1:A:309:ALA:O	1:A:313:GLY:HA2	2.12	0.49
1:B:673:LEU:C	1:B:675:PRO:HD3	2.33	0.49
1:A:286:ASP:OD1	1:A:286:ASP:N	2.46	0.48
1:A:343:ASP:HB3	1:A:345:SER:H	1.78	0.48
1:B:419:ARG:HD3	1:B:446:PRO:HG2	1.95	0.48
1:B:468:ARG:HG2	1:B:468:ARG:HH11	1.78	0.48
1:B:618:GLY:O	1:B:692:ALA:HB2	2.14	0.48
1:A:223:ILE:CG2	1:A:224:ARG:N	2.76	0.48
1:B:407:THR:O	1:B:481:LEU:HB2	2.13	0.48
1:B:567:SER:O	1:B:571:VAL:HG23	2.14	0.48
1:A:268:GLU:OE1	1:A:268:GLU:HA	2.11	0.47
1:B:622:GLN:HE21	1:B:699:LEU:HB2	1.79	0.47
1:A:326:LYS:HA	1:A:329:GLN:HE21	1.80	0.47
1:B:546:ASP:O	1:B:700:ARG:NH1	2.41	0.47
1:B:475:PRO:HD2	1:B:515:TYR:CZ	2.49	0.47
1:A:216:VAL:HG21	1:A:288:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:MET:CE	1:B:740:GLN:NE2	2.66	0.46
1:B:635:ALA:O	1:B:639:VAL:HG23	2.15	0.46
1:A:97:PHE:O	1:A:101:ASN:HB2	2.15	0.46
1:A:201:ILE:N	1:A:202:PRO:CD	2.79	0.46
1:B:546:ASP:N	1:B:546:ASP:OD1	2.26	0.46
1:B:600:LEU:HD12	1:B:600:LEU:C	2.37	0.46
1:B:660:LEU:O	1:B:664:GLU:HG2	2.16	0.46
1:A:213:SER:C	1:A:215:PRO:HD3	2.37	0.45
1:A:290:PHE:CD1	1:A:290:PHE:N	2.84	0.45
1:B:427:ASP:O	1:B:452:ARG:HD2	2.16	0.45
1:B:637:TYR:CZ	1:B:641:THR:HG21	2.52	0.45
1:A:136:GLU:HA	3:A:562:HOH:O	2.16	0.45
1:A:343:ASP:HB3	1:A:345:SER:OG	2.16	0.45
1:B:675:PRO:O	1:B:677:LYS:HG3	2.16	0.45
1:B:618:GLY:HA2	1:B:692:ALA:HB1	1.99	0.45
1:A:262:VAL:HG22	1:A:320:PHE:CZ	2.52	0.45
1:B:720:PHE:O	1:B:724:MET:HG2	2.17	0.45
1:A:283:HIS:HB2	1:A:286:ASP:OD2	2.17	0.44
1:A:197:PRO:CD	1:A:341:VAL:HG11	2.47	0.44
1:A:35:LEU:HD12	1:A:57:LYS:HD2	1.99	0.44
1:B:703:ILE:CG2	1:B:704:ASP:N	2.79	0.44
1:B:654:HIS:HD2	1:B:716:PRO:HD2	1.83	0.44
1:A:141:LEU:HD13	1:A:146:ASP:O	2.16	0.44
1:B:615:PRO:CB	1:B:691:VAL:HG12	2.48	0.44
1:A:263:VAL:CG1	1:A:264:GLU:H	2.28	0.44
1:B:419:ARG:CD	1:B:446:PRO:HG2	2.47	0.44
1:A:146:ASP:OD1	1:A:146:ASP:N	2.34	0.43
1:A:42:MET:CG	1:A:349:GLU:HG3	2.49	0.43
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.82	0.43
1:A:164:LYS:HE3	3:A:412:HOH:O	2.17	0.43
1:B:687:LEU:HD23	1:B:687:LEU:HA	1.72	0.43
1:A:216:VAL:HG23	1:A:288:ILE:HG23	1.99	0.43
1:B:622:GLN:CD	1:B:624:ARG:NH1	2.71	0.43
1:A:260:LEU:HD21	1:A:264:GLU:CD	2.39	0.43
1:B:609:LEU:HA	1:B:609:LEU:HD23	1.79	0.43
1:B:639:VAL:O	1:B:643:GLY:HA3	2.19	0.42
1:B:434:LYS:NZ	3:B:341:HOH:O	2.50	0.42
1:B:468:ARG:NH1	1:B:468:ARG:HG2	2.34	0.42
1:B:403:LYS:HE3	1:B:473:HIS:O	2.19	0.42
1:A:244:LYS:HB3	1:A:247:GLU:CG	2.50	0.42
1:A:335:GLU:HA	1:A:338:TRP:NE1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:ILE:HD13	1:B:651:ILE:HG21	1.85	0.41
1:B:710:ARG:HH11	1:B:710:ARG:HD2	1.64	0.41
1:B:441:LEU:HD23	1:B:441:LEU:HA	1.90	0.41
1:A:275:PRO:O	1:A:277:LYS:HE3	2.20	0.41
1:B:619:ASN:CB	1:B:621:GLN:HG3	2.47	0.41
1:B:703:ILE:HG22	1:B:704:ASP:N	2.36	0.41
1:A:201:ILE:N	1:A:202:PRO:HD2	2.36	0.41
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.78	0.41
1:A:260:LEU:O	1:A:264:GLU:HB2	2.20	0.41
1:B:408:GLY:HA2	1:B:433:ASP:OD2	2.21	0.40
1:B:601:ILE:HB	1:B:602:PRO:HD3	2.03	0.40
1:B:603:LEU:HD12	1:B:603:LEU:HA	1.82	0.40
1:A:165:ALA:O	1:A:168:ASP:HB2	2.21	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	339/355 (96%)	318 (94%)	20 (6%)	1 (0%)	41	31
1	B	340/355 (96%)	320 (94%)	19 (6%)	1 (0%)	41	31
All	All	679/710 (96%)	638 (94%)	39 (6%)	2 (0%)	41	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	600	LEU
1	A	214	LEU

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	287/296 (97%)	261 (91%)	26 (9%)	9 3
1	B	287/296 (97%)	267 (93%)	20 (7%)	15 7
All	All	574/592 (97%)	528 (92%)	46 (8%)	12 5

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	74	GLN
1	A	123	LYS
1	A	151	THR
1	A	157	SER
1	A	164	LYS
1	A	174	TRP
1	A	190	ASN
1	A	198[A]	GLU
1	A	198[B]	GLU
1	A	204	MET
1	A	214	LEU
1	A	219	ASN
1	A	224	ARG
1	A	244	LYS
1	A	257	ARG
1	A	260	LEU
1	A	268	GLU
1	A	276	ASN
1	A	277	LYS
1	A	286	ASP
1	A	289	THR
1	A	306	SER
1	A	314	CYS
1	A	339	LYS
1	A	345	SER
1	B	402	ARG

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Mol	Chain	Res	Type
1	B	403	LYS
1	B	426	SER
1	B	434	LYS
1	B	491	ILE
1	B	528	ARG
1	B	563	SER
1	B	574	TRP
1	B	583	LEU
1	B	617	TYR
1	B	619	ASN
1	B	624	ARG
1	B	627	LEU
1	B	657	ARG
1	B	659	ASN
1	B	717	GLN
1	B	739	LYS
1	B	740	GLN
1	B	743	ASP
1	B	749	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	ASN
1	A	190	ASN
1	A	207	ASN
1	A	219	ASN
1	A	221	GLN
1	A	259	ASN
1	A	276	ASN
1	A	329	GLN
1	B	607	ASN
1	B	622	GLN
1	B	654	HIS
1	B	740	GLN

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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	A	380	-	42,48,48	1.26	5 (11%)	50,73,73	2.70	16 (32%)
2	NAD	B	780	-	42,48,48	1.50	8 (19%)	50,73,73	2.08	13 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	380	-	-	2/26/62/62	0/5/5/5
2	NAD	B	780	-	-	4/26/62/62	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	780	NAD	C4N-C3N	4.31	1.46	1.39
2	B	780	NAD	C2N-N1N	3.36	1.39	1.35
2	A	380	NAD	C4N-C3N	3.05	1.44	1.39
2	A	380	NAD	C2A-N1A	2.92	1.39	1.33
2	B	780	NAD	C3N-C7N	2.79	1.54	1.50
2	B	780	NAD	C6N-N1N	2.59	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	780	NAD	O7N-C7N	-2.50	1.19	1.24
2	A	380	NAD	PA-O2A	-2.36	1.44	1.55
2	B	780	NAD	PN-O2N	-2.32	1.44	1.55
2	A	380	NAD	O7N-C7N	-2.26	1.19	1.24
2	B	780	NAD	O2D-C2D	2.24	1.48	1.43
2	A	380	NAD	O4B-C1B	-2.16	1.38	1.41
2	B	780	NAD	C5N-C4N	2.16	1.43	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	380	NAD	C5N-C4N-C3N	-7.02	112.04	120.34
2	A	380	NAD	C3N-C7N-N7N	-6.38	110.10	117.75
2	A	380	NAD	C5A-C6A-N6A	5.99	129.45	120.35
2	A	380	NAD	C2N-C3N-C4N	5.88	124.93	118.26
2	A	380	NAD	C4N-C3N-C7N	-5.79	105.54	121.04
2	B	780	NAD	C5N-C6N-N1N	-5.47	112.56	120.40
2	A	380	NAD	C3N-C2N-N1N	-4.98	115.56	120.43
2	B	780	NAD	C6N-N1N-C2N	4.88	126.42	121.97
2	B	780	NAD	C6N-C5N-C4N	4.55	126.05	119.44
2	B	780	NAD	C5N-C4N-C3N	-4.53	114.98	120.34
2	B	780	NAD	C4N-C3N-C7N	-4.45	109.12	121.04
2	A	380	NAD	C6N-C5N-C4N	4.33	125.74	119.44
2	A	380	NAD	C6N-N1N-C2N	4.27	125.87	121.97
2	A	380	NAD	O7N-C7N-C3N	4.25	124.72	119.63
2	A	380	NAD	O4B-C1B-C2B	-4.22	100.77	106.93
2	B	780	NAD	C2N-N1N-C1D	-3.49	111.35	119.14
2	A	380	NAD	C5N-C6N-N1N	-3.45	115.46	120.40
2	B	780	NAD	C2N-C3N-C7N	3.44	129.45	119.46
2	A	380	NAD	C2N-C3N-C7N	3.41	129.35	119.46
2	B	780	NAD	O7N-C7N-C3N	3.36	123.66	119.63
2	B	780	NAD	O5D-C5D-C4D	-2.70	99.70	108.99
2	B	780	NAD	C2N-C3N-C4N	2.65	121.26	118.26
2	A	380	NAD	C5A-C6A-N1A	-2.41	114.88	120.35
2	A	380	NAD	C2N-N1N-C1D	-2.37	113.87	119.14
2	A	380	NAD	N3A-C2A-N1A	2.29	132.26	128.68
2	B	780	NAD	PN-O5D-C5D	-2.15	109.05	121.68
2	A	380	NAD	O3D-C3D-C4D	2.12	117.17	111.05
2	B	780	NAD	C3N-C2N-N1N	-2.10	118.37	120.43
2	B	780	NAD	C4A-C5A-N7A	2.10	111.59	109.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	380	NAD	PN-O3-PA-O2A
2	B	780	NAD	PN-O3-PA-O2A
2	B	780	NAD	C5D-O5D-PN-O3
2	B	780	NAD	O4B-C4B-C5B-O5B
2	B	780	NAD	PN-O3-PA-O1A
2	A	380	NAD	O4B-C4B-C5B-O5B

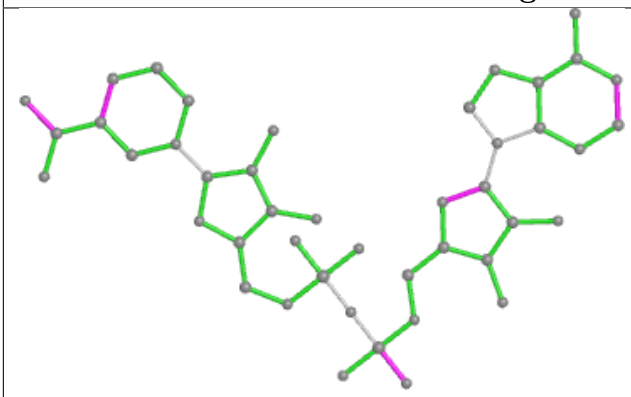
There are no ring outliers.

1 monomer is involved in 1 short contact:

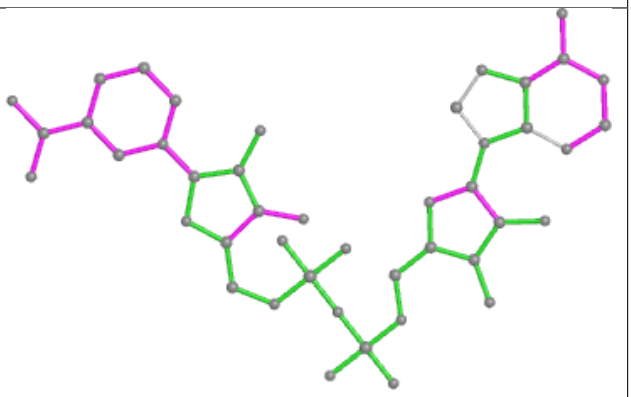
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	780	NAD	1	0

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 then 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.

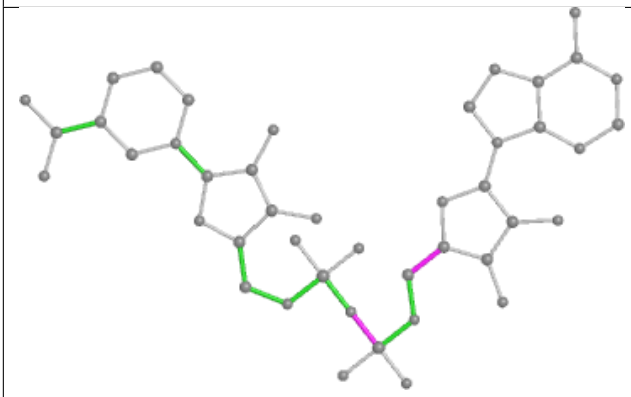
Ligand NAD A 380



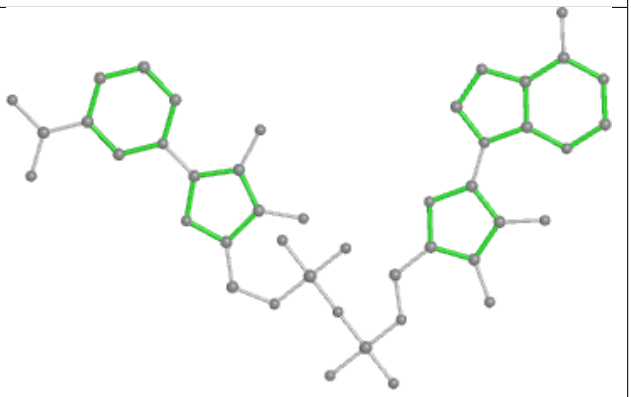
Bond lengths



Bond angles

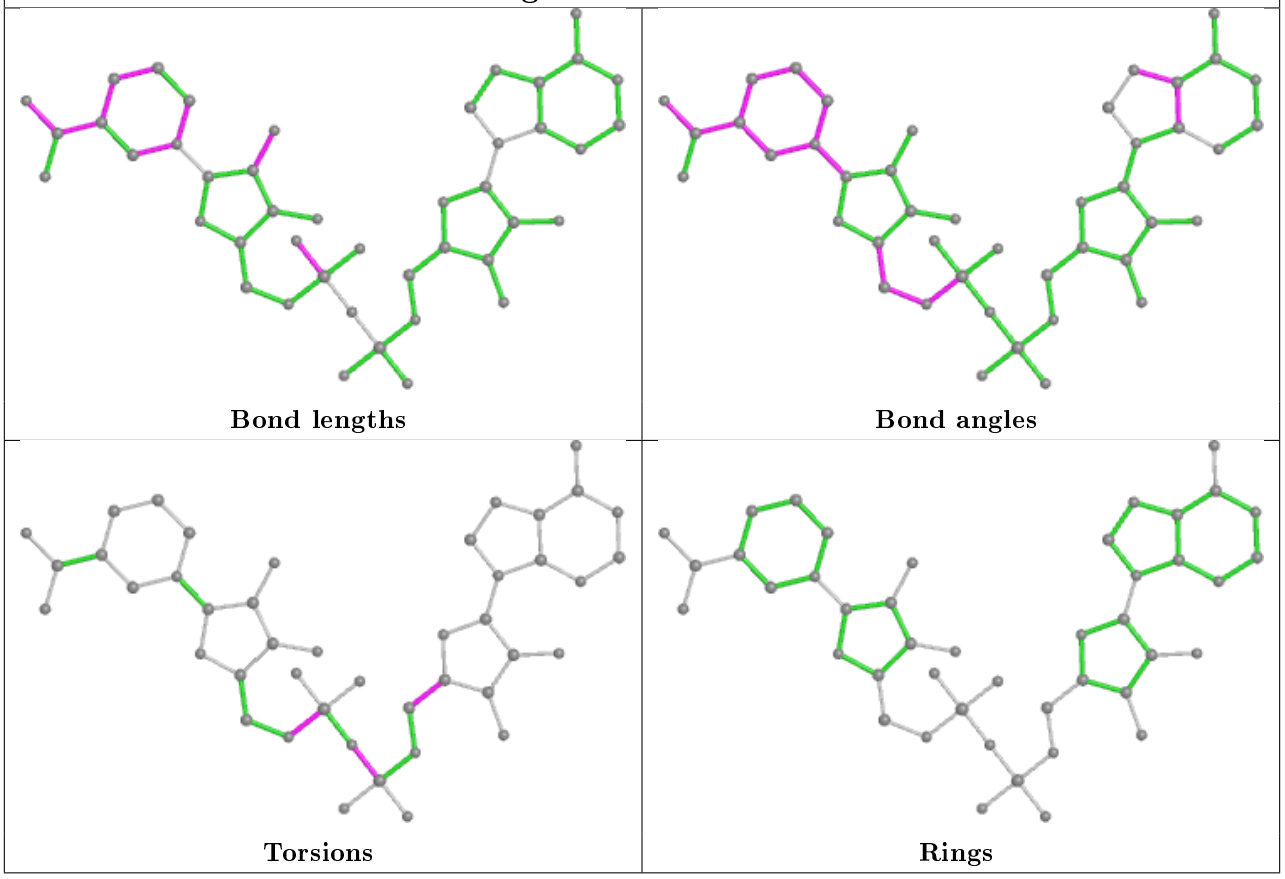


Torsions



Rings

Ligand NAD B 780



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.