



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:01 PM UTC

PDB ID : 6DFT / pdb_00006dft
Title : Trypanosoma brucei deoxyhypusine synthase
Authors : Tomchick, D.R.; Phillips, M.A.; Afanador, G.A.
Deposited on : 2018-05-15
Resolution : 3.50 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

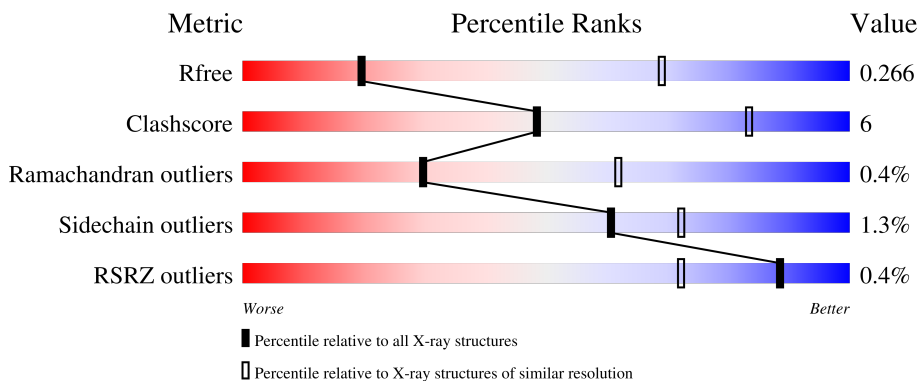
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	461	
1	C	461	
1	E	461	
1	G	461	
1	I	461	

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Mol	Chain	Length	Quality of chain
1	K	461	 70% 13% 17%
2	B	342	 81% 11% 7%
2	D	342	 82% 12% 6%
2	F	342	 81% 13% 6%
2	H	342	 79% 13% 7%
2	J	342	 81% 11% 8%
2	L	342	 79% 13% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32329 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 Deoxyhypusine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	384	Total 2927	C 1841	N 519	O 542	S 25	0	0	0
1	C	369	Total 2839	C 1787	N 504	O 523	S 25	0	0	0
1	E	370	Total 2845	C 1795	N 503	O 522	S 25	0	0	0
1	G	367	Total 2817	C 1770	N 503	O 520	S 24	0	0	0
1	I	364	Total 2792	C 1757	N 498	O 513	S 24	0	0	0
1	K	381	Total 2918	C 1840	N 516	O 537	S 25	0	0	0

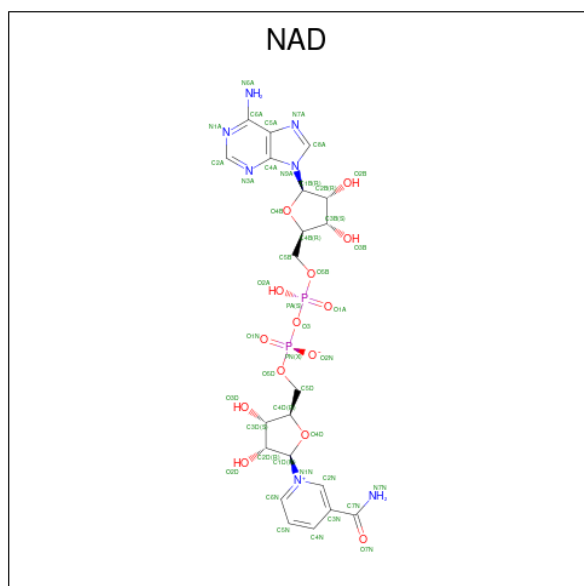
- Molecule 2 is a protein called Deoxyhypusine synthase regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	318	Total 2445	C 1517	N 449	O 464	S 15	0	0	0
2	D	320	Total 2460	C 1525	N 452	O 468	S 15	0	0	0
2	F	321	Total 2464	C 1527	N 452	O 470	S 15	0	0	0
2	H	317	Total 2428	C 1504	N 445	O 464	S 15	0	0	0
2	J	316	Total 2429	C 1506	N 446	O 462	S 15	0	0	0
2	L	317	Total 2436	C 1511	N 447	O 463	S 15	0	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 44 21 7 14 2	0	0
4	B	1	Total C N O P 44 21 7 14 2	0	0
4	C	1	Total C N O P 44 21 7 14 2	0	0
4	D	1	Total C N O P 44 21 7 14 2	0	0
4	E	1	Total C N O P 44 21 7 14 2	0	0
4	F	1	Total C N O P 44 21 7 14 2	0	0
4	G	1	Total C N O P 44 21 7 14 2	0	0
4	H	1	Total C N O P 44 21 7 14 2	0	0
4	I	1	Total C N O P 44 21 7 14 2	0	0
4	J	1	Total C N O P 44 21 7 14 2	0	0

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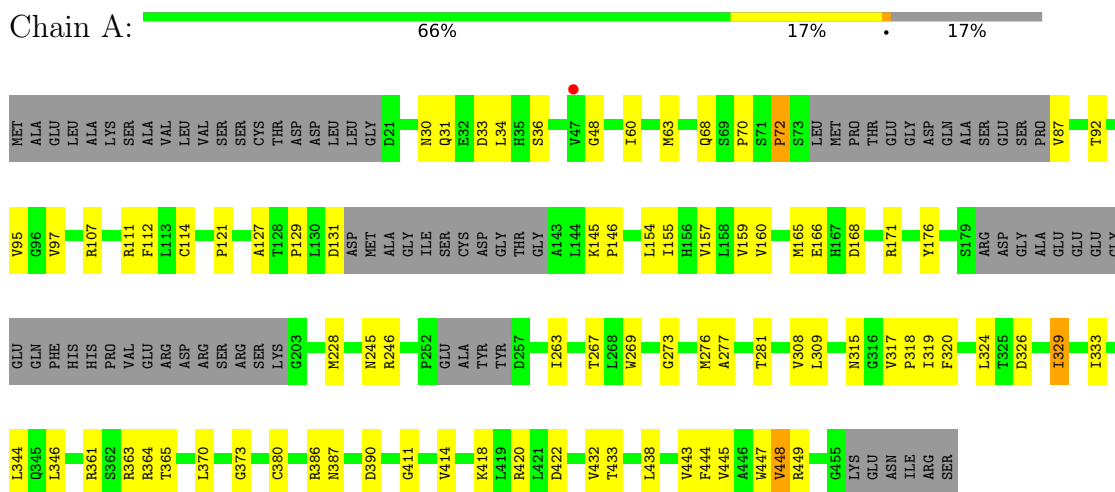
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	L	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

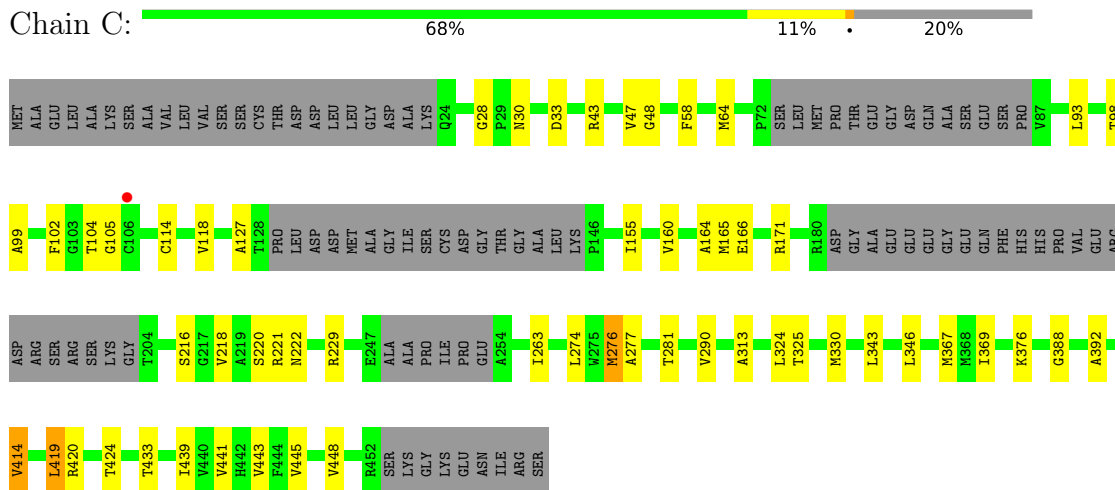
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: Deoxyhypusine synthase

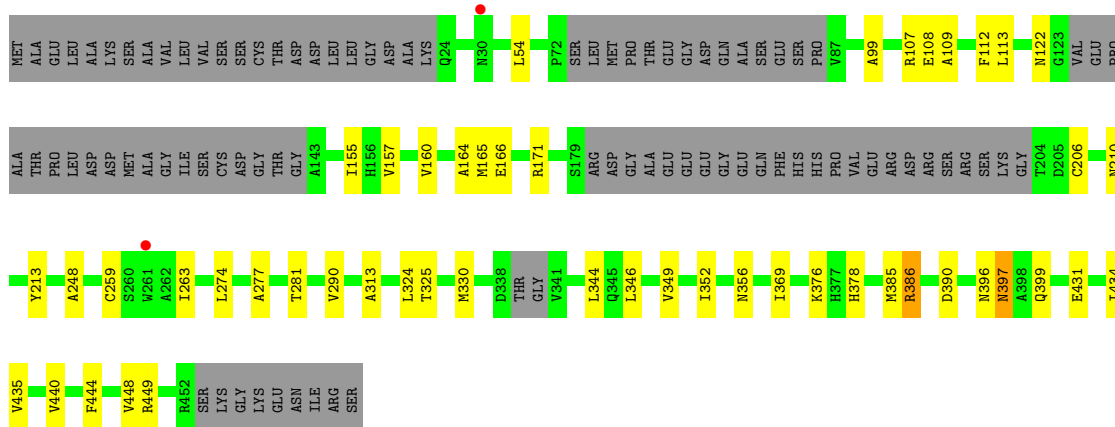


- Molecule 1: Deoxyhypusine synthase



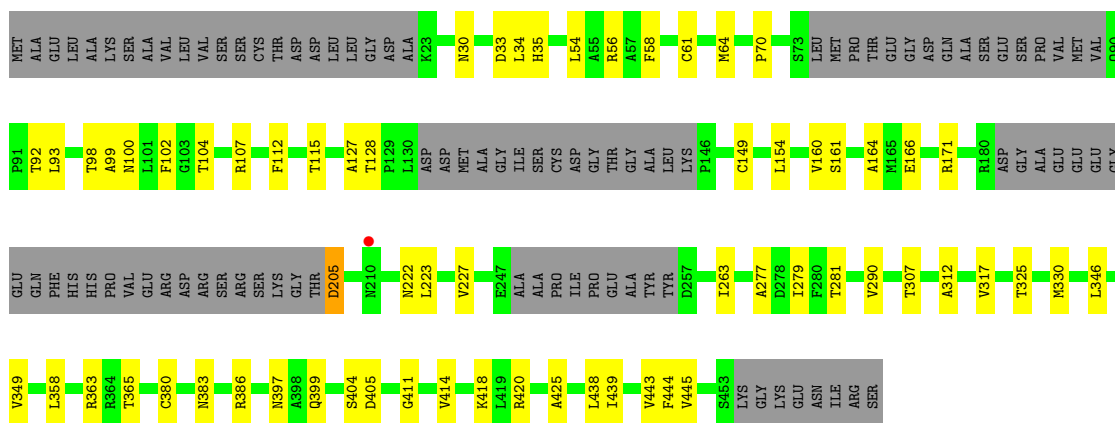
- Molecule 1: Deoxyhypusine synthase





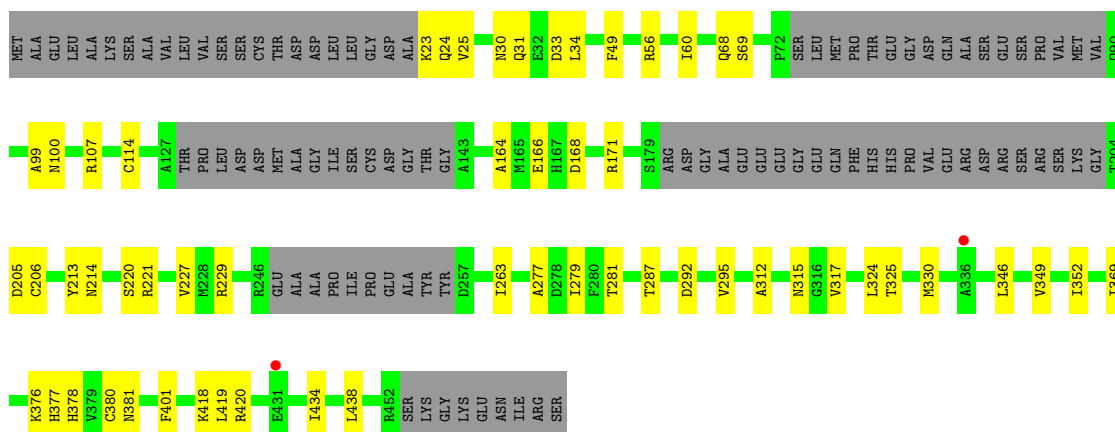
- Molecule 1: Deoxyhypusine synthase

Chain G: 66% 14% 20%



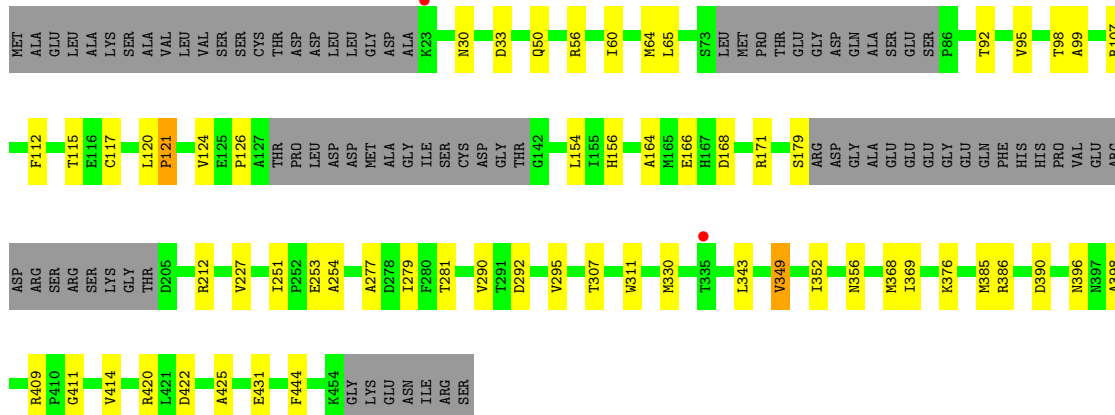
- Molecule 1: Deoxyhypusine synthase

Chain I: 67% 12% 21%




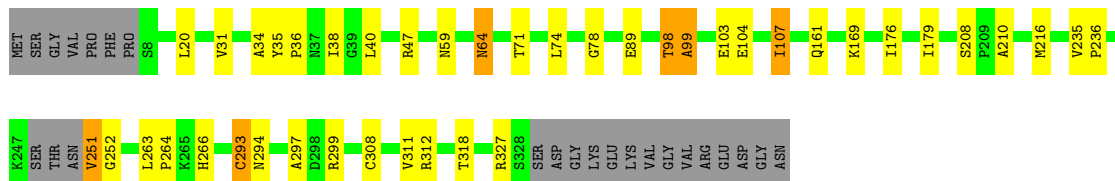
- Molecule 1: Deoxyhypusine synthase

Chain K:  70% 13% 17%




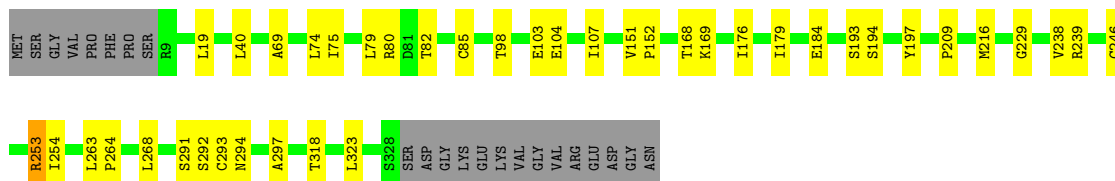
- Molecule 2: Deoxyhypusine synthase regulatory subunit

Chain B:  81% 11% 7%




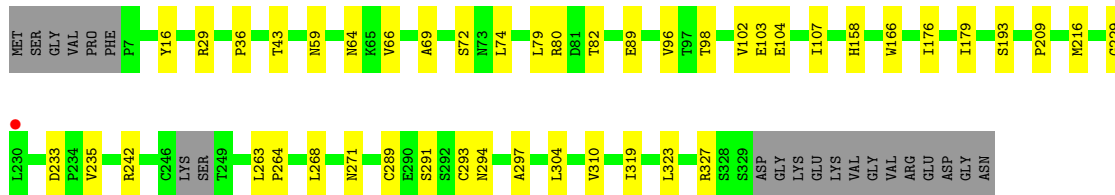
- Molecule 2: Deoxyhypusine synthase regulatory subunit

Chain D:  82% 12% 6%




- Molecule 2: Deoxyhypusine synthase regulatory subunit

Chain F:  81% 13% 6%

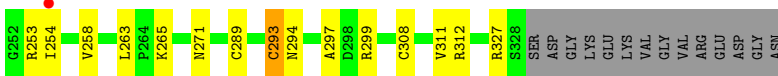
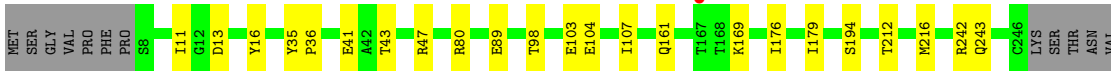
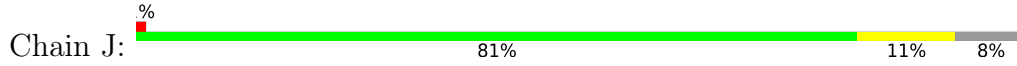


- Molecule 2: Deoxyhypusine synthase regulatory subunit

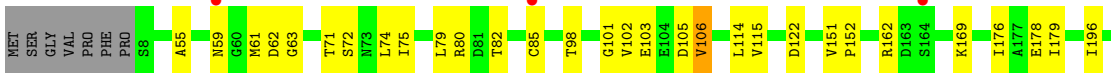
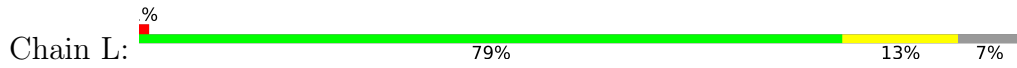
Chain H:  79% 13% 7%



• Molecule 2: Deoxyhypusine synthase regulatory subunit



• Molecule 2: Deoxyhypusine synthase regulatory subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.36Å 242.16Å 266.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 3.50 48.75 – 3.50	Depositor EDS
% Data completeness (in resolution range)	91.5 (48.75-3.50) 91.4 (48.75-3.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.48Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.222 , 0.262 0.225 , 0.266	Depositor DCC
R_{free} test set	1956 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtrriage
Anisotropy	0.079	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	32329	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, NA

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	0.12	0/2982	0.33	0/4042
1	C	0.12	0/2893	0.33	0/3920
1	E	0.12	0/2900	0.32	0/3931
1	G	0.11	0/2870	0.30	0/3887
1	I	0.14	0/2844	0.31	0/3852
1	K	0.11	0/2976	0.31	0/4034
2	B	0.13	0/2482	0.33	1/3368 (0.0%)
2	D	0.14	0/2498	0.35	0/3392
2	F	0.11	0/2502	0.33	0/3397
2	H	0.12	0/2463	0.31	0/3341
2	J	0.12	0/2466	0.32	0/3347
2	L	0.12	0/2473	0.33	0/3357
All	All	0.12	0/32349	0.32	1/43868 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	40	LEU	CB-CA-C	-5.37	110.36	116.54

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	2927	0	2923	50	0
1	C	2839	0	2823	36	0
1	E	2845	0	2835	31	0
1	G	2817	0	2807	39	0
1	I	2792	0	2788	35	0
1	K	2918	0	2913	39	0
2	B	2445	0	2433	27	0
2	D	2460	0	2447	28	0
2	F	2464	0	2446	30	0
2	H	2428	0	2413	27	0
2	J	2429	0	2411	23	0
2	L	2436	0	2420	36	0
3	A	1	0	0	0	0
4	A	44	0	26	1	0
4	B	44	0	26	3	0
4	C	44	0	26	4	0
4	D	44	0	26	3	0
4	E	44	0	26	2	0
4	F	44	0	26	0	0
4	G	44	0	26	2	0
4	H	44	0	26	3	0
4	I	44	0	26	2	0
4	J	44	0	26	0	0
4	K	44	0	26	3	0
4	L	44	0	26	1	0
All	All	32329	0	31971	355	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 (355) 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:G:99:ALA:HA	1:G:164:ALA:HB2	1.69	0.75
2:B:98:THR:HG23	2:B:264:PRO:HD3	1.69	0.74
2:B:64:ASN:N	2:B:64:ASN:OD1	2.21	0.73
1:E:107:ARG:HE	1:E:171:ARG:HD3	1.52	0.72
1:I:99:ALA:HA	1:I:164:ALA:HB2	1.71	0.70
1:E:449:ARG:NH2	2:H:22:ILE:O	2.26	0.69
1:E:113:LEU:HB3	1:E:155:ILE:HG12	1.75	0.68
2:L:55:ALA:HA	2:L:59:ASN:HD22	1.60	0.66
2:L:61:MET:O	2:L:63:GLY:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:386:ARG:NH2	1:K:390:ASP:OD2	2.30	0.65
1:A:165:MET:HE2	1:A:319:ILE:HD13	1.80	0.64
1:A:146:PRO:HA	1:A:267:THR:HG22	1.81	0.63
2:F:98:THR:HG22	2:F:263:LEU:HD23	1.80	0.62
4:G:500:NAD:O5D	4:G:500:NAD:H6N	2.00	0.62
1:A:63:MET:O	1:A:68:GLN:NE2	2.32	0.62
2:J:41:GLU:HB2	1:K:431:GLU:HG2	1.82	0.62
1:A:114:CYS:O	1:A:315:ASN:ND2	2.28	0.61
2:H:313:VAL:HG21	2:H:320:ILE:HG21	1.82	0.60
1:G:205:ASP:OD1	1:G:205:ASP:N	2.34	0.60
2:F:294:ASN:HB3	2:F:297:ALA:HB3	1.84	0.59
2:D:294:ASN:HB3	2:D:297:ALA:HB3	1.83	0.59
1:G:397:ASN:O	1:G:397:ASN:ND2	2.36	0.58
1:A:34:LEU:HD11	2:D:82:THR:HG23	1.84	0.58
2:L:75:ILE:HG13	2:L:80:ARG:HB3	1.85	0.58
1:A:131:ASP:HB3	1:A:361:ARG:HH12	1.68	0.58
2:H:64:ASN:OD1	2:H:253:ARG:HB3	2.04	0.58
2:B:294:ASN:HB3	2:B:297:ALA:HB3	1.86	0.58
2:F:89:GLU:OE2	2:F:327:ARG:NH2	2.36	0.58
2:H:98:THR:HG22	2:H:263:LEU:HD23	1.84	0.57
2:L:299:ARG:NH2	2:L:308:CYS:O	2.37	0.57
1:C:218:VAL:O	1:C:229:ARG:NH1	2.37	0.57
1:A:129:PRO:HD3	1:A:363:ARG:HH11	1.70	0.56
1:K:292:ASP:HB3	1:K:295:VAL:HG12	1.88	0.56
1:C:414:VAL:HG12	1:C:419:LEU:HB3	1.86	0.56
1:A:92:THR:HG23	1:A:127:ALA:HB3	1.86	0.56
2:D:98:THR:HG22	2:D:263:LEU:HD23	1.88	0.56
1:K:154:LEU:HD23	1:K:444:PHE:HD2	1.71	0.56
1:I:352:ILE:HG21	2:J:212:THR:HB	1.88	0.56
1:A:30:ASN:N	1:A:33:ASP:OD1	2.38	0.55
1:C:104:THR:O	1:C:171:ARG:NH1	2.39	0.55
1:C:343:LEU:HD11	2:D:239:ARG:HH21	1.72	0.55
1:C:276:MET:HE2	1:C:276:MET:HA	1.89	0.55
2:B:98:THR:O	2:B:208:SER:OG	2.18	0.55
1:K:107:ARG:NH1	1:K:168:ASP:O	2.40	0.55
4:E:500:NAD:O2A	2:F:291:SER:OG	2.24	0.55
2:J:103:GLU:HG2	2:J:216:MET:HG3	1.87	0.55
1:K:166:GLU:OE1	1:K:166:GLU:N	2.37	0.54
2:B:104:GLU:HA	2:B:107:ILE:HB	1.90	0.54
1:K:99:ALA:HA	1:K:164:ALA:HB2	1.89	0.54
1:G:92:THR:HG21	1:G:128:THR:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:294:ASN:HB3	2:J:297:ALA:HB3	1.90	0.54
1:G:405:ASP:HB2	4:H:500:NAD:H71N	1.73	0.53
2:B:31:VAL:HG21	1:C:441:VAL:HG21	1.90	0.53
1:I:380:CYS:HB3	1:I:418:LYS:HD3	1.91	0.53
1:G:92:THR:HG23	1:G:127:ALA:HB3	1.90	0.53
2:D:98:THR:HG23	2:D:264:PRO:HD3	1.91	0.53
1:G:102:PHE:CD2	1:G:164:ALA:HB1	2.44	0.53
2:L:75:ILE:HD11	2:L:105:ASP:HB2	1.90	0.53
2:B:59:ASN:OD1	2:B:64:ASN:HB2	2.08	0.53
2:J:98:THR:HG22	2:J:263:LEU:HD23	1.91	0.53
2:F:72:SER:OG	2:F:98:THR:OG1	2.23	0.53
4:A:502:NAD:O3B	4:B:500:NAD:O3B	2.24	0.52
2:H:96:VAL:HG22	2:H:207:PHE:HB2	1.92	0.52
2:H:242:ARG:NH1	2:H:271:ASN:OD1	2.42	0.52
1:A:326:ASP:OD2	2:B:266:HIS:ND1	2.42	0.52
1:A:386:ARG:NH2	1:A:390:ASP:OD2	2.41	0.52
1:E:210:ASN:HB3	2:H:40:LEU:HA	1.91	0.52
2:L:72:SER:O	2:L:75:ILE:HG22	2.09	0.52
2:J:89:GLU:OE2	2:J:327:ARG:NH2	2.43	0.52
1:K:121:PRO:HD2	1:K:124:VAL:HG21	1.92	0.52
1:C:99:ALA:HA	1:C:164:ALA:HB2	1.92	0.52
4:C:500:NAD:O3B	4:D:500:NAD:O3B	2.23	0.52
2:D:98:THR:OG1	4:D:500:NAD:O2N	2.27	0.52
2:F:98:THR:HG23	2:F:264:PRO:HD3	1.91	0.51
1:G:404:SER:HB2	4:H:500:NAD:O1A	2.10	0.51
1:A:107:ARG:NE	1:A:168:ASP:OD1	2.37	0.51
2:B:161:GLN:NE2	2:B:169:LYS:O	2.34	0.51
1:G:61:CYS:HA	1:G:64:MET:HE3	1.91	0.51
2:H:72:SER:OG	2:H:98:THR:OG1	2.28	0.51
1:I:377:HIS:O	1:I:381:ASN:N	2.32	0.51
4:I:500:NAD:H3D	4:I:500:NAD:O1N	2.10	0.51
1:A:165:MET:HB3	1:A:309:LEU:HD11	1.91	0.51
1:C:274:LEU:HD12	1:C:313:ALA:HB1	1.92	0.51
2:D:104:GLU:HA	2:D:107:ILE:HB	1.91	0.51
2:L:103:GLU:HG2	2:L:216:MET:HG3	1.92	0.51
1:A:228:MET:HE1	1:A:329:ILE:HG12	1.93	0.51
2:B:38:ILE:HG23	1:C:105:GLY:HA3	1.93	0.51
2:D:197:TYR:OH	2:J:243:GLN:NE2	2.37	0.51
1:I:114:CYS:O	1:I:315:ASN:ND2	2.32	0.51
1:I:369:ILE:HD13	1:I:376:LYS:HA	1.93	0.51
2:J:242:ARG:NH1	2:J:271:ASN:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:369:ILE:HD13	1:K:376:LYS:HA	1.93	0.51
2:F:59:ASN:HA	2:F:64:ASN:HB2	1.92	0.50
2:H:103:GLU:HG2	2:H:216:MET:HG3	1.92	0.50
1:K:253:GLU:HG2	1:K:254:ALA:H	1.75	0.50
2:L:169:LYS:NZ	2:L:178:GLU:OE2	2.42	0.50
1:A:333:ILE:HD12	1:A:344:LEU:HD12	1.94	0.50
1:I:221:ARG:NH1	1:I:287:THR:O	2.45	0.50
2:J:47:ARG:HB2	2:J:311:VAL:HG21	1.93	0.50
2:D:103:GLU:HG2	2:D:216:MET:HG3	1.94	0.50
2:L:176:ILE:HA	2:L:179:ILE:HD12	1.93	0.50
2:F:323:LEU:HD11	1:G:438:LEU:HD11	1.94	0.50
2:F:104:GLU:HA	2:F:107:ILE:HB	1.93	0.49
2:B:176:ILE:HA	2:B:179:ILE:HD12	1.95	0.49
4:E:500:NAD:O1A	2:F:289:CYS:HB2	2.12	0.49
2:J:258:VAL:HG11	2:J:265:LYS:HG3	1.94	0.49
2:H:74:LEU:HD22	2:H:79:LEU:HD12	1.93	0.49
1:K:98:THR:OG1	4:K:500:NAD:O2N	2.29	0.49
1:K:115:THR:HG22	1:K:311:TRP:CD2	2.47	0.49
2:F:103:GLU:HG2	2:F:216:MET:HG3	1.94	0.49
2:B:103:GLU:HG2	2:B:216:MET:HG3	1.93	0.49
1:A:159:VAL:HG22	1:A:320:PHE:HB2	1.93	0.49
2:D:80:ARG:NH2	2:D:193:SER:O	2.46	0.49
1:E:160:VAL:HG11	1:E:165:MET:HE3	1.94	0.49
1:G:166:GLU:OE1	1:G:166:GLU:N	2.39	0.49
2:J:176:ILE:HA	2:J:179:ILE:HD12	1.95	0.49
2:B:78:GLY:H	1:C:47:VAL:HG13	1.78	0.49
1:A:166:GLU:OE1	1:A:166:GLU:N	2.43	0.48
1:K:396:ASN:OD1	1:K:398:ALA:N	2.41	0.48
2:J:36:PRO:HA	2:J:43:THR:HA	1.95	0.48
2:F:209:PRO:HG2	2:F:263:LEU:HD21	1.94	0.48
1:G:56:ARG:NH1	1:G:425:ALA:O	2.45	0.48
1:C:43:ARG:O	1:C:47:VAL:HG23	2.13	0.48
1:C:221:ARG:NH1	1:G:35:HIS:O	2.47	0.48
1:C:325:THR:O	1:C:330:MET:HG3	2.14	0.48
1:I:49:PHE:HB2	2:L:318:THR:HG21	1.96	0.48
2:B:89:GLU:OE2	2:B:327:ARG:NH2	2.47	0.48
2:F:69:ALA:HB2	2:F:268:LEU:HD22	1.96	0.48
1:E:248:ALA:O	2:J:13:ASP:N	2.46	0.48
1:G:127:ALA:O	1:G:363:ARG:HG2	2.14	0.48
1:E:397:ASN:O	1:E:397:ASN:ND2	2.42	0.48
1:K:343:LEU:HD11	2:L:239:ARG:HE	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:THR:HG21	1:C:48:GLY:O	2.14	0.48
1:G:386:ARG:HH12	1:G:420:ARG:HD2	1.79	0.48
1:A:112:PHE:CZ	1:A:445:VAL:HG12	2.49	0.47
1:K:251:ILE:HG22	2:L:162:ARG:HH22	1.77	0.47
2:B:38:ILE:O	1:C:105:GLY:N	2.47	0.47
2:D:151:VAL:HG12	2:D:152:PRO:HD3	1.96	0.47
2:B:251:VAL:HG13	2:B:252:GLY:H	1.78	0.47
1:I:30:ASN:N	1:I:33:ASP:OD1	2.47	0.47
1:A:145:LYS:HD2	1:A:146:PRO:HD2	1.95	0.47
1:C:160:VAL:HG21	1:C:165:MET:HE3	1.95	0.47
1:E:99:ALA:HA	1:E:164:ALA:HB2	1.97	0.47
1:E:206:CYS:N	1:E:213:TYR:O	2.47	0.47
1:I:227:VAL:HG23	1:I:279:ILE:HG22	1.97	0.47
1:I:292:ASP:HB3	1:I:295:VAL:HG12	1.97	0.47
2:L:55:ALA:HA	2:L:59:ASN:ND2	2.27	0.47
2:B:99:ALA:HB2	2:B:210:ALA:O	2.14	0.47
1:G:30:ASN:N	1:G:33:ASP:OD1	2.44	0.47
1:G:439:ILE:O	1:G:443:VAL:HG12	2.15	0.47
1:A:273:GLY:HA2	1:A:276:MET:HG2	1.97	0.47
1:C:28:GLY:HA2	1:C:47:VAL:HG22	1.96	0.47
1:E:324:LEU:HD22	1:E:346:LEU:HD11	1.96	0.47
2:F:82:THR:HG23	1:G:34:LEU:HD11	1.97	0.47
1:I:107:ARG:NE	1:I:168:ASP:OD1	2.39	0.47
1:I:220:SER:O	1:I:229:ARG:NH2	2.47	0.47
2:J:104:GLU:HA	2:J:107:ILE:HB	1.95	0.47
1:K:369:ILE:HG21	1:K:376:LYS:HB2	1.97	0.47
4:C:500:NAD:O2A	2:D:291:SER:HB2	2.14	0.47
1:A:411:GLY:O	1:A:414:VAL:HG12	2.15	0.47
1:K:356:ASN:HB3	1:K:385:MET:HG3	1.97	0.47
1:C:324:LEU:HD22	1:C:346:LEU:HD11	1.97	0.46
1:G:365:THR:HG21	1:G:383:ASN:OD1	2.15	0.46
2:B:47:ARG:HB2	2:B:311:VAL:HG21	1.95	0.46
1:E:259:CYS:HB2	2:F:166:TRP:CE2	2.49	0.46
2:F:319:ILE:HD13	1:G:54:LEU:HD12	1.98	0.46
1:A:277:ALA:O	1:A:281:THR:HG23	2.15	0.46
1:C:220:SER:O	1:C:229:ARG:NH2	2.49	0.46
2:L:151:VAL:HG12	2:L:152:PRO:HD3	1.97	0.46
1:A:438:LEU:HD11	2:D:323:LEU:HD11	1.97	0.46
2:D:74:LEU:HD22	2:D:79:LEU:HD12	1.98	0.46
1:G:154:LEU:HD23	1:G:444:PHE:HD1	1.79	0.46
1:C:330:MET:HE2	2:D:238:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:176:ILE:HA	2:D:179:ILE:HD12	1.97	0.46
1:A:157:VAL:HG23	1:A:318:PRO:HG2	1.97	0.46
2:B:299:ARG:NH2	2:B:308:CYS:O	2.49	0.46
2:H:59:ASN:HB2	2:H:66:VAL:HG23	1.97	0.46
2:J:16:TYR:HB2	1:K:112:PHE:HB2	1.98	0.46
1:K:330:MET:HE2	2:L:238:VAL:HG21	1.98	0.46
1:G:277:ALA:O	1:G:281:THR:HG23	2.15	0.46
2:H:35:TYR:HA	2:H:38:ILE:HG13	1.98	0.46
1:K:349:VAL:HA	1:K:352:ILE:HG22	1.97	0.46
1:A:444:PHE:O	1:A:448:VAL:HG13	2.16	0.46
1:I:24:GLN:HB2	2:L:115:VAL:HG22	1.97	0.46
1:A:443:VAL:O	1:A:447:TRP:N	2.46	0.45
1:I:23:LYS:HD3	2:L:114:LEU:HD13	1.98	0.45
1:A:373:GLY:HA2	4:B:500:NAD:O2A	2.15	0.45
1:C:277:ALA:O	1:C:281:THR:HG23	2.16	0.45
2:F:304:LEU:HD21	2:F:310:VAL:HG21	1.99	0.45
2:H:69:ALA:HB2	2:H:268:LEU:HD22	1.98	0.45
2:F:29:ARG:NH2	2:F:327:ARG:O	2.46	0.45
1:I:31:GLN:HG2	2:L:85:CYS:SG	2.56	0.45
1:K:409:ARG:NH2	2:L:122:ASP:OD2	2.49	0.45
1:K:107:ARG:NH1	1:K:168:ASP:OD1	2.50	0.45
2:L:75:ILE:HG13	2:L:80:ARG:CB	2.46	0.45
1:A:246:ARG:HD3	1:A:246:ARG:HA	1.77	0.45
2:B:35:TYR:N	2:B:36:PRO:HD2	2.31	0.45
1:E:112:PHE:HB2	2:H:16:TYR:HB2	1.99	0.45
1:I:277:ALA:O	1:I:281:THR:HG23	2.16	0.45
1:A:380:CYS:SG	1:A:418:LYS:HD3	2.57	0.45
4:C:500:NAD:H4D	2:D:263:LEU:HA	1.99	0.45
1:A:370:LEU:HD22	1:A:432:VAL:HG13	1.99	0.45
1:C:166:GLU:OE2	1:C:166:GLU:N	2.49	0.45
2:D:75:ILE:HD12	2:D:104:GLU:HB2	1.99	0.45
1:G:411:GLY:O	1:G:414:VAL:HG12	2.16	0.45
1:I:434:ILE:HD13	2:L:320:ILE:HD11	1.98	0.45
2:J:11:ILE:O	1:K:171:ARG:NH2	2.50	0.45
1:A:449:ARG:NH1	2:D:19:LEU:O	2.50	0.44
1:G:149:CYS:HB3	1:G:358:LEU:HD21	1.99	0.44
1:G:380:CYS:HB3	1:G:418:LYS:HD3	1.99	0.44
1:K:115:THR:HG22	1:K:311:TRP:CG	2.53	0.44
2:D:168:THR:HG22	2:D:169:LYS:HG3	1.99	0.44
2:D:209:PRO:HG2	2:D:263:LEU:HD21	1.99	0.44
1:K:65:LEU:HD11	1:K:444:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:254:ILE:HG23	2:L:274:ALA:HA	1.99	0.44
1:I:56:ARG:O	1:I:60:ILE:HG12	2.17	0.44
1:I:263:ILE:O	1:I:346:LEU:HA	2.17	0.44
2:H:294:ASN:HB3	2:H:297:ALA:HB3	1.99	0.44
1:I:100:ASN:HD22	2:J:289:CYS:HA	1.81	0.44
1:K:385:MET:HE2	2:L:221:TYR:CD2	2.53	0.44
2:L:209:PRO:HG2	2:L:263:LEU:HD21	1.99	0.44
1:A:48:GLY:O	2:D:318:THR:HG21	2.16	0.44
2:B:293:CYS:O	2:B:312:ARG:NH1	2.51	0.44
1:E:349:VAL:HA	1:E:352:ILE:HG22	1.99	0.44
1:A:154:LEU:HD23	1:A:444:PHE:HD1	1.83	0.44
1:C:369:ILE:HG21	1:C:376:LYS:HB2	2.00	0.44
1:E:54:LEU:HD12	2:H:319:ILE:HD13	1.98	0.44
1:G:107:ARG:HH21	1:G:307:THR:HA	1.82	0.44
1:K:179:SER:HB2	1:K:212:ARG:NH1	2.33	0.44
1:E:449:ARG:NH1	2:H:24:GLN:OE1	2.50	0.44
2:H:35:TYR:N	2:H:36:PRO:HD2	2.33	0.44
2:H:293:CYS:O	2:H:312:ARG:NH1	2.39	0.44
1:K:30:ASN:N	1:K:33:ASP:OD1	2.50	0.44
1:E:399:GLN:HG2	1:G:399:GLN:CD	2.42	0.43
1:E:434:ILE:HG13	1:E:435:VAL:HG23	1.99	0.43
2:F:59:ASN:HB2	2:F:66:VAL:HG23	2.00	0.43
2:H:304:LEU:HD21	2:H:310:VAL:HG21	2.00	0.43
1:K:411:GLY:O	1:K:414:VAL:HG12	2.18	0.43
1:A:171:ARG:HG3	1:A:176:TYR:CD1	2.54	0.43
2:H:104:GLU:HA	2:H:107:ILE:HB	2.00	0.43
1:I:324:LEU:HD22	1:I:346:LEU:HD11	2.00	0.43
1:K:92:THR:HA	1:K:156:HIS:ND1	2.33	0.43
1:C:114:CYS:SG	1:C:155:ILE:HD11	2.59	0.43
1:G:64:MET:HB3	1:G:93:LEU:HD11	1.99	0.43
1:G:160:VAL:HG12	1:G:161:SER:O	2.19	0.43
1:G:222:ASN:OD1	1:G:223:LEU:N	2.51	0.43
2:H:265:LYS:HE2	2:H:290:GLU:O	2.19	0.43
1:A:97:VAL:HB	1:A:160:VAL:HG12	2.00	0.43
2:B:20:LEU:HD23	1:C:445:VAL:HG13	2.01	0.43
1:C:263:ILE:O	1:C:346:LEU:HA	2.18	0.43
1:E:325:THR:O	1:E:330:MET:HG3	2.18	0.43
1:A:165:MET:HB2	1:A:269:TRP:CZ3	2.54	0.43
1:C:30:ASN:N	1:C:33:ASP:OD1	2.36	0.43
1:E:396:ASN:OD1	1:E:397:ASN:N	2.52	0.43
1:I:325:THR:O	1:I:330:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:227:VAL:HG23	1:K:279:ILE:HG22	2.01	0.43
1:A:95:VAL:HG11	1:A:155:ILE:HD12	1.99	0.43
1:A:263:ILE:HD11	1:A:344:LEU:HD13	2.01	0.43
1:A:263:ILE:O	1:A:346:LEU:HA	2.19	0.43
2:F:80:ARG:NH2	2:F:193:SER:O	2.52	0.43
2:D:69:ALA:HB2	2:D:268:LEU:HD22	2.01	0.43
1:I:420:ARG:HA	1:I:420:ARG:HD2	1.78	0.43
1:K:420:ARG:NH1	1:K:422:ASP:OD2	2.52	0.43
1:A:380:CYS:HB2	1:A:418:LYS:HB3	2.01	0.43
1:I:438:LEU:HD11	2:L:323:LEU:HD11	2.01	0.43
2:F:96:VAL:HG21	2:F:268:LEU:HD13	2.01	0.42
1:K:277:ALA:O	1:K:281:THR:HG23	2.19	0.42
1:I:206:CYS:N	1:I:213:TYR:O	2.51	0.42
1:A:30:ASN:OD1	1:A:31:GLN:N	2.44	0.42
1:E:431:GLU:HG2	2:H:41:GLU:HB2	2.01	0.42
1:G:112:PHE:HA	1:G:115:THR:HG22	2.00	0.42
1:A:31:GLN:HG2	2:D:85:CYS:SG	2.59	0.42
2:D:184:GLU:HB2	2:D:197:TYR:HE1	1.85	0.42
2:H:47:ARG:HB2	2:H:311:VAL:HG21	2.02	0.42
2:J:161:GLN:NE2	2:J:169:LYS:O	2.52	0.42
1:C:58:PHE:HE1	1:C:439:ILE:HA	1.84	0.42
1:C:439:ILE:O	1:C:443:VAL:HG22	2.19	0.42
1:E:344:LEU:O	2:F:235:VAL:HG21	2.19	0.42
1:E:369:ILE:HG21	1:E:376:LYS:HB2	2.00	0.42
1:I:205:ASP:OD1	1:I:205:ASP:N	2.52	0.42
4:I:500:NAD:H52A	2:J:289:CYS:SG	2.60	0.42
4:D:500:NAD:H8A	4:D:500:NAD:O5B	2.20	0.42
1:I:205:ASP:HA	1:I:214:ASN:HA	2.01	0.42
1:K:95:VAL:HA	1:K:368:MET:O	2.19	0.42
2:F:16:TYR:HB2	1:G:112:PHE:HB2	2.02	0.42
2:F:74:LEU:HD22	2:F:79:LEU:HD12	2.02	0.42
2:F:242:ARG:NH1	2:F:271:ASN:OD1	2.53	0.42
2:L:75:ILE:HG21	2:L:101:GLY:HA2	2.02	0.42
1:E:277:ALA:O	1:E:281:THR:HG23	2.19	0.42
2:H:49:ARG:NH1	2:H:323:LEU:O	2.53	0.42
2:H:176:ILE:HA	2:H:179:ILE:HD12	2.02	0.42
1:A:228:MET:HE2	1:A:228:MET:HB3	1.88	0.42
1:A:420:ARG:NE	1:A:422:ASP:OD1	2.51	0.42
1:I:34:LEU:HD11	2:L:82:THR:HG23	2.00	0.42
1:I:107:ARG:HD3	1:I:171:ARG:HD3	2.02	0.42
2:F:176:ILE:HA	2:F:179:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:GLU:OE1	1:I:166:GLU:N	2.43	0.41
2:J:80:ARG:NH2	2:J:194:SER:HA	2.35	0.41
2:B:98:THR:HG21	4:B:500:NAD:O1N	2.20	0.41
1:E:263:ILE:O	1:E:346:LEU:HA	2.20	0.41
1:I:401:PHE:HB2	1:K:50:GLN:HG3	2.02	0.41
1:K:56:ARG:NH1	1:K:425:ALA:O	2.54	0.41
1:G:227:VAL:HG23	1:G:279:ILE:HG22	2.03	0.41
1:G:312:ALA:HA	1:G:317:VAL:HG22	2.01	0.41
1:G:325:THR:O	1:G:330:MET:HG3	2.20	0.41
2:L:279:TYR:HB2	2:L:312:ARG:HA	2.02	0.41
1:A:36:SER:HB3	1:I:221:ARG:HE	1.84	0.41
1:C:64:MET:HB3	1:C:93:LEU:HD11	2.02	0.41
2:J:299:ARG:NH2	2:J:308:CYS:O	2.53	0.41
2:L:71:THR:OG1	4:L:500:NAD:O2N	2.34	0.41
2:L:102:VAL:O	2:L:106:VAL:HG23	2.20	0.41
2:F:102:VAL:HG11	2:F:176:ILE:HG12	2.03	0.41
1:I:68:GLN:HG2	1:I:69:SER:H	1.85	0.41
2:L:105:ASP:OD2	2:L:196:ILE:HG12	2.21	0.41
2:B:71:THR:HG22	2:B:74:LEU:HG	2.01	0.41
1:E:444:PHE:O	1:E:448:VAL:HG23	2.21	0.41
1:K:385:MET:HE2	2:L:221:TYR:HD2	1.85	0.41
4:K:500:NAD:O2A	2:L:291:SER:OG	2.32	0.41
1:E:274:LEU:HD12	1:E:313:ALA:HB1	2.01	0.41
1:E:356:ASN:HB3	1:E:385:MET:HG3	2.02	0.41
1:C:98:THR:HG23	4:C:500:NAD:O2N	2.20	0.41
1:C:104:THR:OG1	1:C:105:GLY:N	2.53	0.41
1:G:100:ASN:OD1	4:G:500:NAD:H5N	2.21	0.41
4:K:500:NAD:H4D	2:L:263:LEU:HA	2.02	0.41
2:L:72:SER:HB3	2:L:98:THR:OG1	2.21	0.41
1:A:72:PRO:HD3	1:A:364:ARG:NH2	2.36	0.41
2:B:34:ALA:O	2:B:38:ILE:HG13	2.21	0.41
2:B:235:VAL:HG22	2:B:236:PRO:HD3	2.03	0.41
2:D:80:ARG:NH2	2:D:194:SER:HA	2.36	0.41
1:E:171:ARG:NH2	2:H:12:GLY:O	2.54	0.41
4:H:500:NAD:H3D	4:H:500:NAD:PN	2.60	0.41
1:I:312:ALA:HA	1:I:317:VAL:HG22	2.02	0.41
2:L:74:LEU:HD22	2:L:79:LEU:HD12	2.03	0.41
1:A:111:ARG:HB2	1:A:308:VAL:HG12	2.03	0.41
1:C:367:MET:O	1:C:392:ALA:HA	2.21	0.41
1:E:166:GLU:OE1	1:E:166:GLU:N	2.52	0.41
2:J:293:CYS:O	2:J:312:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:GLY:C	1:C:420:ARG:HG3	2.46	0.40
2:D:253:ARG:HE	2:D:253:ARG:HB2	1.44	0.40
1:E:109:ALA:HB1	1:E:440:VAL:HG21	2.02	0.40
1:K:60:ILE:HG22	1:K:64:MET:HE3	2.04	0.40
1:A:324:LEU:HD22	1:A:346:LEU:HD11	2.03	0.40
2:F:233:ASP:OD1	2:F:235:VAL:HG22	2.22	0.40
1:G:104:THR:O	1:G:171:ARG:NH1	2.54	0.40
1:C:102:PHE:CD2	1:C:164:ALA:HB1	2.56	0.40
1:E:386:ARG:NH2	1:E:390:ASP:OD2	2.54	0.40
1:G:58:PHE:HE1	1:G:439:ILE:HA	1.85	0.40
1:G:263:ILE:O	1:G:346:LEU:HA	2.21	0.40
1:A:433:THR:HG21	2:D:40:LEU:HB2	2.02	0.40
1:C:118:VAL:HG22	1:C:448:VAL:HG23	2.04	0.40
2:F:158:HIS:NE2	2:F:229:GLY:HA3	2.36	0.40
2:J:35:TYR:N	2:J:36:PRO:HD2	2.36	0.40
1:A:70:PRO:HD3	1:A:87:VAL:O	2.22	0.40
2:F:36:PRO:HA	2:F:43:THR:HA	2.02	0.40
1:K:120:LEU:HD13	1:K:126:PRO:HD3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	374/461 (81%)	358 (96%)	14 (4%)	2 (0%)	24	57
1	C	359/461 (78%)	345 (96%)	13 (4%)	1 (0%)	36	67
1	E	360/461 (78%)	343 (95%)	16 (4%)	1 (0%)	36	67
1	G	357/461 (77%)	344 (96%)	12 (3%)	1 (0%)	36	67
1	I	354/461 (77%)	341 (96%)	13 (4%)	0	100	100
1	K	373/461 (81%)	354 (95%)	18 (5%)	1 (0%)	36	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	314/342 (92%)	289 (92%)	23 (7%)	2 (1%)	21	54
2	D	318/342 (93%)	295 (93%)	20 (6%)	3 (1%)	14	47
2	F	317/342 (93%)	300 (95%)	16 (5%)	1 (0%)	36	67
2	H	311/342 (91%)	286 (92%)	24 (8%)	1 (0%)	36	67
2	J	312/342 (91%)	292 (94%)	18 (6%)	2 (1%)	21	54
2	L	313/342 (92%)	292 (93%)	19 (6%)	2 (1%)	21	54
All	All	4062/4818 (84%)	3839 (94%)	206 (5%)	17 (0%)	30	62

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	62	ASP
2	B	293	CYS
1	C	127	ALA
2	D	292	SER
1	E	122	ASN
2	H	293	CYS
2	J	293	CYS
2	F	293	CYS
1	G	70	PRO
2	J	253	ARG
2	B	99	ALA
2	L	293	CYS
1	A	121	PRO
2	D	293	CYS
2	D	229	GLY
1	K	121	PRO
1	A	72	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/380 (83%)	310 (98%)	7 (2%)	45	65
1	C	307/380 (81%)	299 (97%)	8 (3%)	40	62
1	E	307/380 (81%)	301 (98%)	6 (2%)	48	67
1	G	306/380 (80%)	301 (98%)	5 (2%)	55	70
1	I	302/380 (80%)	298 (99%)	4 (1%)	61	72
1	K	315/380 (83%)	311 (99%)	4 (1%)	61	72
2	B	268/288 (93%)	263 (98%)	5 (2%)	50	68
2	D	270/288 (94%)	267 (99%)	3 (1%)	65	74
2	F	271/288 (94%)	271 (100%)	0	100	100
2	H	267/288 (93%)	265 (99%)	2 (1%)	76	78
2	J	266/288 (92%)	265 (100%)	1 (0%)	84	81
2	L	267/288 (93%)	266 (100%)	1 (0%)	84	81
All	All	3463/4008 (86%)	3417 (99%)	46 (1%)	61	72

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

Mol	Chain	Res	Type
1	A	60	ILE
1	A	245	ASN
1	A	317	VAL
1	A	329	ILE
1	A	365	THR
1	A	387	ASN
1	A	448	VAL
2	B	64	ASN
2	B	98	THR
2	B	107	ILE
2	B	251	VAL
2	B	263	LEU
1	C	216	SER
1	C	222	ASN
1	C	276	MET
1	C	290	VAL
1	C	414	VAL
1	C	419	LEU
1	C	424	THR

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Mol	Chain	Res	Type
1	C	433	THR
2	D	246	CYS
2	D	253	ARG
2	D	254	ILE
1	E	108	GLU
1	E	157	VAL
1	E	290	VAL
1	E	378	HIS
1	E	386	ARG
1	E	397	ASN
1	G	98	THR
1	G	205	ASP
1	G	290	VAL
1	G	349	VAL
1	G	445	VAL
2	H	22	ILE
2	H	318	THR
1	I	25	VAL
1	I	349	VAL
1	I	378	HIS
1	I	419	LEU
2	J	254	ILE
1	K	117	CYS
1	K	290	VAL
1	K	307	THR
1	K	349	VAL
2	L	106	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	HIS
1	A	378	HIS
2	B	37	ASN
2	B	127	ASN
1	C	50	GLN
1	C	53	ASN
1	C	442	HIS
2	D	21	ASN
2	D	140	ASN
2	D	267	HIS
1	E	100	ASN

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Mol	Chain	Res	Type
1	E	122	ASN
1	E	207	HIS
1	G	35	HIS
2	H	267	HIS
2	H	314	HIS
1	I	100	ASN
1	I	156	HIS
1	I	210	ASN
2	J	33	ASN
2	J	73	ASN
2	J	140	ASN
1	K	35	HIS
1	K	377	HIS
1	K	383	ASN
2	L	59	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](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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
4	NAD	E	500	-	46,48,48	3.03	18 (39%)	64,73,73	2.30	16 (25%)
4	NAD	A	502	-	46,48,48	2.97	17 (36%)	64,73,73	2.30	15 (23%)
4	NAD	D	500	-	46,48,48	3.01	18 (39%)	64,73,73	2.34	15 (23%)
4	NAD	H	500	-	46,48,48	3.03	18 (39%)	64,73,73	2.35	15 (23%)
4	NAD	L	500	-	46,48,48	3.03	17 (36%)	64,73,73	2.35	15 (23%)
4	NAD	K	500	-	46,48,48	3.00	19 (41%)	64,73,73	2.34	15 (23%)
4	NAD	B	500	-	46,48,48	2.98	19 (41%)	64,73,73	2.34	15 (23%)
4	NAD	I	500	-	46,48,48	2.97	16 (34%)	64,73,73	2.43	15 (23%)
4	NAD	C	500	-	46,48,48	2.94	18 (39%)	64,73,73	2.37	15 (23%)
4	NAD	J	500	-	46,48,48	3.05	17 (36%)	64,73,73	2.33	14 (21%)
4	NAD	G	500	-	46,48,48	3.03	19 (41%)	64,73,73	2.32	16 (25%)
4	NAD	F	500	-	46,48,48	3.04	19 (41%)	64,73,73	2.35	15 (23%)

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
4	NAD	E	500	-	-	10/30/62/62	0/5/5/5
4	NAD	A	502	-	-	13/30/62/62	0/5/5/5
4	NAD	D	500	-	-	13/30/62/62	0/5/5/5
4	NAD	H	500	-	-	9/30/62/62	0/5/5/5
4	NAD	L	500	-	-	8/30/62/62	0/5/5/5
4	NAD	K	500	-	-	5/30/62/62	0/5/5/5
4	NAD	B	500	-	-	7/30/62/62	0/5/5/5
4	NAD	I	500	-	-	8/30/62/62	0/5/5/5
4	NAD	C	500	-	-	6/30/62/62	0/5/5/5
4	NAD	J	500	-	-	6/30/62/62	0/5/5/5
4	NAD	G	500	-	-	3/30/62/62	0/5/5/5
4	NAD	F	500	-	-	6/30/62/62	0/5/5/5

All (215) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	500	NAD	PA-O3	8.67	1.68	1.59
4	F	500	NAD	PA-O3	8.63	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	500	NAD	PA-O3	8.46	1.68	1.59
4	L	500	NAD	PA-O3	8.46	1.68	1.59
4	E	500	NAD	PA-O3	8.45	1.68	1.59
4	G	500	NAD	PA-O3	8.45	1.68	1.59
4	K	500	NAD	PA-O3	8.45	1.68	1.59
4	A	502	NAD	PA-O3	8.33	1.68	1.59
4	G	500	NAD	O4D-C1D	8.27	1.51	1.40
4	C	500	NAD	O4D-C1D	8.26	1.51	1.40
4	D	500	NAD	O4D-C1D	8.18	1.51	1.40
4	B	500	NAD	PA-O3	8.18	1.68	1.59
4	D	500	NAD	PA-O3	8.17	1.68	1.59
4	L	500	NAD	O4D-C1D	8.17	1.51	1.40
4	I	500	NAD	PA-O3	8.16	1.68	1.59
4	A	502	NAD	O4D-C1D	8.13	1.51	1.40
4	E	500	NAD	O4D-C1D	8.08	1.51	1.40
4	K	500	NAD	O4D-C1D	8.06	1.51	1.40
4	H	500	NAD	O4D-C1D	8.04	1.51	1.40
4	B	500	NAD	O4D-C1D	8.02	1.51	1.40
4	J	500	NAD	O4D-C1D	7.99	1.51	1.40
4	F	500	NAD	O4D-C1D	7.96	1.51	1.40
4	I	500	NAD	O4D-C1D	7.94	1.51	1.40
4	C	500	NAD	PA-O3	7.87	1.68	1.59
4	L	500	NAD	C7N-N7N	7.48	1.46	1.33
4	I	500	NAD	C7N-N7N	7.48	1.46	1.33
4	J	500	NAD	C7N-N7N	7.47	1.46	1.33
4	H	500	NAD	C7N-N7N	7.47	1.46	1.33
4	D	500	NAD	C7N-N7N	7.44	1.46	1.33
4	K	500	NAD	C7N-N7N	7.44	1.46	1.33
4	E	500	NAD	C7N-N7N	7.44	1.46	1.33
4	F	500	NAD	C7N-N7N	7.43	1.46	1.33
4	B	500	NAD	C7N-N7N	7.40	1.46	1.33
4	G	500	NAD	C7N-N7N	7.36	1.46	1.33
4	C	500	NAD	C7N-N7N	7.29	1.46	1.33
4	A	502	NAD	C7N-N7N	7.29	1.46	1.33
4	J	500	NAD	PN-O3	7.06	1.67	1.59
4	F	500	NAD	PN-O3	6.98	1.67	1.59
4	E	500	NAD	PN-O3	6.92	1.67	1.59
4	H	500	NAD	PN-O3	6.88	1.66	1.59
4	L	500	NAD	PN-O3	6.79	1.66	1.59
4	G	500	NAD	PN-O3	6.74	1.66	1.59
4	K	500	NAD	PN-O3	6.71	1.66	1.59
4	B	500	NAD	PN-O3	6.66	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	500	NAD	C8A-N9A	-6.56	1.26	1.37
4	D	500	NAD	PN-O3	6.55	1.66	1.59
4	C	500	NAD	C8A-N9A	-6.53	1.26	1.37
4	I	500	NAD	PN-O3	6.51	1.66	1.59
4	E	500	NAD	C8A-N9A	-6.50	1.26	1.37
4	J	500	NAD	C8A-N9A	-6.49	1.26	1.37
4	F	500	NAD	C8A-N9A	-6.47	1.26	1.37
4	H	500	NAD	C8A-N9A	-6.47	1.26	1.37
4	G	500	NAD	C8A-N9A	-6.45	1.26	1.37
4	A	502	NAD	PN-O3	6.45	1.66	1.59
4	K	500	NAD	C8A-N9A	-6.42	1.26	1.37
4	L	500	NAD	C8A-N9A	-6.41	1.26	1.37
4	I	500	NAD	C8A-N9A	-6.38	1.26	1.37
4	A	502	NAD	C8A-N9A	-6.28	1.26	1.37
4	B	500	NAD	C8A-N9A	-6.25	1.26	1.37
4	C	500	NAD	PN-O3	5.99	1.66	1.59
4	K	500	NAD	C6A-N6A	4.91	1.46	1.34
4	L	500	NAD	C6A-N6A	4.88	1.46	1.34
4	J	500	NAD	C6A-N6A	4.86	1.46	1.34
4	G	500	NAD	C6A-N6A	4.85	1.46	1.34
4	I	500	NAD	C6A-N6A	4.84	1.46	1.34
4	H	500	NAD	C6A-N6A	4.83	1.46	1.34
4	E	500	NAD	C6A-N6A	4.83	1.46	1.34
4	F	500	NAD	C6A-N6A	4.81	1.46	1.34
4	D	500	NAD	C6A-N6A	4.80	1.46	1.34
4	C	500	NAD	C6A-N6A	4.77	1.46	1.34
4	A	502	NAD	C6A-N6A	4.75	1.46	1.34
4	B	500	NAD	C6A-N6A	4.72	1.46	1.34
4	D	500	NAD	O4B-C1B	3.81	1.50	1.42
4	L	500	NAD	O4B-C1B	3.77	1.50	1.42
4	J	500	NAD	O4B-C1B	3.69	1.50	1.42
4	B	500	NAD	O4B-C1B	3.68	1.50	1.42
4	H	500	NAD	O4B-C1B	3.64	1.50	1.42
4	K	500	NAD	O4B-C1B	3.62	1.50	1.42
4	A	502	NAD	O4B-C1B	3.60	1.50	1.42
4	E	500	NAD	O4B-C1B	3.59	1.50	1.42
4	C	500	NAD	O4B-C1B	3.56	1.50	1.42
4	I	500	NAD	O4B-C1B	3.56	1.50	1.42
4	G	500	NAD	O4B-C1B	3.55	1.50	1.42
4	F	500	NAD	O4B-C1B	3.55	1.50	1.42
4	E	500	NAD	O4D-C4D	3.49	1.52	1.45
4	G	500	NAD	O4D-C4D	3.45	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	500	NAD	O4D-C4D	3.39	1.52	1.45
4	J	500	NAD	O4D-C4D	3.37	1.52	1.45
4	K	500	NAD	O4D-C4D	3.34	1.52	1.45
4	B	500	NAD	O4D-C4D	3.33	1.52	1.45
4	F	500	NAD	O4D-C4D	3.33	1.52	1.45
4	A	502	NAD	O7N-C7N	-3.32	1.17	1.24
4	A	502	NAD	O4D-C4D	3.31	1.52	1.45
4	L	500	NAD	O4D-C4D	3.31	1.52	1.45
4	D	500	NAD	O4D-C4D	3.28	1.52	1.45
4	H	500	NAD	O4D-C4D	3.26	1.52	1.45
4	D	500	NAD	O7N-C7N	-3.25	1.18	1.24
4	C	500	NAD	O7N-C7N	-3.22	1.18	1.24
4	C	500	NAD	O4D-C4D	3.20	1.52	1.45
4	G	500	NAD	O7N-C7N	-3.19	1.18	1.24
4	E	500	NAD	O7N-C7N	-3.17	1.18	1.24
4	K	500	NAD	O7N-C7N	-3.16	1.18	1.24
4	B	500	NAD	O7N-C7N	-3.13	1.18	1.24
4	I	500	NAD	O7N-C7N	-3.11	1.18	1.24
4	F	500	NAD	O7N-C7N	-3.10	1.18	1.24
4	H	500	NAD	O7N-C7N	-3.10	1.18	1.24
4	L	500	NAD	O7N-C7N	-3.08	1.18	1.24
4	J	500	NAD	O7N-C7N	-3.05	1.18	1.24
4	C	500	NAD	C4A-N9A	-2.97	1.31	1.37
4	F	500	NAD	C4A-N9A	-2.86	1.31	1.37
4	E	500	NAD	C4A-N9A	-2.85	1.31	1.37
4	G	500	NAD	C4A-N9A	-2.83	1.31	1.37
4	D	500	NAD	C4A-N9A	-2.83	1.31	1.37
4	H	500	NAD	C4A-N9A	-2.78	1.31	1.37
4	A	502	NAD	C4A-N9A	-2.77	1.31	1.37
4	E	500	NAD	PN-O5D	2.73	1.70	1.59
4	K	500	NAD	C4A-N9A	-2.72	1.32	1.37
4	I	500	NAD	C4A-N9A	-2.68	1.32	1.37
4	L	500	NAD	C4A-N9A	-2.68	1.32	1.37
4	J	500	NAD	PN-O5D	2.68	1.69	1.59
4	J	500	NAD	C4A-N9A	-2.67	1.32	1.37
4	H	500	NAD	PN-O5D	2.66	1.69	1.59
4	B	500	NAD	C4A-N9A	-2.65	1.32	1.37
4	L	500	NAD	PN-O5D	2.62	1.69	1.59
4	G	500	NAD	PN-O5D	2.61	1.69	1.59
4	F	500	NAD	PN-O5D	2.59	1.69	1.59
4	K	500	NAD	PN-O5D	2.57	1.69	1.59
4	I	500	NAD	PN-O5D	2.56	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	500	NAD	PN-O5D	2.49	1.69	1.59
4	D	500	NAD	PN-O5D	2.48	1.69	1.59
4	A	502	NAD	PN-O5D	2.47	1.69	1.59
4	C	500	NAD	C2D-C3D	-2.45	1.46	1.53
4	I	500	NAD	C3B-C4B	-2.44	1.46	1.53
4	D	500	NAD	C2B-C3B	-2.38	1.46	1.53
4	A	502	NAD	C2D-C3D	-2.38	1.46	1.53
4	C	500	NAD	PN-O5D	2.37	1.68	1.59
4	G	500	NAD	C3B-C4B	-2.37	1.47	1.53
4	G	500	NAD	C2D-C3D	-2.36	1.47	1.53
4	H	500	NAD	C3B-C4B	-2.35	1.47	1.53
4	H	500	NAD	C2D-C3D	-2.33	1.47	1.53
4	L	500	NAD	C3B-C4B	-2.33	1.47	1.53
4	J	500	NAD	C3B-C4B	-2.33	1.47	1.53
4	B	500	NAD	C2B-C3B	-2.32	1.47	1.53
4	I	500	NAD	C2D-C3D	-2.32	1.47	1.53
4	D	500	NAD	C2D-C3D	-2.31	1.47	1.53
4	K	500	NAD	C2D-C3D	-2.30	1.47	1.53
4	B	500	NAD	C2D-C3D	-2.30	1.47	1.53
4	J	500	NAD	C2D-C3D	-2.29	1.47	1.53
4	F	500	NAD	C2D-C3D	-2.29	1.47	1.53
4	C	500	NAD	C2B-C3B	-2.27	1.47	1.53
4	G	500	NAD	C3D-C4D	-2.27	1.47	1.53
4	F	500	NAD	C3B-C4B	-2.27	1.47	1.53
4	C	500	NAD	C3D-C4D	-2.26	1.47	1.53
4	E	500	NAD	C2D-C3D	-2.26	1.47	1.53
4	L	500	NAD	PA-O5B	2.24	1.68	1.59
4	F	500	NAD	PA-O5B	2.24	1.68	1.59
4	L	500	NAD	C3D-C4D	-2.23	1.47	1.53
4	L	500	NAD	C2D-C3D	-2.22	1.47	1.53
4	H	500	NAD	O4B-C4B	2.22	1.49	1.45
4	K	500	NAD	C3D-C4D	-2.22	1.47	1.53
4	A	502	NAD	C3D-C4D	-2.22	1.47	1.53
4	D	500	NAD	PA-O5B	2.22	1.68	1.59
4	E	500	NAD	PA-O5B	2.21	1.68	1.59
4	K	500	NAD	PA-O5B	2.21	1.68	1.59
4	F	500	NAD	C3D-C4D	-2.21	1.47	1.53
4	F	500	NAD	C2B-C3B	-2.21	1.47	1.53
4	D	500	NAD	O4B-C4B	2.21	1.49	1.45
4	K	500	NAD	C3B-C4B	-2.21	1.47	1.53
4	A	502	NAD	C2B-C3B	-2.21	1.47	1.53
4	G	500	NAD	O4B-C4B	2.20	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	500	NAD	C3D-C4D	-2.20	1.47	1.53
4	J	500	NAD	PA-O5B	2.20	1.68	1.59
4	E	500	NAD	C3B-C4B	-2.20	1.47	1.53
4	L	500	NAD	O4B-C4B	2.20	1.49	1.45
4	B	500	NAD	O4B-C4B	2.19	1.49	1.45
4	D	500	NAD	C3B-C4B	-2.19	1.47	1.53
4	E	500	NAD	C2B-C3B	-2.19	1.47	1.53
4	H	500	NAD	PA-O5B	2.19	1.67	1.59
4	J	500	NAD	O4B-C4B	2.18	1.49	1.45
4	H	500	NAD	C2N-N1N	2.18	1.37	1.35
4	I	500	NAD	O4B-C4B	2.18	1.49	1.45
4	K	500	NAD	O4B-C4B	2.18	1.49	1.45
4	B	500	NAD	PA-O5B	2.17	1.67	1.59
4	J	500	NAD	C3D-C4D	-2.17	1.47	1.53
4	F	500	NAD	O4B-C4B	2.16	1.49	1.45
4	L	500	NAD	C2B-C3B	-2.16	1.47	1.53
4	C	500	NAD	PA-O5B	2.16	1.67	1.59
4	H	500	NAD	C2B-C3B	-2.15	1.47	1.53
4	A	502	NAD	C3B-C4B	-2.15	1.47	1.53
4	G	500	NAD	PA-O5B	2.15	1.67	1.59
4	C	500	NAD	C2B-C1B	-2.14	1.46	1.53
4	E	500	NAD	C3D-C4D	-2.14	1.47	1.53
4	I	500	NAD	PA-O5B	2.14	1.67	1.59
4	E	500	NAD	O4B-C4B	2.13	1.49	1.45
4	A	502	NAD	O4B-C4B	2.13	1.49	1.45
4	B	500	NAD	C3N-C7N	2.13	1.53	1.50
4	H	500	NAD	C3D-C4D	-2.13	1.47	1.53
4	C	500	NAD	C3B-C4B	-2.12	1.47	1.53
4	C	500	NAD	O4B-C4B	2.11	1.49	1.45
4	A	502	NAD	PA-O5B	2.10	1.67	1.59
4	D	500	NAD	C3D-C4D	-2.10	1.47	1.53
4	G	500	NAD	C4N-C3N	-2.07	1.36	1.39
4	E	500	NAD	C2B-C1B	-2.07	1.47	1.53
4	B	500	NAD	C2B-C1B	-2.07	1.47	1.53
4	F	500	NAD	C2B-C1B	-2.07	1.47	1.53
4	J	500	NAD	C2B-C3B	-2.07	1.47	1.53
4	B	500	NAD	C2N-N1N	2.06	1.37	1.35
4	F	500	NAD	C2N-N1N	2.04	1.37	1.35
4	K	500	NAD	C3N-C7N	2.03	1.53	1.50
4	K	500	NAD	C2B-C3B	-2.03	1.47	1.53
4	K	500	NAD	C2B-C1B	-2.03	1.47	1.53
4	G	500	NAD	C2B-C3B	-2.02	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	500	NAD	C2B-C1B	-2.01	1.47	1.53
4	G	500	NAD	C2B-C1B	-2.01	1.47	1.53
4	B	500	NAD	C3B-C4B	-2.01	1.47	1.53

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	500	NAD	C4A-N9A-C8A	8.81	114.99	105.74
4	F	500	NAD	C4A-N9A-C8A	8.79	114.97	105.74
4	I	500	NAD	C4D-O4D-C1D	-8.78	101.88	109.92
4	E	500	NAD	C4A-N9A-C8A	8.77	114.94	105.74
4	G	500	NAD	C4A-N9A-C8A	8.70	114.87	105.74
4	L	500	NAD	C4A-N9A-C8A	8.56	114.73	105.74
4	K	500	NAD	C4A-N9A-C8A	8.56	114.72	105.74
4	I	500	NAD	C4A-N9A-C8A	8.50	114.66	105.74
4	A	502	NAD	C4A-N9A-C8A	8.46	114.62	105.74
4	H	500	NAD	C4A-N9A-C8A	8.44	114.60	105.74
4	D	500	NAD	C4A-N9A-C8A	8.42	114.58	105.74
4	J	500	NAD	C4A-N9A-C8A	8.42	114.58	105.74
4	B	500	NAD	C4A-N9A-C8A	8.41	114.56	105.74
4	C	500	NAD	C4D-O4D-C1D	-8.33	102.30	109.92
4	D	500	NAD	C4D-O4D-C1D	-8.29	102.34	109.92
4	H	500	NAD	C4D-O4D-C1D	-8.25	102.37	109.92
4	L	500	NAD	C4D-O4D-C1D	-7.98	102.61	109.92
4	J	500	NAD	C4D-O4D-C1D	-7.97	102.63	109.92
4	B	500	NAD	C4D-O4D-C1D	-7.79	102.79	109.92
4	K	500	NAD	C4D-O4D-C1D	-7.50	103.05	109.92
4	F	500	NAD	C4D-O4D-C1D	-7.46	103.09	109.92
4	A	502	NAD	C4D-O4D-C1D	-7.19	103.34	109.92
4	B	500	NAD	N3A-C4A-N9A	6.19	137.70	127.17
4	I	500	NAD	N3A-C4A-N9A	6.02	137.40	127.17
4	L	500	NAD	N3A-C4A-N9A	5.96	137.30	127.17
4	B	500	NAD	C5A-C4A-N3A	-5.92	118.57	126.72
4	A	502	NAD	N3A-C4A-N9A	5.91	137.22	127.17
4	F	500	NAD	N3A-C4A-N9A	5.87	137.15	127.17
4	I	500	NAD	C5A-C4A-N3A	-5.84	118.67	126.72
4	J	500	NAD	N3A-C4A-N9A	5.83	137.09	127.17
4	K	500	NAD	N3A-C4A-N9A	5.82	137.07	127.17
4	L	500	NAD	C5A-C4A-N3A	-5.80	118.74	126.72
4	J	500	NAD	C5A-C4A-N3A	-5.78	118.76	126.72
4	G	500	NAD	N3A-C4A-N9A	5.72	136.90	127.17
4	H	500	NAD	N3A-C4A-N9A	5.72	136.89	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	500	NAD	N3A-C4A-N9A	5.71	136.88	127.17
4	D	500	NAD	N3A-C4A-N9A	5.69	136.84	127.17
4	A	502	NAD	C5A-C4A-N3A	-5.67	118.91	126.72
4	E	500	NAD	N3A-C4A-N9A	5.67	136.81	127.17
4	K	500	NAD	C5A-C4A-N3A	-5.64	118.94	126.72
4	F	500	NAD	C5A-C4A-N3A	-5.62	118.98	126.72
4	H	500	NAD	C5A-C4A-N3A	-5.61	118.99	126.72
4	G	500	NAD	C5A-C4A-N3A	-5.57	119.05	126.72
4	E	500	NAD	C5A-C4A-N3A	-5.51	119.13	126.72
4	D	500	NAD	C5A-C4A-N3A	-5.48	119.17	126.72
4	C	500	NAD	C5A-C4A-N3A	-5.44	119.22	126.72
4	E	500	NAD	C4D-O4D-C1D	-5.33	105.04	109.92
4	G	500	NAD	C4D-O4D-C1D	-5.20	105.16	109.92
4	J	500	NAD	C4A-C5A-N7A	-4.48	105.47	110.58
4	E	500	NAD	C4A-C5A-N7A	-4.45	105.49	110.58
4	G	500	NAD	C4A-C5A-N7A	-4.40	105.55	110.58
4	H	500	NAD	C4A-C5A-N7A	-4.37	105.58	110.58
4	L	500	NAD	C4A-C5A-N7A	-4.37	105.58	110.58
4	F	500	NAD	C4A-C5A-N7A	-4.36	105.60	110.58
4	K	500	NAD	C4A-C5A-N7A	-4.33	105.63	110.58
4	F	500	NAD	N9A-C8A-N7A	-4.31	107.82	113.94
4	E	500	NAD	N9A-C8A-N7A	-4.31	107.83	113.94
4	G	500	NAD	N9A-C8A-N7A	-4.29	107.85	113.94
4	C	500	NAD	N9A-C8A-N7A	-4.27	107.87	113.94
4	H	500	NAD	N3A-C2A-N1A	-4.26	122.13	128.58
4	I	500	NAD	C4A-C5A-N7A	-4.25	105.72	110.58
4	D	500	NAD	C4A-C5A-N7A	-4.21	105.76	110.58
4	C	500	NAD	C4A-C5A-N7A	-4.21	105.77	110.58
4	L	500	NAD	N9A-C8A-N7A	-4.17	108.01	113.94
4	E	500	NAD	N3A-C2A-N1A	-4.17	122.26	128.58
4	D	500	NAD	N3A-C2A-N1A	-4.16	122.28	128.58
4	G	500	NAD	N3A-C2A-N1A	-4.16	122.29	128.58
4	A	502	NAD	N9A-C8A-N7A	-4.15	108.06	113.94
4	K	500	NAD	N9A-C8A-N7A	-4.12	108.09	113.94
4	I	500	NAD	N9A-C8A-N7A	-4.12	108.09	113.94
4	B	500	NAD	N9A-C8A-N7A	-4.11	108.10	113.94
4	K	500	NAD	N3A-C2A-N1A	-4.10	122.37	128.58
4	J	500	NAD	N9A-C8A-N7A	-4.09	108.13	113.94
4	L	500	NAD	N3A-C2A-N1A	-4.09	122.40	128.58
4	J	500	NAD	N3A-C2A-N1A	-4.08	122.41	128.58
4	F	500	NAD	N3A-C2A-N1A	-4.07	122.42	128.58
4	H	500	NAD	N9A-C8A-N7A	-4.07	108.17	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	500	NAD	N3A-C2A-N1A	-4.04	122.47	128.58
4	A	502	NAD	C4A-C5A-N7A	-4.02	105.98	110.58
4	C	500	NAD	N3A-C2A-N1A	-4.01	122.52	128.58
4	B	500	NAD	C4A-C5A-N7A	-3.98	106.03	110.58
4	D	500	NAD	N9A-C8A-N7A	-3.95	108.33	113.94
4	A	502	NAD	N3A-C2A-N1A	-3.88	122.70	128.58
4	B	500	NAD	N3A-C2A-N1A	-3.69	123.00	128.58
4	I	500	NAD	C3B-C2B-C1B	3.68	108.43	101.46
4	J	500	NAD	C2A-N3A-C4A	3.57	120.55	111.83
4	G	500	NAD	C3B-C2B-C1B	3.57	108.21	101.46
4	L	500	NAD	C2A-N3A-C4A	3.56	120.52	111.83
4	I	500	NAD	C2A-N3A-C4A	3.55	120.50	111.83
4	E	500	NAD	C2A-N3A-C4A	3.53	120.44	111.83
4	G	500	NAD	C2A-N3A-C4A	3.53	120.44	111.83
4	H	500	NAD	C2A-N3A-C4A	3.52	120.43	111.83
4	F	500	NAD	C2A-N3A-C4A	3.51	120.41	111.83
4	K	500	NAD	C2A-N3A-C4A	3.51	120.39	111.83
4	D	500	NAD	C2A-N3A-C4A	3.50	120.38	111.83
4	C	500	NAD	C2A-N3A-C4A	3.41	120.17	111.83
4	A	502	NAD	C2A-N3A-C4A	3.39	120.11	111.83
4	B	500	NAD	C2A-N3A-C4A	3.36	120.05	111.83
4	G	500	NAD	C6N-N1N-C2N	-3.35	119.02	121.88
4	K	500	NAD	C3B-C2B-C1B	3.32	107.75	101.46
4	C	500	NAD	C3B-C2B-C1B	3.30	107.70	101.46
4	E	500	NAD	C3B-C2B-C1B	3.26	107.63	101.46
4	E	500	NAD	C2D-C3D-C4D	3.13	108.67	102.61
4	E	500	NAD	C6N-N1N-C2N	-3.05	119.28	121.88
4	F	500	NAD	C3B-C2B-C1B	3.05	107.23	101.46
4	B	500	NAD	O7N-C7N-N7N	-2.95	118.35	122.62
4	B	500	NAD	C3N-C7N-N7N	2.94	121.36	117.74
4	H	500	NAD	C2D-C3D-C4D	2.92	108.24	102.61
4	G	500	NAD	C2D-C3D-C4D	2.92	108.24	102.61
4	L	500	NAD	C2D-C3D-C4D	2.85	108.11	102.61
4	G	500	NAD	C2B-C3B-C4B	2.84	108.10	102.61
4	J	500	NAD	C2D-C3D-C4D	2.82	108.05	102.61
4	L	500	NAD	C3B-C2B-C1B	2.77	106.71	101.46
4	K	500	NAD	C2B-C3B-C4B	2.75	107.92	102.61
4	D	500	NAD	C2D-C3D-C4D	2.74	107.90	102.61
4	C	500	NAD	C2B-C3B-C4B	2.73	107.89	102.61
4	F	500	NAD	C5A-N7A-C8A	2.73	107.73	103.45
4	L	500	NAD	C5A-N7A-C8A	2.71	107.71	103.45
4	E	500	NAD	C5A-N7A-C8A	2.69	107.68	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	500	NAD	C5A-N7A-C8A	2.69	107.68	103.45
4	G	500	NAD	C5A-N7A-C8A	2.69	107.67	103.45
4	I	500	NAD	C2D-C3D-C4D	2.67	107.77	102.61
4	H	500	NAD	C3B-C2B-C1B	2.65	106.48	101.46
4	I	500	NAD	C5A-N7A-C8A	2.64	107.60	103.45
4	K	500	NAD	C5A-N7A-C8A	2.63	107.58	103.45
4	B	500	NAD	C5A-N7A-C8A	2.62	107.56	103.45
4	K	500	NAD	C2D-C3D-C4D	2.60	107.64	102.61
4	F	500	NAD	C2D-C3D-C4D	2.60	107.63	102.61
4	J	500	NAD	C3B-C2B-C1B	2.60	106.38	101.46
4	H	500	NAD	C5A-N7A-C8A	2.60	107.53	103.45
4	B	500	NAD	C2D-C3D-C4D	2.58	107.59	102.61
4	I	500	NAD	C2B-C3B-C4B	2.56	107.56	102.61
4	C	500	NAD	C5A-N7A-C8A	2.56	107.47	103.45
4	A	502	NAD	C5A-N7A-C8A	2.56	107.47	103.45
4	I	500	NAD	C5B-C4B-C3B	-2.51	106.17	115.21
4	D	500	NAD	O7N-C7N-N7N	-2.48	119.03	122.62
4	E	500	NAD	C2B-C3B-C4B	2.48	107.40	102.61
4	D	500	NAD	C5A-N7A-C8A	2.48	107.34	103.45
4	A	502	NAD	O7N-C7N-N7N	-2.43	119.11	122.62
4	A	502	NAD	C2D-C3D-C4D	2.41	107.27	102.61
4	E	500	NAD	C6A-C5A-N7A	2.39	136.70	132.09
4	G	500	NAD	C6A-C5A-N7A	2.34	136.60	132.09
4	D	500	NAD	C4B-O4B-C1B	-2.31	104.36	109.47
4	D	500	NAD	C3B-C2B-C1B	2.30	105.81	101.46
4	A	502	NAD	C6N-N1N-C2N	-2.30	119.92	121.88
4	J	500	NAD	C4B-O4B-C1B	-2.29	104.41	109.47
4	F	500	NAD	C2B-C3B-C4B	2.28	107.02	102.61
4	A	502	NAD	C3B-C2B-C1B	2.28	105.78	101.46
4	F	500	NAD	C6A-C5A-N7A	2.28	136.48	132.09
4	D	500	NAD	C3N-C7N-N7N	2.28	120.54	117.74
4	J	500	NAD	C6A-C5A-N7A	2.27	136.47	132.09
4	C	500	NAD	C4A-N9A-C1B	-2.26	121.34	126.63
4	A	502	NAD	C4A-N9A-C1B	-2.26	121.34	126.63
4	E	500	NAD	C4A-N9A-C1B	-2.26	121.36	126.63
4	H	500	NAD	C6A-C5A-N7A	2.24	136.41	132.09
4	D	500	NAD	C6A-C5A-N7A	2.21	136.36	132.09
4	L	500	NAD	C6N-N1N-C2N	-2.21	120.00	121.88
4	C	500	NAD	C6A-C5A-N7A	2.20	136.34	132.09
4	K	500	NAD	C6N-N1N-C2N	-2.20	120.01	121.88
4	K	500	NAD	C6A-C5A-N7A	2.19	136.32	132.09
4	L	500	NAD	C6A-C5A-N7A	2.18	136.30	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	500	NAD	C3B-C2B-C1B	2.18	105.58	101.46
4	G	500	NAD	C4A-N9A-C1B	-2.15	121.60	126.63
4	L	500	NAD	C4B-O4B-C1B	-2.13	104.77	109.47
4	C	500	NAD	O7N-C7N-N7N	-2.12	119.56	122.62
4	H	500	NAD	C4B-O4B-C1B	-2.11	104.80	109.47
4	L	500	NAD	C1B-N9A-C8A	-2.09	122.47	127.09
4	F	500	NAD	C6N-N1N-C2N	-2.08	120.11	121.88
4	C	500	NAD	C3N-C7N-N7N	2.08	120.30	117.74
4	I	500	NAD	C6A-C5A-N7A	2.06	136.06	132.09
4	I	500	NAD	C6N-N1N-C2N	-2.05	120.13	121.88
4	K	500	NAD	C4A-N9A-C1B	-2.04	121.85	126.63
4	J	500	NAD	C6N-N1N-C2N	-2.03	120.15	121.88
4	B	500	NAD	C5A-C6A-N6A	-2.03	118.26	123.29
4	H	500	NAD	O7N-C7N-N7N	-2.03	119.68	122.62
4	B	500	NAD	C4A-N9A-C1B	-2.02	121.90	126.63
4	A	502	NAD	C5A-C6A-N6A	-2.01	118.30	123.29
4	E	500	NAD	C2B-C1B-N9A	-2.01	108.30	113.30
4	G	500	NAD	C5B-C4B-C3B	-2.01	107.97	115.21
4	H	500	NAD	C6N-N1N-C2N	-2.00	120.17	121.88
4	F	500	NAD	C3N-C7N-N7N	2.00	120.21	117.74

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	NAD	C5D-O5D-PN-O3
4	A	502	NAD	C5D-O5D-PN-O1N
4	A	502	NAD	C2N-C3N-C7N-N7N
4	B	500	NAD	C5B-O5B-PA-O1A
4	C	500	NAD	C5B-O5B-PA-O1A
4	C	500	NAD	C5B-O5B-PA-O2A
4	C	500	NAD	C5B-O5B-PA-O3
4	C	500	NAD	O4B-C4B-C5B-O5B
4	D	500	NAD	C5B-O5B-PA-O1A
4	D	500	NAD	C5B-O5B-PA-O2A
4	D	500	NAD	C5B-O5B-PA-O3
4	D	500	NAD	C5D-O5D-PN-O3
4	D	500	NAD	C5D-O5D-PN-O1N
4	D	500	NAD	C2N-C3N-C7N-O7N
4	D	500	NAD	C2N-C3N-C7N-N7N
4	E	500	NAD	PA-O3-PN-O5D
4	E	500	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
4	F	500	NAD	C5D-O5D-PN-O3
4	F	500	NAD	C5D-O5D-PN-O1N
4	G	500	NAD	O4B-C4B-C5B-O5B
4	H	500	NAD	C5B-O5B-PA-O1A
4	H	500	NAD	C5B-O5B-PA-O2A
4	H	500	NAD	C5B-O5B-PA-O3
4	H	500	NAD	O4B-C4B-C5B-O5B
4	I	500	NAD	C5B-O5B-PA-O1A
4	J	500	NAD	C5B-O5B-PA-O1A
4	J	500	NAD	C5B-O5B-PA-O2A
4	J	500	NAD	C5B-O5B-PA-O3
4	J	500	NAD	O4B-C4B-C5B-O5B
4	L	500	NAD	C5B-O5B-PA-O3
4	L	500	NAD	O4B-C4B-C5B-O5B
4	L	500	NAD	C5D-O5D-PN-O3
4	L	500	NAD	C5D-O5D-PN-O1N
4	D	500	NAD	C4N-C3N-C7N-O7N
4	D	500	NAD	C4N-C3N-C7N-N7N
4	A	502	NAD	C2N-C3N-C7N-O7N
4	A	502	NAD	O4B-C4B-C5B-O5B
4	A	502	NAD	C3B-C4B-C5B-O5B
4	A	502	NAD	O4D-C4D-C5D-O5D
4	B	500	NAD	O4B-C4B-C5B-O5B
4	B	500	NAD	C3B-C4B-C5B-O5B
4	D	500	NAD	O4B-C4B-C5B-O5B
4	F	500	NAD	O4B-C4B-C5B-O5B
4	F	500	NAD	C3B-C4B-C5B-O5B
4	G	500	NAD	C3B-C4B-C5B-O5B
4	I	500	NAD	C3B-C4B-C5B-O5B
4	C	500	NAD	C3B-C4B-C5B-O5B
4	E	500	NAD	O4D-C4D-C5D-O5D
4	E	500	NAD	C3D-C4D-C5D-O5D
4	I	500	NAD	O4B-C4B-C5B-O5B
4	I	500	NAD	O4D-C4D-C5D-O5D
4	K	500	NAD	O4B-C4B-C5B-O5B
4	K	500	NAD	C3B-C4B-C5B-O5B
4	A	502	NAD	C4N-C3N-C7N-N7N
4	A	502	NAD	C4N-C3N-C7N-O7N
4	H	500	NAD	C3B-C4B-C5B-O5B
4	J	500	NAD	C3B-C4B-C5B-O5B
4	L	500	NAD	C3B-C4B-C5B-O5B
4	D	500	NAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	A	502	NAD	C3D-C4D-C5D-O5D
4	K	500	NAD	O4D-C4D-C5D-O5D
4	E	500	NAD	C4N-C3N-C7N-N7N
4	E	500	NAD	C4N-C3N-C7N-O7N
4	E	500	NAD	C2N-C3N-C7N-O7N
4	A	502	NAD	PA-O3-PN-O5D
4	C	500	NAD	PA-O3-PN-O5D
4	D	500	NAD	PA-O3-PN-O5D
4	G	500	NAD	PA-O3-PN-O5D
4	H	500	NAD	PA-O3-PN-O5D
4	I	500	NAD	PA-O3-PN-O5D
4	J	500	NAD	PA-O3-PN-O5D
4	K	500	NAD	PA-O3-PN-O5D
4	I	500	NAD	C3D-C4D-C5D-O5D
4	E	500	NAD	C2N-C3N-C7N-N7N
4	E	500	NAD	C4D-C5D-O5D-PN
4	A	502	NAD	C5D-O5D-PN-O2N
4	B	500	NAD	C5D-O5D-PN-O3
4	B	500	NAD	C5D-O5D-PN-O1N
4	B	500	NAD	C5D-O5D-PN-O2N
4	D	500	NAD	C5D-O5D-PN-O2N
4	F	500	NAD	C5D-O5D-PN-O2N
4	H	500	NAD	C5D-O5D-PN-O2N
4	I	500	NAD	C5B-O5B-PA-O3
4	L	500	NAD	C5B-O5B-PA-O1A
4	L	500	NAD	C5D-O5D-PN-O2N
4	I	500	NAD	C4D-C5D-O5D-PN
4	H	500	NAD	C4D-C5D-O5D-PN
4	E	500	NAD	O4D-C1D-N1N-C2N
4	L	500	NAD	C4D-C5D-O5D-PN
4	B	500	NAD	PN-O3-PA-O2A
4	K	500	NAD	C3D-C4D-C5D-O5D
4	A	502	NAD	PA-O3-PN-O2N
4	F	500	NAD	PN-O3-PA-O2A
4	H	500	NAD	PA-O3-PN-O2N

There are no ring outliers.

10 monomers are involved in 22 short contacts:

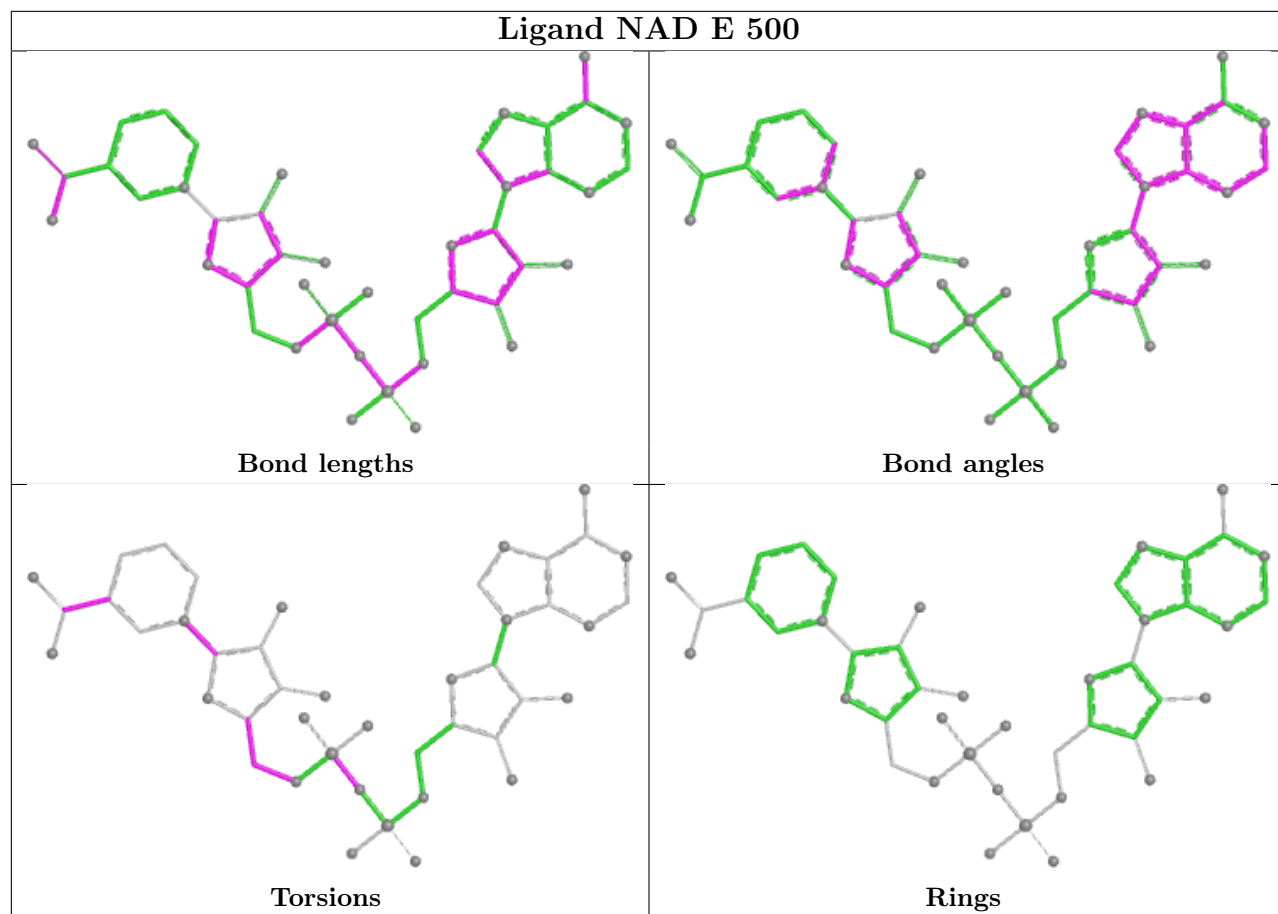
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	500	NAD	2	0
4	A	502	NAD	1	0

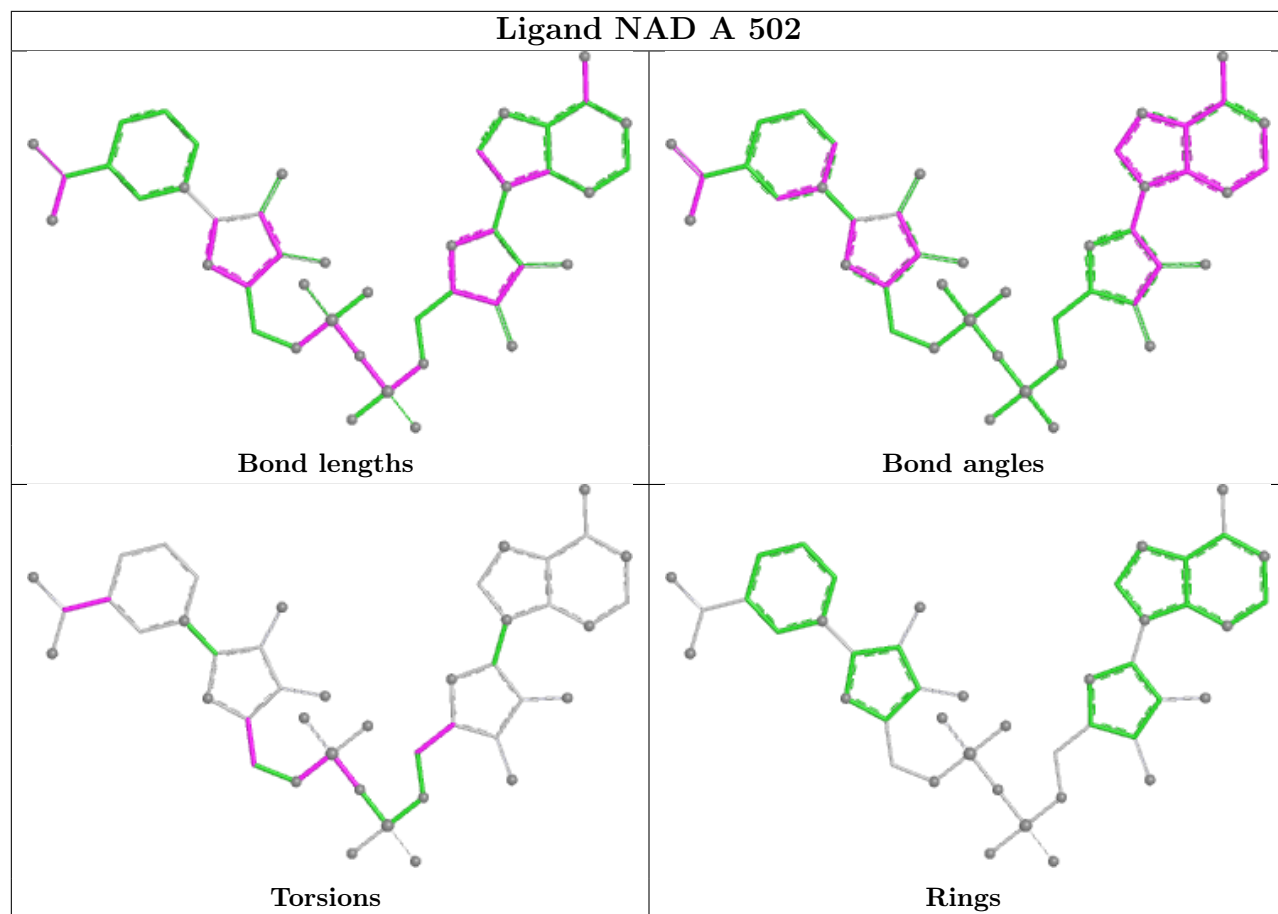
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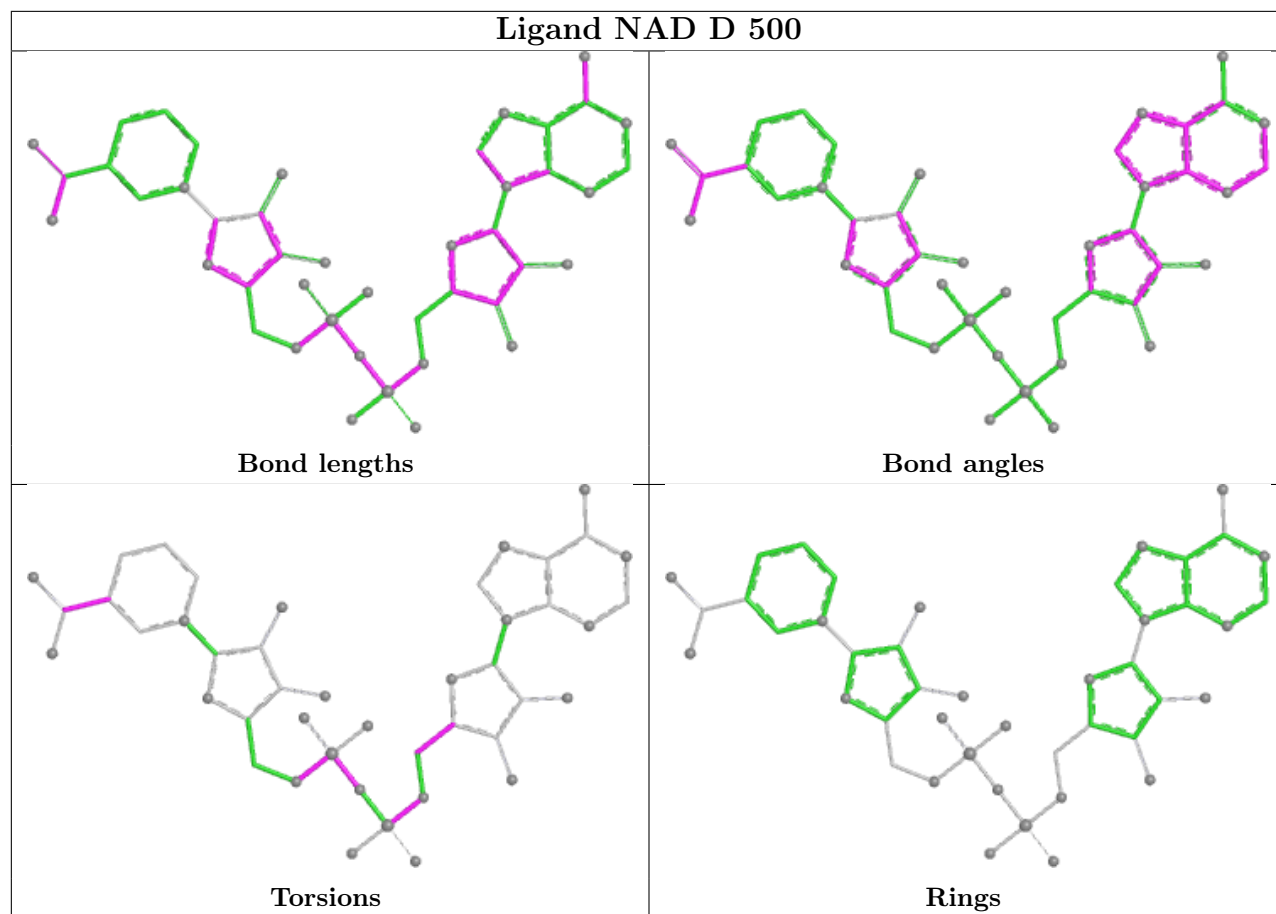
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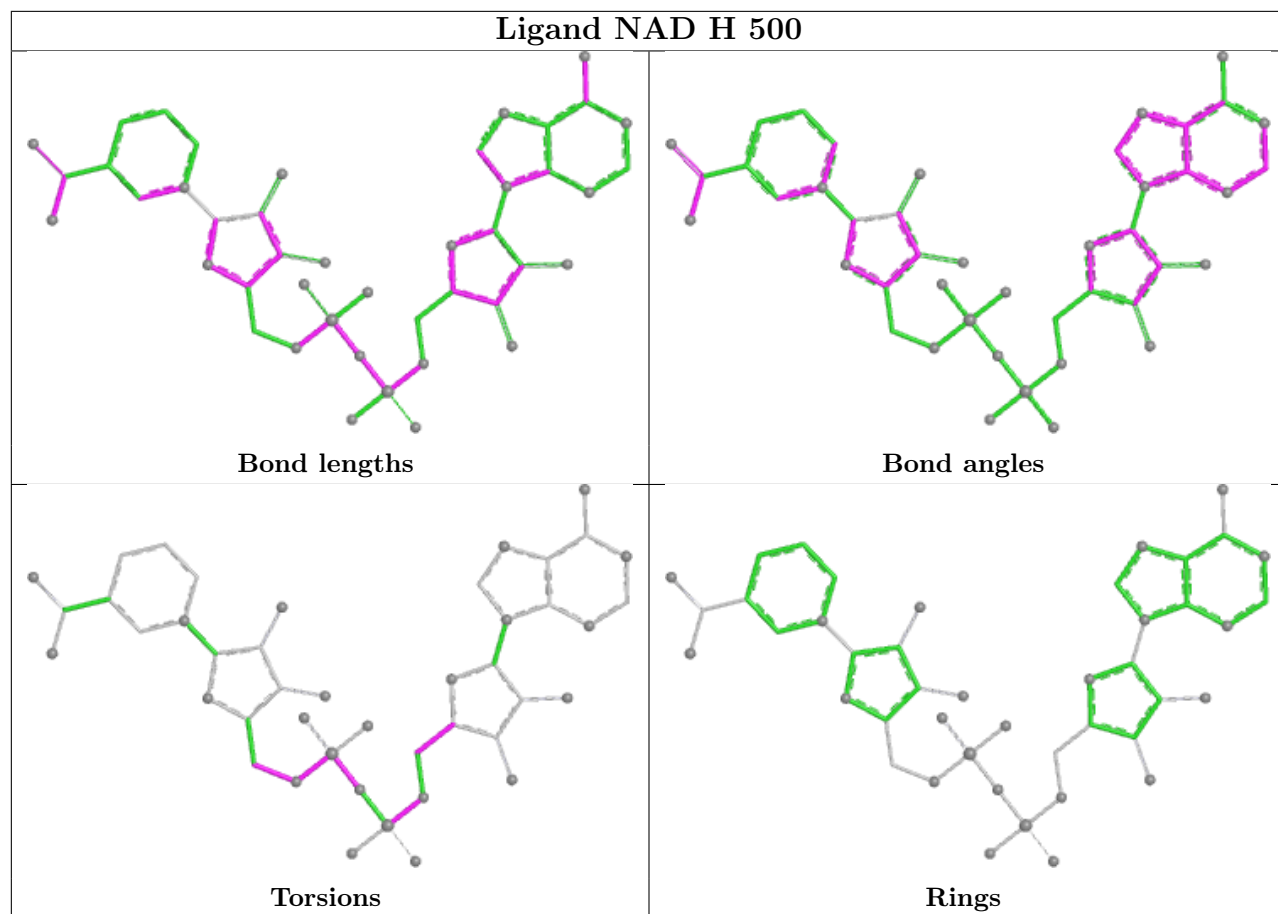
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	500	NAD	3	0
4	H	500	NAD	3	0
4	L	500	NAD	1	0
4	K	500	NAD	3	0
4	B	500	NAD	3	0
4	I	500	NAD	2	0
4	C	500	NAD	4	0
4	G	500	NAD	2	0

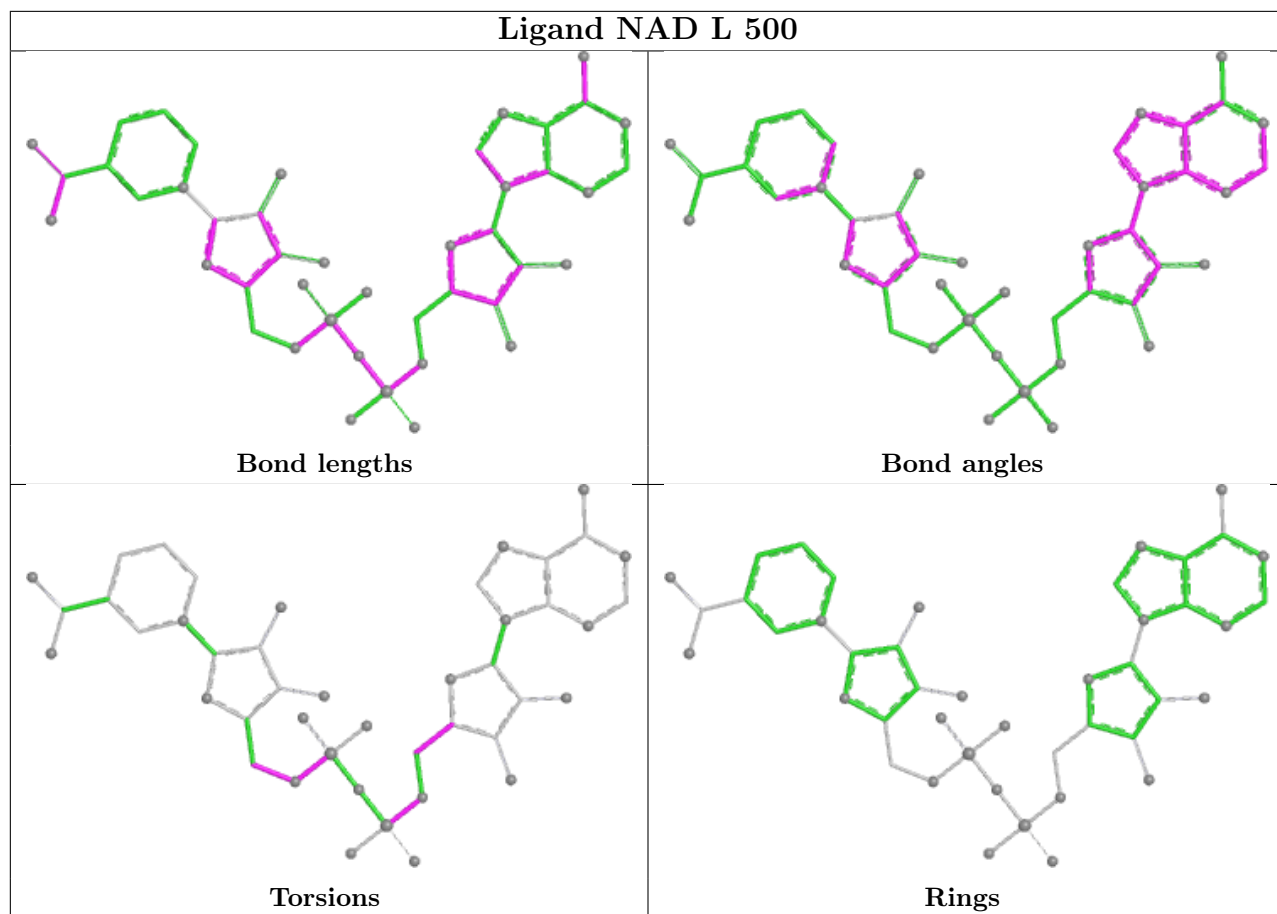
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

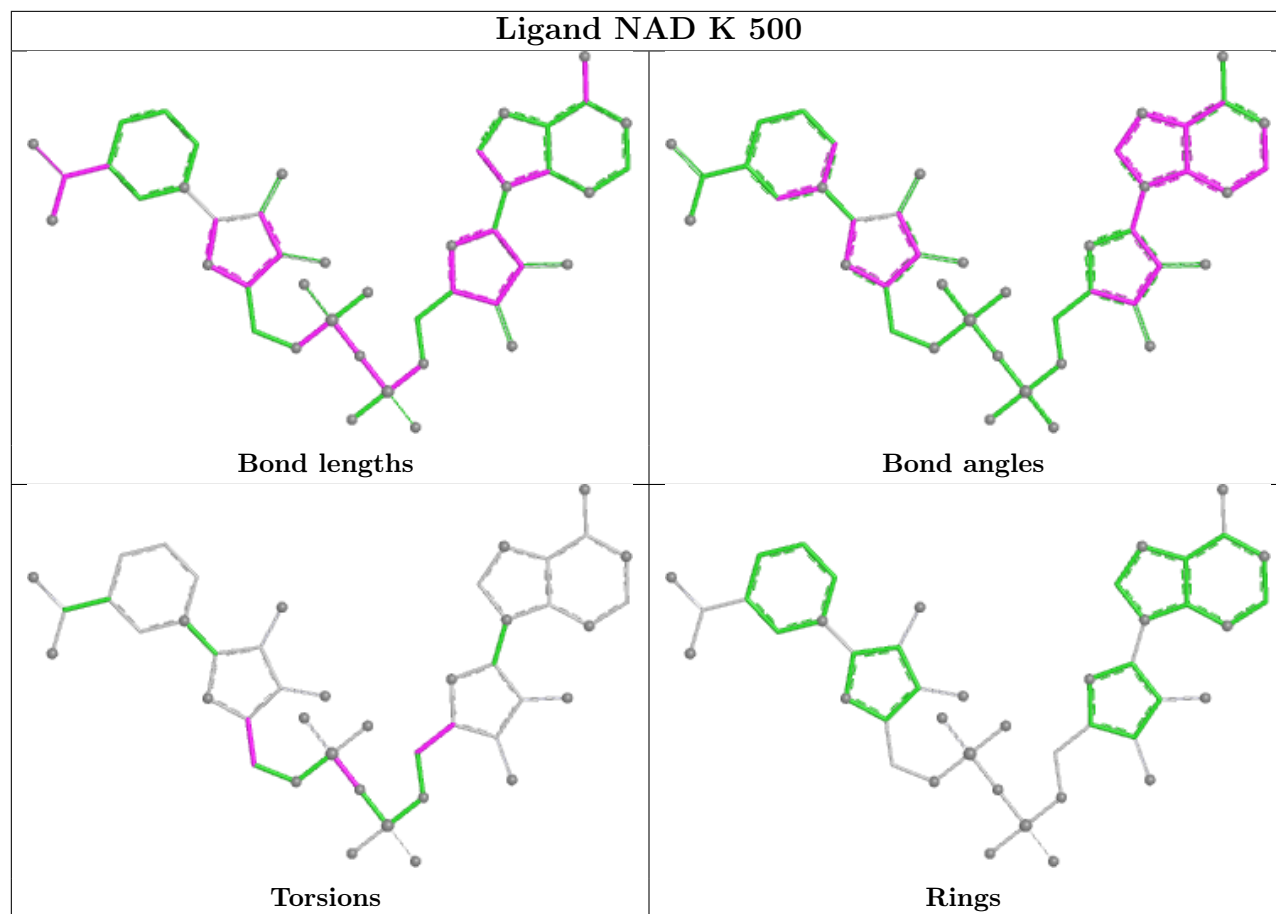


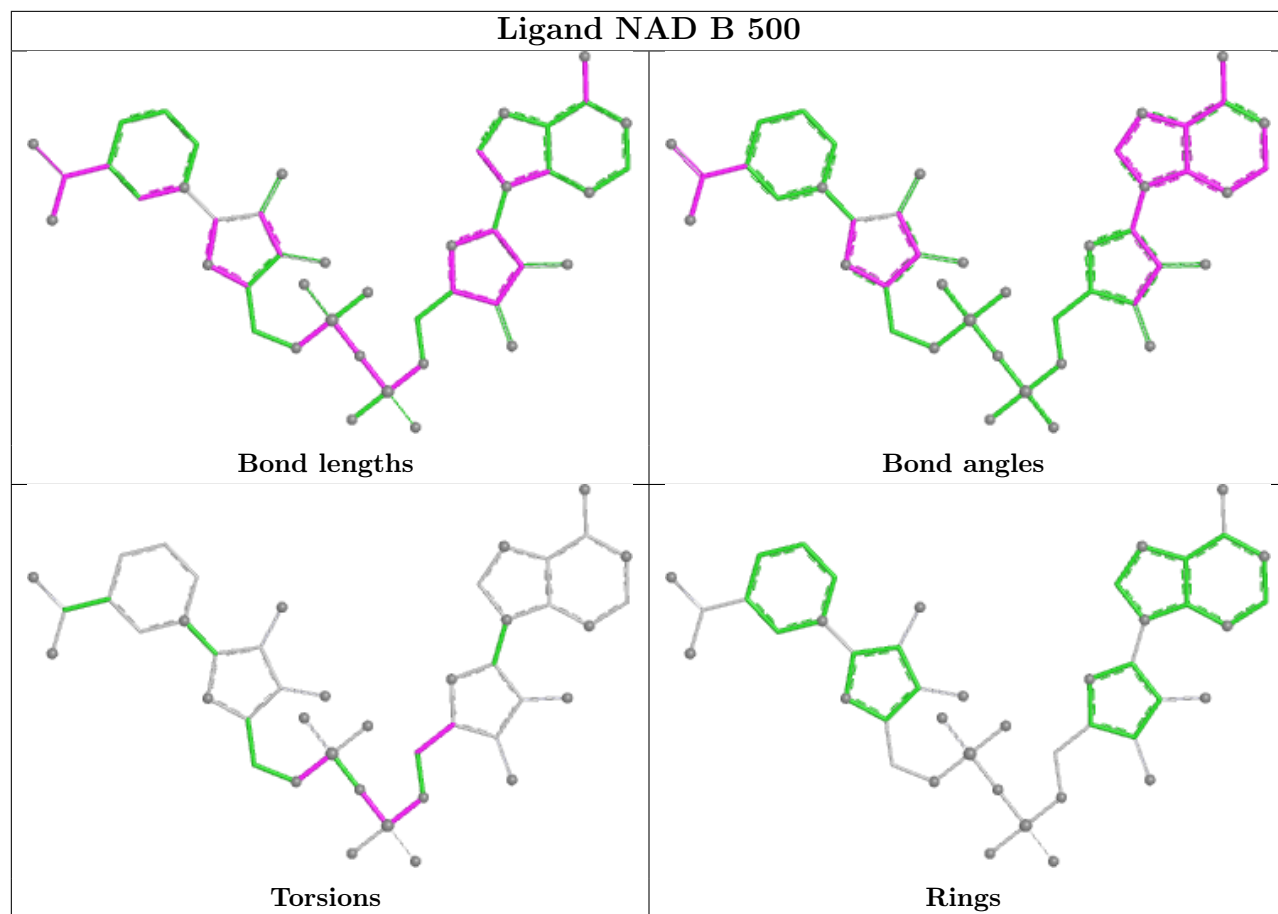


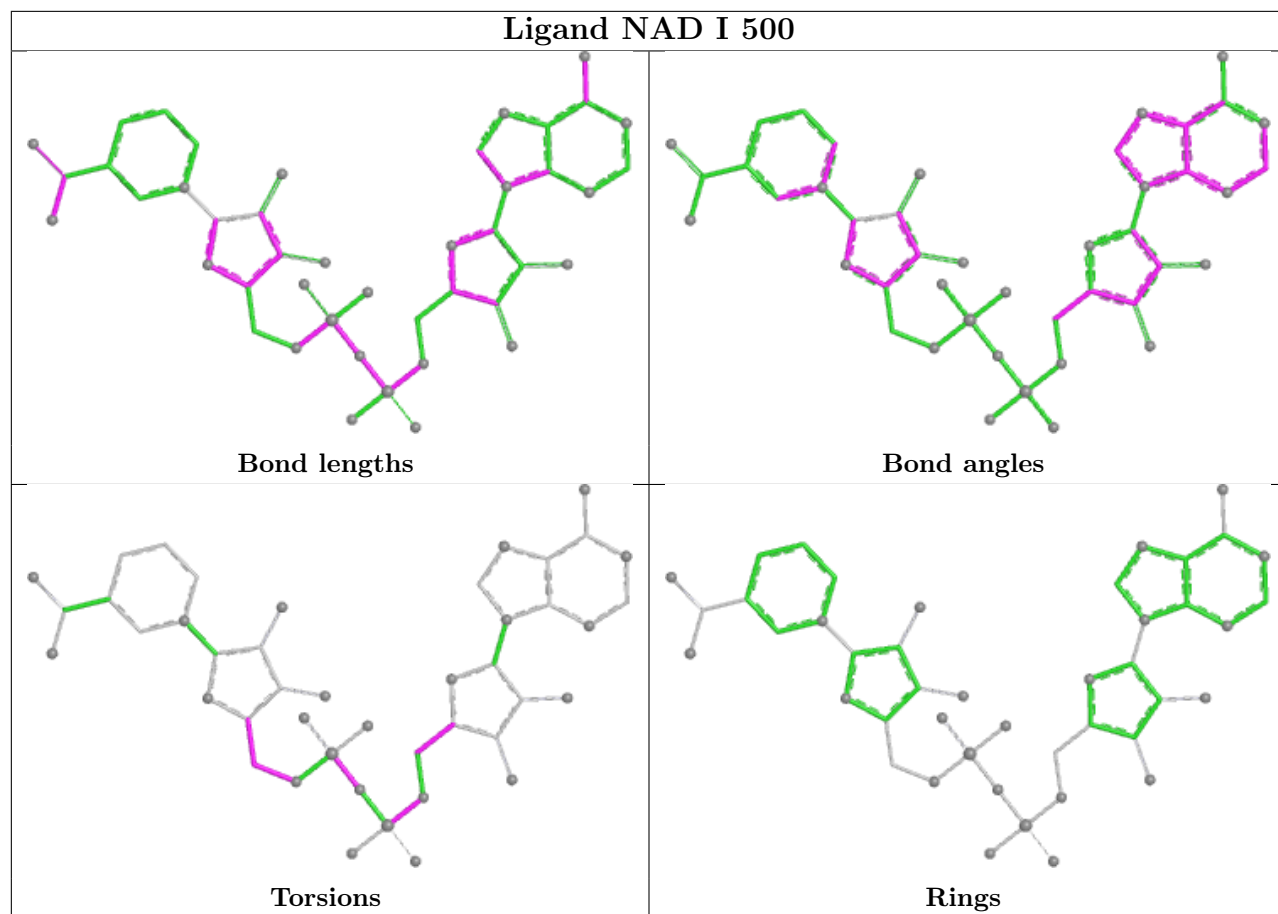


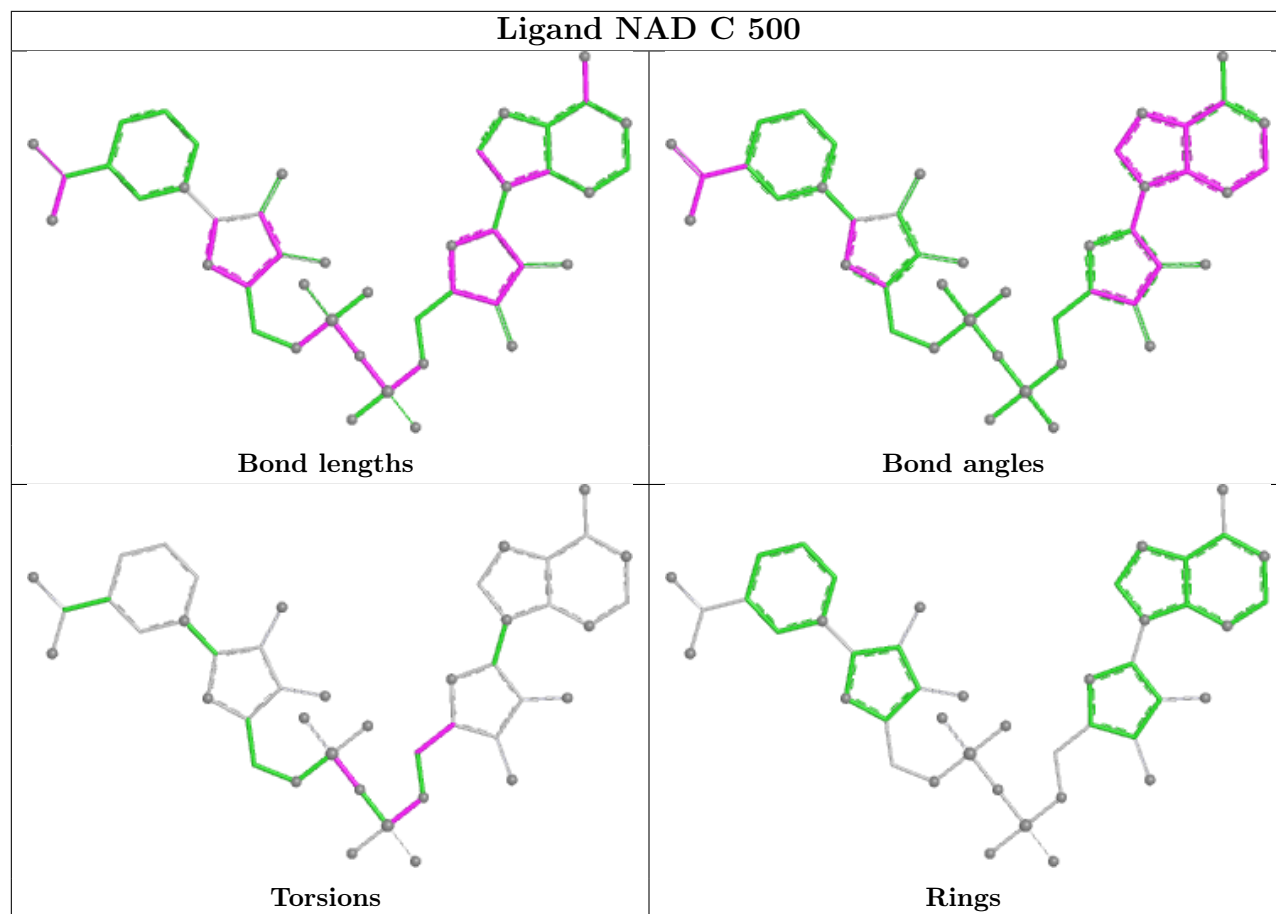


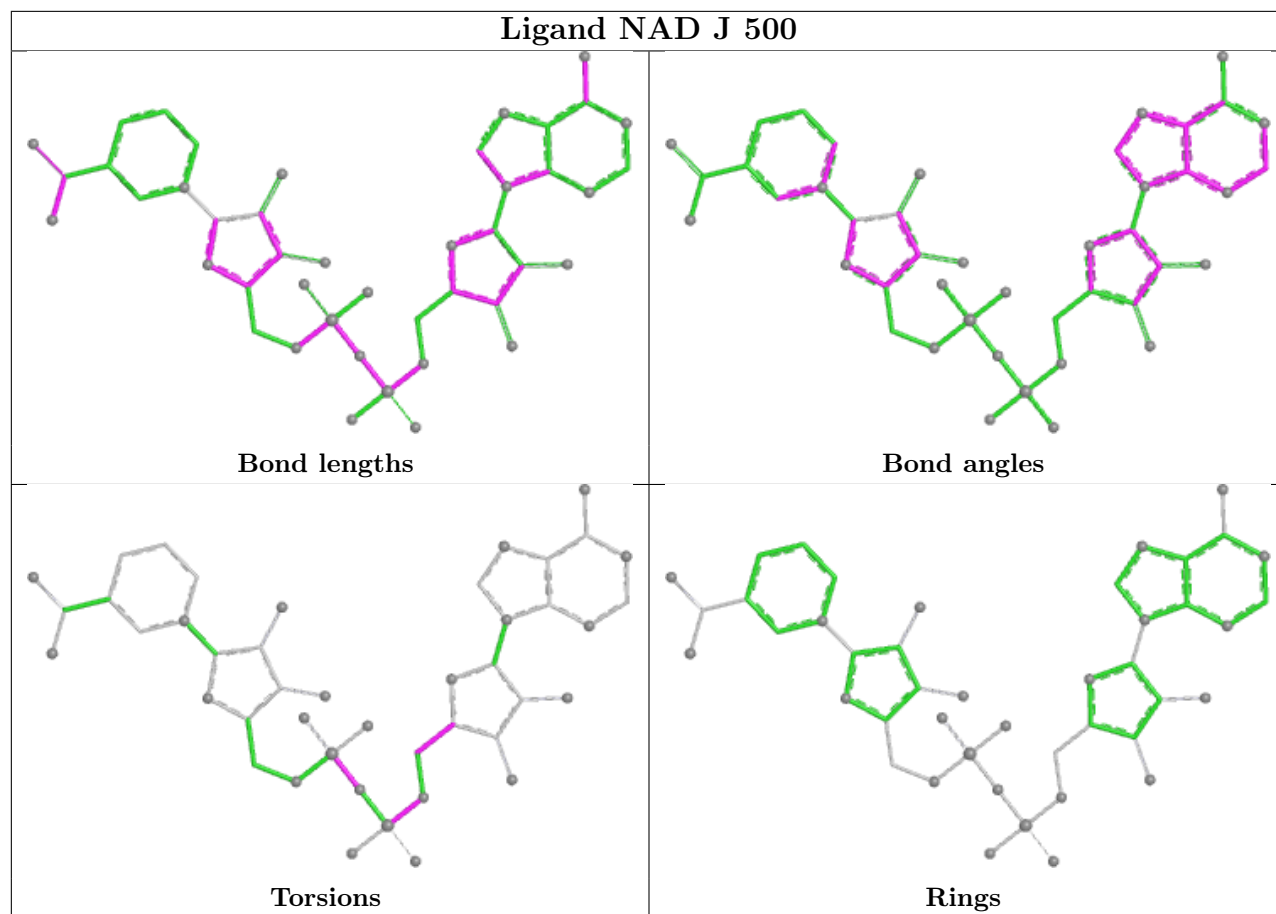


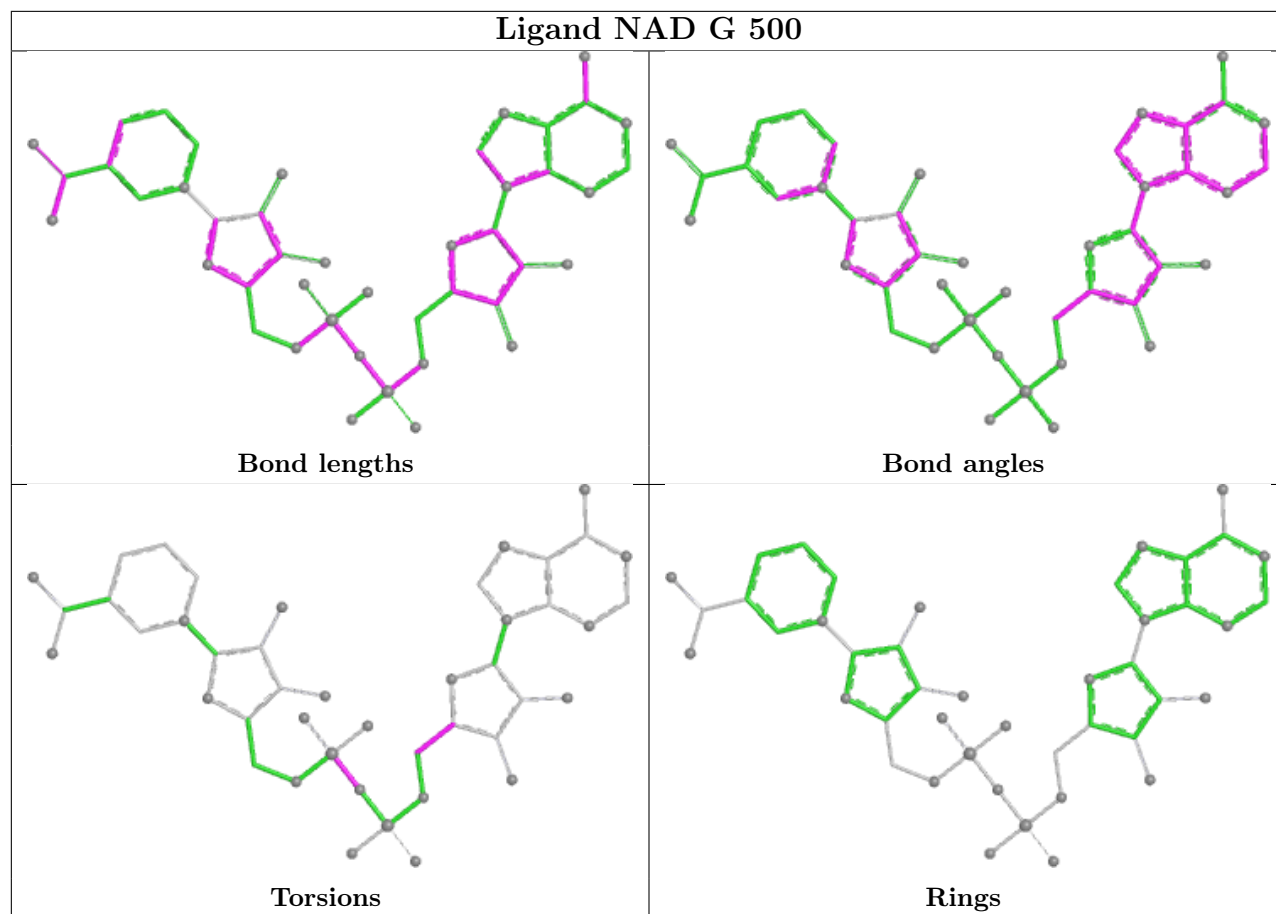


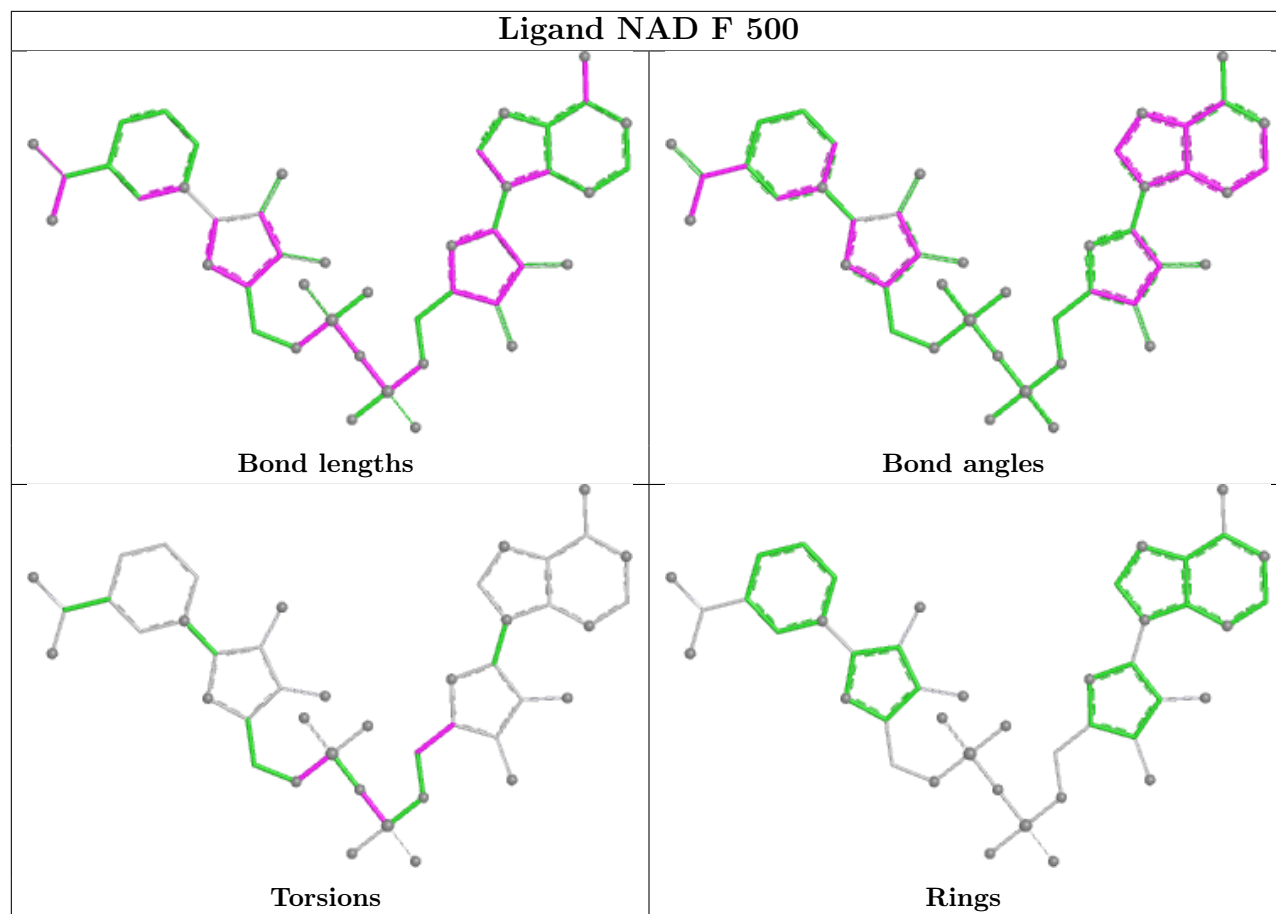












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	384/461 (83%)	0.11	1 (0%) 90 76	29, 50, 74, 87	0
1	C	369/461 (80%)	0.08	1 (0%) 90 76	30, 50, 74, 91	0
1	E	370/461 (80%)	0.17	2 (0%) 87 68	37, 64, 88, 113	0
1	G	367/461 (79%)	0.12	1 (0%) 90 76	36, 55, 78, 92	0
1	I	364/461 (78%)	0.14	2 (0%) 87 68	39, 60, 82, 95	0
1	K	381/461 (82%)	0.09	2 (0%) 87 68	35, 55, 83, 99	0
2	B	318/342 (92%)	0.08	0 100 100	33, 48, 71, 111	0
2	D	320/342 (93%)	0.09	0 100 100	34, 48, 76, 127	0
2	F	321/342 (93%)	0.12	1 (0%) 90 76	38, 60, 81, 102	0
2	H	317/342 (92%)	0.18	1 (0%) 90 76	37, 60, 89, 113	0
2	J	316/342 (92%)	0.09	2 (0%) 85 65	31, 57, 82, 101	0
2	L	317/342 (92%)	0.08	4 (1%) 75 50	35, 51, 78, 107	0
All	All	4144/4818 (86%)	0.11	17 (0%) 88 72	29, 55, 82, 127	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	254	ILE	2.9
1	A	47	VAL	2.6
1	I	431	GLU	2.6
1	E	30	ASN	2.6
2	L	59	ASN	2.5
1	G	210	ASN	2.5
2	L	85	CYS	2.5
1	I	336	ALA	2.5
2	H	185	SER	2.3
1	K	335	THR	2.2
2	J	167	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	217	GLY	2.2
1	K	23	LYS	2.1
1	E	261	TRP	2.1
2	F	230	LEU	2.1
2	L	164	SER	2.0
1	C	106	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

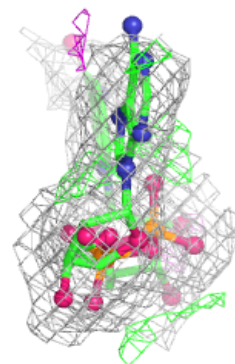
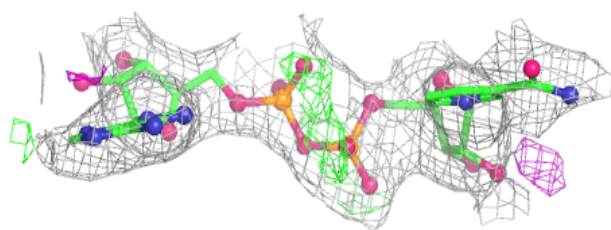
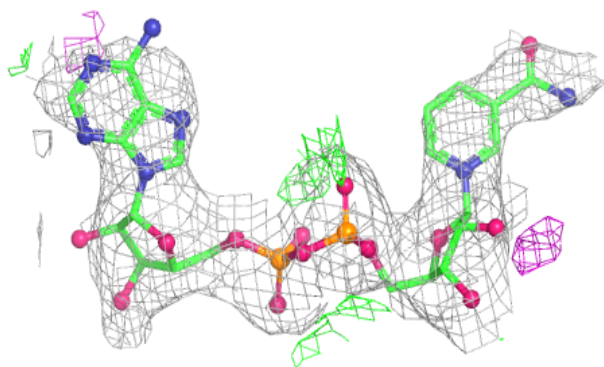
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	A	501	1/1	0.56	0.28	27,27,27,27	0
4	NAD	I	500	44/44	0.88	0.12	35,47,54,68	0
4	NAD	G	500	44/44	0.89	0.12	40,47,57,63	0
4	NAD	K	500	44/44	0.89	0.11	34,48,54,59	0
4	NAD	A	502	44/44	0.90	0.11	31,42,49,63	0
4	NAD	J	500	44/44	0.90	0.12	32,48,63,71	0
4	NAD	H	500	44/44	0.90	0.11	34,47,58,62	0
4	NAD	D	500	44/44	0.91	0.10	38,47,53,56	0
4	NAD	B	500	44/44	0.92	0.12	32,39,50,52	0
4	NAD	E	500	44/44	0.92	0.11	43,54,66,75	0
4	NAD	F	500	44/44	0.92	0.10	34,49,62,72	0
4	NAD	C	500	44/44	0.92	0.11	33,42,48,50	0
4	NAD	L	500	44/44	0.92	0.09	32,41,47,49	0

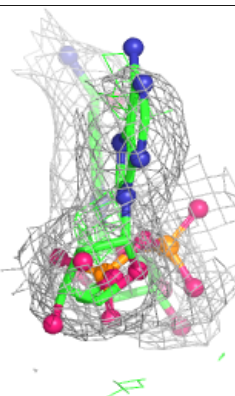
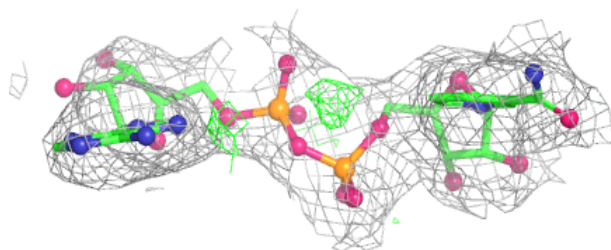
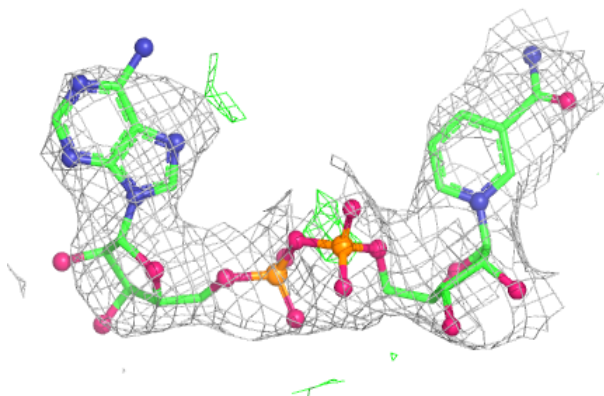
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAD I 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

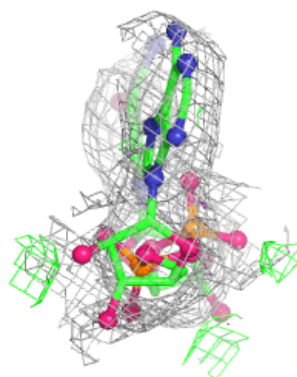
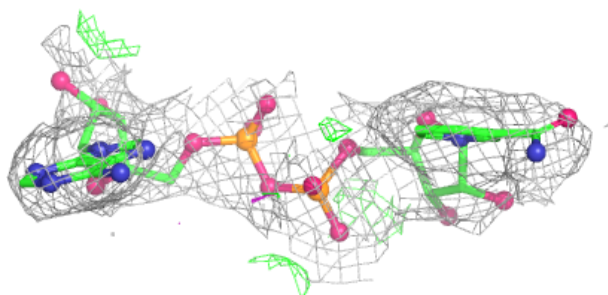
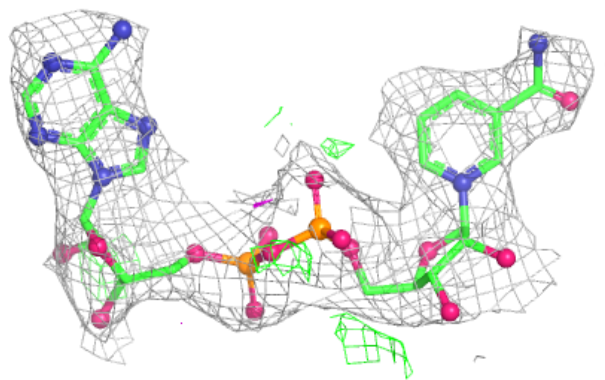
**Electron density around NAD G 500:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

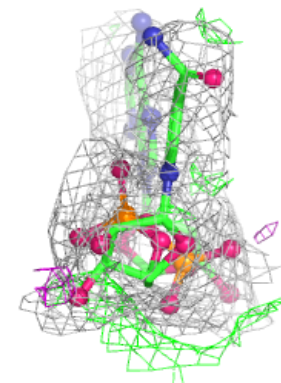
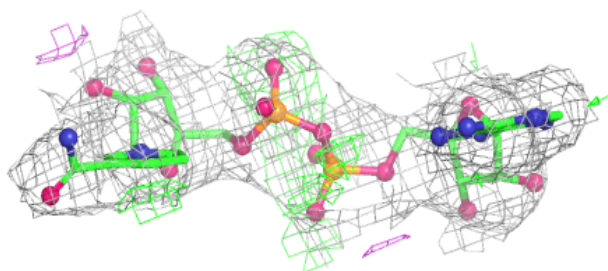
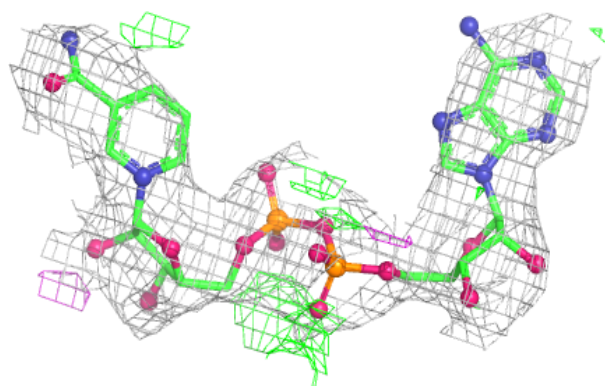


Electron density around NAD K 500:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

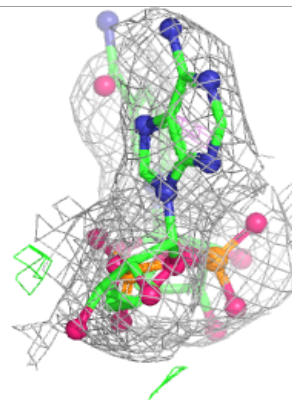
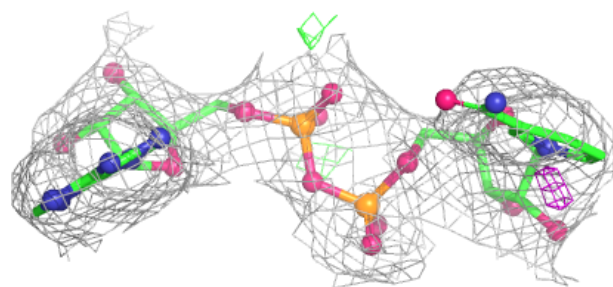
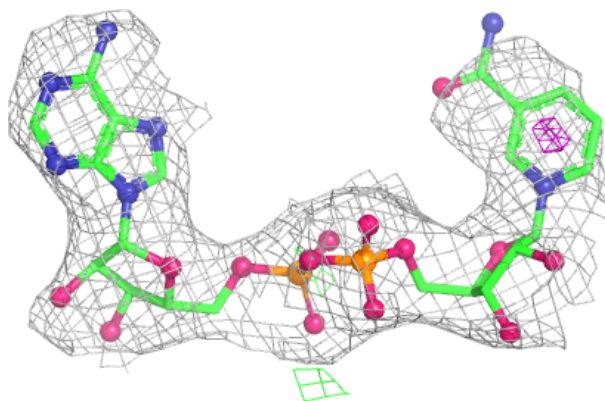
**Electron density around NAD A 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

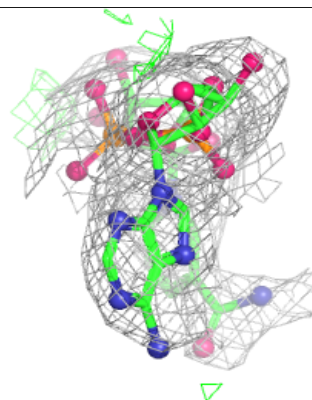
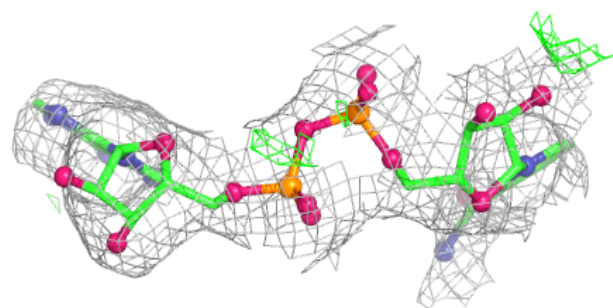
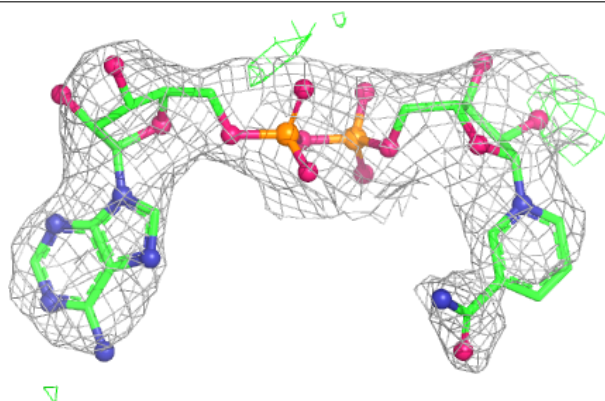


Electron density around NAD J 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

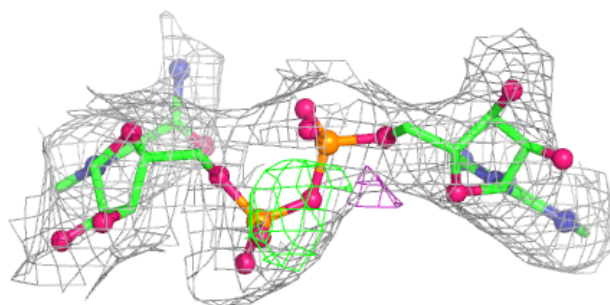
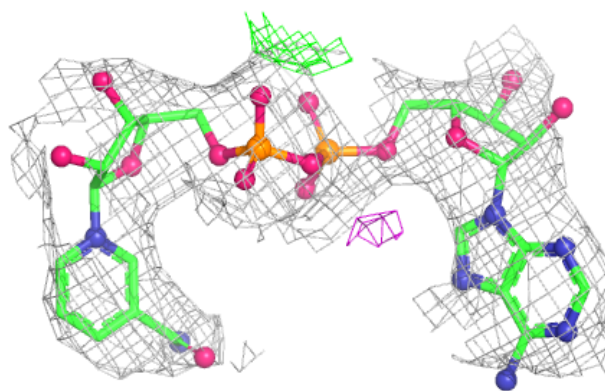
**Electron density around NAD H 500:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

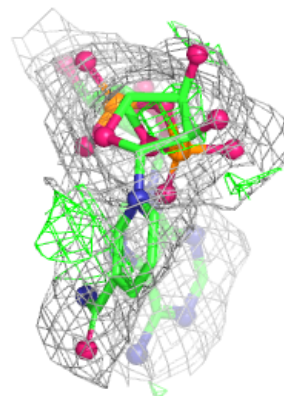
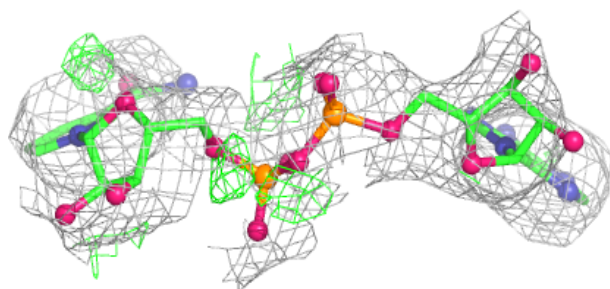
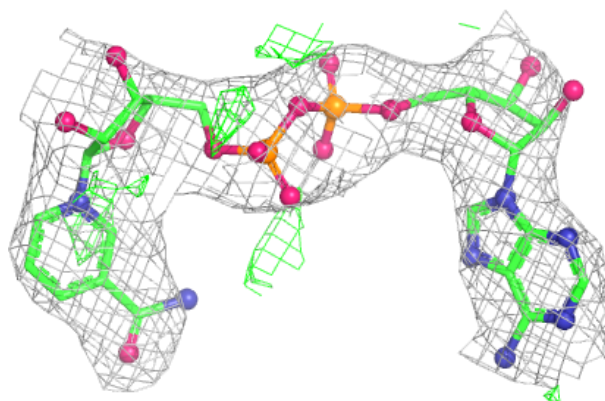


Electron density around NAD D 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

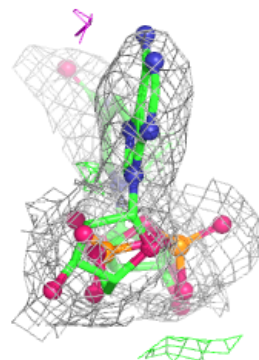
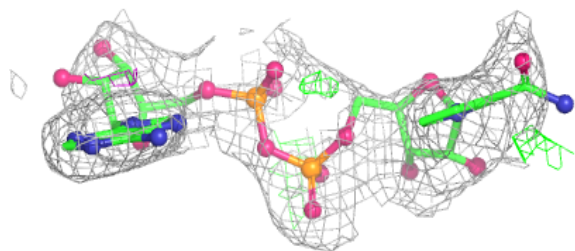
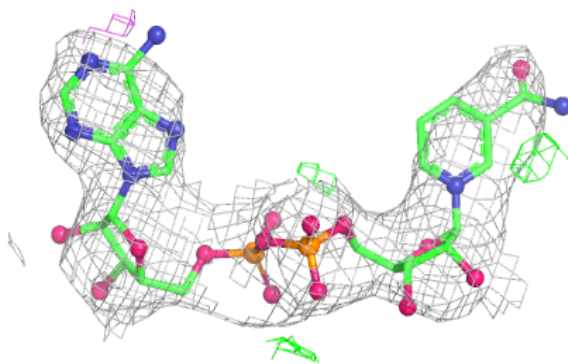
**Electron density around NAD B 500:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

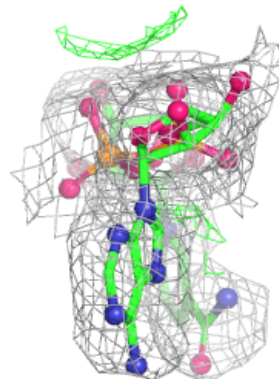
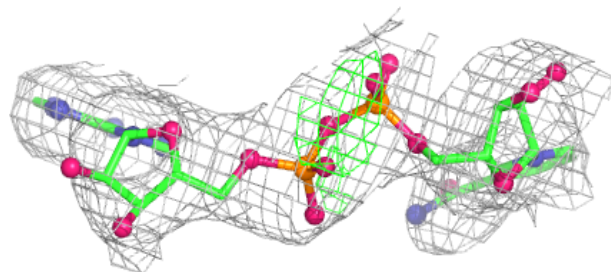
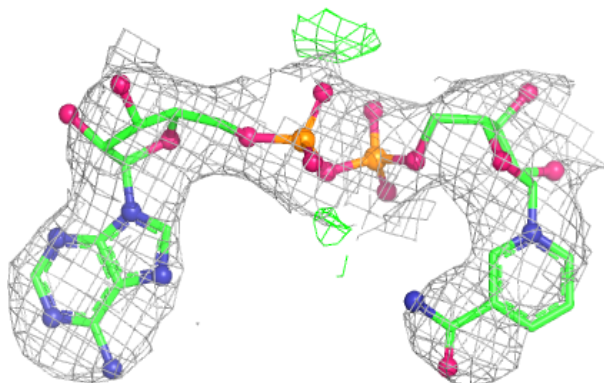


Electron density around NAD E 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

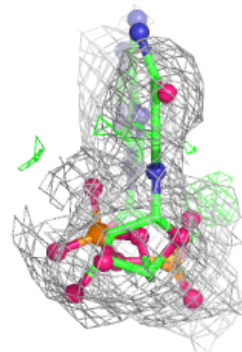
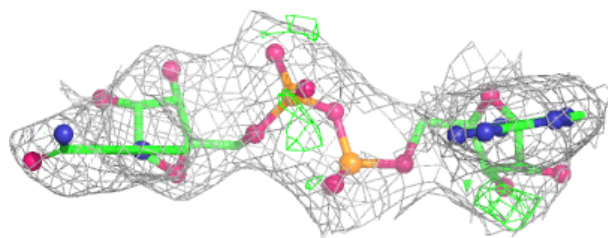
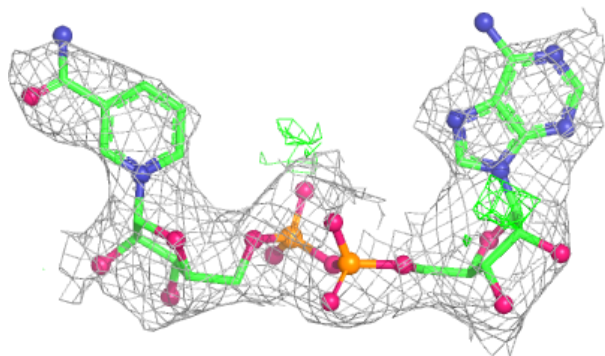
**Electron density around NAD F 500:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

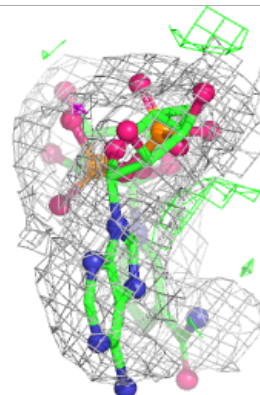
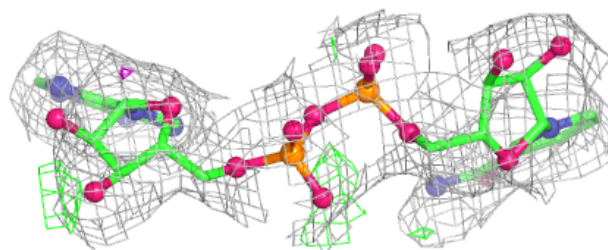
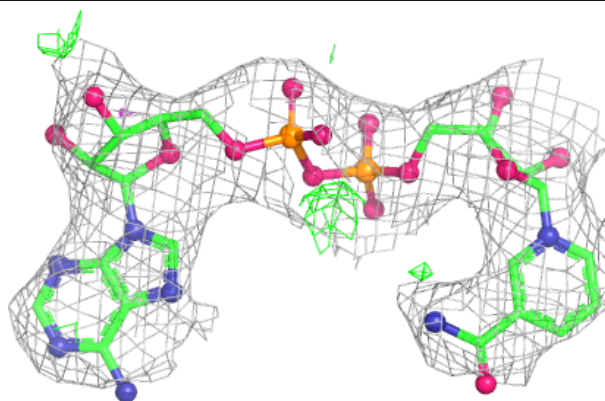


Electron density around NAD C 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAD L 500:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.