



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:30 pm BST

PDB ID : 6DFT
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 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) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

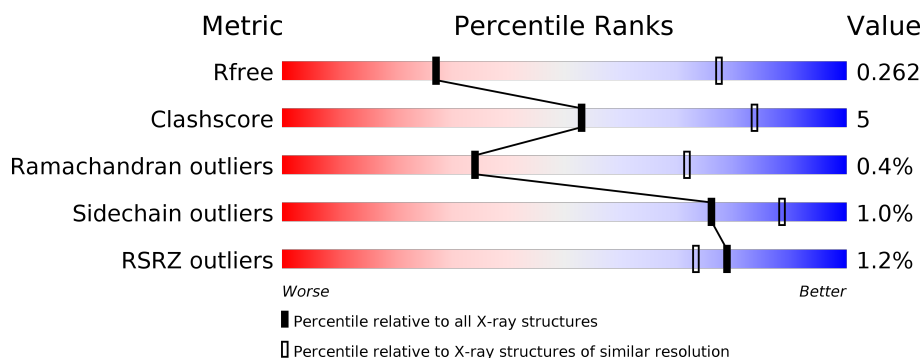
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>66%</div> <div>16%</div> <div>•</div> <div>17%</div> </div>
1	C	461	<div> <div>69%</div> <div>11%</div> <div>20%</div> </div>
1	E	461	<div> <div>2%</div> <div>70%</div> <div>10%</div> <div>20%</div> </div>
1	G	461	<div> <div>66%</div> <div>13%</div> <div>20%</div> </div>
1	I	461	<div> <div>%</div> <div>67%</div> <div>12%</div> <div>21%</div> </div>
1	K	461	<div> <div>%</div> <div>70%</div> <div>13%</div> <div>17%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	342	
2	D	342	
2	F	342	
2	H	342	
2	J	342	
2	L	342	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	A	501	-	-	-	X

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

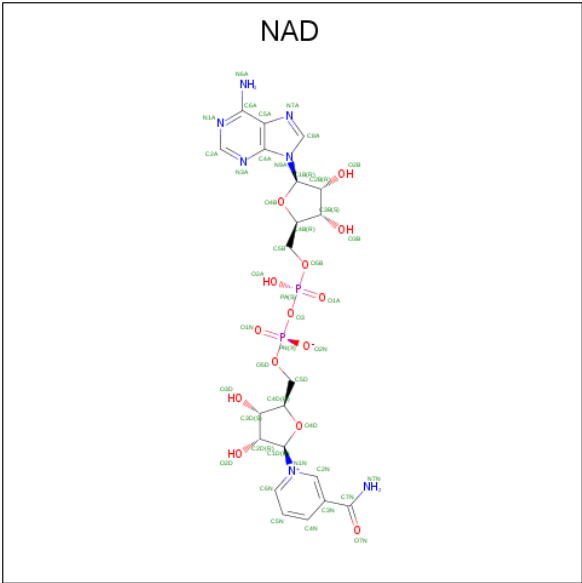
- Molecule 2 is a protein called Deoxyhypusine synthase regulatory subunit.

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by author).



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

Continued on next page...

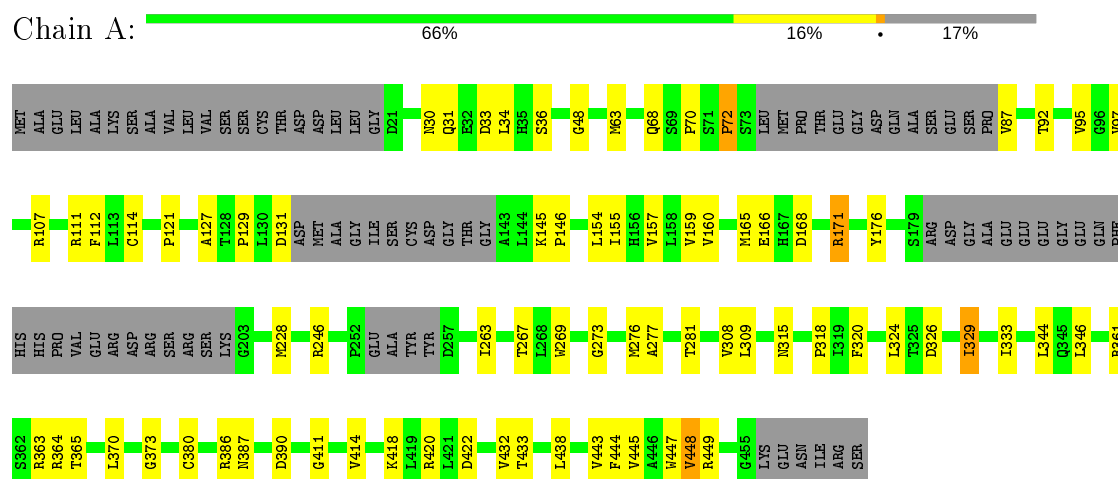
Continued from previous page...

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		

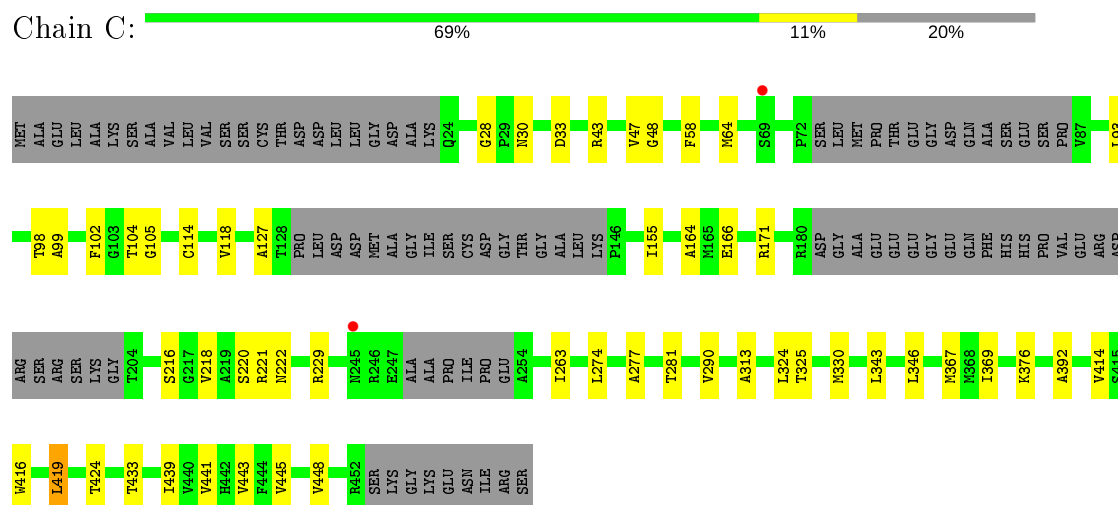
3 Residue-property plots

These plots are drawn for all protein, RNA 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 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

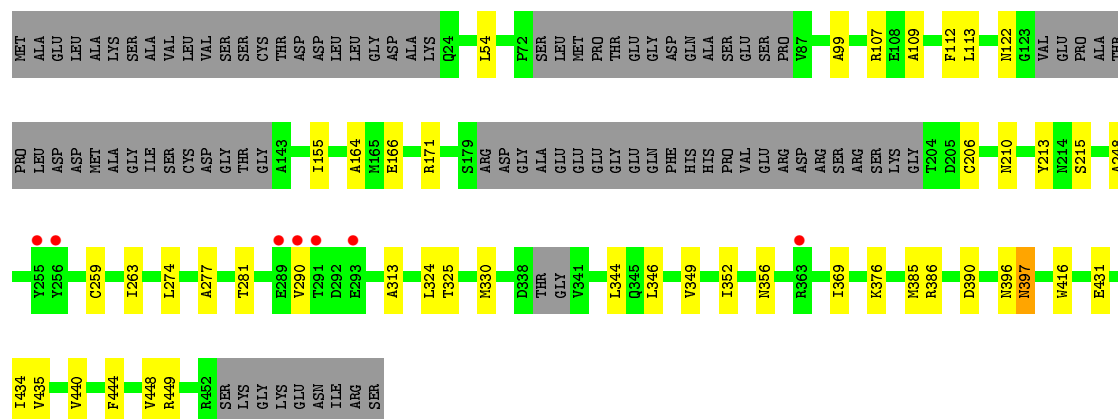


• Molecule 1: Deoxyhypusine synthase

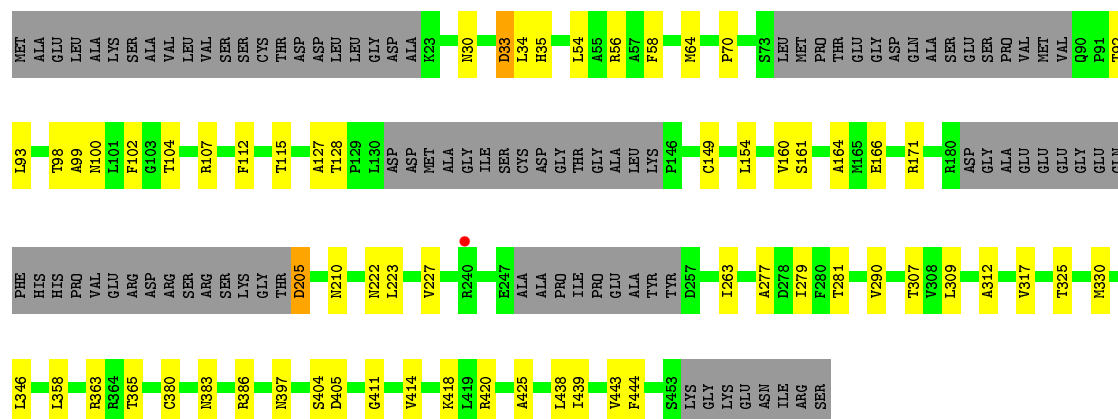


• Molecule 1: Deoxyhypusine synthase

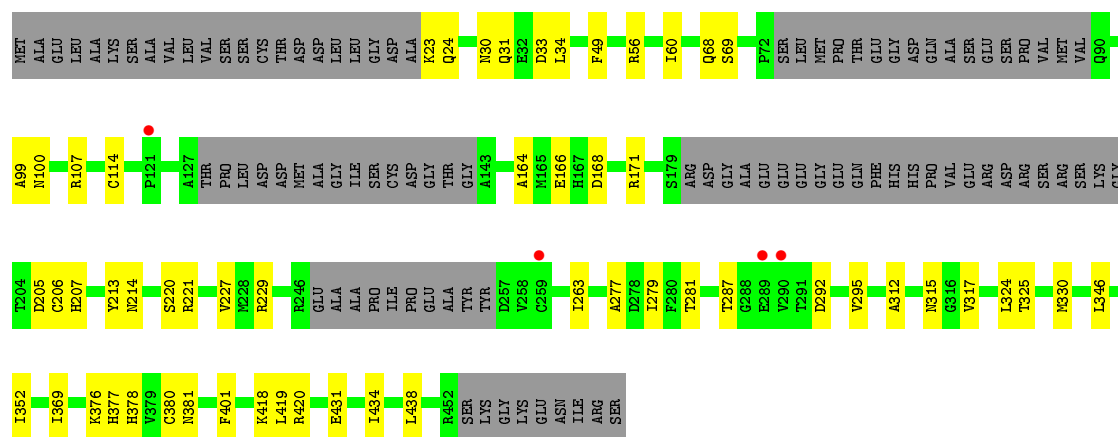




• Molecule 1: Deoxyhypusine synthase

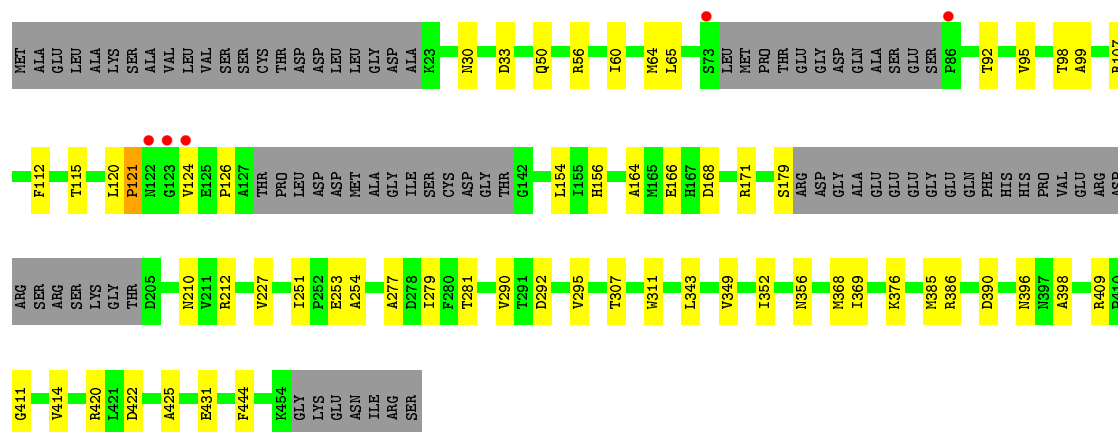


• Molecule 1: Deoxyhypusine synthase

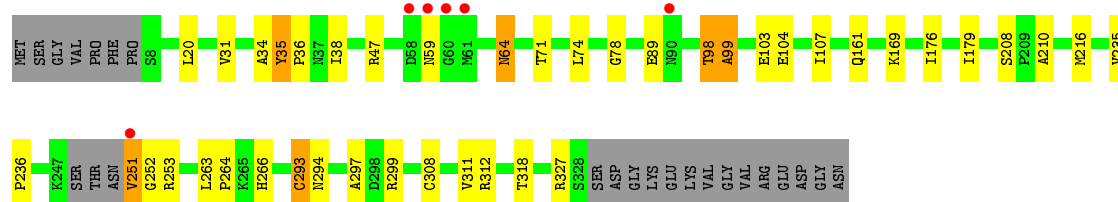
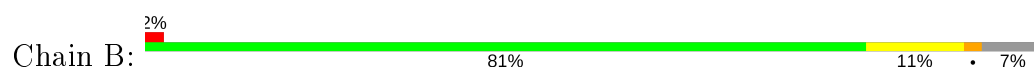


• Molecule 1: Deoxyhypusine synthase

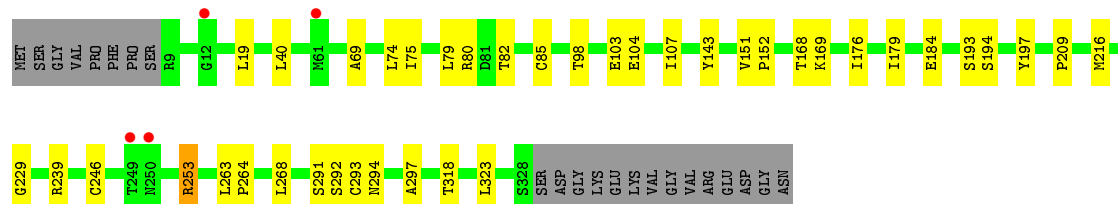
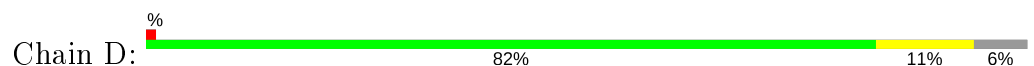




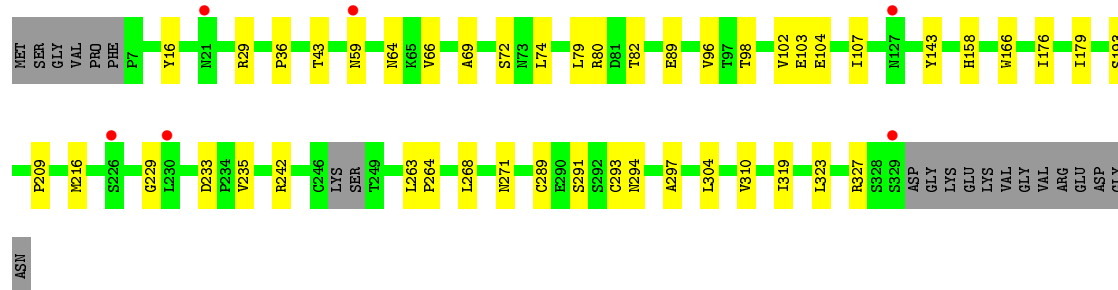
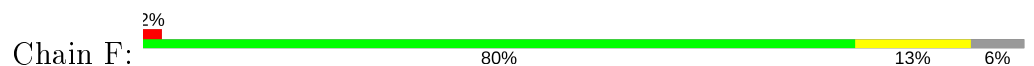
• Molecule 2: Deoxyhypusine synthase regulatory subunit




• Molecule 2: Deoxyhypusine synthase regulatory subunit

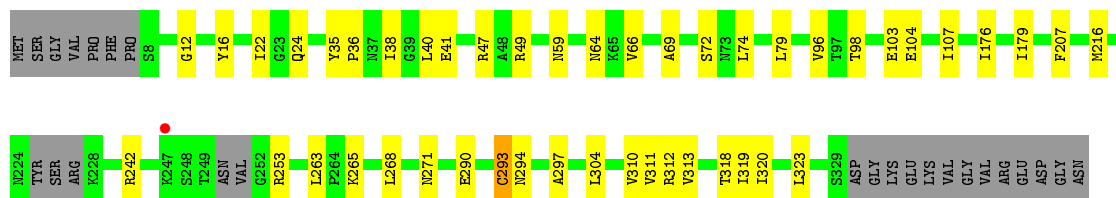


• Molecule 2: Deoxyhypusine synthase regulatory subunit




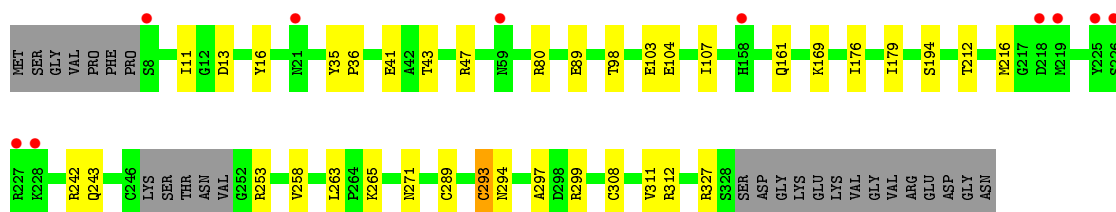
• Molecule 2: Deoxyhypusine synthase regulatory subunit

Chain H:  79% 13% 7%




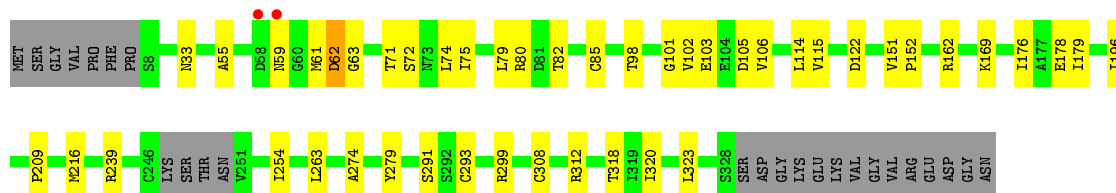
- Molecule 2: Deoxyhypusine synthase regulatory subunit

Chain J:  3% 82% 11% 8%



- Molecule 2: Deoxyhypusine synthase regulatory subunit

Chain L:  79% 13% 7%



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) 91.5 (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)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.222 , 0.262 0.222 , 0.262	Depositor DCC
R_{free} test set	1956 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 18.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	32329	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage'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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.25	0/2982	0.42	0/4042
1	C	0.24	0/2893	0.42	0/3920
1	E	0.25	0/2900	0.42	0/3931
1	G	0.24	0/2870	0.41	0/3887
1	I	0.27	1/2844 (0.0%)	0.41	0/3852
1	K	0.25	0/2976	0.41	0/4034
2	B	0.25	0/2482	0.42	0/3368
2	D	0.25	0/2498	0.43	0/3392
2	F	0.24	0/2502	0.42	0/3397
2	H	0.24	0/2463	0.43	0/3341
2	J	0.24	0/2466	0.42	0/3347
2	L	0.24	0/2473	0.41	0/3357
All	All	0.25	1/32349 (0.0%)	0.42	0/43868

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	431	GLU	CD-OE2	6.68	1.33	1.25

There are no bond angle outliers.

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	2927	0	2923	48	0
1	C	2839	0	2823	33	0
1	E	2845	0	2835	31	0
1	G	2817	0	2807	37	0
1	I	2792	0	2788	35	0
1	K	2918	0	2913	36	0
2	B	2445	0	2433	27	0
2	D	2460	0	2447	28	0
2	F	2464	0	2446	31	0
2	H	2428	0	2413	27	0
2	J	2429	0	2411	23	0
2	L	2436	0	2420	33	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	346	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 5.

All (346) 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:OD1	2:B:64:ASN:N	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

Continued on next page...

Continued from previous page...

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: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:H6N	4:G:500:NAD:O5D	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:ND2	1:G:397:ASN:O	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:228:MET:HE1	1:A:329:ILE:HG12	1.86	0.56
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
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:N	1:K:166:GLU:OE1	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
2:J:294:ASN:HB3	2:J:297:ALA:HB3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:98:THR:OG1	4:D:500:NAD:O2N	2.27	0.52
4:C:500:NAD:O3B	4:D:500:NAD:O3B	2.23	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
2:H:72:SER:OG	2:H:98:THR:OG1	2.28	0.51
1:E:416:TRP:HH2	2:F:143:TYR:HH	1.59	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:G:166:GLU:N	1:G:166:GLU:OE1	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:325:THR:O	1:C:330:MET:HG3	2.14	0.48
1:C:221:ARG:NH1	1:G:35:HIS:O	2.47	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:ND2	1:E:397:ASN:O	2.42	0.48
1:K:343:LEU:HD11	2:L:239:ARG:HE	1.78	0.48
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:28:GLY:HA2	1:C:47:VAL:HG22	1.96	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
1:A:273:GLY:HA2	1:A:276:MET:HG2	1.97	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
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
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:G:277:ALA:O	1:G:281:THR:HG23	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:246:ARG:HD3	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:N	1:C:166:GLU:OE2	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
2:L:254:ILE:HG23	2:L:274:ALA:HA	1.99	0.44
1:I:263:ILE:O	1:I:346:LEU:HA	2.17	0.44
1:I:56:ARG:O	1:I:60:ILE:HG12	2.17	0.44
2:L:169:LYS:NZ	2:L:178:GLU:OE2	2.42	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
2:L:209:PRO:HG2	2:L:263:LEU:HD21	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:CYS:O	2:B:312:ARG:NH1	2.51	0.44
1:A:48:GLY:O	2:D:318:THR:HG21	2.16	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:293:CYS:O	2:H:312:ARG:NH1	2.39	0.44
2:H:35:TYR:N	2:H:36:PRO:HD2	2.33	0.44
1:K:30:ASN:N	1:K:33:ASP:OD1	2.50	0.44
1:K:60:ILE:HG22	1:K:64:MET:HE3	2.00	0.44
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
1:C:263:ILE:O	1:C:346:LEU:HA	2.18	0.43
2:B:20:LEU:HD23	1:C:445:VAL:HG13	2.01	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
1:K:227:VAL:HG23	1:K:279:ILE:HG22	2.01	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
1:A:95:VAL:HG11	1:A:155:ILE:HD12	1.99	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:HD2	1:I:420:ARG:HA	1.78	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:184:GLU:HB2	2:D:197:TYR:HE1	1.85	0.42
1:A:31:GLN:HG2	2:D:85:CYS:SG	2.59	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:439:ILE:O	1:C:443:VAL:HG22	2.19	0.42
1:C:58:PHE:HE1	1:C:439:ILE:HA	1.84	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:N	1:I:205:ASP:OD1	2.52	0.42
4:I:500:NAD:H52A	2:J:289:CYS:SG	2.60	0.42
4:D:500:NAD:O5B	4:D:500:NAD:H8A	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:242:ARG:NH1	2:F:271:ASN:OD1	2.53	0.42
2:F:74:LEU:HD22	2:F:79:LEU:HD12	2.02	0.42
2:F:16:TYR:HB2	1:G:112:PHE:HB2	2.02	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:176:ILE:HA	2:H:179:ILE:HD12	2.02	0.42
2:H:49:ARG:NH1	2:H:323:LEU:O	2.53	0.42
1:A:420:ARG:NE	1:A:422:ASP:OD1	2.51	0.42
1:I:107:ARG:HD3	1:I:171:ARG:HD3	2.02	0.42
1:I:34:LEU:HD11	2:L:82:THR:HG23	2.00	0.42
2:F:176:ILE:HA	2:F:179:ILE:HD12	2.01	0.41
1:I:166:GLU:N	1:I:166:GLU:OE1	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:K:56:ARG:NH1	1:K:425:ALA:O	2.54	0.41
1:I:401:PHE:HB2	1:K:50:GLN:HG3	2.02	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:64:MET:HB3	1:C:93:LEU:HD11	2.02	0.41
1:A:36:SER:HB3	1:I:221:ARG:HE	1.84	0.41
2:J:299:ARG:NH2	2:J:308:CYS:O	2.53	0.41
2:L:102:VAL:O	2:L:106:VAL:HG23	2.20	0.41
2:L:71:THR:OG1	4:L:500:NAD:O2N	2.34	0.41
1:E:206:CYS:HG	1:E:215:SER:HG	1.64	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
4:K:500:NAD:O2A	2:L:291:SER:OG	2.32	0.41
1:C:416:TRP:HH2	2:D:143:TYR:HH	1.67	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:104:THR:OG1	1:C:105:GLY:N	2.53	0.41
1:C:98:THR:HG23	4:C:500:NAD:O2N	2.20	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:235:VAL:HG22	2:B:236:PRO:HD3	2.03	0.41
2:B:34:ALA:O	2:B:38:ILE:HG13	2.21	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
2:D:80:ARG:NH2	2:D:194:SER:HA	2.36	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:263:ILE:O	1:G:346:LEU:HA	2.21	0.40
1:G:58:PHE:HE1	1:G:439:ILE:HA	1.85	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%)	29	68
1	C	359/461 (78%)	345 (96%)	13 (4%)	1 (0%)	41	75
1	E	360/461 (78%)	343 (95%)	16 (4%)	1 (0%)	41	75
1	G	357/461 (77%)	344 (96%)	12 (3%)	1 (0%)	41	75
1	I	354/461 (77%)	341 (96%)	13 (4%)	0	100	100
1	K	373/461 (81%)	354 (95%)	18 (5%)	1 (0%)	41	75
2	B	314/342 (92%)	289 (92%)	23 (7%)	2 (1%)	25	64
2	D	318/342 (93%)	295 (93%)	20 (6%)	3 (1%)	17	56
2	F	317/342 (93%)	300 (95%)	16 (5%)	1 (0%)	41	75
2	H	311/342 (91%)	286 (92%)	24 (8%)	1 (0%)	41	75
2	J	312/342 (91%)	292 (94%)	18 (6%)	2 (1%)	25	64
2	L	313/342 (92%)	292 (93%)	19 (6%)	2 (1%)	25	64
All	All	4062/4818 (84%)	3839 (94%)	206 (5%)	17 (0%)	34	72

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 ⓘ

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	317/380 (83%)	312 (98%)	5 (2%)	62	83
1	C	307/380 (81%)	301 (98%)	6 (2%)	55	79
1	E	307/380 (81%)	305 (99%)	2 (1%)	84	93
1	G	306/380 (80%)	300 (98%)	6 (2%)	55	79
1	I	302/380 (80%)	299 (99%)	3 (1%)	76	88
1	K	315/380 (83%)	312 (99%)	3 (1%)	76	88
2	B	268/288 (93%)	262 (98%)	6 (2%)	52	78
2	D	270/288 (94%)	268 (99%)	2 (1%)	84	93
2	F	271/288 (94%)	271 (100%)	0	100	100
2	H	267/288 (93%)	266 (100%)	1 (0%)	91	96

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	266/288 (92%)	266 (100%)	0	100	100
2	L	267/288 (93%)	265 (99%)	2 (1%)	84	93
All	All	3463/4008 (86%)	3427 (99%)	36 (1%)	76	88

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	ARG
1	A	329	ILE
1	A	365	THR
1	A	387	ASN
1	A	448	VAL
2	B	35	TYR
2	B	64	ASN
2	B	98	THR
2	B	251	VAL
2	B	253	ARG
2	B	263	LEU
1	C	216	SER
1	C	222	ASN
1	C	290	VAL
1	C	419	LEU
1	C	424	THR
1	C	433	THR
2	D	246	CYS
2	D	253	ARG
1	E	290	VAL
1	E	397	ASN
1	G	33	ASP
1	G	98	THR
1	G	205	ASP
1	G	210	ASN
1	G	290	VAL
1	G	309	LEU
2	H	318	THR
1	I	207	HIS
1	I	378	HIS
1	I	419	LEU
1	K	210	ASN
1	K	290	VAL
1	K	307	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	33	ASN
2	L	62	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	160	GLN
1	G	207	HIS

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 carbohydrates 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	-	42,48,48	2.60	16 (38%)	50,73,73	1.70	9 (18%)
4	NAD	A	502	-	42,48,48	2.57	16 (38%)	50,73,73	1.57	9 (18%)
4	NAD	L	500	-	42,48,48	2.62	16 (38%)	50,73,73	1.52	9 (18%)
4	NAD	I	500	-	42,48,48	2.58	15 (35%)	50,73,73	1.63	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAD	K	500	-	42,48,48	2.58	16 (38%)	50,73,73	1.66	9 (18%)
4	NAD	H	500	-	42,48,48	2.61	16 (38%)	50,73,73	1.55	9 (18%)
4	NAD	J	500	-	42,48,48	2.60	16 (38%)	50,73,73	1.46	8 (16%)
4	NAD	G	500	-	42,48,48	2.60	15 (35%)	50,73,73	1.74	10 (20%)
4	NAD	D	500	-	42,48,48	2.64	16 (38%)	50,73,73	1.52	9 (18%)
4	NAD	F	500	-	42,48,48	2.60	16 (38%)	50,73,73	1.53	10 (20%)
4	NAD	C	500	-	42,48,48	2.58	16 (38%)	50,73,73	1.59	9 (18%)
4	NAD	B	500	-	42,48,48	2.61	15 (35%)	50,73,73	1.52	9 (18%)

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	-	-	9/26/62/62	0/5/5/5
4	NAD	A	502	-	-	12/26/62/62	0/5/5/5
4	NAD	L	500	-	-	8/26/62/62	0/5/5/5
4	NAD	I	500	-	-	8/26/62/62	0/5/5/5
4	NAD	K	500	-	-	5/26/62/62	0/5/5/5
4	NAD	H	500	-	-	9/26/62/62	0/5/5/5
4	NAD	J	500	-	-	6/26/62/62	0/5/5/5
4	NAD	G	500	-	-	3/26/62/62	0/5/5/5
4	NAD	D	500	-	-	13/26/62/62	0/5/5/5
4	NAD	F	500	-	-	6/26/62/62	0/5/5/5
4	NAD	C	500	-	-	6/26/62/62	0/5/5/5
4	NAD	B	500	-	-	8/26/62/62	0/5/5/5

All (189) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	500	NAD	O4D-C1D	7.64	1.51	1.41
4	C	500	NAD	O4D-C1D	7.63	1.51	1.41
4	D	500	NAD	O4D-C1D	7.56	1.51	1.41
4	L	500	NAD	O4D-C1D	7.55	1.51	1.41
4	A	502	NAD	O4D-C1D	7.51	1.51	1.41
4	E	500	NAD	O4D-C1D	7.47	1.51	1.41
4	K	500	NAD	O4D-C1D	7.45	1.51	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	500	NAD	O4D-C1D	7.42	1.51	1.41
4	B	500	NAD	O4D-C1D	7.41	1.51	1.41
4	J	500	NAD	O4D-C1D	7.38	1.51	1.41
4	F	500	NAD	O4D-C1D	7.35	1.51	1.41
4	I	500	NAD	O4D-C1D	7.33	1.51	1.41
4	L	500	NAD	C7N-N7N	7.22	1.46	1.33
4	I	500	NAD	C7N-N7N	7.22	1.46	1.33
4	J	500	NAD	C7N-N7N	7.21	1.46	1.33
4	H	500	NAD	C7N-N7N	7.20	1.46	1.33
4	D	500	NAD	C7N-N7N	7.18	1.46	1.33
4	K	500	NAD	C7N-N7N	7.17	1.46	1.33
4	E	500	NAD	C7N-N7N	7.17	1.46	1.33
4	F	500	NAD	C7N-N7N	7.17	1.46	1.33
4	B	500	NAD	C7N-N7N	7.13	1.46	1.33
4	G	500	NAD	C7N-N7N	7.10	1.46	1.33
4	C	500	NAD	C7N-N7N	7.04	1.46	1.33
4	A	502	NAD	C7N-N7N	7.03	1.46	1.33
4	D	500	NAD	O4B-C1B	6.98	1.50	1.41
4	L	500	NAD	O4B-C1B	6.91	1.50	1.41
4	J	500	NAD	O4B-C1B	6.77	1.50	1.41
4	B	500	NAD	O4B-C1B	6.75	1.50	1.41
4	H	500	NAD	O4B-C1B	6.69	1.50	1.41
4	K	500	NAD	O4B-C1B	6.65	1.50	1.41
4	A	502	NAD	O4B-C1B	6.61	1.50	1.41
4	E	500	NAD	O4B-C1B	6.60	1.50	1.41
4	C	500	NAD	O4B-C1B	6.56	1.50	1.41
4	I	500	NAD	O4B-C1B	6.56	1.50	1.41
4	G	500	NAD	O4B-C1B	6.54	1.50	1.41
4	F	500	NAD	O4B-C1B	6.54	1.50	1.41
4	C	500	NAD	C2B-C1B	-4.61	1.46	1.53
4	E	500	NAD	C2B-C1B	-4.47	1.47	1.53
4	B	500	NAD	C2B-C1B	-4.46	1.47	1.53
4	F	500	NAD	C2B-C1B	-4.46	1.47	1.53
4	K	500	NAD	C2B-C1B	-4.38	1.47	1.53
4	D	500	NAD	C2B-C1B	-4.35	1.47	1.53
4	G	500	NAD	C2B-C1B	-4.34	1.47	1.53
4	L	500	NAD	C2B-C1B	-4.28	1.47	1.53
4	I	500	NAD	C2B-C1B	-4.25	1.47	1.53
4	H	500	NAD	C2B-C1B	-4.25	1.47	1.53
4	A	502	NAD	C2B-C1B	-4.14	1.47	1.53
4	J	500	NAD	C2B-C1B	-4.11	1.47	1.53
4	J	500	NAD	C2D-C1D	-4.06	1.47	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	500	NAD	C2D-C1D	-4.05	1.47	1.53
4	D	500	NAD	C2D-C1D	-3.94	1.47	1.53
4	I	500	NAD	C2D-C1D	-3.92	1.47	1.53
4	B	500	NAD	C2D-C1D	-3.88	1.47	1.53
4	H	500	NAD	C2D-C1D	-3.86	1.47	1.53
4	L	500	NAD	C2D-C1D	-3.81	1.48	1.53
4	K	500	NAD	C2D-C1D	-3.75	1.48	1.53
4	E	500	NAD	C2D-C1D	-3.64	1.48	1.53
4	C	500	NAD	C2D-C1D	-3.57	1.48	1.53
4	G	500	NAD	C2D-C1D	-3.53	1.48	1.53
4	K	500	NAD	C6A-N6A	3.48	1.46	1.34
4	E	500	NAD	O4D-C4D	3.47	1.52	1.45
4	L	500	NAD	C6A-N6A	3.46	1.46	1.34
4	J	500	NAD	C6A-N6A	3.44	1.46	1.34
4	G	500	NAD	C6A-N6A	3.44	1.46	1.34
4	A	502	NAD	C2D-C1D	-3.44	1.48	1.53
4	I	500	NAD	C6A-N6A	3.43	1.46	1.34
4	G	500	NAD	O4D-C4D	3.43	1.52	1.45
4	H	500	NAD	C6A-N6A	3.43	1.46	1.34
4	E	500	NAD	C6A-N6A	3.43	1.46	1.34
4	F	500	NAD	C6A-N6A	3.41	1.46	1.34
4	D	500	NAD	C6A-N6A	3.41	1.46	1.34
4	C	500	NAD	C6A-N6A	3.39	1.46	1.34
4	I	500	NAD	O4D-C4D	3.37	1.52	1.45
4	A	502	NAD	C6A-N6A	3.37	1.46	1.34
4	B	500	NAD	C6A-N6A	3.35	1.46	1.34
4	J	500	NAD	O4D-C4D	3.35	1.52	1.45
4	K	500	NAD	O4D-C4D	3.32	1.52	1.45
4	B	500	NAD	O4D-C4D	3.32	1.52	1.45
4	F	500	NAD	O4D-C4D	3.31	1.52	1.45
4	A	502	NAD	O4D-C4D	3.29	1.52	1.45
4	L	500	NAD	O4D-C4D	3.29	1.52	1.45
4	D	500	NAD	O4D-C4D	3.26	1.52	1.45
4	A	502	NAD	O7N-C7N	-3.24	1.17	1.24
4	H	500	NAD	O4D-C4D	3.24	1.52	1.45
4	C	500	NAD	O4D-C4D	3.18	1.52	1.45
4	D	500	NAD	O7N-C7N	-3.17	1.18	1.24
4	C	500	NAD	O7N-C7N	-3.14	1.18	1.24
4	G	500	NAD	O7N-C7N	-3.11	1.18	1.24
4	E	500	NAD	O7N-C7N	-3.09	1.18	1.24
4	K	500	NAD	O7N-C7N	-3.08	1.18	1.24
4	B	500	NAD	O7N-C7N	-3.05	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	500	NAD	O7N-C7N	-3.04	1.18	1.24
4	F	500	NAD	O7N-C7N	-3.03	1.18	1.24
4	H	500	NAD	O7N-C7N	-3.03	1.18	1.24
4	L	500	NAD	O7N-C7N	-3.00	1.18	1.24
4	J	500	NAD	O7N-C7N	-2.98	1.18	1.24
4	E	500	NAD	PN-O5D	2.66	1.70	1.59
4	J	500	NAD	PN-O5D	2.61	1.69	1.59
4	H	500	NAD	PN-O5D	2.60	1.69	1.59
4	D	500	NAD	C4A-N3A	-2.57	1.32	1.35
4	A	502	NAD	C4A-N3A	-2.57	1.32	1.35
4	L	500	NAD	PN-O5D	2.56	1.69	1.59
4	G	500	NAD	PN-O5D	2.55	1.69	1.59
4	C	500	NAD	C4A-N3A	-2.54	1.32	1.35
4	F	500	NAD	PN-O5D	2.53	1.69	1.59
4	K	500	NAD	PN-O5D	2.51	1.69	1.59
4	I	500	NAD	PN-O5D	2.50	1.69	1.59
4	B	500	NAD	C4A-N3A	-2.44	1.32	1.35
4	F	500	NAD	C4A-N3A	-2.44	1.32	1.35
4	B	500	NAD	PN-O5D	2.43	1.69	1.59
4	I	500	NAD	C3B-C4B	-2.42	1.46	1.53
4	G	500	NAD	C4A-N3A	-2.42	1.32	1.35
4	J	500	NAD	C4A-N3A	-2.42	1.32	1.35
4	D	500	NAD	PN-O5D	2.42	1.69	1.59
4	H	500	NAD	C4A-N3A	-2.42	1.32	1.35
4	C	500	NAD	C2D-C3D	-2.42	1.46	1.53
4	A	502	NAD	PN-O5D	2.41	1.69	1.59
4	E	500	NAD	C4A-N3A	-2.36	1.32	1.35
4	G	500	NAD	C3B-C4B	-2.35	1.47	1.53
4	D	500	NAD	C2B-C3B	-2.34	1.46	1.53
4	A	502	NAD	C2D-C3D	-2.34	1.46	1.53
4	H	500	NAD	C3B-C4B	-2.34	1.47	1.53
4	I	500	NAD	C4A-N3A	-2.33	1.32	1.35
4	L	500	NAD	C4A-N3A	-2.33	1.32	1.35
4	G	500	NAD	C2D-C3D	-2.32	1.47	1.53
4	C	500	NAD	PN-O5D	2.32	1.68	1.59
4	L	500	NAD	C3B-C4B	-2.31	1.47	1.53
4	J	500	NAD	C3B-C4B	-2.31	1.47	1.53
4	H	500	NAD	C2D-C3D	-2.30	1.47	1.53
4	B	500	NAD	C2B-C3B	-2.29	1.47	1.53
4	I	500	NAD	C2D-C3D	-2.29	1.47	1.53
4	D	500	NAD	C2D-C3D	-2.28	1.47	1.53
4	K	500	NAD	C2D-C3D	-2.27	1.47	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	500	NAD	C2D-C3D	-2.27	1.47	1.53
4	J	500	NAD	C2D-C3D	-2.26	1.47	1.53
4	G	500	NAD	C3D-C4D	-2.25	1.47	1.53
4	F	500	NAD	C2D-C3D	-2.25	1.47	1.53
4	F	500	NAD	C3B-C4B	-2.25	1.47	1.53
4	K	500	NAD	C4A-N3A	-2.25	1.32	1.35
4	C	500	NAD	C3D-C4D	-2.24	1.47	1.53
4	C	500	NAD	C2B-C3B	-2.24	1.47	1.53
4	E	500	NAD	C2D-C3D	-2.23	1.47	1.53
4	L	500	NAD	C3D-C4D	-2.21	1.47	1.53
4	H	500	NAD	O4B-C4B	2.21	1.49	1.45
4	K	500	NAD	C3D-C4D	-2.20	1.47	1.53
4	A	502	NAD	C3D-C4D	-2.20	1.47	1.53
4	D	500	NAD	O4B-C4B	2.20	1.49	1.45
4	F	500	NAD	C3D-C4D	-2.20	1.47	1.53
4	L	500	NAD	C2D-C3D	-2.19	1.47	1.53
4	L	500	NAD	PA-O5B	2.19	1.68	1.59
4	K	500	NAD	C3B-C4B	-2.19	1.47	1.53
4	G	500	NAD	O4B-C4B	2.19	1.49	1.45
4	F	500	NAD	PA-O5B	2.18	1.68	1.59
4	I	500	NAD	C3D-C4D	-2.18	1.47	1.53
4	L	500	NAD	O4B-C4B	2.18	1.49	1.45
4	F	500	NAD	C2B-C3B	-2.18	1.47	1.53
4	E	500	NAD	C3B-C4B	-2.18	1.47	1.53
4	B	500	NAD	O4B-C4B	2.18	1.49	1.45
4	A	502	NAD	C2B-C3B	-2.18	1.47	1.53
4	D	500	NAD	C3B-C4B	-2.17	1.47	1.53
4	J	500	NAD	O4B-C4B	2.17	1.49	1.45
4	D	500	NAD	PA-O5B	2.17	1.68	1.59
4	E	500	NAD	PA-O5B	2.17	1.68	1.59
4	I	500	NAD	O4B-C4B	2.16	1.49	1.45
4	K	500	NAD	O4B-C4B	2.16	1.49	1.45
4	K	500	NAD	PA-O5B	2.16	1.68	1.59
4	E	500	NAD	C2B-C3B	-2.15	1.47	1.53
4	J	500	NAD	PA-O5B	2.15	1.68	1.59
4	F	500	NAD	O4B-C4B	2.15	1.49	1.45
4	J	500	NAD	C3D-C4D	-2.15	1.47	1.53
4	H	500	NAD	PA-O5B	2.14	1.67	1.59
4	A	502	NAD	C3B-C4B	-2.14	1.47	1.53
4	L	500	NAD	C2B-C3B	-2.13	1.47	1.53
4	B	500	NAD	C3N-C7N	2.13	1.53	1.50
4	H	500	NAD	C2B-C3B	-2.12	1.47	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	500	NAD	C3D-C4D	-2.12	1.47	1.53
4	B	500	NAD	PA-O5B	2.12	1.67	1.59
4	E	500	NAD	O4B-C4B	2.12	1.49	1.45
4	A	502	NAD	O4B-C4B	2.12	1.49	1.45
4	H	500	NAD	C3D-C4D	-2.11	1.47	1.53
4	C	500	NAD	C3B-C4B	-2.11	1.47	1.53
4	C	500	NAD	PA-O5B	2.11	1.67	1.59
4	G	500	NAD	PA-O5B	2.10	1.67	1.59
4	C	500	NAD	O4B-C4B	2.10	1.49	1.45
4	I	500	NAD	PA-O5B	2.09	1.67	1.59
4	D	500	NAD	C3D-C4D	-2.08	1.47	1.53
4	A	502	NAD	PA-O5B	2.05	1.67	1.59
4	J	500	NAD	C2B-C3B	-2.03	1.47	1.53
4	K	500	NAD	C3N-C7N	2.03	1.53	1.50

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	500	NAD	C3B-C2B-C1B	4.95	108.43	100.98
4	G	500	NAD	C3B-C2B-C1B	4.80	108.21	100.98
4	A	502	NAD	C3D-C2D-C1D	4.79	108.19	100.98
4	K	500	NAD	C3D-C2D-C1D	4.61	107.92	100.98
4	E	500	NAD	C3D-C2D-C1D	4.60	107.90	100.98
4	G	500	NAD	C3D-C2D-C1D	4.53	107.80	100.98
4	K	500	NAD	C3B-C2B-C1B	4.50	107.75	100.98
4	C	500	NAD	C3B-C2B-C1B	4.46	107.70	100.98
4	E	500	NAD	C3B-C2B-C1B	4.42	107.63	100.98
4	H	500	NAD	N3A-C2A-N1A	-4.19	122.13	128.68
4	L	500	NAD	C3D-C2D-C1D	4.17	107.26	100.98
4	F	500	NAD	C3B-C2B-C1B	4.15	107.23	100.98
4	E	500	NAD	N3A-C2A-N1A	-4.10	122.26	128.68
4	D	500	NAD	N3A-C2A-N1A	-4.09	122.28	128.68
4	G	500	NAD	N3A-C2A-N1A	-4.09	122.29	128.68
4	K	500	NAD	N3A-C2A-N1A	-4.04	122.37	128.68
4	L	500	NAD	N3A-C2A-N1A	-4.02	122.40	128.68
4	J	500	NAD	N3A-C2A-N1A	-4.01	122.41	128.68
4	F	500	NAD	N3A-C2A-N1A	-4.00	122.42	128.68
4	I	500	NAD	N3A-C2A-N1A	-3.97	122.47	128.68
4	B	500	NAD	C3D-C2D-C1D	3.96	106.94	100.98
4	C	500	NAD	N3A-C2A-N1A	-3.94	122.52	128.68
4	H	500	NAD	C3D-C2D-C1D	3.89	106.84	100.98
4	C	500	NAD	C3D-C2D-C1D	3.87	106.81	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	500	NAD	C3D-C2D-C1D	3.87	106.80	100.98
4	A	502	NAD	N3A-C2A-N1A	-3.82	122.70	128.68
4	L	500	NAD	C3B-C2B-C1B	3.81	106.71	100.98
4	J	500	NAD	C4A-C5A-N7A	-3.77	105.47	109.40
4	E	500	NAD	C4A-C5A-N7A	-3.75	105.49	109.40
4	G	500	NAD	C4A-C5A-N7A	-3.69	105.55	109.40
4	H	500	NAD	C4A-C5A-N7A	-3.66	105.58	109.40
4	L	500	NAD	C4A-C5A-N7A	-3.66	105.58	109.40
4	H	500	NAD	C3B-C2B-C1B	3.65	106.48	100.98
4	F	500	NAD	C4A-C5A-N7A	-3.64	105.60	109.40
4	B	500	NAD	N3A-C2A-N1A	-3.64	123.00	128.68
4	I	500	NAD	PN-O3-PA	-3.63	120.36	132.83
4	K	500	NAD	C4A-C5A-N7A	-3.62	105.63	109.40
4	J	500	NAD	C3B-C2B-C1B	3.59	106.38	100.98
4	I	500	NAD	C3D-C2D-C1D	3.57	106.36	100.98
4	I	500	NAD	C4A-C5A-N7A	-3.53	105.72	109.40
4	D	500	NAD	C4A-C5A-N7A	-3.49	105.76	109.40
4	C	500	NAD	C4A-C5A-N7A	-3.49	105.77	109.40
4	D	500	NAD	PN-O3-PA	-3.30	121.50	132.83
4	C	500	NAD	PN-O3-PA	-3.29	121.52	132.83
4	A	502	NAD	C4A-C5A-N7A	-3.28	105.98	109.40
4	K	500	NAD	PN-O3-PA	-3.27	121.59	132.83
4	F	500	NAD	C3D-C2D-C1D	3.25	105.87	100.98
4	G	500	NAD	C6N-N1N-C2N	-3.24	119.02	121.97
4	B	500	NAD	C4A-C5A-N7A	-3.23	106.03	109.40
4	D	500	NAD	C3B-C2B-C1B	3.21	105.81	100.98
4	A	502	NAD	C3B-C2B-C1B	3.19	105.78	100.98
4	H	500	NAD	PN-O3-PA	-3.17	121.93	132.83
4	J	500	NAD	C3D-C2D-C1D	3.14	105.71	100.98
4	J	500	NAD	PN-O3-PA	-3.14	122.05	132.83
4	E	500	NAD	C2D-C3D-C4D	3.10	108.67	102.64
4	B	500	NAD	C3B-C2B-C1B	3.06	105.58	100.98
4	L	500	NAD	PN-O3-PA	-3.04	122.39	132.83
4	F	500	NAD	PN-O3-PA	-3.03	122.42	132.83
4	E	500	NAD	PN-O3-PA	-3.03	122.43	132.83
4	C	500	NAD	C1B-N9A-C4A	-3.02	121.34	126.64
4	A	502	NAD	C1B-N9A-C4A	-3.01	121.34	126.64
4	E	500	NAD	C1B-N9A-C4A	-3.01	121.36	126.64
4	B	500	NAD	C3N-C7N-N7N	3.00	121.36	117.75
4	B	500	NAD	O7N-C7N-N7N	-2.98	118.35	122.58
4	E	500	NAD	C6N-N1N-C2N	-2.95	119.28	121.97
4	H	500	NAD	C2D-C3D-C4D	2.88	108.24	102.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	500	NAD	C2D-C3D-C4D	2.88	108.24	102.64
4	G	500	NAD	C1B-N9A-C4A	-2.87	121.60	126.64
4	A	502	NAD	PN-O3-PA	-2.87	122.98	132.83
4	G	500	NAD	PN-O3-PA	-2.86	123.02	132.83
4	L	500	NAD	C2D-C3D-C4D	2.81	108.11	102.64
4	G	500	NAD	C2B-C3B-C4B	2.81	108.10	102.64
4	J	500	NAD	C2D-C3D-C4D	2.78	108.05	102.64
4	B	500	NAD	PN-O3-PA	-2.75	123.38	132.83
4	K	500	NAD	C1B-N9A-C4A	-2.73	121.85	126.64
4	K	500	NAD	C2B-C3B-C4B	2.72	107.92	102.64
4	D	500	NAD	C2D-C3D-C4D	2.71	107.90	102.64
4	C	500	NAD	C2B-C3B-C4B	2.70	107.89	102.64
4	B	500	NAD	C1B-N9A-C4A	-2.70	121.90	126.64
4	I	500	NAD	C2D-C3D-C4D	2.64	107.77	102.64
4	K	500	NAD	C2D-C3D-C4D	2.57	107.64	102.64
4	H	500	NAD	C1B-N9A-C4A	-2.57	122.12	126.64
4	F	500	NAD	C2D-C3D-C4D	2.57	107.63	102.64
4	B	500	NAD	C2D-C3D-C4D	2.54	107.59	102.64
4	I	500	NAD	C2B-C3B-C4B	2.53	107.56	102.64
4	D	500	NAD	O7N-C7N-N7N	-2.50	119.03	122.58
4	E	500	NAD	C2B-C3B-C4B	2.45	107.40	102.64
4	A	502	NAD	O7N-C7N-N7N	-2.44	119.11	122.58
4	F	500	NAD	C1B-N9A-C4A	-2.44	122.35	126.64
4	I	500	NAD	C5B-C4B-C3B	-2.41	106.17	115.18
4	A	502	NAD	C2D-C3D-C4D	2.38	107.27	102.64
4	I	500	NAD	C1B-N9A-C4A	-2.36	122.49	126.64
4	J	500	NAD	C1B-N9A-C4A	-2.35	122.51	126.64
4	D	500	NAD	C3N-C7N-N7N	2.33	120.54	117.75
4	D	500	NAD	C1B-N9A-C4A	-2.31	122.58	126.64
4	F	500	NAD	C2B-C3B-C4B	2.25	107.02	102.64
4	A	502	NAD	C6N-N1N-C2N	-2.25	119.92	121.97
4	L	500	NAD	C1B-N9A-C4A	-2.18	122.81	126.64
4	L	500	NAD	C6N-N1N-C2N	-2.17	120.00	121.97
4	K	500	NAD	C6N-N1N-C2N	-2.16	120.01	121.97
4	C	500	NAD	O7N-C7N-N7N	-2.13	119.56	122.58
4	C	500	NAD	C3N-C7N-N7N	2.12	120.30	117.75
4	F	500	NAD	C6N-N1N-C2N	-2.05	120.11	121.97
4	F	500	NAD	C3N-C7N-N7N	2.05	120.21	117.75
4	H	500	NAD	C3N-C7N-N7N	2.04	120.20	117.75
4	H	500	NAD	O7N-C7N-N7N	-2.04	119.68	122.58
4	G	500	NAD	C2N-C3N-C4N	2.03	120.56	118.26
4	I	500	NAD	C6N-N1N-C2N	-2.02	120.13	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	500	NAD	C6N-N1N-C2N	-2.00	120.15	121.97
4	L	500	NAD	C3N-C7N-N7N	2.00	120.15	117.75

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	500	NAD	PA-O3-PN-O5D
4	E	500	NAD	O4D-C1D-N1N-C6N
4	A	502	NAD	C5D-O5D-PN-O1N
4	A	502	NAD	C2N-C3N-C7N-O7N
4	A	502	NAD	C2N-C3N-C7N-N7N
4	L	500	NAD	C5B-O5B-PA-O3
4	L	500	NAD	O4B-C4B-C5B-O5B
4	L	500	NAD	C5D-O5D-PN-O1N
4	I	500	NAD	C5B-O5B-PA-O1A
4	H	500	NAD	C5B-O5B-PA-O1A
4	H	500	NAD	C5B-O5B-PA-O2A
4	H	500	NAD	O4B-C4B-C5B-O5B
4	J	500	NAD	C5B-O5B-PA-O1A
4	J	500	NAD	C5B-O5B-PA-O2A
4	J	500	NAD	O4B-C4B-C5B-O5B
4	G	500	NAD	O4B-C4B-C5B-O5B
4	G	500	NAD	C3B-C4B-C5B-O5B
4	D	500	NAD	C5B-O5B-PA-O1A
4	D	500	NAD	C5B-O5B-PA-O2A
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	F	500	NAD	C3B-C4B-C5B-O5B
4	F	500	NAD	C5D-O5D-PN-O1N
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	B	500	NAD	C5B-O5B-PA-O1A
4	B	500	NAD	C3B-C4B-C5B-O5B
4	B	500	NAD	C5D-O5D-PN-O3
4	D	500	NAD	C4N-C3N-C7N-O7N
4	D	500	NAD	C4N-C3N-C7N-N7N
4	A	502	NAD	O4B-C4B-C5B-O5B
4	A	502	NAD	C3B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	502	NAD	O4D-C4D-C5D-O5D
4	L	500	NAD	C3B-C4B-C5B-O5B
4	I	500	NAD	C3B-C4B-C5B-O5B
4	H	500	NAD	C3B-C4B-C5B-O5B
4	J	500	NAD	C3B-C4B-C5B-O5B
4	D	500	NAD	O4B-C4B-C5B-O5B
4	F	500	NAD	O4B-C4B-C5B-O5B
4	B	500	NAD	O4B-C4B-C5B-O5B
4	A	502	NAD	C4N-C3N-C7N-N7N
4	E	500	NAD	O4D-C4D-C5D-O5D
4	E	500	NAD	C3D-C4D-C5D-O5D
4	A	502	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	D	500	NAD	C3B-C4B-C5B-O5B
4	C	500	NAD	C3B-C4B-C5B-O5B
4	A	502	NAD	C4N-C3N-C7N-O7N
4	I	500	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	I	500	NAD	PA-O3-PN-O5D
4	K	500	NAD	PA-O3-PN-O5D
4	H	500	NAD	PA-O3-PN-O5D
4	J	500	NAD	PA-O3-PN-O5D
4	G	500	NAD	PA-O3-PN-O5D
4	D	500	NAD	PA-O3-PN-O5D
4	C	500	NAD	PA-O3-PN-O5D
4	E	500	NAD	C4D-C5D-O5D-PN
4	I	500	NAD	C4D-C5D-O5D-PN
4	A	502	NAD	C5D-O5D-PN-O3
4	L	500	NAD	C5D-O5D-PN-O3
4	H	500	NAD	C5B-O5B-PA-O3
4	J	500	NAD	C5B-O5B-PA-O3
4	D	500	NAD	C5D-O5D-PN-O3
4	F	500	NAD	C5D-O5D-PN-O3
4	E	500	NAD	C2N-C3N-C7N-N7N
4	A	502	NAD	C5D-O5D-PN-O2N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	L	500	NAD	C5B-O5B-PA-O1A
4	L	500	NAD	C5D-O5D-PN-O2N
4	H	500	NAD	C5D-O5D-PN-O2N
4	D	500	NAD	C5D-O5D-PN-O2N
4	F	500	NAD	C5D-O5D-PN-O2N
4	B	500	NAD	C5D-O5D-PN-O1N
4	B	500	NAD	C5D-O5D-PN-O2N
4	H	500	NAD	C4D-C5D-O5D-PN
4	L	500	NAD	C4D-C5D-O5D-PN
4	K	500	NAD	C3D-C4D-C5D-O5D
4	I	500	NAD	C5B-O5B-PA-O3
4	H	500	NAD	C5D-O5D-PN-O3
4	D	500	NAD	C5B-O5B-PA-O3
4	F	500	NAD	C5B-O5B-PA-O3
4	B	500	NAD	C5B-O5B-PA-O3
4	B	500	NAD	PN-O3-PA-O2A

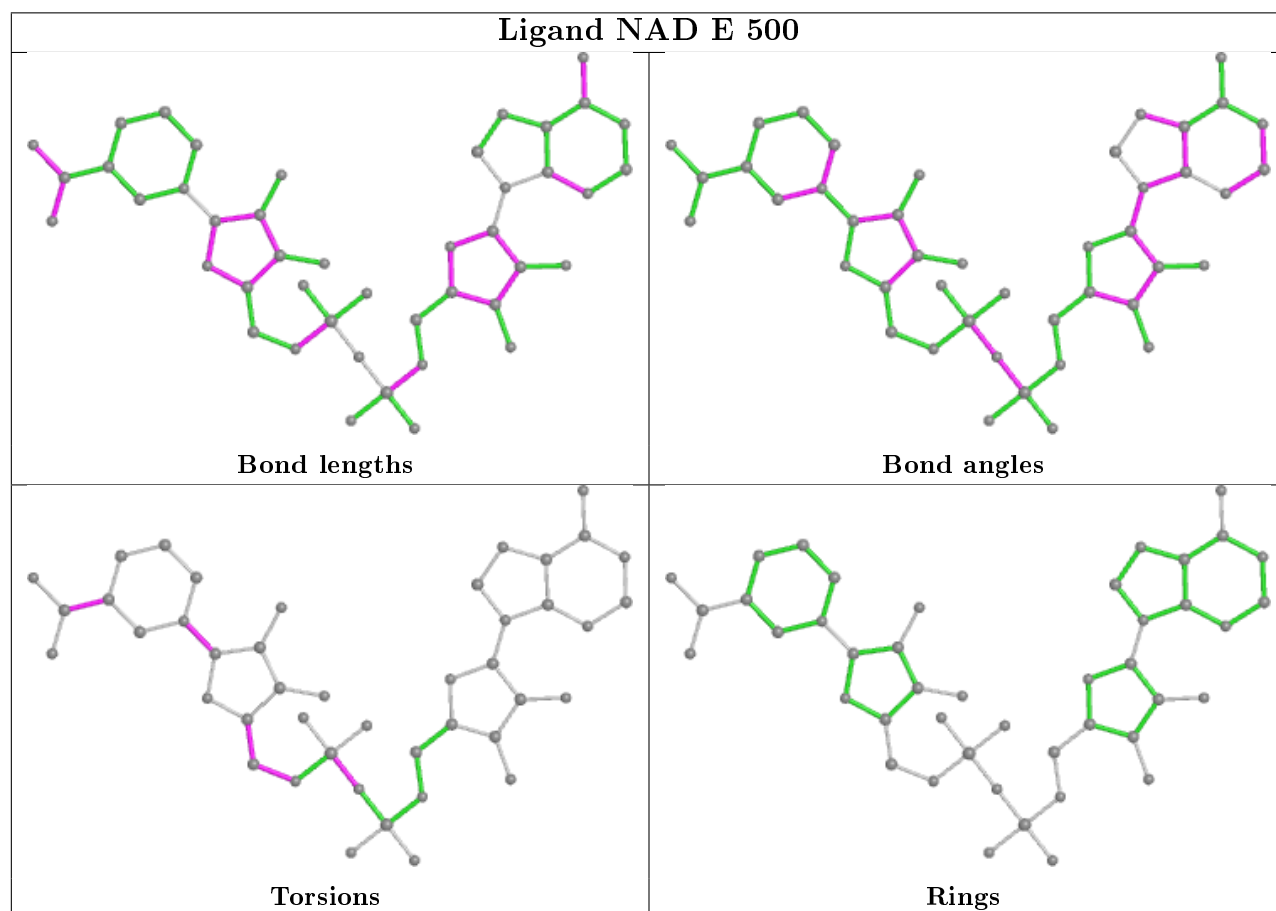
There are no ring outliers.

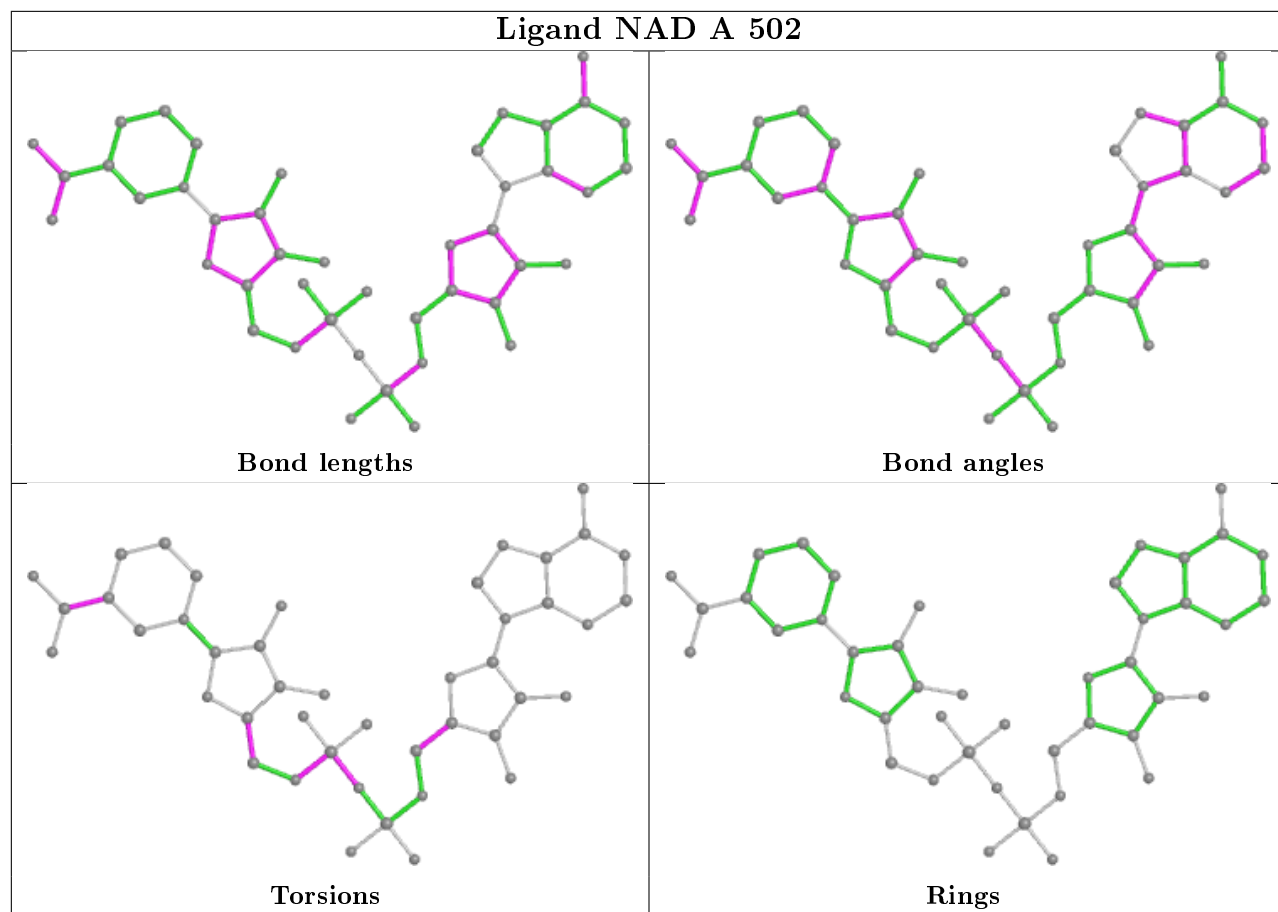
10 monomers are involved in 22 short contacts:

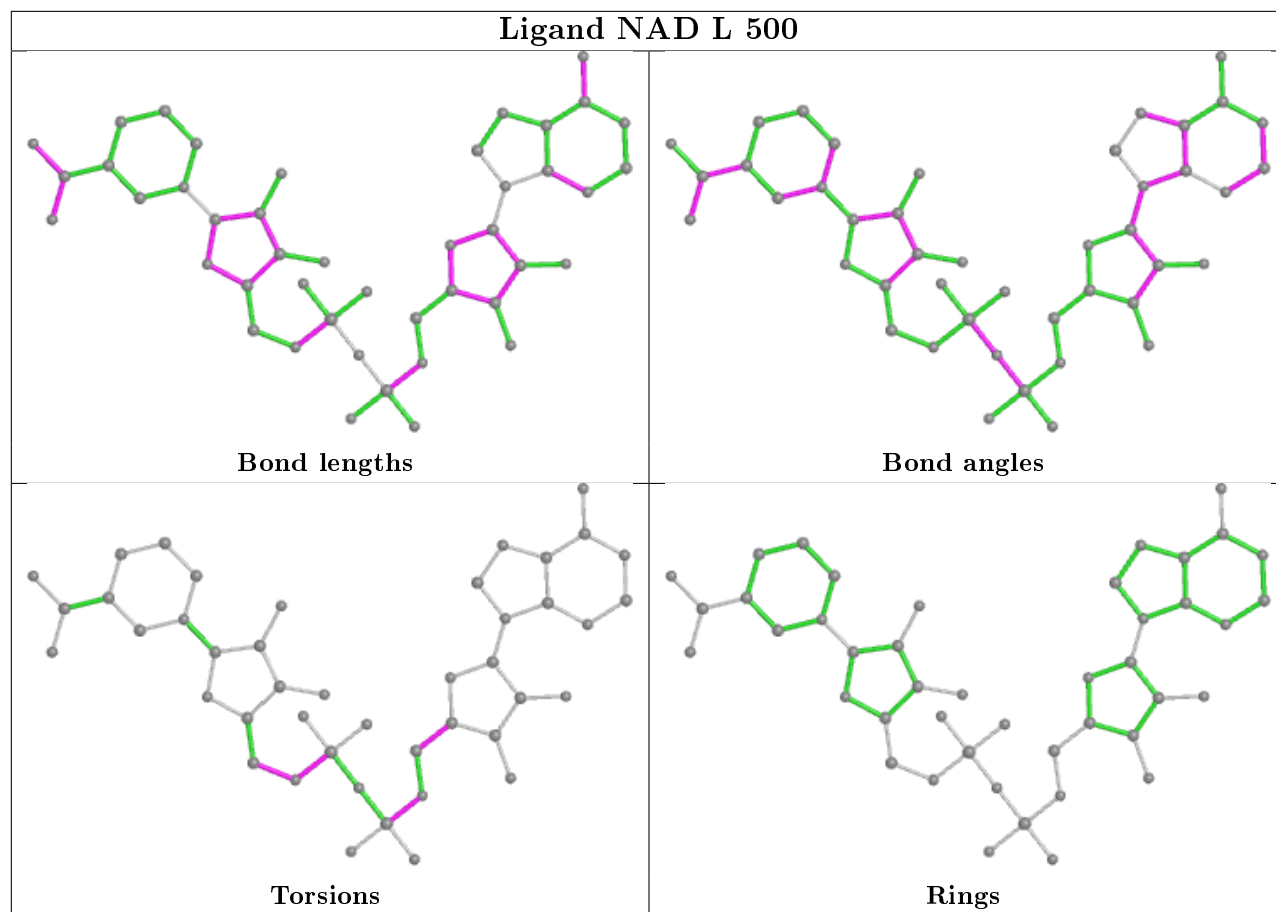
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	500	NAD	2	0
4	A	502	NAD	1	0
4	L	500	NAD	1	0
4	I	500	NAD	2	0
4	K	500	NAD	3	0
4	H	500	NAD	3	0
4	G	500	NAD	2	0
4	D	500	NAD	3	0
4	C	500	NAD	4	0
4	B	500	NAD	3	0

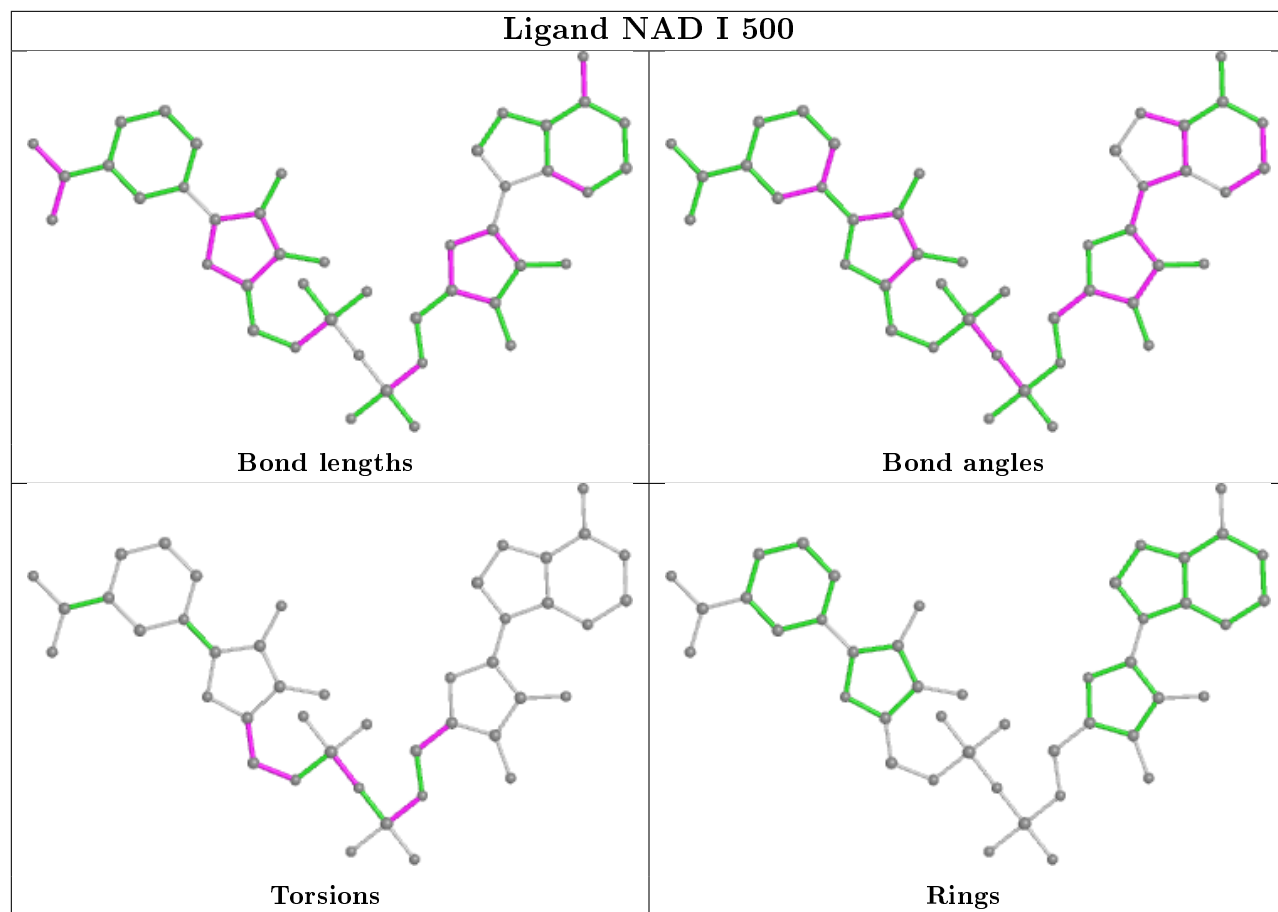
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

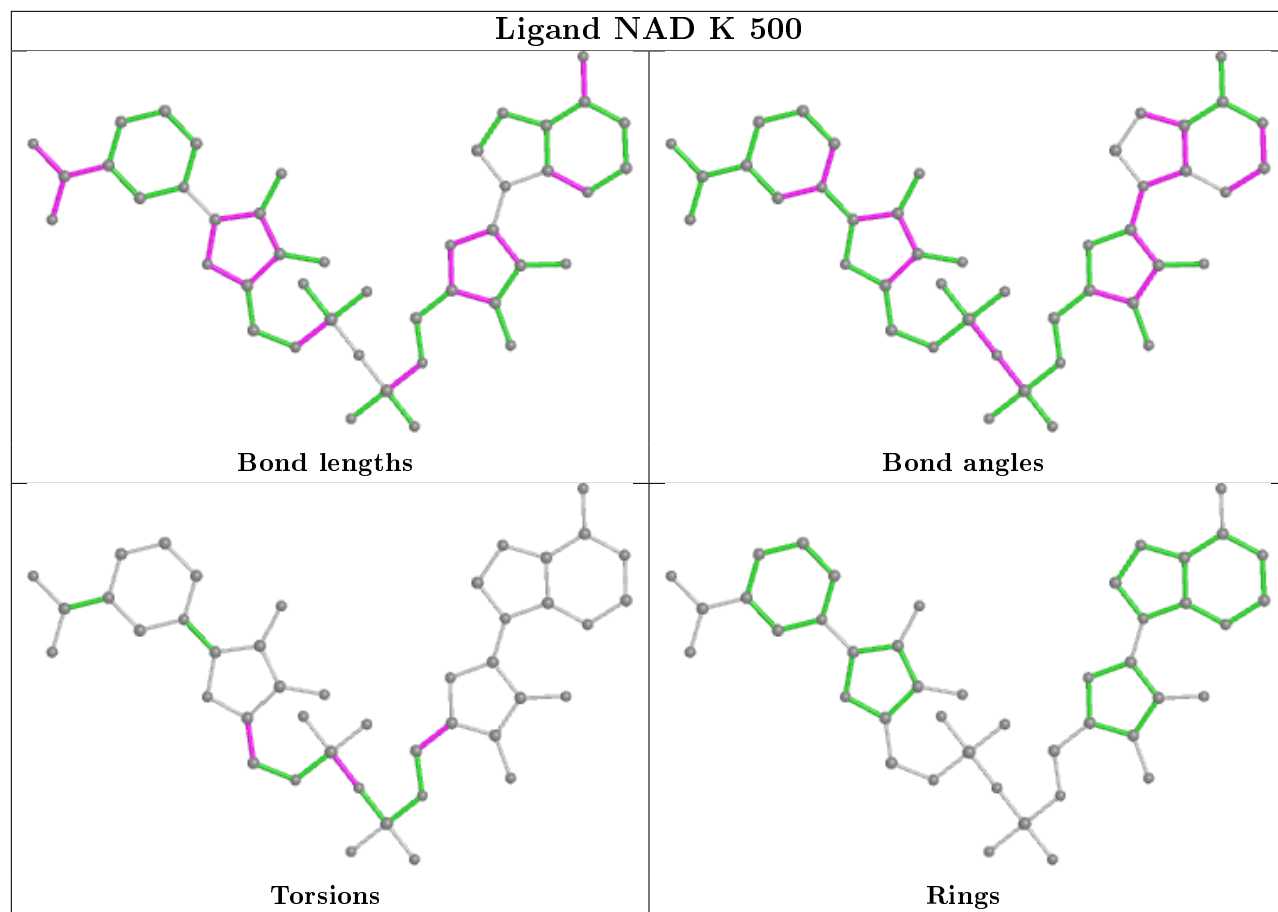
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

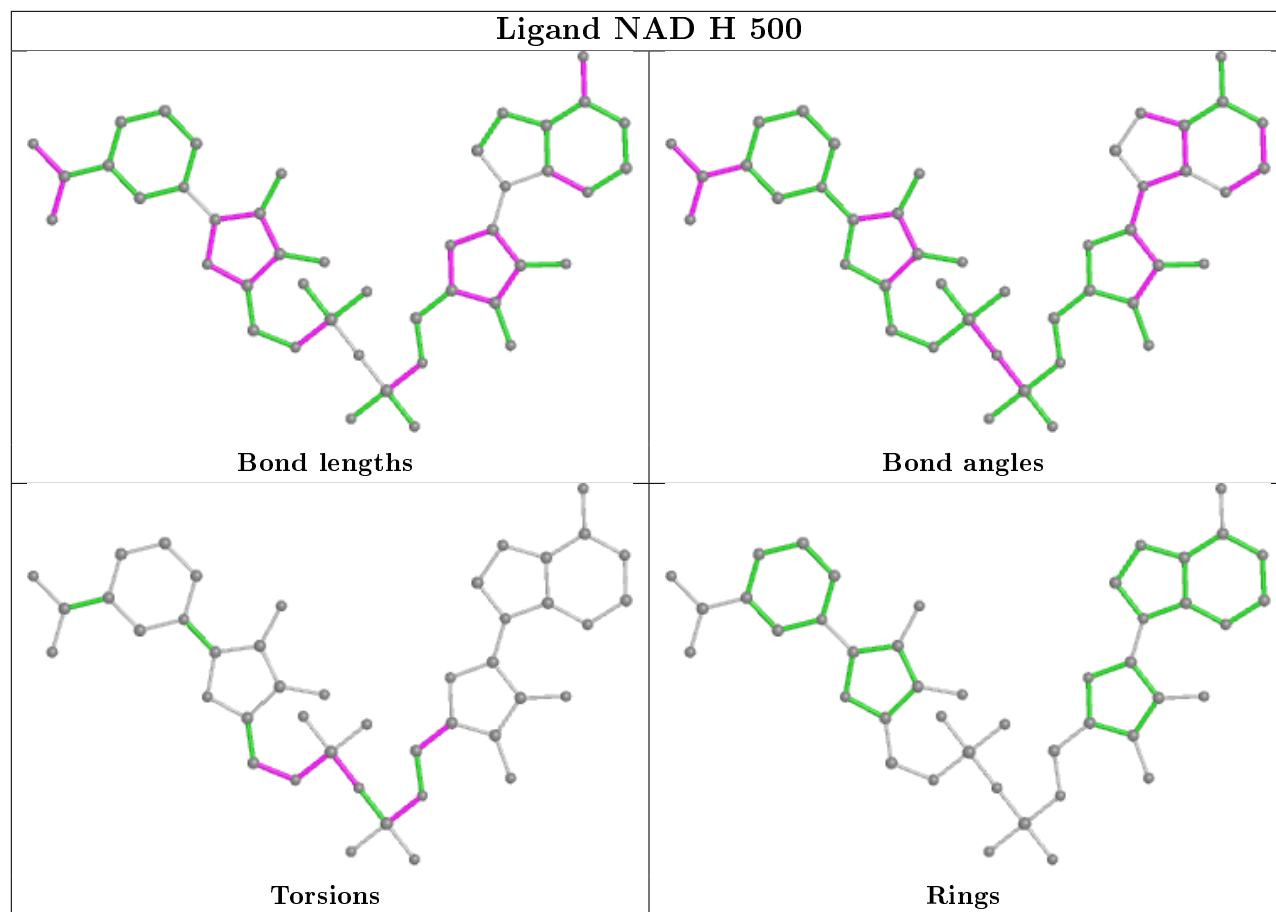


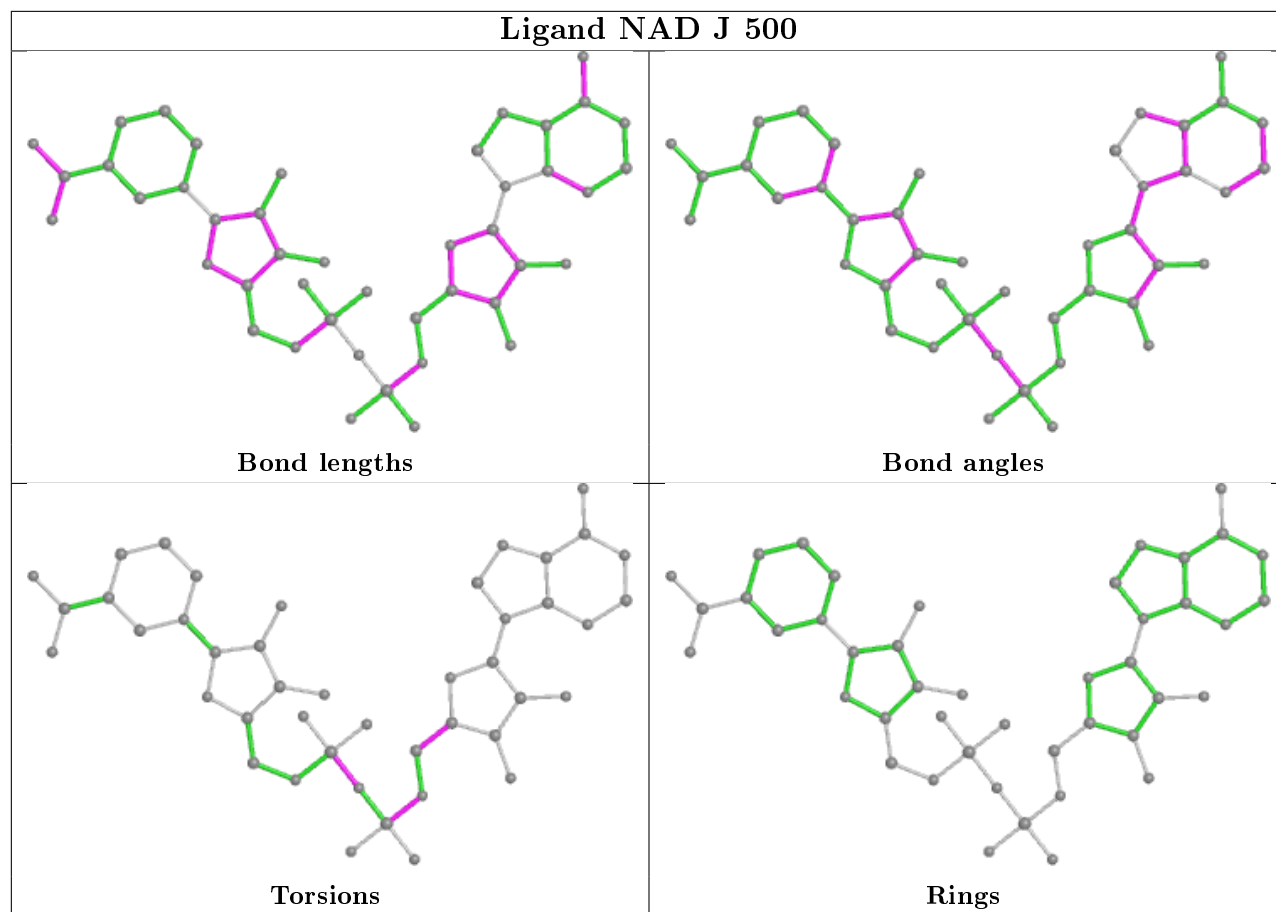


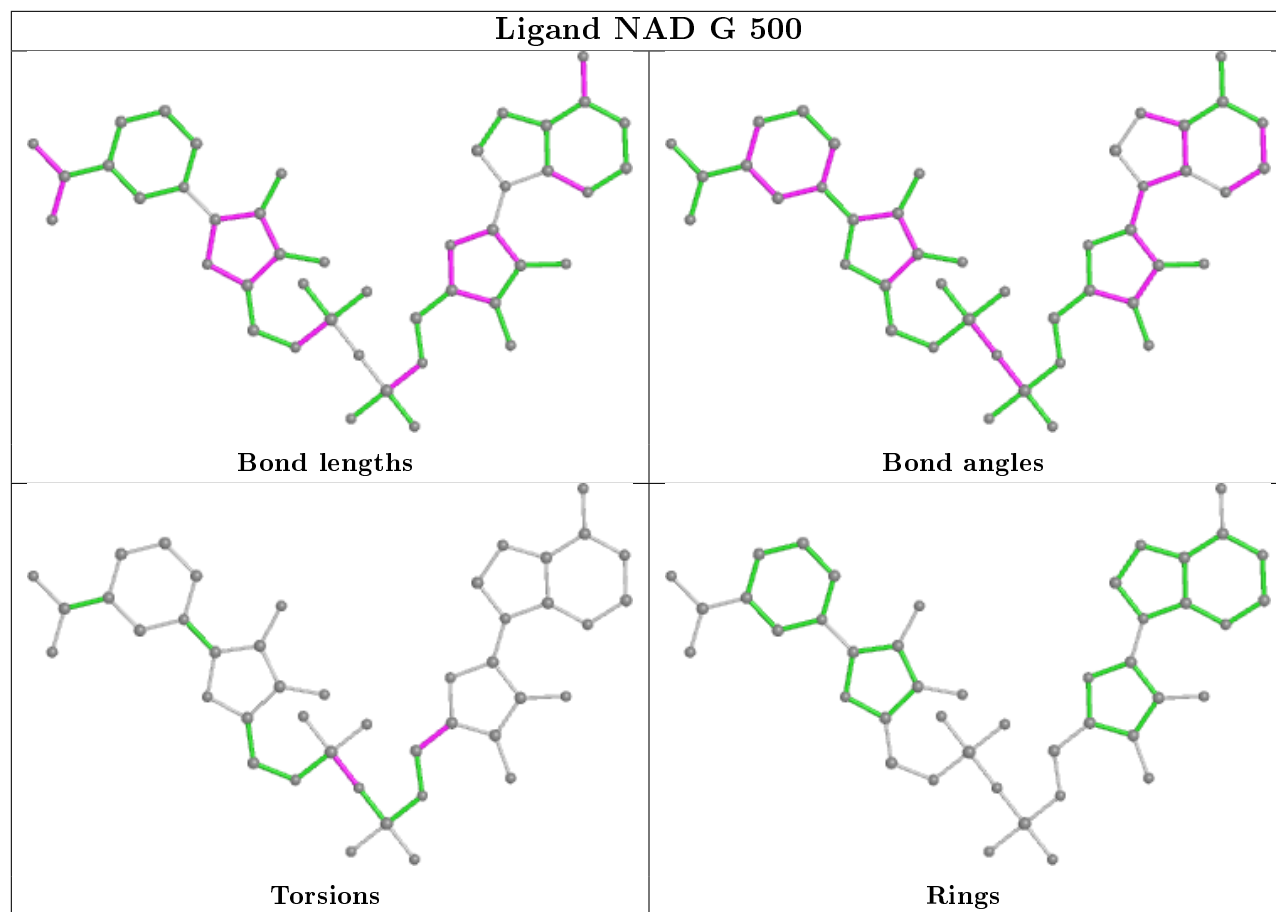


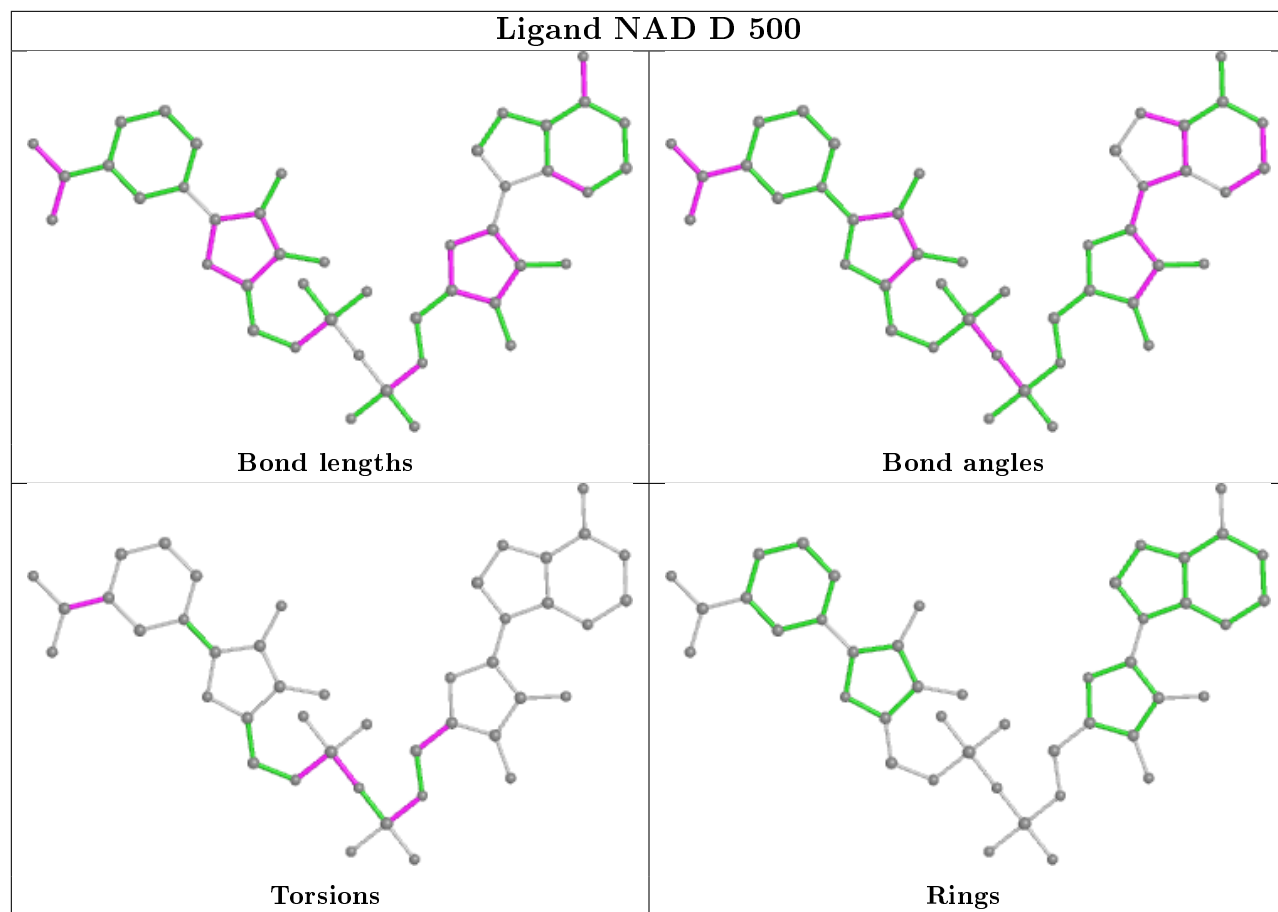


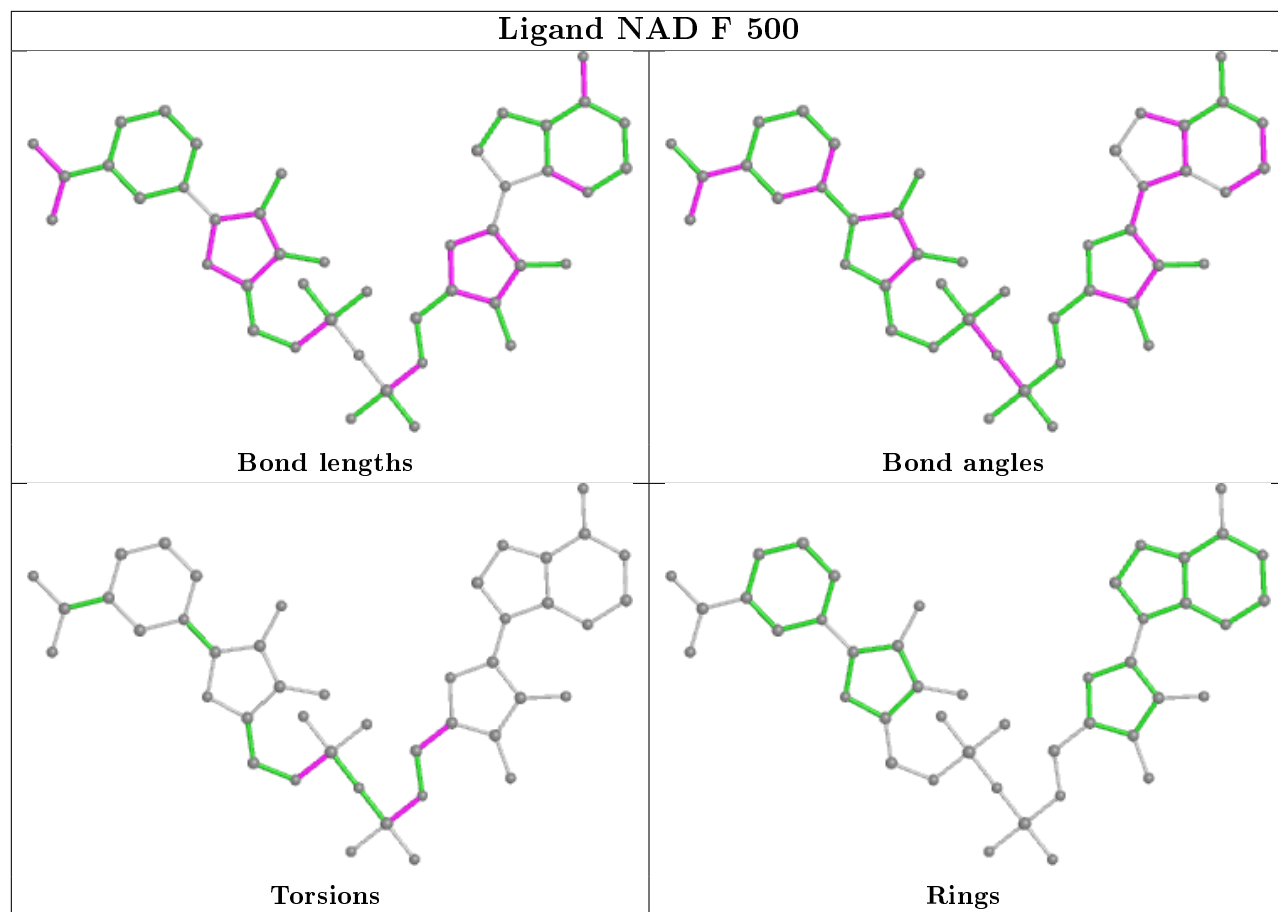


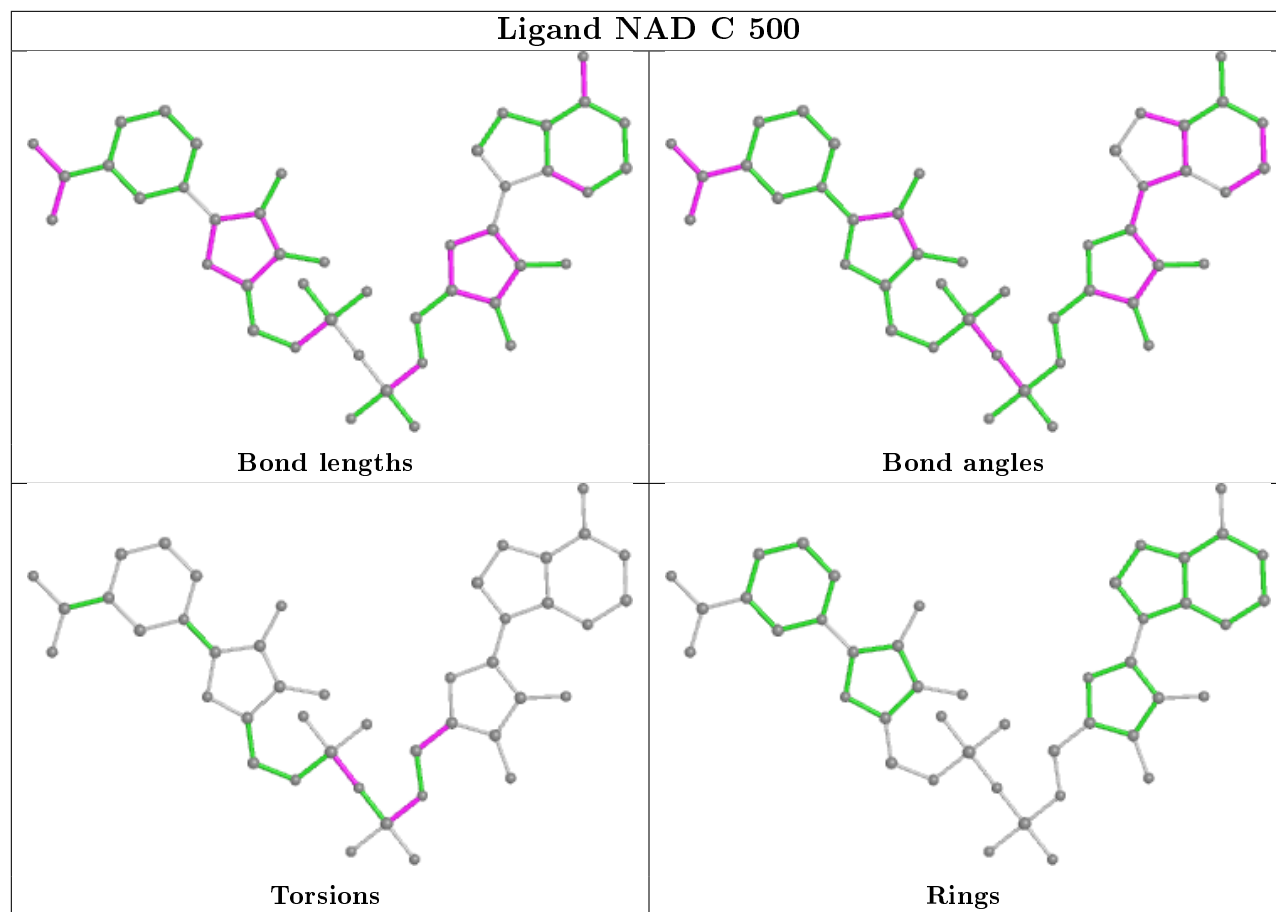


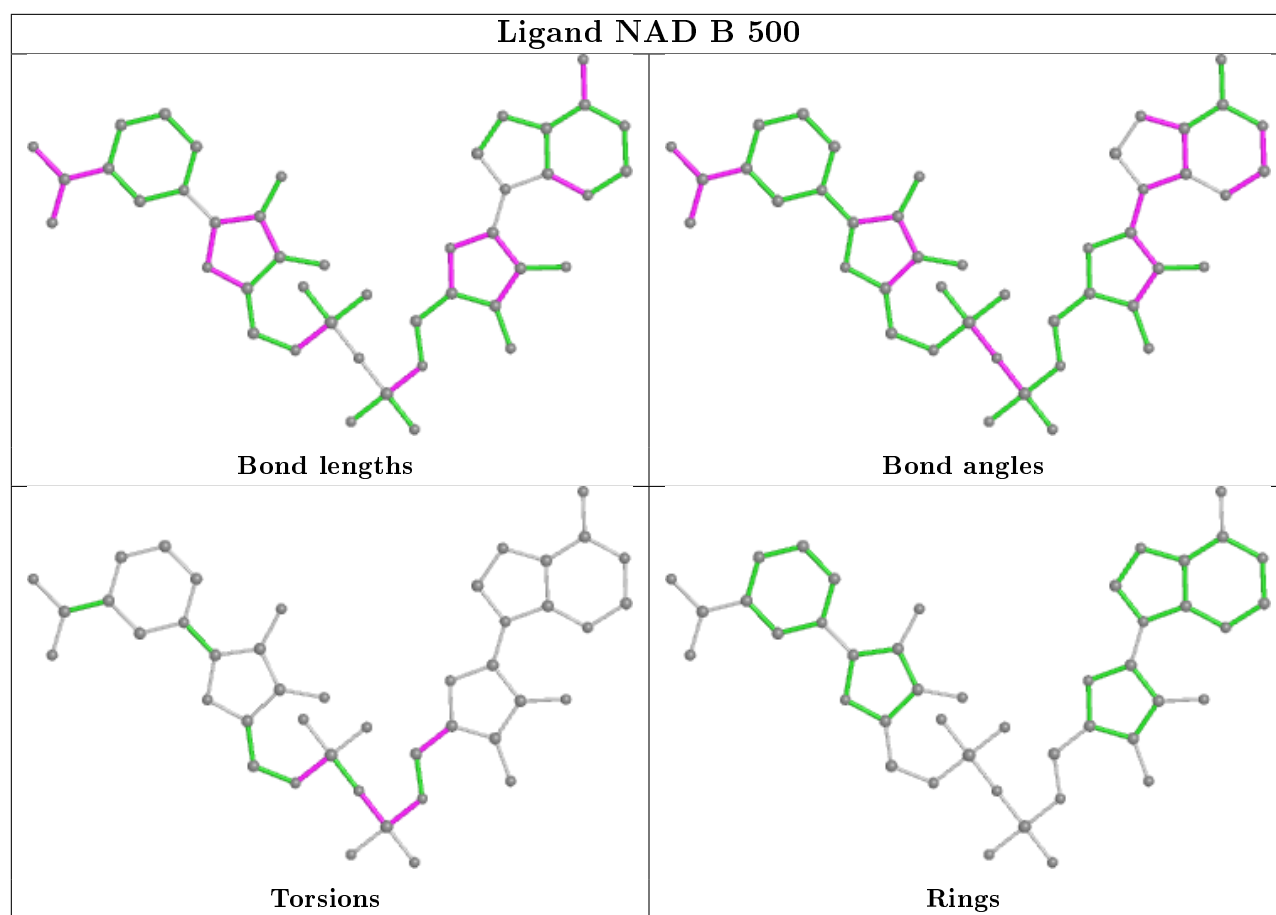












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.21	0 100 100	29, 50, 74, 87	0
1	C	369/461 (80%)	-0.18	2 (0%) 91 88	30, 50, 74, 91	0
1	E	370/461 (80%)	0.05	7 (1%) 66 61	37, 64, 88, 113	0
1	G	367/461 (79%)	-0.05	1 (0%) 94 91	36, 55, 78, 92	0
1	I	364/461 (78%)	-0.12	4 (1%) 80 75	39, 60, 82, 95	0
1	K	381/461 (82%)	-0.20	5 (1%) 77 71	35, 55, 83, 99	0
2	B	318/342 (92%)	-0.23	6 (1%) 66 61	33, 48, 71, 111	0
2	D	320/342 (93%)	-0.18	4 (1%) 77 71	34, 48, 76, 127	0
2	F	321/342 (93%)	0.06	6 (1%) 66 61	38, 60, 81, 102	0
2	H	317/342 (92%)	-0.07	1 (0%) 94 91	37, 60, 89, 113	0
2	J	316/342 (92%)	0.01	10 (3%) 47 42	31, 57, 82, 101	0
2	L	317/342 (92%)	-0.22	2 (0%) 89 86	35, 51, 78, 107	0
All	All	4144/4818 (86%)	-0.11	48 (1%) 79 73	29, 55, 82, 127	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	290	VAL	3.2
2	L	59	ASN	3.2
1	K	86	PRO	3.1
2	J	227	ARG	3.0
2	J	228	LYS	3.0
1	G	240	ARG	2.8
2	F	21	ASN	2.7
1	I	290	VAL	2.7
2	B	61	MET	2.7
2	J	21	ASN	2.6
2	B	251	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	291	THR	2.6
2	J	59	ASN	2.5
2	J	226	SER	2.5
1	I	289	GLU	2.5
1	I	259	CYS	2.5
2	F	226	SER	2.4
2	L	58	ASP	2.4
1	K	73	SER	2.4
2	J	8	SER	2.4
2	B	59	ASN	2.4
2	F	230	LEU	2.3
1	E	363	ARG	2.3
1	E	289	GLU	2.3
2	H	247	LYS	2.3
1	K	122	ASN	2.3
2	D	12	GLY	2.3
2	F	59	ASN	2.3
2	D	250	ASN	2.3
2	F	127	ASN	2.3
1	E	256	TYR	2.3
2	J	225	TYR	2.2
2	D	61	MET	2.2
2	B	60	GLY	2.2
1	K	123	GLY	2.2
2	D	249	THR	2.2
1	E	255	TYR	2.1
1	I	121	PRO	2.1
1	K	124	VAL	2.1
2	J	219	MET	2.1
2	B	58	ASP	2.1
2	F	329	SER	2.1
2	J	158	HIS	2.1
1	E	293	GLU	2.1
1	C	69	SER	2.1
2	B	90	ASN	2.0
1	C	245	ASN	2.0
2	J	218	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

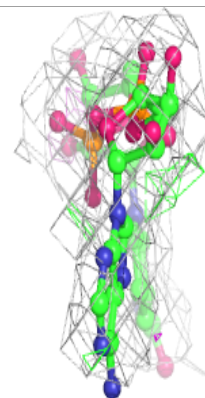
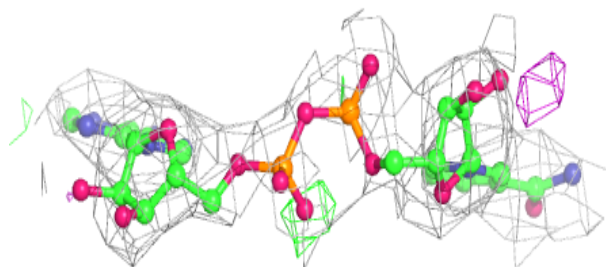
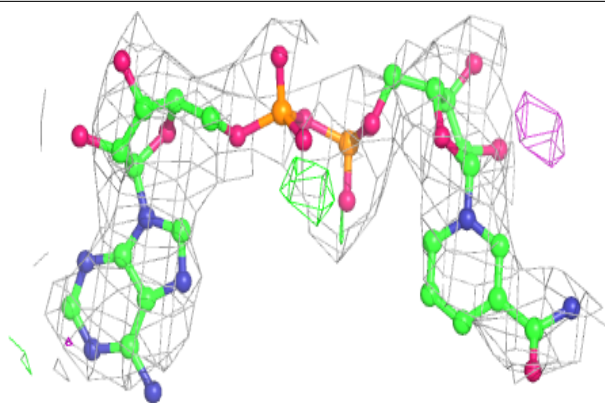
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.80	0.72	27,27,27,27	0
4	NAD	I	500	44/44	0.93	0.24	35,47,54,68	0
4	NAD	K	500	44/44	0.93	0.22	34,48,54,59	0
4	NAD	H	500	44/44	0.93	0.30	34,47,58,62	0
4	NAD	J	500	44/44	0.93	0.23	32,48,63,71	0
4	NAD	D	500	44/44	0.93	0.24	38,47,53,56	0
4	NAD	C	500	44/44	0.93	0.25	33,42,48,50	0
4	NAD	G	500	44/44	0.94	0.27	40,47,57,63	0
4	NAD	E	500	44/44	0.94	0.31	43,54,66,75	0
4	NAD	F	500	44/44	0.94	0.27	34,49,62,72	0
4	NAD	A	502	44/44	0.94	0.25	31,42,49,63	0
4	NAD	B	500	44/44	0.94	0.26	32,39,50,52	0
4	NAD	L	500	44/44	0.95	0.23	32,41,47,49	0

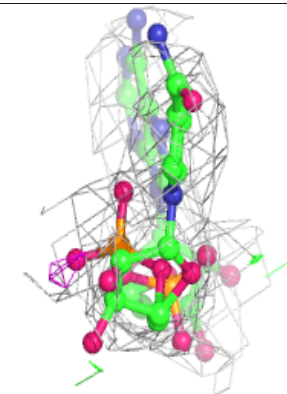
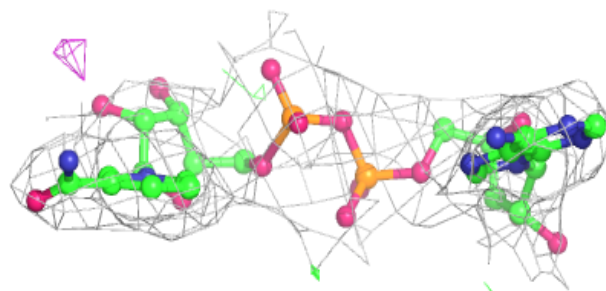
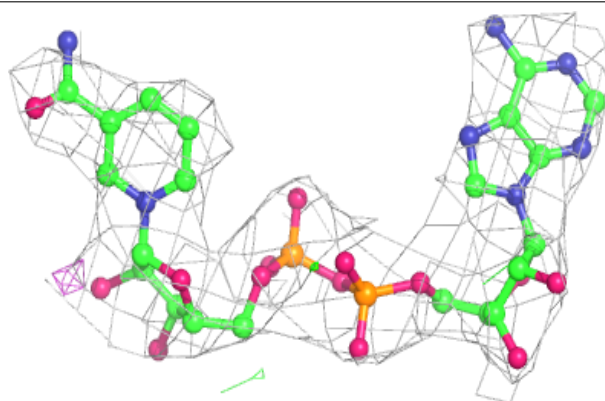
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

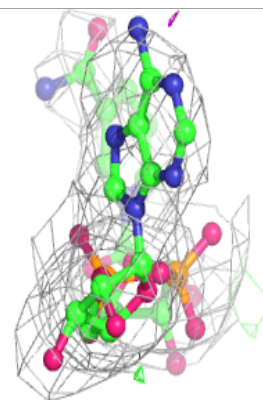
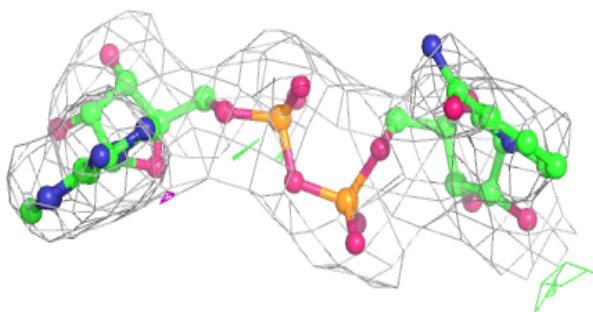
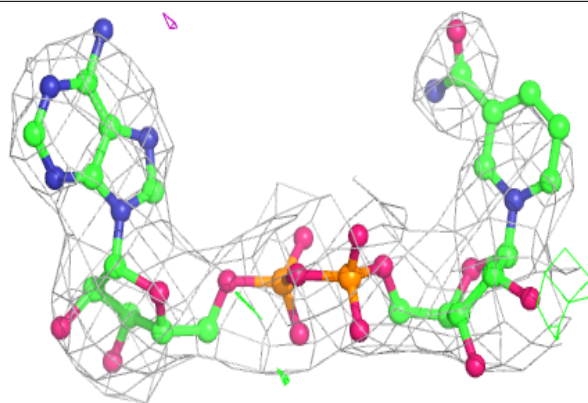
**Electron density around NAD K 500:**

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

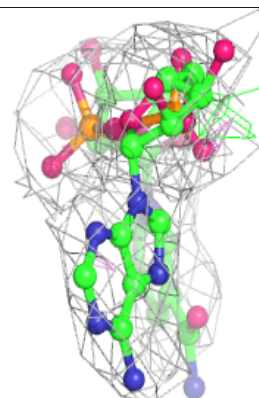
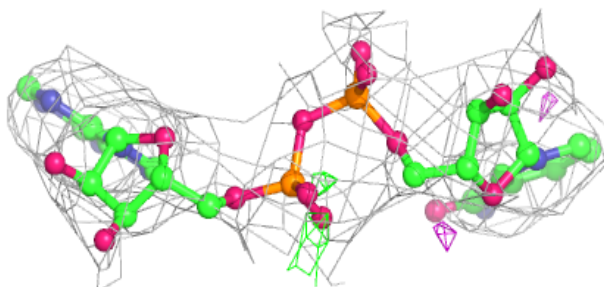
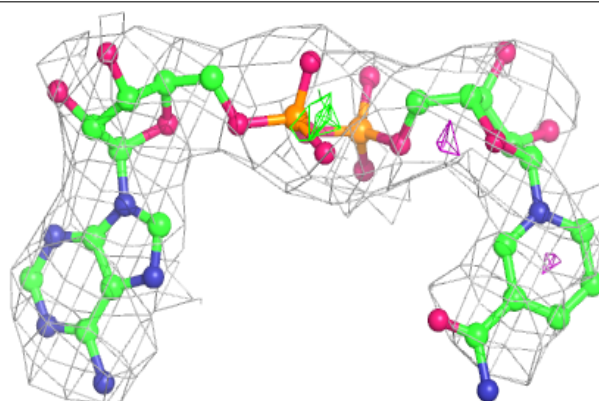


Electron density around NAD H 500:

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

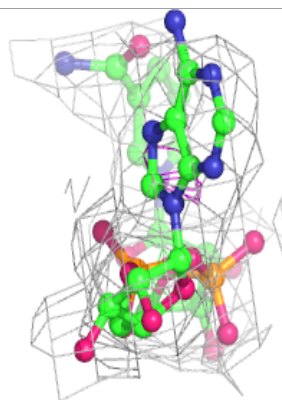
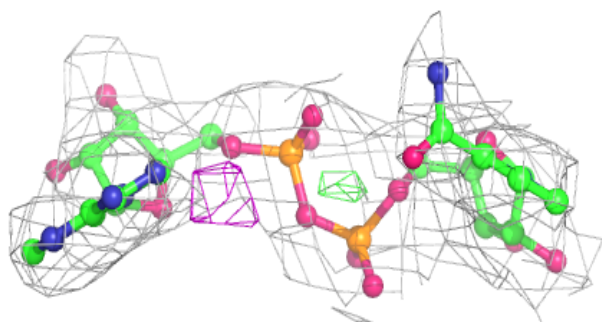
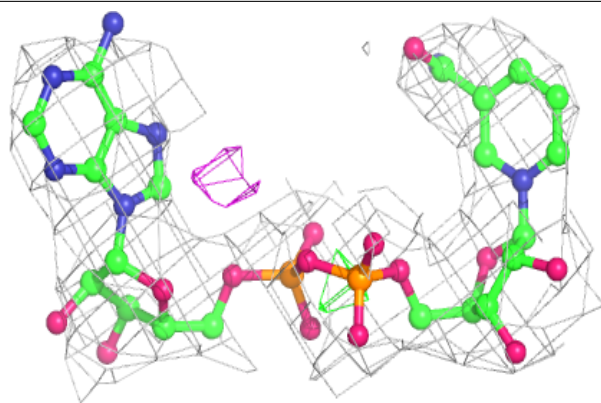
**Electron density around NAD J 500:**

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

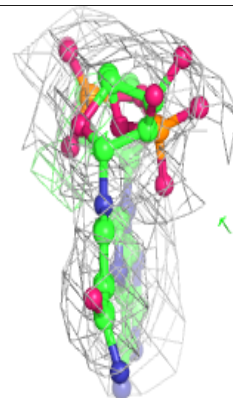
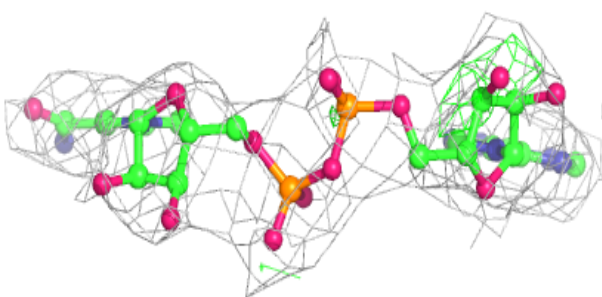
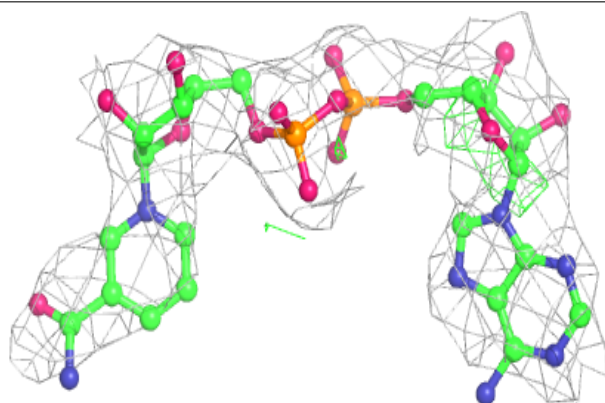


Electron density around NAD D 500:

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

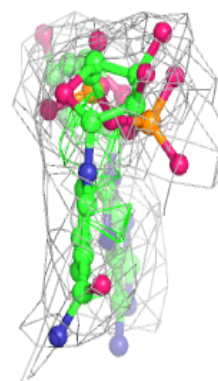
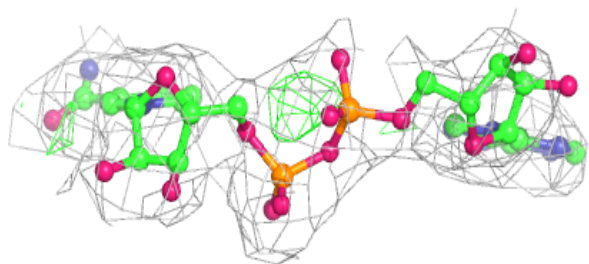
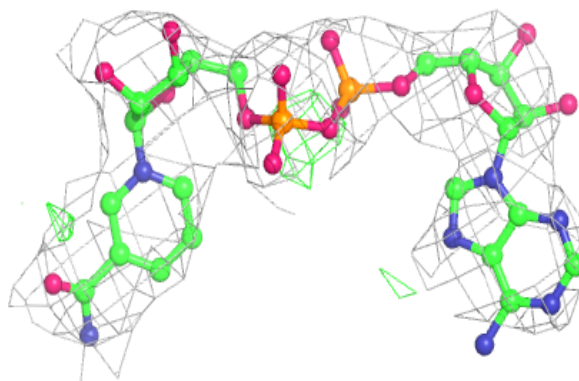
**Electron density around NAD C 500:**

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

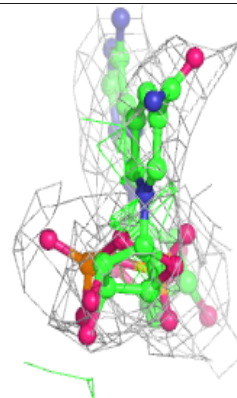
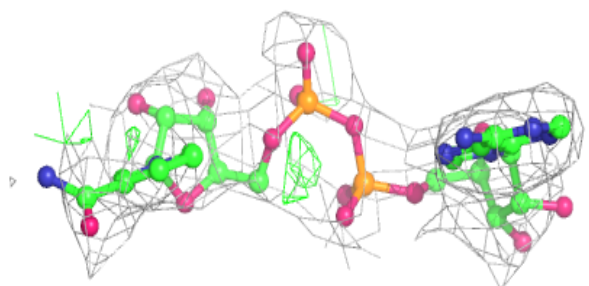
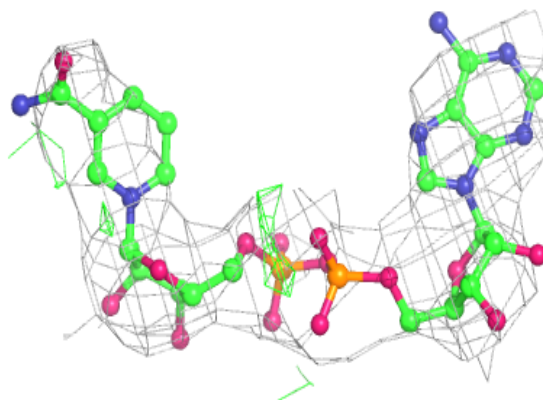


Electron density around NAD G 500:

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

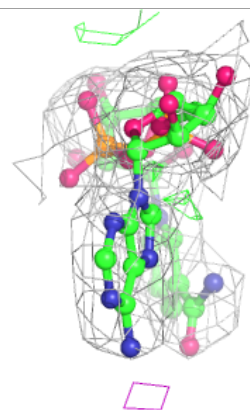
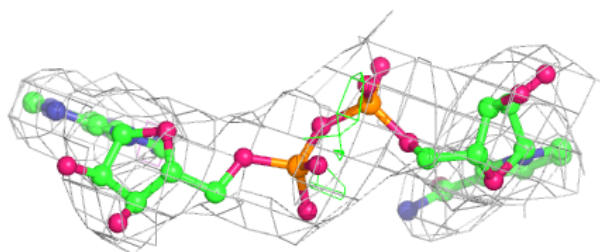
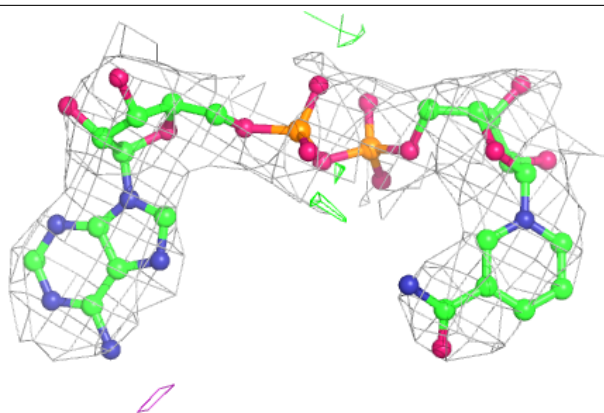
**Electron density around NAD E 500:**

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

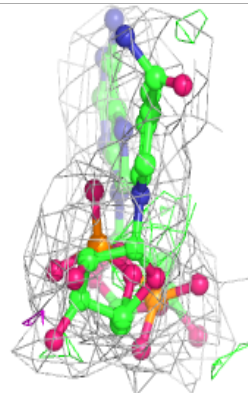
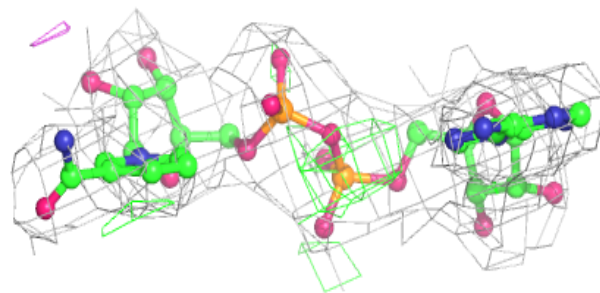
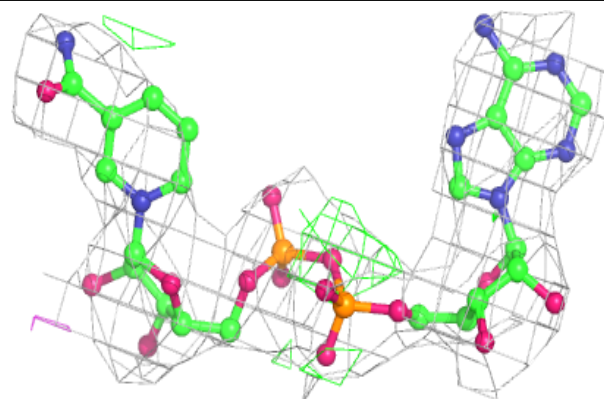


Electron density around NAD F 500:

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

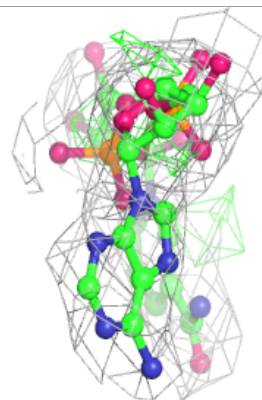
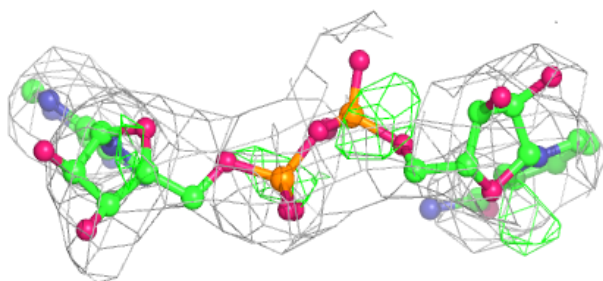
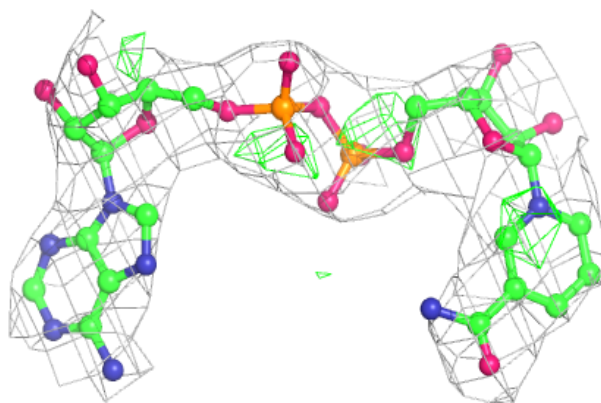
**Electron density around NAD A 502:**

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

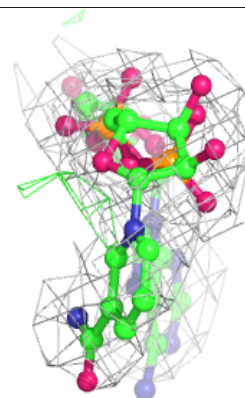
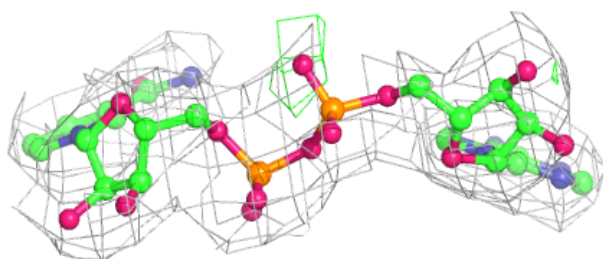
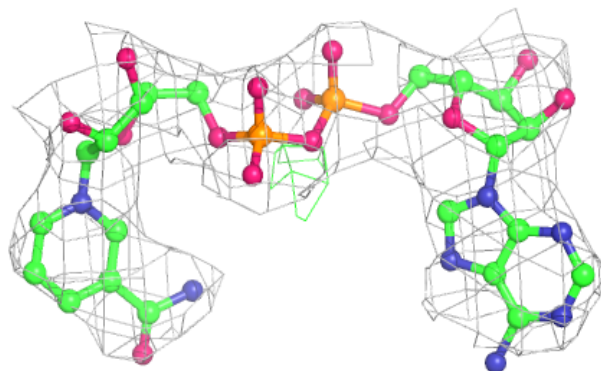


Electron density around NAD B 500:

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

**Electron density around NAD 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.