



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:50 AM UTC

PDB ID : 2CNB / pdb_00002cnb
Title : Trypanosoma brucei UDP-galactose-4-epimerase in ternary complex with NAD and the substrate analogue UDP-4-deoxy-4-fluoro-alpha-D-galactose
Authors : Alpey, M.S.; Ferguson, M.A.J.; Hunter, W.N.
Deposited on : 2006-05-18
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

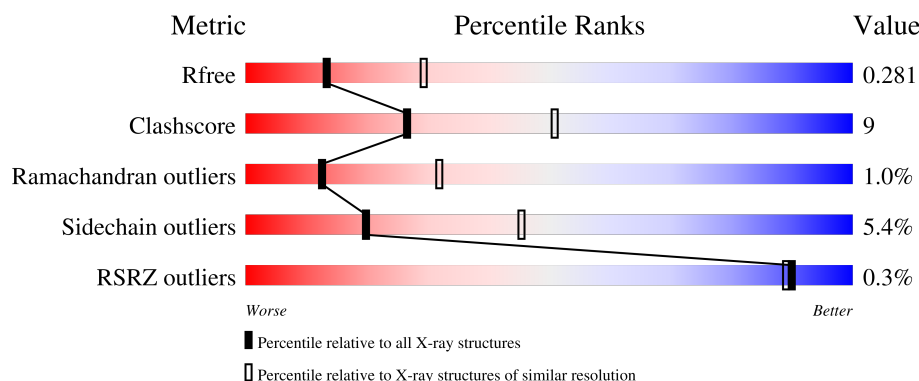
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	397	
1	B	397	
1	C	397	
1	D	397	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UFG	A	1382	X	-	-	-
2	UFG	B	1382	X	-	-	-
2	UFG	C	1382	X	-	-	-
2	UFG	D	1382	X	-	-	-

2 Entry composition [i](#)

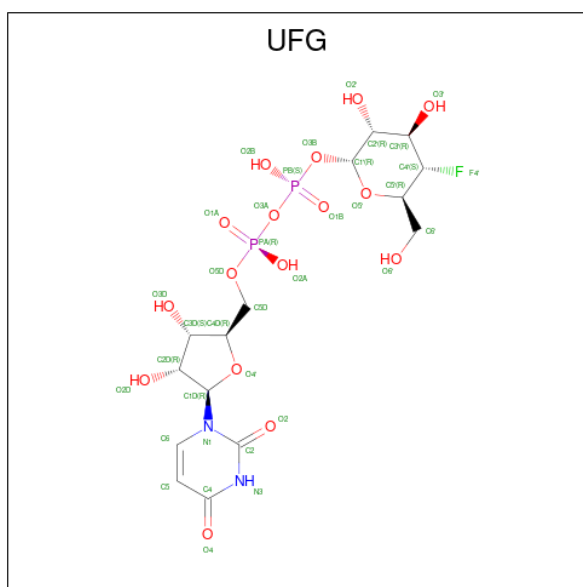
There are 4 unique types of molecules in this entry. The entry contains 12168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-GALACTOSE-4-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	3	0
			2863	1803	508	535	17			
1	B	363	Total	C	N	O	S	0	4	0
			2855	1800	512	527	16			
1	C	366	Total	C	N	O	S	0	3	0
			2863	1803	510	533	17			
1	D	364	Total	C	N	O	S	0	4	0
			2851	1796	506	533	16			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-4-DEOXY-4-FLUORO-ALPHA-D-GALACTOSE (CCD ID: UFG) (formula: C₁₅H₂₃FN₂O₁₆P₂).



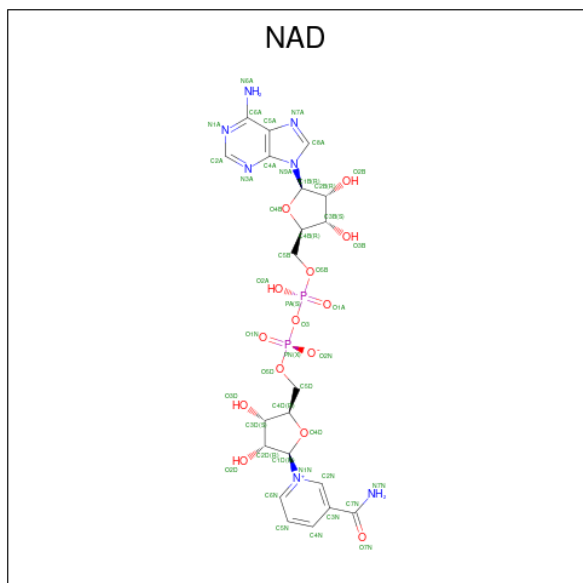
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0
			36	15	1	2	16	2	
2	B	1	Total	C	F	N	O	P	0
			36	15	1	2	16	2	

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		
2	D	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	101	Total	O	0	0
			101	101		
4	C	118	Total	O	0	0
			118	118		

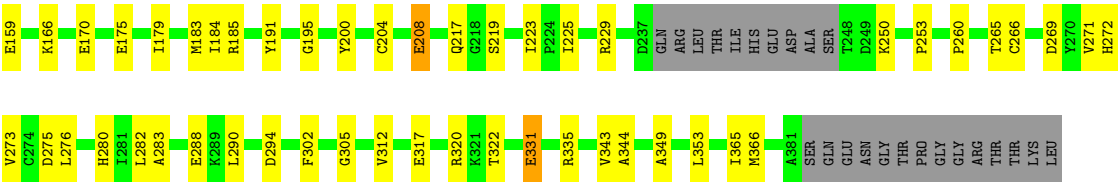
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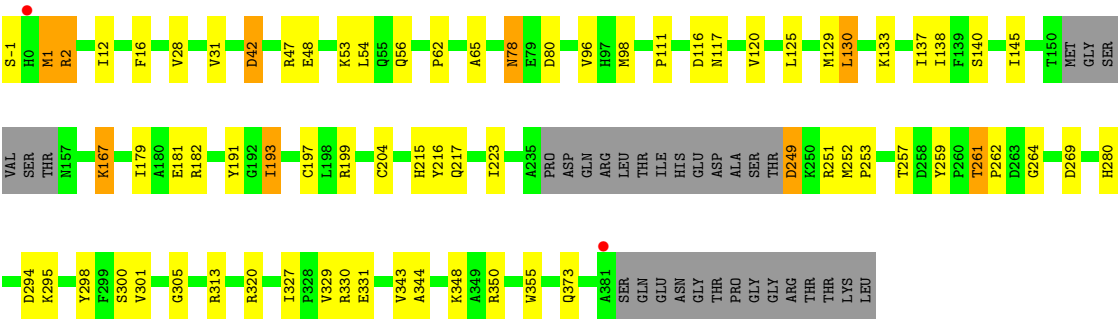
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	94	Total	O	0	0
			94	94		

● Molecule 1: UDP-GALACTOSE-4-EPIMERASE





• Molecule 1: UDP-GALACTOSE-4-EPIMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.72Å 111.69Å 160.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.67 – 2.70 91.67 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.3 (91.67-2.70) 95.3 (91.67-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.199 , 0.281 0.203 , 0.281	Depositor DCC
R_{free} test set	2462 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12168	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.5215e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: UFG, 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	0.73	0/2937	1.01	7/3978 (0.2%)
1	B	0.72	0/2929	0.99	5/3964 (0.1%)
1	C	0.74	0/2937	1.00	2/3978 (0.1%)
1	D	0.68	0/2926	0.96	4/3962 (0.1%)
All	All	0.72	0/11729	0.99	18/15882 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ARG	N-CA-C	8.49	121.38	111.02
1	A	47	ARG	CA-C-N	7.14	134.56	121.70
1	A	47	ARG	C-N-CA	7.14	134.56	121.70
1	D	28	VAL	N-CA-C	6.20	116.81	107.75
1	A	233	ASP	N-CA-C	-5.85	105.04	111.82
1	B	161	ILE	N-CA-C	5.83	116.97	108.58
1	D	261	THR	CA-C-N	-5.69	112.83	119.32
1	D	261	THR	C-N-CA	-5.69	112.83	119.32
1	A	235	ALA	CA-C-N	5.44	126.64	119.84
1	A	235	ALA	C-N-CA	5.44	126.64	119.84
1	B	28	VAL	N-CA-C	5.32	115.70	107.78
1	C	73	VAL	N-CA-C	5.31	114.95	106.88
1	A	344	ALA	N-CA-C	5.24	118.10	109.76
1	B	296	SER	N-CA-C	5.18	121.84	110.80
1	D	137	ILE	N-CA-C	5.07	115.41	108.12
1	B	325	HIS	CA-C-N	5.02	124.63	119.56
1	B	325	HIS	C-N-CA	5.02	124.63	119.56
1	C	5	VAL	N-CA-C	5.02	113.98	106.85

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	2863	0	2815	58	0
1	B	2855	0	2821	58	0
1	C	2863	0	2821	50	0
1	D	2851	0	2808	48	0
2	A	36	0	21	4	0
2	B	36	0	21	2	0
2	C	36	0	21	5	0
2	D	36	0	21	2	0
3	A	44	0	26	2	0
3	B	44	0	26	2	0
3	C	44	0	26	1	0
3	D	44	0	26	2	0
4	A	103	0	0	6	0
4	B	101	0	0	10	0
4	C	118	0	0	8	0
4	D	94	0	0	5	0
All	All	12168	0	11453	216	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 9.

All (216) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:PRO:HD2	1:B:65:ALA:HB2	1.44	0.98
1:C:159:GLU:HA	4:C:2048:HOH:O	1.67	0.94
2:D:1382:UFG:H4'	3:D:1383:NAD:C4N	2.00	0.92
1:B:308:ARG:HD2	4:B:2073:HOH:O	1.68	0.91
1:D:78:ASN:HD22	1:D:78:ASN:C	1.77	0.91
1:B:56[A]:GLN:HG3	4:B:2016:HOH:O	1.76	0.84
1:C:271:VAL:HG22	4:C:2087:HOH:O	1.77	0.84
1:B:295:LYS:O	1:B:297:LYS:N	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HD11	1:A:31:VAL:HG12	1.64	0.79
1:C:204[B]:CYS:SG	1:C:365:ILE:HG21	2.23	0.78
1:C:204[A]:CYS:SG	1:C:223:ILE:HD12	2.24	0.78
1:A:46:THR:OG1	1:A:49:ASN:HB2	1.84	0.78
1:A:306:THR:O	1:A:307:SER:HB2	1.84	0.75
1:D:116:ASP:O	1:D:120:VAL:HB	1.88	0.73
2:A:1382:UFG:H4'	3:A:1383:NAD:C4N	2.18	0.73
1:A:47:ARG:CA	1:A:48:GLU:HB2	2.19	0.72
1:B:78:ASN:C	1:B:78:ASN:HD22	1.97	0.72
2:B:1382:UFG:H4'	3:B:1383:NAD:C4N	2.19	0.71
1:C:335:ARG:HH22	2:C:1382:UFG:C2D	2.03	0.71
1:A:72:GLU:OE1	1:A:88:ARG:NH2	2.23	0.71
1:A:202:ASN:OD1	1:A:268:ARG:HB3	1.91	0.70
1:B:86:PHE:HB3	1:B:132:HIS:ND1	2.07	0.70
1:A:263:ASP:OD1	1:A:265:THR:OG1	2.12	0.68
1:B:53:LYS:O	1:B:57:SER:HB2	1.94	0.68
1:D:78:ASN:C	1:D:78:ASN:ND2	2.51	0.68
1:A:78:ASN:HD22	1:A:78:ASN:C	2.04	0.65
1:B:1:MET:HG3	1:B:93:ASP:HB2	1.79	0.65
1:D:295:LYS:HA	1:D:298:TYR:CD1	2.32	0.64
1:A:47:ARG:HB3	1:A:48:GLU:HB2	1.78	0.63
1:A:172:PRO:HD3	4:A:2050:HOH:O	1.98	0.63
1:D:305:GLY:HA3	1:D:344:ALA:HB3	1.80	0.63
1:B:313:ARG:HH11	1:B:313:ARG:HG3	1.63	0.62
2:D:1382:UFG:H4'	3:D:1383:NAD:H4N	1.79	0.62
1:B:196:ILE:HD11	1:B:286:TYR:HD2	1.64	0.62
1:A:47:ARG:CB	1:A:48:GLU:HB2	2.30	0.61
1:A:204[B]:CYS:SG	1:A:270:TYR:HB3	2.41	0.60
1:B:197:CYS:HB2	1:B:301:VAL:HG12	1.83	0.60
1:B:249:ASP:HB3	1:B:251:ARG:HB2	1.84	0.60
1:B:48:GLU:O	1:B:52[B]:ARG:HD2	2.02	0.60
1:A:4:LEU:HD11	1:A:31:VAL:CG1	2.32	0.60
1:B:119:VAL:HG13	1:B:179:ILE:HD11	1.84	0.59
1:B:175:GLU:O	1:B:179:ILE:HG23	2.02	0.59
1:D:96:VAL:HG22	1:D:138:ILE:HB	1.84	0.58
1:B:360:ASP:HB3	4:B:2091:HOH:O	2.03	0.58
1:C:335:ARG:HH22	2:C:1382:UFG:H2D	1.66	0.58
1:B:95:VAL:HG11	1:B:125:LEU:CD1	2.33	0.58
1:B:259:TYR:CZ	1:B:334:ARG:HG2	2.38	0.58
1:B:17:VAL:HG21	1:B:30:ILE:HD11	1.85	0.58
1:D:16:PHE:CE1	1:D:280:HIS:CB	2.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ARG:NH2	4:B:2074:HOH:O	2.37	0.57
1:D:313:ARG:NH2	1:D:331:GLU:OE2	2.37	0.57
1:C:2:ARG:HD3	1:C:27:SER:HB2	1.86	0.57
1:D:261:THR:O	1:D:262:PRO:C	2.46	0.57
1:D:215:HIS:CD2	1:D:217[A]:GLN:H	2.23	0.57
1:D:215:HIS:CD2	1:D:217[B]:GLN:H	2.22	0.57
1:D:2:ARG:HH11	1:D:2:ARG:HB2	1.70	0.56
1:D:269:ASP:HB2	1:D:343:VAL:HA	1.87	0.56
1:B:107:SER:O	1:B:172:PRO:HG2	2.06	0.56
2:C:1382:UFG:H4'	3:C:1383:NAD:C4N	2.34	0.55
1:B:95:VAL:HG11	1:B:125:LEU:HD12	1.88	0.55
1:D:204:CYS:SG	1:D:223:ILE:HD13	2.46	0.55
1:A:297:LYS:HE2	4:A:2075:HOH:O	2.05	0.55
1:C:79:GLU:HB2	4:C:2040:HOH:O	2.07	0.55
1:D:249:ASP:HB3	1:D:251:ARG:HG3	1.88	0.55
1:A:225:ILE:HG22	1:A:252:MET:HE1	1.89	0.55
1:D:12:ILE:HG22	1:D:98:MET:HE1	1.89	0.55
1:A:294:ASP:HB2	1:A:295:LYS:HA	1.90	0.54
1:C:219:SER:O	1:C:225:ILE:HD11	2.08	0.54
1:A:47:ARG:N	1:A:48:GLU:HB2	2.23	0.54
1:D:117:ASN:HB2	4:D:2025:HOH:O	2.08	0.54
1:A:72:GLU:CD	1:A:88:ARG:NH2	2.65	0.54
1:C:111:PRO:HD2	1:D:191:TYR:CZ	2.43	0.53
1:D:320:ARG:HG3	1:D:327:ILE:HD12	1.90	0.53
1:C:78:ASN:C	1:C:78:ASN:HD22	2.16	0.53
1:C:113:LYS:HE3	4:C:2038:HOH:O	2.07	0.53
1:D:53:LYS:HB2	4:D:2008:HOH:O	2.06	0.53
1:B:216:TYR:H	1:B:373:GLN:HE22	1.57	0.53
1:C:272:HIS:O	4:C:2087:HOH:O	2.19	0.53
1:D:16:PHE:CE1	1:D:280:HIS:HB2	2.44	0.53
1:D:42:ASP:OD2	1:D:42:ASP:N	2.41	0.53
1:D:16:PHE:CE1	1:D:280:HIS:HB3	2.44	0.53
1:B:2:ARG:HG3	1:B:27:SER:HB2	1.91	0.52
1:B:52[A]:ARG:HD2	4:B:2011:HOH:O	2.09	0.52
1:B:181:GLU:HG2	1:B:197:CYS:SG	2.49	0.52
1:C:72:GLU:OE1	1:C:88:ARG:NH2	2.42	0.52
1:C:335:ARG:NH2	2:C:1382:UFG:O2D	2.40	0.52
1:B:325:HIS:CG	1:B:326:PRO:HD2	2.44	0.52
1:C:269:ASP:HB2	1:C:343:VAL:HA	1.91	0.52
1:D:145:ILE:HD12	1:D:167:LYS:HD2	1.91	0.52
1:B:123:LEU:HB2	1:B:183:MET:HE1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:PRO:HD2	1:D:65:ALA:HB2	1.90	0.52
1:D:98:MET:HA	1:D:140:SER:OG	2.09	0.51
1:B:350:ARG:HG2	1:B:355:TRP:O	2.10	0.51
1:B:97:HIS:HD2	1:B:139:PHE:CE1	2.29	0.51
1:A:56:GLN:O	1:A:57:SER:HB3	2.10	0.51
1:C:276:LEU:HG	4:C:2087:HOH:O	2.10	0.51
1:A:232:SER:HB2	4:A:2065:HOH:O	2.10	0.51
1:A:119:VAL:O	1:A:122:ILE:HG22	2.10	0.50
1:D:78:ASN:HD21	1:D:80:ASP:HB2	1.76	0.50
1:B:269:ASP:HB2	1:B:343:VAL:HA	1.92	0.50
1:D:80:ASP:HA	4:D:2015:HOH:O	2.11	0.50
1:B:119:VAL:CG1	1:B:179:ILE:HD11	2.42	0.50
1:C:2:ARG:HB2	1:C:2:ARG:HH11	1.77	0.50
1:B:20:LEU:O	1:B:24:THR:OG1	2.29	0.50
1:B:229:ARG:NH1	4:B:2061:HOH:O	2.43	0.49
1:B:313:ARG:HG3	1:B:313:ARG:NH1	2.26	0.49
1:C:142:SER:O	1:C:145:ILE:HG23	2.12	0.49
1:A:204[A]:CYS:SG	1:A:223:ILE:HD13	2.53	0.49
1:B:78:ASN:C	1:B:78:ASN:ND2	2.65	0.49
1:A:123:LEU:HA	1:A:183:MET:HE1	1.95	0.49
1:B:308:ARG:CD	4:B:2073:HOH:O	2.43	0.49
1:A:202:ASN:ND2	2:A:1382:UFG:H3'	2.27	0.48
1:D:252:MET:HE3	1:D:253:PRO:O	2.12	0.48
1:A:150:THR:HG22	4:A:2042:HOH:O	2.13	0.48
1:B:97:HIS:HD2	1:B:139:PHE:HE1	1.61	0.48
2:A:1382:UFG:H4'	3:A:1383:NAD:H4N	1.93	0.48
1:B:116:ASP:O	1:B:120:VAL:HB	2.14	0.48
1:A:112:LEU:HD12	1:B:130:LEU:HD22	1.96	0.47
1:C:138:ILE:HD12	1:C:283:ALA:HB1	1.95	0.47
1:D:47:ARG:HB3	4:D:2007:HOH:O	2.13	0.47
1:A:226:ILE:O	1:A:229:ARG:N	2.47	0.47
1:B:0[B]:HIS:HE1	4:B:2005:HOH:O	1.96	0.47
1:A:130:LEU:HD12	1:A:130:LEU:HA	1.69	0.47
1:C:170:GLU:O	1:C:170:GLU:HG3	2.14	0.47
1:B:249:ASP:OD2	1:B:251:ARG:NH2	2.42	0.47
1:B:306:THR:O	1:B:307:SER:HB2	2.15	0.47
1:D:249:ASP:OD2	1:D:251:ARG:NE	2.42	0.47
1:D:216:TYR:H	1:D:373:GLN:HE22	1.63	0.47
1:D:181:GLU:HG2	1:D:197:CYS:SG	2.54	0.47
1:D:129:MET:HE2	1:D:193:ILE:HD13	1.97	0.47
1:A:105:GLY:HA3	1:A:335:ARG:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:PHE:HB3	1:B:132:HIS:CE1	2.50	0.46
1:C:179:ILE:HG12	1:D:179:ILE:HG12	1.98	0.46
1:A:269:ASP:HB2	1:A:343:VAL:HA	1.98	0.46
1:D:350:ARG:HA	1:D:355:TRP:H	1.81	0.46
1:C:200:TYR:OH	1:C:280:HIS:NE2	2.46	0.46
1:A:145:ILE:HD12	1:A:167:LYS:HD2	1.98	0.46
1:C:282:LEU:HD13	1:C:353:LEU:O	2.16	0.46
1:A:370:TRP:CD1	1:A:374:ARG:HH11	2.34	0.46
1:C:208:GLU:H	1:C:208:GLU:CD	2.24	0.46
1:A:123:LEU:HB2	1:A:183:MET:HE1	1.97	0.45
1:A:216:TYR:H	1:A:373:GLN:HE22	1.64	0.45
1:A:202:ASN:HD22	2:A:1382:UFG:H3'	1.80	0.45
1:D:167:LYS:HE3	1:D:199:ARG:HH22	1.82	0.45
1:A:46:THR:HG1	1:A:49:ASN:HB2	1.80	0.45
1:A:159:GLU:HB2	1:A:160:PRO:CD	2.47	0.45
1:C:317:GLU:OE1	1:C:320:ARG:NH1	2.49	0.45
1:B:204:CYS:SG	1:B:223:ILE:HD13	2.57	0.45
1:A:216:TYR:CD2	1:A:228:GLY:HA2	2.52	0.45
1:B:339:PRO:HG2	1:B:342:LEU:HD11	1.98	0.45
1:B:294:ASP:O	1:B:295:LYS:HB3	2.16	0.44
1:C:124:ARG:HD3	4:C:2041:HOH:O	2.16	0.44
1:C:191:TYR:CZ	1:D:111:PRO:HD2	2.53	0.44
1:A:163:ILE:HB	1:A:301:VAL:HG23	2.00	0.44
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.84	0.44
1:C:290:LEU:HD22	1:C:294:ASP:HB3	1.98	0.44
1:A:201:PHE:HB3	4:A:2056:HOH:O	2.18	0.44
1:D:96:VAL:HG12	1:D:98:MET:HG3	1.99	0.44
1:A:32:ASP:O	1:A:73:VAL:HA	2.18	0.44
1:B:196:ILE:HD11	1:B:286:TYR:CD2	2.49	0.44
1:C:184:ILE:O	1:C:185:ARG:C	2.61	0.44
1:B:215:HIS:CD2	1:B:217:GLN:H	2.36	0.43
1:A:215:HIS:HA	1:A:373:GLN:HE22	1.84	0.43
1:C:200:TYR:OH	1:C:280:HIS:CE1	2.71	0.43
1:A:78:ASN:HD22	1:A:80:ASP:H	1.67	0.43
1:A:201:PHE:CE1	1:A:344:ALA:HB2	2.53	0.43
1:A:253:PRO:HA	1:A:330:ARG:O	2.18	0.43
1:B:62:PRO:C	1:B:64:TRP:H	2.27	0.43
1:C:16:PHE:CZ	1:C:20:LEU:HD11	2.53	0.43
1:B:378:ASN:HB3	4:B:2096:HOH:O	2.18	0.43
1:A:251:ARG:HG2	1:A:328:PRO:HB2	2.01	0.43
1:C:266:CYS:HB2	2:C:1382:UFG:O3D	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ASP:O	1:B:351:GLU:HG3	2.19	0.42
1:C:166:LYS:HE2	1:C:166:LYS:HB3	1.79	0.42
1:C:54:LEU:HD11	1:C:65:ALA:HB1	2.00	0.42
1:D:182:ARG:HG3	1:D:182:ARG:HH11	1.84	0.42
1:A:32:ASP:OD1	1:A:33:SER:N	2.51	0.42
1:A:177:LYS:HD3	1:A:177:LYS:HA	1.88	0.42
1:D:182:ARG:HG3	1:D:182:ARG:NH1	2.34	0.42
1:A:197:CYS:HB2	1:A:301:VAL:HG12	2.02	0.42
1:C:229:ARG:HH21	1:C:253:PRO:HD3	1.84	0.42
1:D:216:TYR:N	1:D:373:GLN:HE22	2.17	0.42
1:C:265:THR:HB	1:C:312:VAL:HB	2.02	0.42
1:D:130:LEU:HD12	1:D:130:LEU:HA	1.93	0.42
1:C:302:PHE:HB3	1:C:349:ALA:HB2	2.01	0.42
1:C:331:GLU:H	1:C:331:GLU:HG2	1.70	0.42
1:A:56:GLN:O	1:A:57:SER:CB	2.67	0.42
1:A:78:ASN:ND2	1:A:81:PHE:H	2.18	0.41
1:A:294:ASP:CB	1:A:295:LYS:HA	2.49	0.41
1:A:306:THR:O	1:A:307:SER:CB	2.59	0.41
1:B:93:ASP:O	1:B:136:LYS:HE2	2.20	0.41
1:C:250:LYS:HA	1:C:250:LYS:HE2	2.03	0.41
1:A:83:ASN:OD1	1:A:132:HIS:NE2	2.52	0.41
1:C:322:THR:HG21	1:C:366:MET:HG3	2.01	0.41
2:B:1382:UFG:H4'	3:B:1383:NAD:H4N	2.00	0.41
1:C:130:LEU:HD12	1:C:130:LEU:HA	1.94	0.41
1:A:200:TYR:OH	1:A:280:HIS:NE2	2.50	0.41
1:C:111:PRO:HD2	1:D:191:TYR:OH	2.20	0.41
1:C:137:ILE:O	1:C:195:GLY:HA2	2.20	0.41
1:D:-1:SER:C	1:D:1:MET:H	2.27	0.41
1:A:141:SER:OG	1:A:142:SER:N	2.53	0.41
1:B:202:ASN:O	1:B:270:TYR:HA	2.20	0.41
1:B:95:VAL:HG11	1:B:125:LEU:HD11	2.03	0.41
1:B:27:SER:HB3	4:B:2002:HOH:O	2.20	0.41
1:C:183:MET:HE2	1:C:183:MET:HB3	1.91	0.41
1:C:305:GLY:HA3	1:C:344:ALA:HB3	2.01	0.41
1:C:175:GLU:HG2	4:D:2041:HOH:O	2.21	0.40
1:D:259:TYR:O	1:D:264:GLY:HA2	2.20	0.40
1:B:1:MET:HG3	1:B:93:ASP:CB	2.49	0.40
1:D:197:CYS:HB2	1:D:301:VAL:HG12	2.03	0.40
1:D:251:ARG:HH21	1:D:330:ARG:HD3	1.86	0.40
1:A:18:ARG:HD2	1:A:207:HIS:CD2	2.57	0.40
1:A:66:ASP:HB2	4:A:2016:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ASP:O	1:C:136:LYS:HE2	2.21	0.40
1:C:275:ASP:HB2	4:C:2087:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	363/397 (91%)	330 (91%)	25 (7%)	8 (2%)	5	14
1	B	361/397 (91%)	337 (93%)	19 (5%)	5 (1%)	9	23
1	C	363/397 (91%)	338 (93%)	23 (6%)	2 (1%)	21	44
1	D	362/397 (91%)	329 (91%)	32 (9%)	1 (0%)	36	60
All	All	1449/1588 (91%)	1334 (92%)	99 (7%)	16 (1%)	12	29

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	0[A]	HIS
1	B	0[B]	HIS
1	B	295	LYS
1	B	296	SER
1	D	1	MET
1	A	48	GLU
1	A	55	GLN
1	A	57	SER
1	A	334	ARG
1	A	49	ASN
1	A	56	GLN
1	A	236	PRO
1	A	294	ASP

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Mol	Chain	Res	Type
1	C	273	VAL
1	B	63	PRO
1	C	260	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	308/331 (93%)	297 (96%)	11 (4%)	31	60
1	B	306/331 (92%)	279 (91%)	27 (9%)	9	23
1	C	308/331 (93%)	296 (96%)	12 (4%)	28	57
1	D	306/331 (92%)	287 (94%)	19 (6%)	16	39
All	All	1228/1324 (93%)	1159 (94%)	69 (6%)	20	44

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	VAL
1	A	125	LEU
1	A	130	LEU
1	A	131	LEU
1	A	168	SER
1	A	223	ILE
1	A	288	GLU
1	A	293	ASN
1	A	335	ARG
1	A	358	LYS
1	A	360	ASP
1	B	31	VAL
1	B	40[A]	LYS
1	B	40[B]	LYS
1	B	41	SER
1	B	47	ARG
1	B	52[A]	ARG
1	B	52[B]	ARG

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Mol	Chain	Res	Type
1	B	55	GLN
1	B	56[A]	GLN
1	B	56[B]	GLN
1	B	61	LYS
1	B	78	ASN
1	B	125	LEU
1	B	135	ASP
1	B	159	GLU
1	B	166	LYS
1	B	167	LYS
1	B	179	ILE
1	B	194	LYS
1	B	212	ILE
1	B	217	GLN
1	B	233	ASP
1	B	273	VAL
1	B	297	LYS
1	B	300	SER
1	B	308	ARG
1	B	329	VAL
1	C	1	MET
1	C	2	ARG
1	C	40	LYS
1	C	54	LEU
1	C	56	GLN
1	C	58	ASP
1	C	87	THR
1	C	125	LEU
1	C	208	GLU
1	C	217	GLN
1	C	288	GLU
1	C	331	GLU
1	D	2	ARG
1	D	31	VAL
1	D	42	ASP
1	D	48	GLU
1	D	54	LEU
1	D	56[A]	GLN
1	D	56[B]	GLN
1	D	78	ASN
1	D	125	LEU
1	D	130	LEU

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Mol	Chain	Res	Type
1	D	133	LYS
1	D	167	LYS
1	D	193	ILE
1	D	249	ASP
1	D	257	THR
1	D	294	ASP
1	D	300	SER
1	D	329	VAL
1	D	348	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	78	ASN
1	A	97	HIS
1	A	373	GLN
1	B	55	GLN
1	B	78	ASN
1	B	97	HIS
1	B	373	GLN
1	C	49	ASN
1	C	78	ASN
1	C	83	ASN
1	D	49	ASN
1	D	78	ASN
1	D	97	HIS
1	D	373	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UFG	D	1382	-	37,38,38	1.62	4 (10%)	52,58,58	1.85	8 (15%)
3	NAD	B	1383	-	46,48,48	1.72	3 (6%)	64,73,73	1.77	12 (18%)
2	UFG	A	1382	-	37,38,38	1.30	6 (16%)	52,58,58	1.75	11 (21%)
2	UFG	B	1382	-	37,38,38	1.16	3 (8%)	52,58,58	1.58	6 (11%)
3	NAD	A	1383	-	46,48,48	1.79	8 (17%)	64,73,73	1.60	9 (14%)
3	NAD	D	1383	-	46,48,48	1.71	3 (6%)	64,73,73	1.50	10 (15%)
3	NAD	C	1383	-	46,48,48	1.78	7 (15%)	64,73,73	1.76	15 (23%)
2	UFG	C	1382	-	37,38,38	1.11	4 (10%)	52,58,58	1.59	7 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UFG	D	1382	-	1/1/11/11	3/23/59/59	0/3/3/3
3	NAD	B	1383	-	-	14/30/62/62	0/5/5/5
2	UFG	A	1382	-	1/1/11/11	2/23/59/59	0/3/3/3
2	UFG	B	1382	-	1/1/11/11	4/23/59/59	0/3/3/3
3	NAD	A	1383	-	-	4/30/62/62	0/5/5/5
3	NAD	D	1383	-	-	5/30/62/62	0/5/5/5
3	NAD	C	1383	-	-	6/30/62/62	0/5/5/5
2	UFG	C	1382	-	1/1/11/11	3/23/59/59	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1383	NAD	O7N-C7N	9.42	1.41	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1383	NAD	O7N-C7N	9.26	1.41	1.24
3	C	1383	NAD	O7N-C7N	9.06	1.41	1.24
3	A	1383	NAD	O7N-C7N	9.03	1.40	1.24
2	D	1382	UFG	PA-O3A	6.39	1.66	1.59
2	D	1382	UFG	PB-O3A	4.84	1.64	1.59
2	B	1382	UFG	PA-O3A	4.14	1.64	1.59
3	B	1383	NAD	C2N-N1N	3.04	1.38	1.35
2	C	1382	UFG	C2-N1	2.94	1.43	1.38
3	A	1383	NAD	PN-O3	2.89	1.62	1.59
3	A	1383	NAD	C2A-N1A	2.83	1.39	1.33
3	C	1383	NAD	C2N-N1N	2.81	1.38	1.35
3	D	1383	NAD	C2A-N1A	2.72	1.38	1.33
3	A	1383	NAD	PA-O3	2.64	1.62	1.59
2	A	1382	UFG	O4'-C1D	2.63	1.48	1.42
3	C	1383	NAD	C8A-N7A	2.61	1.36	1.31
3	C	1383	NAD	C2A-N1A	2.52	1.38	1.33
3	A	1383	NAD	C2A-N3A	2.44	1.38	1.33
2	B	1382	UFG	C5-C4	-2.42	1.38	1.43
3	C	1383	NAD	C2A-N3A	2.37	1.38	1.33
3	D	1383	NAD	C2N-N1N	2.37	1.37	1.35
2	A	1382	UFG	PA-O3A	2.36	1.62	1.59
2	A	1382	UFG	C2-N1	2.27	1.42	1.38
3	A	1383	NAD	C2N-N1N	2.24	1.37	1.35
3	A	1383	NAD	C8A-N7A	2.22	1.35	1.31
3	A	1383	NAD	O4B-C4B	-2.18	1.40	1.45
3	C	1383	NAD	C5A-N7A	-2.16	1.35	1.39
3	B	1383	NAD	C2A-N3A	2.15	1.37	1.33
2	A	1382	UFG	C6-N1	2.15	1.43	1.38
2	D	1382	UFG	C4'-C5'	-2.15	1.50	1.52
2	D	1382	UFG	C5-C4	-2.15	1.39	1.43
2	C	1382	UFG	C6-C5	2.15	1.40	1.35
2	A	1382	UFG	C6-C5	2.14	1.40	1.35
3	C	1383	NAD	O4D-C1D	2.06	1.43	1.40
2	C	1382	UFG	C4'-C3'	2.06	1.54	1.52
2	A	1382	UFG	PB-O3A	-2.05	1.57	1.59
2	C	1382	UFG	C4'-C5'	2.01	1.54	1.52
2	B	1382	UFG	C2-N1	2.00	1.41	1.38

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1382	UFG	C4-N3-C2	-6.17	118.95	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1382	UFG	C4-N3-C2	-6.12	119.02	126.61
2	A	1382	UFG	O5'-C1'-O3B	-6.02	103.50	111.36
3	B	1383	NAD	N3A-C2A-N1A	-5.84	119.74	128.58
3	C	1383	NAD	N3A-C2A-N1A	-5.84	119.75	128.58
3	D	1383	NAD	N3A-C2A-N1A	-5.64	120.05	128.58
2	D	1382	UFG	O5'-C1'-O3B	-5.53	104.13	111.36
3	A	1383	NAD	N3A-C2A-N1A	-5.49	120.28	128.58
2	B	1382	UFG	C4-N3-C2	-5.25	120.10	126.61
2	D	1382	UFG	N3-C2-N1	5.08	121.51	114.89
2	B	1382	UFG	O5'-C1'-O3B	-4.97	104.87	111.36
2	A	1382	UFG	C4-N3-C2	-4.57	120.94	126.61
3	A	1383	NAD	N9A-C8A-N7A	-4.47	107.59	113.94
2	A	1382	UFG	C5-C4-N3	4.40	120.97	114.80
3	B	1383	NAD	C5A-C4A-N3A	-4.38	120.68	126.72
2	B	1382	UFG	C5-C4-N3	4.36	120.91	114.80
2	C	1382	UFG	N3-C2-N1	4.35	120.55	114.89
3	B	1383	NAD	N9A-C8A-N7A	-4.30	107.83	113.94
3	C	1383	NAD	C5A-C4A-N3A	-4.17	120.98	126.72
2	C	1382	UFG	C5-C4-N3	4.04	120.46	114.80
2	D	1382	UFG	O2-C2-N1	-4.01	117.58	122.80
3	D	1383	NAD	N9A-C8A-N7A	-3.88	108.42	113.94
3	B	1383	NAD	O3B-C3B-C4B	-3.85	100.03	111.08
3	C	1383	NAD	O3D-C3D-C4D	-3.83	100.08	111.08
3	C	1383	NAD	N9A-C8A-N7A	-3.78	108.58	113.94
3	B	1383	NAD	C5A-N7A-C8A	3.74	109.33	103.45
3	B	1383	NAD	C2A-N3A-C4A	3.62	120.67	111.83
3	A	1383	NAD	C5A-C4A-N3A	-3.54	121.84	126.72
3	A	1383	NAD	C5A-N7A-C8A	3.52	108.99	103.45
2	A	1382	UFG	O5'-C5'-C4'	3.51	114.68	108.83
3	C	1383	NAD	C2A-N3A-C4A	3.48	120.34	111.83
3	D	1383	NAD	C5A-C4A-N3A	-3.42	122.01	126.72
2	B	1382	UFG	O4-C4-C5	-3.41	119.27	125.16
2	C	1382	UFG	F4'-C4'-C3'	3.36	111.72	108.81
2	D	1382	UFG	O4-C4-C5	-3.31	119.46	125.16
3	D	1383	NAD	O3D-C3D-C4D	-3.26	101.73	111.08
2	A	1382	UFG	C2D-C1D-N1	3.24	122.28	113.25
3	B	1383	NAD	C4A-C5A-N7A	-3.18	106.95	110.58
3	D	1383	NAD	C2A-N3A-C4A	3.16	119.54	111.83
3	A	1383	NAD	C2A-N3A-C4A	3.15	119.52	111.83
3	B	1383	NAD	C3N-C7N-N7N	3.13	121.59	117.74
3	D	1383	NAD	C5A-N7A-C8A	3.12	108.36	103.45
2	D	1382	UFG	C5-C4-N3	3.12	119.16	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1383	NAD	C4D-O4D-C1D	2.98	112.66	109.92
3	C	1383	NAD	C5A-N7A-C8A	2.96	108.11	103.45
3	C	1383	NAD	C4D-O4D-C1D	2.93	112.61	109.92
3	A	1383	NAD	O3D-C3D-C4D	-2.90	102.75	111.08
3	C	1383	NAD	O7N-C7N-C3N	-2.84	116.13	119.60
2	A	1382	UFG	N3-C2-N1	2.81	118.55	114.89
3	A	1383	NAD	C4A-N9A-C8A	2.78	108.66	105.74
2	C	1382	UFG	O5'-C5'-C4'	2.68	113.30	108.83
2	C	1382	UFG	O4-C4-C5	-2.62	120.64	125.16
2	B	1382	UFG	N3-C2-N1	2.57	118.23	114.89
3	A	1383	NAD	C4A-C5A-N7A	-2.55	107.67	110.58
2	D	1382	UFG	O5'-C5'-C4'	-2.49	104.69	108.83
2	C	1382	UFG	O5'-C1'-O3B	-2.44	108.17	111.36
3	C	1383	NAD	O2A-PA-O3	2.40	113.75	107.27
3	D	1383	NAD	C4A-N9A-C8A	2.36	108.22	105.74
3	C	1383	NAD	N3A-C4A-N9A	2.35	131.17	127.17
3	C	1383	NAD	C2B-C3B-C4B	2.34	107.14	102.61
3	B	1383	NAD	C5A-C4A-N9A	2.32	108.34	105.81
3	A	1383	NAD	N3A-C4A-N9A	2.31	131.09	127.17
3	D	1383	NAD	C4A-C5A-N7A	-2.27	107.98	110.58
3	D	1383	NAD	C4D-O4D-C1D	2.25	111.99	109.92
2	A	1382	UFG	C3D-C2D-C1D	-2.24	97.22	101.46
3	D	1383	NAD	N3A-C4A-N9A	2.24	130.97	127.17
3	B	1383	NAD	N3A-C4A-N9A	2.24	130.97	127.17
2	A	1382	UFG	O5'-C1'-C2'	2.22	114.93	110.37
3	C	1383	NAD	O3-PN-O1N	-2.20	104.08	110.70
2	D	1382	UFG	O5'-C5'-C6'	2.18	111.85	106.44
3	B	1383	NAD	O3-PN-O1N	-2.18	104.14	110.70
3	C	1383	NAD	C2D-C3D-C4D	2.12	106.70	102.61
3	C	1383	NAD	C2N-C3N-C4N	2.12	120.72	118.26
2	A	1382	UFG	O4-C4-C5	-2.12	121.51	125.16
2	A	1382	UFG	O2A-PA-O3A	-2.09	101.62	107.27
3	C	1383	NAD	C3N-C7N-N7N	2.05	120.27	117.74
2	B	1382	UFG	C1'-O5'-C5'	-2.03	109.75	113.72
2	A	1382	UFG	O4'-C1D-C2D	-2.01	102.31	106.62

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1382	UFG	C4'
2	B	1382	UFG	C4'
2	C	1382	UFG	C4'

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Mol	Chain	Res	Type	Atom
2	D	1382	UFG	C4'

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1382	UFG	PB-O3A-PA-O5D
2	A	1382	UFG	C1'-O3B-PB-O3A
2	C	1382	UFG	C1'-O3B-PB-O3A
2	D	1382	UFG	PB-O3A-PA-O5D
3	B	1383	NAD	C5B-O5B-PA-O1A
3	B	1383	NAD	C5B-O5B-PA-O3
3	B	1383	NAD	PN-O3-PA-O5B
3	B	1383	NAD	C5D-O5D-PN-O3
3	B	1383	NAD	C5D-O5D-PN-O1N
3	B	1383	NAD	C5D-O5D-PN-O2N
3	C	1383	NAD	O4D-C1D-N1N-C2N
3	C	1383	NAD	O4D-C1D-N1N-C6N
3	D	1383	NAD	O4D-C1D-N1N-C2N
3	B	1383	NAD	PA-O3-PN-O1N
3	B	1383	NAD	O4D-C4D-C5D-O5D
2	C	1382	UFG	PB-O3A-PA-O5D
2	D	1382	UFG	C1'-O3B-PB-O1B
3	A	1383	NAD	O4D-C4D-C5D-O5D
3	B	1383	NAD	C3D-C4D-C5D-O5D
2	B	1382	UFG	C5D-O5D-PA-O3A
2	D	1382	UFG	C1'-O3B-PB-O3A
3	B	1383	NAD	C5B-O5B-PA-O2A
3	B	1383	NAD	PA-O3-PN-O2N
2	B	1382	UFG	O5'-C1'-O3B-PB
3	C	1383	NAD	C2D-C1D-N1N-C6N
3	B	1383	NAD	C4B-C5B-O5B-PA
3	A	1383	NAD	O4D-C1D-N1N-C6N
3	B	1383	NAD	O4D-C1D-N1N-C2N
3	B	1383	NAD	O4D-C1D-N1N-C6N
3	D	1383	NAD	O4D-C1D-N1N-C6N
3	A	1383	NAD	PA-O3-PN-O2N
3	C	1383	NAD	PA-O3-PN-O2N
3	C	1383	NAD	C4B-C5B-O5B-PA
2	B	1382	UFG	C1'-O3B-PB-O1B
2	C	1382	UFG	C1'-O3B-PB-O1B
2	B	1382	UFG	PA-O3A-PB-O1B
3	D	1383	NAD	PA-O3-PN-O1N

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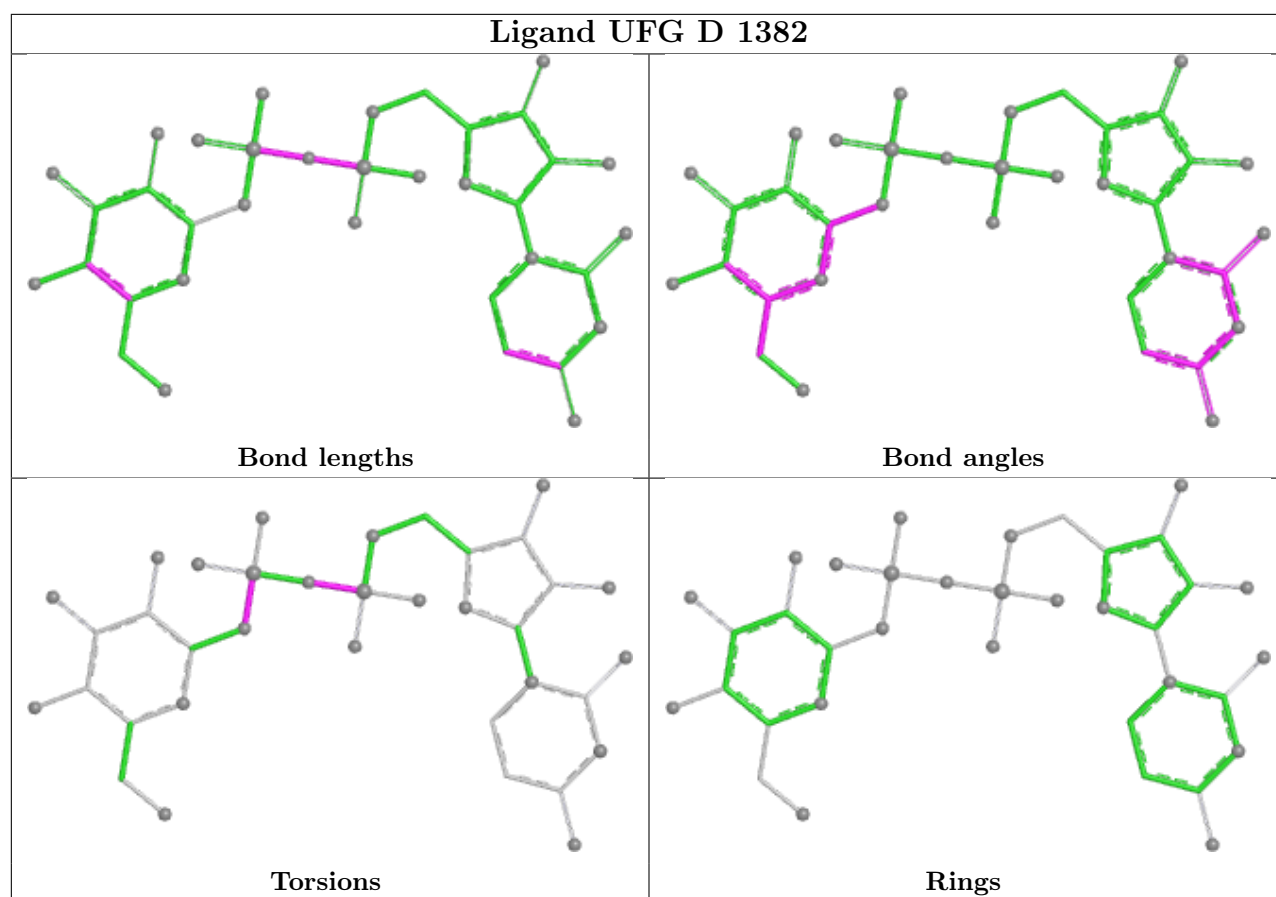
Mol	Chain	Res	Type	Atoms
3	D	1383	NAD	PA-O3-PN-O2N
3	A	1383	NAD	C3D-C4D-C5D-O5D
3	C	1383	NAD	O4B-C4B-C5B-O5B
3	D	1383	NAD	O4B-C4B-C5B-O5B

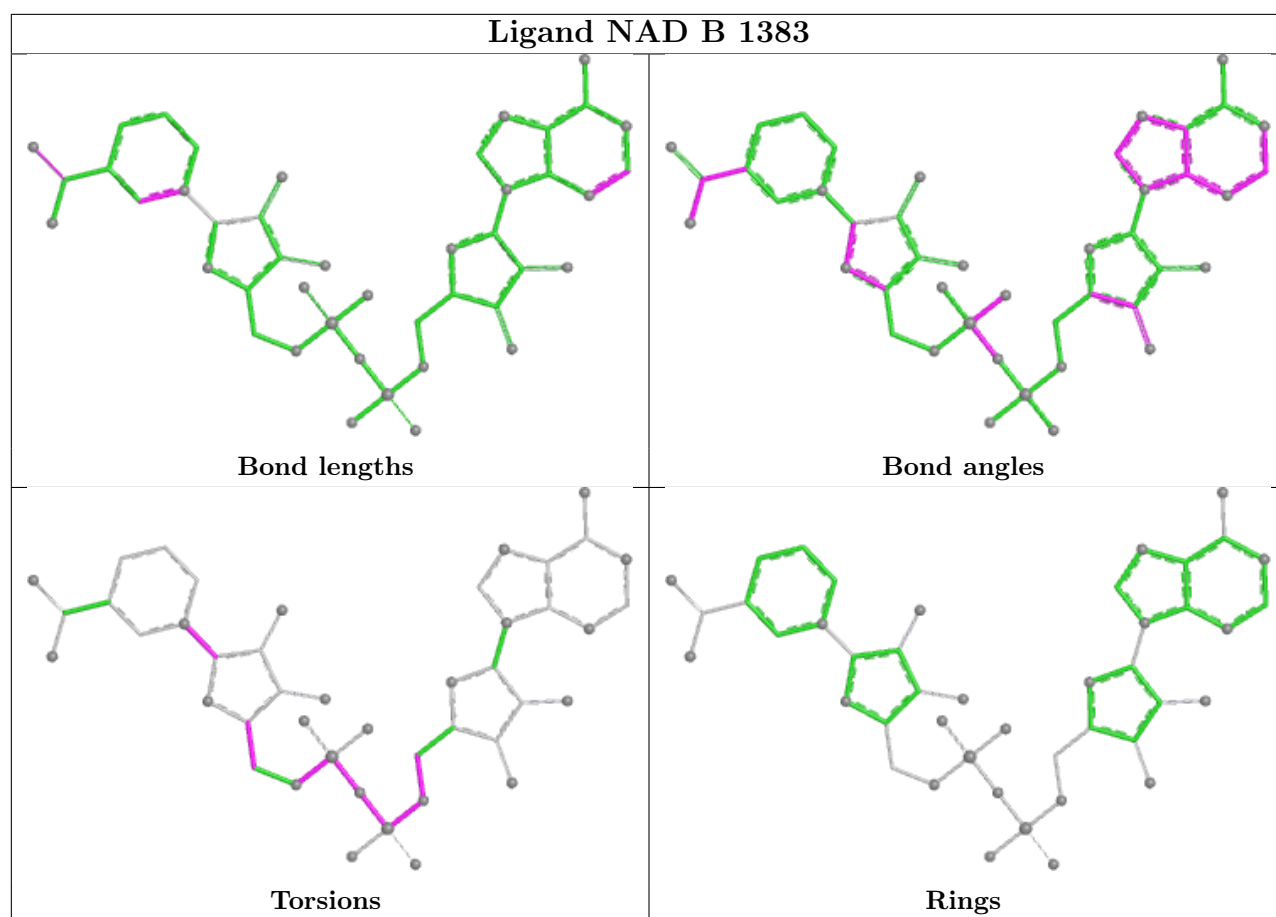
There are no ring outliers.

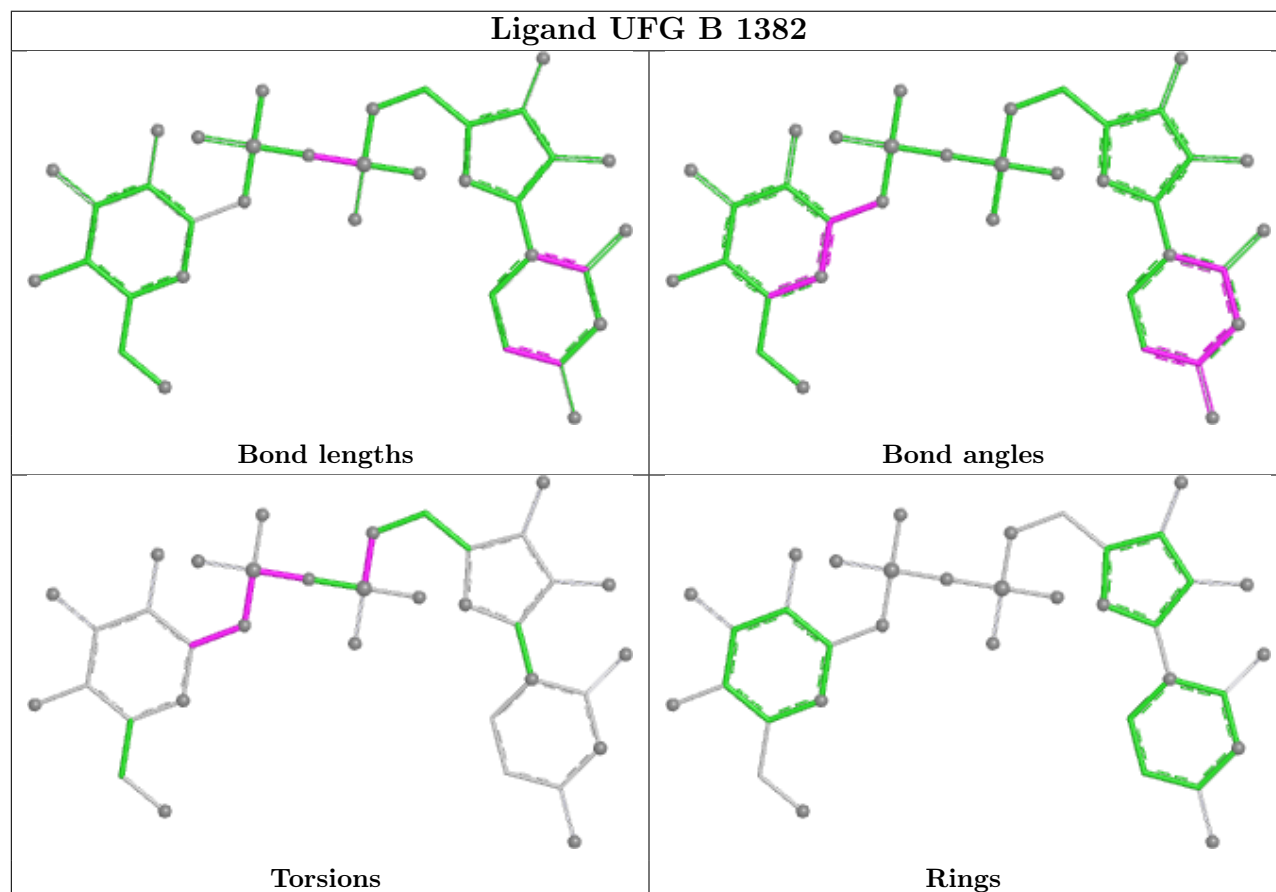
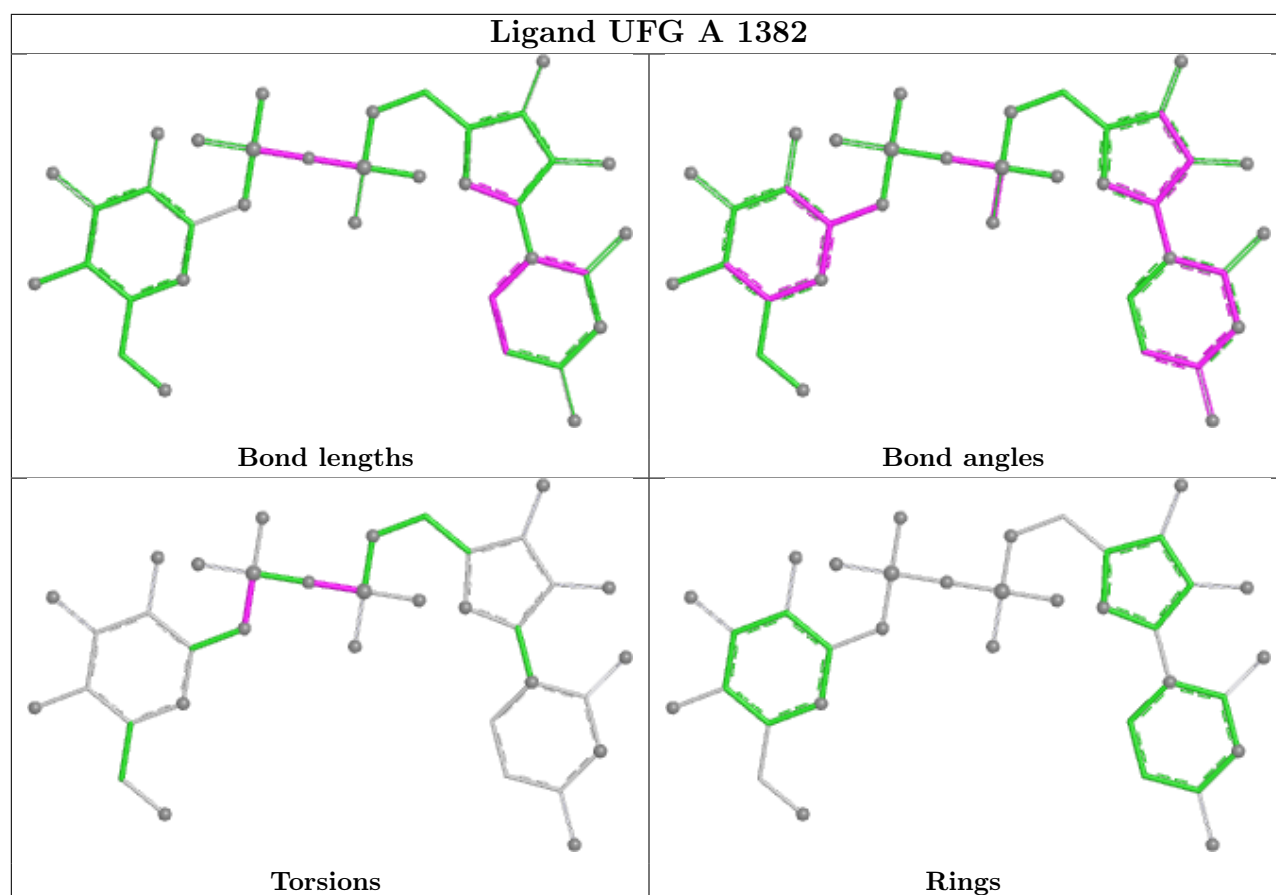
8 monomers are involved in 13 short contacts:

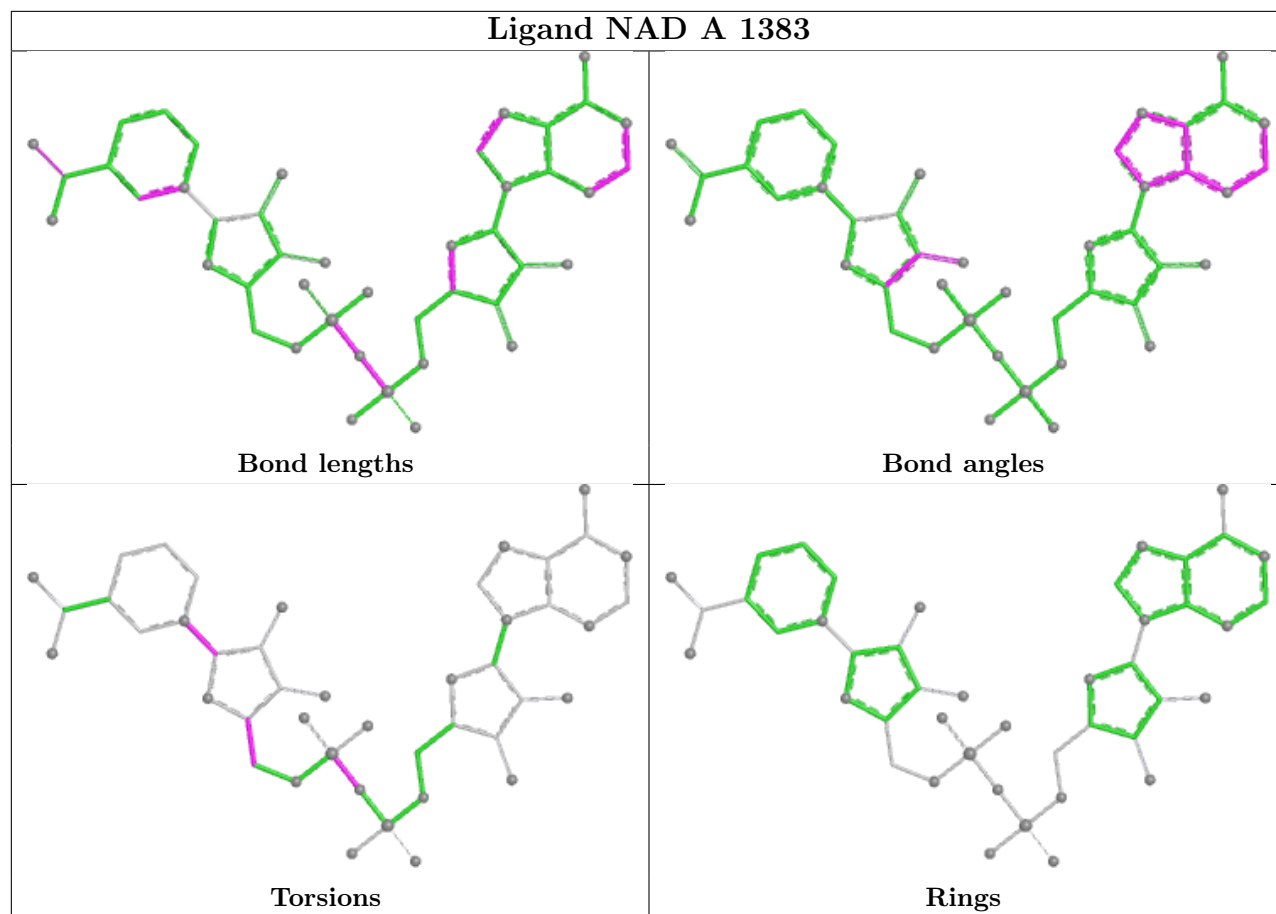
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1382	UFG	2	0
3	B	1383	NAD	2	0
2	A	1382	UFG	4	0
2	B	1382	UFG	2	0
3	A	1383	NAD	2	0
3	D	1383	NAD	2	0
3	C	1383	NAD	1	0
2	C	1382	UFG	5	0

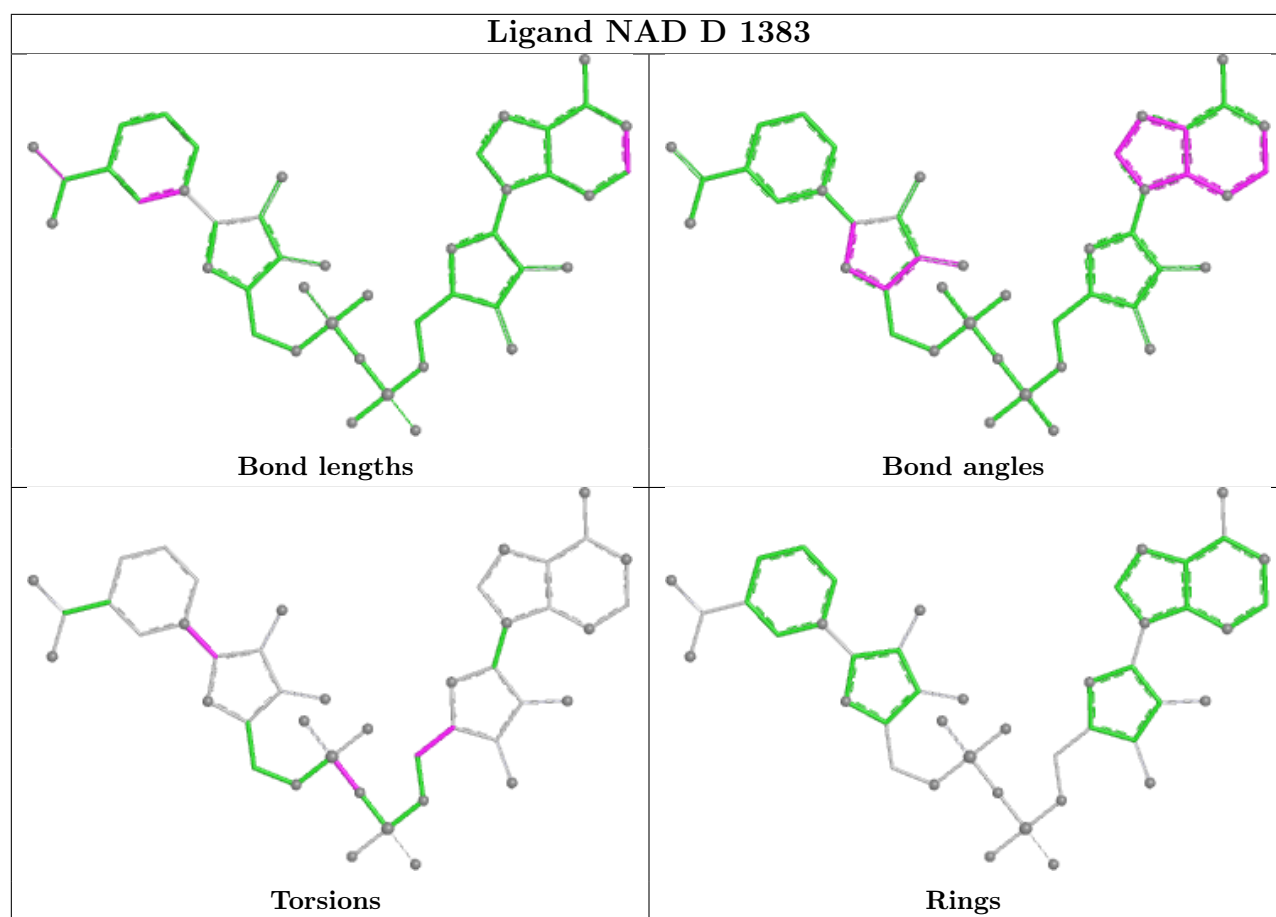
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

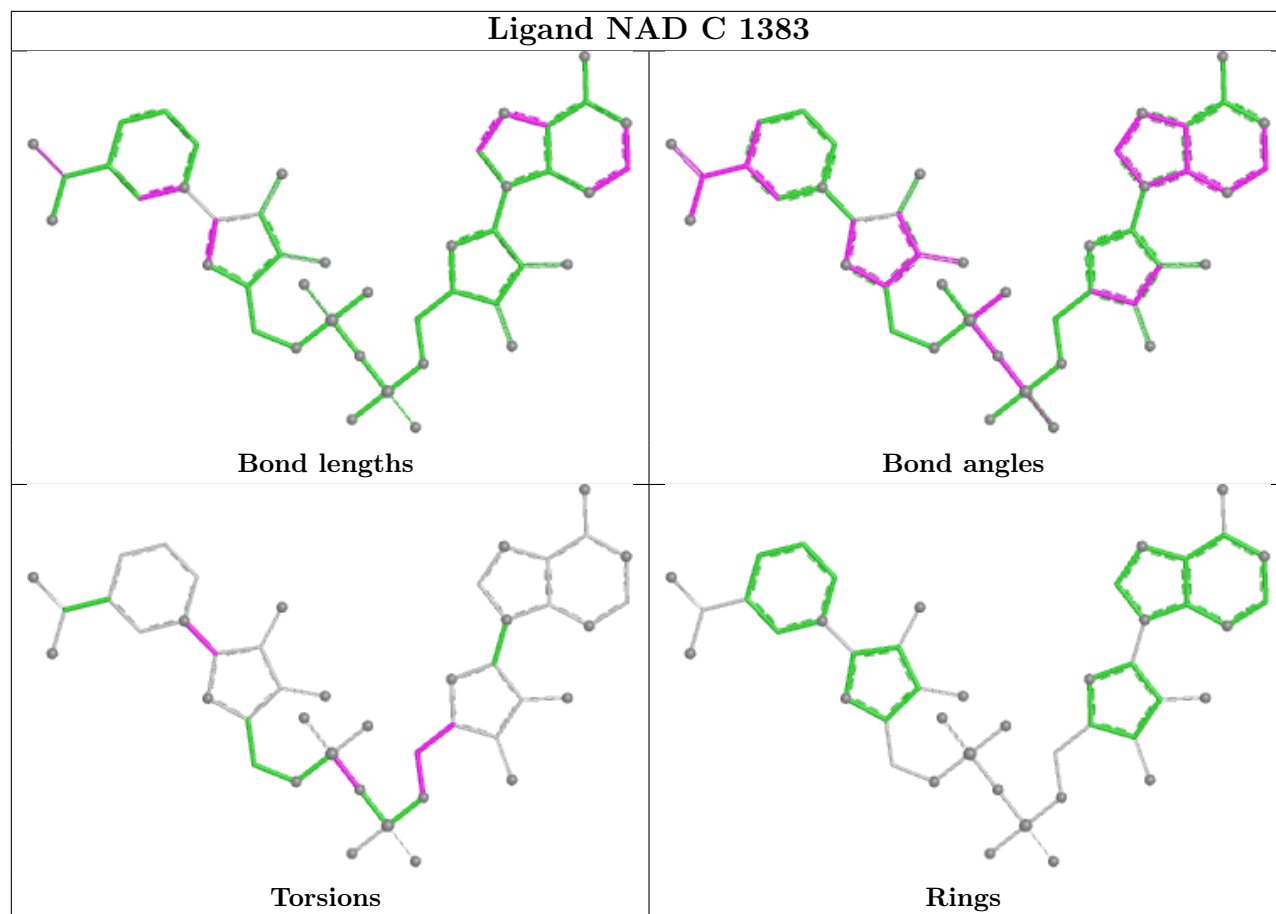


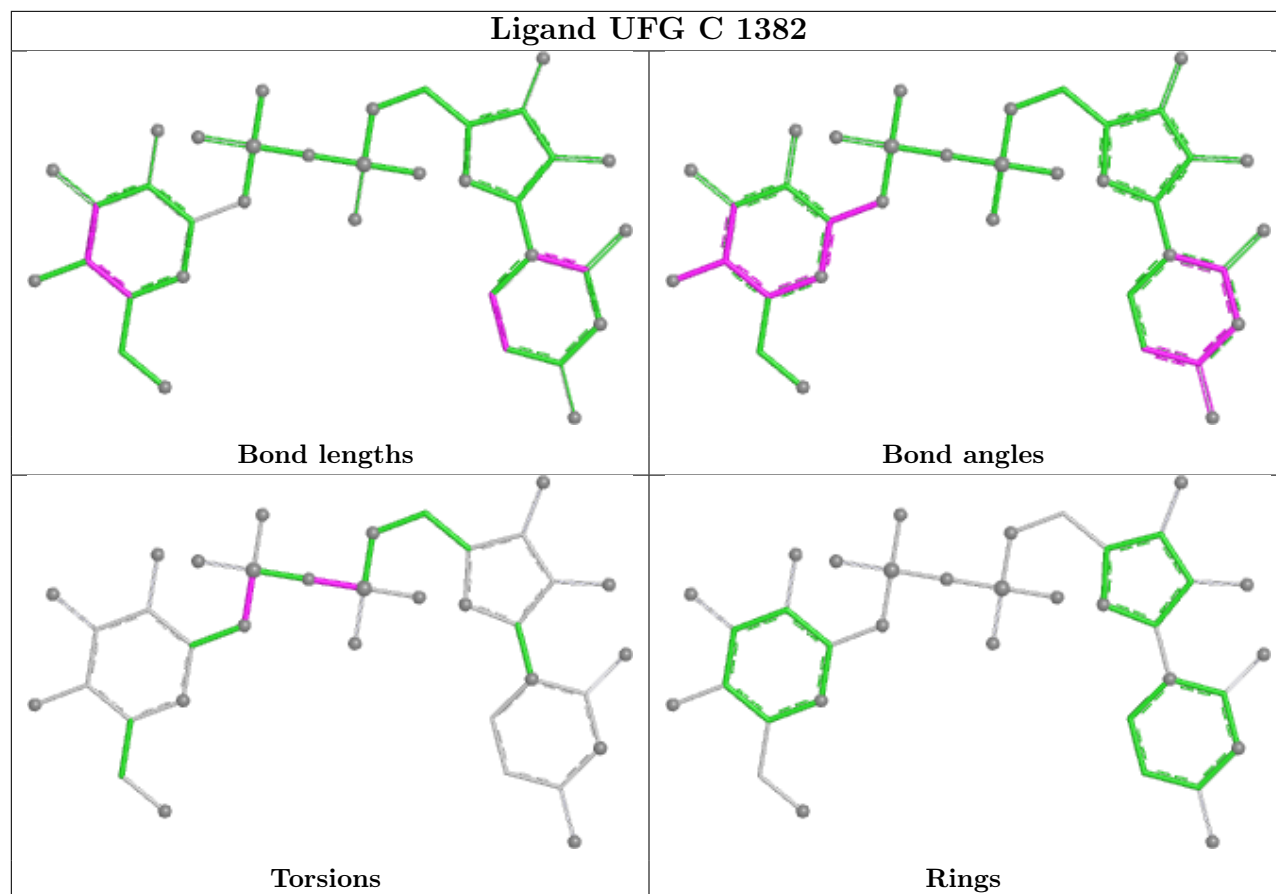












5.7 Other polymers [i](#)

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	366/397 (92%)	-0.38	0 100 100	23, 44, 70, 91	4 (1%)
1	B	363/397 (91%)	-0.27	3 (0%) 82 81	32, 49, 68, 81	4 (1%)
1	C	366/397 (92%)	-0.37	0 100 100	23, 43, 66, 79	3 (0%)
1	D	364/397 (91%)	-0.27	2 (0%) 87 86	27, 49, 66, 78	4 (1%)
All	All	1459/1588 (91%)	-0.32	5 (0%) 90 89	23, 47, 68, 91	15 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	381	ALA	2.9
1	B	292	PRO	2.6
1	D	0	HIS	2.2
1	B	381	ALA	2.2
1	B	291	GLY	2.2

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,

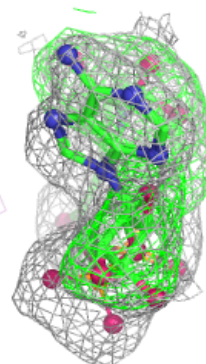
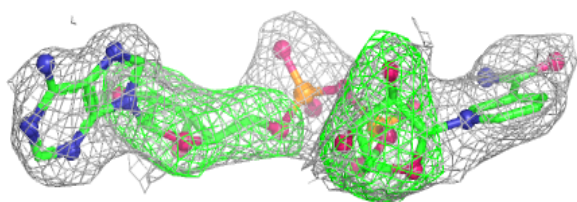
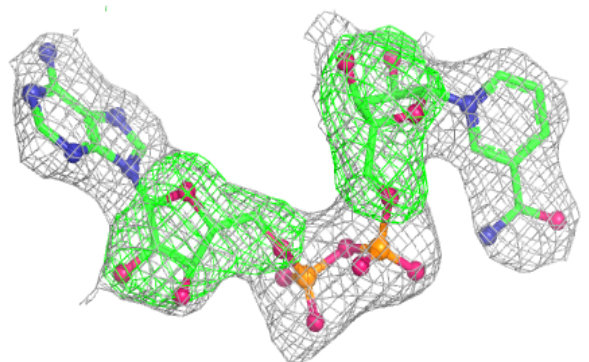
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAD	D	1383	44/44	0.86	0.20	38,44,49,50	18
3	NAD	C	1383	44/44	0.87	0.19	23,33,37,38	18
3	NAD	A	1383	44/44	0.87	0.18	29,38,41,43	18
3	NAD	B	1383	44/44	0.88	0.18	37,41,44,45	18
2	UFG	A	1382	36/36	0.94	0.08	43,47,50,50	0
2	UFG	C	1382	36/36	0.95	0.07	46,52,55,56	0
2	UFG	B	1382	36/36	0.96	0.06	31,34,37,39	0
2	UFG	D	1382	36/36	0.97	0.06	33,37,41,43	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.

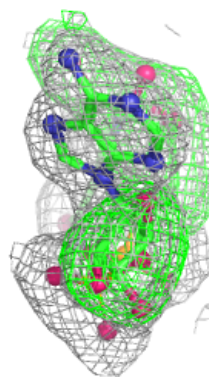
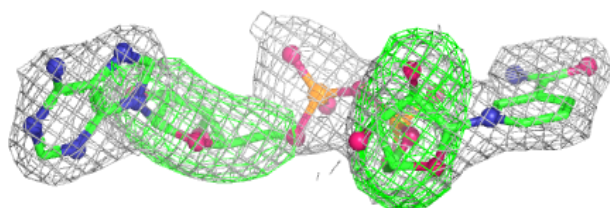
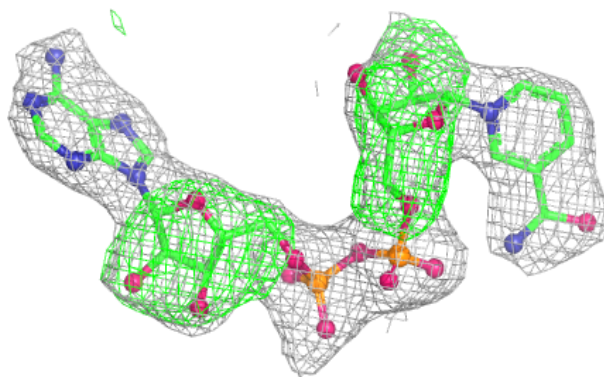
Electron density around NAD D 1383:

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

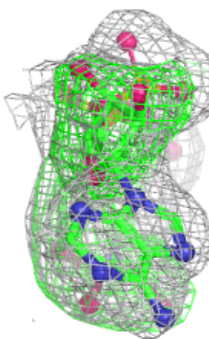
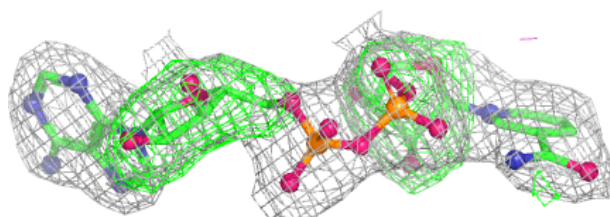
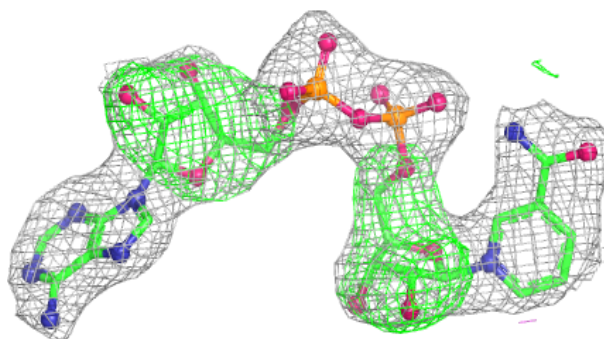


Electron density around NAD C 1383:

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

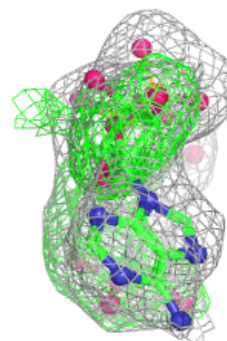
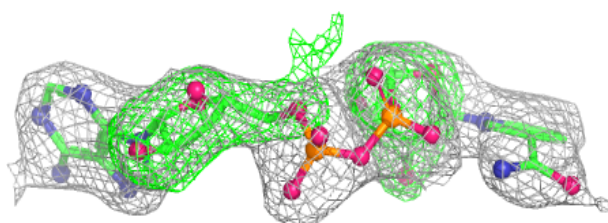
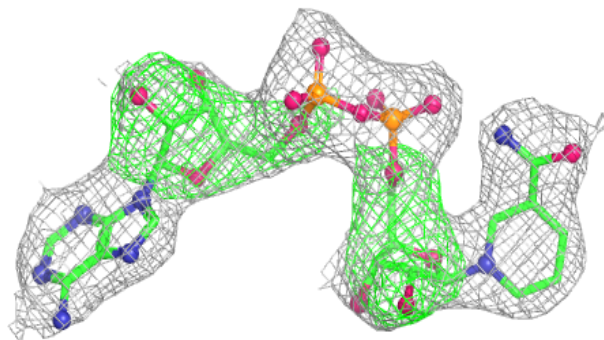
**Electron density around NAD A 1383:**

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

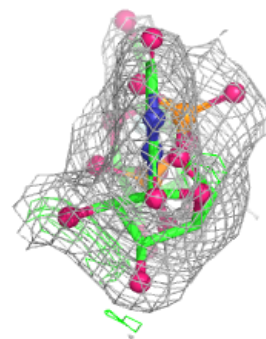
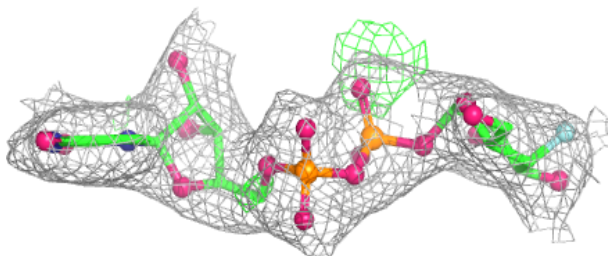
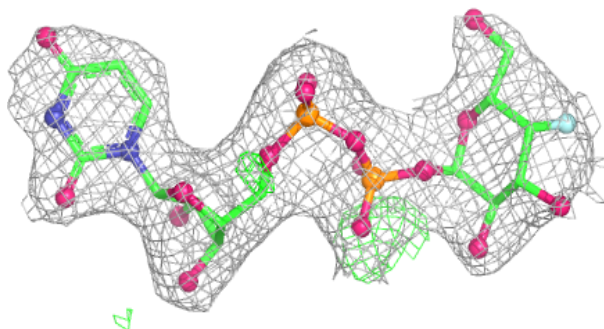


Electron density around NAD B 1383:

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

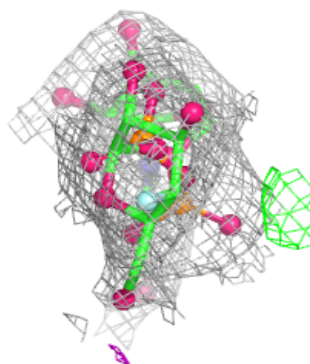
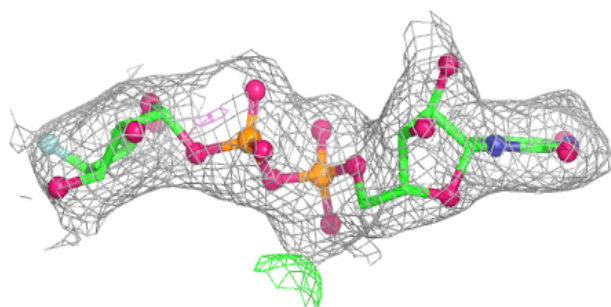
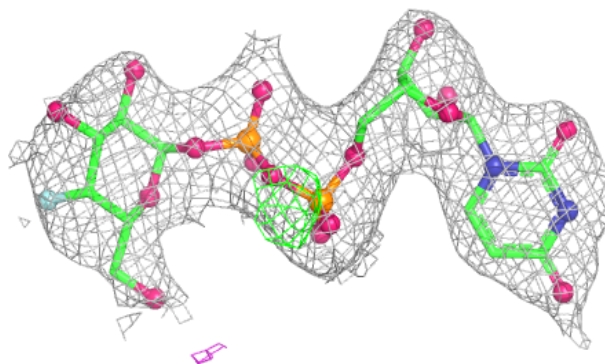
**Electron density around UFG A 1382:**

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

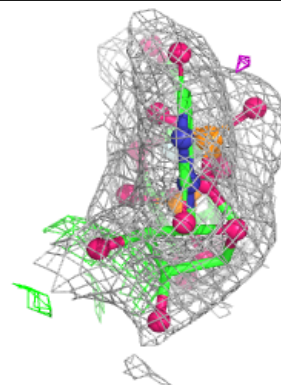
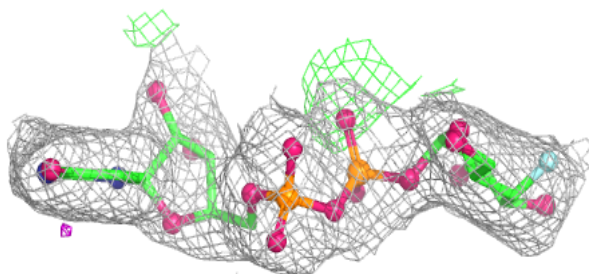
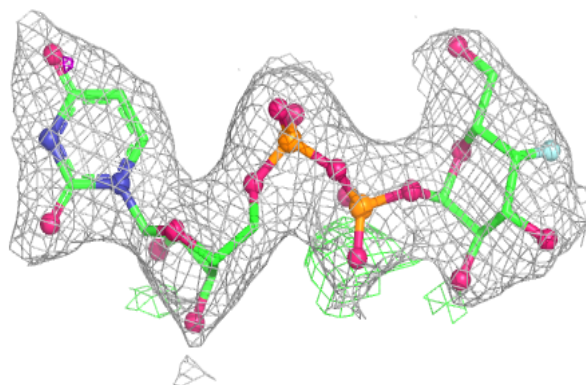


Electron density around UFG C 1382:

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

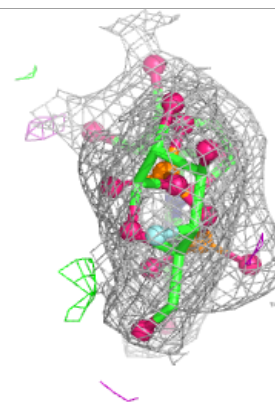
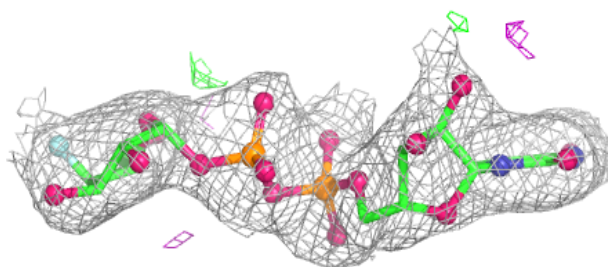
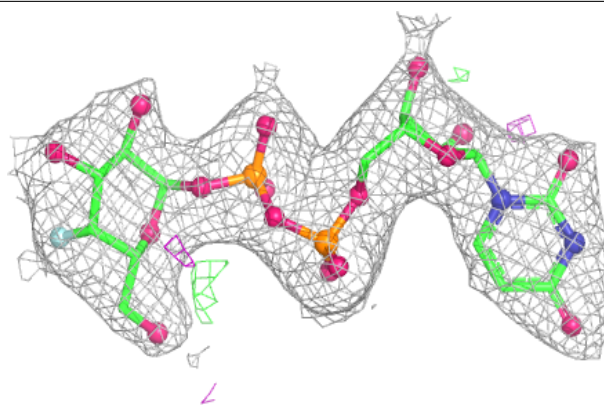
**Electron density around UFG B 1382:**

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



Electron density around UFG D 1382:

$2mF_o-DF_c$ (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.