Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 03:39 AM EDT

PDB ID	:	3PTZ
Title	:	Role of Packing Defects in the Evolution of Allostery and Induced Fit in Human UDP-Glucose Dehydrogenase.
Authors	:	Kadirvelraj, R.; Wood, Z.A.
Deposited on	:	2010-12-03
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

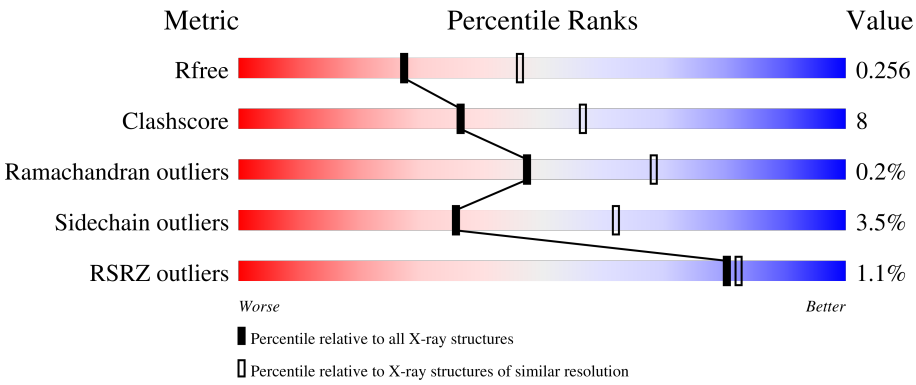
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	494	79% 13% 7%
1	B	494	81% 11% 7%
1	C	494	2% 77% 14% • 7%
1	D	494	.% 75% 16% • 7%
1	E	494	77% 15% • 7%

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Mol	Chain	Length	Quality of chain
1	F	494	3% 73% 18% 7%

2 Entry composition (i)

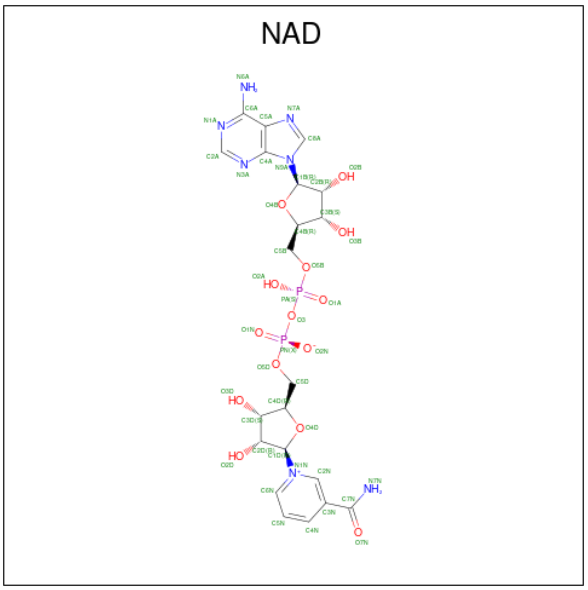
There are 4 unique types of molecules in this entry. The entry contains 22753 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-glucose 6-dehydrogenase.

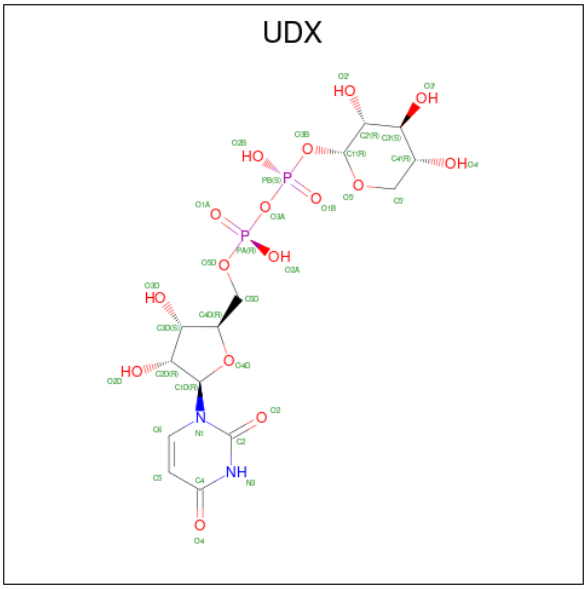
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	458	3589	2271	619	679	20	0	0	0
1	B	457	3581	2266	618	678	19	0	0	0
1	C	457	3581	2266	618	678	19	0	0	0
1	D	457	3581	2266	618	678	19	0	0	0
1	E	458	3589	2271	619	679	20	0	0	0
1	F	457	3581	2266	618	678	19	0	0	0

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



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

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-XYLOPYRANOSE (three-letter code: UDX) (formula: $C_{14}H_{22}N_2O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	34	14	2	16	2	0	0
3	B	1	34	14	2	16	2	0	0
3	C	1	34	14	2	16	2	0	0
3	D	1	34	14	2	16	2	0	0
3	E	1	34	14	2	16	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	F	1	34	14	2	16	2	0	0

- Molecule 4 is water.

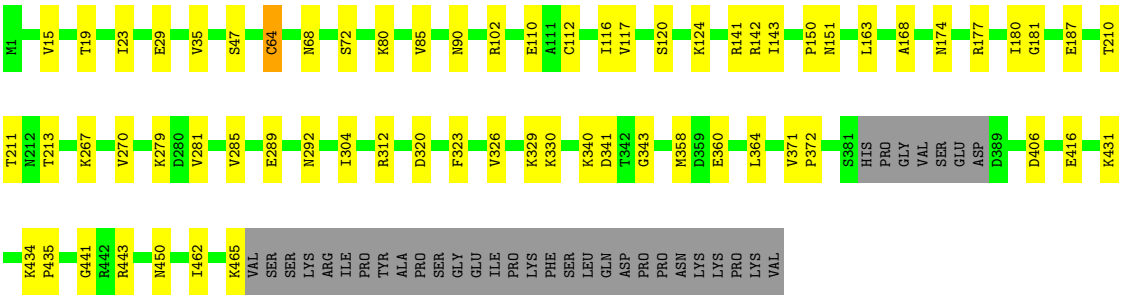
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	164	164	164	0	0
4	B	141	141	141	0	0
4	C	121	121	121	0	0
4	D	87	87	87	0	0
4	E	161	161	161	0	0
4	F	109	109	109	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

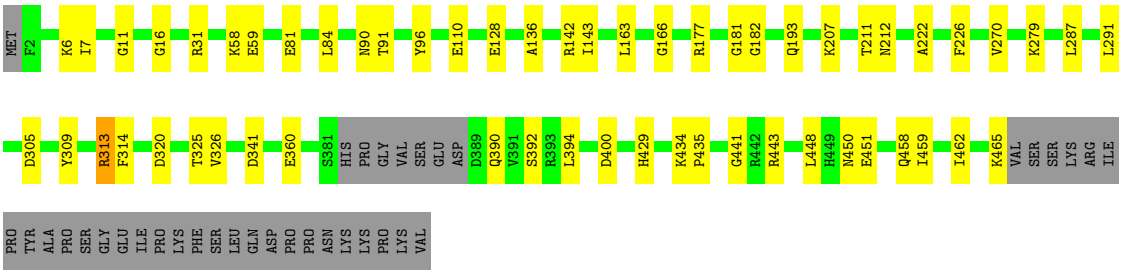
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain A: 79% 13% 7%



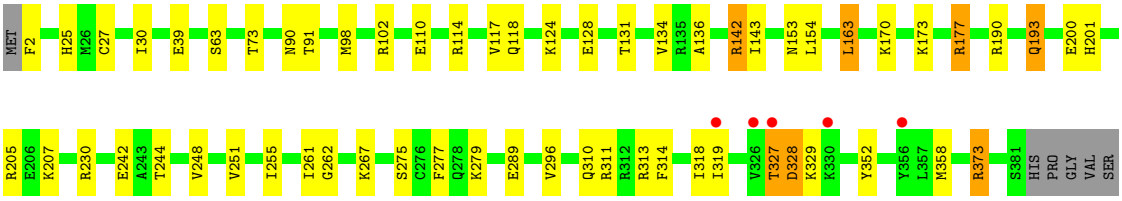
• Molecule 1: UDP-glucose 6-dehydrogenase

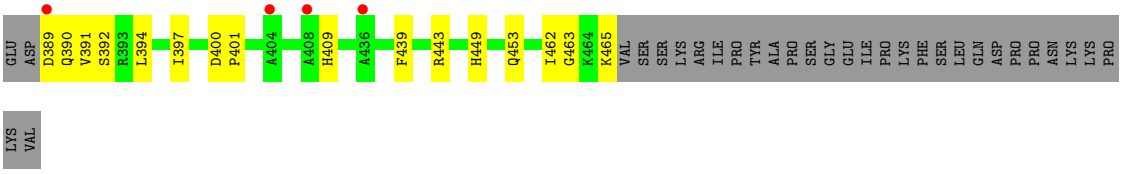
Chain B: 81% 11% 7%



• Molecule 1: UDP-glucose 6-dehydrogenase

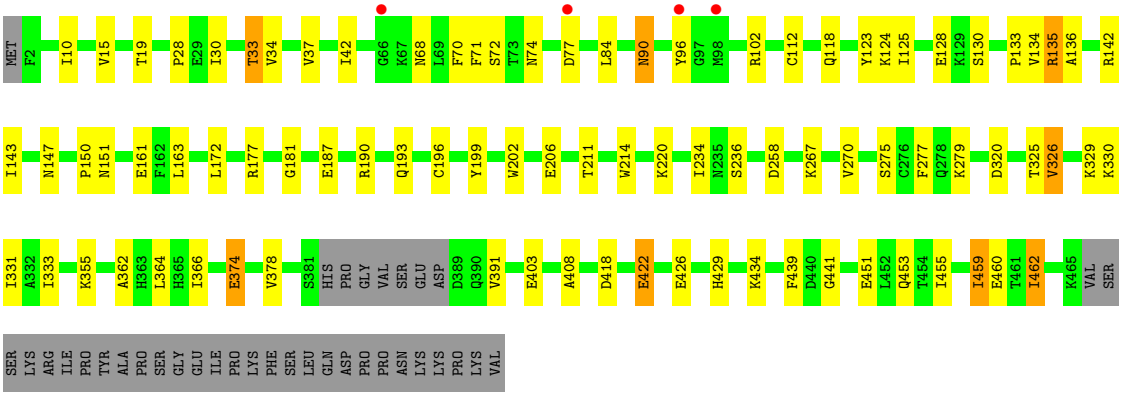
Chain C: 2% 77% 14% • 7%





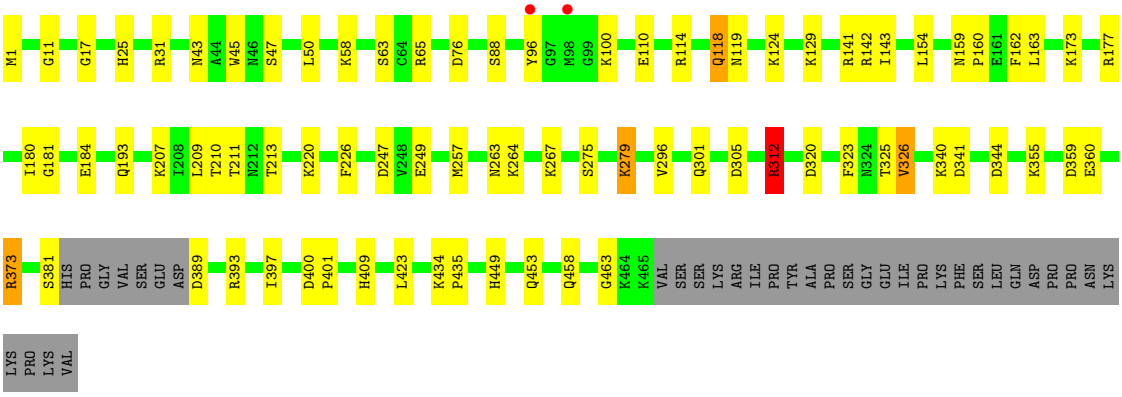
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain D:



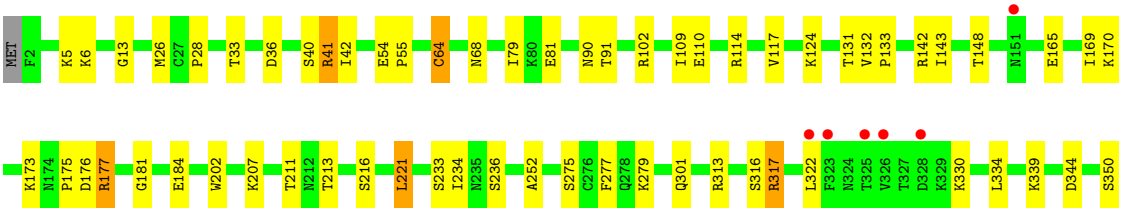
• Molecule 1: UDP-glucose 6-dehydrogenase

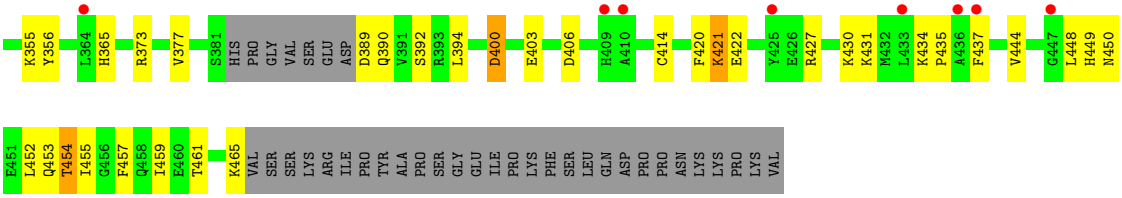
Chain E:



• Molecule 1: UDP-glucose 6-dehydrogenase

Chain F:




K355
Y356
L364
H365
R373
V377
S381
HIS
PRO
GLY
VAL
SER
GLU
ASP
D389
Q390
V391
S392
R393
L394
D400
E403
D406
H409
A410
C414
F420
K421
E422
Y425
E426
R427
K430
K431
M432
L433
K434
P435
A436
F437
V444
G447
L448
H449
N450
E451
L452
Q453
T454
I455
G456
F457
Q458
I459
E460
T461
K465
VAL
SER
SER
LYS
ARG
ILE
PRO
TYR
ALA
PRO
SER
GLY
GLU
ILE
PRO
LYS
PHE
SER
LEU
GLN
ASP
PRO
PRO
ASN
LYS
LYS
PRO
LYS
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.10Å 196.67Å 111.74Å 90.00° 111.88° 90.00°	Depositor
Resolution (Å)	49.17 – 2.50 49.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.17-2.50) 97.3 (49.17-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.258 0.190 , 0.256	Depositor DCC
R_{free} test set	6018 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22753	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAD, UDX

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	0.93	1/3653 (0.0%)	0.87	0/4941
1	B	0.89	1/3645 (0.0%)	0.86	4/4931 (0.1%)
1	C	0.84	0/3645	0.81	1/4931 (0.0%)
1	D	0.84	1/3645 (0.0%)	0.79	0/4931
1	E	0.88	0/3653	0.86	6/4941 (0.1%)
1	F	0.84	0/3645	0.81	2/4931 (0.0%)
All	All	0.87	3/21886 (0.0%)	0.83	13/29606 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	59	GLU	CG-CD	5.17	1.59	1.51
1	A	64	CYS	CB-SG	-5.16	1.73	1.81
1	D	196	CYS	CB-SG	-5.01	1.73	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	313	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	E	312	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	E	209	LEU	CA-CB-CG	7.07	131.56	115.30
1	F	344	ASP	CB-CG-OD1	6.20	123.88	118.30
1	E	1	MET	CG-SD-CE	-5.89	90.77	100.20
1	B	31	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	C	311	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	E	305	ASP	CB-CG-OD1	5.61	123.35	118.30
1	F	102	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	E	31	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	B	305	ASP	CB-CG-OD1	5.12	122.91	118.30
1	E	344	ASP	CB-CG-OD1	5.02	122.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	448	LEU	CA-CB-CG	5.01	126.83	115.30

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	3589	0	3611	60	0
1	B	3581	0	3599	51	0
1	C	3581	0	3599	59	0
1	D	3581	0	3599	50	0
1	E	3589	0	3611	66	0
1	F	3581	0	3599	67	0
2	A	44	0	26	12	0
2	B	44	0	26	18	0
2	C	44	0	26	13	0
2	D	44	0	26	10	0
2	E	44	0	26	11	0
2	F	44	0	26	14	0
3	A	34	0	20	0	0
3	B	34	0	20	0	0
3	C	34	0	20	1	0
3	D	34	0	20	1	0
3	E	34	0	20	0	0
3	F	34	0	20	1	0
4	A	164	0	0	11	0
4	B	141	0	0	6	0
4	C	121	0	0	10	0
4	D	87	0	0	4	0
4	E	161	0	0	19	0
4	F	109	0	0	16	0
All	All	22753	0	21894	347	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 8.

All (347) 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:279:LYS:CE	2:B:500:NAD:H6N	1.63	1.28
1:A:279:LYS:HE3	2:A:500:NAD:C6N	1.67	1.24
1:D:90:ASN:HB2	2:D:500:NAD:N7N	1.51	1.24
1:C:90:ASN:HB2	2:C:500:NAD:N7N	1.54	1.21
1:B:279:LYS:HE2	2:B:500:NAD:H6N	1.23	1.14
4:A:778:HOH:O	1:C:142:ARG:HD2	1.52	1.10
1:B:279:LYS:NZ	2:B:500:NAD:H6N	1.67	1.09
1:B:451:GLU:HB2	4:B:596:HOH:O	1.50	1.09
1:D:90:ASN:HB2	2:D:500:NAD:H71N	1.01	1.08
1:A:279:LYS:HE3	2:A:500:NAD:H6N	1.28	1.06
1:F:356:TYR:HB3	4:F:553:HOH:O	1.53	1.05
2:B:500:NAD:O1A	2:B:500:NAD:N7N	1.94	1.00
1:A:279:LYS:CE	2:A:500:NAD:C6N	2.39	0.99
1:A:279:LYS:HZ2	2:A:500:NAD:H1D	1.25	0.99
1:C:90:ASN:HB2	2:C:500:NAD:H71N	0.86	0.98
1:E:193:GLN:HG2	4:E:608:HOH:O	1.59	0.98
1:B:279:LYS:HZ3	2:B:500:NAD:C6N	1.81	0.94
1:F:421:LYS:HB3	4:F:542:HOH:O	1.68	0.94
1:A:90:ASN:HB2	2:A:500:NAD:H71N	1.31	0.93
1:D:90:ASN:CB	2:D:500:NAD:H71N	1.81	0.92
1:B:279:LYS:NZ	2:B:500:NAD:H1D	1.86	0.91
1:B:279:LYS:HE2	2:B:500:NAD:C6N	1.99	0.91
1:C:90:ASN:CB	2:C:500:NAD:H71N	1.80	0.90
1:B:279:LYS:HZ3	2:B:500:NAD:H6N	1.28	0.88
1:B:279:LYS:HZ1	2:B:500:NAD:H1D	1.38	0.88
1:A:279:LYS:NZ	2:A:500:NAD:H1D	1.89	0.87
1:D:90:ASN:CB	2:D:500:NAD:N7N	2.36	0.86
1:F:389:ASP:HB2	4:F:670:HOH:O	1.75	0.85
1:F:275:SER:O	2:F:500:NAD:H5N	1.77	0.84
1:C:279:LYS:HZ3	2:C:500:NAD:C6N	1.92	0.82
1:F:90:ASN:HB2	2:F:500:NAD:H71N	1.43	0.81
1:A:142:ARG:HD2	4:E:579:HOH:O	1.80	0.81
1:A:292:ASN:HB3	4:F:520:HOH:O	1.79	0.80
1:E:320:ASP:HB3	4:E:513:HOH:O	1.81	0.80
1:F:330:LYS:HE2	1:F:406:ASP:O	1.82	0.80
1:C:275:SER:O	2:C:500:NAD:H5N	1.85	0.76
1:B:326:VAL:CG2	1:B:360:GLU:HB3	2.16	0.76
1:C:200:GLU:OE1	1:C:205:ARG:HD3	1.86	0.76
1:C:373:ARG:HB3	1:C:397:ILE:HG21	1.68	0.75
1:B:193:GLN:HG3	4:B:565:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:LYS:HE2	2:E:500:NAD:C6N	2.18	0.74
1:E:359:ASP:HB3	4:E:587:HOH:O	1.88	0.74
1:A:326:VAL:HG22	1:A:360:GLU:HB3	1.69	0.74
1:E:326:VAL:HG22	1:E:360:GLU:HB3	1.71	0.73
1:E:173:LYS:HD2	4:E:643:HOH:O	1.87	0.73
1:F:427:ARG:CD	4:F:558:HOH:O	2.36	0.72
1:F:90:ASN:HB2	2:F:500:NAD:N7N	2.06	0.71
1:A:110:GLU:HG3	1:A:143:ILE:HD11	1.73	0.70
1:F:313:ARG:O	1:F:317:ARG:HB2	1.92	0.70
1:E:355:LYS:HE2	4:E:784:HOH:O	1.92	0.69
1:E:76:ASP:HB3	1:E:119:ASN:OD1	1.92	0.69
1:C:27:CYS:HB3	1:C:30:ILE:HD12	1.75	0.69
1:D:33:THR:HG23	1:D:70:PHE:HB2	1.74	0.68
1:B:314:PHE:CD1	1:B:462:ILE:HD11	2.28	0.68
1:B:326:VAL:CG2	1:B:360:GLU:CB	2.71	0.68
1:D:15:VAL:O	1:D:19:THR:HG23	1.92	0.68
1:F:390:GLN:HG2	1:F:394:LEU:HD12	1.77	0.67
1:B:90:ASN:HB2	2:B:500:NAD:C2N	2.25	0.67
1:C:110:GLU:HG3	1:C:143:ILE:HD11	1.77	0.66
1:D:275:SER:HB2	2:D:500:NAD:C5N	2.26	0.66
1:D:355:LYS:HE3	4:D:529:HOH:O	1.95	0.66
1:E:389:ASP:HB3	4:E:506:HOH:O	1.95	0.66
1:E:184:GLU:HG2	4:E:605:HOH:O	1.96	0.65
1:C:352:TYR:HB3	4:C:568:HOH:O	1.96	0.65
1:D:19:THR:HG22	1:D:172:LEU:HD21	1.76	0.64
1:E:279:LYS:HZ3	2:E:500:NAD:C5N	2.10	0.64
1:E:275:SER:HB2	2:E:500:NAD:C6N	2.28	0.64
1:B:465:LYS:HE3	4:B:779:HOH:O	1.99	0.62
1:E:279:LYS:NZ	2:E:500:NAD:C6N	2.63	0.62
1:E:275:SER:O	2:E:500:NAD:H6N	1.98	0.62
1:F:91:THR:H	2:F:500:NAD:H2N	1.64	0.62
1:B:390:GLN:HB3	1:B:394:LEU:HD12	1.82	0.62
1:A:90:ASN:CB	2:A:500:NAD:H71N	2.07	0.61
1:F:427:ARG:HD2	4:F:558:HOH:O	1.95	0.61
1:A:102:ARG:HD2	4:A:665:HOH:O	1.99	0.61
1:E:296:VAL:HG13	1:F:236:SER:HB2	1.82	0.61
1:A:90:ASN:HB2	2:A:500:NAD:N7N	2.09	0.61
1:F:449:HIS:O	1:F:453:GLN:HG3	2.01	0.60
1:A:80:LYS:HE2	4:A:609:HOH:O	2.00	0.60
2:B:500:NAD:H51N	2:B:500:NAD:H2N	1.84	0.60
1:E:58:LYS:HE2	4:E:626:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:LYS:CE	2:E:500:NAD:C6N	2.79	0.60
1:C:153:ASN:HA	4:C:593:HOH:O	2.02	0.60
1:B:279:LYS:NZ	2:B:500:NAD:C6N	2.46	0.59
1:D:422:GLU:HA	4:D:707:HOH:O	2.00	0.59
1:C:114:ARG:O	1:C:117:VAL:HG12	2.02	0.59
1:F:90:ASN:HA	2:F:500:NAD:H2D	1.85	0.59
1:B:309:TYR:CZ	1:B:313:ARG:HD3	2.38	0.59
1:C:163:LEU:HD12	1:C:163:LEU:C	2.23	0.59
1:E:458:GLN:HG2	4:E:578:HOH:O	2.02	0.58
1:C:296:VAL:HG13	1:D:236:SER:HB2	1.86	0.58
1:F:427:ARG:HD3	4:F:558:HOH:O	2.00	0.58
1:A:326:VAL:HG22	1:A:360:GLU:CB	2.33	0.58
1:B:458:GLN:NE2	1:F:142:ARG:HH12	2.02	0.58
1:D:325:THR:O	1:D:329:LYS:HE3	2.04	0.57
1:F:301:GLN:NE2	4:F:507:HOH:O	2.37	0.57
1:D:331:ILE:HD12	1:D:362:ALA:HB1	1.86	0.57
1:D:451:GLU:O	1:D:455:ILE:HG13	2.05	0.57
1:A:187:GLU:HG2	4:A:563:HOH:O	2.04	0.56
1:D:441:GLY:HA2	1:D:462:ILE:HD12	1.85	0.56
1:C:279:LYS:HD3	2:C:500:NAD:C5N	2.35	0.56
1:C:279:LYS:NZ	2:C:500:NAD:C6N	2.67	0.56
1:F:450:ASN:O	1:F:454:THR:HB	2.05	0.56
1:D:10:ILE:HG21	1:D:112:CYS:SG	2.46	0.55
1:B:326:VAL:HG23	1:B:360:GLU:CB	2.36	0.55
1:E:279:LYS:NZ	2:E:500:NAD:C5N	2.68	0.55
1:B:110:GLU:HG2	1:B:143:ILE:HD11	1.88	0.55
1:F:6:LYS:NZ	4:F:525:HOH:O	2.39	0.55
1:D:74:ASN:ND2	1:D:77:ASP:HB2	2.22	0.55
1:C:131:THR:HG21	4:C:541:HOH:O	2.07	0.55
1:D:199:TYR:HA	1:D:202:TRP:CZ3	2.41	0.55
1:B:279:LYS:NZ	2:B:500:NAD:C1D	2.65	0.55
1:B:90:ASN:HB2	2:B:500:NAD:C3N	2.38	0.54
1:F:79:ILE:O	1:F:124:LYS:HE3	2.06	0.54
1:A:292:ASN:CB	4:F:520:HOH:O	2.47	0.54
1:A:326:VAL:HA	1:A:329:LYS:HD2	1.89	0.54
1:B:279:LYS:HZ3	2:B:500:NAD:H1D	1.68	0.54
1:E:279:LYS:HE2	2:E:500:NAD:H6N	1.89	0.54
1:C:389:ASP:O	1:C:392:SER:HB2	2.08	0.54
2:B:500:NAD:C2N	2:B:500:NAD:H51N	2.36	0.54
1:A:279:LYS:NZ	2:A:500:NAD:C1D	2.65	0.53
1:C:170:LYS:HG2	4:C:530:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:PHE:CZ	1:F:233:SER:HB3	2.44	0.53
1:D:34:VAL:O	1:D:71:PHE:HA	2.09	0.53
1:C:390:GLN:HG2	1:C:394:LEU:HD12	1.91	0.53
1:F:181:GLY:HA2	1:F:211:THR:O	2.08	0.53
4:A:579:HOH:O	1:E:409:HIS:HD2	1.91	0.53
1:C:244:THR:HG1	1:D:214:TRP:HE1	1.57	0.53
1:C:262:GLY:HA2	4:C:584:HOH:O	2.08	0.53
1:F:317:ARG:NH2	1:F:461:THR:O	2.41	0.53
1:A:181:GLY:HA2	1:A:211:THR:O	2.09	0.53
1:B:279:LYS:HZ1	2:B:500:NAD:C1D	2.17	0.53
1:C:90:ASN:HA	2:C:500:NAD:H2D	1.91	0.53
1:D:134:VAL:O	1:D:135:ARG:HB2	2.09	0.52
1:A:141:ARG:NH2	1:A:213:THR:OG1	2.42	0.52
1:B:279:LYS:CE	2:B:500:NAD:C6N	2.57	0.52
1:C:242:GLU:OE1	1:C:313:ARG:NH1	2.42	0.52
1:F:334:LEU:HB3	1:F:420:PHE:CZ	2.44	0.52
1:C:201:HIS:HD2	4:C:518:HOH:O	1.92	0.52
1:A:180:ILE:O	1:A:210:THR:HA	2.09	0.52
1:C:90:ASN:HA	2:C:500:NAD:H2N	1.90	0.52
1:A:416:GLU:HG2	1:A:416:GLU:O	2.08	0.52
1:B:443:ARG:HD3	1:B:462:ILE:O	2.09	0.52
1:E:301:GLN:NE2	4:E:593:HOH:O	2.43	0.52
1:B:326:VAL:HG23	1:B:360:GLU:HB3	1.88	0.52
1:C:449:HIS:O	1:C:453:GLN:HG3	2.10	0.51
1:A:320:ASP:O	1:A:323:PHE:N	2.42	0.51
1:B:182:GLY:O	1:B:212:ASN:HA	2.10	0.51
1:D:429:HIS:CE1	1:D:434:LYS:HE3	2.45	0.51
1:B:326:VAL:HG22	1:B:360:GLU:HB3	1.92	0.51
1:D:130:SER:HB2	2:D:500:NAD:O3D	2.10	0.51
1:F:169:ILE:HG12	4:F:499:HOH:O	2.10	0.51
1:A:270:VAL:HG22	1:A:270:VAL:O	2.10	0.51
1:E:160:PRO:HB3	1:E:220:LYS:HG2	1.92	0.51
1:A:29:GLU:HB3	4:A:587:HOH:O	2.10	0.50
1:D:161:GLU:CG	1:D:163:LEU:HD23	2.42	0.50
2:D:500:NAD:H4N	4:D:764:HOH:O	2.11	0.50
1:F:373:ARG:O	1:F:377:VAL:HG23	2.11	0.50
1:C:39:GLU:HG3	1:C:73:THR:HG21	1.94	0.50
1:D:326:VAL:CG1	1:D:331:ILE:HD11	2.42	0.50
1:F:133:PRO:O	1:F:221:LEU:HD11	2.11	0.50
1:C:110:GLU:CG	1:C:143:ILE:HD11	2.42	0.50
1:E:163:LEU:C	1:E:163:LEU:HD12	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:GLU:CG	1:F:143:ILE:HD11	2.42	0.50
1:F:184:GLU:HG3	4:F:554:HOH:O	2.10	0.50
1:B:326:VAL:CG2	1:B:360:GLU:HB2	2.39	0.50
1:B:441:GLY:HA2	1:B:462:ILE:HD13	1.94	0.50
1:C:230:ARG:NH1	1:C:261:ILE:O	2.37	0.50
1:C:2:PHE:HB2	1:C:190:ARG:NH1	2.26	0.49
1:B:287:LEU:HD11	1:B:291:LEU:HD11	1.94	0.49
1:C:310:GLN:OE1	1:C:313:ARG:NH2	2.45	0.49
1:E:162:PHE:CD1	1:E:220:LYS:HE2	2.47	0.49
1:C:207:LYS:HE3	4:C:533:HOH:O	2.12	0.49
1:E:400:ASP:HB2	1:E:401:PRO:CD	2.43	0.49
1:B:166:GLY:HA2	1:B:341:ASP:O	2.12	0.49
1:B:181:GLY:HA2	1:B:211:THR:O	2.13	0.49
1:A:279:LYS:NZ	2:A:500:NAD:N1N	2.60	0.49
1:C:128:GLU:HG3	1:C:136:ALA:HB1	1.93	0.49
1:E:110:GLU:HB3	1:E:143:ILE:HD11	1.95	0.49
1:E:96:TYR:HA	1:E:100:LYS:HB2	1.94	0.49
1:E:312:ARG:CG	1:E:312:ARG:HH11	2.26	0.49
1:F:279:LYS:HD2	2:F:500:NAD:C5N	2.43	0.49
1:E:373:ARG:HB2	1:E:397:ILE:HG21	1.95	0.49
1:F:400:ASP:OD1	1:F:403:GLU:HB2	2.13	0.49
1:E:124:LYS:HB2	1:E:154:LEU:CD2	2.43	0.48
1:F:275:SER:HB2	2:F:500:NAD:C5N	2.43	0.48
1:B:314:PHE:CD1	1:B:462:ILE:CD1	2.96	0.48
1:F:91:THR:CG2	1:F:109:ILE:HD12	2.43	0.48
1:C:110:GLU:HG3	1:C:143:ILE:CD1	2.43	0.48
1:F:177:ARG:HD3	4:F:562:HOH:O	2.13	0.48
1:C:318:ILE:HA	1:C:439:PHE:CE1	2.48	0.48
1:D:123:TYR:O	1:D:124:LYS:HG3	2.12	0.48
1:B:450:ASN:O	1:B:451:GLU:C	2.51	0.48
1:D:130:SER:HB2	2:D:500:NAD:C3D	2.44	0.48
1:F:36:ASP:HB3	1:F:42:ILE:HD11	1.96	0.48
1:C:25:HIS:CE1	1:C:173:LYS:HZ1	2.32	0.48
1:E:325:THR:HG23	1:E:325:THR:O	2.14	0.48
1:A:443:ARG:HD3	1:A:462:ILE:O	2.13	0.48
1:F:91:THR:O	1:F:279:LYS:NZ	2.47	0.48
1:E:118:GLN:HB3	1:E:119:ASN:ND2	2.29	0.47
1:F:175:PRO:O	1:F:207:LYS:HE2	2.14	0.47
1:D:150:PRO:O	1:D:151:ASN:HB2	2.14	0.47
1:C:314:PHE:CD1	1:C:462:ILE:HD11	2.49	0.47
1:F:26:MET:HG3	1:F:202:TRP:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:350:SER:OG	1:F:414:CYS:HB3	2.15	0.47
1:A:343:GLY:O	1:A:371:VAL:HG22	2.14	0.47
1:C:190:ARG:HD3	4:C:521:HOH:O	2.15	0.47
1:C:329:LYS:HD3	1:C:409:HIS:ND1	2.29	0.47
1:E:381:SER:C	4:E:777:HOH:O	2.53	0.47
1:A:281:VAL:HG11	1:A:304:ILE:HG12	1.96	0.47
1:A:431:LYS:HD2	4:A:646:HOH:O	2.14	0.47
1:D:277:PHE:CE2	3:D:501:UDX:H5A1	2.49	0.47
1:E:326:VAL:HG22	1:E:360:GLU:CB	2.42	0.47
1:E:434:LYS:HA	1:E:435:PRO:C	2.33	0.47
1:F:169:ILE:HG22	1:F:173:LYS:HD2	1.97	0.47
1:A:187:GLU:CG	4:A:563:HOH:O	2.63	0.46
1:C:248:VAL:HG12	1:C:463:GLY:HA3	1.96	0.46
1:E:401:PRO:HG2	1:E:423:LEU:HD21	1.95	0.46
1:E:181:GLY:HA2	1:E:211:THR:O	2.15	0.46
1:B:458:GLN:HE21	1:F:142:ARG:HH12	1.63	0.46
1:B:6:LYS:HD2	4:B:601:HOH:O	2.16	0.46
1:C:318:ILE:HG12	1:C:439:PHE:CD1	2.51	0.46
1:D:90:ASN:HB2	2:D:500:NAD:H72N	1.64	0.46
1:E:114:ARG:NH2	4:E:541:HOH:O	2.36	0.46
1:A:441:GLY:HA2	1:A:462:ILE:HG13	1.98	0.46
1:D:128:GLU:HG3	1:D:136:ALA:HB1	1.96	0.46
1:E:45:TRP:O	1:E:65:ARG:NH1	2.49	0.46
1:F:452:LEU:O	1:F:457:PHE:HB2	2.16	0.46
1:D:333:ILE:HB	1:D:366:ILE:HG12	1.97	0.46
1:E:393:ARG:HD2	4:E:695:HOH:O	2.15	0.46
1:E:449:HIS:O	1:E:453:GLN:HG3	2.16	0.46
1:D:84:LEU:HD12	1:D:125:ILE:O	2.16	0.45
1:D:181:GLY:HA2	1:D:211:THR:O	2.16	0.45
1:A:120:SER:HB3	1:A:124:LYS:HE2	1.98	0.45
1:B:222:ALA:O	1:B:226:PHE:HD1	1.99	0.45
1:E:275:SER:O	2:E:500:NAD:C6N	2.64	0.45
1:E:279:LYS:HE3	2:E:500:NAD:O2D	2.16	0.45
1:B:325:THR:HB	4:F:523:HOH:O	2.16	0.45
1:D:439:PHE:CE1	1:D:460:GLU:HG3	2.51	0.45
1:E:114:ARG:NE	4:E:541:HOH:O	2.36	0.45
1:F:131:THR:H	2:F:500:NAD:H4D	1.81	0.45
1:A:163:LEU:HD13	1:A:168:ALA:HB2	1.99	0.45
1:C:102:ARG:NH1	1:C:289:GLU:OE2	2.43	0.45
1:A:142:ARG:HD3	1:E:323:PHE:HE2	1.81	0.45
1:D:374:GLU:O	1:D:378:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LYS:NZ	2:A:500:NAD:C6N	2.79	0.45
1:B:207:LYS:HE3	4:B:556:HOH:O	2.17	0.45
1:A:142:ARG:HD3	1:E:323:PHE:CE2	2.53	0.44
1:C:279:LYS:NZ	2:C:500:NAD:C5N	2.81	0.44
1:D:206:GLU:CD	1:D:206:GLU:H	2.19	0.44
1:E:110:GLU:CD	4:E:570:HOH:O	2.54	0.44
1:A:330:LYS:NZ	1:A:406:ASP:O	2.41	0.44
1:A:326:VAL:CG2	1:A:360:GLU:HB2	2.47	0.44
1:E:50:LEU:HD11	1:E:58:LYS:HA	2.00	0.44
1:B:11:GLY:O	1:B:16:GLY:HA3	2.18	0.44
1:B:429:HIS:CE1	1:B:434:LYS:HE3	2.52	0.44
1:E:340:LYS:O	1:E:341:ASP:HB2	2.18	0.44
1:F:234:ILE:HD11	1:F:252:ALA:HB2	2.00	0.44
1:A:434:LYS:HA	1:A:435:PRO:C	2.39	0.44
1:F:13:GLY:HA2	1:F:41:ARG:NH2	2.33	0.44
1:A:90:ASN:HD22	2:A:500:NAD:H72N	1.66	0.44
2:E:500:NAD:H3D	4:E:535:HOH:O	2.17	0.44
1:F:28:PRO:HA	1:F:68:ASN:ND2	2.33	0.44
1:F:455:ILE:O	1:F:455:ILE:CG2	2.66	0.44
1:B:163:LEU:C	1:B:163:LEU:HD12	2.38	0.43
1:A:281:VAL:O	1:A:285:VAL:HG23	2.18	0.43
1:A:326:VAL:CG2	1:A:360:GLU:CB	2.95	0.43
1:E:263:ASN:OD1	1:E:264:LYS:HD3	2.17	0.43
1:C:251:VAL:O	1:C:255:ILE:HG13	2.18	0.43
1:B:58:LYS:HD2	4:B:573:HOH:O	2.18	0.43
1:F:64:CYS:HB2	1:F:68:ASN:OD1	2.17	0.43
1:F:170:LYS:HG2	4:F:571:HOH:O	2.19	0.43
1:C:443:ARG:HD3	1:C:462:ILE:O	2.18	0.43
1:D:453:GLN:HG3	1:D:459:ILE:HD11	2.00	0.43
1:F:165:GLU:O	1:F:339:LYS:NZ	2.50	0.43
1:A:292:ASN:CA	4:F:520:HOH:O	2.66	0.43
1:D:143:ILE:O	1:D:147:ASN:ND2	2.37	0.43
1:C:134:VAL:HB	4:C:610:HOH:O	2.18	0.43
1:A:150:PRO:O	1:A:151:ASN:HB2	2.19	0.42
1:A:312:ARG:NH2	1:C:98:MET:SD	2.92	0.42
1:B:270:VAL:O	1:B:270:VAL:HG22	2.18	0.42
1:C:193:GLN:HG3	4:C:553:HOH:O	2.18	0.42
1:F:90:ASN:HD22	2:F:500:NAD:H72N	1.65	0.42
1:F:91:THR:HG21	1:F:109:ILE:HD12	2.01	0.42
1:A:340:LYS:O	1:A:341:ASP:HB2	2.19	0.42
1:D:234:ILE:HD12	1:D:234:ILE:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:GLU:O	1:F:55:PRO:C	2.58	0.42
1:F:213:THR:O	1:F:216:SER:HB3	2.19	0.42
1:B:7:ILE:HG12	1:B:84:LEU:HD23	2.00	0.42
1:D:364:LEU:HA	1:D:364:LEU:HD23	1.75	0.42
1:E:43:ASN:O	1:E:47:SER:HB3	2.20	0.42
1:E:207:LYS:HD3	4:E:607:HOH:O	2.19	0.42
1:E:129:LYS:HG3	1:E:159:ASN:O	2.20	0.42
1:F:427:ARG:HA	1:F:430:LYS:HD2	2.02	0.42
1:A:371:VAL:HA	1:A:372:PRO:HD3	1.90	0.42
1:E:247:ASP:HA	1:E:463:GLY:O	2.20	0.42
1:A:15:VAL:O	1:A:19:THR:OG1	2.29	0.42
1:F:90:ASN:CB	2:F:500:NAD:H71N	2.23	0.42
1:C:358:MET:HB3	1:C:390:GLN:NE2	2.35	0.42
1:A:358:MET:HG3	1:A:364:LEU:HD11	2.01	0.42
1:C:177:ARG:CZ	1:D:258:ASP:HB2	2.49	0.42
1:D:30:ILE:O	1:D:68:ASN:HB2	2.20	0.42
1:F:91:THR:N	2:F:500:NAD:H2N	2.33	0.42
1:F:277:PHE:CE2	3:F:501:UDX:H5A1	2.55	0.42
1:A:465:LYS:HB2	4:A:582:HOH:O	2.20	0.41
1:B:128:GLU:HG3	1:B:136:ALA:HB1	2.02	0.41
1:C:124:LYS:HB2	1:C:154:LEU:HD23	2.01	0.41
1:D:161:GLU:O	1:D:220:LYS:CE	2.68	0.41
1:D:330:LYS:HG2	1:D:408:ALA:HA	2.01	0.41
1:E:257:MET:O	1:F:176:ASP:HB3	2.20	0.41
1:E:312:ARG:HH11	1:E:312:ARG:HG3	1.84	0.41
1:F:434:LYS:HA	1:F:435:PRO:C	2.39	0.41
1:A:289:GLU:HG2	4:A:783:HOH:O	2.19	0.41
1:B:434:LYS:HA	1:B:435:PRO:C	2.40	0.41
1:C:329:LYS:HB3	1:C:409:HIS:CD2	2.55	0.41
1:E:141:ARG:NH2	1:E:213:THR:OG1	2.54	0.41
1:F:110:GLU:HG3	1:F:143:ILE:HD11	2.01	0.41
1:A:35:VAL:HA	1:A:72:SER:O	2.20	0.41
1:F:90:ASN:ND2	2:F:500:NAD:N7N	2.67	0.41
1:C:91:THR:H	2:C:500:NAD:C2N	2.33	0.41
1:D:270:VAL:O	1:D:270:VAL:HG22	2.20	0.41
1:E:124:LYS:HB2	1:E:154:LEU:HD23	2.02	0.41
1:F:114:ARG:HG3	1:F:143:ILE:HD13	2.02	0.41
1:F:279:LYS:HD2	2:F:500:NAD:C6N	2.51	0.41
1:A:85:VAL:HG11	1:A:116:ILE:CD1	2.50	0.41
1:C:277:PHE:CE2	3:C:501:UDX:H5A1	2.56	0.41
1:C:279:LYS:HD3	2:C:500:NAD:H5N	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:ASP:HB3	4:D:531:HOH:O	2.20	0.41
1:F:322:LEU:HD23	1:F:437:PHE:CD1	2.55	0.41
1:E:320:ASP:CB	4:E:513:HOH:O	2.51	0.41
1:A:19:THR:O	1:A:23:ILE:HG13	2.21	0.41
1:A:64:CYS:HB2	1:A:68:ASN:OD1	2.21	0.41
1:A:112:CYS:O	1:A:116:ILE:HG13	2.21	0.41
1:B:91:THR:OG1	1:B:279:LYS:NZ	2.54	0.41
1:E:17:GLY:HA3	1:E:45:TRP:CZ2	2.56	0.41
1:E:279:LYS:HZ3	1:E:279:LYS:HG3	1.63	0.41
1:E:180:ILE:O	1:E:210:THR:HA	2.20	0.41
1:E:249:GLU:OE2	1:E:267:LYS:HE2	2.20	0.40
1:D:28:PRO:HA	1:D:68:ASN:ND2	2.35	0.40
1:A:29:GLU:CB	4:A:587:HOH:O	2.69	0.40
1:A:326:VAL:HA	1:A:329:LYS:CD	2.52	0.40
1:C:91:THR:H	2:C:500:NAD:H2N	1.86	0.40
1:C:400:ASP:HB2	1:C:401:PRO:CD	2.51	0.40
1:E:11:GLY:HA3	1:E:88:SER:O	2.21	0.40
1:D:42:ILE:HD13	1:D:42:ILE:HA	1.93	0.40
1:F:279:LYS:HE2	2:F:500:NAD:C6N	2.51	0.40
1:D:37:VAL:HG13	2:D:500:NAD:C2A	2.51	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	454/494 (92%)	428 (94%)	26 (6%)	0	100	100
1	B	453/494 (92%)	434 (96%)	19 (4%)	0	100	100
1	C	453/494 (92%)	428 (94%)	23 (5%)	2 (0%)	34	54
1	D	453/494 (92%)	426 (94%)	25 (6%)	2 (0%)	34	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	454/494 (92%)	435 (96%)	19 (4%)	0	100	100
1	F	453/494 (92%)	423 (93%)	29 (6%)	1 (0%)	47	68
All	All	2720/2964 (92%)	2574 (95%)	141 (5%)	5 (0%)	47	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	327	THR
1	C	328	ASP
1	D	118	GLN
1	D	133	PRO
1	F	448	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/426 (92%)	387 (98%)	6 (2%)	65	85
1	B	392/426 (92%)	384 (98%)	8 (2%)	55	79
1	C	392/426 (92%)	379 (97%)	13 (3%)	38	64
1	D	392/426 (92%)	370 (94%)	22 (6%)	21	40
1	E	393/426 (92%)	384 (98%)	9 (2%)	50	76
1	F	392/426 (92%)	368 (94%)	24 (6%)	18	36
All	All	2354/2556 (92%)	2272 (96%)	82 (4%)	36	62

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	A	117	VAL
1	A	174	ASN
1	A	177	ARG
1	A	267	LYS

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Mol	Chain	Res	Type
1	A	450	ASN
1	B	81	GLU
1	B	96	TYR
1	B	142	ARG
1	B	177	ARG
1	B	320	ASP
1	B	392	SER
1	B	400	ASP
1	B	459	ILE
1	C	63	SER
1	C	118	GLN
1	C	142	ARG
1	C	163	LEU
1	C	177	ARG
1	C	193	GLN
1	C	267	LYS
1	C	319	ILE
1	C	327	THR
1	C	328	ASP
1	C	373	ARG
1	C	391	VAL
1	C	465	LYS
1	D	33	THR
1	D	72	SER
1	D	90	ASN
1	D	96	TYR
1	D	102	ARG
1	D	135	ARG
1	D	142	ARG
1	D	177	ARG
1	D	187	GLU
1	D	190	ARG
1	D	193	GLN
1	D	267	LYS
1	D	279	LYS
1	D	320	ASP
1	D	326	VAL
1	D	374	GLU
1	D	391	VAL
1	D	403	GLU
1	D	422	GLU
1	D	426	GLU

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Mol	Chain	Res	Type
1	D	459	ILE
1	D	462	ILE
1	E	25	HIS
1	E	63	SER
1	E	118	GLN
1	E	142	ARG
1	E	177	ARG
1	E	279	LYS
1	E	312	ARG
1	E	326	VAL
1	E	373	ARG
1	F	5	LYS
1	F	33	THR
1	F	40	SER
1	F	41	ARG
1	F	64	CYS
1	F	81	GLU
1	F	117	VAL
1	F	132	VAL
1	F	148	THR
1	F	177	ARG
1	F	221	LEU
1	F	316	SER
1	F	317	ARG
1	F	355	LYS
1	F	365	HIS
1	F	392	SER
1	F	400	ASP
1	F	421	LYS
1	F	422	GLU
1	F	431	LYS
1	F	444	VAL
1	F	454	THR
1	F	459	ILE
1	F	465	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	HIS
1	A	453	GLN
1	B	324	ASN

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Mol	Chain	Res	Type
1	B	429	HIS
1	B	458	GLN
1	C	301	GLN
1	E	278	GLN
1	E	301	GLN
1	E	302	GLN
1	E	409	HIS
1	F	229	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	A	500	-	42,48,48	2.58	8 (19%)	50,73,73	2.70	16 (32%)
2	NAD	B	500	-	42,48,48	3.18	9 (21%)	50,73,73	3.14	18 (36%)
2	NAD	D	500	-	42,48,48	2.42	8 (19%)	50,73,73	1.99	11 (22%)
3	UDX	A	501	-	33,36,36	1.20	4 (12%)	50,55,55	2.02	13 (26%)
3	UDX	E	501	-	33,36,36	1.17	2 (6%)	50,55,55	1.85	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	UDX	B	501	-	33,36,36	1.43	3 (9%)	50,55,55	1.75	8 (16%)
3	UDX	C	501	-	33,36,36	1.01	1 (3%)	50,55,55	1.70	12 (24%)
2	NAD	E	500	-	42,48,48	3.02	8 (19%)	50,73,73	2.19	12 (24%)
3	UDX	D	501	-	33,36,36	1.14	1 (3%)	50,55,55	1.91	11 (22%)
2	NAD	C	500	-	42,48,48	2.37	9 (21%)	50,73,73	2.00	16 (32%)
3	UDX	F	501	-	33,36,36	1.05	2 (6%)	50,55,55	1.82	11 (22%)
2	NAD	F	500	-	42,48,48	2.57	8 (19%)	50,73,73	2.35	15 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	500	-	-	7/26/62/62	0/5/5/5
2	NAD	B	500	-	-	10/26/62/62	0/5/5/5
2	NAD	D	500	-	-	5/26/62/62	0/5/5/5
3	UDX	A	501	-	-	4/21/54/54	0/3/3/3
3	UDX	E	501	-	-	3/21/54/54	0/3/3/3
3	UDX	B	501	-	-	2/21/54/54	0/3/3/3
3	UDX	C	501	-	-	4/21/54/54	0/3/3/3
2	NAD	E	500	-	-	7/26/62/62	0/5/5/5
3	UDX	D	501	-	-	1/21/54/54	0/3/3/3
2	NAD	C	500	-	-	8/26/62/62	0/5/5/5
3	UDX	F	501	-	-	2/21/54/54	0/3/3/3
2	NAD	F	500	-	-	11/26/62/62	0/5/5/5

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	NAD	O4D-C1D	12.27	1.58	1.41
2	B	500	NAD	C2N-N1N	10.66	1.47	1.35
2	E	500	NAD	C4N-C3N	10.43	1.57	1.39
2	B	500	NAD	C4N-C3N	10.34	1.57	1.39
2	A	500	NAD	C4N-C3N	9.60	1.55	1.39
2	C	500	NAD	C4N-C3N	9.04	1.54	1.39
2	D	500	NAD	C4N-C3N	8.90	1.54	1.39
2	F	500	NAD	C4N-C3N	8.88	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NAD	C2N-N1N	8.30	1.45	1.35
2	D	500	NAD	C2N-N1N	8.21	1.45	1.35
2	F	500	NAD	C2N-N1N	8.02	1.44	1.35
2	E	500	NAD	C2N-N1N	7.84	1.44	1.35
2	B	500	NAD	C3N-C7N	7.76	1.62	1.50
2	F	500	NAD	O4D-C1D	7.04	1.50	1.41
2	C	500	NAD	C2N-N1N	6.99	1.43	1.35
2	B	500	NAD	O4D-C1D	6.98	1.50	1.41
2	A	500	NAD	O4D-C1D	5.60	1.48	1.41
2	D	500	NAD	O4D-C1D	5.37	1.48	1.41
2	C	500	NAD	C3N-C7N	4.72	1.57	1.50
2	B	500	NAD	C2N-C3N	4.71	1.46	1.39
2	F	500	NAD	C3N-C7N	4.38	1.57	1.50
3	B	501	UDX	C2-N1	4.16	1.45	1.38
2	C	500	NAD	O4D-C1D	4.09	1.46	1.41
3	B	501	UDX	O4D-C4D	3.93	1.53	1.45
2	F	500	NAD	C2N-C3N	3.87	1.45	1.39
2	E	500	NAD	C6N-N1N	3.84	1.44	1.35
2	A	500	NAD	C6N-N1N	3.81	1.44	1.35
2	B	500	NAD	C6N-N1N	3.77	1.44	1.35
2	D	500	NAD	C3N-C7N	3.57	1.55	1.50
2	A	500	NAD	C3N-C7N	3.56	1.55	1.50
2	B	500	NAD	O4D-C4D	3.45	1.52	1.45
2	A	500	NAD	C2N-C3N	3.42	1.44	1.39
2	D	500	NAD	PN-O1N	3.42	1.63	1.50
2	C	500	NAD	O2D-C2D	3.33	1.50	1.43
3	D	501	UDX	C2-N1	3.29	1.43	1.38
2	C	500	NAD	C2N-C3N	3.25	1.44	1.39
3	E	501	UDX	O5'-C5'	3.22	1.48	1.43
2	F	500	NAD	PN-O1N	3.17	1.62	1.50
2	C	500	NAD	C2D-C3D	3.05	1.61	1.53
2	F	500	NAD	C2D-C3D	3.02	1.61	1.53
2	B	500	NAD	C2D-C1D	2.97	1.58	1.53
2	A	500	NAD	O4B-C1B	2.91	1.45	1.41
2	D	500	NAD	O4B-C1B	2.89	1.45	1.41
2	C	500	NAD	PN-O1N	2.79	1.60	1.50
3	A	501	UDX	C4'-C3'	2.65	1.56	1.52
3	A	501	UDX	C2-N1	2.62	1.42	1.38
2	E	500	NAD	C3N-C7N	2.61	1.54	1.50
3	C	501	UDX	O5'-C5'	2.61	1.47	1.43
2	B	500	NAD	PN-O1N	2.54	1.59	1.50
3	A	501	UDX	O4D-C4D	2.54	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	UDX	O5'-C5'	-2.50	1.39	1.43
2	D	500	NAD	C6N-N1N	2.49	1.41	1.35
2	D	500	NAD	C2N-C3N	2.48	1.42	1.39
3	A	501	UDX	O5'-C1'	2.48	1.47	1.41
3	F	501	UDX	C5-C4	-2.30	1.38	1.43
2	C	500	NAD	O4B-C1B	2.29	1.44	1.41
2	E	500	NAD	C2B-C1B	-2.25	1.50	1.53
3	F	501	UDX	O2D-C2D	2.24	1.48	1.43
2	A	500	NAD	C2B-C1B	-2.24	1.50	1.53
2	E	500	NAD	C6N-C5N	2.13	1.43	1.38
3	E	501	UDX	C6-C5	2.12	1.40	1.35
2	E	500	NAD	C2N-C3N	2.05	1.42	1.39
2	F	500	NAD	C6N-N1N	2.01	1.40	1.35

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	NAD	C6N-N1N-C2N	-10.72	112.20	121.97
2	B	500	NAD	O4D-C1D-C2D	-8.59	94.38	106.93
2	E	500	NAD	C6N-N1N-C2N	-8.37	114.34	121.97
2	A	500	NAD	C6N-N1N-C2N	-7.81	114.86	121.97
2	F	500	NAD	C5N-C4N-C3N	-7.16	111.88	120.34
2	E	500	NAD	C5N-C4N-C3N	-6.77	112.33	120.34
3	F	501	UDX	O5'-C1'-O3B	-6.73	102.57	111.36
2	B	500	NAD	C5D-C4D-C3D	-6.65	90.27	115.18
3	D	501	UDX	O5'-C1'-O3B	-6.48	102.90	111.36
2	F	500	NAD	C6N-N1N-C2N	-6.40	116.14	121.97
3	A	501	UDX	C4-N3-C2	-6.37	118.18	126.58
2	C	500	NAD	C5N-C4N-C3N	-6.22	112.98	120.34
2	A	500	NAD	C2N-N1N-C1D	6.12	132.76	119.14
2	B	500	NAD	C2N-N1N-C1D	5.89	132.25	119.14
3	B	501	UDX	C4-N3-C2	-5.89	118.81	126.58
3	E	501	UDX	C4-N3-C2	-5.81	118.91	126.58
2	A	500	NAD	C5N-C4N-C3N	-5.79	113.49	120.34
2	D	500	NAD	C5N-C4N-C3N	-5.73	113.57	120.34
3	D	501	UDX	C4-N3-C2	-5.69	119.07	126.58
3	C	501	UDX	C4-N3-C2	-5.62	119.16	126.58
2	A	500	NAD	C5D-C4D-C3D	-5.51	94.54	115.18
2	D	500	NAD	C6N-N1N-C2N	-5.13	117.30	121.97
3	A	501	UDX	C5-C4-N3	5.06	122.41	114.84
2	B	500	NAD	C5N-C4N-C3N	-5.06	114.35	120.34
2	B	500	NAD	N3A-C2A-N1A	-4.86	121.08	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	501	UDX	N3-C2-N1	4.81	121.27	114.89
2	A	500	NAD	C2N-C3N-C4N	4.74	123.64	118.26
2	F	500	NAD	C2N-N1N-C1D	4.74	129.70	119.14
2	A	500	NAD	O4D-C1D-C2D	-4.61	100.19	106.93
2	B	500	NAD	C5N-C6N-N1N	4.61	127.01	120.40
2	C	500	NAD	N3A-C2A-N1A	-4.54	121.58	128.68
2	A	500	NAD	C3D-C2D-C1D	4.53	107.80	100.98
2	F	500	NAD	N3A-C2A-N1A	-4.52	121.62	128.68
2	F	500	NAD	C6N-C5N-C4N	4.51	125.99	119.44
2	A	500	NAD	C5N-C6N-N1N	4.49	126.84	120.40
3	F	501	UDX	C4-N3-C2	-4.47	120.68	126.58
2	D	500	NAD	N3A-C2A-N1A	-4.47	121.70	128.68
2	E	500	NAD	O4D-C1D-C2D	-4.45	100.42	106.93
3	F	501	UDX	N3-C2-N1	4.44	120.79	114.89
3	A	501	UDX	C5'-O5'-C1'	4.44	121.35	112.38
3	B	501	UDX	C5-C4-N3	4.41	121.43	114.84
2	A	500	NAD	O3D-C3D-C4D	-4.39	98.36	111.05
2	F	500	NAD	C5D-C4D-C3D	-4.32	99.01	115.18
2	B	500	NAD	C3D-C2D-C1D	4.21	107.32	100.98
2	B	500	NAD	O4D-C4D-C5D	4.19	123.16	109.37
2	B	500	NAD	C5B-C4B-C3B	-4.17	99.55	115.18
2	D	500	NAD	O4D-C1D-C2D	-4.14	100.88	106.93
2	A	500	NAD	O4B-C1B-C2B	-4.03	101.03	106.93
3	B	501	UDX	PA-O3A-PB	-4.03	118.99	132.83
3	D	501	UDX	C5-C4-N3	4.01	120.84	114.84
3	C	501	UDX	C5-C4-N3	3.98	120.79	114.84
2	C	500	NAD	C2N-N1N-C1D	3.95	127.94	119.14
2	C	500	NAD	C6N-C5N-C4N	3.95	125.18	119.44
3	B	501	UDX	N3-C2-N1	3.93	120.11	114.89
3	E	501	UDX	O3A-PB-O3B	3.88	110.30	102.48
2	E	500	NAD	C2N-C3N-C4N	3.86	122.63	118.26
2	B	500	NAD	O7N-C7N-C3N	3.83	124.22	119.63
3	E	501	UDX	O5'-C1'-C2'	-3.72	104.33	110.04
2	D	500	NAD	C6N-C5N-C4N	3.65	124.74	119.44
2	A	500	NAD	N3A-C2A-N1A	-3.64	122.98	128.68
2	C	500	NAD	C4N-C3N-C7N	-3.63	111.32	121.04
3	E	501	UDX	C5-C4-N3	3.60	120.23	114.84
3	E	501	UDX	O5'-C5'-C4'	-3.59	105.22	110.77
2	C	500	NAD	O4B-C1B-C2B	-3.57	101.71	106.93
2	D	500	NAD	PN-O3-PA	-3.54	120.68	132.83
2	F	500	NAD	C4N-C3N-C7N	-3.54	111.57	121.04
3	D	501	UDX	N3-C2-N1	3.51	119.55	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	NAD	O7N-C7N-N7N	-3.51	117.59	122.58
3	C	501	UDX	N3-C2-N1	3.50	119.53	114.89
2	F	500	NAD	O4D-C1D-C2D	-3.41	101.94	106.93
2	E	500	NAD	N3A-C2A-N1A	-3.39	123.38	128.68
2	E	500	NAD	C5N-C6N-N1N	3.36	125.22	120.40
2	C	500	NAD	C5D-C4D-C3D	-3.36	102.61	115.18
2	B	500	NAD	C3N-C2N-N1N	3.34	123.69	120.43
3	D	501	UDX	O5'-C5'-C4'	-3.32	105.64	110.77
3	A	501	UDX	O4'-C4'-C5'	-3.28	102.44	109.15
2	E	500	NAD	O4B-C1B-C2B	-3.28	102.14	106.93
3	C	501	UDX	O5'-C1'-O3B	-3.26	107.11	111.36
3	F	501	UDX	O2-C2-N1	-3.25	118.47	122.79
2	A	500	NAD	PN-O3-PA	-3.20	121.85	132.83
2	A	500	NAD	C4N-C3N-C7N	-3.16	112.59	121.04
3	A	501	UDX	O4-C4-C5	-3.11	119.69	125.16
3	B	501	UDX	O5'-C1'-O3B	-3.11	107.30	111.36
3	C	501	UDX	O4-C4-C5	-3.08	119.75	125.16
3	D	501	UDX	O3D-C3D-C4D	-3.07	102.16	111.05
3	A	501	UDX	O5'-C1'-C2'	3.07	114.76	110.04
3	B	501	UDX	O3A-PB-O3B	3.06	108.65	102.48
3	A	501	UDX	N3-C2-N1	3.05	118.94	114.89
2	F	500	NAD	O4D-C4D-C5D	3.05	119.40	109.37
3	B	501	UDX	O5'-C5'-C4'	2.98	115.36	110.77
2	D	500	NAD	C2N-N1N-C1D	2.97	125.75	119.14
3	A	501	UDX	O5'-C5'-C4'	-2.97	106.19	110.77
2	C	500	NAD	C2N-C3N-C7N	2.94	128.01	119.46
3	F	501	UDX	C5-C4-N3	2.90	119.18	114.84
3	D	501	UDX	O4-C4-C5	-2.81	120.22	125.16
3	A	501	UDX	PA-O3A-PB	-2.78	123.28	132.83
3	A	501	UDX	O3A-PB-O3B	2.77	108.07	102.48
2	B	500	NAD	O3D-C3D-C4D	-2.76	103.06	111.05
3	C	501	UDX	O2-C2-N1	-2.75	119.13	122.79
2	E	500	NAD	C6N-C5N-C4N	2.69	123.34	119.44
2	F	500	NAD	C2N-C3N-C7N	2.65	127.17	119.46
2	F	500	NAD	C2N-C3N-C4N	2.64	121.25	118.26
2	D	500	NAD	O4B-C1B-C2B	-2.64	103.07	106.93
2	F	500	NAD	C3D-C2D-C1D	2.63	104.94	100.98
2	B	500	NAD	C6N-C5N-C4N	2.61	123.24	119.44
2	C	500	NAD	C3D-C2D-C1D	2.49	104.73	100.98
2	C	500	NAD	C6N-N1N-C2N	-2.48	119.72	121.97
3	F	501	UDX	O3D-C3D-C4D	-2.46	103.94	111.05
3	D	501	UDX	O5'-C1'-C2'	2.45	113.80	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	501	UDX	O4-C4-C5	-2.43	120.89	125.16
3	A	501	UDX	C5-C6-N1	-2.42	117.76	121.81
3	E	501	UDX	PA-O3A-PB	-2.41	124.57	132.83
3	C	501	UDX	C5'-C4'-C3'	2.40	112.61	109.67
2	E	500	NAD	C5B-C4B-C3B	-2.39	106.22	115.18
2	B	500	NAD	C1B-N9A-C4A	-2.39	122.44	126.64
3	F	501	UDX	O3B-PB-O1B	2.39	118.42	109.47
3	C	501	UDX	O4'-C4'-C3'	-2.38	105.36	110.14
3	F	501	UDX	C6-N1-C2	-2.34	118.00	120.99
3	C	501	UDX	O4D-C1D-N1	-2.31	103.08	108.36
2	A	500	NAD	O2D-C2D-C3D	-2.30	104.40	111.82
3	C	501	UDX	O5'-C1'-C2'	2.28	113.54	110.04
2	D	500	NAD	C2N-C3N-C4N	2.27	120.83	118.26
3	C	501	UDX	C5-C6-N1	-2.26	118.02	121.81
2	F	500	NAD	O3D-C3D-C2D	2.25	119.08	111.82
2	D	500	NAD	C4A-C5A-N7A	-2.21	107.09	109.40
2	C	500	NAD	O2A-PA-O1A	-2.21	101.31	112.24
3	F	501	UDX	O3B-C1'-C2'	2.21	112.42	108.38
2	A	500	NAD	PN-O5D-C5D	-2.20	108.76	121.68
2	C	500	NAD	PN-O3-PA	-2.20	125.27	132.83
3	B	501	UDX	O4-C4-C5	-2.20	121.29	125.16
3	E	501	UDX	C5'-O5'-C1'	2.20	116.82	112.38
3	F	501	UDX	PA-O3A-PB	-2.18	125.35	132.83
2	E	500	NAD	C2N-N1N-C1D	2.18	123.98	119.14
3	C	501	UDX	O3A-PB-O3B	2.17	106.85	102.48
3	E	501	UDX	C5-C6-N1	-2.16	118.19	121.81
3	D	501	UDX	C4'-C3'-C2'	-2.16	107.16	110.89
3	E	501	UDX	O3B-C1'-C2'	2.15	112.32	108.38
2	C	500	NAD	C2N-C3N-C4N	2.13	120.67	118.26
2	E	500	NAD	C4A-C5A-N7A	-2.12	107.19	109.40
2	C	500	NAD	O2D-C2D-C3D	2.12	118.67	111.82
3	D	501	UDX	O4'-C4'-C3'	2.11	114.36	110.14
3	A	501	UDX	O4D-C1D-C2D	-2.10	102.05	106.64
2	D	500	NAD	C3D-C2D-C1D	-2.10	97.82	100.98
2	E	500	NAD	C1B-N9A-C4A	-2.10	122.96	126.64
2	B	500	NAD	O2N-PN-O5D	2.09	117.47	107.75
2	F	500	NAD	O3D-C3D-C4D	-2.09	105.00	111.05
3	E	501	UDX	O2-C2-N3	-2.08	117.62	121.50
2	F	500	NAD	C5N-C6N-N1N	2.07	123.38	120.40
2	A	500	NAD	O4D-C4D-C5D	2.06	116.16	109.37
3	D	501	UDX	O3A-PB-O3B	2.05	106.62	102.48
2	B	500	NAD	O5D-C5D-C4D	2.05	116.05	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	UDX	C5D-C4D-C3D	-2.03	107.58	115.18
2	C	500	NAD	C4A-C5A-N7A	-2.03	107.29	109.40
2	C	500	NAD	O4D-C4D-C5D	2.01	115.98	109.37

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	NAD	O4D-C1D-N1N-C2N
2	A	500	NAD	O4D-C1D-N1N-C6N
2	A	500	NAD	C2D-C1D-N1N-C6N
2	B	500	NAD	O4D-C1D-N1N-C2N
2	B	500	NAD	O4D-C1D-N1N-C6N
2	B	500	NAD	C2D-C1D-N1N-C2N
2	B	500	NAD	C2D-C1D-N1N-C6N
2	C	500	NAD	C5D-O5D-PN-O1N
2	C	500	NAD	O4D-C4D-C5D-O5D
2	C	500	NAD	O4D-C1D-N1N-C6N
2	C	500	NAD	C2D-C1D-N1N-C6N
2	D	500	NAD	O4D-C1D-N1N-C2N
2	D	500	NAD	O4D-C1D-N1N-C6N
2	D	500	NAD	C2D-C1D-N1N-C2N
2	D	500	NAD	C2D-C1D-N1N-C6N
2	E	500	NAD	C5D-O5D-PN-O3
2	E	500	NAD	O4D-C1D-N1N-C2N
2	F	500	NAD	C5D-O5D-PN-O1N
2	F	500	NAD	C5D-O5D-PN-O2N
2	F	500	NAD	C2D-C1D-N1N-C2N
2	F	500	NAD	C2D-C1D-N1N-C6N
3	A	501	UDX	PA-O3A-PB-O3B
2	B	500	NAD	O4D-C4D-C5D-O5D
2	F	500	NAD	O4D-C4D-C5D-O5D
2	B	500	NAD	C3B-C4B-C5B-O5B
2	F	500	NAD	C3D-C4D-C5D-O5D
3	A	501	UDX	C1'-O3B-PB-O3A
2	E	500	NAD	O4D-C4D-C5D-O5D
3	B	501	UDX	C1'-O3B-PB-O3A
3	C	501	UDX	C1'-O3B-PB-O3A
3	D	501	UDX	C1'-O3B-PB-O3A
2	B	500	NAD	O4B-C4B-C5B-O5B
2	E	500	NAD	C3D-C4D-C5D-O5D
3	E	501	UDX	C1'-O3B-PB-O3A

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Mol	Chain	Res	Type	Atoms
3	F	501	UDX	C1'-O3B-PB-O3A
2	A	500	NAD	PN-O3-PA-O5B
2	F	500	NAD	PN-O3-PA-O5B
3	C	501	UDX	PA-O3A-PB-O3B
3	E	501	UDX	PA-O3A-PB-O3B
2	A	500	NAD	O4D-C4D-C5D-O5D
2	C	500	NAD	C5D-O5D-PN-O3
2	F	500	NAD	C5D-O5D-PN-O3
3	A	501	UDX	PB-O3A-PA-O2A
2	B	500	NAD	C5D-O5D-PN-O1N
2	B	500	NAD	C5D-O5D-PN-O2N
2	C	500	NAD	C5D-O5D-PN-O2N
2	E	500	NAD	C5D-O5D-PN-O1N
2	E	500	NAD	C5D-O5D-PN-O2N
2	F	500	NAD	O4B-C4B-C5B-O5B
2	F	500	NAD	PA-O3-PN-O2N
2	B	500	NAD	C3D-C4D-C5D-O5D
3	A	501	UDX	PB-O3A-PA-O1A
3	B	501	UDX	PB-O3A-PA-O1A
3	C	501	UDX	PB-O3A-PA-O1A
3	E	501	UDX	PB-O3A-PA-O1A
2	A	500	NAD	C2D-C1D-N1N-C2N
2	C	500	NAD	C2D-C1D-N1N-C2N
2	A	500	NAD	O4B-C4B-C5B-O5B
2	C	500	NAD	O4B-C4B-C5B-O5B
2	D	500	NAD	O4B-C4B-C5B-O5B
2	F	500	NAD	PA-O3-PN-O1N
3	C	501	UDX	C5D-O5D-PA-O1A
3	F	501	UDX	C5D-O5D-PA-O1A
2	E	500	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

9 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NAD	12	0
2	B	500	NAD	18	0
2	D	500	NAD	10	0
3	C	501	UDX	1	0
2	E	500	NAD	11	0
3	D	501	UDX	1	0
2	C	500	NAD	13	0

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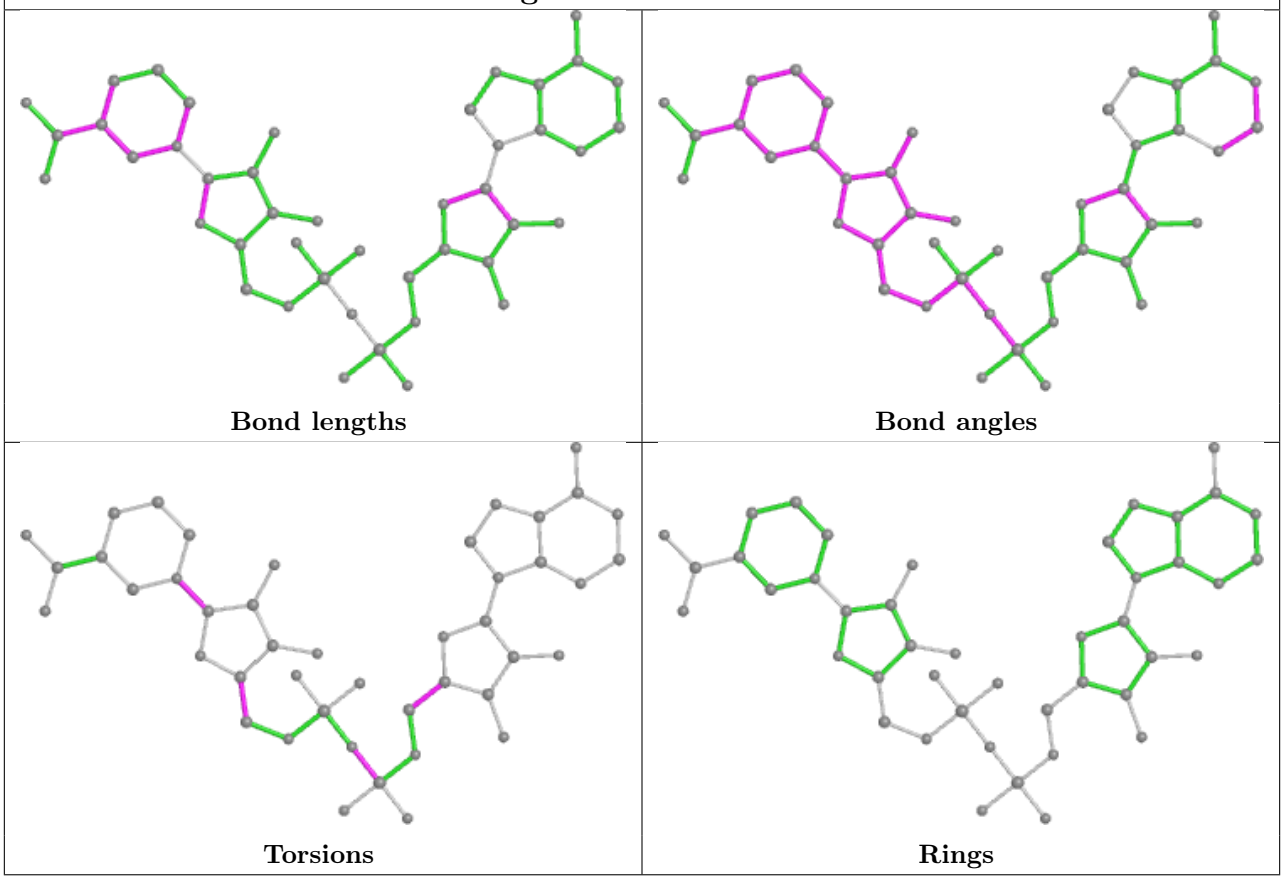
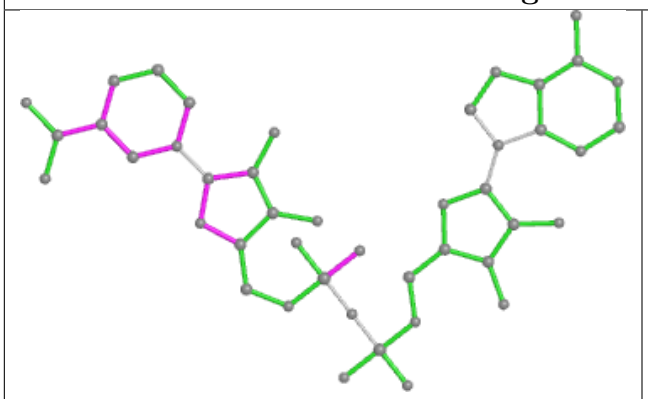
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	501	UDX	1	0
2	F	500	NAD	14	0

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

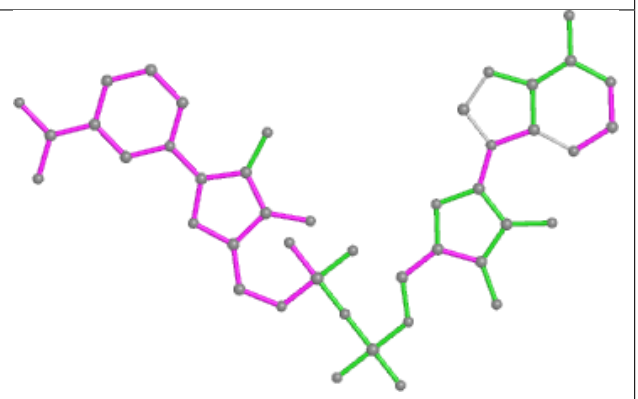
Ligand NAD A 500



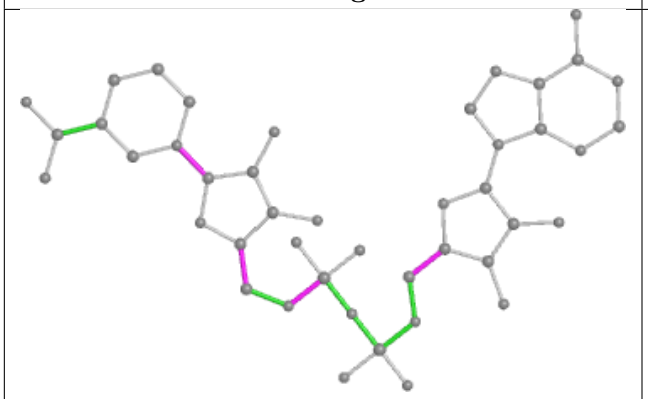
Ligand NAD B 500



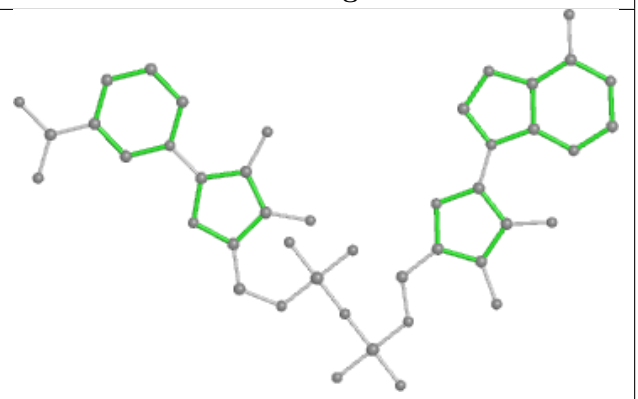
Bond lengths



Bond angles

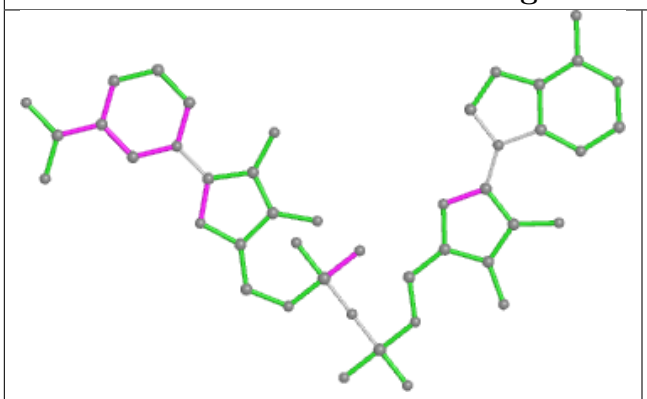


Torsions



Rings

Ligand NAD D 500



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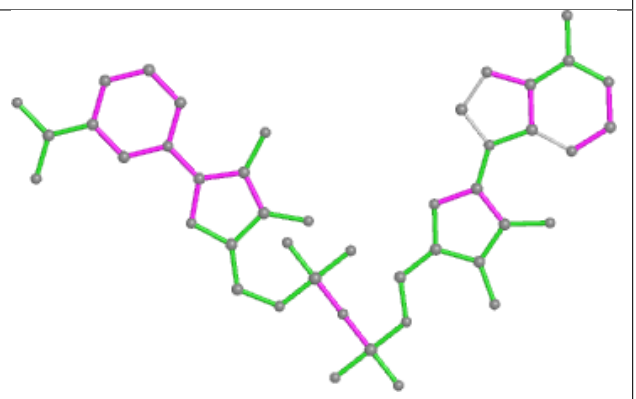
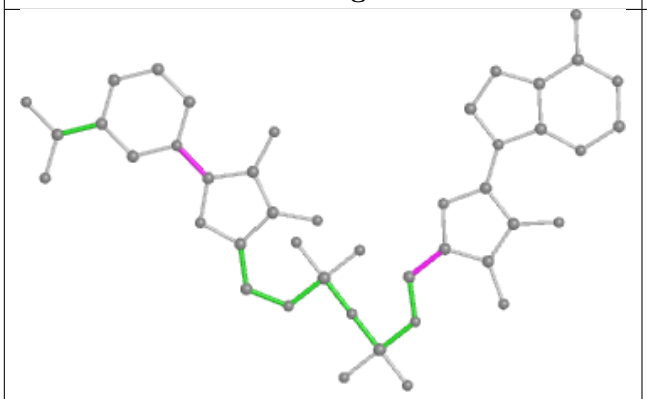


Bond angles



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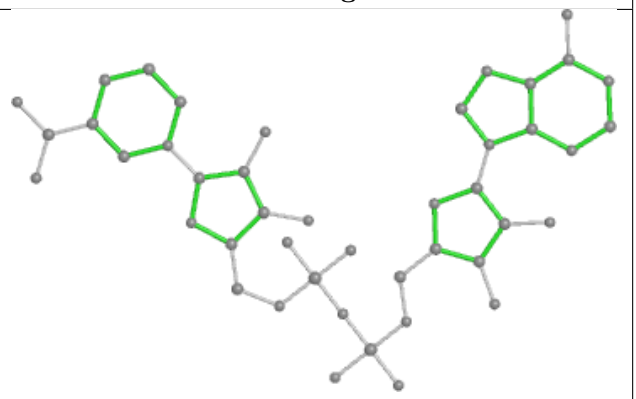
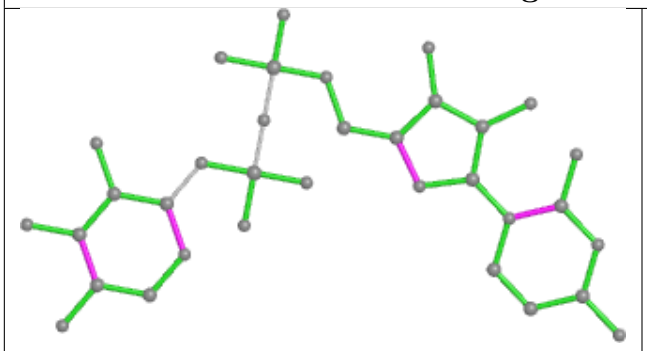
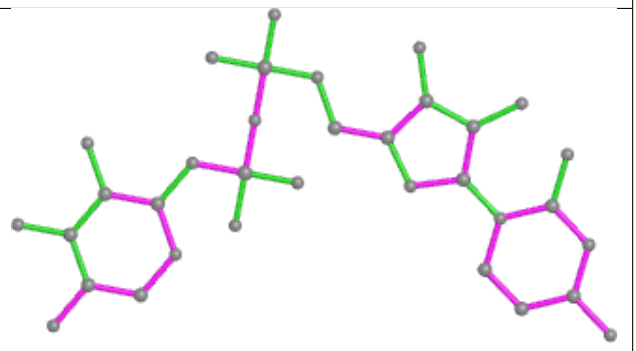


Rings

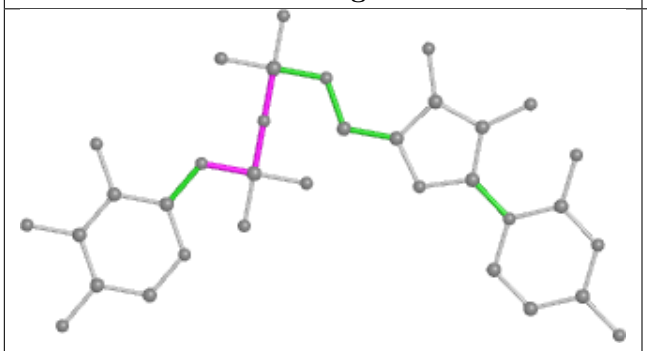
Ligand UDX A 501



Bond lengths



Bond angles



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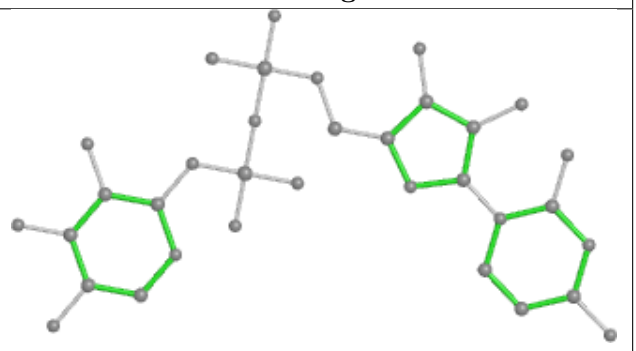
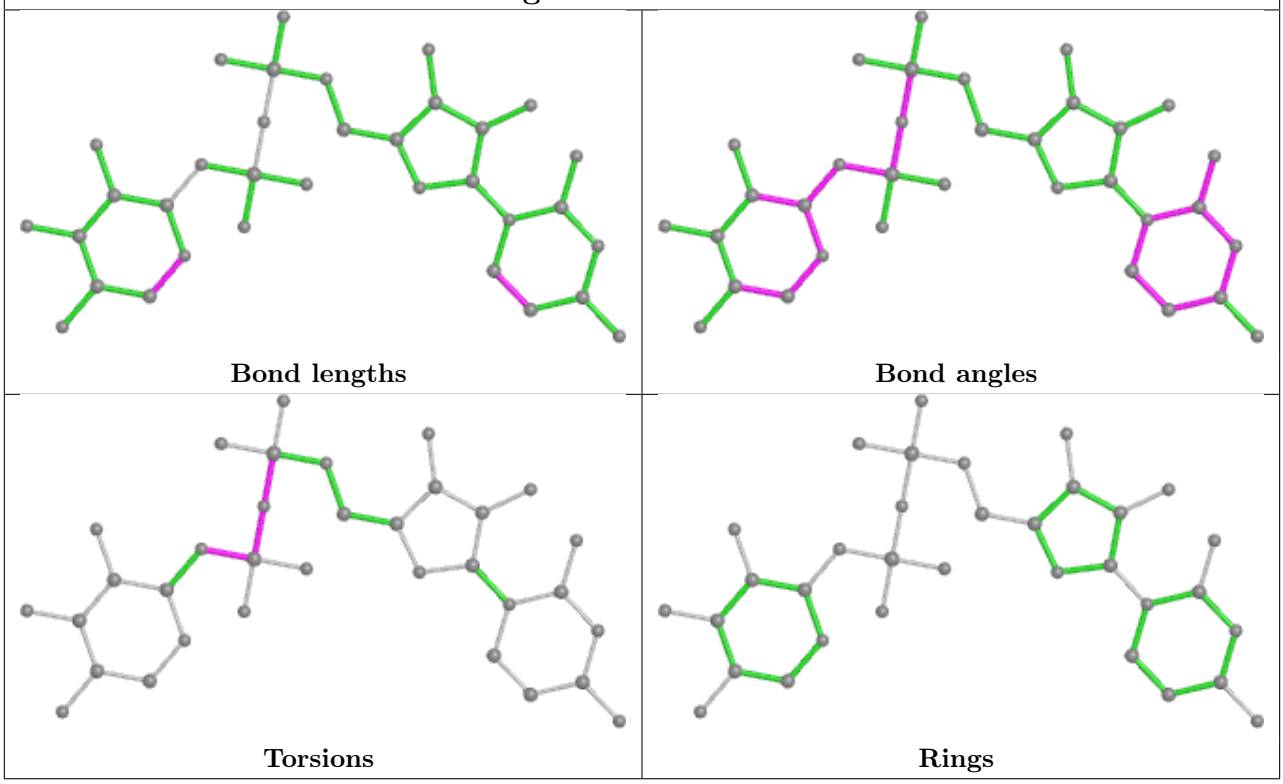
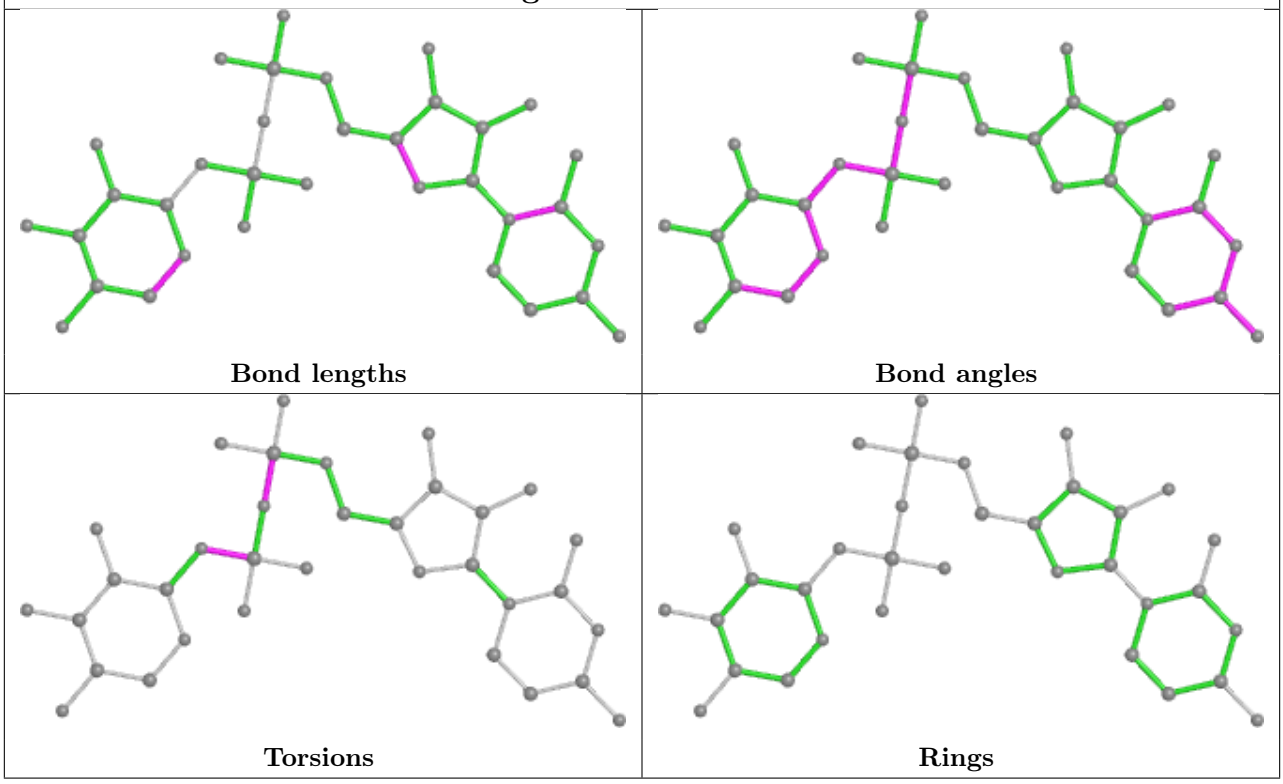


Rings

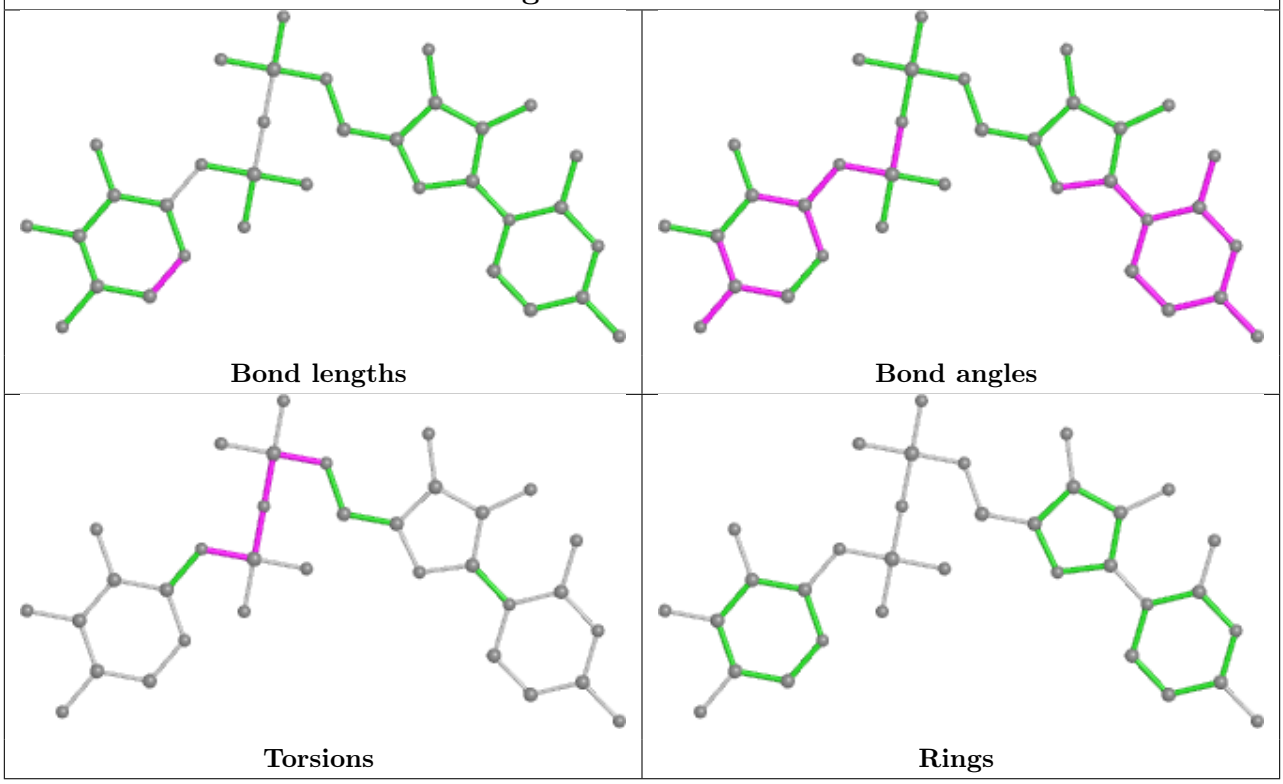
Ligand UDX E 501



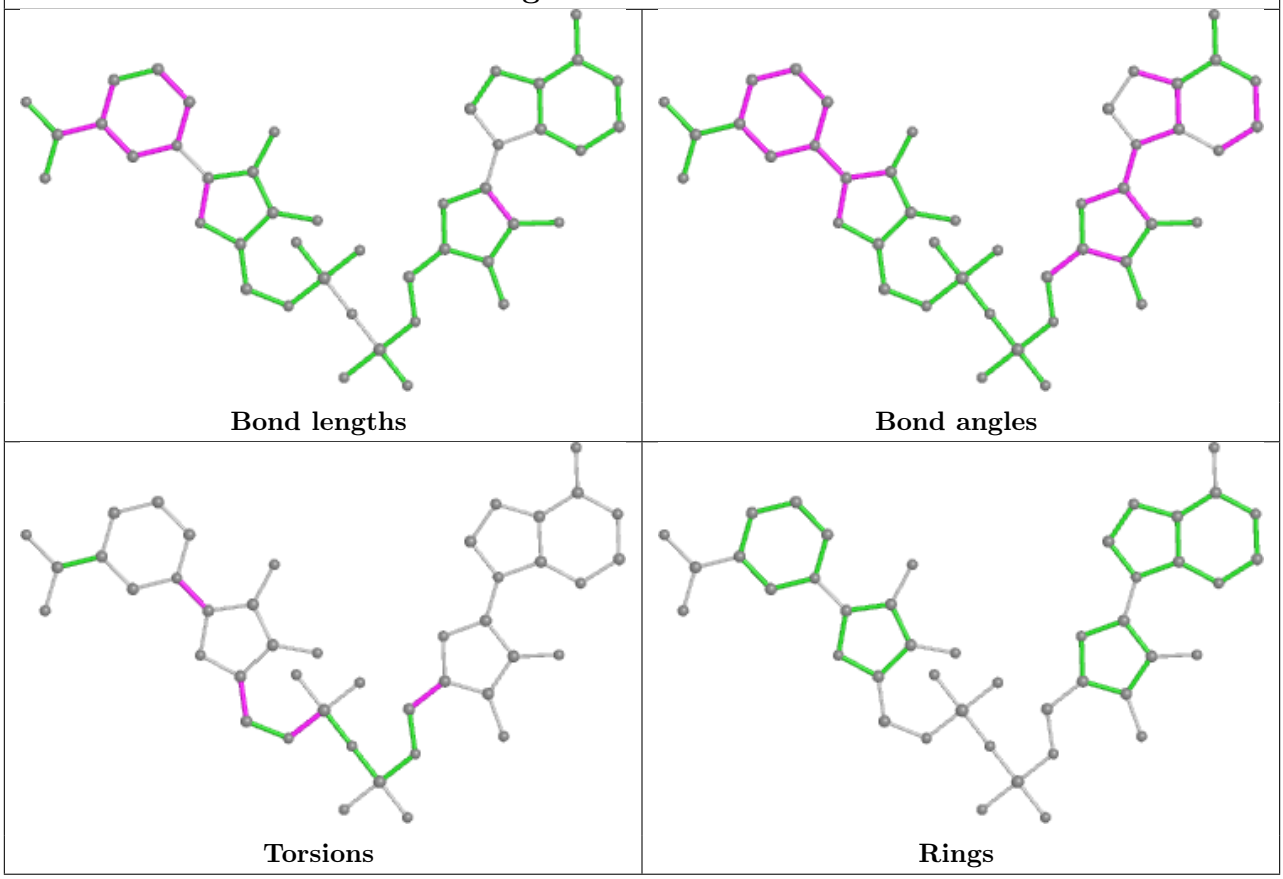
Ligand UDX B 501



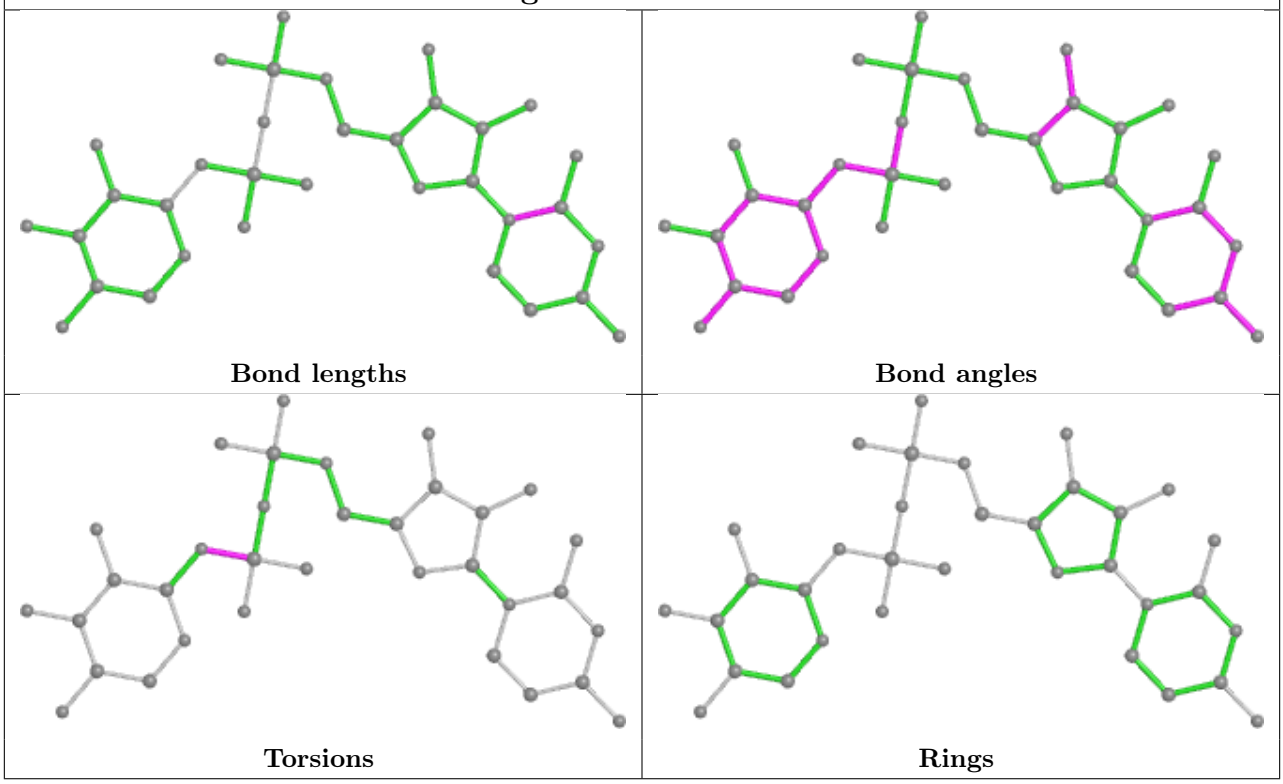
Ligand UDX C 501



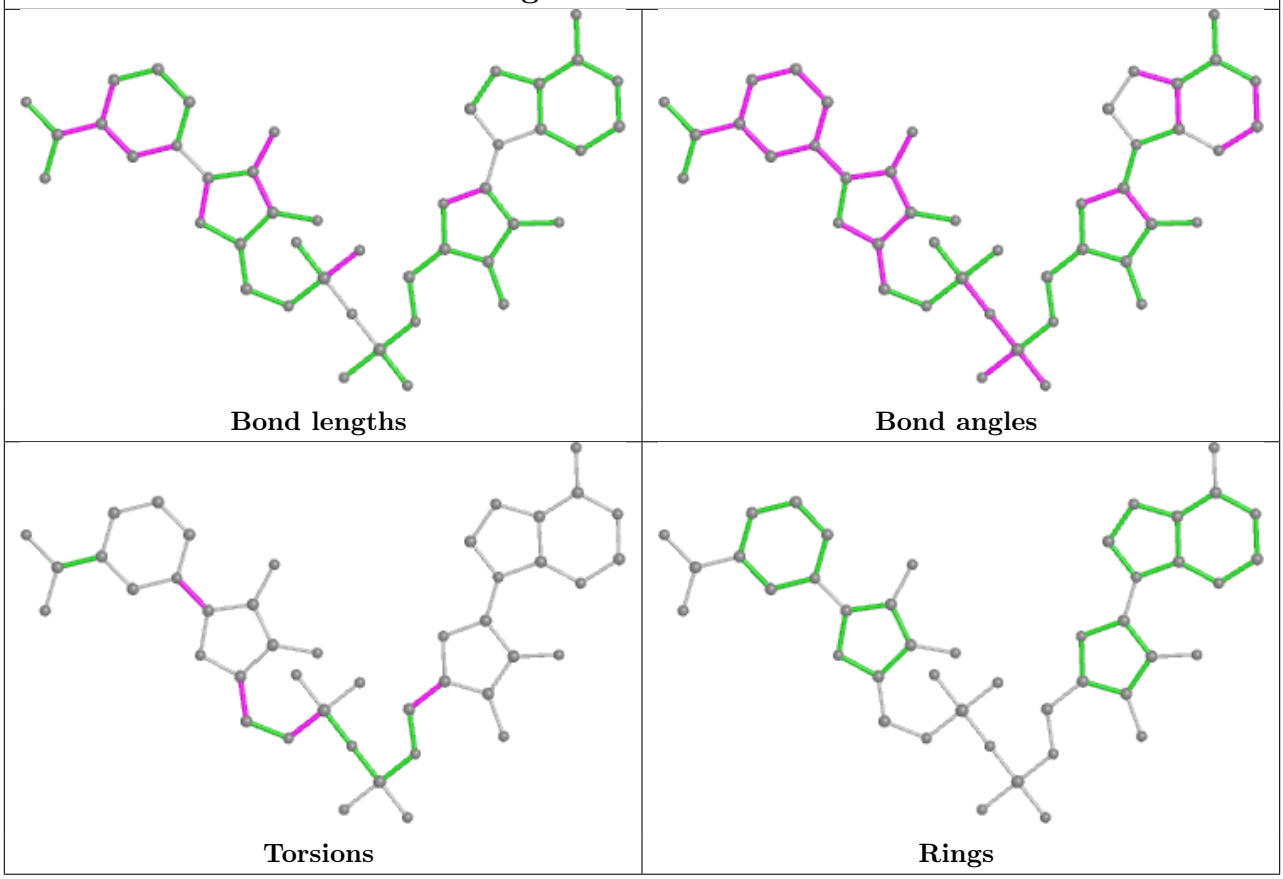
Ligand NAD E 500



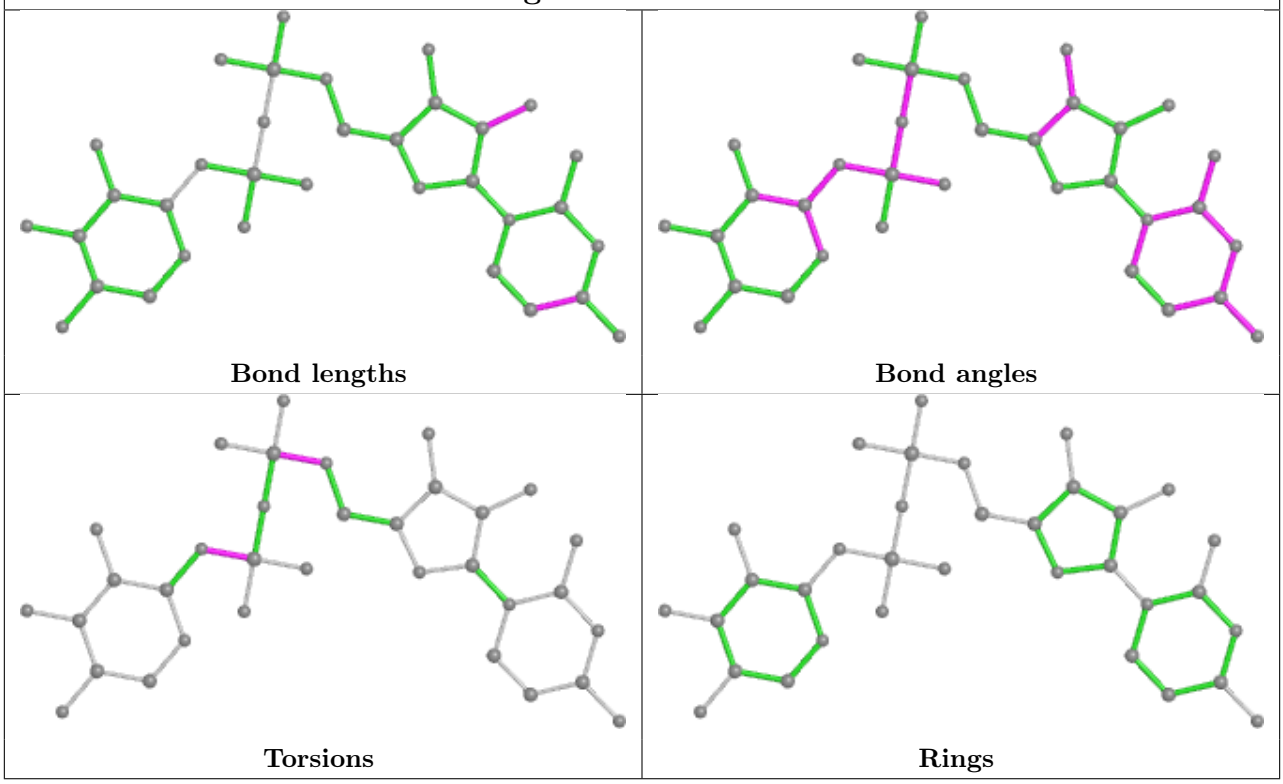
Ligand UDX D 501



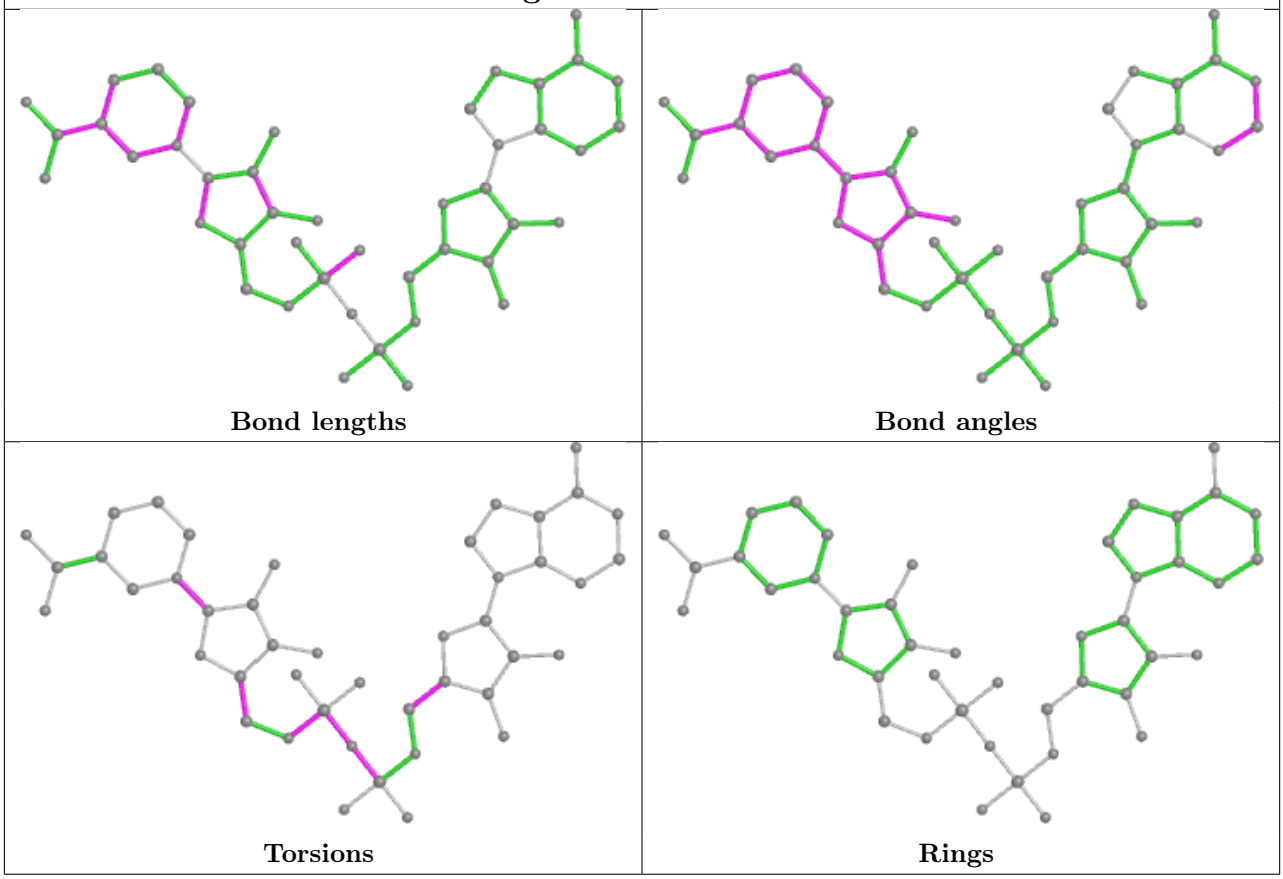
Ligand NAD C 500



Ligand UDX F 501



Ligand NAD F 500



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	458/494 (92%)	-0.51	0	100	100	14, 23, 39, 53	0
1	B	457/494 (92%)	-0.45	0	100	100	14, 27, 41, 51	0
1	C	457/494 (92%)	-0.23	9 (1%)	65	68	19, 30, 58, 68	0
1	D	457/494 (92%)	-0.27	4 (0%)	84	86	20, 38, 53, 66	0
1	E	458/494 (92%)	-0.39	2 (0%)	92	93	15, 26, 43, 60	0
1	F	457/494 (92%)	-0.03	14 (3%)	49	52	18, 32, 54, 62	0
All	All	2744/2964 (92%)	-0.31	29 (1%)	80	82	14, 29, 52, 68	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	98	MET	3.7
1	C	389	ASP	3.5
1	F	447	GLY	3.4
1	D	96	TYR	3.3
1	F	410	ALA	3.2
1	C	327	THR	3.0
1	E	98	MET	2.9
1	F	326	VAL	2.7
1	C	436	ALA	2.7
1	F	323	PHE	2.6
1	C	356	TYR	2.6
1	D	66	GLY	2.3
1	C	408	ALA	2.2
1	F	436	ALA	2.2
1	F	325	THR	2.2
1	F	322	LEU	2.2
1	F	433	LEU	2.2
1	F	409	HIS	2.2
1	F	437	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	425	TYR	2.1
1	C	319	ILE	2.1
1	E	96	TYR	2.1
1	F	364	LEU	2.1
1	C	330	LYS	2.1
1	F	151	ASN	2.1
1	F	328	ASP	2.1
1	D	77	ASP	2.0
1	C	326	VAL	2.0
1	C	404	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

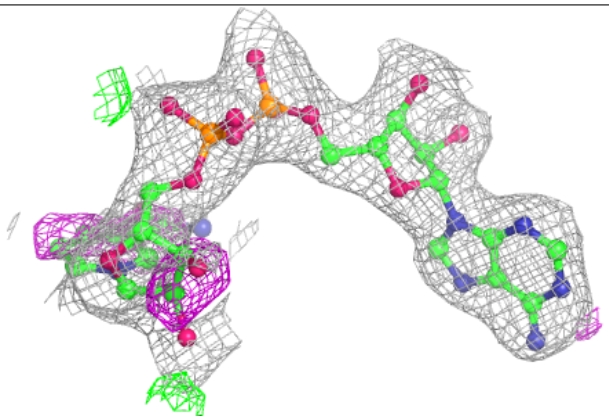
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

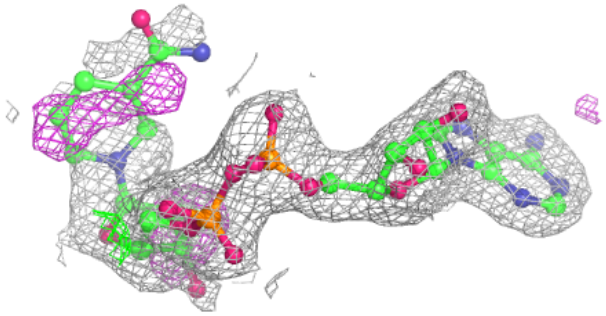
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	C	500	44/44	0.95	0.18	23,32,69,71	0
2	NAD	D	500	44/44	0.95	0.17	33,40,77,79	0
2	NAD	E	500	44/44	0.96	0.16	19,29,73,78	0
2	NAD	F	500	44/44	0.96	0.17	23,32,70,72	0
2	NAD	A	500	44/44	0.97	0.15	14,21,66,68	0
2	NAD	B	500	44/44	0.97	0.16	18,28,58,60	0
3	UDX	B	501	34/34	0.98	0.11	11,16,19,22	0
3	UDX	C	501	34/34	0.98	0.11	18,23,27,31	0
3	UDX	D	501	34/34	0.98	0.12	20,28,32,37	0
3	UDX	F	501	34/34	0.98	0.15	17,23,26,29	0
3	UDX	E	501	34/34	0.99	0.14	11,16,18,19	0
3	UDX	A	501	34/34	0.99	0.11	6,11,15,17	0

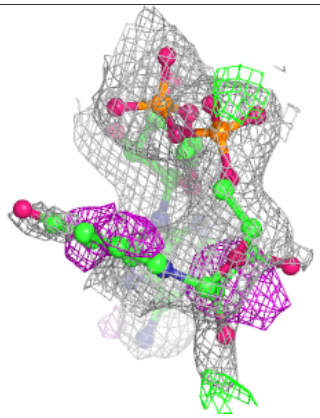
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD 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)

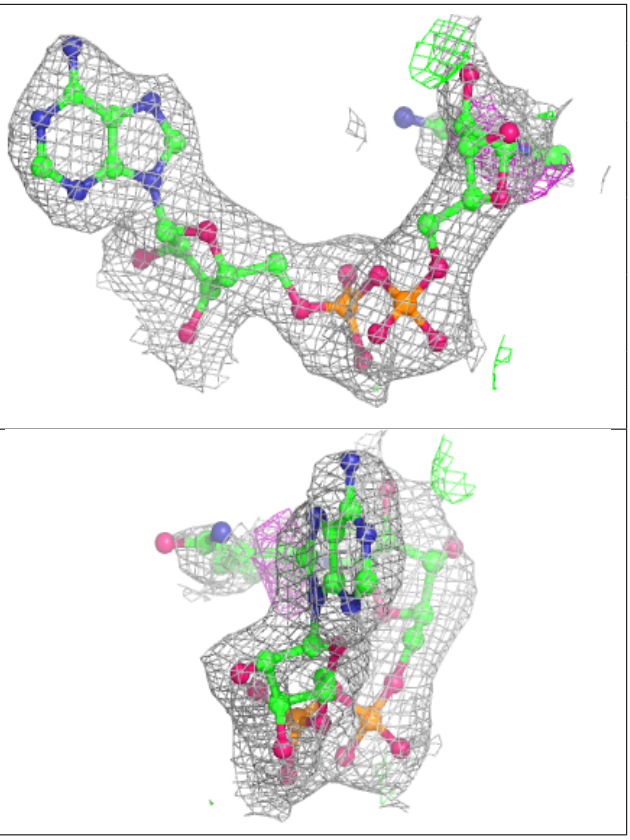






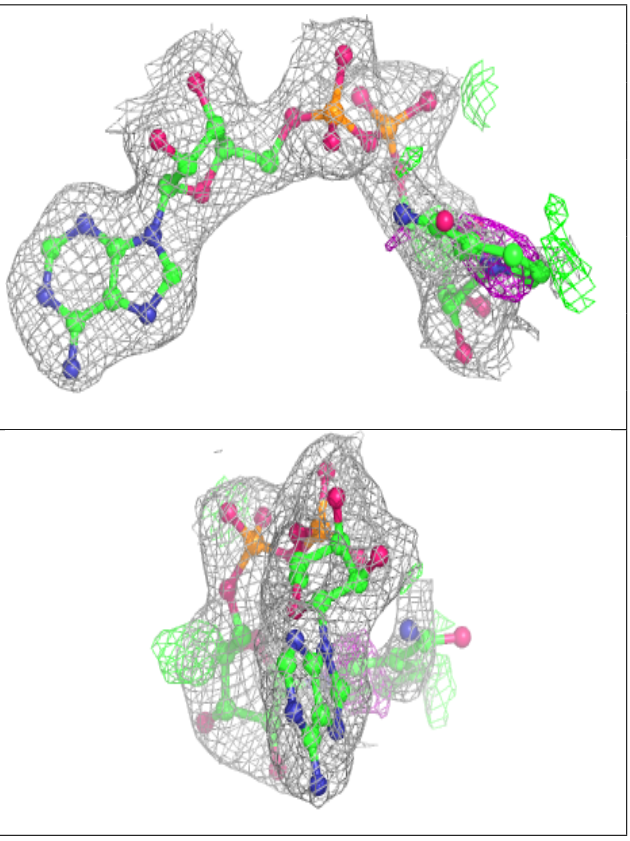
Electron density around NAD D 500:

$2mF_o$-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 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:

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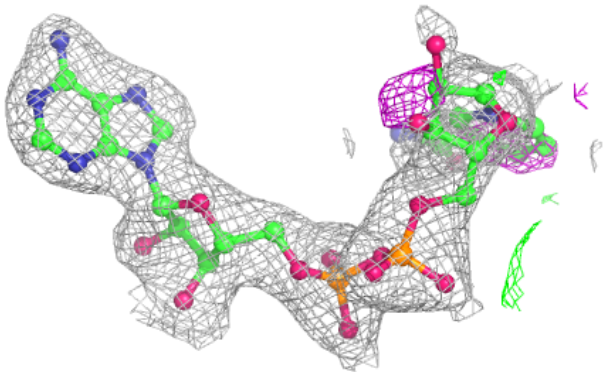
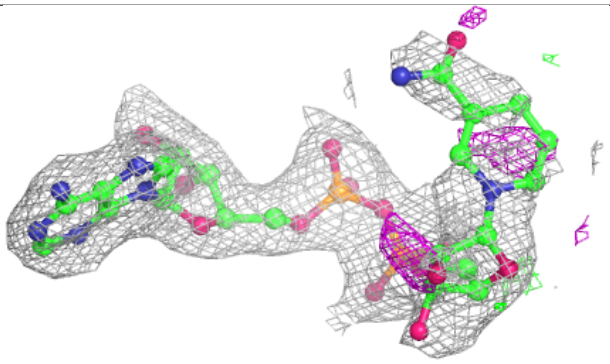
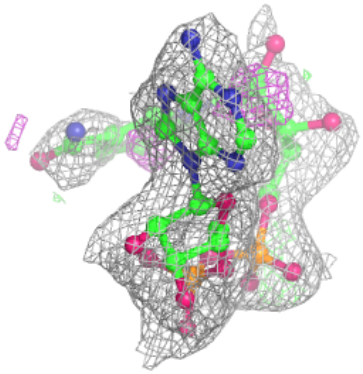
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

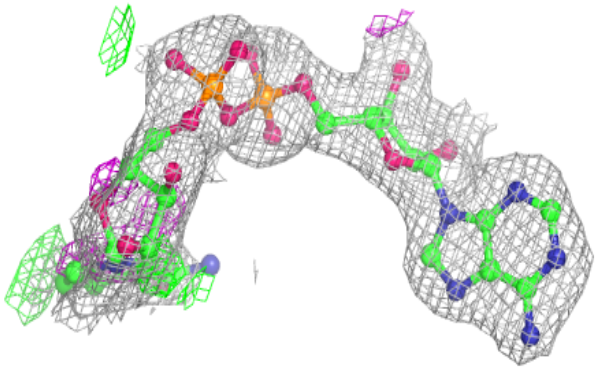


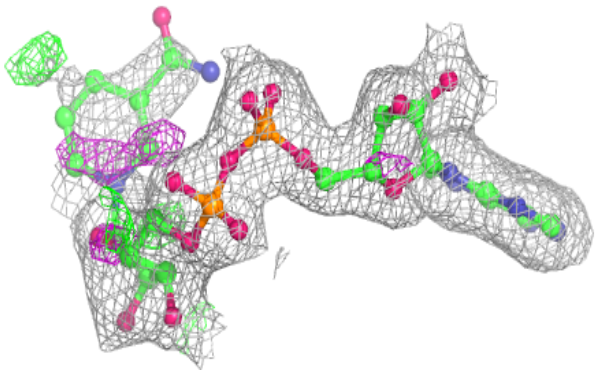


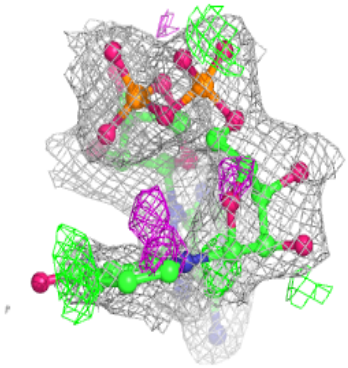


Electron density around NAD A 500:

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







Electron density around NAD B 500:

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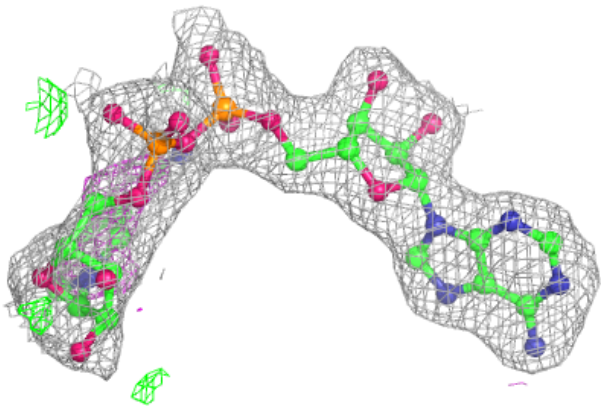
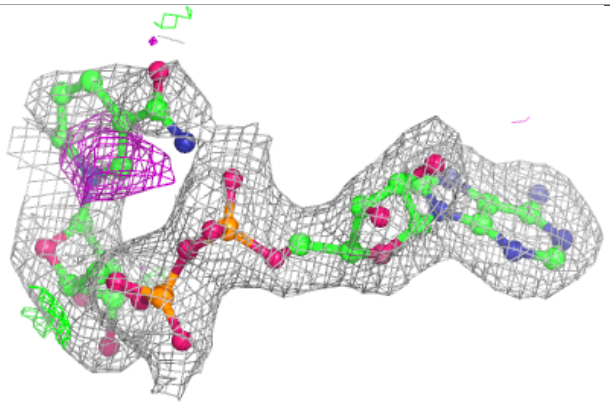
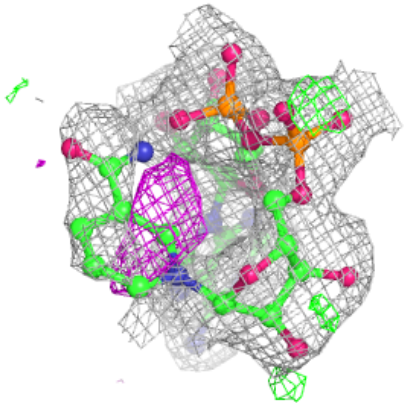
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

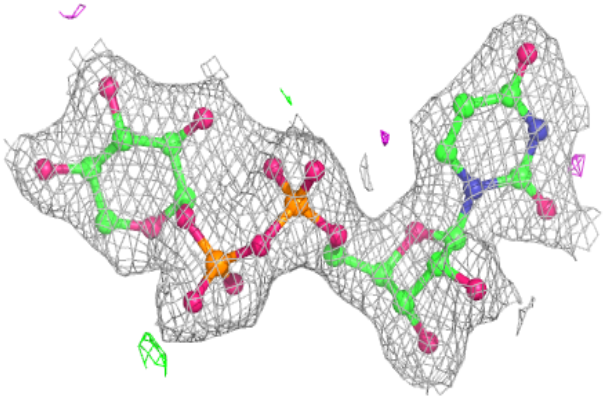


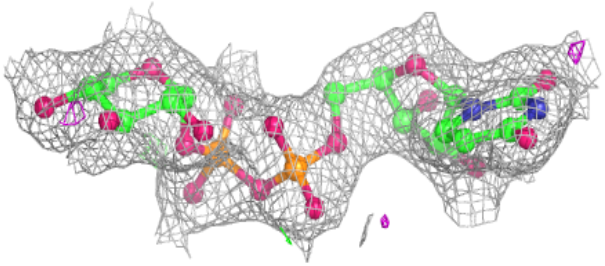


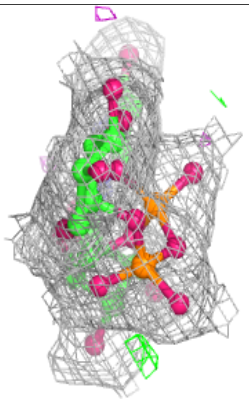


Electron density around UDX B 501:

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







Electron density around UDX C 501:

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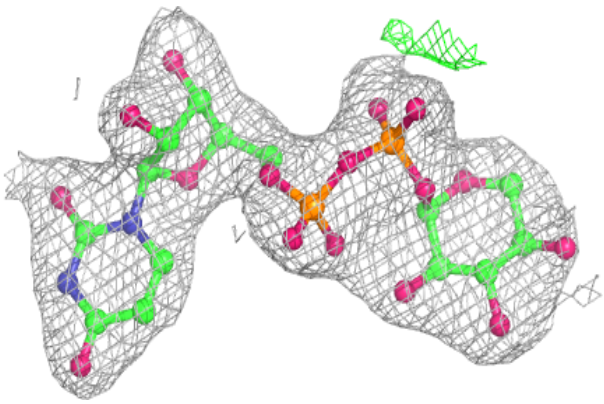
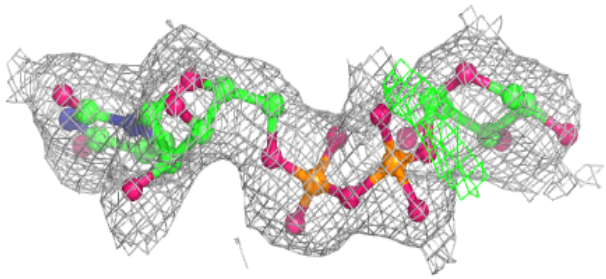
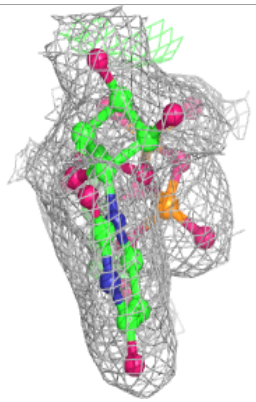
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around UDX D 501:

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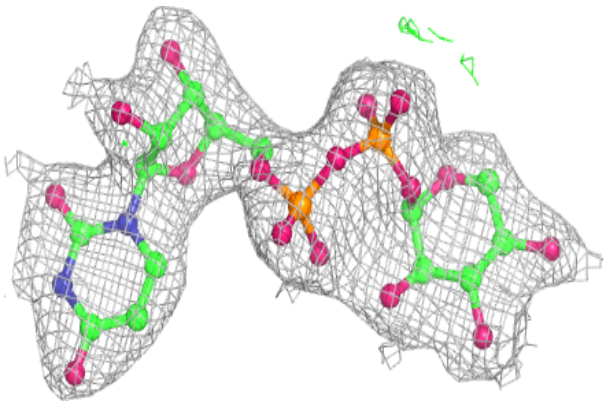
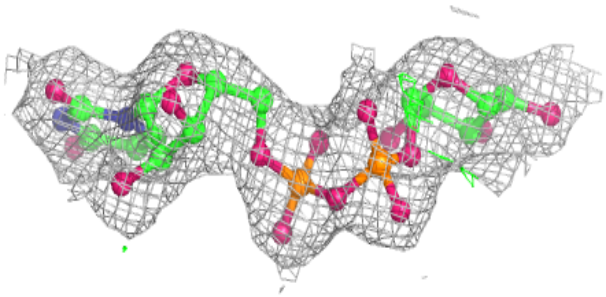
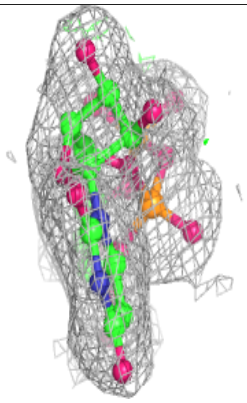
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

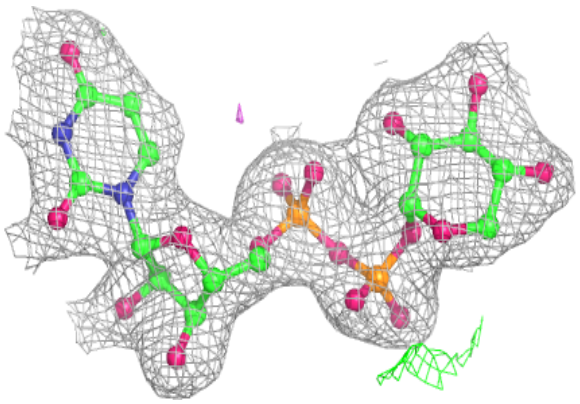


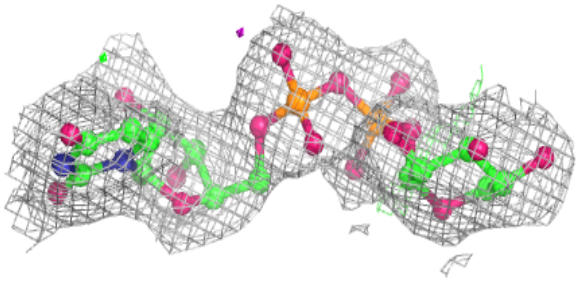


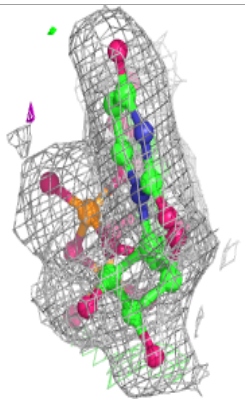


Electron density around UDX F 501:

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







Electron density around UDX E 501:

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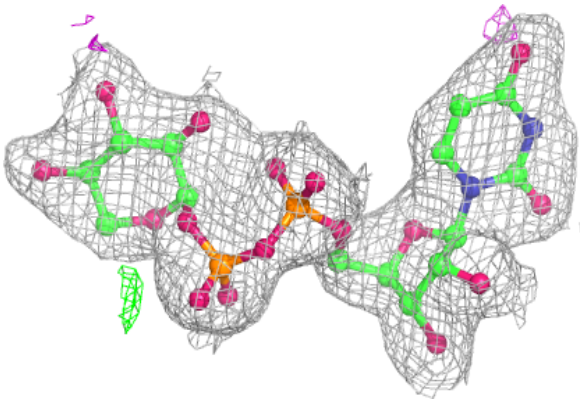
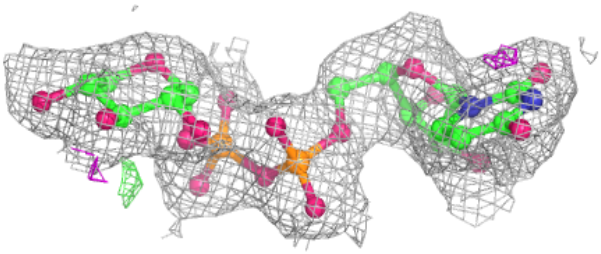
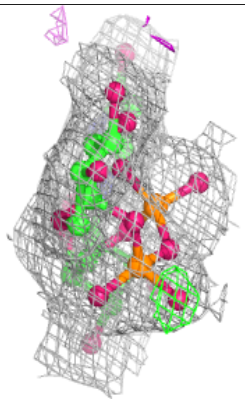
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around UDX A 501:

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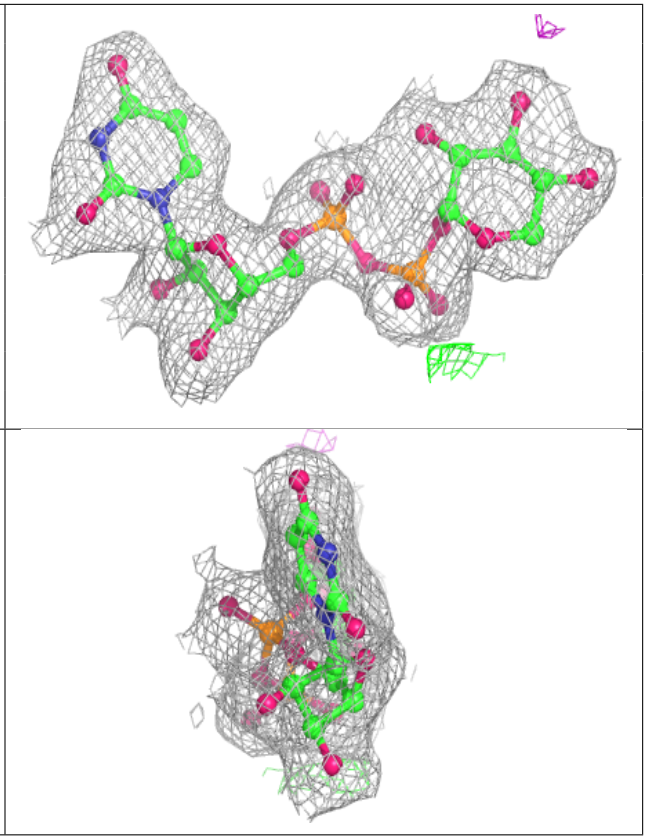
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.