



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:21 pm BST

PDB ID : 1ZEM
Title : Crystal Structure of NAD⁺-Bound Xylitol Dehydrogenase
Authors : Ehrensberger, A.H.; Elling, R.A.; Wilson, D.K.
Deposited on : 2005-04-19
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

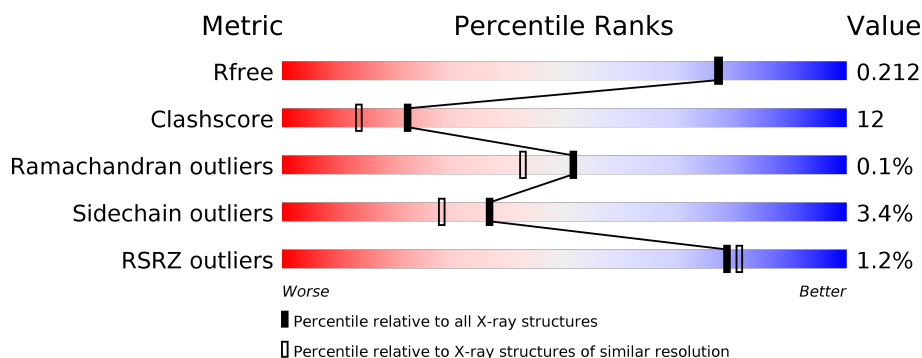
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	262	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>21%</div> <div>.</div> </div> </div>
1	B	262	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>.</div> </div> </div>
1	C	262	<div> <div></div> <div> <div></div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div>
1	D	262	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>...</div> </div> </div>
1	E	262	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	F	262	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	262	<div><div><div>%</div><div><div></div><div>84%</div><div>14%</div><div>..</div></div></div></div>
1	H	262	<div><div><div>%</div><div><div></div><div>79%</div><div>19%</div><div>..</div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17517 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 xylitol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1939	1224	332	372	11			
1	B	260	Total	C	N	O	S	0	0	0
			1939	1224	332	372	11			
1	C	260	Total	C	N	O	S	0	0	0
			1939	1224	332	372	11			
1	D	260	Total	C	N	O	S	0	0	0
			1939	1224	332	372	11			
1	E	260	Total	C	N	O	S	0	0	0
			1939	1224	332	372	11			
1	F	260	Total	C	N	O	S	0	0	0
			1939	1224	332	372	11			
1	G	260	Total	C	N	O	S	0	0	0
			1939	1224	332	372	11			
1	H	260	Total	C	N	O	S	0	0	0
			1939	1224	332	372	11			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		
3	F	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

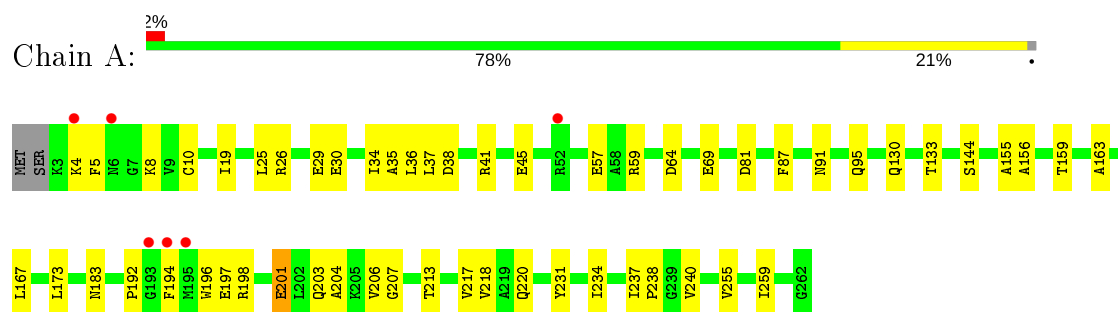
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	164	Total 164	O 164	0	0
4	B	199	Total 199	O 199	0	0
4	C	252	Total 252	O 252	0	0
4	D	203	Total 203	O 203	0	0
4	E	183	Total 183	O 183	0	0
4	F	226	Total 226	O 226	0	0
4	G	201	Total 201	O 201	0	0
4	H	220	Total 220	O 220	0	0

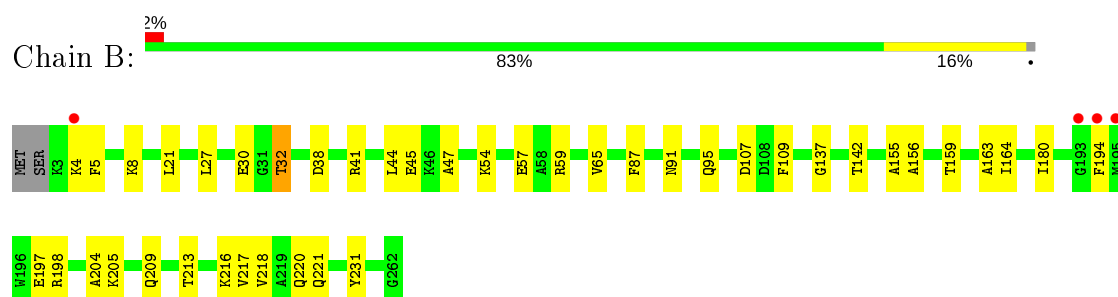
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

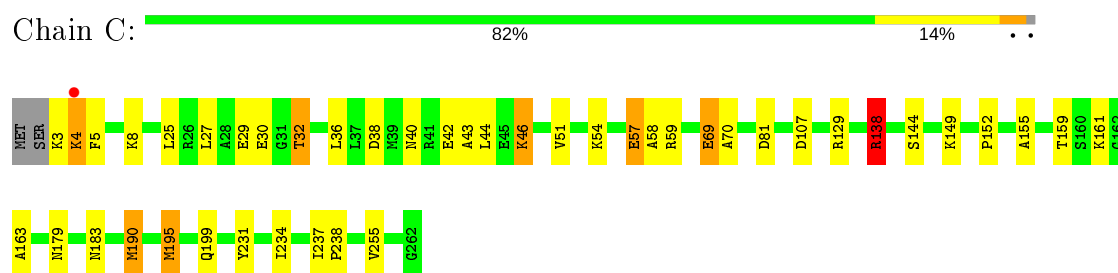
- Molecule 1: xylitol dehydrogenase



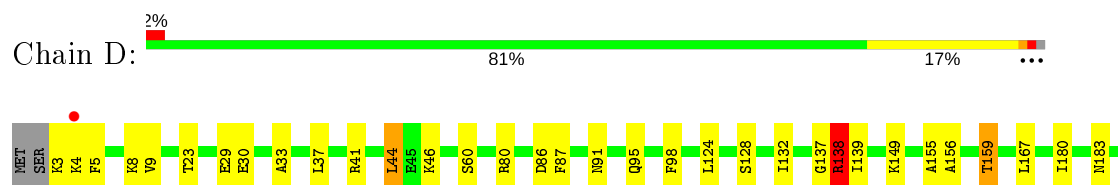
- Molecule 1: xylitol dehydrogenase



- Molecule 1: xylitol dehydrogenase

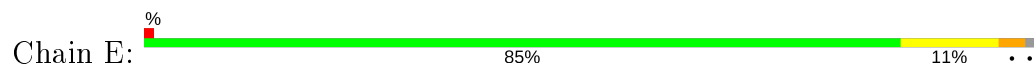


- Molecule 1: xylitol dehydrogenase

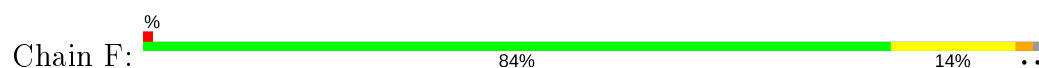




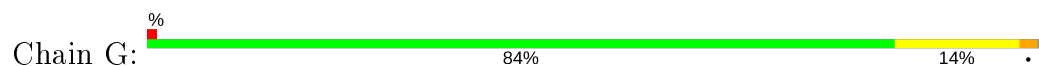
- Molecule 1: xylitol dehydrogenase



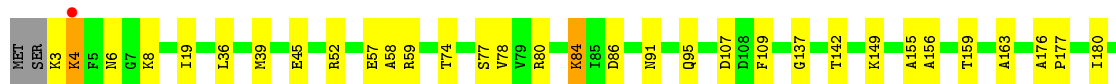
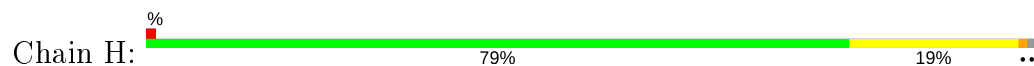
- Molecule 1: xylitol dehydrogenase



- Molecule 1: xylitol dehydrogenase



- Molecule 1: xylitol dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.96 Å 64.72 Å 168.24 Å 90.00° 93.06° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.0 (30.00-1.90) 87.0 (29.98-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.12 (at 1.91 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.167 , 0.218 0.163 , 0.212	Depositor DCC
R_{free} test set	6553 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17517	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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 32.62 % 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 9.1227e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MG, 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	0.82	2/1972 (0.1%)	0.85	2/2671 (0.1%)
1	B	0.86	0/1972	0.90	0/2671
1	C	0.84	1/1972 (0.1%)	0.89	3/2671 (0.1%)
1	D	0.84	0/1972	0.87	2/2671 (0.1%)
1	E	0.82	0/1972	0.89	1/2671 (0.0%)
1	F	0.90	1/1972 (0.1%)	0.92	0/2671
1	G	0.85	0/1972	0.88	1/2671 (0.0%)
1	H	0.87	0/1972	0.90	1/2671 (0.0%)
All	All	0.85	4/15776 (0.0%)	0.89	10/21368 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	190	MET	SD-CE	-5.90	1.44	1.77
1	F	190	MET	SD-CE	-5.31	1.48	1.77
1	A	201	GLU	CG-CD	5.28	1.59	1.51
1	A	69	GLU	CG-CD	5.08	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	ARG	NE-CZ-NH2	-10.18	115.21	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	190	MET	CG-SD-CE	-8.54	86.53	100.20
1	D	138	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	E	195	MET	N-CA-C	-6.76	92.75	111.00
1	C	138	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	C	107	ASP	CB-CG-OD1	6.17	123.85	118.30
1	H	190	MET	CG-SD-CE	-5.66	91.15	100.20
1	D	196	TRP	N-CA-C	-5.42	96.35	111.00
1	A	64	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	35	ALA	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	210	TYR	Sidechain

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	1939	0	1936	45	0
1	B	1939	0	1936	43	0
1	C	1939	0	1936	60	0
1	D	1939	0	1936	59	0
1	E	1939	0	1936	51	0
1	F	1939	0	1936	50	0
1	G	1939	0	1936	34	0
1	H	1939	0	1936	40	0
2	A	44	0	26	3	0
2	B	44	0	26	3	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0
2	E	44	0	26	1	0
2	F	44	0	26	1	0
2	G	44	0	26	1	0
2	H	44	0	26	4	0
3	C	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	164	0	0	3	0
4	B	199	0	0	2	0
4	C	252	0	0	11	0
4	D	203	0	0	11	0
4	E	183	0	0	6	0
4	F	226	0	0	3	0
4	G	201	0	0	4	0
4	H	220	0	0	5	0
All	All	17517	0	15696	368	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 12.

All (368) 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:C:4:LYS:HD3	1:C:5:PHE:N	1.38	1.35
1:C:4:LYS:CD	1:C:5:PHE:H	1.50	1.25
1:D:155:ALA:O	1:D:159:THR:HG22	1.52	1.09
1:F:27:LEU:HB3	1:F:32:THR:HG21	1.12	1.07
1:E:156:ALA:O	1:E:159:THR:HG22	1.58	1.03
1:G:4:LYS:CD	1:G:5:PHE:H	1.75	0.98
1:C:155:ALA:O	1:C:159:THR:HG23	1.65	0.97
1:C:4:LYS:HD2	4:C:4347:HOH:O	1.63	0.97
1:F:27:LEU:CB	1:F:32:THR:HG21	1.96	0.94
1:G:155:ALA:O	1:G:159:THR:HG22	1.66	0.94
1:E:205:LYS:HA	1:E:205:LYS:HE3	1.49	0.93
1:F:27:LEU:C	1:F:32:THR:HG22	1.89	0.93
1:C:43:ALA:O	1:C:46:LYS:HD3	1.67	0.92
1:H:149:LYS:HE2	4:H:9359:HOH:O	1.68	0.92
1:G:4:LYS:HD2	1:G:5:PHE:H	1.33	0.92
1:C:4:LYS:HD3	1:C:5:PHE:H	0.74	0.91
1:B:27:LEU:O	1:B:32:THR:HG23	1.69	0.90
1:F:27:LEU:O	1:F:32:THR:HG22	1.71	0.90
1:B:4:LYS:CD	1:B:5:PHE:H	1.85	0.89
1:F:4:LYS:O	1:F:30:GLU:O	1.92	0.86
1:E:27:LEU:O	1:E:32:THR:HG23	1.75	0.86
1:C:27:LEU:O	1:C:32:THR:HG23	1.77	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:ASN:HB2	4:F:7281:HOH:O	1.76	0.85
1:A:203:GLN:HA	4:A:2267:HOH:O	1.77	0.85
1:H:155:ALA:O	1:H:159:THR:HG23	1.76	0.85
1:B:4:LYS:O	1:B:30:GLU:O	1.93	0.84
1:F:27:LEU:HB3	1:F:32:THR:CG2	2.04	0.82
1:H:4:LYS:NZ	1:H:247:ASP:H	1.77	0.82
1:A:167:LEU:HB2	1:C:159:THR:HG22	1.61	0.81
1:F:4:LYS:CG	1:F:5:PHE:H	1.91	0.81
1:A:95:GLN:HB3	1:A:198:ARG:HH12	1.45	0.81
1:C:4:LYS:O	1:C:30:GLU:O	1.97	0.81
1:E:194:PHE:HD2	1:E:194:PHE:N	1.80	0.79
1:D:41:ARG:HD3	1:H:45:GLU:OE1	1.81	0.79
1:H:3:LYS:HB3	1:H:6:ASN:ND2	1.96	0.79
1:C:4:LYS:NZ	1:C:8:LYS:HZ1	1.81	0.79
1:C:190:MET:CE	1:C:234:ILE:HA	2.12	0.79
1:D:3:LYS:HG2	1:D:3:LYS:O	1.83	0.79
1:A:159:THR:OG1	1:C:163:ALA:HB1	1.83	0.78
1:F:167:LEU:HB2	1:H:159:THR:HG21	1.65	0.78
1:D:4:LYS:O	1:D:30:GLU:O	2.02	0.78
1:C:4:LYS:NZ	1:C:8:LYS:NZ	2.34	0.76
1:A:155:ALA:O	1:A:159:THR:HG22	1.85	0.76
1:G:155:ALA:O	1:G:159:THR:CG2	2.33	0.76
1:G:5:PHE:HA	1:G:8:LYS:HG3	1.66	0.75
1:C:4:LYS:HA	4:C:4404:HOH:O	1.85	0.75
1:E:48:GLU:CD	1:E:52:ARG:HH21	1.89	0.75
1:D:4:LYS:CD	1:D:5:PHE:H	1.99	0.74
1:E:194:PHE:HD2	1:E:194:PHE:H	1.33	0.74
1:F:4:LYS:CD	1:F:5:PHE:H	2.00	0.74
1:C:59:ARG:N	4:C:4273:HOH:O	2.21	0.73
1:A:4:LYS:O	1:A:5:PHE:HB2	1.88	0.73
1:D:156:ALA:O	1:D:159:THR:HG23	1.89	0.72
1:E:138:ARG:HG3	1:E:138:ARG:HH11	1.54	0.72
1:B:41:ARG:O	1:B:45:GLU:HG3	1.89	0.72
1:H:95:GLN:OE1	1:H:198:ARG:NH1	2.23	0.72
1:F:183:ASN:OD1	1:F:255:VAL:HG22	1.90	0.71
1:B:4:LYS:CE	1:B:5:PHE:H	2.03	0.71
1:F:167:LEU:HB2	1:H:159:THR:CG2	2.21	0.71
1:F:4:LYS:O	1:F:5:PHE:HB2	1.91	0.71
1:A:217:VAL:HA	1:A:220:GLN:HE21	1.57	0.70
1:B:8:LYS:HD3	1:B:87:PHE:CZ	2.26	0.70
1:D:4:LYS:CG	1:D:5:PHE:H	2.04	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:ARG:CG	1:E:138:ARG:HH11	2.01	0.70
1:E:194:PHE:CD2	1:E:194:PHE:N	2.52	0.70
1:H:57:GLU:OE1	1:H:59:ARG:NH1	2.23	0.70
1:E:5:PHE:HA	1:E:8:LYS:HG3	1.74	0.70
1:F:4:LYS:CG	1:F:5:PHE:N	2.55	0.69
1:F:4:LYS:HG3	1:F:5:PHE:H	1.55	0.69
1:G:4:LYS:HD3	1:G:5:PHE:H	1.55	0.69
1:A:41:ARG:O	1:A:45:GLU:HG3	1.93	0.69
1:F:113:LEU:HD21	1:F:159:THR:CG2	2.23	0.69
1:F:98:PHE:HD2	4:F:7281:HOH:O	1.76	0.68
1:C:4:LYS:O	1:C:5:PHE:HB2	1.93	0.68
1:F:4:LYS:HD3	1:F:5:PHE:H	1.57	0.68
1:C:4:LYS:HD3	1:C:5:PHE:CA	2.23	0.68
1:B:4:LYS:HG3	1:B:5:PHE:CD2	2.29	0.68
1:A:167:LEU:HB2	1:C:159:THR:CG2	2.23	0.68
1:E:159:THR:CG2	1:E:160:SER:N	2.56	0.68
1:C:183:ASN:OD1	1:C:255:VAL:HG22	1.93	0.68
1:F:156:ALA:O	1:F:159:THR:HG22	1.94	0.67
1:G:4:LYS:O	1:G:5:PHE:HB2	1.93	0.67
1:F:27:LEU:C	1:F:32:THR:CG2	2.63	0.66
1:D:220:GLN:CG	4:D:5379:HOH:O	2.42	0.66
1:C:190:MET:HE2	1:C:237:ILE:HD11	1.77	0.66
1:F:113:LEU:HD21	1:F:159:THR:HG23	1.77	0.66
1:F:190:MET:HE2	1:F:234:ILE:HD12	1.78	0.66
1:H:3:LYS:HB3	1:H:6:ASN:HD21	1.58	0.66
1:E:4:LYS:O	1:E:30:GLU:O	2.12	0.66
1:E:26:ARG:HD3	4:E:6365:HOH:O	1.97	0.65
1:E:183:ASN:OD1	1:E:255:VAL:HG22	1.97	0.65
1:G:5:PHE:HA	1:G:8:LYS:CG	2.26	0.65
1:B:155:ALA:O	1:B:159:THR:HG23	1.97	0.64
1:G:4:LYS:CD	1:G:5:PHE:N	2.54	0.64
1:E:5:PHE:HB3	1:E:32:THR:HG22	1.78	0.64
1:G:4:LYS:HD3	1:G:5:PHE:N	2.13	0.64
1:F:194:PHE:O	1:F:194:PHE:CD2	2.51	0.63
1:D:194:PHE:O	1:D:195:MET:HB2	1.98	0.63
1:D:4:LYS:CG	1:D:5:PHE:N	2.62	0.63
1:H:217:VAL:O	1:H:221:GLN:HG3	1.97	0.63
1:C:190:MET:HE1	1:C:234:ILE:HA	1.81	0.63
1:D:4:LYS:HD2	1:D:5:PHE:H	1.61	0.63
1:C:36:LEU:CD1	4:C:4273:HOH:O	2.46	0.63
1:F:52:ARG:HG2	1:F:52:ARG:HH11	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:PHE:CD1	1:D:195:MET:N	2.66	0.62
1:H:183:ASN:OD1	1:H:255:VAL:HG22	2.00	0.62
1:F:4:LYS:HG3	1:F:5:PHE:N	2.14	0.62
1:A:95:GLN:OE1	1:A:198:ARG:NH1	2.33	0.62
1:B:163:ALA:HB1	1:D:159:THR:OG1	2.00	0.61
1:G:59:ARG:NH1	1:G:81:ASP:HB3	2.15	0.61
1:B:4:LYS:CD	1:B:5:PHE:N	2.61	0.61
1:E:95:GLN:HB3	1:E:198:ARG:NH1	2.15	0.61
1:B:4:LYS:HE3	1:B:5:PHE:H	1.65	0.61
1:G:197:GLU:O	1:G:201:GLU:HG2	2.01	0.61
1:F:57:GLU:OE1	1:F:59:ARG:NH1	2.34	0.60
1:C:4:LYS:CD	1:C:5:PHE:N	2.29	0.60
1:C:5:PHE:HB3	1:C:32:THR:HG22	1.82	0.60
1:B:4:LYS:CG	1:B:5:PHE:H	2.15	0.60
1:F:4:LYS:HD3	1:F:5:PHE:N	2.17	0.60
1:B:4:LYS:CG	1:B:5:PHE:N	2.65	0.60
1:B:38:ASP:HB3	1:B:44:LEU:HG	1.84	0.60
1:C:195:MET:HA	1:C:195:MET:HE2	1.83	0.60
1:C:36:LEU:HD12	4:C:4273:HOH:O	2.02	0.60
1:E:95:GLN:OE1	1:E:198:ARG:NH1	2.34	0.59
1:B:5:PHE:HB3	1:B:32:THR:HG22	1.83	0.59
1:F:32:THR:HG23	1:F:34:ILE:HD11	1.85	0.59
1:E:95:GLN:HB3	1:E:198:ARG:HH12	1.67	0.59
1:D:220:GLN:HG2	4:D:5379:HOH:O	2.00	0.59
1:D:4:LYS:HG3	1:D:5:PHE:H	1.68	0.59
1:D:4:LYS:HG3	1:D:5:PHE:N	2.18	0.58
1:A:91:ASN:ND2	2:A:2263:NAD:H4D	2.18	0.58
1:E:113:LEU:HD21	1:E:159:THR:CG2	2.34	0.58
1:A:156:ALA:O	1:A:159:THR:CG2	2.52	0.57
1:E:194:PHE:O	1:E:195:MET:HB3	2.02	0.57
1:G:51:VAL:O	1:G:54:LYS:HB2	2.04	0.57
1:C:27:LEU:C	1:C:32:THR:HG23	2.24	0.57
1:F:52:ARG:NH2	1:F:58:ALA:O	2.37	0.57
1:D:4:LYS:HA	4:D:5397:HOH:O	2.05	0.57
1:E:5:PHE:HA	1:E:8:LYS:CG	2.34	0.57
1:G:4:LYS:O	1:G:30:GLU:O	2.22	0.57
1:H:203:GLN:OE1	4:H:9290:HOH:O	2.18	0.57
1:A:156:ALA:O	1:A:159:THR:HG23	2.05	0.57
1:E:4:LYS:O	1:E:5:PHE:HB2	2.04	0.57
1:B:4:LYS:HD2	1:B:5:PHE:H	1.68	0.57
1:D:138:ARG:HD2	4:D:5317:HOH:O	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:LEU:O	1:B:32:THR:CG2	2.48	0.56
1:C:4:LYS:O	1:C:30:GLU:HB3	2.05	0.56
1:F:4:LYS:O	1:F:5:PHE:CB	2.53	0.56
1:G:217:VAL:HA	1:G:220:GLN:HE21	1.70	0.56
1:C:27:LEU:O	1:C:32:THR:CG2	2.52	0.56
1:D:44:LEU:HD22	1:D:60:SER:HB3	1.88	0.56
1:A:4:LYS:HD3	1:A:5:PHE:H	1.71	0.56
1:C:59:ARG:NH1	1:C:81:ASP:HB3	2.21	0.55
1:D:183:ASN:OD1	1:D:255:VAL:HG22	2.06	0.55
1:B:57:GLU:CG	1:B:59:ARG:HH12	2.19	0.55
1:A:4:LYS:O	1:A:5:PHE:CB	2.53	0.55
1:G:4:LYS:O	1:G:5:PHE:CB	2.54	0.55
1:A:26:ARG:HD3	4:A:2358:HOH:O	2.07	0.55
1:B:194:PHE:HA	1:B:197:GLU:HB2	1.88	0.55
1:B:159:THR:HG22	1:D:167:LEU:HB2	1.88	0.55
1:D:155:ALA:O	1:D:159:THR:CG2	2.42	0.55
1:A:10:CYS:HB2	1:A:87:PHE:HB2	1.87	0.55
1:C:51:VAL:O	1:C:54:LYS:HB2	2.07	0.55
1:D:4:LYS:O	1:D:5:PHE:HB2	2.07	0.55
1:C:4:LYS:HZ2	1:C:8:LYS:HZ1	1.55	0.55
1:C:59:ARG:HH11	1:C:81:ASP:HB3	1.72	0.55
1:C:190:MET:CE	1:C:237:ILE:HD11	2.37	0.54
1:D:9:VAL:N	1:D:86:ASP:OD1	2.36	0.54
1:A:19:ILE:HD12	2:A:2263:NAD:H51N	1.89	0.54
1:C:4:LYS:HZ3	1:C:8:LYS:NZ	2.06	0.54
1:A:5:PHE:HA	1:A:8:LYS:CG	2.38	0.54
1:F:262:GLY:C	4:F:7449:HOH:O	2.46	0.54
1:C:138:ARG:HD2	4:C:4296:HOH:O	2.08	0.54
1:H:195:MET:HB2	4:H:9322:HOH:O	2.08	0.54
1:C:138:ARG:NH2	1:C:179:ASN:O	2.40	0.54
1:E:159:THR:HG23	1:E:160:SER:N	2.23	0.54
1:E:138:ARG:NH1	4:E:6308:HOH:O	2.41	0.54
1:B:159:THR:CG2	1:D:167:LEU:HB2	2.38	0.53
1:E:27:LEU:C	1:E:32:THR:HG23	2.28	0.53
1:F:52:ARG:HG2	1:F:52:ARG:NH1	2.23	0.53
1:H:109:PHE:CD1	1:H:156:ALA:HB2	2.42	0.53
1:A:25:LEU:O	1:A:29:GLU:HG3	2.08	0.53
1:D:5:PHE:O	1:D:8:LYS:HB2	2.07	0.53
1:F:197:GLU:O	1:F:201:GLU:HG2	2.09	0.53
1:B:4:LYS:O	1:B:5:PHE:HB2	2.09	0.53
1:D:80:ARG:CZ	4:D:5369:HOH:O	2.56	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:GLN:HA	4:D:5274:HOH:O	2.08	0.53
1:D:4:LYS:HD2	1:D:5:PHE:N	2.22	0.53
1:H:137:GLY:O	1:H:180:ILE:HA	2.08	0.53
1:H:84:LYS:HE2	1:H:86:ASP:OD2	2.08	0.53
1:H:95:GLN:HB3	1:H:198:ARG:HH12	1.73	0.53
1:D:192:PRO:HG2	1:D:193:GLY:N	2.24	0.52
1:H:142:THR:HG21	2:H:9263:NAD:O4D	2.09	0.52
1:C:195:MET:HA	1:C:195:MET:CE	2.39	0.52
1:C:59:ARG:NH1	1:C:81:ASP:O	2.42	0.52
1:E:57:GLU:HG2	4:E:6354:HOH:O	2.09	0.52
1:F:23:THR:HA	1:F:238:PRO:HB3	1.92	0.52
1:H:107:ASP:HB3	4:H:9468:HOH:O	2.09	0.52
1:H:91:ASN:ND2	2:H:9263:NAD:H4D	2.25	0.52
1:B:142:THR:HG21	2:B:3263:NAD:O4D	2.10	0.52
1:B:57:GLU:OE1	1:B:59:ARG:NH1	2.43	0.51
1:A:198:ARG:HA	1:A:201:GLU:HG2	1.92	0.51
1:D:128:SER:O	1:D:132:ILE:HG13	2.10	0.51
1:H:4:LYS:HZ1	1:H:247:ASP:H	1.57	0.51
1:E:138:ARG:CG	1:E:138:ARG:NH1	2.66	0.51
1:E:194:PHE:O	1:E:195:MET:CB	2.58	0.51
1:F:15:ALA:HB1	1:F:36:LEU:HD12	1.92	0.51
1:D:23:THR:HA	1:D:238:PRO:HB3	1.93	0.51
1:D:220:GLN:HA	4:D:5379:HOH:O	2.10	0.50
1:H:74:THR:O	1:H:78:VAL:HG23	2.11	0.50
1:F:159:THR:CG2	1:F:160:SER:N	2.74	0.50
1:C:4:LYS:CE	1:C:5:PHE:H	2.20	0.50
1:D:91:ASN:ND2	2:D:5263:NAD:H4D	2.26	0.50
1:E:205:LYS:CA	1:E:205:LYS:HE3	2.27	0.50
1:G:194:PHE:HA	1:G:197:GLU:HB2	1.94	0.50
1:G:23:THR:HA	1:G:238:PRO:HB3	1.93	0.50
1:F:8:LYS:HD3	1:F:87:PHE:CZ	2.47	0.50
1:A:57:GLU:OE2	1:A:59:ARG:NH2	2.45	0.50
1:G:59:ARG:NH1	1:G:81:ASP:CB	2.75	0.50
1:B:54:LYS:NZ	4:B:3396:HOH:O	2.45	0.50
1:A:37:LEU:HD23	1:A:37:LEU:C	2.32	0.50
1:C:58:ALA:HB1	4:C:4273:HOH:O	2.11	0.50
1:A:173:LEU:CD1	1:C:152:PRO:HD3	2.42	0.49
1:C:5:PHE:HB3	1:C:32:THR:CG2	2.43	0.49
1:A:194:PHE:HA	1:A:197:GLU:HB2	1.93	0.49
1:E:80:ARG:NH2	4:E:6345:HOH:O	2.45	0.49
1:H:206:VAL:HB	4:H:9290:HOH:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:LEU:N	1:H:36:LEU:HD12	2.27	0.49
1:D:137:GLY:O	1:D:180:ILE:HA	2.11	0.49
1:F:27:LEU:CB	1:F:32:THR:CG2	2.79	0.49
1:E:159:THR:HG22	1:E:160:SER:H	1.78	0.49
1:H:19:ILE:HB	2:H:9263:NAD:H51N	1.94	0.49
1:C:149:LYS:HG2	4:C:4467:HOH:O	2.13	0.48
1:C:190:MET:HE2	1:C:237:ILE:CD1	2.42	0.48
1:A:156:ALA:HA	1:A:159:THR:CG2	2.44	0.48
1:A:240:VAL:HG11	1:A:259:ILE:HD11	1.95	0.48
1:A:5:PHE:HA	1:A:8:LYS:HG3	1.93	0.48
1:D:217:VAL:O	1:D:221:GLN:HG3	2.14	0.48
1:E:48:GLU:OE1	1:E:52:ARG:NH2	2.32	0.48
1:B:4:LYS:HG3	1:B:5:PHE:N	2.29	0.48
1:C:4:LYS:O	1:C:5:PHE:CB	2.61	0.48
1:E:113:LEU:HD21	1:E:159:THR:HG23	1.95	0.48
1:C:38:ASP:HB3	1:C:44:LEU:HG	1.94	0.48
1:B:4:LYS:HG3	1:B:5:PHE:HD2	1.78	0.48
1:G:195:MET:CE	1:G:198:ARG:HD3	2.44	0.47
1:D:194:PHE:O	1:D:195:MET:CB	2.62	0.47
1:C:8:LYS:HE2	4:C:4455:HOH:O	2.14	0.47
1:D:237:ILE:N	1:D:238:PRO:CD	2.76	0.47
1:B:194:PHE:CD1	1:B:197:GLU:HB2	2.49	0.47
1:C:5:PHE:CB	1:C:32:THR:HG22	2.43	0.47
1:A:130:GLN:O	1:A:133:THR:HB	2.15	0.47
1:G:4:LYS:HA	4:G:8418:HOH:O	2.13	0.47
1:G:149:LYS:HE3	4:G:8431:HOH:O	2.15	0.47
1:B:4:LYS:HD2	1:B:5:PHE:N	2.26	0.47
1:H:176:ALA:N	1:H:177:PRO:CD	2.79	0.46
1:F:190:MET:HB3	1:F:234:ILE:CD1	2.45	0.46
1:B:91:ASN:ND2	2:B:3263:NAD:H4D	2.31	0.46
1:D:87:PHE:CE1	1:D:138:ARG:HG3	2.50	0.46
1:B:109:PHE:CD1	1:B:156:ALA:HB2	2.51	0.46
1:E:52:ARG:CZ	1:E:58:ALA:O	2.64	0.46
1:E:4:LYS:HE3	4:E:6343:HOH:O	2.14	0.46
1:F:159:THR:OG1	1:H:163:ALA:HB1	2.15	0.46
1:H:211:PHE:HB3	1:H:218:VAL:HG22	1.98	0.46
1:A:59:ARG:HH11	1:A:81:ASP:HB3	1.81	0.46
1:E:159:THR:HG22	1:E:160:SER:N	2.29	0.46
1:H:226:VAL:O	1:H:229:ARG:HD3	2.16	0.46
1:F:91:ASN:ND2	2:F:7263:NAD:H4D	2.30	0.46
1:B:137:GLY:O	1:B:180:ILE:HA	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ARG:NH2	4:C:4341:HOH:O	2.49	0.45
1:C:57:GLU:OE1	1:C:59:ARG:CZ	2.65	0.45
1:D:29:GLU:OE1	1:D:29:GLU:HA	2.16	0.45
1:D:194:PHE:HD1	1:D:195:MET:H	1.60	0.45
1:D:4:LYS:HG3	1:D:5:PHE:CD2	2.51	0.45
1:G:137:GLY:O	1:G:180:ILE:HA	2.17	0.45
1:E:176:ALA:N	1:E:177:PRO:CD	2.79	0.45
1:G:211:PHE:HB3	1:G:218:VAL:HG22	1.99	0.45
1:G:6:ASN:HB2	4:G:8418:HOH:O	2.17	0.45
1:H:52:ARG:CZ	1:H:58:ALA:O	2.65	0.45
1:A:234:ILE:O	1:A:238:PRO:HD3	2.18	0.44
1:A:4:LYS:O	1:A:30:GLU:O	2.35	0.44
1:D:124:LEU:HD12	1:D:139:ILE:HD13	1.99	0.44
1:D:192:PRO:CG	1:D:193:GLY:N	2.76	0.44
1:B:216:LYS:O	1:B:220:GLN:HG3	2.18	0.44
1:C:40:ASN:HB2	4:C:4507:HOH:O	2.18	0.44
1:H:91:ASN:HD21	2:H:9263:NAD:C5D	2.31	0.44
1:E:109:PHE:CD1	1:E:156:ALA:HB2	2.52	0.44
1:F:32:THR:HG23	1:F:34:ILE:CD1	2.48	0.44
1:C:25:LEU:O	1:C:29:GLU:HG3	2.17	0.44
1:D:95:GLN:HB3	1:D:198:ARG:NH1	2.33	0.44
1:E:194:PHE:C	1:E:196:TRP:H	2.17	0.44
1:F:109:PHE:CD1	1:F:156:ALA:HB2	2.53	0.44
1:C:237:ILE:N	1:C:238:PRO:CD	2.81	0.43
1:G:3:LYS:O	4:G:8418:HOH:O	2.21	0.43
1:C:4:LYS:NZ	1:C:8:LYS:HZ3	2.13	0.43
1:F:34:ILE:CG2	1:F:36:LEU:HD13	2.48	0.43
1:H:77:SER:O	1:H:80:ARG:HG2	2.18	0.43
1:E:5:PHE:N	1:E:5:PHE:CD2	2.87	0.43
1:F:34:ILE:HG22	1:F:36:LEU:HD13	2.01	0.43
1:H:77:SER:HA	1:H:80:ARG:HG2	2.01	0.43
1:D:44:LEU:CD2	1:D:60:SER:HB3	2.48	0.43
1:F:36:LEU:HD22	1:F:36:LEU:N	2.33	0.43
1:H:237:ILE:N	1:H:238:PRO:CD	2.82	0.43
1:A:10:CYS:CB	1:A:87:PHE:HB2	2.48	0.43
1:B:57:GLU:HG2	1:B:59:ARG:NH1	2.32	0.43
1:E:91:ASN:ND2	2:E:6263:NAD:H4D	2.33	0.43
1:F:167:LEU:CA	1:H:159:THR:HG22	2.48	0.43
1:G:91:ASN:ND2	2:G:8263:NAD:H4D	2.33	0.43
1:H:194:PHE:HA	1:H:197:GLU:HB2	1.99	0.43
1:G:11:LEU:HD12	1:G:35:ALA:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PHE:HA	1:A:8:LYS:HG2	1.99	0.43
1:F:48:GLU:O	1:F:52:ARG:HG3	2.19	0.43
1:A:237:ILE:N	1:A:238:PRO:CD	2.82	0.43
1:A:37:LEU:HD23	1:A:38:ASP:N	2.34	0.43
1:E:5:PHE:CB	1:E:32:THR:HG22	2.46	0.43
1:A:183:ASN:OD1	1:A:255:VAL:HG22	2.19	0.42
1:D:9:VAL:HG22	1:D:33:ALA:HB3	2.00	0.42
1:G:5:PHE:HB3	1:G:32:THR:OG1	2.19	0.42
1:D:98:PHE:HB3	4:D:5274:HOH:O	2.18	0.42
1:E:113:LEU:HD21	1:E:159:THR:HG21	1.99	0.42
1:A:207:GLY:HA2	1:A:213:THR:HG22	2.00	0.42
1:E:144:SER:HB3	1:E:161:LYS:HG3	2.00	0.42
1:H:4:LYS:HZ2	1:H:247:ASP:H	1.65	0.42
1:A:34:ILE:HG22	1:A:36:LEU:HD12	2.00	0.42
1:G:217:VAL:O	1:G:221:GLN:HG3	2.18	0.42
1:D:237:ILE:H	1:D:238:PRO:HD3	1.85	0.42
1:A:163:ALA:HB1	1:C:159:THR:HB	2.02	0.42
1:A:144:SER:HB2	2:A:2263:NAD:H6N	2.01	0.42
1:C:144:SER:HB3	1:C:161:LYS:HG3	2.01	0.42
1:D:220:GLN:HG3	4:D:5379:HOH:O	2.16	0.42
1:D:44:LEU:HD22	1:D:60:SER:CB	2.50	0.42
1:D:192:PRO:HB3	1:D:231:TYR:OH	2.20	0.42
1:D:37:LEU:HD23	1:D:37:LEU:C	2.41	0.42
1:B:4:LYS:HA	1:B:4:LYS:HD2	1.64	0.42
1:F:211:PHE:HB3	1:F:218:VAL:HG22	2.01	0.42
1:C:3:LYS:HG2	1:C:3:LYS:O	2.20	0.41
1:E:8:LYS:HE2	4:E:6424:HOH:O	2.19	0.41
1:E:27:LEU:HB3	1:E:32:THR:CG2	2.50	0.41
1:E:4:LYS:O	1:E:5:PHE:CB	2.68	0.41
1:A:156:ALA:O	1:A:159:THR:HG22	2.19	0.41
1:B:164:ILE:HA	1:B:164:ILE:HD13	1.92	0.41
1:B:21:LEU:HD13	1:B:47:ALA:HB1	2.01	0.41
1:E:4:LYS:CD	1:E:5:PHE:H	2.32	0.41
1:G:156:ALA:HA	1:G:159:THR:HG23	2.02	0.41
1:G:36:LEU:HD12	1:G:36:LEU:N	2.36	0.41
1:D:149:LYS:NZ	4:D:5387:HOH:O	2.38	0.41
1:B:217:VAL:O	1:B:221:GLN:HG3	2.21	0.41
1:D:156:ALA:HA	1:D:159:THR:CG2	2.51	0.41
1:B:204:ALA:HB2	1:B:218:VAL:HG21	2.03	0.41
1:C:237:ILE:H	1:C:238:PRO:CD	2.33	0.41
1:D:8:LYS:HG3	1:D:8:LYS:HZ2	1.71	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:ILE:H	1:D:238:PRO:CD	2.33	0.41
1:B:95:GLN:OE1	1:B:198:ARG:HD3	2.20	0.41
1:E:27:LEU:O	1:E:32:THR:CG2	2.56	0.41
1:D:211:PHE:HB3	1:D:218:VAL:HG22	2.03	0.41
1:E:29:GLU:HG3	1:E:54:LYS:HE2	2.03	0.41
1:B:209:GLN:NE2	4:B:3453:HOH:O	2.51	0.40
1:F:217:VAL:HA	1:F:220:GLN:HE21	1.86	0.40
1:A:206:VAL:CG2	4:A:2267:HOH:O	2.69	0.40
1:A:204:ALA:HB2	1:A:218:VAL:HG21	2.03	0.40
1:B:107:ASP:N	1:B:107:ASP:OD1	2.54	0.40
1:C:69:GLU:HG3	1:C:70:ALA:N	2.34	0.40
1:G:244:LEU:HD11	1:G:257:LEU:HD22	2.04	0.40
1:H:176:ALA:N	1:H:177:PRO:HD3	2.36	0.40
1:H:192:PRO:HB3	1:H:231:TYR:OH	2.21	0.40
1:B:65:VAL:HG22	2:B:3263:NAD:N1A	2.35	0.40
1:D:220:GLN:CA	4:D:5379:HOH:O	2.68	0.40
1:E:173:LEU:CD1	1:G:152:PRO:HD3	2.51	0.40
1:A:59:ARG:NH1	1:A:81:ASP:HB3	2.36	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	258/262 (98%)	249 (96%)	9 (4%)	0	100	100
1	B	258/262 (98%)	250 (97%)	8 (3%)	0	100	100
1	C	258/262 (98%)	250 (97%)	8 (3%)	0	100	100
1	D	258/262 (98%)	247 (96%)	10 (4%)	1 (0%)	34	24
1	E	258/262 (98%)	251 (97%)	6 (2%)	1 (0%)	34	24
1	F	258/262 (98%)	249 (96%)	9 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	258/262 (98%)	252 (98%)	6 (2%)	0	100	100
1	H	258/262 (98%)	252 (98%)	6 (2%)	0	100	100
All	All	2064/2096 (98%)	2000 (97%)	62 (3%)	2 (0%)	51	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	192	PRO
1	E	195	MET

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	201/203 (99%)	198 (98%)	3 (2%)	65	62
1	B	201/203 (99%)	197 (98%)	4 (2%)	55	51
1	C	201/203 (99%)	191 (95%)	10 (5%)	24	15
1	D	201/203 (99%)	195 (97%)	6 (3%)	41	33
1	E	201/203 (99%)	189 (94%)	12 (6%)	19	9
1	F	201/203 (99%)	196 (98%)	5 (2%)	47	41
1	G	201/203 (99%)	194 (96%)	7 (4%)	36	27
1	H	201/203 (99%)	194 (96%)	7 (4%)	36	27
All	All	1608/1624 (99%)	1554 (97%)	54 (3%)	37	28

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	PRO
1	A	196	TRP
1	A	231	TYR
1	B	32	THR
1	B	205	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	213	THR
1	B	231	TYR
1	C	4	LYS
1	C	32	THR
1	C	42	GLU
1	C	46	LYS
1	C	57	GLU
1	C	69	GLU
1	C	138	ARG
1	C	195	MET
1	C	199	GLN
1	C	231	TYR
1	D	44	LEU
1	D	46	LYS
1	D	138	ARG
1	D	159	THR
1	D	192	PRO
1	D	231	TYR
1	E	32	THR
1	E	39	MET
1	E	46	LYS
1	E	57	GLU
1	E	80	ARG
1	E	138	ARG
1	E	159	THR
1	E	194	PHE
1	E	195	MET
1	E	205	LYS
1	E	231	TYR
1	E	234	ILE
1	F	36	LEU
1	F	57	GLU
1	F	159	THR
1	F	195	MET
1	F	231	TYR
1	G	4	LYS
1	G	54	LYS
1	G	138	ARG
1	G	159	THR
1	G	194	PHE
1	G	231	TYR
1	G	234	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	4	LYS
1	H	8	LYS
1	H	39	MET
1	H	84	LYS
1	H	205	LYS
1	H	213	THR
1	H	231	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	199	GLN
1	A	209	GLN
1	A	220	GLN
1	A	235	ASN
1	A	256	ASN
1	B	91	ASN
1	B	209	GLN
1	C	209	GLN
1	C	220	GLN
1	C	235	ASN
1	D	91	ASN
1	D	209	GLN
1	D	220	GLN
1	D	235	ASN
1	D	256	ASN
1	E	18	ASN
1	E	91	ASN
1	E	199	GLN
1	E	209	GLN
1	E	256	ASN
1	F	199	GLN
1	F	209	GLN
1	F	220	GLN
1	G	6	ASN
1	G	91	ASN
1	G	199	GLN
1	G	209	GLN
1	G	220	GLN
1	G	256	ASN
1	H	91	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	199	GLN
1	H	209	GLN
1	H	220	GLN
1	H	256	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	E	6263	-	42,48,48	2.27	13 (30%)	50,73,73	1.71	9 (18%)
2	NAD	B	3263	-	42,48,48	2.28	14 (33%)	50,73,73	1.69	12 (24%)
2	NAD	A	2263	-	42,48,48	2.21	15 (35%)	50,73,73	1.73	9 (18%)
2	NAD	D	5263	-	42,48,48	2.21	14 (33%)	50,73,73	1.71	10 (20%)
2	NAD	C	4263	-	42,48,48	2.17	13 (30%)	50,73,73	1.72	11 (22%)
2	NAD	F	7263	-	42,48,48	2.33	15 (35%)	50,73,73	1.70	10 (20%)
2	NAD	H	9263	-	42,48,48	2.44	15 (35%)	50,73,73	1.73	11 (22%)
2	NAD	G	8263	-	42,48,48	2.16	13 (30%)	50,73,73	1.76	10 (20%)

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	E	6263	-	-	5/26/62/62	0/5/5/5
2	NAD	B	3263	-	-	8/26/62/62	0/5/5/5
2	NAD	A	2263	-	-	7/26/62/62	0/5/5/5
2	NAD	D	5263	-	-	8/26/62/62	0/5/5/5
2	NAD	C	4263	-	-	4/26/62/62	0/5/5/5
2	NAD	F	7263	-	-	4/26/62/62	0/5/5/5
2	NAD	H	9263	-	-	5/26/62/62	0/5/5/5
2	NAD	G	8263	-	-	5/26/62/62	0/5/5/5

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4263	NAD	C2N-N1N	6.53	1.42	1.35
2	F	7263	NAD	C2N-N1N	6.42	1.42	1.35
2	H	9263	NAD	C2N-N1N	6.39	1.42	1.35
2	B	3263	NAD	C2N-N1N	6.38	1.42	1.35
2	D	5263	NAD	C2N-N1N	6.19	1.42	1.35
2	G	8263	NAD	C2N-N1N	5.74	1.42	1.35
2	F	7263	NAD	C4N-C3N	5.72	1.49	1.39
2	E	6263	NAD	C2N-N1N	5.57	1.41	1.35
2	H	9263	NAD	C4N-C3N	5.47	1.48	1.39
2	B	3263	NAD	C4N-C3N	5.46	1.48	1.39
2	A	2263	NAD	C4N-C3N	5.32	1.48	1.39
2	A	2263	NAD	C2A-N3A	5.29	1.40	1.32
2	E	6263	NAD	C2D-C1D	-5.23	1.45	1.53
2	B	3263	NAD	C2A-N3A	5.06	1.40	1.32
2	E	6263	NAD	C4N-C3N	5.04	1.47	1.39
2	H	9263	NAD	C2A-N3A	4.94	1.40	1.32
2	G	8263	NAD	C4N-C3N	4.93	1.47	1.39
2	E	6263	NAD	C2A-N3A	4.81	1.39	1.32
2	F	7263	NAD	C6N-N1N	4.80	1.47	1.35
2	D	5263	NAD	C4N-C3N	4.80	1.47	1.39
2	D	5263	NAD	C2D-C1D	-4.66	1.46	1.53
2	A	2263	NAD	C2N-N1N	4.60	1.40	1.35
2	E	6263	NAD	C6N-N1N	4.60	1.46	1.35
2	H	9263	NAD	C6N-N1N	4.59	1.46	1.35
2	F	7263	NAD	C2A-N3A	4.59	1.39	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4263	NAD	C4N-C3N	4.56	1.47	1.39
2	H	9263	NAD	O4D-C1D	4.52	1.47	1.41
2	C	4263	NAD	C2A-N3A	4.30	1.39	1.32
2	G	8263	NAD	C2A-N3A	4.06	1.38	1.32
2	G	8263	NAD	C6N-N1N	4.05	1.45	1.35
2	E	6263	NAD	C4A-N3A	4.02	1.41	1.35
2	A	2263	NAD	O4D-C1D	4.01	1.46	1.41
2	C	4263	NAD	C4A-N3A	3.96	1.41	1.35
2	A	2263	NAD	C2A-N1A	3.95	1.41	1.33
2	B	3263	NAD	O4D-C1D	3.94	1.46	1.41
2	H	9263	NAD	C2A-N1A	3.83	1.41	1.33
2	B	3263	NAD	C2D-C1D	-3.80	1.48	1.53
2	C	4263	NAD	C2D-C1D	-3.80	1.48	1.53
2	D	5263	NAD	C6N-N1N	3.79	1.44	1.35
2	D	5263	NAD	C2A-N3A	3.79	1.38	1.32
2	F	7263	NAD	O4D-C1D	3.78	1.46	1.41
2	D	5263	NAD	C2A-N1A	3.67	1.40	1.33
2	B	3263	NAD	C6N-N1N	3.64	1.44	1.35
2	H	9263	NAD	C3D-C4D	3.61	1.62	1.53
2	B	3263	NAD	O4B-C4B	3.59	1.53	1.45
2	A	2263	NAD	C2D-C1D	-3.45	1.48	1.53
2	H	9263	NAD	C5N-C4N	3.45	1.46	1.38
2	A	2263	NAD	C4A-N3A	3.40	1.40	1.35
2	C	4263	NAD	C6N-N1N	3.34	1.43	1.35
2	F	7263	NAD	C6N-C5N	3.33	1.46	1.38
2	G	8263	NAD	C2D-C1D	-3.29	1.48	1.53
2	H	9263	NAD	PN-O2N	-3.27	1.40	1.55
2	F	7263	NAD	C5N-C4N	3.26	1.45	1.38
2	G	8263	NAD	C3B-C4B	3.26	1.61	1.53
2	A	2263	NAD	PN-O2N	-3.23	1.40	1.55
2	A	2263	NAD	C6N-N1N	3.19	1.43	1.35
2	G	8263	NAD	C3D-C4D	3.16	1.61	1.53
2	G	8263	NAD	PN-O2N	-3.16	1.40	1.55
2	E	6263	NAD	C2A-N1A	3.15	1.39	1.33
2	E	6263	NAD	PN-O2N	-3.12	1.40	1.55
2	D	5263	NAD	PN-O2N	-3.12	1.40	1.55
2	B	3263	NAD	C3B-C4B	3.12	1.61	1.53
2	G	8263	NAD	O4D-C1D	3.10	1.45	1.41
2	D	5263	NAD	C4A-N3A	3.05	1.39	1.35
2	F	7263	NAD	C2A-N1A	3.05	1.39	1.33
2	C	4263	NAD	PN-O2N	-3.00	1.41	1.55
2	G	8263	NAD	O4B-C4B	2.98	1.51	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	6263	NAD	O4D-C1D	2.89	1.45	1.41
2	F	7263	NAD	C3B-C4B	2.82	1.60	1.53
2	H	9263	NAD	O7N-C7N	-2.79	1.18	1.24
2	B	3263	NAD	C2A-N1A	2.70	1.38	1.33
2	F	7263	NAD	C3D-C4D	2.68	1.59	1.53
2	D	5263	NAD	O4B-C1B	-2.68	1.37	1.41
2	E	6263	NAD	C5N-C4N	2.67	1.44	1.38
2	C	4263	NAD	C3B-C4B	2.64	1.59	1.53
2	D	5263	NAD	C6N-C5N	2.63	1.44	1.38
2	H	9263	NAD	O4B-C4B	2.57	1.50	1.45
2	G	8263	NAD	C8A-N7A	-2.56	1.30	1.34
2	F	7263	NAD	C2D-C1D	-2.56	1.49	1.53
2	B	3263	NAD	C3D-C4D	2.54	1.59	1.53
2	D	5263	NAD	C5N-C4N	2.53	1.44	1.38
2	C	4263	NAD	O4B-C4B	2.53	1.50	1.45
2	A	2263	NAD	O4B-C4B	2.52	1.50	1.45
2	G	8263	NAD	C2A-N1A	2.51	1.38	1.33
2	C	4263	NAD	C5N-C4N	2.51	1.44	1.38
2	E	6263	NAD	PA-O1A	-2.51	1.42	1.50
2	H	9263	NAD	C6N-C5N	2.49	1.44	1.38
2	F	7263	NAD	PN-O2N	-2.49	1.43	1.55
2	H	9263	NAD	C4A-N3A	2.45	1.39	1.35
2	G	8263	NAD	PA-O1A	-2.44	1.42	1.50
2	D	5263	NAD	O4B-C4B	2.43	1.50	1.45
2	A	2263	NAD	C5N-C4N	2.43	1.44	1.38
2	C	4263	NAD	O4D-C1D	2.42	1.44	1.41
2	A	2263	NAD	PA-O1A	-2.41	1.42	1.50
2	F	7263	NAD	C3N-C7N	2.35	1.54	1.50
2	B	3263	NAD	PN-O2N	-2.33	1.44	1.55
2	C	4263	NAD	C3N-C7N	2.31	1.54	1.50
2	B	3263	NAD	C3N-C7N	2.24	1.53	1.50
2	C	4263	NAD	C2A-N1A	2.21	1.38	1.33
2	H	9263	NAD	C3B-C4B	2.21	1.58	1.53
2	E	6263	NAD	C3D-C4D	2.20	1.58	1.53
2	F	7263	NAD	C4A-N3A	2.18	1.38	1.35
2	D	5263	NAD	C3N-C7N	2.16	1.53	1.50
2	F	7263	NAD	O4B-C4B	2.16	1.49	1.45
2	A	2263	NAD	C3B-C4B	2.16	1.58	1.53
2	B	3263	NAD	C5N-C4N	2.15	1.43	1.38
2	A	2263	NAD	C6N-C5N	2.13	1.43	1.38
2	H	9263	NAD	C2D-C1D	-2.09	1.50	1.53
2	B	3263	NAD	C6N-C5N	2.07	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2263	NAD	C3D-C4D	2.07	1.58	1.53
2	D	5263	NAD	PA-O1A	-2.06	1.43	1.50
2	E	6263	NAD	C6N-C5N	2.04	1.43	1.38

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2263	NAD	O5D-PN-O1N	-5.10	89.14	109.07
2	D	5263	NAD	C5A-C6A-N6A	4.78	127.61	120.35
2	H	9263	NAD	O5D-PN-O1N	-4.76	90.46	109.07
2	A	2263	NAD	C5A-C6A-N6A	4.65	127.42	120.35
2	D	5263	NAD	O5D-PN-O1N	-4.65	90.91	109.07
2	E	6263	NAD	O5D-PN-O1N	-4.54	91.33	109.07
2	B	3263	NAD	C5A-C6A-N6A	4.52	127.22	120.35
2	B	3263	NAD	O5D-PN-O1N	-4.48	91.58	109.07
2	F	7263	NAD	O5D-PN-O1N	-4.42	91.79	109.07
2	G	8263	NAD	C5A-C6A-N6A	4.41	127.05	120.35
2	F	7263	NAD	C5A-C6A-N6A	4.39	127.03	120.35
2	C	4263	NAD	C5A-C6A-N6A	4.32	126.92	120.35
2	C	4263	NAD	O5D-PN-O1N	-4.30	92.26	109.07
2	G	8263	NAD	O5D-PN-O1N	-4.23	92.54	109.07
2	G	8263	NAD	O7N-C7N-C3N	-4.19	114.61	119.63
2	H	9263	NAD	C3N-C7N-N7N	4.11	122.68	117.75
2	G	8263	NAD	C3N-C7N-N7N	4.05	122.61	117.75
2	H	9263	NAD	C5A-C6A-N6A	4.00	126.43	120.35
2	E	6263	NAD	C5A-C6A-N6A	3.98	126.41	120.35
2	E	6263	NAD	N3A-C2A-N1A	-3.96	122.48	128.68
2	E	6263	NAD	O5B-C5B-C4B	-3.96	95.36	108.99
2	C	4263	NAD	N3A-C2A-N1A	-3.82	122.71	128.68
2	C	4263	NAD	O5B-C5B-C4B	-3.68	96.32	108.99
2	H	9263	NAD	O7N-C7N-C3N	-3.67	115.24	119.63
2	F	7263	NAD	C2N-C3N-C4N	3.65	122.39	118.26
2	G	8263	NAD	N3A-C2A-N1A	-3.63	123.01	128.68
2	F	7263	NAD	C3N-C7N-N7N	3.51	121.96	117.75
2	F	7263	NAD	O5B-C5B-C4B	-3.45	97.13	108.99
2	F	7263	NAD	O7N-C7N-C3N	-3.38	115.59	119.63
2	A	2263	NAD	O5B-C5B-C4B	-3.37	97.40	108.99
2	D	5263	NAD	O5B-C5B-C4B	-3.35	97.45	108.99
2	B	3263	NAD	O5B-C5B-C4B	-3.33	97.52	108.99
2	B	3263	NAD	C3N-C7N-N7N	3.31	121.72	117.75
2	B	3263	NAD	N3A-C2A-N1A	-3.31	123.51	128.68
2	D	5263	NAD	N3A-C2A-N1A	-3.30	123.51	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2263	NAD	C2N-C3N-C4N	3.28	121.97	118.26
2	F	7263	NAD	N3A-C2A-N1A	-3.26	123.58	128.68
2	D	5263	NAD	O7N-C7N-C3N	-3.23	115.77	119.63
2	E	6263	NAD	C2N-C3N-C4N	3.21	121.90	118.26
2	D	5263	NAD	C3N-C7N-N7N	3.20	121.59	117.75
2	G	8263	NAD	O5B-C5B-C4B	-3.17	98.07	108.99
2	H	9263	NAD	N3A-C2A-N1A	-3.15	123.75	128.68
2	B	3263	NAD	O7N-C7N-C3N	-3.11	115.91	119.63
2	G	8263	NAD	C2N-C3N-C4N	3.10	121.77	118.26
2	H	9263	NAD	C2N-C3N-C4N	3.08	121.75	118.26
2	A	2263	NAD	C3N-C7N-N7N	3.05	121.41	117.75
2	C	4263	NAD	O7N-C7N-C3N	-3.04	115.99	119.63
2	D	5263	NAD	C2N-C3N-C4N	3.02	121.68	118.26
2	C	4263	NAD	C3N-C7N-N7N	3.02	121.37	117.75
2	A	2263	NAD	O7N-C7N-C3N	-3.01	116.03	119.63
2	B	3263	NAD	C2N-C3N-C4N	3.01	121.67	118.26
2	C	4263	NAD	C2N-C3N-C4N	3.00	121.66	118.26
2	E	6263	NAD	C3N-C7N-N7N	2.96	121.31	117.75
2	A	2263	NAD	N3A-C2A-N1A	-2.96	124.05	128.68
2	A	2263	NAD	C5N-C4N-C3N	-2.96	116.84	120.34
2	H	9263	NAD	C1B-N9A-C4A	-2.91	121.53	126.64
2	H	9263	NAD	O5B-C5B-C4B	-2.88	99.06	108.99
2	D	5263	NAD	C1B-N9A-C4A	-2.87	121.59	126.64
2	A	2263	NAD	C1B-N9A-C4A	-2.87	121.61	126.64
2	C	4263	NAD	C1B-N9A-C4A	-2.79	121.74	126.64
2	E	6263	NAD	O7N-C7N-C3N	-2.77	116.31	119.63
2	B	3263	NAD	C1B-N9A-C4A	-2.76	121.80	126.64
2	F	7263	NAD	C1B-N9A-C4A	-2.71	121.87	126.64
2	C	4263	NAD	C5N-C6N-N1N	-2.71	116.51	120.40
2	F	7263	NAD	C5N-C4N-C3N	-2.62	117.24	120.34
2	E	6263	NAD	C1B-N9A-C4A	-2.61	122.06	126.64
2	H	9263	NAD	C5N-C4N-C3N	-2.61	117.26	120.34
2	G	8263	NAD	C3N-C2N-N1N	-2.50	117.98	120.43
2	B	3263	NAD	C2N-N1N-C1D	2.44	124.58	119.14
2	F	7263	NAD	C2N-N1N-C1D	2.41	124.49	119.14
2	G	8263	NAD	C5N-C6N-N1N	-2.38	116.99	120.40
2	G	8263	NAD	C2N-N1N-C1D	2.28	124.21	119.14
2	D	5263	NAD	C2N-N1N-C1D	2.27	124.19	119.14
2	H	9263	NAD	C3B-C2B-C1B	2.18	104.26	100.98
2	B	3263	NAD	C5N-C4N-C3N	-2.15	117.79	120.34
2	E	6263	NAD	C5N-C6N-N1N	-2.13	117.35	120.40
2	B	3263	NAD	C3N-C2N-N1N	-2.11	118.37	120.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3263	NAD	C3B-C2B-C1B	2.10	104.14	100.98
2	H	9263	NAD	C5N-C6N-N1N	-2.10	117.40	120.40
2	D	5263	NAD	C5N-C6N-N1N	-2.03	117.50	120.40
2	C	4263	NAD	C3N-C2N-N1N	-2.02	118.45	120.43
2	C	4263	NAD	C6N-N1N-C2N	2.01	123.81	121.97

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	6263	NAD	C5D-O5D-PN-O1N
2	E	6263	NAD	C5D-O5D-PN-O2N
2	E	6263	NAD	O4D-C1D-N1N-C2N
2	D	5263	NAD	PN-O3-PA-O5B
2	D	5263	NAD	C5D-O5D-PN-O1N
2	D	5263	NAD	C5D-O5D-PN-O2N
2	D	5263	NAD	O4D-C1D-N1N-C2N
2	G	8263	NAD	C5D-O5D-PN-O1N
2	G	8263	NAD	C5D-O5D-PN-O2N
2	G	8263	NAD	O4D-C1D-N1N-C2N
2	A	2263	NAD	PN-O3-PA-O5B
2	A	2263	NAD	C5D-O5D-PN-O3
2	A	2263	NAD	O4D-C1D-N1N-C2N
2	F	7263	NAD	C5D-O5D-PN-O1N
2	C	4263	NAD	C5D-O5D-PN-O1N
2	H	9263	NAD	C5D-O5D-PN-O1N
2	H	9263	NAD	C5D-O5D-PN-O2N
2	H	9263	NAD	O4D-C1D-N1N-C2N
2	B	3263	NAD	C5D-O5D-PN-O1N
2	B	3263	NAD	C5D-O5D-PN-O2N
2	B	3263	NAD	O4D-C1D-N1N-C2N
2	B	3263	NAD	PN-O3-PA-O5B
2	E	6263	NAD	C5D-O5D-PN-O3
2	D	5263	NAD	C5D-O5D-PN-O3
2	G	8263	NAD	C5D-O5D-PN-O3
2	F	7263	NAD	C5D-O5D-PN-O3
2	D	5263	NAD	PA-O3-PN-O1N
2	A	2263	NAD	PA-O3-PN-O1N
2	A	2263	NAD	C5D-O5D-PN-O2N
2	F	7263	NAD	C5D-O5D-PN-O2N
2	C	4263	NAD	C5D-O5D-PN-O2N
2	B	3263	NAD	PA-O3-PN-O1N

Continued on next page...

Continued from previous page...

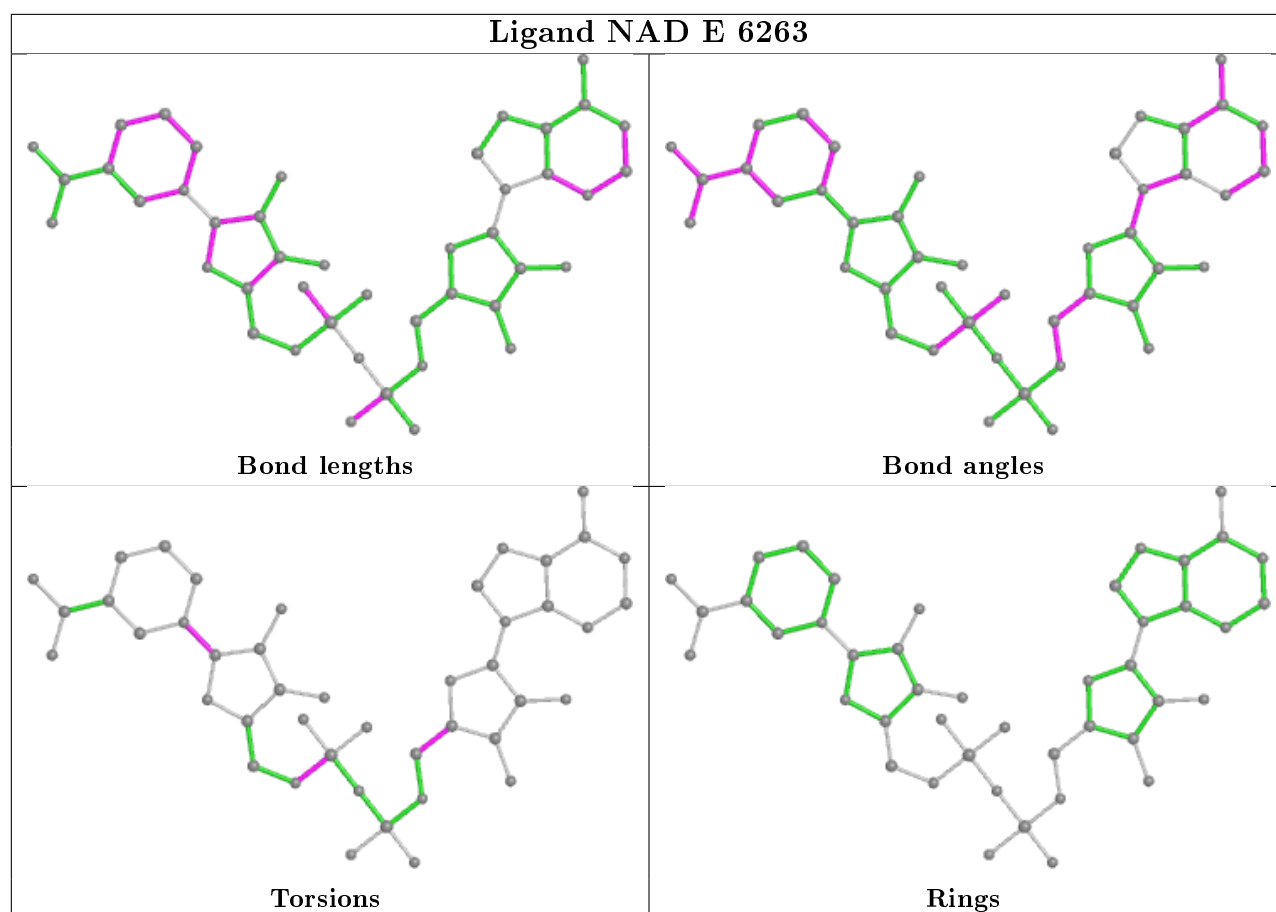
Mol	Chain	Res	Type	Atoms
2	H	9263	NAD	O4B-C4B-C5B-O5B
2	C	4263	NAD	C5D-O5D-PN-O3
2	H	9263	NAD	C5D-O5D-PN-O3
2	B	3263	NAD	C5D-O5D-PN-O3
2	E	6263	NAD	O4B-C4B-C5B-O5B
2	D	5263	NAD	O4B-C4B-C5B-O5B
2	G	8263	NAD	O4B-C4B-C5B-O5B
2	A	2263	NAD	O4B-C4B-C5B-O5B
2	F	7263	NAD	O4B-C4B-C5B-O5B
2	C	4263	NAD	O4B-C4B-C5B-O5B
2	B	3263	NAD	O4B-C4B-C5B-O5B
2	D	5263	NAD	PA-O3-PN-O2N
2	A	2263	NAD	PA-O3-PN-O2N
2	B	3263	NAD	PA-O3-PN-O2N

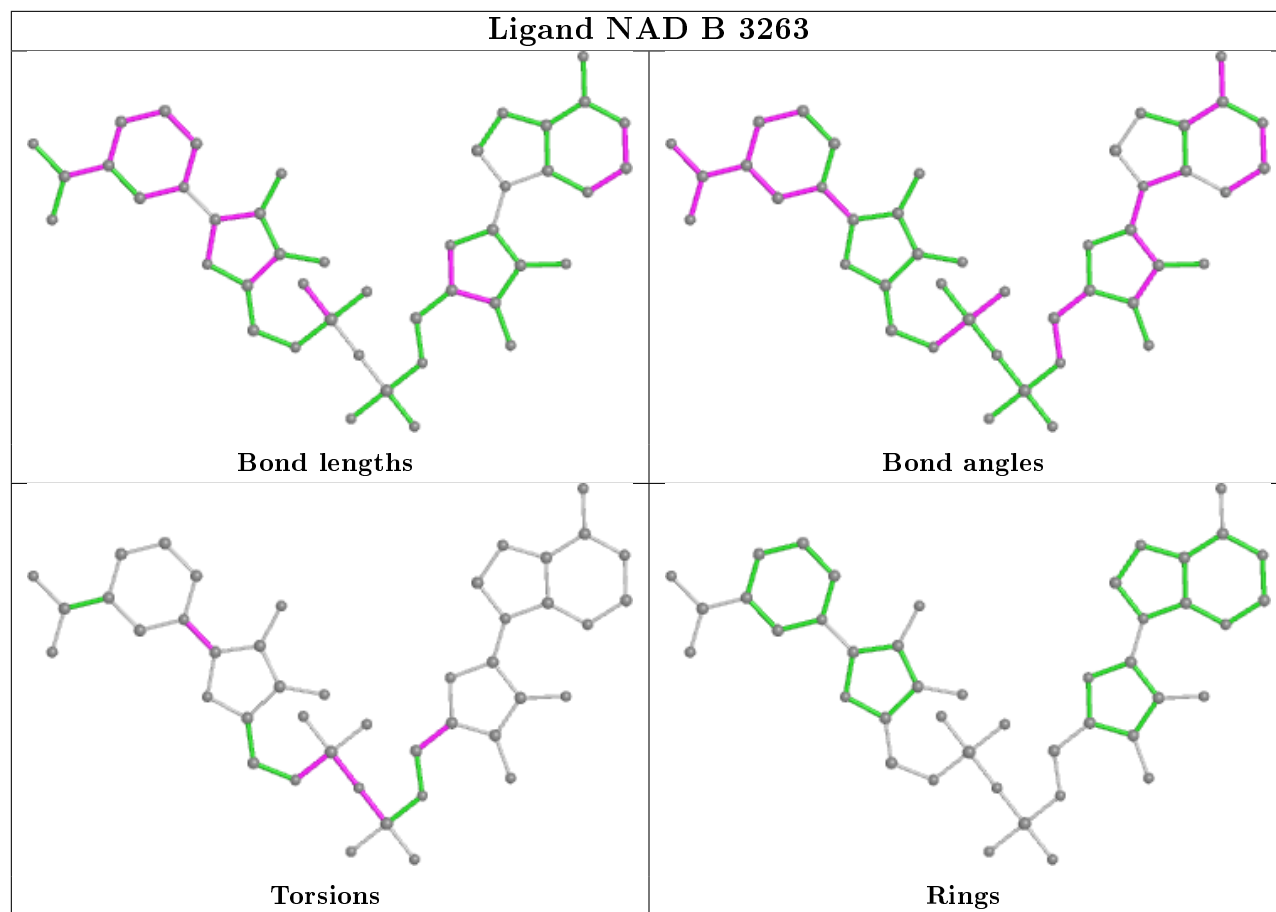
There are no ring outliers.

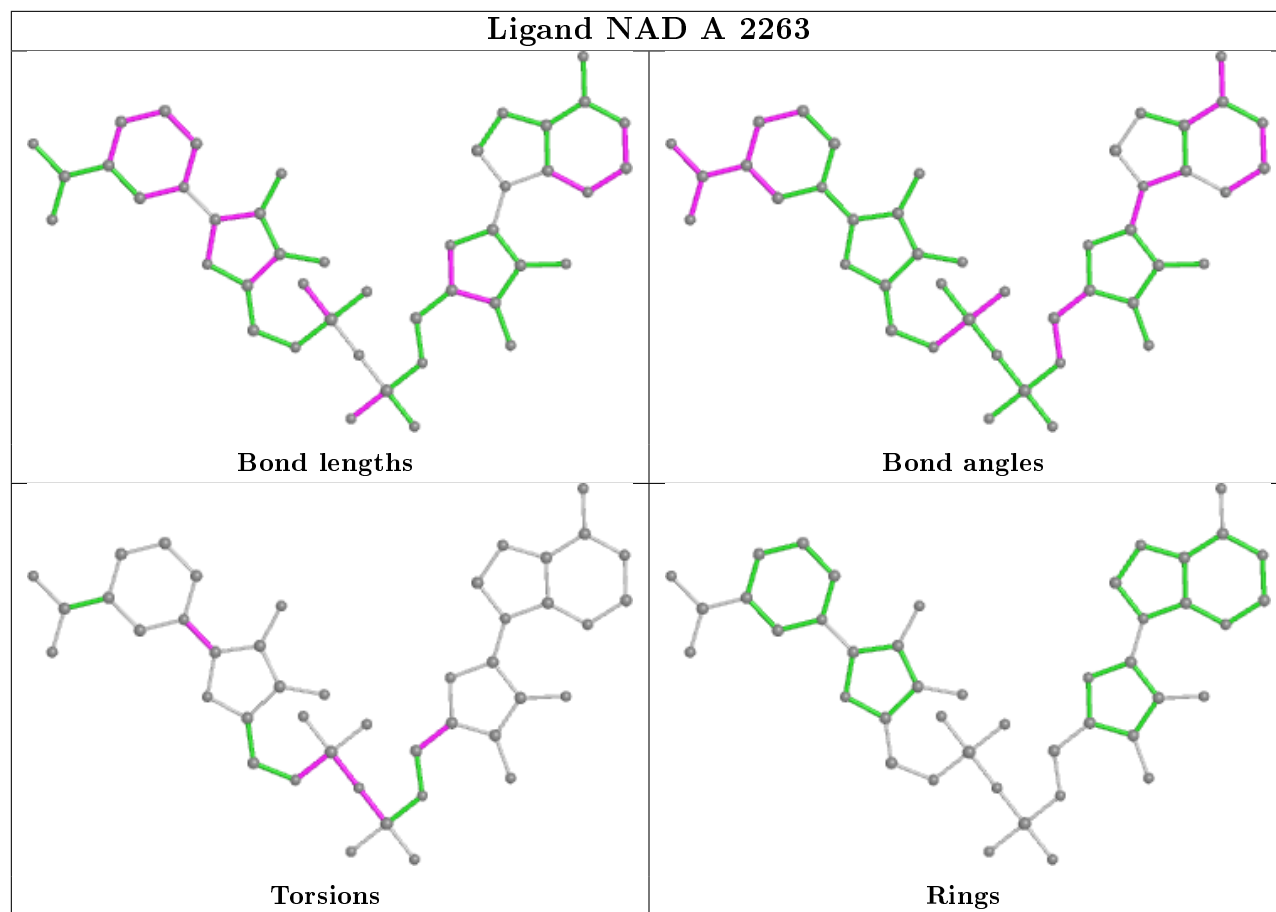
7 monomers are involved in 14 short contacts:

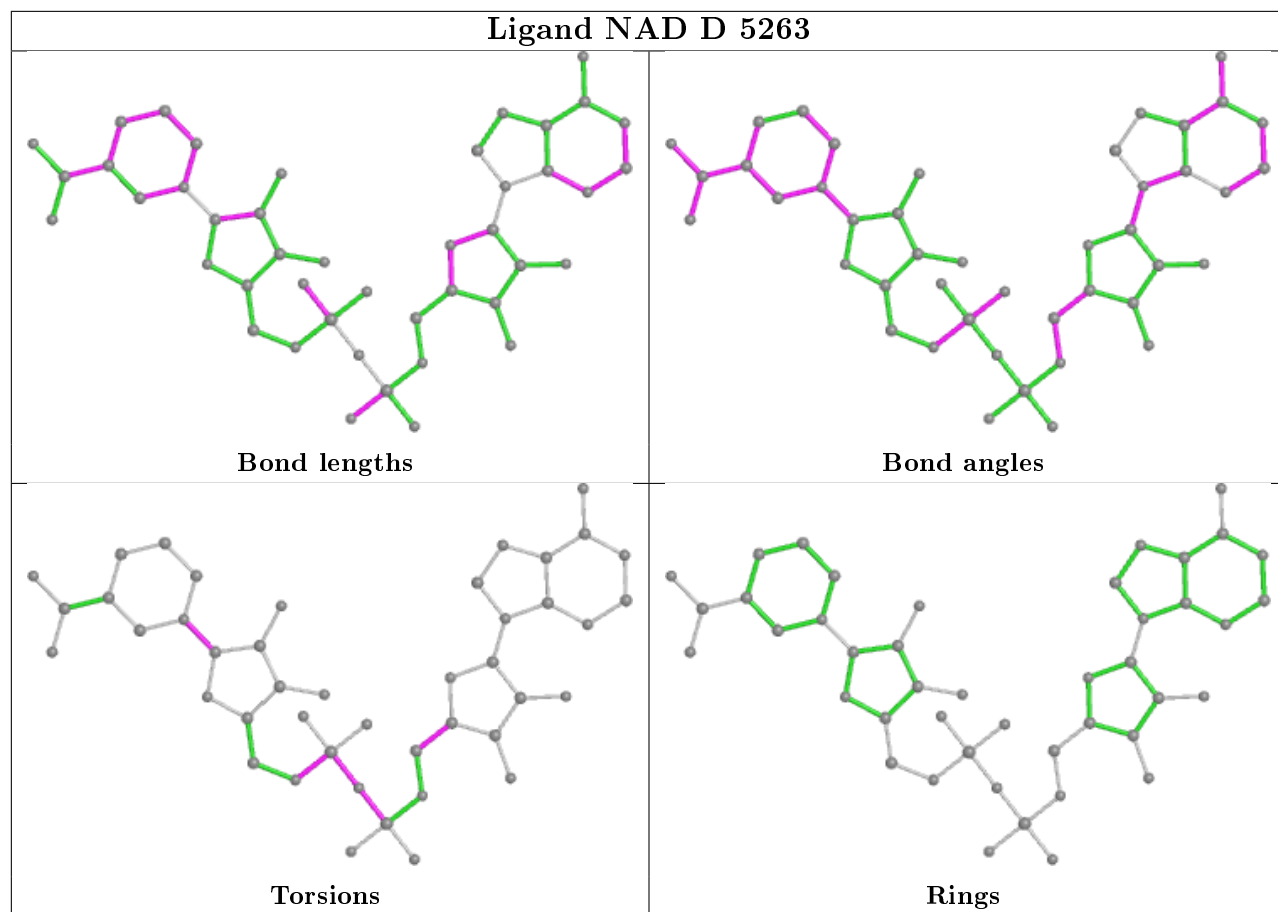
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	6263	NAD	1	0
2	B	3263	NAD	3	0
2	A	2263	NAD	3	0
2	D	5263	NAD	1	0
2	F	7263	NAD	1	0
2	H	9263	NAD	4	0
2	G	8263	NAD	1	0

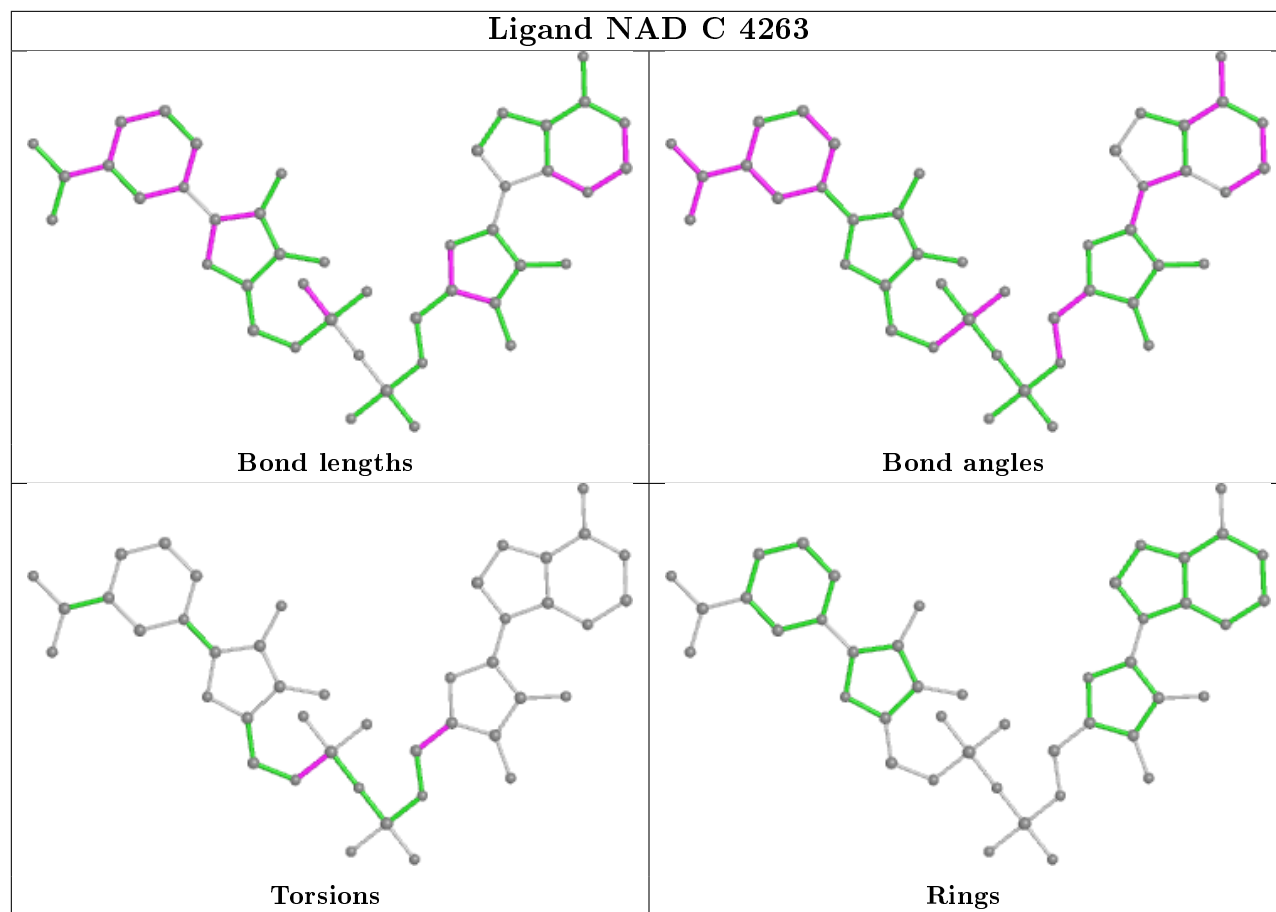
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

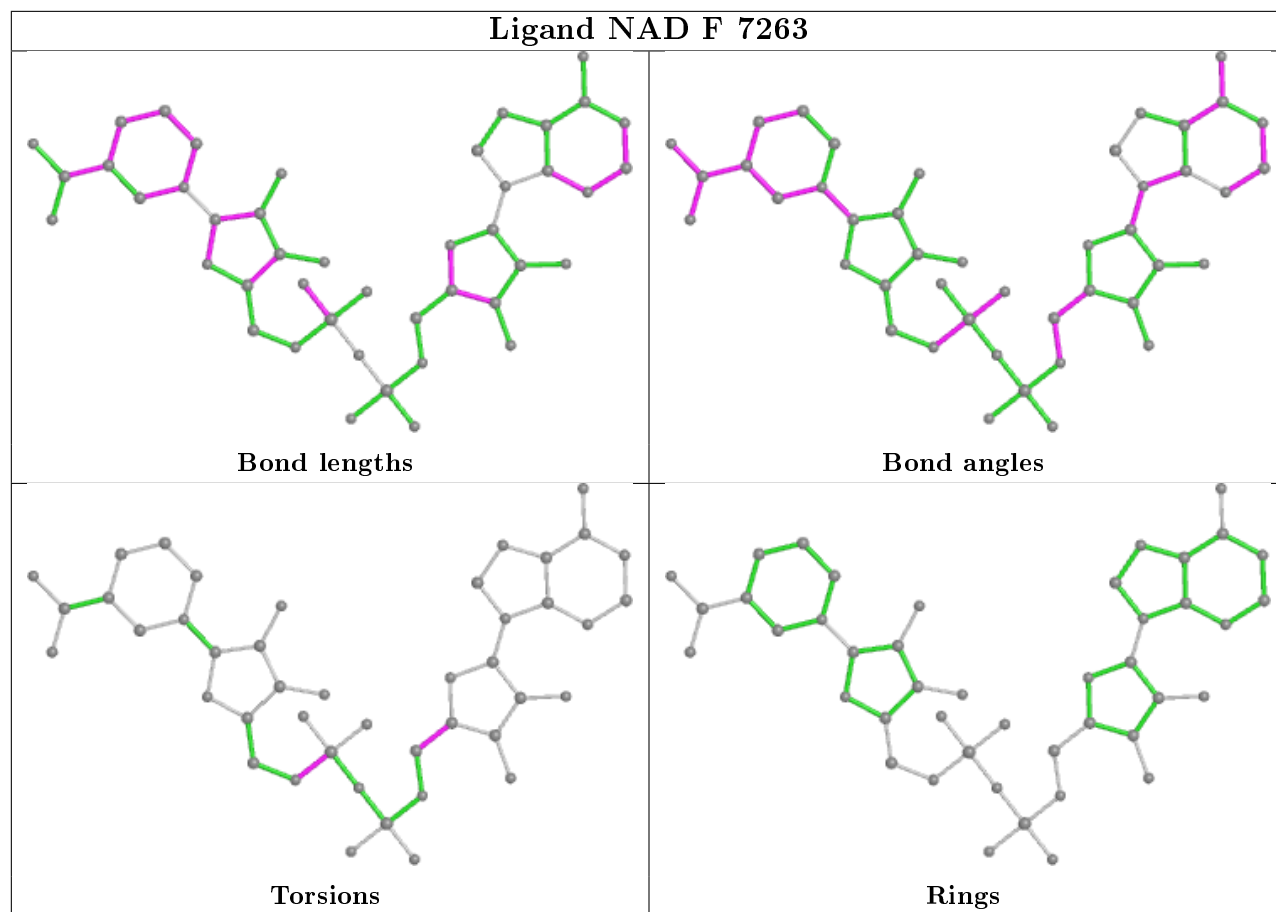


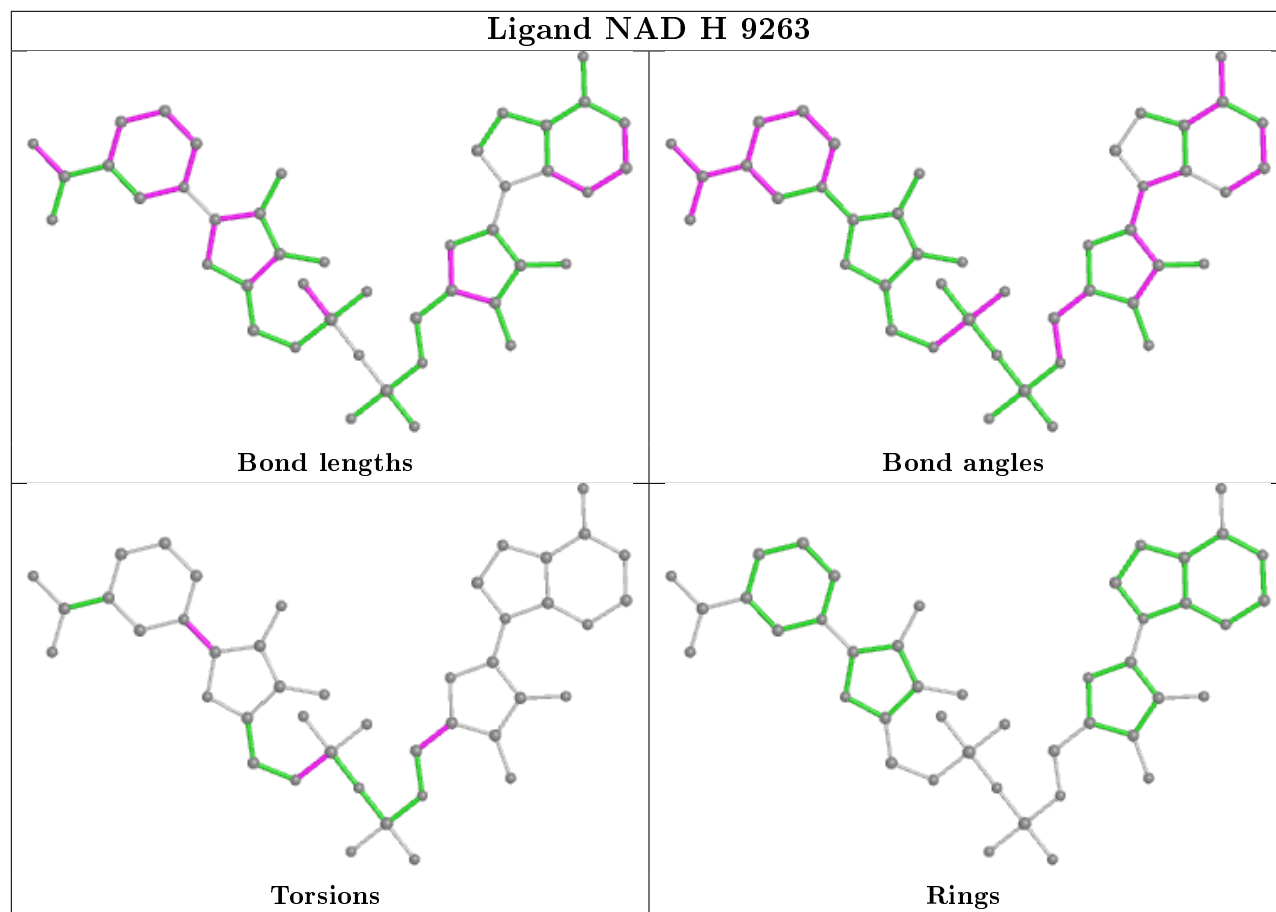


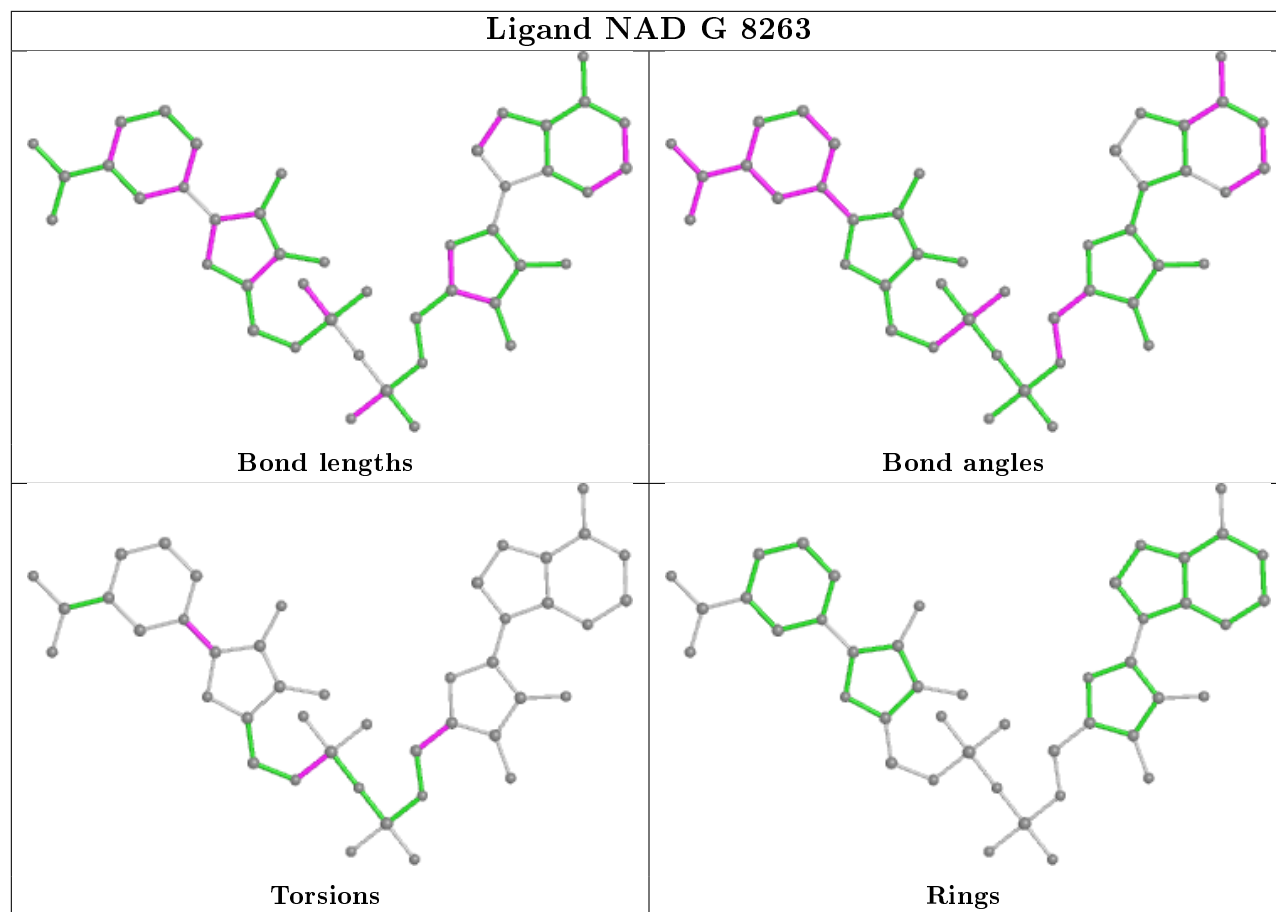












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	260/262 (99%)	-0.14	6 (2%) 60 63	8, 18, 34, 52	0
1	B	260/262 (99%)	-0.36	4 (1%) 73 76	7, 14, 28, 46	0
1	C	260/262 (99%)	-0.36	1 (0%) 92 93	7, 15, 28, 42	0
1	D	260/262 (99%)	-0.23	4 (1%) 73 76	7, 15, 31, 55	0
1	E	260/262 (99%)	-0.16	3 (1%) 79 81	9, 18, 34, 56	0
1	F	260/262 (99%)	-0.50	2 (0%) 86 87	4, 12, 23, 42	0
1	G	260/262 (99%)	-0.28	2 (0%) 86 87	6, 15, 28, 44	0
1	H	260/262 (99%)	-0.32	2 (0%) 86 87	5, 14, 29, 45	0
All	All	2080/2096 (99%)	-0.29	24 (1%) 79 81	4, 15, 30, 56	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	194	PHE	9.0
1	E	194	PHE	7.9
1	D	194	PHE	7.2
1	A	194	PHE	7.1
1	G	194	PHE	7.0
1	B	194	PHE	6.0
1	D	193	GLY	5.0
1	E	193	GLY	4.1
1	B	193	GLY	3.9
1	A	193	GLY	3.4
1	A	4	LYS	3.4
1	E	4	LYS	3.1
1	G	4	LYS	2.9
1	F	194	PHE	2.9
1	D	4	LYS	2.8
1	A	52	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	4	LYS	2.5
1	F	4	LYS	2.5
1	A	6	ASN	2.4
1	H	4	LYS	2.3
1	A	195	MET	2.3
1	D	195	MET	2.1
1	B	195	MET	2.1
1	B	4	LYS	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

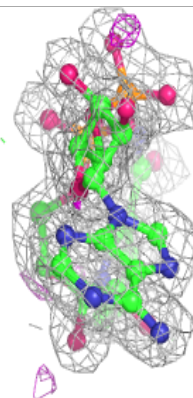
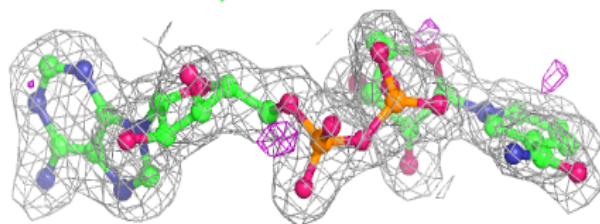
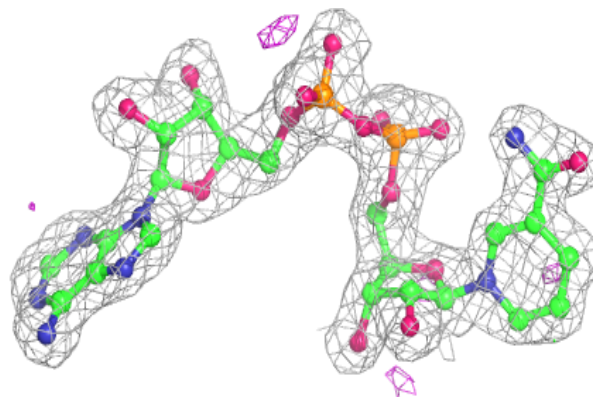
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAD	E	6263	44/44	0.95	0.09	19,23,27,30	0
2	NAD	A	2263	44/44	0.95	0.09	18,23,26,29	0
2	NAD	G	8263	44/44	0.96	0.09	14,18,22,23	0
2	NAD	D	5263	44/44	0.96	0.09	12,19,23,26	0
2	NAD	F	7263	44/44	0.96	0.10	14,18,22,25	0
2	NAD	C	4263	44/44	0.96	0.09	12,16,19,21	0
2	NAD	H	9263	44/44	0.96	0.09	16,21,26,27	0
2	NAD	B	3263	44/44	0.96	0.08	13,19,28,29	0
3	MG	C	3268	1/1	0.98	0.04	17,17,17,17	0
3	MG	E	3266	1/1	0.99	0.12	13,13,13,13	0
3	MG	F	3267	1/1	0.99	0.07	12,12,12,12	0
3	MG	D	3264	1/1	0.99	0.07	11,11,11,11	0
3	MG	C	3265	1/1	1.00	0.09	13,13,13,13	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.

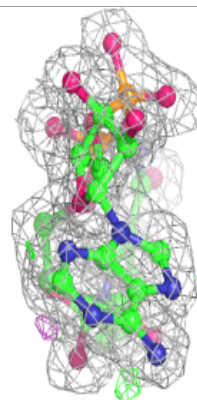
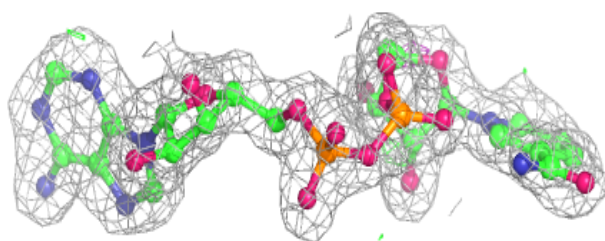
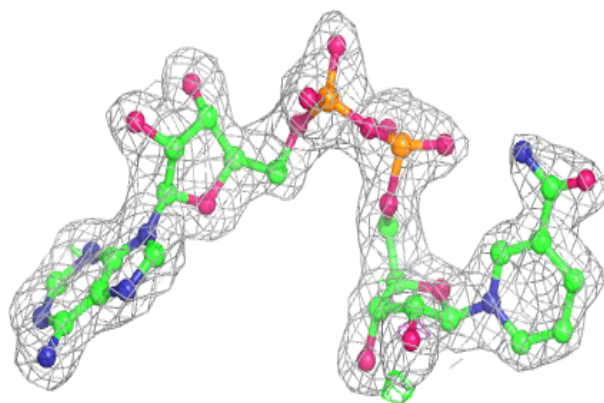
Electron density around NAD E 6263:

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

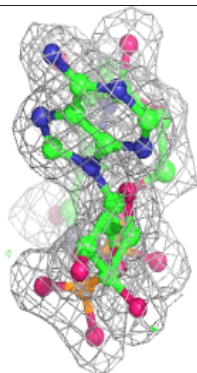
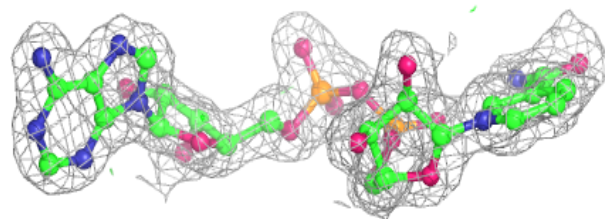
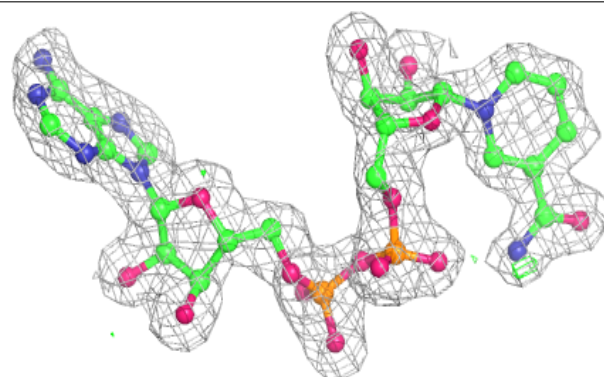


Electron density around NAD A 2263:

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

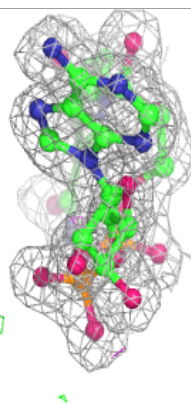
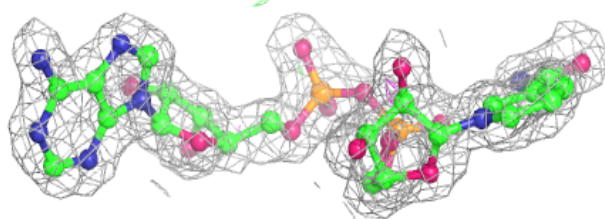
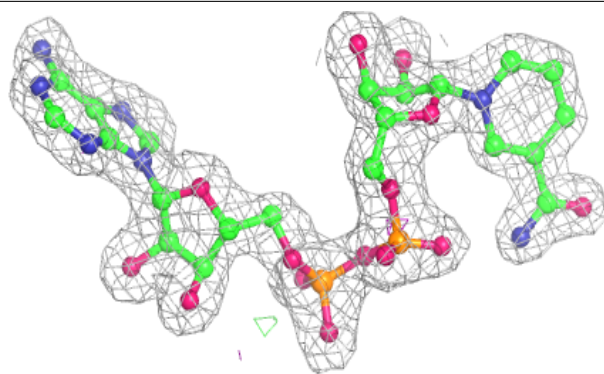
**Electron density around NAD G 8263:**

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

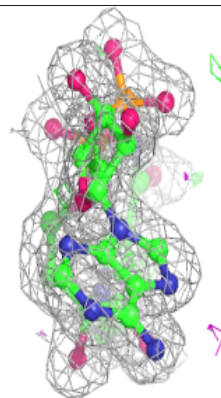
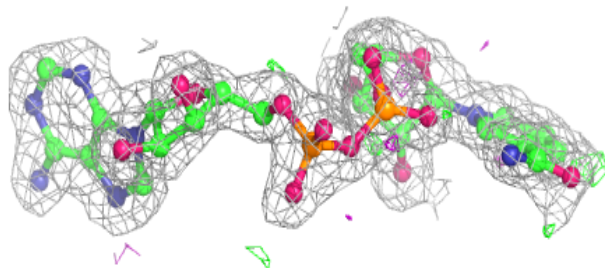
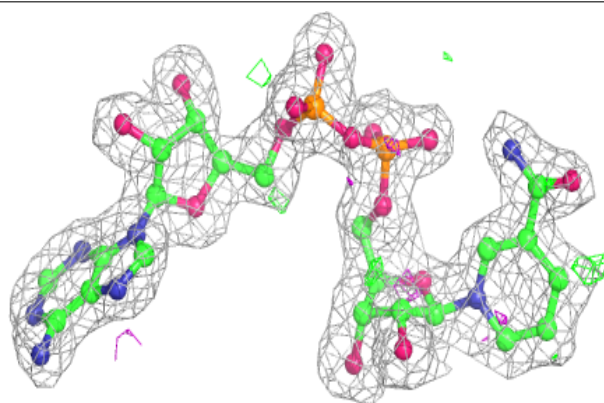


Electron density around NAD D 5263:

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

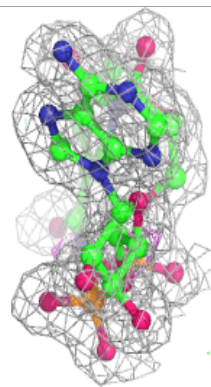
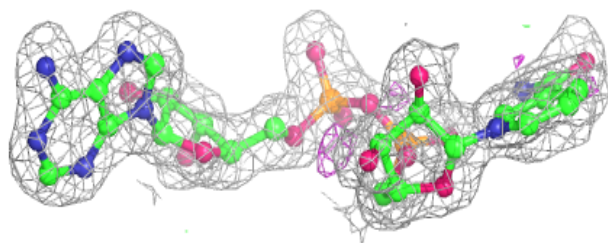
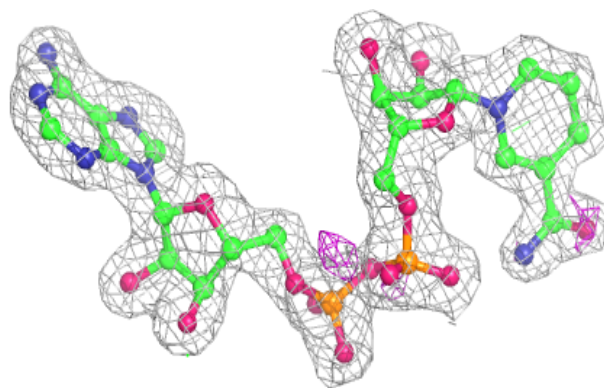
**Electron density around NAD F 7263:**

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

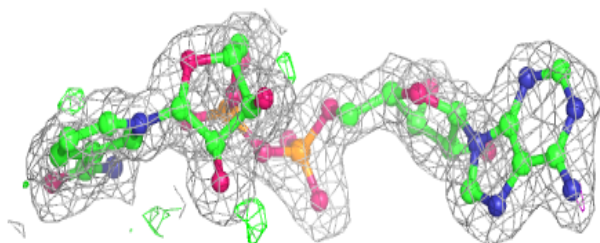
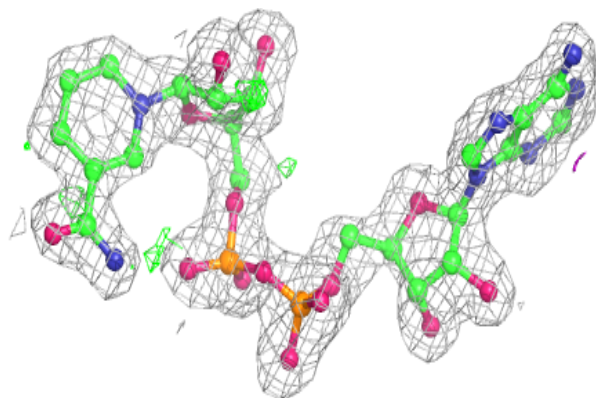


Electron density around NAD C 4263:

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

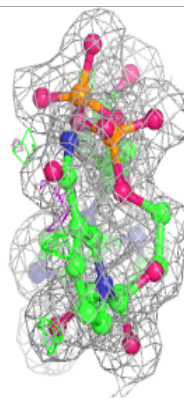
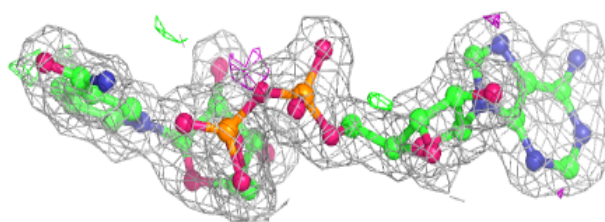
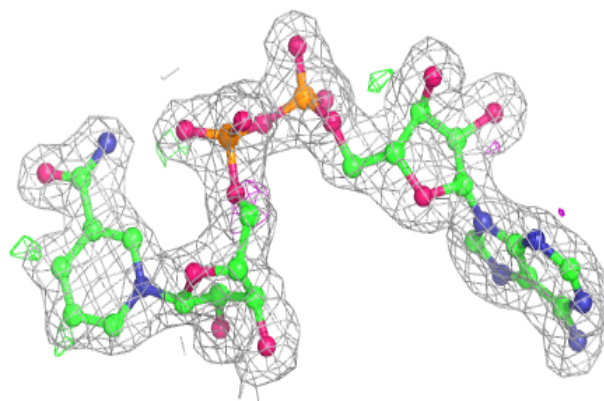
**Electron density around NAD H 9263:**

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



Electron density around NAD B 3263:

$2mF_o-DF_c$ (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.