



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2020 – 10:20 AM BST

PDB ID : 3N7U
Title : NAD-dependent formate dehydrogenase from higher-plant *Arabidopsis thaliana* in complex with NAD and azide
Authors : Shabalin, I.G.; Polyakov, K.M.; Serov, A.E.; Skirgello, O.E.; Sadykhov, E.G.; Dorovatovskiy, P.V.; Tishkov, V.I.; Popov, V.O.
Deposited on : 2010-05-27
Resolution : 2.00 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 : 2.13
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) : 2.13

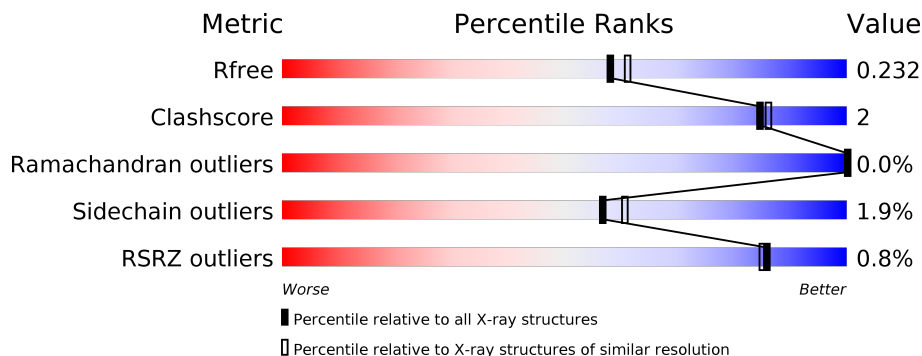
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	351	
1	B	351	
1	C	351	
1	D	351	
1	E	351	
1	F	351	

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Mol	Chain	Length	Quality of chain
1	G	351	 92% 8%
1	H	351	 % 92% 8%
1	I	351	 2% 91% 8%
1	J	351	 2% 91% 9%
1	K	351	 % 92% 8%
1	L	351	 % 92% 8%

2 Entry composition [i](#)

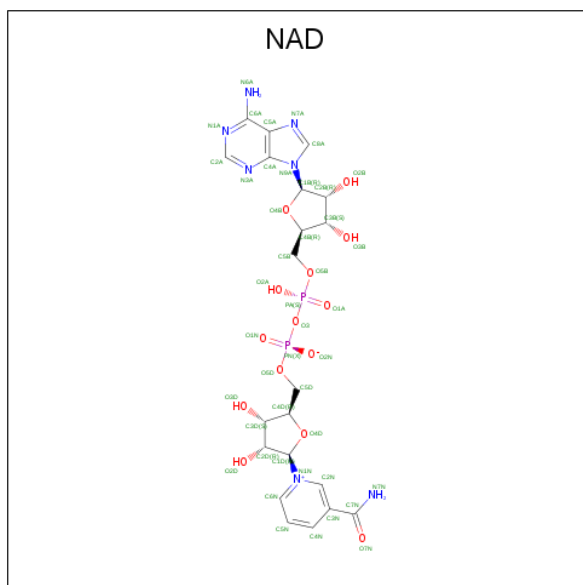
There are 6 unique types of molecules in this entry. The entry contains 37338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Formate dehydrogenase.

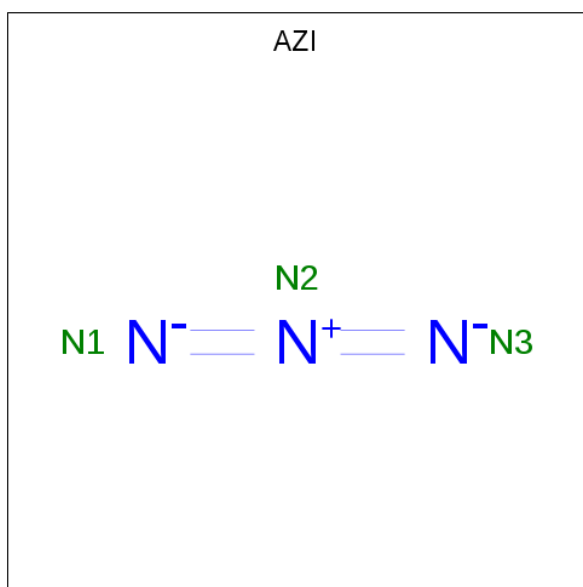
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	351	2740	1741	472	513	14	0	1	0
1	B	351	2739	1740	472	513	14	0	0	0
1	C	351	2740	1741	472	513	14	0	1	0
1	D	351	2739	1740	472	513	14	0	0	0
1	E	351	2739	1740	472	513	14	0	0	0
1	F	351	2739	1740	472	513	14	0	0	0
1	G	351	2739	1740	472	513	14	0	0	0
1	H	351	2739	1740	472	513	14	0	0	0
1	I	351	2739	1740	472	513	14	0	0	0
1	J	351	2739	1740	472	513	14	0	0	0
1	K	351	2739	1740	472	513	14	0	0	0
1	L	351	2739	1740	472	513	14	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
2	G	1	44	21	7	14	2	0	0
2	H	1	44	21	7	14	2	0	0
2	I	1	44	21	7	14	2	0	0
2	J	1	44	21	7	14	2	0	0
2	K	1	44	21	7	14	2	0	0
2	L	1	44	21	7	14	2	0	0

- Molecule 3 is AZIDE ION (three-letter code: AZI) (formula: N₃).



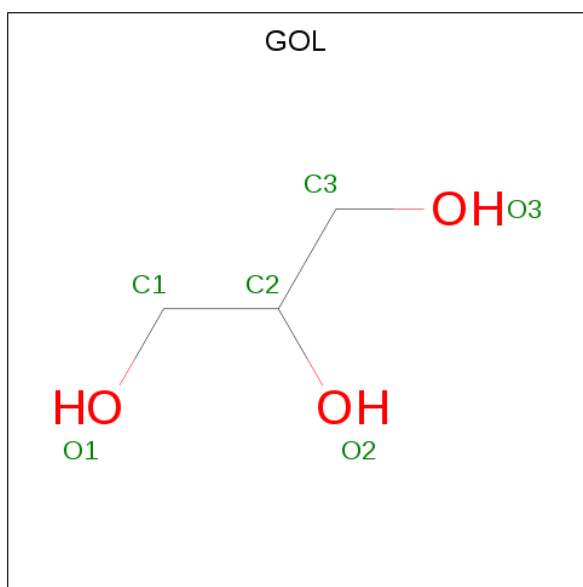
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N 3 3	0	0
3	B	1	Total N 3 3	0	0
3	C	1	Total N 3 3	0	0
3	D	1	Total N 3 3	0	0
3	E	1	Total N 3 3	0	0
3	F	1	Total N 3 3	0	0
3	G	1	Total N 3 3	0	0
3	H	1	Total N 3 3	0	0
3	I	1	Total N 3 3	0	0
3	J	1	Total N 3 3	0	0
3	K	1	Total N 3 3	0	0
3	L	1	Total N 3 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0
5	I	1	Total C O 6 3 3	0	0
5	I	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	355	Total	O	0	0
			355	355		
6	B	353	Total	O	0	0
			353	353		
6	C	332	Total	O	0	0
			332	332		
6	D	344	Total	O	0	0
			344	344		
6	E	353	Total	O	0	0
			353	353		
6	F	275	Total	O	0	0
			275	275		
6	G	311	Total	O	0	0
			311	311		
6	H	293	Total	O	0	0
			293	293		
6	I	276	Total	O	0	0
			276	276		
6	J	233	Total	O	0	0
			233	233		
6	K	315	Total	O	0	0
			315	315		
6	L	305	Total	O	0	0
			305	305		

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: Formate dehydrogenase

Chain A: 



- Molecule 1: Formate dehydrogenase

Chain B: 



- Molecule 1: Formate dehydrogenase

Chain C: 



- Molecule 1: Formate dehydrogenase

Chain D: 

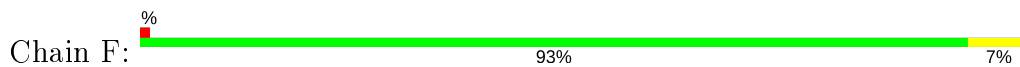


- Molecule 1: Formate dehydrogenase

Chain E: 



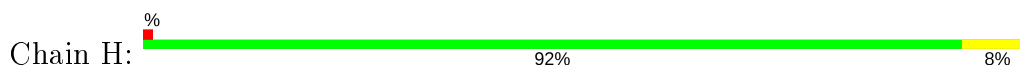
- Molecule 1: Formate dehydrogenase



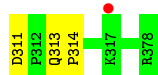
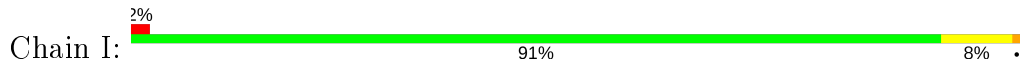
• Molecule 1: Formate dehydrogenase



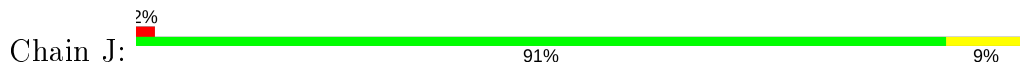
• Molecule 1: Formate dehydrogenase



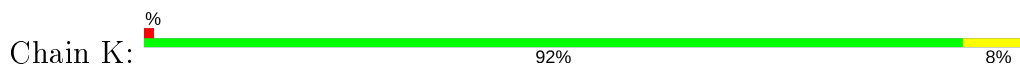
• Molecule 1: Formate dehydrogenase



• Molecule 1: Formate dehydrogenase

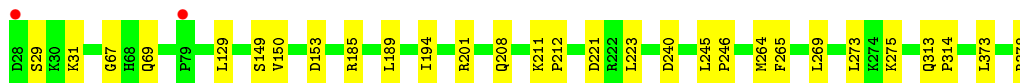
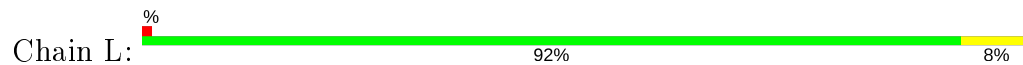


• Molecule 1: Formate dehydrogenase





- Molecule 1: Formate dehydrogenase



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.62Å 217.68Å 139.11Å 90.00° 92.62° 90.00°	Depositor
Resolution (Å)	19.99 – 2.00 19.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.99-2.00) 96.9 (19.88-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.01Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.231 0.191 , 0.232	Depositor DCC
R_{free} test set	22264 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtrriage
Anisotropy	0.264	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	37338	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.10 % 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 3.3212e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, SO4, NAD, GOL

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	0.91	1/2804 (0.0%)	0.77	2/3796 (0.1%)
1	B	0.91	0/2796	0.77	0/3785
1	C	0.87	0/2804	0.74	0/3796
1	D	0.90	0/2796	0.76	1/3785 (0.0%)
1	E	0.98	0/2796	0.78	0/3785
1	F	0.87	0/2796	0.72	0/3785
1	G	0.95	0/2796	0.75	2/3785 (0.1%)
1	H	0.90	0/2796	0.75	1/3785 (0.0%)
1	I	0.87	0/2796	0.75	1/3785 (0.0%)
1	J	0.87	0/2796	0.77	0/3785
1	K	0.87	0/2796	0.74	1/3785 (0.0%)
1	L	0.92	0/2796	0.76	1/3785 (0.0%)
All	All	0.90	1/33568 (0.0%)	0.76	9/45442 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	ALA	CA-CB	5.08	1.63	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	373	LEU	CA-CB-CG	5.86	128.78	115.30
1	I	240	ASP	CB-CG-OD2	5.67	123.41	118.30
1	G	188	ASP	CB-CG-OD1	5.54	123.29	118.30
1	K	163	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	163	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	L	240	ASP	CB-CG-OD1	5.09	122.88	118.30
1	G	185	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	157	ARG	NE-CZ-NH2	-5.03	117.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
1	H	342	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2740	0	2743	8	0
1	B	2739	0	2744	10	0
1	C	2740	0	2743	11	0
1	D	2739	0	2744	8	0
1	E	2739	0	2744	14	0
1	F	2739	0	2744	11	0
1	G	2739	0	2744	19	0
1	H	2739	0	2744	15	0
1	I	2739	0	2744	16	0
1	J	2739	0	2744	15	0
1	K	2739	0	2744	12	0
1	L	2739	0	2744	15	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	2	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	1	0
2	I	44	0	26	1	0
2	J	44	0	26	1	0
2	K	44	0	26	1	0
2	L	44	0	26	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
4	K	5	0	0	0	0
5	B	6	0	8	1	0
5	C	12	0	16	1	0
5	D	24	0	32	2	0
5	E	6	0	8	0	0
5	F	6	0	8	0	0
5	G	6	0	8	3	0
5	H	12	0	16	0	0
5	I	18	0	24	0	0
5	K	18	0	24	1	0
5	L	6	0	8	0	0
6	A	355	0	0	2	0
6	B	353	0	0	3	0
6	C	332	0	0	3	0
6	D	344	0	0	1	0
6	E	353	0	0	4	0
6	F	275	0	0	0	0
6	G	311	0	0	0	0
6	H	293	0	0	2	0
6	I	276	0	0	1	0
6	J	233	0	0	2	0
6	K	315	0	0	0	0
6	L	305	0	0	1	0
All	All	37338	0	33390	151	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 2.

All (151) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:ASP:HB2	5:G:9:GOL:H11	1.64	0.77
1:I:41:GLU:HG3	6:I:447:HOH:O	1.84	0.77
1:D:378:ARG:HH22	5:D:11:GOL:H32	1.52	0.75
1:L:211:LYS:HG2	1:L:212:PRO:HD3	1.71	0.72
1:H:291:GLN:NE2	1:H:295:ASP:OD2	2.24	0.69
1:I:175:GLY:O	1:J:317:LYS:HG2	1.93	0.67
1:E:28:ASP:N	6:E:1:HOH:O	2.29	0.66
1:G:61:ASP:HB2	5:G:9:GOL:C1	2.25	0.66
1:H:219:TYR:CZ	1:H:225:MET:HG3	2.30	0.66
1:G:211:LYS:HD3	1:G:232:GLU:O	1.96	0.65
1:I:87:ILE:HD13	1:I:107:ARG:HG2	1.78	0.65
1:E:245:LEU:HD23	1:E:251:ILE:HD11	1.79	0.65
1:C:184:TYR:CE1	1:C:185:ARG:HG3	2.35	0.62
1:G:31:LYS:HD3	1:G:69:GLN:OE1	1.99	0.62
1:H:150:VAL:HG21	2:H:401:NAD:C4N	2.30	0.62
1:H:62:TRP:HZ2	1:H:353:GLU:HG2	1.65	0.61
1:J:327:GLN:N	6:J:411:HOH:O	2.33	0.61
1:I:84:GLU:HA	1:I:87:ILE:HD12	1.82	0.61
1:F:164:ASN:HD21	1:F:185:ARG:NE	1.98	0.61
1:J:189:LEU:HD11	1:J:194:ILE:HD11	1.82	0.61
1:C:150:VAL:HG21	2:C:401:NAD:C4N	2.33	0.59
1:B:189:LEU:HD11	1:B:194:ILE:HD11	1.86	0.58
5:C:10:GOL:H31	6:C:688:HOH:O	2.04	0.57
1:K:128:ASP:HB2	5:K:24:GOL:H2	1.85	0.57
1:L:189:LEU:HD11	1:L:194:ILE:HD11	1.86	0.56
1:A:46:ASN:ND2	1:B:187:TYR:OH	2.37	0.56
5:B:16:GOL:H11	6:B:611:HOH:O	2.06	0.55
1:D:150:VAL:HG21	2:D:401:NAD:C4N	2.38	0.54
1:I:45:LYS:HD3	1:I:45:LYS:O	2.08	0.54
1:C:62:TRP:HE1	1:H:41:GLU:HB2	1.72	0.54
1:J:150:VAL:HG21	2:J:401:NAD:C4N	2.38	0.54
1:A:194[B]:ILE:HD12	1:A:250:VAL:HB	1.90	0.54
1:E:31:LYS:HG3	1:E:90:LEU:HA	1.89	0.53
1:G:31:LYS:CG	1:G:90:LEU:HA	2.38	0.53
1:C:38:LYS:HE3	1:C:40:ASN:HD21	1.74	0.52
1:G:150:VAL:HG21	2:G:401:NAD:C4N	2.39	0.52
1:L:245:LEU:HB2	1:L:246:PRO:HD3	1.92	0.52
1:H:85:LYS:HD2	6:H:507:HOH:O	2.09	0.52
1:E:274:LYS:HD3	6:E:464:HOH:O	2.08	0.52
1:G:93:LEU:HB3	1:G:117:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:31:LYS:HE3	1:K:71:ILE:HD12	1.91	0.52
1:K:93:LEU:HB3	1:K:117:LEU:HD23	1.92	0.52
1:I:227:PRO:HD2	1:I:228:GLU:OE2	2.10	0.51
1:H:62:TRP:CZ2	1:H:353:GLU:HG2	2.45	0.51
1:E:150:VAL:HG21	2:E:401:NAD:C4N	2.40	0.51
1:I:172:VAL:HG11	1:J:329:MET:HB2	1.92	0.51
1:F:189:LEU:HD11	1:F:194:ILE:HD11	1.93	0.51
1:B:130:GLN:HG3	6:B:513:HOH:O	2.09	0.51
1:B:62:TRP:CZ2	1:B:353:GLU:HG2	2.45	0.50
1:H:189:LEU:HD11	1:H:194:ILE:HD11	1.93	0.50
1:I:238:VAL:HG11	1:I:244:MET:HB2	1.93	0.50
1:J:201:ARG:O	1:J:205:LEU:HG	2.11	0.50
1:G:189:LEU:HD11	1:G:194:ILE:HD11	1.94	0.50
1:K:150:VAL:HG21	2:K:401:NAD:C4N	2.42	0.49
1:E:31:LYS:HD3	1:E:69:GLN:OE1	2.12	0.49
1:F:313:GLN:HA	1:F:314:PRO:C	2.32	0.49
1:G:245:LEU:HB3	1:G:273:LEU:HD23	1.94	0.49
1:L:373:LEU:O	1:L:378:ARG:NH2	2.46	0.49
1:G:31:LYS:HG2	1:G:90:LEU:HA	1.95	0.48
1:I:313:GLN:HA	1:I:314:PRO:C	2.33	0.48
1:L:313:GLN:HA	1:L:314:PRO:C	2.34	0.48
1:J:93:LEU:HB3	1:J:117:LEU:HD23	1.96	0.48
1:B:62:TRP:HZ2	1:B:353:GLU:HG2	1.79	0.48
1:B:150:VAL:HG21	2:B:401:NAD:C4N	2.44	0.48
1:J:245:LEU:HB3	1:J:273:LEU:HD23	1.97	0.47
1:L:150:VAL:HG21	2:L:401:NAD:C4N	2.45	0.47
1:F:28:ASP:O	1:F:30:LYS:HD3	2.14	0.47
1:F:150:VAL:HG21	2:F:401:NAD:C4N	2.43	0.47
1:D:30:LYS:NZ	6:D:673:HOH:O	2.48	0.47
1:I:46:ASN:ND2	1:I:48:ASN:H	2.13	0.47
1:K:269:LEU:HD12	1:K:272:LYS:HD2	1.96	0.47
1:A:378:ARG:NH2	6:A:508:HOH:O	2.47	0.47
1:G:28:ASP:OD1	1:G:28:ASP:N	2.48	0.47
1:H:232:GLU:HG2	6:H:602:HOH:O	2.14	0.47
1:J:123:GLY:HA3	1:J:284:ARG:NH2	2.30	0.47
1:K:189:LEU:HD11	1:K:194:ILE:HD11	1.96	0.47
1:I:170:ASN:O	1:I:174:LYS:HG3	2.16	0.46
1:K:313:GLN:HA	1:K:314:PRO:C	2.36	0.46
1:C:122:ILE:HD12	1:C:146:ASN:OD1	2.16	0.46
1:D:142:VAL:HG12	1:D:145:SER:HB3	1.97	0.46
1:L:269:LEU:O	1:L:269:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:142:VAL:HG12	1:H:145:SER:HB3	1.98	0.46
1:I:150:VAL:HG21	2:I:401:NAD:C4N	2.46	0.46
1:I:189:LEU:HD11	1:I:194:ILE:HD11	1.97	0.46
1:F:219:TYR:CZ	1:F:225:MET:HG3	2.51	0.46
1:F:71:ILE:HD13	1:F:86:HIS:CE1	2.51	0.46
1:A:31:LYS:HE3	1:A:71:ILE:HD12	1.97	0.45
1:L:201:ARG:HD2	6:L:610:HOH:O	2.15	0.45
1:I:311:ASP:OD1	1:I:311:ASP:C	2.54	0.45
1:I:46:ASN:HD21	1:I:48:ASN:HB2	1.82	0.45
1:A:150:VAL:HG21	2:A:401:NAD:C4N	2.46	0.45
1:G:84:GLU:HA	1:G:87:ILE:HD12	1.98	0.45
1:L:269:LEU:C	1:L:269:LEU:HD23	2.37	0.45
1:B:313:GLN:HA	1:B:314:PRO:C	2.37	0.45
1:J:35:VAL:HA	1:J:73:THR:O	2.17	0.45
1:E:364:GLU:HB2	6:E:504:HOH:O	2.16	0.44
1:E:46:ASN:HA	1:E:47:PRO:HD2	1.90	0.44
1:L:31:LYS:HG3	1:L:69:GLN:OE1	2.18	0.44
1:K:71:ILE:HD13	1:K:86:HIS:CE1	2.53	0.44
1:E:31:LYS:HE3	1:E:71:ILE:HD12	2.00	0.44
1:H:313:GLN:HA	1:H:314:PRO:C	2.37	0.44
1:I:82:GLU:HA	1:I:82:GLU:OE1	2.17	0.44
6:C:654:HOH:O	1:G:275:LYS:HD2	2.16	0.44
1:E:201:ARG:NH2	6:E:515:HOH:O	2.36	0.43
1:L:245:LEU:HB3	1:L:273:LEU:HD23	2.00	0.43
1:A:242:ASN:ND2	1:A:272:LYS:HE2	2.33	0.43
1:B:236:LYS:HD3	6:B:464:HOH:O	2.19	0.43
1:G:31:LYS:HG3	1:G:90:LEU:HA	2.00	0.43
1:H:85:LYS:HB2	1:H:85:LYS:HE3	1.34	0.43
1:J:220:HIS:CD2	1:J:241:LEU:HD13	2.53	0.43
1:B:228:GLU:CD	1:B:228:GLU:H	2.20	0.43
1:C:38:LYS:HE3	1:C:40:ASN:ND2	2.33	0.43
1:H:221:ASP:OD1	1:H:222:ARG:N	2.52	0.43
1:H:35:VAL:HA	1:H:73:THR:O	2.19	0.43
1:L:265:PHE:CD2	1:L:269:LEU:HD22	2.54	0.43
1:C:123:GLY:HA3	1:C:284:ARG:NH2	2.34	0.43
1:D:313:GLN:HA	1:D:314:PRO:C	2.39	0.43
1:E:201:ARG:O	1:E:205:LEU:HG	2.18	0.43
1:D:189:LEU:HD11	1:D:194:ILE:HD11	2.01	0.43
1:K:50:LEU:HD12	1:K:342:LEU:HD23	2.01	0.43
1:E:245:LEU:HD23	1:E:251:ILE:CD1	2.48	0.42
1:G:110:LYS:HB3	1:G:110:LYS:HE2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:129:LEU:HB3	1:L:373:LEU:HD21	2.00	0.42
1:G:31:LYS:CD	1:G:69:GLN:OE1	2.64	0.42
1:J:313:GLN:HA	1:J:314:PRO:C	2.39	0.42
1:F:245:LEU:HB3	1:F:273:LEU:HD23	2.00	0.42
1:C:317:LYS:HE3	6:C:425:HOH:O	2.20	0.42
1:E:313:GLN:HA	1:E:314:PRO:C	2.41	0.42
1:C:227:PRO:HD2	1:C:228:GLU:OE2	2.20	0.42
1:B:195:GLY:HA2	1:B:218:LEU:O	2.19	0.41
1:E:245:LEU:CD2	1:E:251:ILE:CD1	2.98	0.41
1:F:44:THR:HG22	1:F:45:LYS:HG2	2.02	0.41
1:K:29:SER:HB2	1:K:67:GLY:O	2.19	0.41
1:C:256:PRO:HD3	2:C:401:NAD:H52A	2.02	0.41
1:D:104:THR:HG22	5:D:25:GOL:H2	2.01	0.41
1:G:46:ASN:HB3	1:G:49:PHE:HB2	2.01	0.41
1:J:311:ASP:HA	1:J:312:PRO:HA	1.87	0.41
1:J:247:LYS:HG2	1:J:247:LYS:H	1.57	0.41
1:G:60:ARG:HD2	5:G:9:GOL:H31	2.01	0.41
1:J:294:VAL:HG13	6:J:434:HOH:O	2.19	0.41
1:L:29:SER:HB2	1:L:67:GLY:O	2.20	0.41
1:A:219:TYR:CZ	1:A:225:MET:HG3	2.56	0.41
1:L:221:ASP:HB3	1:L:223:LEU:O	2.21	0.41
1:A:106:GLU:HG3	6:A:448:HOH:O	2.20	0.40
1:C:41:GLU:HA	1:G:323:TYR:CZ	2.55	0.40
1:F:50:LEU:CD1	1:F:342:LEU:HD23	2.51	0.40
1:H:306:SER:HB2	1:H:328:ALA:HB3	2.02	0.40
1:K:46:ASN:HA	1:K:47:PRO:HD3	2.00	0.40
1:D:311:ASP:HA	1:D:312:PRO:HA	1.93	0.40
1:K:96:THR:HA	1:K:97:PRO:HD3	1.96	0.40
1:F:50:LEU:HD11	1:F:342:LEU:HD23	2.04	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	350/351 (100%)	340 (97%)	10 (3%)	0	100	100
1	B	349/351 (99%)	339 (97%)	10 (3%)	0	100	100
1	C	350/351 (100%)	340 (97%)	10 (3%)	0	100	100
1	D	349/351 (99%)	338 (97%)	11 (3%)	0	100	100
1	E	349/351 (99%)	339 (97%)	10 (3%)	0	100	100
1	F	349/351 (99%)	337 (97%)	12 (3%)	0	100	100
1	G	349/351 (99%)	339 (97%)	10 (3%)	0	100	100
1	H	349/351 (99%)	340 (97%)	9 (3%)	0	100	100
1	I	349/351 (99%)	339 (97%)	10 (3%)	0	100	100
1	J	349/351 (99%)	329 (94%)	19 (5%)	1 (0%)	41	37
1	K	349/351 (99%)	338 (97%)	11 (3%)	0	100	100
1	L	349/351 (99%)	339 (97%)	10 (3%)	0	100	100
All	All	4190/4212 (100%)	4057 (97%)	132 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	263	GLY

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	291/290 (100%)	288 (99%)	3 (1%)	76	81
1	B	290/290 (100%)	287 (99%)	3 (1%)	76	81
1	C	291/290 (100%)	288 (99%)	3 (1%)	76	81
1	D	290/290 (100%)	286 (99%)	4 (1%)	67	72
1	E	290/290 (100%)	283 (98%)	7 (2%)	49	51
1	F	290/290 (100%)	286 (99%)	4 (1%)	67	72
1	G	290/290 (100%)	285 (98%)	5 (2%)	60	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	290/290 (100%)	284 (98%)	6 (2%)	53	57
1	I	290/290 (100%)	280 (97%)	10 (3%)	37	36
1	J	290/290 (100%)	282 (97%)	8 (3%)	43	44
1	K	290/290 (100%)	284 (98%)	6 (2%)	53	57
1	L	290/290 (100%)	284 (98%)	6 (2%)	53	57
All	All	3482/3480 (100%)	3417 (98%)	65 (2%)	57	61

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	SER
1	A	153	ASP
1	A	236	LYS
1	B	153	ASP
1	B	185	ARG
1	B	268	GLU
1	C	28	ASP
1	C	153	ASP
1	C	268	GLU
1	D	77	GLU
1	D	149	SER
1	D	153	ASP
1	D	268	GLU
1	E	30	LYS
1	E	38	LYS
1	E	69	GLN
1	E	87	ILE
1	E	153	ASP
1	E	185	ARG
1	E	251	ILE
1	F	49	PHE
1	F	153	ASP
1	F	259	GLU
1	F	372	GLU
1	G	30	LYS
1	G	41	GLU
1	G	89	ASP
1	G	109	LYS
1	G	178	ASN
1	H	30	LYS

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Mol	Chain	Res	Type
1	H	49	PHE
1	H	115	LYS
1	H	153	ASP
1	H	357	LYS
1	H	363	THR
1	I	45	LYS
1	I	46	ASN
1	I	74	ASP
1	I	85	LYS
1	I	109	LYS
1	I	115	LYS
1	I	125	ASP
1	I	130	GLN
1	I	153	ASP
1	I	290	ARG
1	J	29	SER
1	J	71	ILE
1	J	106	GLU
1	J	115	LYS
1	J	125	ASP
1	J	185	ARG
1	J	274	LYS
1	J	372	GLU
1	K	30	LYS
1	K	41	GLU
1	K	65	SER
1	K	125	ASP
1	K	153	ASP
1	K	247	LYS
1	L	149	SER
1	L	153	ASP
1	L	185	ARG
1	L	208	GLN
1	L	264	MET
1	L	275	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	ASN
1	B	178	ASN
1	B	254	ASN

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Mol	Chain	Res	Type
1	C	178	ASN
1	C	208	GLN
1	C	254	ASN
1	D	178	ASN
1	E	178	ASN
1	F	164	ASN
1	F	178	ASN
1	F	254	ASN
1	G	178	ASN
1	H	178	ASN
1	H	254	ASN
1	I	46	ASN
1	I	130	GLN
1	I	178	ASN
1	I	254	ASN
1	J	178	ASN
1	K	178	ASN
1	L	208	GLN
1	L	326	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

52 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$
3	AZI	D	403	-	0,2,2	0.00	-	0,1,1	0.00	-
4	SO4	C	3	-	4,4,4	0.22	0	6,6,6	0.43	0
4	SO4	D	4	-	4,4,4	0.19	0	6,6,6	0.22	0
4	SO4	K	8	-	4,4,4	0.38	0	6,6,6	0.23	0
5	GOL	H	27	-	5,5,5	0.52	0	5,5,5	1.01	0
5	GOL	I	13	-	5,5,5	0.43	0	5,5,5	0.85	0
5	GOL	D	11	-	5,5,5	0.59	0	5,5,5	1.30	1 (20%)
2	NAD	B	401	-	42,48,48	0.97	4 (9%)	50,73,73	1.22	4 (8%)
3	AZI	F	403	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	C	10	-	5,5,5	0.58	0	5,5,5	0.62	0
5	GOL	D	18	-	5,5,5	0.62	0	5,5,5	1.00	0
4	SO4	F	20	-	4,4,4	0.20	0	6,6,6	0.38	0
5	GOL	F	26	-	5,5,5	0.31	0	5,5,5	0.77	0
2	NAD	A	401	-	42,48,48	1.08	4 (9%)	50,73,73	1.33	5 (10%)
5	GOL	G	9	-	5,5,5	0.76	0	5,5,5	0.83	0
5	GOL	H	12	-	5,5,5	0.25	0	5,5,5	0.52	0
4	SO4	G	5	-	4,4,4	0.16	0	6,6,6	0.38	0
5	GOL	C	17	-	5,5,5	0.42	0	5,5,5	0.31	0
5	GOL	L	21	-	5,5,5	0.45	0	5,5,5	0.95	0
3	AZI	K	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NAD	K	401	-	42,48,48	1.10	3 (7%)	50,73,73	1.34	8 (16%)
5	GOL	B	16	-	5,5,5	0.46	0	5,5,5	0.69	0
3	AZI	J	403	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	I	19	-	5,5,5	0.63	0	5,5,5	0.51	0
5	GOL	D	22	-	5,5,5	0.43	0	5,5,5	0.39	0
3	AZI	C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
3	AZI	A	403	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	I	23	-	5,5,5	0.46	0	5,5,5	0.62	0
2	NAD	C	401	-	42,48,48	1.16	3 (7%)	50,73,73	1.27	2 (4%)
5	GOL	D	25	-	5,5,5	0.48	0	5,5,5	0.31	0
2	NAD	G	401	-	42,48,48	1.19	5 (11%)	50,73,73	1.41	7 (14%)
2	NAD	E	401	-	42,48,48	1.26	5 (11%)	50,73,73	1.18	5 (10%)
2	NAD	H	401	-	42,48,48	1.13	3 (7%)	50,73,73	1.36	6 (12%)
2	NAD	L	401	-	42,48,48	1.25	3 (7%)	50,73,73	1.42	10 (20%)
4	SO4	I	7	-	4,4,4	0.16	0	6,6,6	0.44	0
2	NAD	F	401	-	42,48,48	1.09	3 (7%)	50,73,73	1.43	6 (12%)
5	GOL	E	379	-	5,5,5	0.33	0	5,5,5	0.31	0
2	NAD	D	401	-	42,48,48	1.07	2 (4%)	50,73,73	1.24	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AZI	I	403	-	0,2,2	0.00	-	0,1,1	0.00	-
3	AZI	H	403	-	0,2,2	0.00	-	0,1,1	0.00	-
3	AZI	E	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NAD	I	401	-	42,48,48	1.07	2 (4%)	50,73,73	1.37	6 (12%)
3	AZI	B	403	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	K	24	-	5,5,5	0.41	0	5,5,5	0.52	0
4	SO4	B	2	-	4,4,4	0.13	0	6,6,6	0.45	0
5	GOL	K	15	-	5,5,5	0.40	0	5,5,5	0.55	0
4	SO4	H	6	-	4,4,4	0.14	0	6,6,6	0.11	0
4	SO4	A	1	-	4,4,4	0.18	0	6,6,6	0.32	0
3	AZI	L	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NAD	J	401	-	42,48,48	1.11	2 (4%)	50,73,73	1.41	5 (10%)
3	AZI	G	403	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	K	14	-	5,5,5	0.23	0	5,5,5	0.96	0

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	B	401	-	-	2/26/62/62	0/5/5/5
5	GOL	D	25	-	-	2/4/4/4	-
5	GOL	K	14	-	-	1/4/4/4	-
5	GOL	I	13	-	-	4/4/4/4	-
5	GOL	D	11	-	-	2/4/4/4	-
5	GOL	C	10	-	-	2/4/4/4	-
5	GOL	E	379	-	-	3/4/4/4	-
5	GOL	F	26	-	-	4/4/4/4	-
2	NAD	A	401	-	-	2/26/62/62	0/5/5/5
5	GOL	G	9	-	-	2/4/4/4	-
5	GOL	H	12	-	-	0/4/4/4	-
5	GOL	B	16	-	-	2/4/4/4	-
5	GOL	I	19	-	-	2/4/4/4	-
5	GOL	D	22	-	-	0/4/4/4	-
5	GOL	C	17	-	-	0/4/4/4	-
5	GOL	I	23	-	-	3/4/4/4	-
2	NAD	C	401	-	-	2/26/62/62	0/5/5/5
2	NAD	G	401	-	-	2/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	E	401	-	-	2/26/62/62	0/5/5/5
2	NAD	H	401	-	-	2/26/62/62	0/5/5/5
2	NAD	L	401	-	-	2/26/62/62	0/5/5/5
2	NAD	F	401	-	-	2/26/62/62	0/5/5/5
5	GOL	D	18	-	-	2/4/4/4	-
2	NAD	D	401	-	-	2/26/62/62	0/5/5/5
2	NAD	K	401	-	-	2/26/62/62	0/5/5/5
5	GOL	L	21	-	-	4/4/4/4	-
2	NAD	I	401	-	-	2/26/62/62	0/5/5/5
5	GOL	K	24	-	-	3/4/4/4	-
5	GOL	K	15	-	-	4/4/4/4	-
5	GOL	H	27	-	-	4/4/4/4	-
2	NAD	J	401	-	-	2/26/62/62	0/5/5/5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	401	NAD	O4D-C1D	3.98	1.46	1.41
2	D	401	NAD	O4B-C1B	3.75	1.46	1.41
2	C	401	NAD	O4D-C1D	3.70	1.46	1.41
2	E	401	NAD	O4B-C1B	3.41	1.45	1.41
2	J	401	NAD	O4B-C1B	3.38	1.45	1.41
2	K	401	NAD	O4B-C1B	3.37	1.45	1.41
2	F	401	NAD	O4D-C1D	3.18	1.45	1.41
2	A	401	NAD	C2N-C3N	3.17	1.43	1.39
2	H	401	NAD	O4D-C1D	3.01	1.45	1.41
2	E	401	NAD	O4D-C1D	2.99	1.45	1.41
2	J	401	NAD	O4D-C1D	2.89	1.45	1.41
2	G	401	NAD	C2N-C3N	2.82	1.43	1.39
2	B	401	NAD	O4B-C1B	2.78	1.45	1.41
2	G	401	NAD	O4D-C1D	2.72	1.44	1.41
2	L	401	NAD	O4B-C1B	2.70	1.44	1.41
2	G	401	NAD	O4B-C1B	2.64	1.44	1.41
2	A	401	NAD	O4B-C1B	2.63	1.44	1.41
2	C	401	NAD	O4B-C1B	2.55	1.44	1.41
2	A	401	NAD	C2D-C1D	2.54	1.57	1.53
2	I	401	NAD	O4D-C1D	2.53	1.44	1.41
2	A	401	NAD	O4D-C1D	2.52	1.44	1.41
2	I	401	NAD	O4B-C1B	2.48	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	NAD	C8A-N7A	-2.37	1.30	1.34
2	F	401	NAD	O4B-C1B	2.35	1.44	1.41
2	K	401	NAD	O4D-C1D	2.35	1.44	1.41
2	E	401	NAD	C2A-N3A	2.31	1.35	1.32
2	K	401	NAD	C7N-N7N	2.25	1.37	1.33
2	E	401	NAD	C7N-N7N	2.19	1.37	1.33
2	C	401	NAD	C2N-N1N	2.18	1.37	1.35
2	H	401	NAD	C7N-N7N	2.18	1.37	1.33
2	G	401	NAD	PA-O2A	-2.18	1.45	1.55
2	B	401	NAD	O4D-C1D	2.16	1.44	1.41
2	D	401	NAD	O4D-C1D	2.15	1.44	1.41
2	B	401	NAD	C2D-C1D	2.14	1.57	1.53
2	F	401	NAD	C4A-N3A	-2.11	1.32	1.35
2	H	401	NAD	O4B-C1B	2.08	1.44	1.41
2	E	401	NAD	C3N-C7N	-2.03	1.47	1.50
2	B	401	NAD	PA-O2A	-2.02	1.45	1.55
2	L	401	NAD	C7N-N7N	2.02	1.36	1.33

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	NAD	N3A-C2A-N1A	-5.03	120.81	128.68
2	F	401	NAD	O4B-C1B-C2B	-4.94	99.70	106.93
2	I	401	NAD	N3A-C2A-N1A	-4.79	121.18	128.68
2	H	401	NAD	N3A-C2A-N1A	-4.73	121.28	128.68
2	D	401	NAD	N3A-C2A-N1A	-4.71	121.31	128.68
2	A	401	NAD	N3A-C2A-N1A	-4.68	121.36	128.68
2	B	401	NAD	N3A-C2A-N1A	-4.67	121.37	128.68
2	J	401	NAD	N3A-C2A-N1A	-4.64	121.43	128.68
2	G	401	NAD	N3A-C2A-N1A	-4.41	121.78	128.68
2	K	401	NAD	N3A-C2A-N1A	-4.35	121.88	128.68
2	E	401	NAD	N3A-C2A-N1A	-4.14	122.21	128.68
2	L	401	NAD	N3A-C2A-N1A	-4.03	122.38	128.68
2	G	401	NAD	O7N-C7N-N7N	-3.94	116.99	122.58
2	F	401	NAD	N3A-C2A-N1A	-3.84	122.67	128.68
2	J	401	NAD	C3N-C7N-N7N	3.73	122.23	117.75
2	H	401	NAD	O4B-C1B-C2B	-3.68	101.55	106.93
2	J	401	NAD	O7N-C7N-N7N	-3.60	117.46	122.58
2	H	401	NAD	C3D-C2D-C1D	3.54	106.31	100.98
2	D	401	NAD	O4B-C1B-C2B	-3.52	101.79	106.93
2	A	401	NAD	O4B-C1B-C2B	-3.46	101.86	106.93
2	C	401	NAD	C3N-C7N-N7N	3.45	121.89	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	401	NAD	O4B-C1B-C2B	-3.39	101.98	106.93
2	L	401	NAD	C3D-C2D-C1D	3.27	105.89	100.98
2	K	401	NAD	C4A-C5A-N7A	-3.24	106.02	109.40
2	G	401	NAD	O7N-C7N-C3N	3.15	123.40	119.63
2	A	401	NAD	O7N-C7N-N7N	-3.12	118.15	122.58
2	F	401	NAD	O4D-C4D-C3D	-3.08	99.02	105.11
2	F	401	NAD	C3N-C7N-N7N	3.08	121.44	117.75
2	A	401	NAD	C3N-C7N-N7N	3.08	121.44	117.75
2	J	401	NAD	O4B-C1B-C2B	-2.88	102.72	106.93
2	F	401	NAD	O7N-C7N-N7N	-2.75	118.67	122.58
2	B	401	NAD	C3D-C2D-C1D	2.72	105.08	100.98
2	D	401	NAD	C3N-C7N-N7N	2.72	121.01	117.75
2	L	401	NAD	O4D-C1D-C2D	-2.67	103.02	106.93
5	D	11	GOL	O1-C1-C2	-2.60	97.74	110.20
2	I	401	NAD	C3D-C2D-C1D	2.50	104.74	100.98
2	L	401	NAD	C6N-N1N-C2N	-2.48	119.72	121.97
2	K	401	NAD	C3N-C7N-N7N	2.45	120.69	117.75
2	L	401	NAD	C4A-C5A-N7A	-2.42	106.87	109.40
2	L	401	NAD	O7N-C7N-N7N	-2.42	119.14	122.58
2	H	401	NAD	C3N-C7N-N7N	2.39	120.62	117.75
2	K	401	NAD	C3N-C2N-N1N	2.39	122.76	120.43
2	B	401	NAD	C1B-N9A-C4A	-2.39	122.44	126.64
2	G	401	NAD	C6N-N1N-C2N	-2.37	119.81	121.97
2	I	401	NAD	O2N-PN-O1N	2.37	123.95	112.24
2	A	401	NAD	C3D-C2D-C1D	2.30	104.45	100.98
2	L	401	NAD	C3N-C7N-N7N	2.29	120.50	117.75
2	L	401	NAD	O4B-C1B-C2B	-2.29	103.58	106.93
2	E	401	NAD	C3N-C7N-N7N	2.25	120.45	117.75
2	E	401	NAD	N6A-C6A-N1A	2.24	123.22	118.57
2	I	401	NAD	C5N-C4N-C3N	-2.20	117.74	120.34
2	B	401	NAD	O4B-C1B-C2B	-2.19	103.72	106.93
2	K	401	NAD	O4B-C4B-C3B	2.19	109.45	105.11
2	K	401	NAD	C6N-N1N-C2N	-2.17	120.00	121.97
2	G	401	NAD	C1B-N9A-C4A	-2.15	122.87	126.64
2	J	401	NAD	C4A-C5A-N7A	-2.13	107.18	109.40
2	K	401	NAD	C3D-C2D-C1D	2.11	104.16	100.98
2	I	401	NAD	N6A-C6A-N1A	2.10	122.94	118.57
2	H	401	NAD	O7N-C7N-N7N	-2.10	119.59	122.58
2	K	401	NAD	C5N-C4N-C3N	-2.10	117.86	120.34
2	G	401	NAD	C3D-C2D-C1D	2.09	104.12	100.98
2	E	401	NAD	C5N-C4N-C3N	-2.07	117.89	120.34
2	L	401	NAD	C5N-C4N-C3N	-2.07	117.89	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	NAD	O2N-PN-O1N	2.07	122.46	112.24
2	G	401	NAD	C4A-C5A-N7A	-2.05	107.26	109.40
2	H	401	NAD	C4A-C5A-N7A	-2.03	107.28	109.40
2	L	401	NAD	C2A-N1A-C6A	2.02	122.22	118.75
2	E	401	NAD	C3D-C2D-C1D	2.01	104.00	100.98

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	NAD	O4D-C1D-N1N-C6N
5	E	379	GOL	C1-C2-C3-O3
5	H	27	GOL	C1-C2-C3-O3
5	H	27	GOL	O2-C2-C3-O3
5	I	13	GOL	C1-C2-C3-O3
5	D	11	GOL	O1-C1-C2-C3
5	F	26	GOL	O1-C1-C2-O2
5	F	26	GOL	O1-C1-C2-C3
2	A	401	NAD	O4D-C1D-N1N-C6N
5	G	9	GOL	O1-C1-C2-C3
5	L	21	GOL	O1-C1-C2-C3
2	K	401	NAD	O4D-C1D-N1N-C6N
5	B	16	GOL	C1-C2-C3-O3
5	I	19	GOL	O1-C1-C2-O2
5	I	19	GOL	O1-C1-C2-C3
5	I	23	GOL	O2-C2-C3-O3
2	C	401	NAD	O4D-C1D-N1N-C6N
5	D	25	GOL	C1-C2-C3-O3
2	G	401	NAD	O4D-C1D-N1N-C6N
2	E	401	NAD	O4D-C1D-N1N-C6N
2	H	401	NAD	O4D-C1D-N1N-C6N
2	L	401	NAD	O4D-C1D-N1N-C6N
2	F	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	I	401	NAD	O4D-C1D-N1N-C6N
5	K	15	GOL	O1-C1-C2-O2
5	K	15	GOL	O1-C1-C2-C3
2	J	401	NAD	O4D-C1D-N1N-C6N
5	E	379	GOL	O1-C1-C2-C3
5	I	13	GOL	O1-C1-C2-C3
5	D	18	GOL	C1-C2-C3-O3
5	L	21	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	I	23	GOL	C1-C2-C3-O3
5	C	10	GOL	O1-C1-C2-C3
5	K	24	GOL	O1-C1-C2-C3
5	K	15	GOL	C1-C2-C3-O3
5	K	14	GOL	O1-C1-C2-C3
5	I	13	GOL	O1-C1-C2-O2
5	I	13	GOL	O2-C2-C3-O3
5	D	11	GOL	O1-C1-C2-O2
5	D	18	GOL	O2-C2-C3-O3
5	L	21	GOL	O1-C1-C2-O2
5	L	21	GOL	O2-C2-C3-O3
5	B	16	GOL	O2-C2-C3-O3
5	D	25	GOL	O2-C2-C3-O3
5	C	10	GOL	O1-C1-C2-O2
5	E	379	GOL	O2-C2-C3-O3
5	K	15	GOL	O2-C2-C3-O3
5	H	27	GOL	O1-C1-C2-O2
5	F	26	GOL	O2-C2-C3-O3
5	G	9	GOL	O1-C1-C2-O2
5	I	23	GOL	O1-C1-C2-O2
5	K	24	GOL	O1-C1-C2-O2
2	E	401	NAD	O4B-C4B-C5B-O5B
2	H	401	NAD	O4B-C4B-C5B-O5B
2	K	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	O4B-C4B-C5B-O5B
2	L	401	NAD	O4B-C4B-C5B-O5B
2	F	401	NAD	O4B-C4B-C5B-O5B
2	D	401	NAD	O4B-C4B-C5B-O5B
2	I	401	NAD	O4B-C4B-C5B-O5B
2	J	401	NAD	O4B-C4B-C5B-O5B
5	H	27	GOL	O1-C1-C2-C3
5	F	26	GOL	C1-C2-C3-O3
5	K	24	GOL	C1-C2-C3-O3
2	B	401	NAD	O4B-C4B-C5B-O5B
2	C	401	NAD	O4B-C4B-C5B-O5B
2	G	401	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

18 monomers are involved in 21 short contacts:

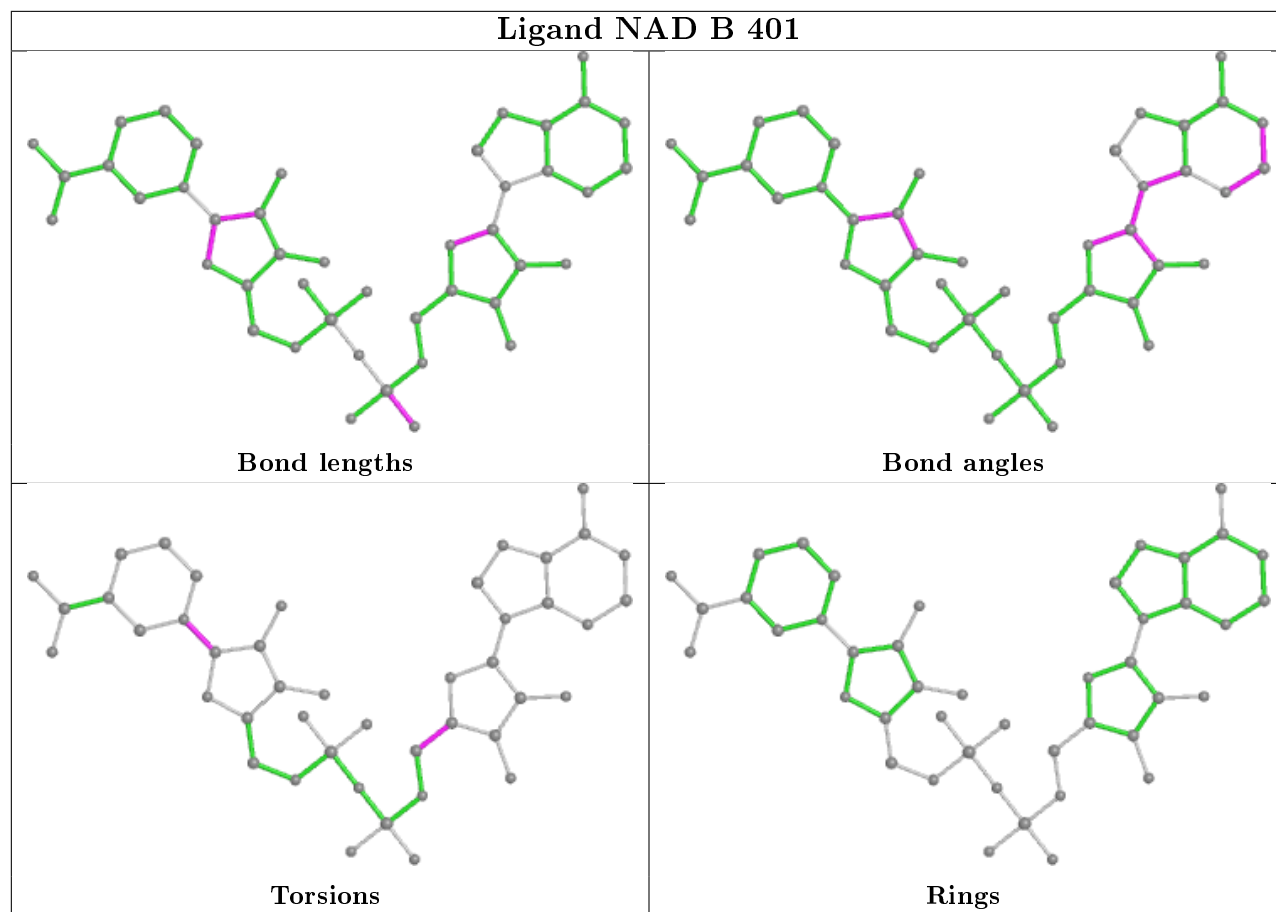
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	11	GOL	1	0

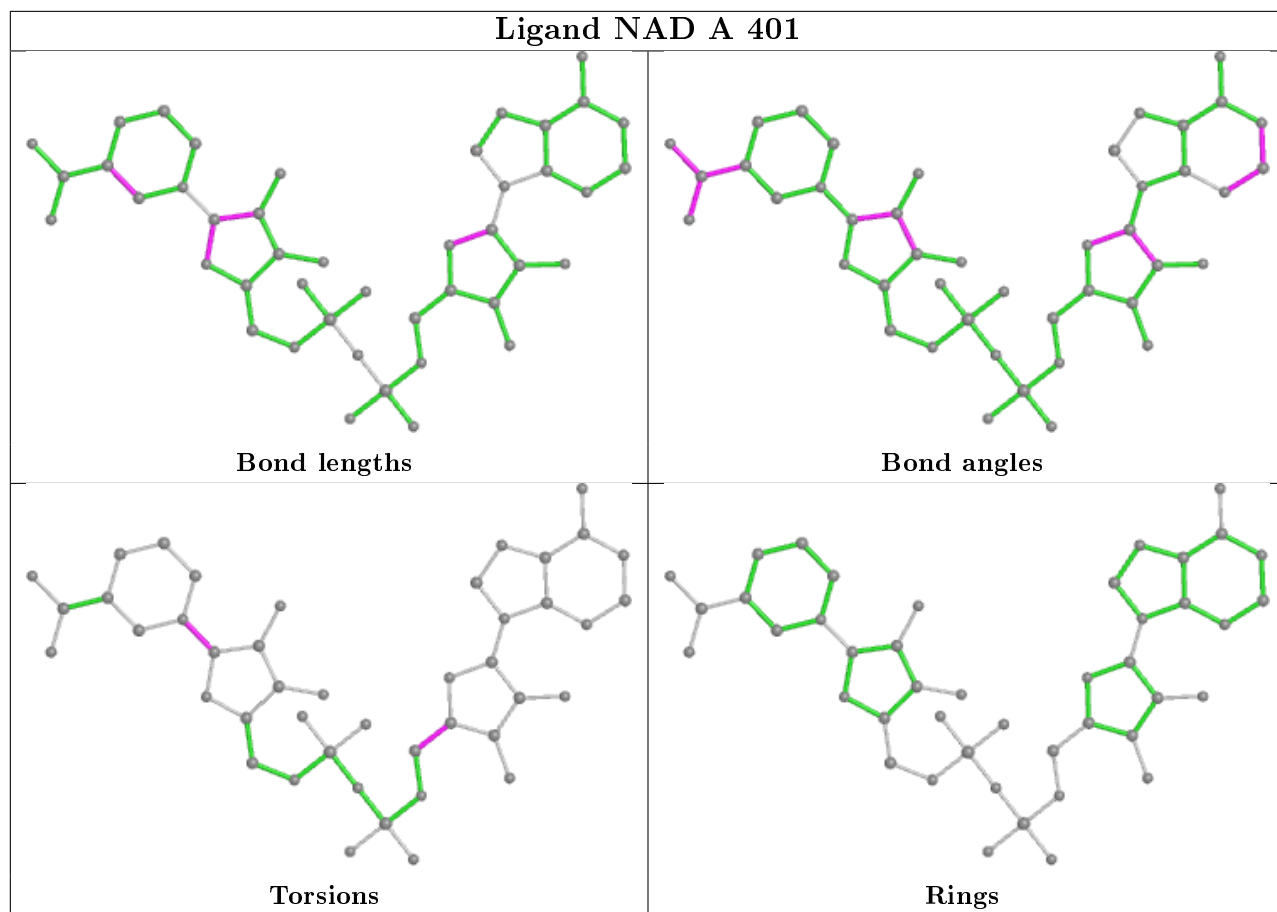
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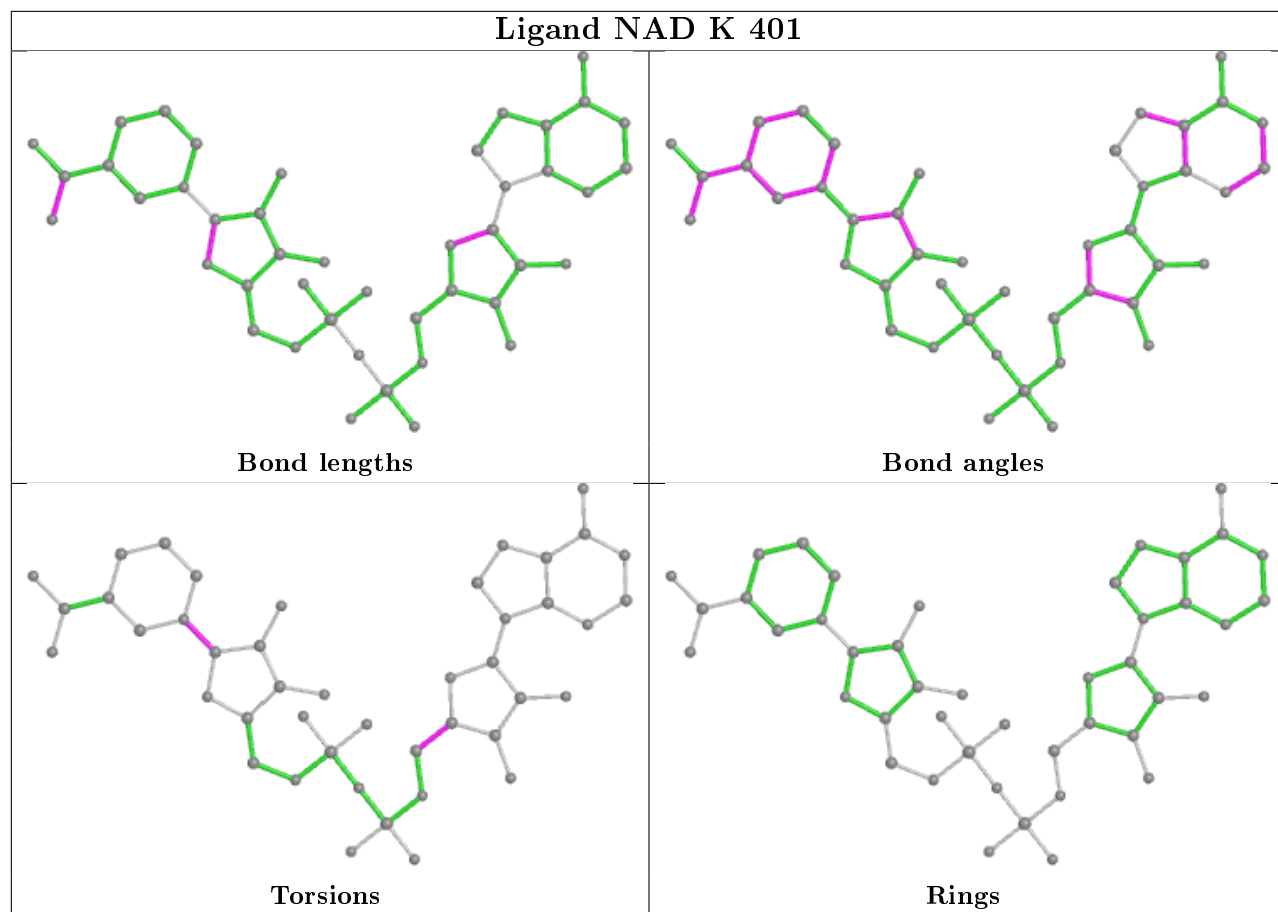
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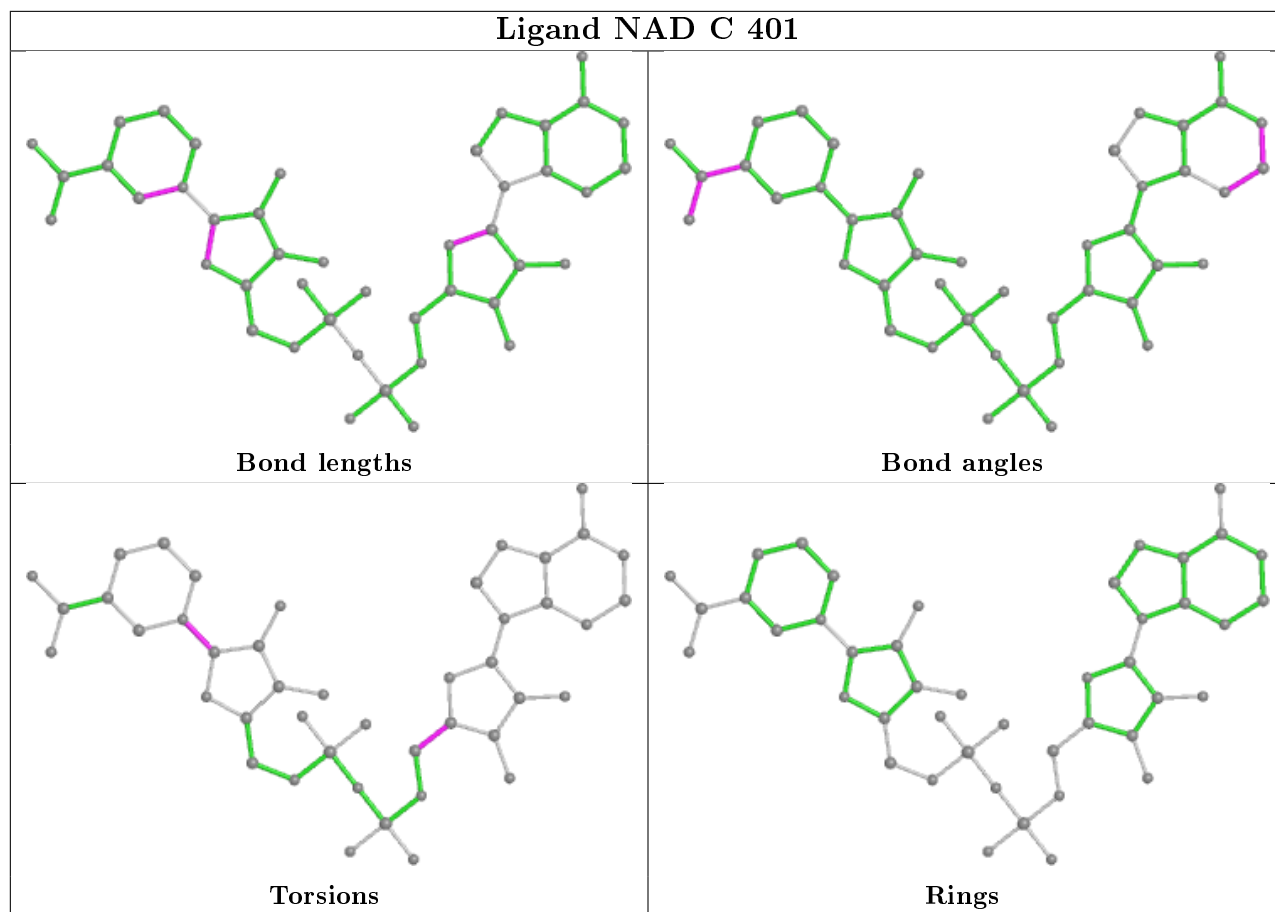
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NAD	1	0
5	C	10	GOL	1	0
2	A	401	NAD	1	0
5	G	9	GOL	3	0
2	K	401	NAD	1	0
5	B	16	GOL	1	0
2	C	401	NAD	2	0
5	D	25	GOL	1	0
2	G	401	NAD	1	0
2	E	401	NAD	1	0
2	H	401	NAD	1	0
2	L	401	NAD	1	0
2	F	401	NAD	1	0
2	D	401	NAD	1	0
2	I	401	NAD	1	0
5	K	24	GOL	1	0
2	J	401	NAD	1	0

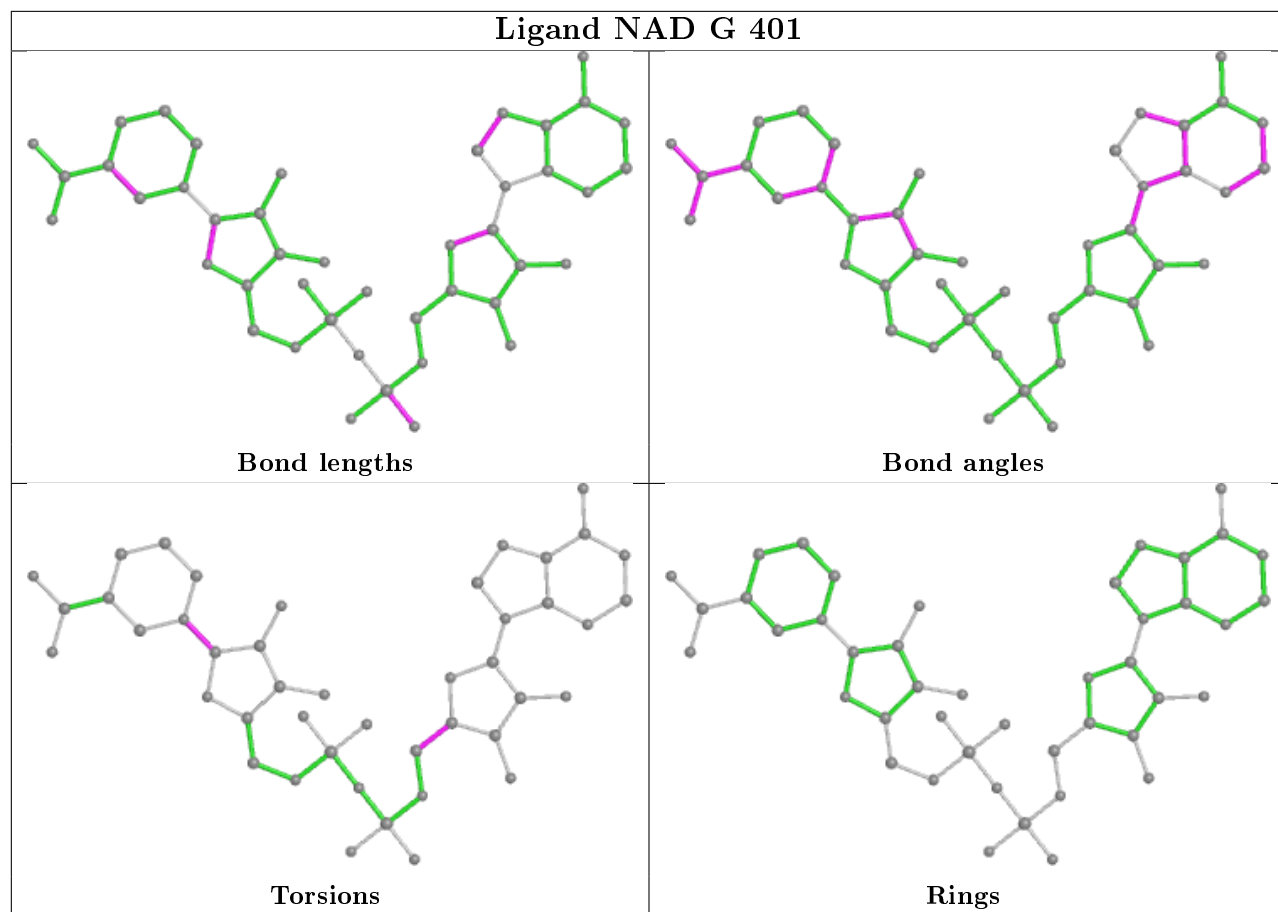
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

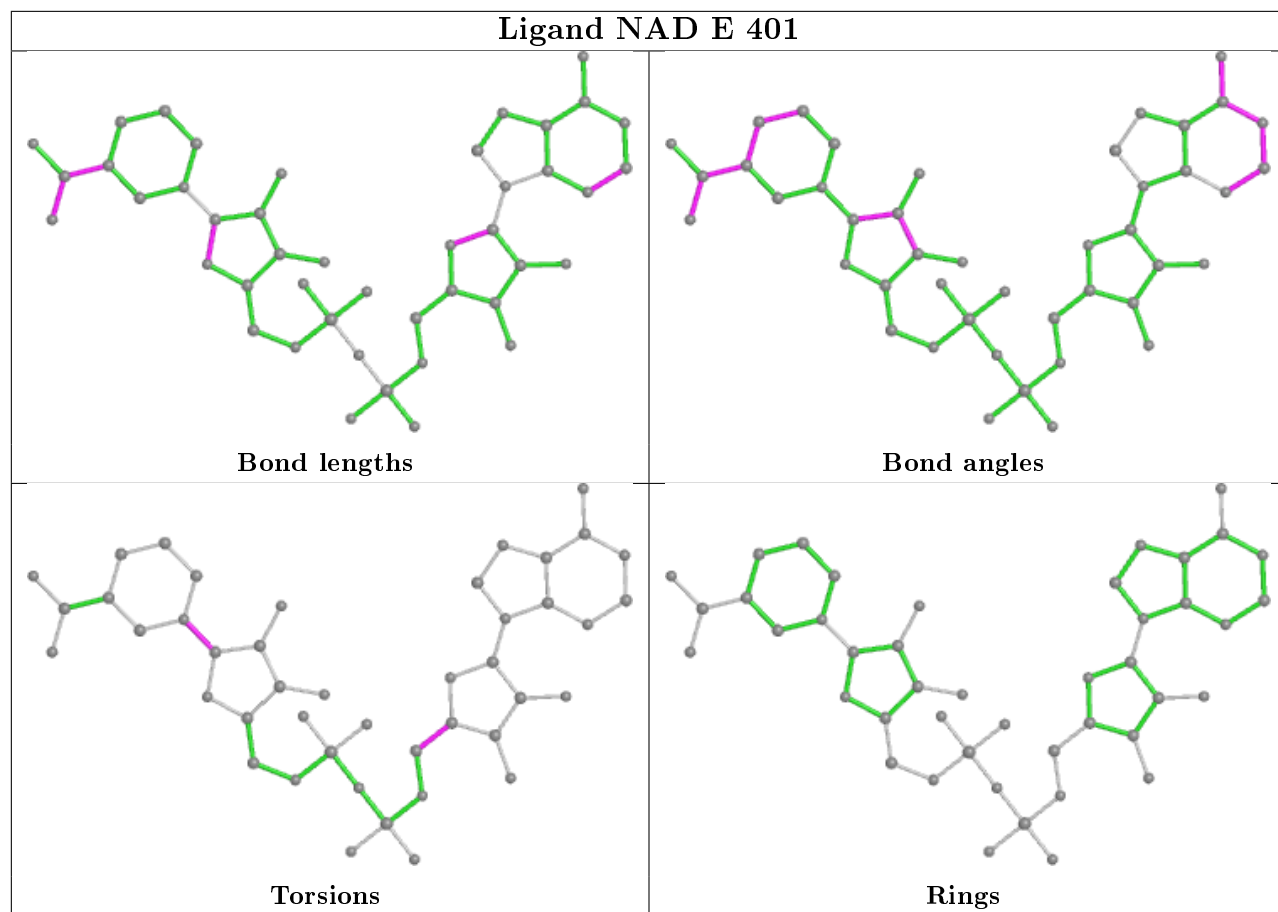


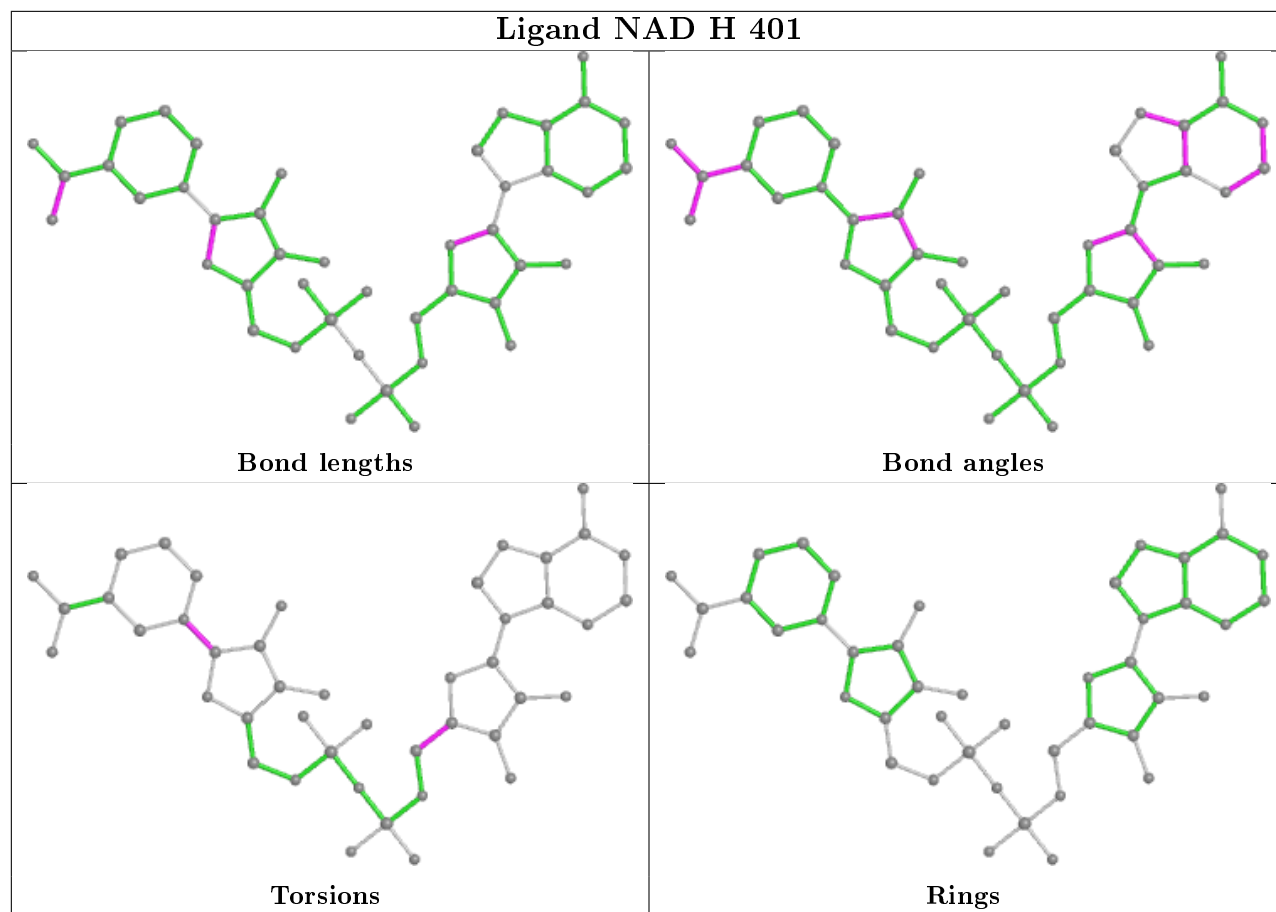


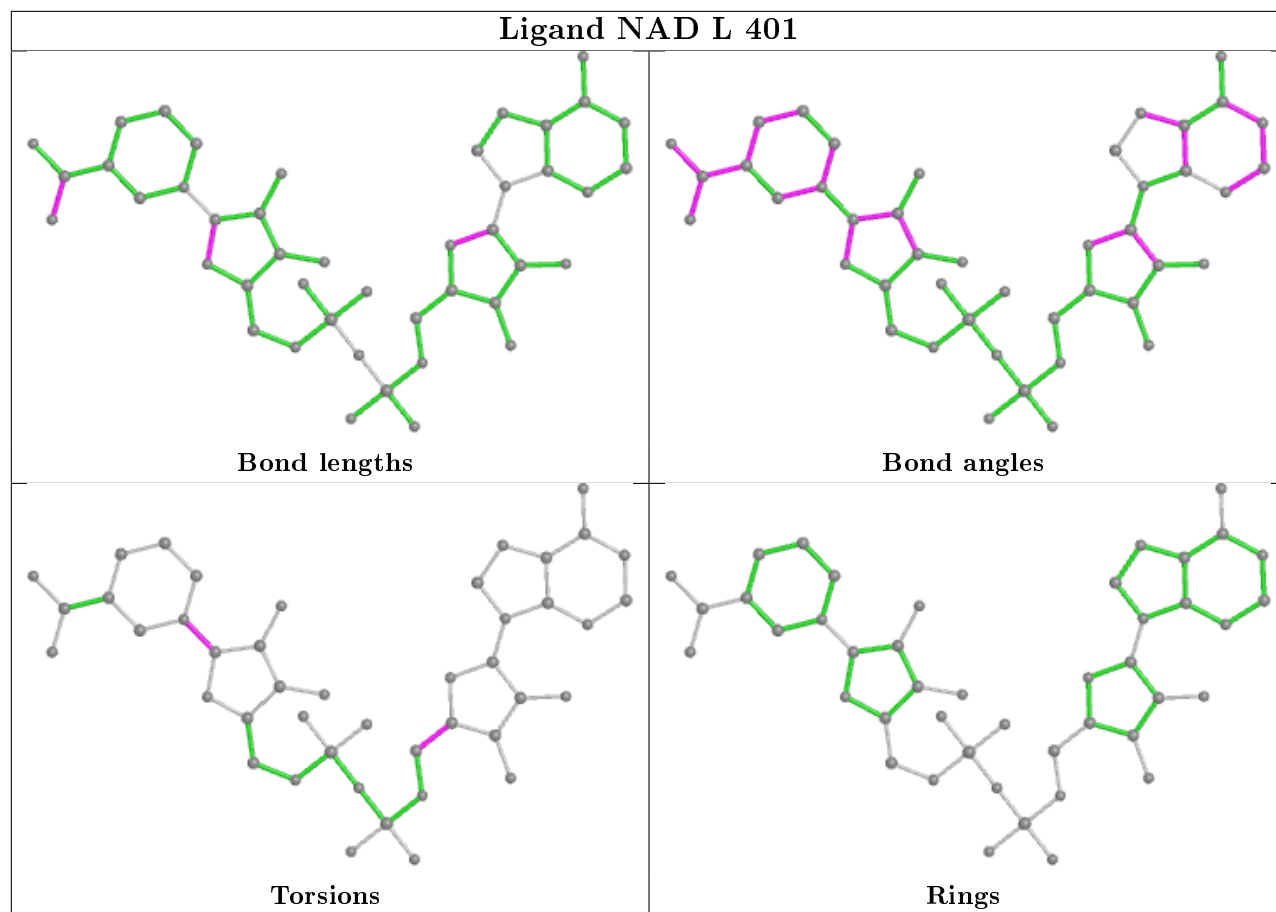


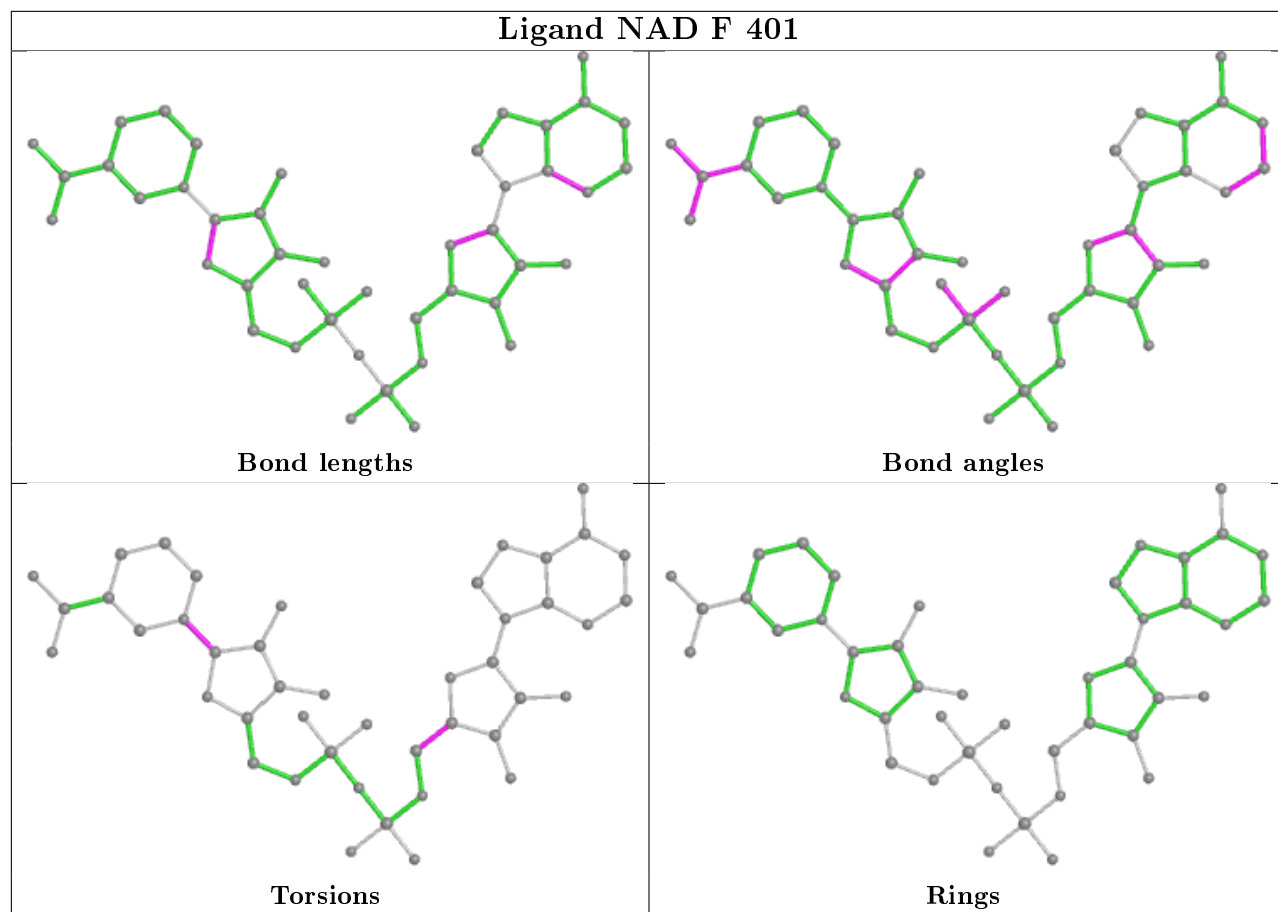


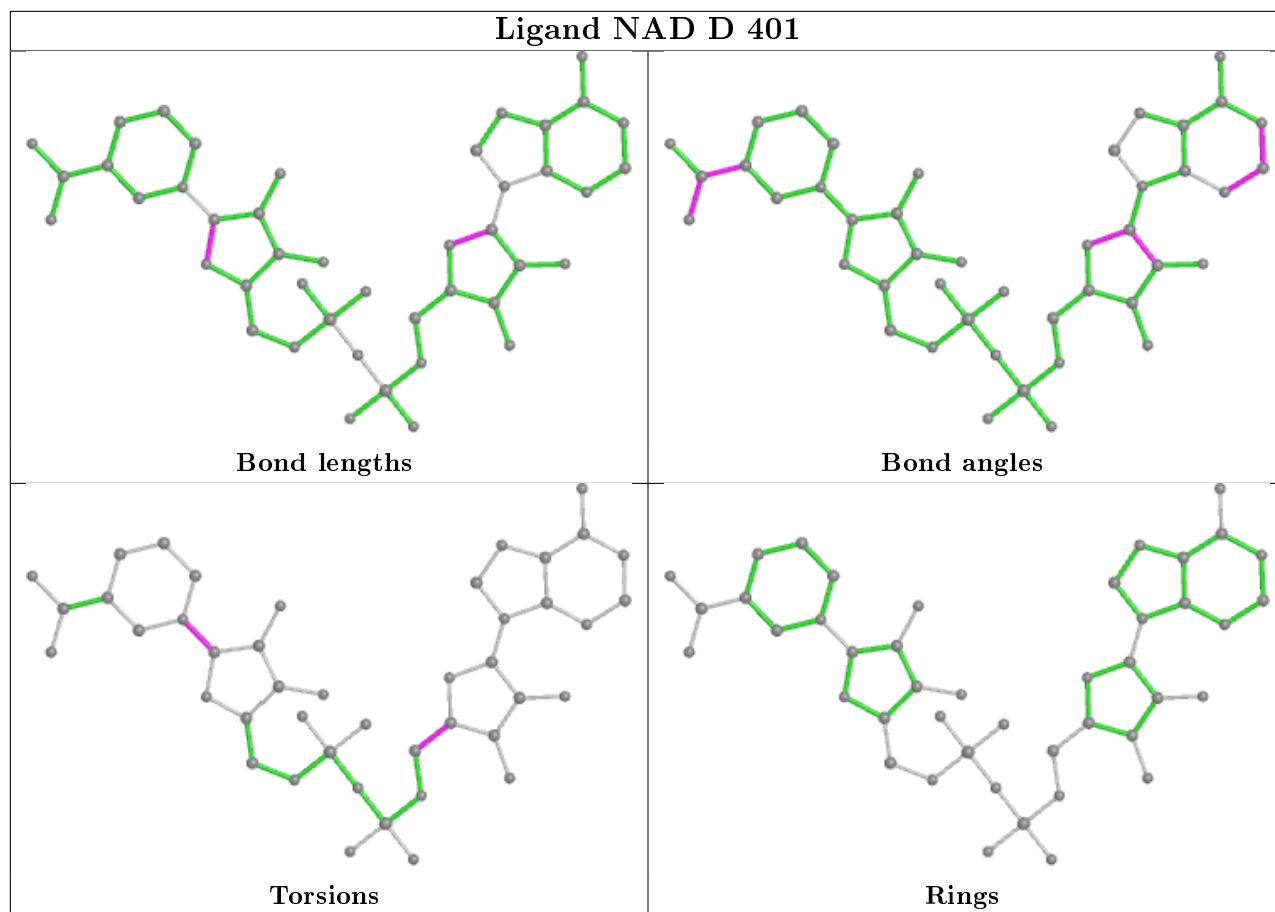


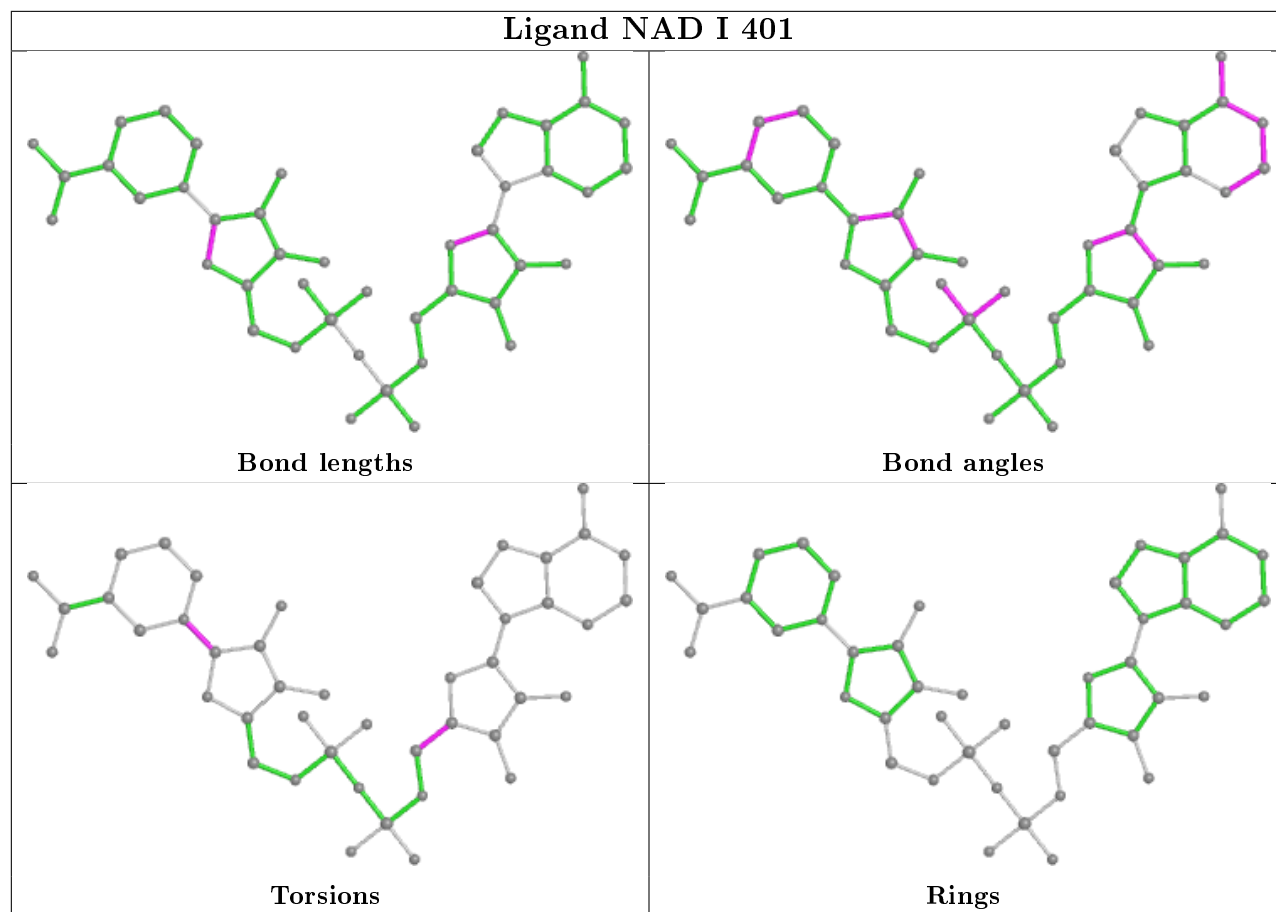


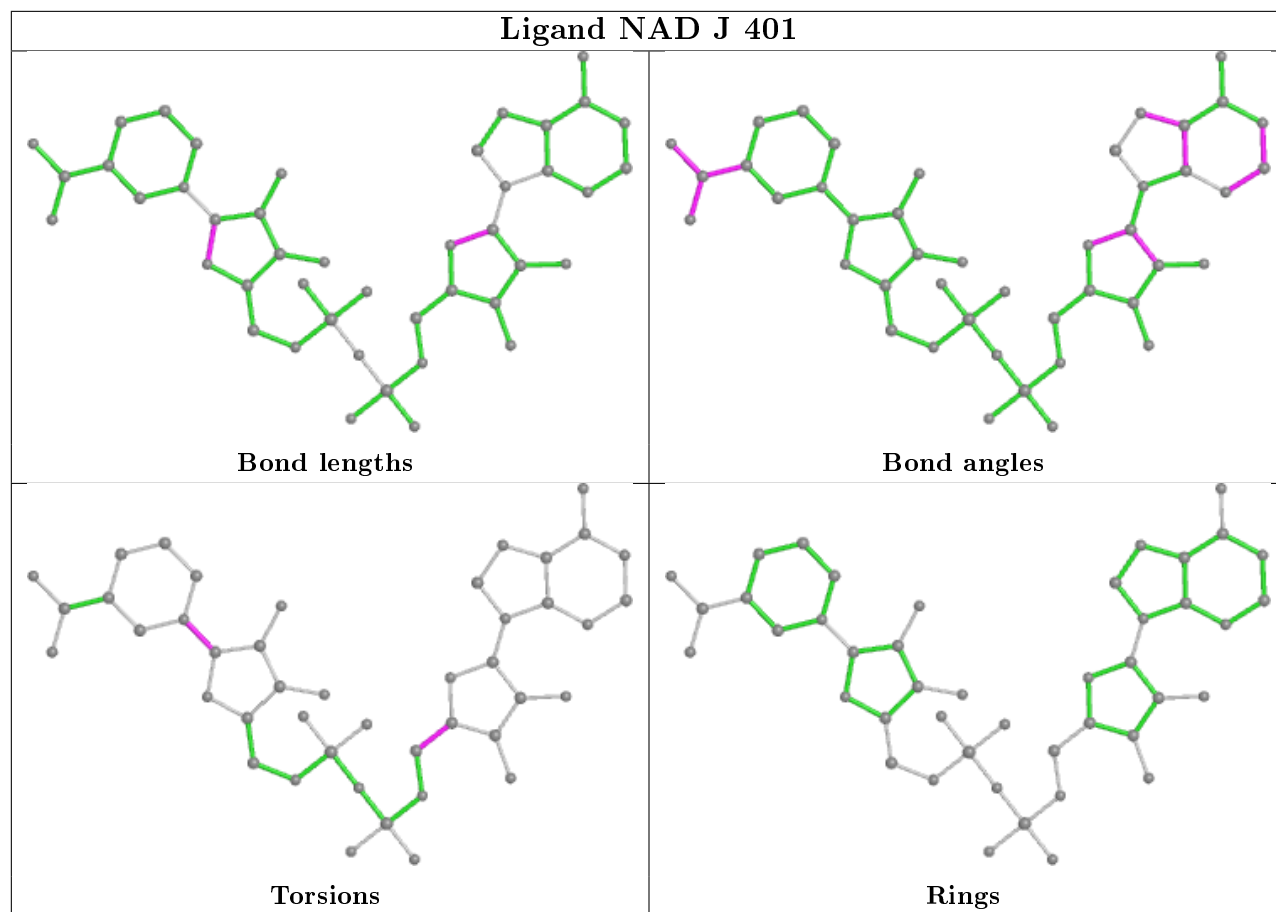












5.7 Other polymers [i](#)

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	351/351 (100%)	-0.57	1 (0%) 94 93	12, 19, 32, 45	0
1	B	351/351 (100%)	-0.55	2 (0%) 89 88	12, 20, 33, 50	0
1	C	351/351 (100%)	-0.48	1 (0%) 94 93	15, 22, 35, 51	0
1	D	351/351 (100%)	-0.61	1 (0%) 94 93	14, 20, 32, 49	0
1	E	351/351 (100%)	-0.58	2 (0%) 89 88	10, 18, 31, 44	0
1	F	351/351 (100%)	-0.27	5 (1%) 75 74	13, 25, 42, 58	0
1	G	351/351 (100%)	-0.47	1 (0%) 94 93	10, 22, 33, 48	0
1	H	351/351 (100%)	-0.39	3 (0%) 84 83	11, 22, 38, 57	0
1	I	351/351 (100%)	-0.18	7 (1%) 65 63	13, 25, 42, 55	0
1	J	351/351 (100%)	-0.09	6 (1%) 70 68	12, 26, 43, 50	0
1	K	351/351 (100%)	-0.46	2 (0%) 89 88	15, 23, 36, 56	0
1	L	351/351 (100%)	-0.54	2 (0%) 89 88	13, 21, 33, 49	0
All	All	4212/4212 (100%)	-0.43	33 (0%) 86 85	10, 22, 37, 58	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	28	ASP	5.2
1	K	28	ASP	4.7
1	I	28	ASP	4.3
1	J	28	ASP	3.9
1	G	28	ASP	3.9
1	F	28	ASP	3.5
1	C	28	ASP	3.5
1	I	79	PRO	3.4
1	I	78	GLY	3.4
1	L	28	ASP	3.1
1	F	29	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	134	ALA	2.9
1	F	79	PRO	2.8
1	J	79	PRO	2.7
1	B	28	ASP	2.7
1	D	28	ASP	2.6
1	I	317	LYS	2.6
1	L	79	PRO	2.6
1	H	47	PRO	2.5
1	K	65	SER	2.5
1	F	65	SER	2.4
1	J	78	GLY	2.4
1	B	29	SER	2.4
1	H	44	THR	2.3
1	A	28	ASP	2.2
1	I	45	LYS	2.2
1	E	47	PRO	2.2
1	I	29	SER	2.2
1	J	109	LYS	2.2
1	E	28	ASP	2.1
1	F	47	PRO	2.1
1	J	289	GLU	2.0
1	I	267	LYS	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
5	GOL	D	11	6/6	0.73	0.21	53,55,56,56	0

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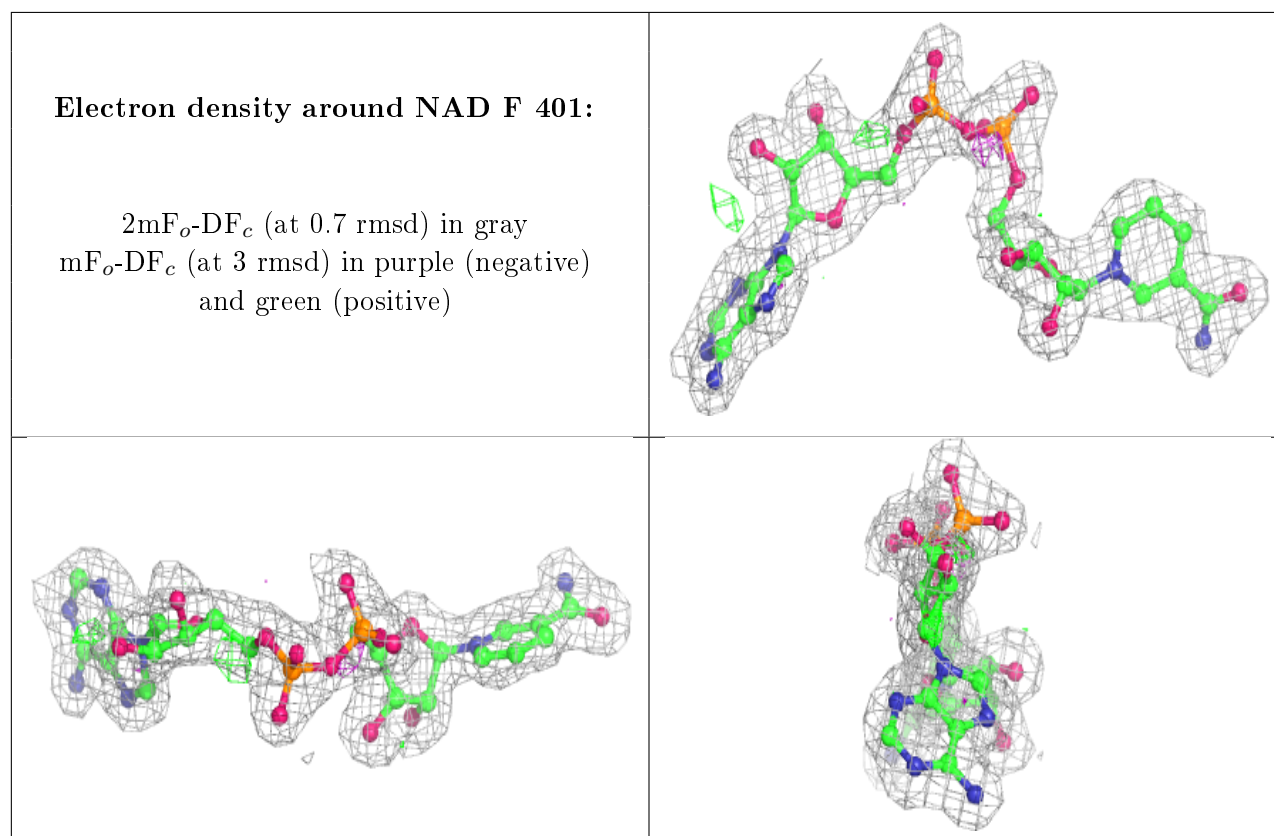
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	L	21	6/6	0.78	0.21	44,47,47,49	0
5	GOL	I	23	6/6	0.81	0.15	41,42,43,45	0
5	GOL	D	25	6/6	0.81	0.26	51,54,55,55	0
5	GOL	K	24	6/6	0.82	0.14	44,44,45,46	0
5	GOL	D	22	6/6	0.85	0.19	50,53,54,54	0
5	GOL	H	27	6/6	0.85	0.17	35,39,40,45	0
5	GOL	C	17	6/6	0.87	0.19	49,50,51,53	0
5	GOL	I	19	6/6	0.87	0.20	36,41,41,43	0
5	GOL	F	26	6/6	0.89	0.14	44,48,49,50	0
5	GOL	B	16	6/6	0.90	0.15	42,43,45,49	0
5	GOL	I	13	6/6	0.90	0.16	26,33,35,36	0
5	GOL	E	379	6/6	0.91	0.19	35,39,40,43	0
5	GOL	C	10	6/6	0.92	0.12	39,42,45,47	0
5	GOL	D	18	6/6	0.92	0.19	43,45,47,47	0
5	GOL	K	15	6/6	0.92	0.11	36,38,39,40	0
4	SO4	G	5	5/5	0.93	0.21	28,28,31,32	5
5	GOL	G	9	6/6	0.93	0.09	31,36,38,38	0
4	SO4	I	7	5/5	0.93	0.16	53,53,56,56	0
4	SO4	F	20	5/5	0.94	0.13	26,28,29,29	5
4	SO4	B	2	5/5	0.96	0.15	45,46,48,48	0
2	NAD	F	401	44/44	0.97	0.08	14,20,26,27	0
2	NAD	C	401	44/44	0.97	0.08	13,21,23,25	0
5	GOL	H	12	6/6	0.97	0.08	24,26,26,29	0
2	NAD	H	401	44/44	0.97	0.07	12,16,21,23	0
4	SO4	C	3	5/5	0.97	0.19	46,46,49,49	0
5	GOL	K	14	6/6	0.97	0.06	23,24,25,26	0
4	SO4	D	4	5/5	0.98	0.13	43,44,45,48	0
2	NAD	A	401	44/44	0.98	0.06	11,17,21,23	0
4	SO4	K	8	5/5	0.98	0.14	32,32,33,34	0
2	NAD	D	401	44/44	0.98	0.06	14,18,23,25	0
3	AZI	E	403	3/3	0.98	0.08	12,12,13,15	0
2	NAD	I	401	44/44	0.98	0.07	12,17,24,26	0
2	NAD	K	401	44/44	0.98	0.07	14,17,23,24	0
2	NAD	B	401	44/44	0.98	0.07	13,17,22,23	0
2	NAD	G	401	44/44	0.98	0.07	14,19,24,25	0
4	SO4	H	6	5/5	0.98	0.15	32,33,34,36	0
4	SO4	A	1	5/5	0.98	0.12	47,48,49,50	0
2	NAD	J	401	44/44	0.98	0.07	13,19,33,35	0
3	AZI	G	403	3/3	0.98	0.06	17,17,18,19	0
3	AZI	J	403	3/3	0.98	0.08	19,19,20,22	0
3	AZI	A	403	3/3	0.99	0.06	14,14,14,15	0
3	AZI	B	403	3/3	0.99	0.07	12,12,13,15	0

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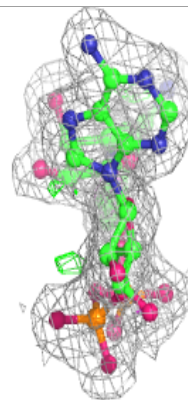
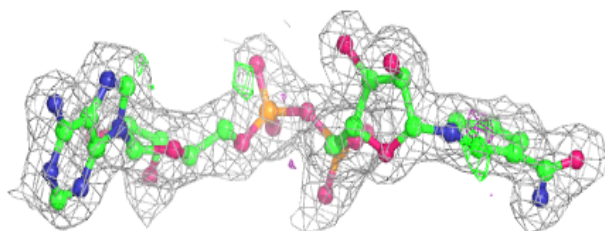
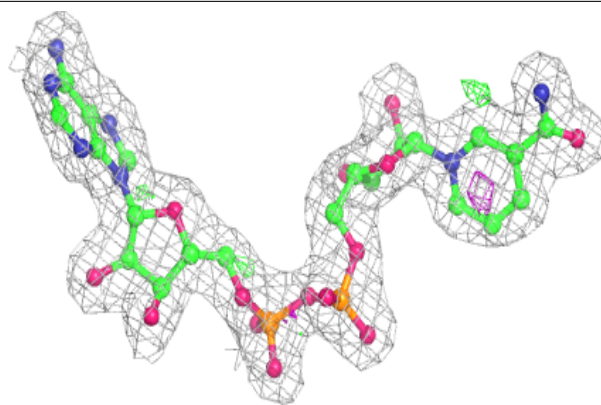
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAD	L	401	44/44	0.99	0.05	11,17,23,25	0
3	AZI	K	403	3/3	0.99	0.05	13,13,17,18	0
3	AZI	F	403	3/3	0.99	0.04	13,13,17,20	0
3	AZI	D	403	3/3	0.99	0.09	16,16,18,18	0
3	AZI	C	403	3/3	0.99	0.07	15,15,16,17	0
3	AZI	L	403	3/3	0.99	0.07	17,17,18,22	0
3	AZI	I	403	3/3	0.99	0.07	18,18,19,19	0
3	AZI	H	403	3/3	0.99	0.07	15,15,15,17	0
2	NAD	E	401	44/44	0.99	0.06	9,14,17,17	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.

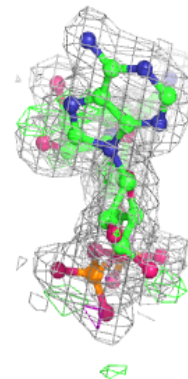
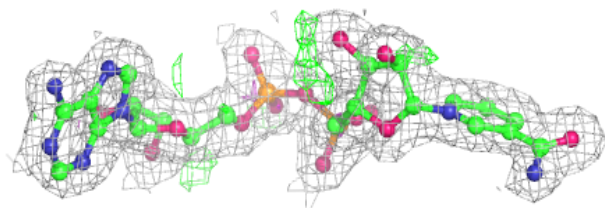
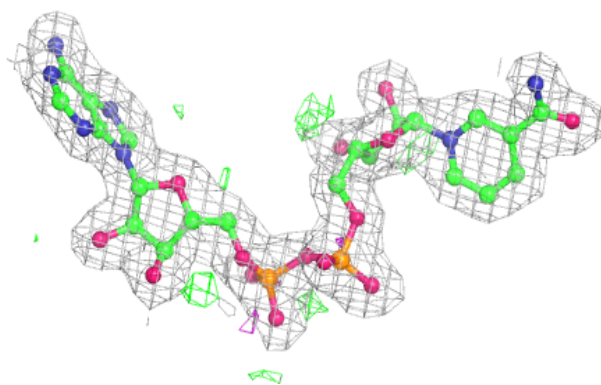


Electron density around NAD C 401:

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

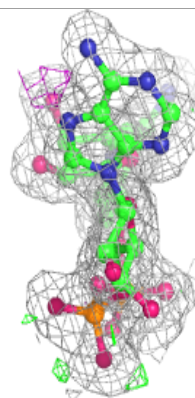
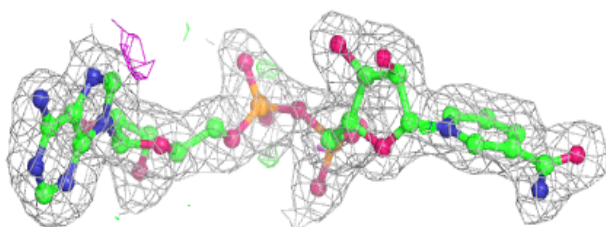
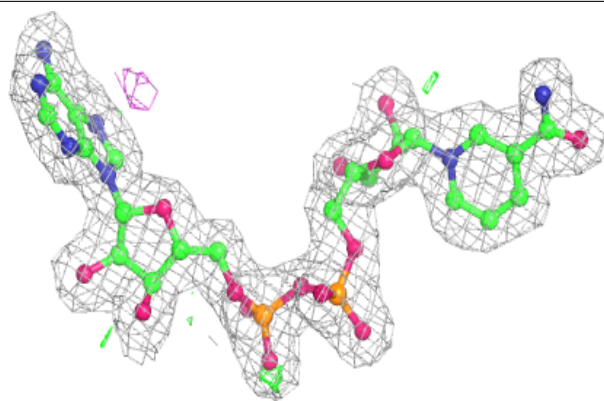
**Electron density around NAD H 401:**

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

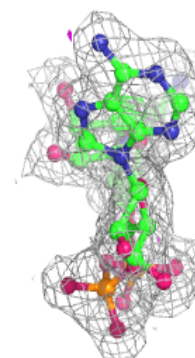
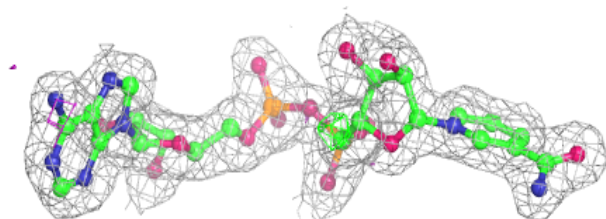
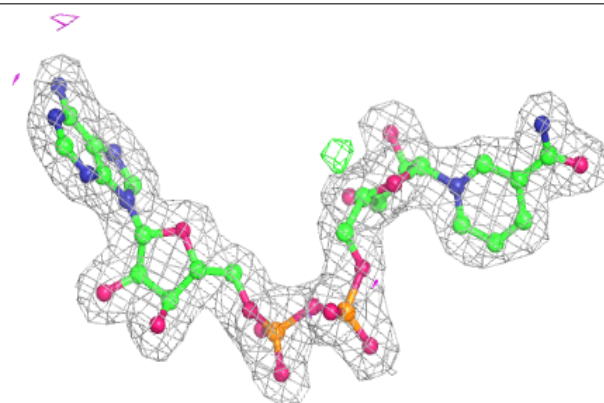


Electron density around NAD A 401:

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

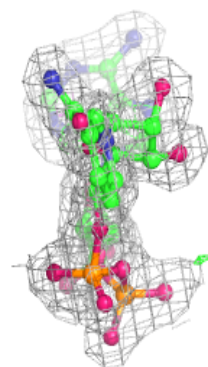
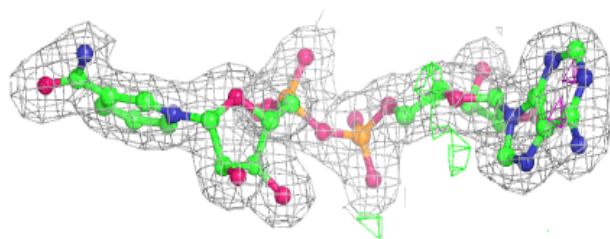
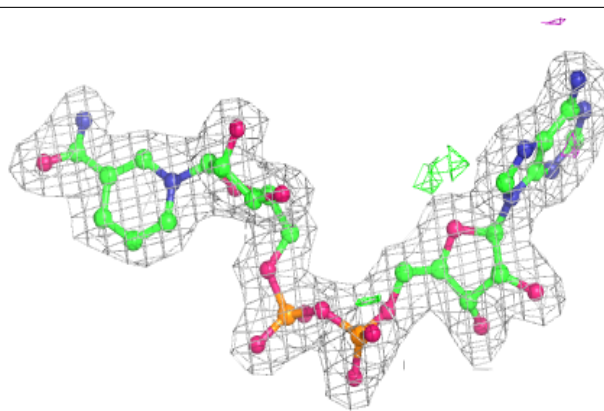
**Electron density around NAD D 401:**

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

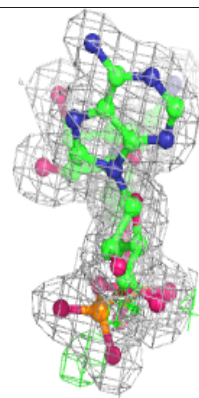
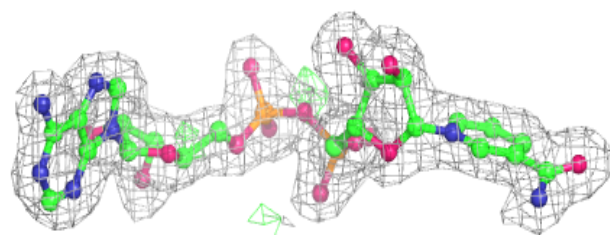
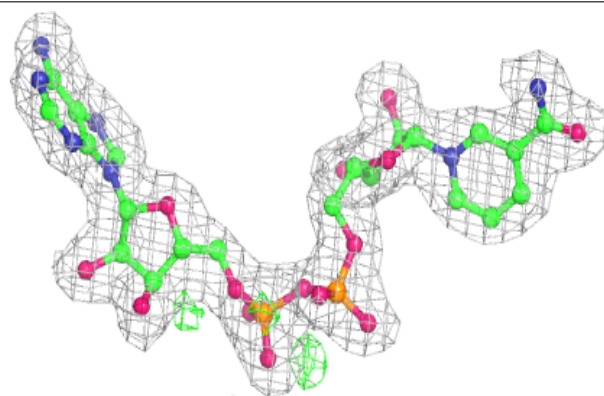


Electron density around NAD I 401:

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

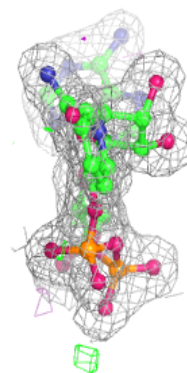
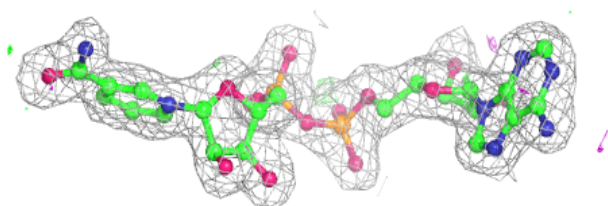
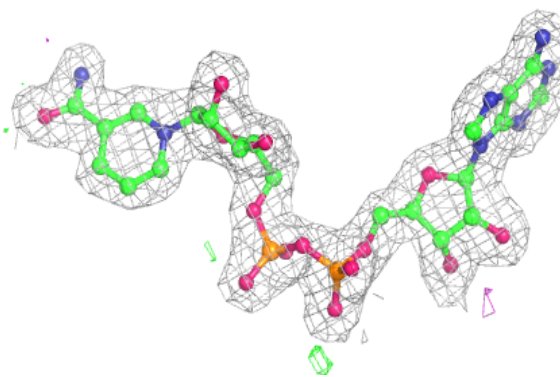
**Electron density around NAD K 401:**

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

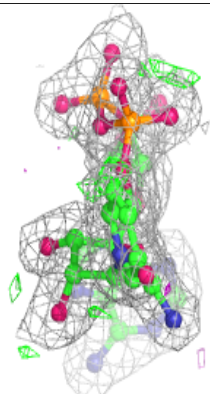
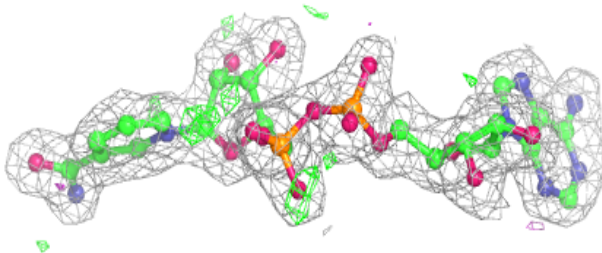
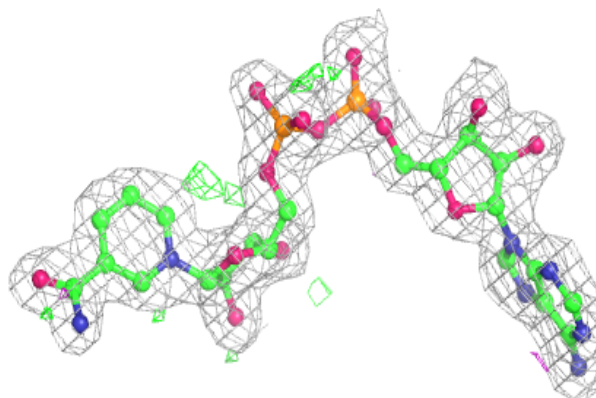


Electron density around NAD B 401:

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

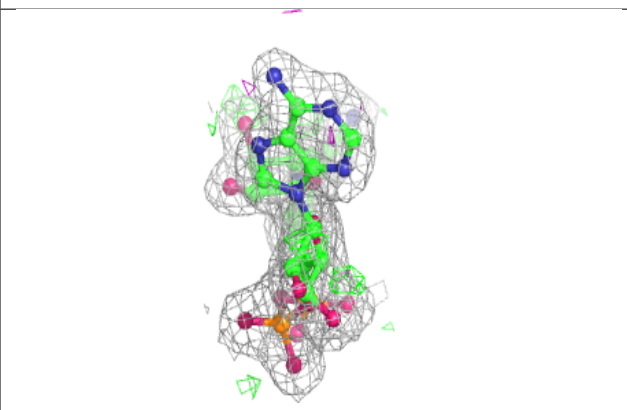
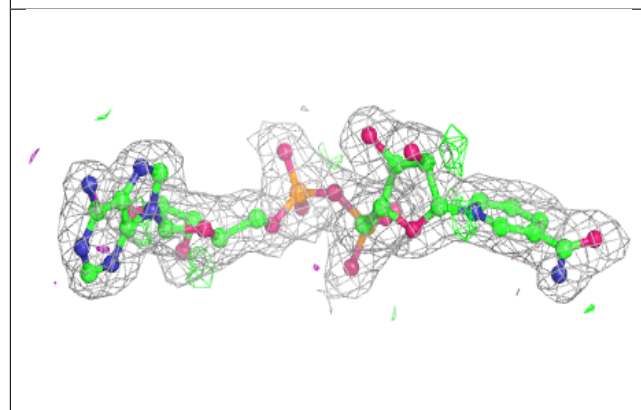
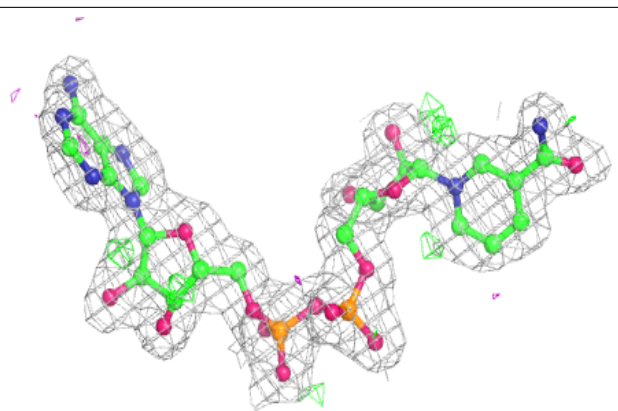
**Electron density around NAD G 401:**

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

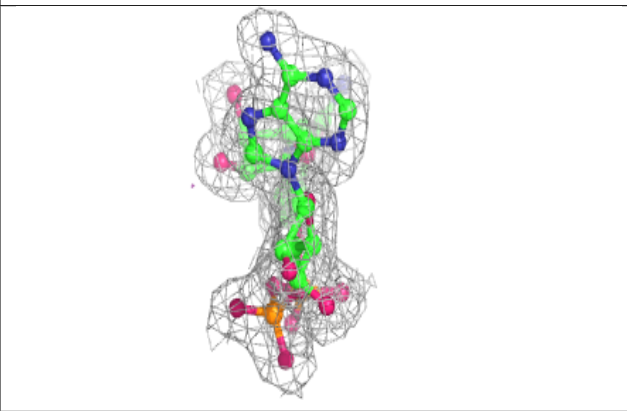
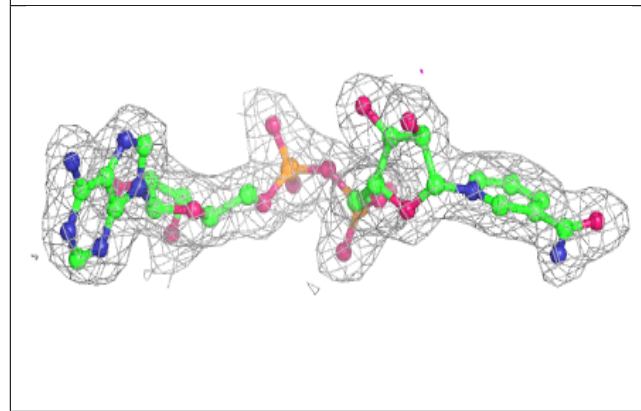
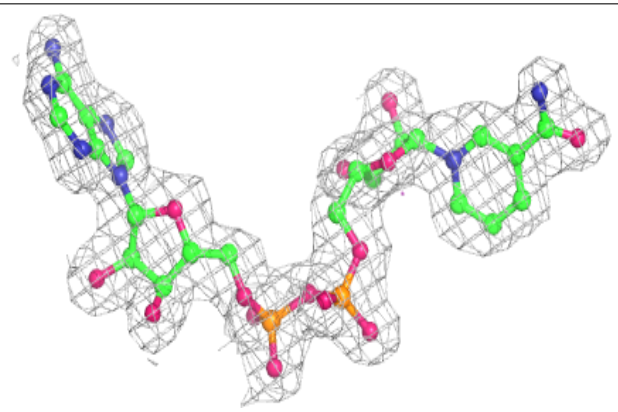


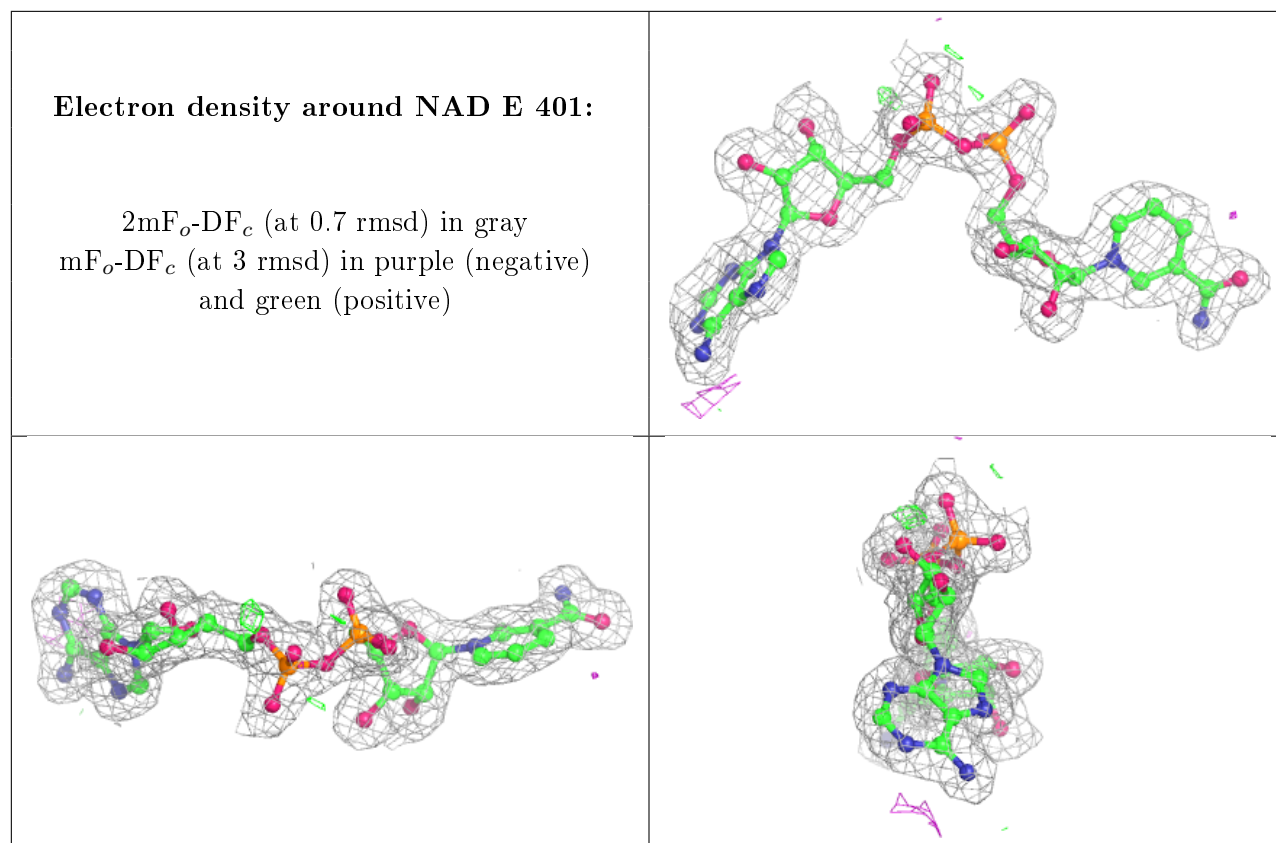
Electron density around NAD J 401:

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

**Electron density around NAD L 401:**

$2mF_o-DF_c$ (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.