



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 01:10 AM UTC

PDB ID : 9W15 / pdb_00009w15
Title : 3-Hydroxybutyryl-CoA dehydrogenase with NAD and acetoacetyl CoA
Authors : Shin, B.M.
Deposited on : 2025-07-25
Resolution : 3.29 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

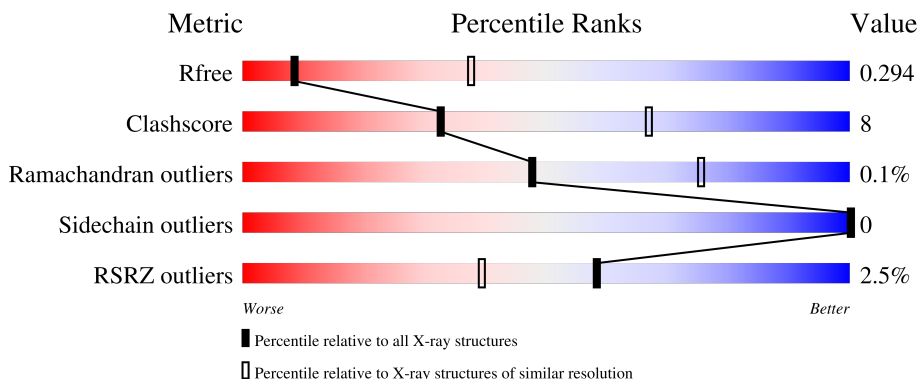
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 Å.

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



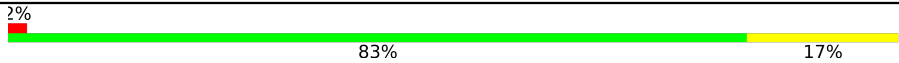
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	290	<div> <div>82%</div> <div>18%</div> </div>
1	B	290	<div> <div>79%</div> <div>21%</div> </div>
1	C	290	<div> <div>8%</div> <div>82%</div> <div>18%</div> </div>
1	D	290	<div> <div>78%</div> <div>22%</div> </div>
1	E	290	<div> <div>79%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	290	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a small red segment at the beginning labeled '2%', a large green segment in the middle labeled '83%', and a yellow segment at the end labeled '17%'. The segments are separated by thin black lines.

2 Entry composition [i](#)

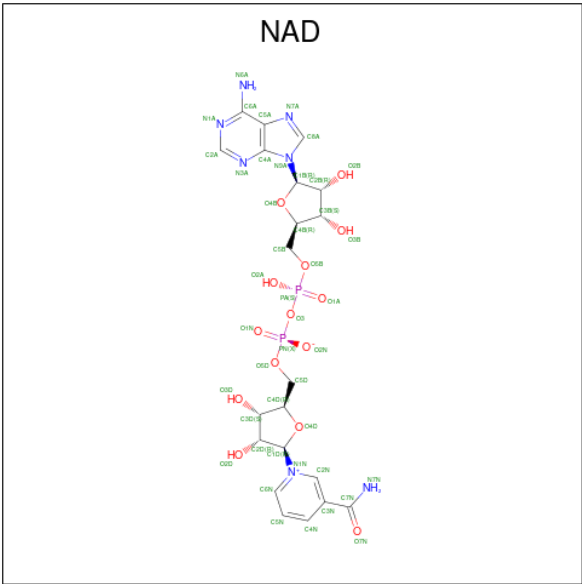
There are 3 unique types of molecules in this entry. The entry contains 13310 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-hydroxyacyl-CoA dehydrogenase, NAD binding domain protein.

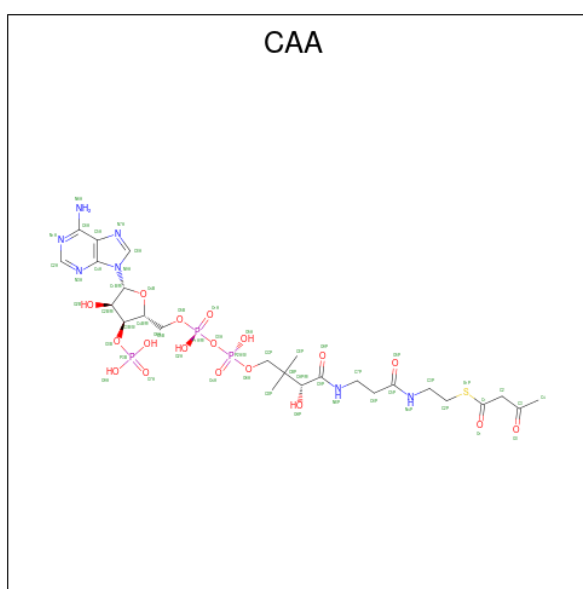
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	289	Total	C	N	O	S	0	0	0
			2153	1364	361	406	22			
1	A	289	Total	C	N	O	S	0	0	0
			2153	1364	361	406	22			
1	C	289	Total	C	N	O	S	0	0	0
			2153	1364	361	406	22			
1	D	289	Total	C	N	O	S	0	0	0
			2153	1364	361	406	22			
1	E	289	Total	C	N	O	S	0	0	0
			2153	1364	361	406	22			
1	F	289	Total	C	N	O	S	0	0	0
			2153	1364	361	406	22			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is ACETOACETYL-COENZYME A (CCD ID: CAA) (formula: $C_{25}H_{40}N_7O_{18}P_3S$) (labeled as "Ligand of Interest" by depositor).

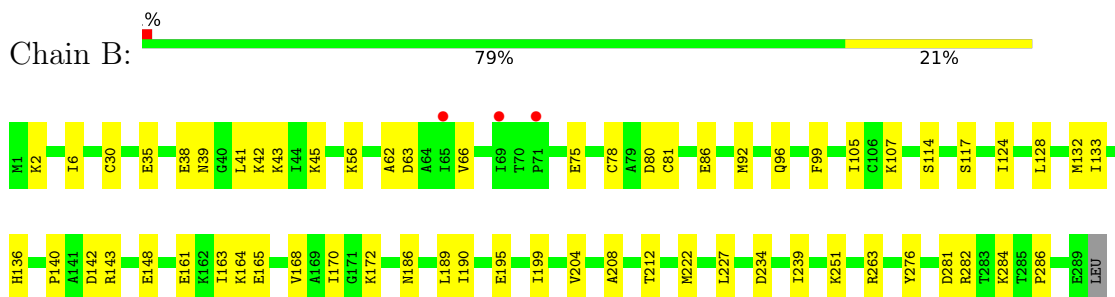


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 54	C 25	N 7	O 18	P 3	S 1	0	0
3	C	1	Total 54	C 25	N 7	O 18	P 3	S 1	0	0
3	D	1	Total 54	C 25	N 7	O 18	P 3	S 1	0	0
3	F	1	Total 54	C 25	N 7	O 18	P 3	S 1	0	0

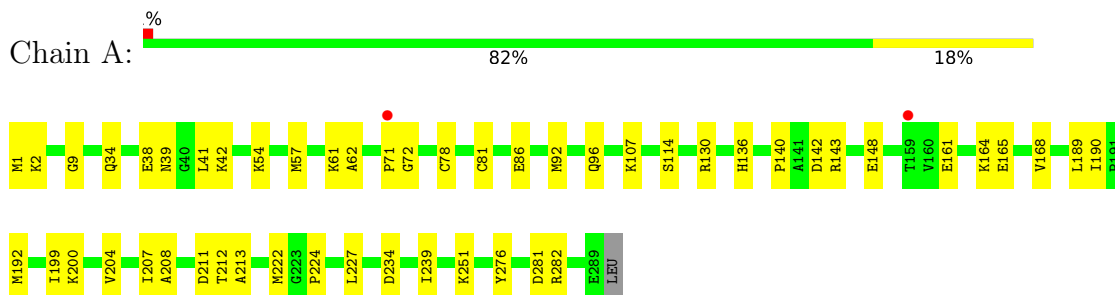
3 Residue-property plots

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.

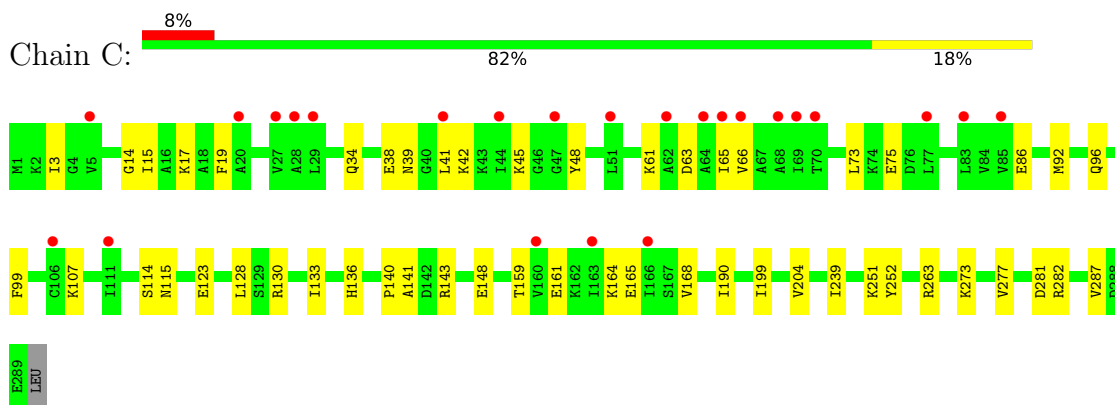
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase, NAD binding domain protein



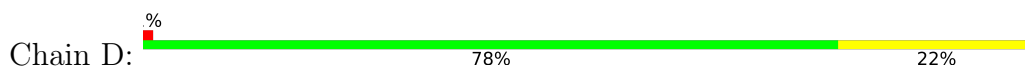
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase, NAD binding domain protein

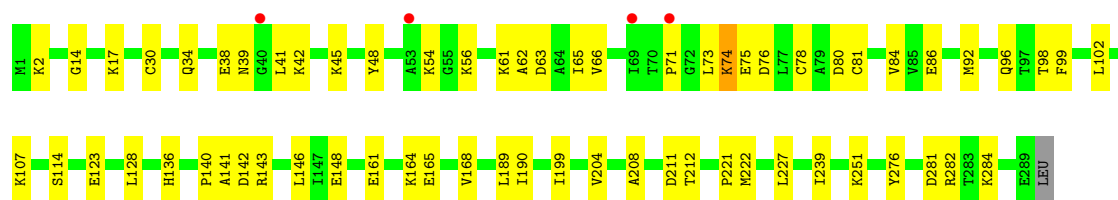


- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase, NAD binding domain protein

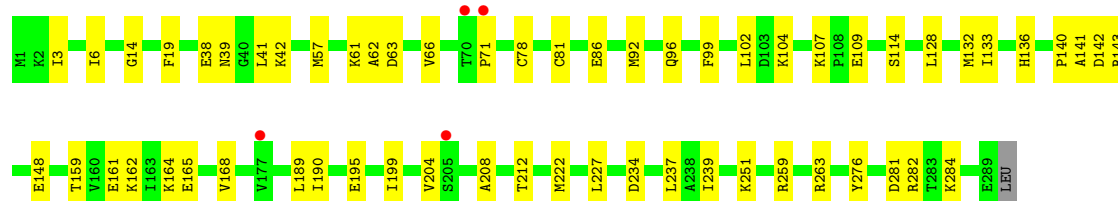
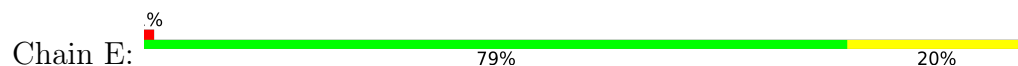


- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase, NAD binding domain protein

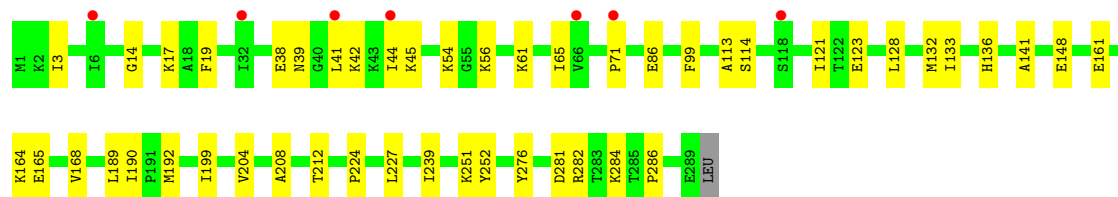
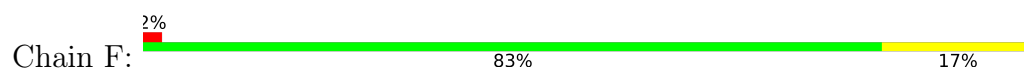




- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase, NAD binding domain protein



- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase, NAD binding domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.62Å 92.14Å 132.47Å 90.00° 100.42° 90.00°	Depositor
Resolution (Å)	48.01 – 3.29 48.01 – 3.29	Depositor EDS
% Data completeness (in resolution range)	89.6 (48.01-3.29) 89.5 (48.01-3.29)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.253 , 0.294 0.253 , 0.294	Depositor DCC
R_{free} test set	2000 reflections (6.63%)	wwPDB-VP
Wilson B-factor (Å ²)	75.2	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13310	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.11	0/2182	0.29	0/2934
1	B	0.11	0/2182	0.30	0/2934
1	C	0.11	0/2182	0.29	0/2934
1	D	0.12	0/2182	0.30	0/2934
1	E	0.11	0/2182	0.31	0/2934
1	F	0.10	0/2182	0.28	0/2934
All	All	0.11	0/13092	0.30	0/17604

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2153	0	2223	32	0
1	B	2153	0	2224	43	0
1	C	2153	0	2223	31	0
1	D	2153	0	2223	44	0
1	E	2153	0	2224	35	0
1	F	2153	0	2223	28	0
2	A	44	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	25	2	0
2	D	44	0	25	2	0
2	E	44	0	25	2	0
3	A	54	0	36	4	0
3	C	54	0	36	2	0
3	D	54	0	36	2	0
3	F	54	0	36	1	0
All	All	13310	0	13584	212	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (212) 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)
2:D:402:NAD:O4D	2:D:402:NAD:C4D	1.68	1.21
2:A:301:NAD:O4D	2:A:301:NAD:C4D	1.68	1.11
2:E:301:NAD:O4D	2:E:301:NAD:C4D	1.68	1.10
2:B:301:NAD:O4D	2:B:301:NAD:C4D	1.68	1.09
1:A:2:LYS:HB2	1:A:81:CYS:HA	1.67	0.76
1:B:136:HIS:HB3	1:B:148:GLU:HB2	1.68	0.74
1:E:136:HIS:HB3	1:E:148:GLU:HB2	1.67	0.74
1:A:136:HIS:HB3	1:A:148:GLU:HB2	1.70	0.74
1:D:136:HIS:HB3	1:D:148:GLU:HB2	1.70	0.73
1:C:136:HIS:HB3	1:C:148:GLU:HB2	1.71	0.73
1:B:199:ILE:HG23	1:B:204:VAL:HB	1.71	0.72
1:F:136:HIS:HB3	1:F:148:GLU:HB2	1.71	0.71
1:B:41:LEU:HG	1:B:45:LYS:HE2	1.71	0.71
1:E:199:ILE:HG23	1:E:204:VAL:HB	1.74	0.70
1:F:199:ILE:HG23	1:F:204:VAL:HB	1.76	0.67
1:A:199:ILE:HG23	1:A:204:VAL:HB	1.77	0.67
1:A:1:MET:SD	1:A:1:MET:N	2.67	0.66
1:C:133:ILE:HD11	1:C:159:THR:HB	1.77	0.66
1:B:86:GLU:HG3	1:B:114:SER:HA	1.77	0.66
3:A:302:CAA:HN8	1:D:222:MET:HE2	1.61	0.66
1:A:86:GLU:HG3	1:A:114:SER:HA	1.78	0.65
1:B:45:LYS:HZ2	1:B:66:VAL:HB	1.62	0.64
1:B:124:ILE:HG22	1:B:132:MET:HE3	1.80	0.64
1:E:190:ILE:HG13	1:E:239:ILE:HG21	1.79	0.64
1:B:222:MET:HE2	3:C:401:CAA:HN8	1.63	0.63
1:D:161:GLU:O	1:D:165:GLU:HG3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:MET:HE2	3:F:401:CAA:HN8	1.64	0.62
1:C:199:ILE:HG23	1:C:204:VAL:HB	1.82	0.62
1:B:63:ASP:HA	1:B:66:VAL:HG22	1.82	0.61
1:C:75:GLU:OE1	1:C:75:GLU:N	2.30	0.61
1:D:63:ASP:HA	1:D:66:VAL:HG22	1.83	0.61
1:D:190:ILE:HG13	1:D:239:ILE:HG21	1.83	0.61
1:B:39:ASN:O	1:B:43:LYS:HG2	2.01	0.61
1:D:199:ILE:HG23	1:D:204:VAL:HB	1.83	0.60
1:B:161:GLU:O	1:B:165:GLU:HG3	2.02	0.60
1:D:73:LEU:H	1:D:76:ASP:HB2	1.66	0.60
1:F:192:MET:HE3	1:F:224:PRO:HB3	1.84	0.60
1:C:161:GLU:O	1:C:165:GLU:HG3	2.02	0.60
1:E:86:GLU:HG3	1:E:114:SER:HA	1.84	0.59
1:E:161:GLU:O	1:E:165:GLU:HG3	2.02	0.59
1:D:86:GLU:HG3	1:D:114:SER:HA	1.82	0.59
1:E:39:ASN:HA	1:E:42:LYS:HD2	1.84	0.59
1:F:161:GLU:O	1:F:165:GLU:HG3	2.03	0.58
1:D:38:GLU:O	1:D:42:LYS:HG3	2.04	0.58
1:F:86:GLU:HG3	1:F:114:SER:HA	1.86	0.58
1:D:73:LEU:O	1:D:75:GLU:N	2.36	0.58
1:A:161:GLU:O	1:A:165:GLU:HG3	2.03	0.57
1:A:140:PRO:HG2	1:A:143:ARG:HB2	1.87	0.57
1:C:140:PRO:HG2	1:C:143:ARG:HB2	1.86	0.57
1:C:38:GLU:O	1:C:42:LYS:HG3	2.04	0.57
1:A:38:GLU:O	1:A:42:LYS:HG3	2.05	0.56
1:F:38:GLU:O	1:F:42:LYS:HG3	2.05	0.56
1:B:35:GLU:O	1:B:39:ASN:ND2	2.35	0.56
1:D:80:ASP:HA	1:D:107:LYS:HG2	1.87	0.56
1:F:54:LYS:HD2	1:F:56:LYS:HG2	1.88	0.56
1:B:140:PRO:HG2	1:B:143:ARG:HB2	1.88	0.56
1:D:2:LYS:HB3	1:D:81:CYS:HA	1.87	0.56
1:F:190:ILE:HG13	1:F:239:ILE:HG21	1.87	0.56
3:A:302:CAA:O9A	1:D:54:LYS:NZ	2.39	0.56
1:E:38:GLU:O	1:E:42:LYS:HG3	2.05	0.56
1:D:39:ASN:HA	1:D:42:LYS:HD2	1.88	0.55
1:C:34:GLN:HB2	1:C:73:LEU:HD22	1.88	0.55
1:A:39:ASN:HA	1:A:42:LYS:HD2	1.87	0.55
1:C:190:ILE:HG13	1:C:239:ILE:HG21	1.89	0.54
1:A:107:LYS:O	1:A:130:ARG:NH1	2.27	0.54
1:B:80:ASP:HA	1:B:107:LYS:HG3	1.89	0.54
1:B:41:LEU:O	1:B:45:LYS:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HG13	1:A:239:ILE:HG21	1.90	0.53
1:C:263:ARG:HG2	1:D:123:GLU:HG3	1.90	0.53
1:D:189:LEU:HD21	1:D:227:LEU:HD21	1.91	0.53
1:B:38:GLU:O	1:B:42:LYS:HG3	2.09	0.52
1:D:61:LYS:O	1:D:65:ILE:HG23	2.10	0.52
1:D:41:LEU:HD22	1:D:71:PRO:HD3	1.92	0.52
1:D:30:CYS:HB3	1:D:74:LYS:H	1.74	0.51
1:A:200:LYS:HD3	1:A:207:ILE:HG13	1.91	0.51
1:F:61:LYS:O	1:F:65:ILE:HG22	2.10	0.51
1:B:45:LYS:NZ	1:B:66:VAL:HB	2.25	0.51
1:B:39:ASN:HA	1:B:42:LYS:HD2	1.93	0.50
1:E:189:LEU:HD21	1:E:227:LEU:HD21	1.92	0.50
1:C:99:PHE:HB3	1:C:128:LEU:HD11	1.93	0.50
1:E:92:MET:O	1:E:96:GLN:HG3	2.12	0.50
1:C:164:LYS:O	1:C:168:VAL:HG13	2.12	0.49
1:D:84:VAL:HG11	1:D:102:LEU:HD13	1.93	0.49
1:F:39:ASN:HA	1:F:42:LYS:HD2	1.93	0.49
1:B:86:GLU:HG2	1:B:99:PHE:CE2	2.47	0.49
1:E:104:LYS:HE3	1:E:104:LYS:HA	1.94	0.49
1:D:34:GLN:HB2	1:D:73:LEU:HD12	1.94	0.49
1:C:61:LYS:O	1:C:65:ILE:HG23	2.13	0.49
1:D:41:LEU:O	1:D:45:LYS:HG2	2.12	0.49
1:B:189:LEU:HD21	1:B:227:LEU:HD21	1.95	0.48
1:C:123:GLU:HG3	1:E:263:ARG:HG2	1.95	0.48
1:F:41:LEU:HG	1:F:45:LYS:HE3	1.95	0.48
1:F:41:LEU:HD22	1:F:71:PRO:HD3	1.95	0.48
1:E:99:PHE:HB3	1:E:128:LEU:HD11	1.96	0.48
1:C:39:ASN:HA	1:C:42:LYS:HD2	1.96	0.48
1:D:276:TYR:HB3	1:D:284:LYS:HB2	1.96	0.48
2:E:301:NAD:H2N	2:E:301:NAD:H2D	1.51	0.48
1:E:164:LYS:O	1:E:168:VAL:HG13	2.14	0.48
1:F:189:LEU:HD21	1:F:227:LEU:HD21	1.96	0.48
1:E:251:LYS:HA	1:F:251:LYS:HB2	1.96	0.48
2:A:301:NAD:H2D	2:A:301:NAD:H2N	1.54	0.47
1:E:107:LYS:HZ1	1:E:109:GLU:HB2	1.79	0.47
1:B:62:ALA:O	1:B:66:VAL:HG13	2.14	0.47
1:A:54:LYS:NZ	3:D:401:CAA:O9A	2.34	0.47
2:B:301:NAD:H2N	2:B:301:NAD:H2D	1.49	0.47
1:A:78:CYS:HA	1:A:81:CYS:SG	2.55	0.47
1:B:164:LYS:O	1:B:168:VAL:HG13	2.15	0.47
1:F:276:TYR:HB3	1:F:284:LYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ILE:HA	1:B:30:CYS:HB2	1.97	0.47
1:D:281:ASP:O	1:D:282:ARG:HB2	2.15	0.47
1:E:133:ILE:HD11	1:E:159:THR:HB	1.96	0.47
1:B:281:ASP:O	1:B:282:ARG:HB2	2.15	0.47
1:D:86:GLU:HG2	1:D:99:PHE:CE2	2.50	0.47
1:B:92:MET:O	1:B:96:GLN:HG3	2.15	0.46
1:B:190:ILE:HG13	1:B:239:ILE:HG21	1.95	0.46
1:D:92:MET:O	1:D:96:GLN:HG3	2.15	0.46
3:A:302:CAA:N8P	1:D:222:MET:HE2	2.30	0.46
1:A:281:ASP:O	1:A:282:ARG:HB2	2.16	0.46
2:D:402:NAD:H2N	2:D:402:NAD:H2D	1.46	0.46
1:D:78:CYS:HA	1:D:81:CYS:SG	2.55	0.46
1:D:142:ASP:OD1	1:D:142:ASP:N	2.43	0.46
1:B:208:ALA:O	1:B:212:THR:HG23	2.16	0.46
1:D:17:LYS:HG2	1:D:48:TYR:CE2	2.51	0.46
1:A:189:LEU:HD21	1:A:227:LEU:HD21	1.99	0.45
1:E:57:MET:HG3	1:E:62:ALA:HB2	1.99	0.45
1:F:113:ALA:HA	1:F:133:ILE:O	2.16	0.45
1:D:140:PRO:HG2	1:D:143:ARG:HB2	1.99	0.45
1:F:281:ASP:O	1:F:282:ARG:HB2	2.16	0.45
1:B:263:ARG:HG2	1:F:123:GLU:HG3	1.99	0.45
1:E:237:LEU:HD21	1:E:259:ARG:HG3	1.97	0.45
1:F:164:LYS:O	1:F:168:VAL:HG13	2.16	0.45
1:B:276:TYR:HB3	1:B:284:LYS:HB2	1.98	0.45
1:A:41:LEU:HD22	1:A:71:PRO:HD3	1.97	0.45
1:A:92:MET:O	1:A:96:GLN:HG3	2.16	0.45
1:A:192:MET:HE3	1:A:224:PRO:HB3	1.99	0.45
1:D:164:LYS:O	1:D:168:VAL:HG13	2.17	0.45
1:A:251:LYS:HB2	1:D:251:LYS:HA	1.98	0.45
1:C:61:LYS:HA	1:C:61:LYS:HD2	1.68	0.45
1:D:99:PHE:HB3	1:D:128:LEU:HD11	1.98	0.45
1:D:211:ASP:OD2	1:D:276:TYR:OH	2.30	0.45
1:E:132:MET:HE3	1:E:133:ILE:O	2.17	0.45
1:B:2:LYS:HB2	1:B:81:CYS:HA	1.99	0.44
1:E:78:CYS:HA	1:E:81:CYS:SG	2.57	0.44
1:D:107:LYS:HD3	1:D:107:LYS:HA	1.84	0.44
1:D:61:LYS:HA	1:D:61:LYS:HD2	1.70	0.44
1:E:6:ILE:HG12	1:E:102:LEU:HD11	1.99	0.44
1:A:9:GLY:HA3	2:A:301:NAD:H4B	1.99	0.44
1:D:208:ALA:O	1:D:212:THR:HG23	2.17	0.44
3:A:302:CAA:OAP	1:D:221:PRO:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:VAL:HG23	1:C:287:VAL:HG12	1.99	0.44
1:E:281:ASP:O	1:E:282:ARG:HB2	2.16	0.44
1:B:78:CYS:HA	1:B:81:CYS:SG	2.57	0.44
1:A:142:ASP:OD1	1:A:142:ASP:N	2.43	0.44
1:C:92:MET:O	1:C:96:GLN:HG3	2.18	0.44
1:E:3:ILE:HD13	1:E:19:PHE:CD1	2.52	0.44
1:F:208:ALA:O	1:F:212:THR:HG23	2.17	0.44
1:E:41:LEU:HD22	1:E:71:PRO:HD3	2.00	0.44
1:E:276:TYR:HB3	1:E:284:LYS:HB2	1.99	0.43
1:A:57:MET:HG3	1:A:62:ALA:HB2	1.99	0.43
1:A:222:MET:HE2	3:D:401:CAA:HN8	1.84	0.43
1:C:41:LEU:HD12	1:C:41:LEU:HA	1.84	0.43
1:D:62:ALA:O	1:D:66:VAL:HG13	2.18	0.43
1:E:140:PRO:HG2	1:E:143:ARG:HB2	2.00	0.43
1:B:251:LYS:HA	1:C:251:LYS:HB2	2.00	0.43
1:D:98:THR:O	1:D:102:LEU:HG	2.18	0.43
1:E:61:LYS:HD2	1:E:61:LYS:HA	1.71	0.43
1:B:133:ILE:HG21	1:B:163:ILE:HG13	2.01	0.43
1:B:170:ILE:HG13	1:B:172:LYS:HG2	2.00	0.43
1:A:41:LEU:HD12	1:A:41:LEU:HA	1.81	0.43
1:A:164:LYS:O	1:A:168:VAL:HG13	2.19	0.43
1:F:121:ILE:HG23	1:F:132:MET:HE3	2.01	0.42
1:D:56:LYS:HA	1:D:56:LYS:HD3	1.74	0.42
1:E:142:ASP:OD1	1:E:142:ASP:N	2.45	0.42
1:F:17:LYS:HD2	1:F:44:ILE:HG12	2.01	0.42
1:F:41:LEU:HD12	1:F:41:LEU:HA	1.87	0.42
1:B:234:ASP:OD1	1:B:234:ASP:N	2.52	0.42
1:C:63:ASP:HA	1:C:66:VAL:HG22	2.01	0.42
1:B:56:LYS:HA	1:B:56:LYS:HD3	1.74	0.42
1:B:142:ASP:OD1	1:B:142:ASP:N	2.43	0.42
1:E:14:GLY:C	1:E:141:ALA:HB3	2.45	0.42
1:B:276:TYR:CE2	1:B:286:PRO:HG3	2.55	0.42
1:C:17:LYS:HG2	1:C:48:TYR:CE2	2.55	0.42
1:C:41:LEU:O	1:C:45:LYS:HG2	2.19	0.42
1:A:208:ALA:O	1:A:212:THR:HG23	2.20	0.42
1:C:14:GLY:C	1:C:141:ALA:HB3	2.45	0.42
1:D:14:GLY:C	1:D:141:ALA:HB3	2.44	0.42
1:E:195:GLU:OE2	1:F:252:TYR:OH	2.34	0.42
1:F:276:TYR:CE2	1:F:286:PRO:HG3	2.54	0.42
1:A:213:ALA:O	1:D:146:LEU:HD22	2.20	0.41
1:B:92:MET:CE	1:B:96:GLN:HE21	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:HD2	1:A:61:LYS:HA	1.71	0.41
1:B:75:GLU:HA	1:B:105:ILE:HD13	2.02	0.41
1:C:273:LYS:HD2	1:C:277:VAL:HG22	2.01	0.41
1:B:117:SER:HB2	1:B:186:ASN:ND2	2.35	0.41
1:B:195:GLU:OE2	1:C:252:TYR:OH	2.38	0.41
1:B:222:MET:HE2	3:C:401:CAA:N8P	2.34	0.41
1:E:63:ASP:HA	1:E:66:VAL:HG22	2.03	0.41
1:B:99:PHE:HB3	1:B:128:LEU:HD11	2.03	0.41
1:F:14:GLY:C	1:F:141:ALA:HB3	2.45	0.41
1:E:162:LYS:HA	1:E:162:LYS:HD2	1.91	0.41
1:E:208:ALA:O	1:E:212:THR:HG23	2.21	0.41
1:A:211:ASP:OD2	1:A:276:TYR:OH	2.34	0.41
1:A:234:ASP:OD1	1:A:234:ASP:N	2.52	0.41
1:E:234:ASP:OD1	1:E:234:ASP:N	2.53	0.41
1:A:34:GLN:OE1	1:A:72:GLY:HA2	2.21	0.40
1:C:107:LYS:O	1:C:130:ARG:NH1	2.38	0.40
1:C:281:ASP:O	1:C:282:ARG:HB2	2.20	0.40
1:C:3:ILE:HD13	1:C:19:PHE:CD1	2.56	0.40
1:F:99:PHE:HB3	1:F:128:LEU:HD11	2.03	0.40
1:C:15:ILE:HD11	1:C:115:ASN:ND2	2.36	0.40
1:C:86:GLU:HG3	1:C:114:SER:HA	2.03	0.40
1:F:3:ILE:HD13	1:F:19:PHE:CD1	2.56	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	287/290 (99%)	277 (96%)	10 (4%)	0	100	100
1	B	287/290 (99%)	280 (98%)	7 (2%)	0	100	100
1	C	287/290 (99%)	282 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	287/290 (99%)	281 (98%)	5 (2%)	1 (0%)	36	65
1	E	287/290 (99%)	282 (98%)	5 (2%)	0	100	100
1	F	287/290 (99%)	282 (98%)	5 (2%)	0	100	100
All	All	1722/1740 (99%)	1684 (98%)	37 (2%)	1 (0%)	48	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	74	LYS

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	229/231 (99%)	229 (100%)	0	100	100
1	B	229/231 (99%)	229 (100%)	0	100	100
1	C	229/231 (99%)	229 (100%)	0	100	100
1	D	229/231 (99%)	229 (100%)	0	100	100
1	E	229/231 (99%)	229 (100%)	0	100	100
1	F	229/231 (99%)	229 (100%)	0	100	100
All	All	1374/1386 (99%)	1374 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	GLN
1	C	34	GLN
1	D	279	ASN
1	E	279	ASN
1	F	186	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAD	B	301	-	46,48,48	3.57	19 (41%)	64,73,73	1.61	8 (12%)
2	NAD	A	301	-	46,48,48	3.57	20 (43%)	64,73,73	1.63	9 (14%)
3	CAA	A	302	1	53,56,56	3.29	18 (33%)	77,83,83	1.73	12 (15%)
3	CAA	C	401	1	53,56,56	3.28	18 (33%)	77,83,83	1.74	13 (16%)
2	NAD	D	402	-	46,48,48	3.57	20 (43%)	64,73,73	1.65	9 (14%)
3	CAA	D	401	1	53,56,56	3.28	18 (33%)	77,83,83	1.73	13 (16%)
3	CAA	F	401	1	53,56,56	3.28	18 (33%)	77,83,83	1.73	12 (15%)
2	NAD	E	301	-	46,48,48	3.56	20 (43%)	64,73,73	1.62	8 (12%)

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	301	-	-	12/30/62/62	0/5/5/5
2	NAD	A	301	-	-	13/30/62/62	0/5/5/5
3	CAA	A	302	1	-	9/55/71/71	0/3/3/3
3	CAA	C	401	1	-	11/55/71/71	0/3/3/3
2	NAD	D	402	-	-	12/30/62/62	0/5/5/5
3	CAA	D	401	1	-	11/55/71/71	0/3/3/3
3	CAA	F	401	1	-	11/55/71/71	0/3/3/3
2	NAD	E	301	-	-	13/30/62/62	0/5/5/5

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	402	NAD	O4D-C4D	10.69	1.68	1.45
2	B	301	NAD	O4D-C4D	10.65	1.68	1.45
2	A	301	NAD	O4D-C4D	10.61	1.68	1.45
2	E	301	NAD	O4D-C4D	10.58	1.68	1.45
2	A	301	NAD	C3D-C4D	-9.96	1.27	1.53
2	B	301	NAD	C3D-C4D	-9.94	1.27	1.53
2	D	402	NAD	C3D-C4D	-9.92	1.27	1.53
2	E	301	NAD	C3D-C4D	-9.87	1.28	1.53
3	A	302	CAA	C3B-C4B	-9.45	1.28	1.52
3	F	401	CAA	C3B-C4B	-9.45	1.28	1.52
3	D	401	CAA	C3B-C4B	-9.39	1.28	1.52
3	C	401	CAA	C3B-C4B	-9.38	1.28	1.52
3	F	401	CAA	C2B-C1B	-8.89	1.25	1.53
3	C	401	CAA	C2B-C1B	-8.88	1.25	1.53
3	D	401	CAA	C2B-C1B	-8.85	1.25	1.53
3	A	302	CAA	C2B-C1B	-8.83	1.25	1.53
3	C	401	CAA	O4B-C1B	7.98	1.60	1.42
3	D	401	CAA	O4B-C1B	7.96	1.60	1.42
3	A	302	CAA	O4B-C1B	7.93	1.60	1.42
3	F	401	CAA	O4B-C1B	7.91	1.60	1.42
3	A	302	CAA	C2B-C3B	7.54	1.69	1.53
3	D	401	CAA	C2B-C3B	7.49	1.69	1.53
2	D	402	NAD	O4D-C1D	-7.49	1.31	1.40
2	E	301	NAD	O4D-C1D	-7.48	1.31	1.40
2	A	301	NAD	O4D-C1D	-7.46	1.31	1.40
3	C	401	CAA	C2B-C3B	7.44	1.69	1.53
2	B	301	NAD	O4D-C1D	-7.44	1.31	1.40
3	F	401	CAA	C2B-C3B	7.42	1.69	1.53
2	B	301	NAD	C3B-C4B	-7.10	1.35	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	NAD	C3B-C4B	-7.08	1.35	1.53
2	D	402	NAD	C3B-C4B	-7.05	1.35	1.53
2	A	301	NAD	C3B-C4B	-7.03	1.35	1.53
2	A	301	NAD	O4B-C4B	6.81	1.60	1.45
2	D	402	NAD	O4B-C4B	6.76	1.60	1.45
2	E	301	NAD	O4B-C4B	6.76	1.60	1.45
3	F	401	CAA	C9P-N8P	6.73	1.49	1.33
2	B	301	NAD	O4B-C4B	6.71	1.59	1.45
3	C	401	CAA	C9P-N8P	6.70	1.49	1.33
3	A	302	CAA	C9P-N8P	6.69	1.49	1.33
3	D	401	CAA	C9P-N8P	6.68	1.49	1.33
2	B	301	NAD	C7N-N7N	6.28	1.44	1.33
2	D	402	NAD	C7N-N7N	6.21	1.44	1.33
2	E	301	NAD	C7N-N7N	6.17	1.44	1.33
2	A	301	NAD	C7N-N7N	6.15	1.44	1.33
3	A	302	CAA	C5P-N4P	5.98	1.47	1.33
3	F	401	CAA	C5P-N4P	5.95	1.47	1.33
3	C	401	CAA	C5P-N4P	5.93	1.47	1.33
3	D	401	CAA	C5P-N4P	5.91	1.47	1.33
3	A	302	CAA	P2A-O3A	5.75	1.65	1.59
3	D	401	CAA	P2A-O3A	5.71	1.65	1.59
3	F	401	CAA	P2A-O3A	5.67	1.65	1.59
3	F	401	CAA	P1A-O3A	5.67	1.65	1.59
3	C	401	CAA	P2A-O3A	5.65	1.65	1.59
3	A	302	CAA	P1A-O3A	5.64	1.65	1.59
3	D	401	CAA	P1A-O3A	5.54	1.65	1.59
3	C	401	CAA	P1A-O3A	5.53	1.65	1.59
2	D	402	NAD	C6A-N6A	5.25	1.47	1.34
2	A	301	NAD	C6A-N6A	5.23	1.47	1.34
2	B	301	NAD	O4B-C1B	-5.23	1.29	1.42
2	D	402	NAD	O4B-C1B	-5.23	1.29	1.42
2	B	301	NAD	C6A-N6A	5.23	1.47	1.34
2	E	301	NAD	C6A-N6A	5.21	1.47	1.34
2	E	301	NAD	O4B-C1B	-5.18	1.30	1.42
2	A	301	NAD	O4B-C1B	-5.17	1.30	1.42
3	C	401	CAA	C6A-N6A	4.81	1.46	1.34
3	F	401	CAA	C6A-N6A	4.77	1.46	1.34
3	D	401	CAA	C6A-N6A	4.76	1.46	1.34
3	A	302	CAA	C6A-N6A	4.74	1.46	1.34
3	D	401	CAA	P3B-O3B	4.54	1.67	1.59
3	A	302	CAA	P3B-O3B	4.50	1.67	1.59
3	C	401	CAA	P3B-O3B	4.48	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	CAA	P3B-O3B	4.37	1.67	1.59
2	A	301	NAD	PA-O3	4.34	1.64	1.59
2	B	301	NAD	PA-O3	4.26	1.64	1.59
2	D	402	NAD	PA-O3	4.25	1.64	1.59
2	A	301	NAD	O2D-C2D	-4.23	1.32	1.43
2	B	301	NAD	O2D-C2D	-4.22	1.32	1.43
2	D	402	NAD	O2D-C2D	-4.21	1.32	1.43
2	E	301	NAD	PA-O3	4.21	1.64	1.59
2	E	301	NAD	O2D-C2D	-4.19	1.32	1.43
2	A	301	NAD	PN-O3	4.01	1.63	1.59
2	D	402	NAD	PN-O3	4.00	1.63	1.59
2	E	301	NAD	PN-O3	3.97	1.63	1.59
2	B	301	NAD	PN-O3	3.95	1.63	1.59
3	D	401	CAA	O4B-C4B	3.88	1.53	1.45
3	C	401	CAA	O4B-C4B	3.87	1.53	1.45
3	A	302	CAA	O4B-C4B	3.84	1.53	1.45
3	F	401	CAA	O4B-C4B	3.84	1.53	1.45
3	F	401	CAA	C6P-C5P	3.50	1.58	1.51
3	D	401	CAA	C6P-C5P	3.45	1.58	1.51
3	A	302	CAA	C6P-C5P	3.45	1.58	1.51
3	C	401	CAA	C6P-C5P	3.44	1.58	1.51
2	D	402	NAD	O3B-C3B	3.25	1.51	1.43
2	B	301	NAD	O3B-C3B	3.23	1.51	1.43
2	A	301	NAD	O3B-C3B	3.20	1.50	1.43
2	E	301	NAD	O3B-C3B	3.19	1.50	1.43
2	A	301	NAD	PA-O5B	2.94	1.70	1.59
2	E	301	NAD	PA-O5B	2.93	1.70	1.59
3	A	302	CAA	C8A-N9A	-2.91	1.32	1.37
2	B	301	NAD	PA-O5B	2.90	1.70	1.59
2	D	402	NAD	PA-O5B	2.86	1.70	1.59
3	F	401	CAA	CCP-CBP	2.86	1.57	1.52
3	F	401	CAA	C8A-N9A	-2.85	1.32	1.37
3	D	401	CAA	C8A-N9A	-2.84	1.32	1.37
3	D	401	CAA	CCP-CBP	2.83	1.57	1.52
3	C	401	CAA	C8A-N9A	-2.83	1.32	1.37
3	A	302	CAA	CCP-CBP	2.80	1.57	1.52
2	E	301	NAD	C8A-N9A	-2.79	1.32	1.37
2	A	301	NAD	C8A-N9A	-2.76	1.32	1.37
2	B	301	NAD	C8A-N9A	-2.76	1.32	1.37
2	D	402	NAD	C8A-N9A	-2.76	1.32	1.37
3	C	401	CAA	C5B-C4B	2.73	1.59	1.51
3	D	401	CAA	C5B-C4B	2.72	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	CAA	C5B-C4B	2.71	1.59	1.51
3	C	401	CAA	CCP-CBP	2.71	1.57	1.52
3	F	401	CAA	C5B-C4B	2.69	1.59	1.51
2	A	301	NAD	O7N-C7N	-2.61	1.19	1.24
2	E	301	NAD	O7N-C7N	-2.61	1.19	1.24
2	B	301	NAD	O7N-C7N	-2.60	1.19	1.24
2	D	402	NAD	O7N-C7N	-2.57	1.19	1.24
2	E	301	NAD	C2D-C3D	2.48	1.60	1.53
2	D	402	NAD	C2D-C3D	2.47	1.60	1.53
3	F	401	CAA	C5A-N7A	-2.47	1.34	1.39
2	B	301	NAD	C2D-C3D	2.46	1.60	1.53
3	A	302	CAA	C5A-N7A	-2.45	1.34	1.39
2	A	301	NAD	C2D-C3D	2.45	1.60	1.53
2	D	402	NAD	C3N-C7N	2.45	1.54	1.50
3	D	401	CAA	C5A-N7A	-2.43	1.34	1.39
3	C	401	CAA	C5A-N7A	-2.41	1.34	1.39
2	B	301	NAD	C3N-C7N	2.40	1.54	1.50
3	F	401	CAA	C1-S1P	2.38	1.81	1.76
3	C	401	CAA	C1-S1P	2.37	1.81	1.76
3	D	401	CAA	C1-S1P	2.37	1.81	1.76
2	A	301	NAD	C3N-C7N	2.36	1.54	1.50
3	A	302	CAA	C1-S1P	2.35	1.81	1.76
2	A	301	NAD	O3D-C3D	2.31	1.48	1.43
2	E	301	NAD	O3D-C3D	2.30	1.48	1.43
2	D	402	NAD	C5A-N7A	-2.29	1.34	1.39
2	B	301	NAD	O3D-C3D	2.28	1.48	1.43
2	E	301	NAD	C5A-N7A	-2.28	1.34	1.39
2	A	301	NAD	C5A-N7A	-2.27	1.34	1.39
2	D	402	NAD	O3D-C3D	2.26	1.48	1.43
2	B	301	NAD	C5A-N7A	-2.25	1.35	1.39
3	D	401	CAA	O9P-C9P	-2.23	1.19	1.23
3	A	302	CAA	O9P-C9P	-2.17	1.19	1.23
3	C	401	CAA	O9P-C9P	-2.17	1.19	1.23
2	E	301	NAD	C3N-C7N	2.16	1.53	1.50
3	F	401	CAA	O9P-C9P	-2.13	1.19	1.23
2	E	301	NAD	C2N-N1N	-2.05	1.32	1.35
2	D	402	NAD	C2N-N1N	-2.02	1.32	1.35
2	A	301	NAD	C2N-N1N	-2.02	1.32	1.35

All (84) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	CAA	C5A-C4A-N3A	-5.96	118.51	126.72
3	D	401	CAA	C5A-C4A-N3A	-5.93	118.56	126.72
3	A	302	CAA	C5A-C4A-N3A	-5.92	118.57	126.72
3	F	401	CAA	C5A-C4A-N3A	-5.79	118.74	126.72
2	D	402	NAD	C5A-C4A-N3A	-5.54	119.09	126.72
2	E	301	NAD	C5A-C4A-N3A	-5.46	119.20	126.72
2	A	301	NAD	C5A-C4A-N3A	-5.38	119.30	126.72
2	B	301	NAD	C5A-C4A-N3A	-5.32	119.39	126.72
3	F	401	CAA	C2-C1-S1P	4.70	119.60	113.63
3	C	401	CAA	C2-C1-S1P	4.68	119.57	113.63
3	C	401	CAA	N3A-C4A-N9A	4.66	135.09	127.17
3	D	401	CAA	N3A-C4A-N9A	4.64	135.05	127.17
3	A	302	CAA	C2-C1-S1P	4.63	119.51	113.63
2	B	301	NAD	N3A-C2A-N1A	-4.62	121.58	128.58
2	A	301	NAD	N3A-C2A-N1A	-4.61	121.60	128.58
3	A	302	CAA	N3A-C4A-N9A	4.61	135.01	127.17
3	F	401	CAA	N3A-C4A-N9A	4.61	135.01	127.17
2	E	301	NAD	N3A-C2A-N1A	-4.60	121.62	128.58
2	D	402	NAD	N3A-C2A-N1A	-4.57	121.66	128.58
3	D	401	CAA	C2-C1-S1P	4.54	119.40	113.63
3	D	401	CAA	N3A-C2A-N1A	-4.51	121.75	128.58
3	F	401	CAA	N3A-C2A-N1A	-4.49	121.78	128.58
3	C	401	CAA	N3A-C2A-N1A	-4.48	121.80	128.58
3	A	302	CAA	N3A-C2A-N1A	-4.47	121.81	128.58
3	A	302	CAA	C4B-O4B-C1B	-4.21	100.17	109.47
3	F	401	CAA	C4B-O4B-C1B	-4.07	100.47	109.47
3	D	401	CAA	C4B-O4B-C1B	-3.97	100.70	109.47
2	E	301	NAD	N3A-C4A-N9A	3.86	133.74	127.17
2	D	402	NAD	N3A-C4A-N9A	3.85	133.71	127.17
2	B	301	NAD	N3A-C4A-N9A	3.79	133.61	127.17
3	C	401	CAA	C4B-O4B-C1B	-3.77	101.15	109.47
2	A	301	NAD	N3A-C4A-N9A	3.73	133.50	127.17
2	D	402	NAD	C2A-N3A-C4A	3.65	120.76	111.83
2	E	301	NAD	C2A-N3A-C4A	3.64	120.73	111.83
3	D	401	CAA	C2A-N3A-C4A	3.62	120.67	111.83
3	C	401	CAA	C2A-N3A-C4A	3.62	120.66	111.83
3	A	302	CAA	C2A-N3A-C4A	3.61	120.65	111.83
2	A	301	NAD	C2A-N3A-C4A	3.60	120.63	111.83
2	B	301	NAD	C2A-N3A-C4A	3.57	120.55	111.83
3	F	401	CAA	C2A-N3A-C4A	3.55	120.50	111.83
2	D	402	NAD	C4A-C5A-N7A	-3.54	106.54	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAD	C4A-C5A-N7A	-3.47	106.61	110.58
2	E	301	NAD	C4A-C5A-N7A	-3.40	106.70	110.58
2	D	402	NAD	C5A-N7A-C8A	3.36	108.73	103.45
2	B	301	NAD	C4A-C5A-N7A	-3.33	106.78	110.58
2	A	301	NAD	C5A-N7A-C8A	3.27	108.59	103.45
2	E	301	NAD	C5A-N7A-C8A	3.26	108.57	103.45
3	C	401	CAA	C3B-C2B-C1B	3.25	107.03	99.89
2	B	301	NAD	C5A-N7A-C8A	3.21	108.50	103.45
3	D	401	CAA	C3B-C2B-C1B	3.20	106.93	99.89
3	A	302	CAA	C3B-C2B-C1B	3.19	106.92	99.89
2	D	402	NAD	N9A-C8A-N7A	-3.17	109.44	113.94
2	B	301	NAD	N9A-C8A-N7A	-3.16	109.45	113.94
2	E	301	NAD	N9A-C8A-N7A	-3.16	109.46	113.94
2	A	301	NAD	N9A-C8A-N7A	-3.13	109.49	113.94
3	F	401	CAA	C3B-C2B-C1B	3.06	106.61	99.89
3	A	302	CAA	C5A-N7A-C8A	2.69	107.67	103.45
3	A	302	CAA	N9A-C8A-N7A	-2.68	110.13	113.94
3	F	401	CAA	N9A-C8A-N7A	-2.66	110.17	113.94
3	C	401	CAA	C5A-N7A-C8A	2.65	107.62	103.45
3	F	401	CAA	C5A-N7A-C8A	2.63	107.58	103.45
3	D	401	CAA	C5A-N7A-C8A	2.63	107.58	103.45
3	C	401	CAA	N9A-C8A-N7A	-2.62	110.22	113.94
3	D	401	CAA	N9A-C8A-N7A	-2.61	110.24	113.94
3	A	302	CAA	C4A-C5A-N7A	-2.51	107.71	110.58
3	C	401	CAA	C4A-C5A-N7A	-2.49	107.74	110.58
3	C	401	CAA	C2P-S1P-C1	2.47	109.14	101.84
3	D	401	CAA	C4A-C5A-N7A	-2.43	107.80	110.58
2	B	301	NAD	C4A-N9A-C8A	2.42	108.28	105.74
3	D	401	CAA	C2P-S1P-C1	2.37	108.84	101.84
3	F	401	CAA	C4A-C5A-N7A	-2.37	107.88	110.58
2	E	301	NAD	C4A-N9A-C8A	2.36	108.22	105.74
3	F	401	CAA	C2P-S1P-C1	2.35	108.79	101.84
3	A	302	CAA	C2P-S1P-C1	2.30	108.64	101.84
3	F	401	CAA	C4A-N9A-C8A	2.27	108.12	105.74
2	A	301	NAD	C4A-N9A-C8A	2.26	108.11	105.74
2	D	402	NAD	C4A-N9A-C8A	2.24	108.09	105.74
3	A	302	CAA	C4A-N9A-C8A	2.21	108.06	105.74
3	C	401	CAA	C4A-N9A-C8A	2.17	108.02	105.74
3	D	401	CAA	C4A-N9A-C8A	2.14	107.99	105.74
2	A	301	NAD	C5N-C4N-C3N	-2.12	118.28	120.36
3	C	401	CAA	O1-C1-S1P	-2.12	119.98	122.68
2	D	402	NAD	C3B-C2B-C1B	2.05	105.34	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	CAA	C3P-N4P-C5P	-2.03	119.04	122.82

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	NAD	C5D-O5D-PN-O3
2	B	301	NAD	C5D-O5D-PN-O1N
2	B	301	NAD	O4D-C1D-N1N-C2N
2	B	301	NAD	O4D-C1D-N1N-C6N
2	B	301	NAD	C2D-C1D-N1N-C6N
2	A	301	NAD	C5D-O5D-PN-O3
2	A	301	NAD	O4D-C1D-N1N-C2N
2	A	301	NAD	O4D-C1D-N1N-C6N
2	A	301	NAD	C2D-C1D-N1N-C2N
2	A	301	NAD	C2D-C1D-N1N-C6N
2	D	402	NAD	C5D-O5D-PN-O3
2	D	402	NAD	O4D-C1D-N1N-C2N
2	D	402	NAD	O4D-C1D-N1N-C6N
2	D	402	NAD	C2D-C1D-N1N-C6N
2	E	301	NAD	C5D-O5D-PN-O3
2	E	301	NAD	C5D-O5D-PN-O2N
2	E	301	NAD	O4D-C1D-N1N-C2N
2	E	301	NAD	O4D-C1D-N1N-C6N
2	E	301	NAD	C2D-C1D-N1N-C6N
3	A	302	CAA	CCP-O6A-P2A-O3A
3	A	302	CAA	CCP-O6A-P2A-O4A
3	A	302	CAA	CCP-O6A-P2A-O5A
3	A	302	CAA	C1-C2-C3-O3
3	A	302	CAA	C1-C2-C3-C4
3	C	401	CAA	CCP-O6A-P2A-O3A
3	C	401	CAA	C1-C2-C3-O3
3	C	401	CAA	C1-C2-C3-C4
3	D	401	CAA	CCP-O6A-P2A-O3A
3	D	401	CAA	CCP-O6A-P2A-O4A
3	D	401	CAA	CCP-O6A-P2A-O5A
3	D	401	CAA	C1-C2-C3-O3
3	F	401	CAA	CCP-O6A-P2A-O3A
3	F	401	CAA	CCP-O6A-P2A-O4A
3	F	401	CAA	CCP-O6A-P2A-O5A
3	F	401	CAA	C1-C2-C3-O3
3	F	401	CAA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	B	301	NAD	O4D-C4D-C5D-O5D
2	B	301	NAD	C3D-C4D-C5D-O5D
2	A	301	NAD	O4D-C4D-C5D-O5D
2	A	301	NAD	C3D-C4D-C5D-O5D
2	D	402	NAD	O4D-C4D-C5D-O5D
2	D	402	NAD	C3D-C4D-C5D-O5D
3	A	302	CAA	O4B-C1B-N9A-C4A
2	E	301	NAD	C3D-C4D-C5D-O5D
3	D	401	CAA	O4B-C1B-N9A-C4A
2	E	301	NAD	O4B-C4B-C5B-O5B
2	E	301	NAD	O4D-C4D-C5D-O5D
3	A	302	CAA	O4B-C1B-N9A-C8A
3	D	401	CAA	C1-C2-C3-C4
3	C	401	CAA	O4B-C1B-N9A-C4A
2	D	402	NAD	C4B-C5B-O5B-PA
3	F	401	CAA	O4B-C1B-N9A-C4A
3	C	401	CAA	O4B-C1B-N9A-C8A
3	D	401	CAA	O4B-C1B-N9A-C8A
3	A	302	CAA	P1A-O3A-P2A-O5A
3	C	401	CAA	P1A-O3A-P2A-O5A
3	D	401	CAA	P1A-O3A-P2A-O4A
3	C	401	CAA	C3P-C2P-S1P-C1
3	F	401	CAA	C3P-C2P-S1P-C1
2	A	301	NAD	C5D-O5D-PN-O1N
2	D	402	NAD	C5D-O5D-PN-O1N
2	E	301	NAD	C5D-O5D-PN-O1N
3	C	401	CAA	CCP-O6A-P2A-O4A
3	C	401	CAA	CCP-O6A-P2A-O5A
2	A	301	NAD	C4B-C5B-O5B-PA
3	F	401	CAA	O4B-C1B-N9A-C8A
2	B	301	NAD	C4B-C5B-O5B-PA
2	B	301	NAD	PA-O3-PN-O2N
2	D	402	NAD	PA-O3-PN-O2N
3	A	302	CAA	C4B-C5B-O5B-P1A
2	B	301	NAD	C2D-C1D-N1N-C2N
2	D	402	NAD	C2D-C1D-N1N-C2N
2	E	301	NAD	C2D-C1D-N1N-C2N
3	D	401	CAA	C4B-C5B-O5B-P1A
2	A	301	NAD	PN-O3-PA-O1A
3	F	401	CAA	P1A-O3A-P2A-O4A
3	C	401	CAA	C4B-C5B-O5B-P1A
3	F	401	CAA	C4B-C5B-O5B-P1A

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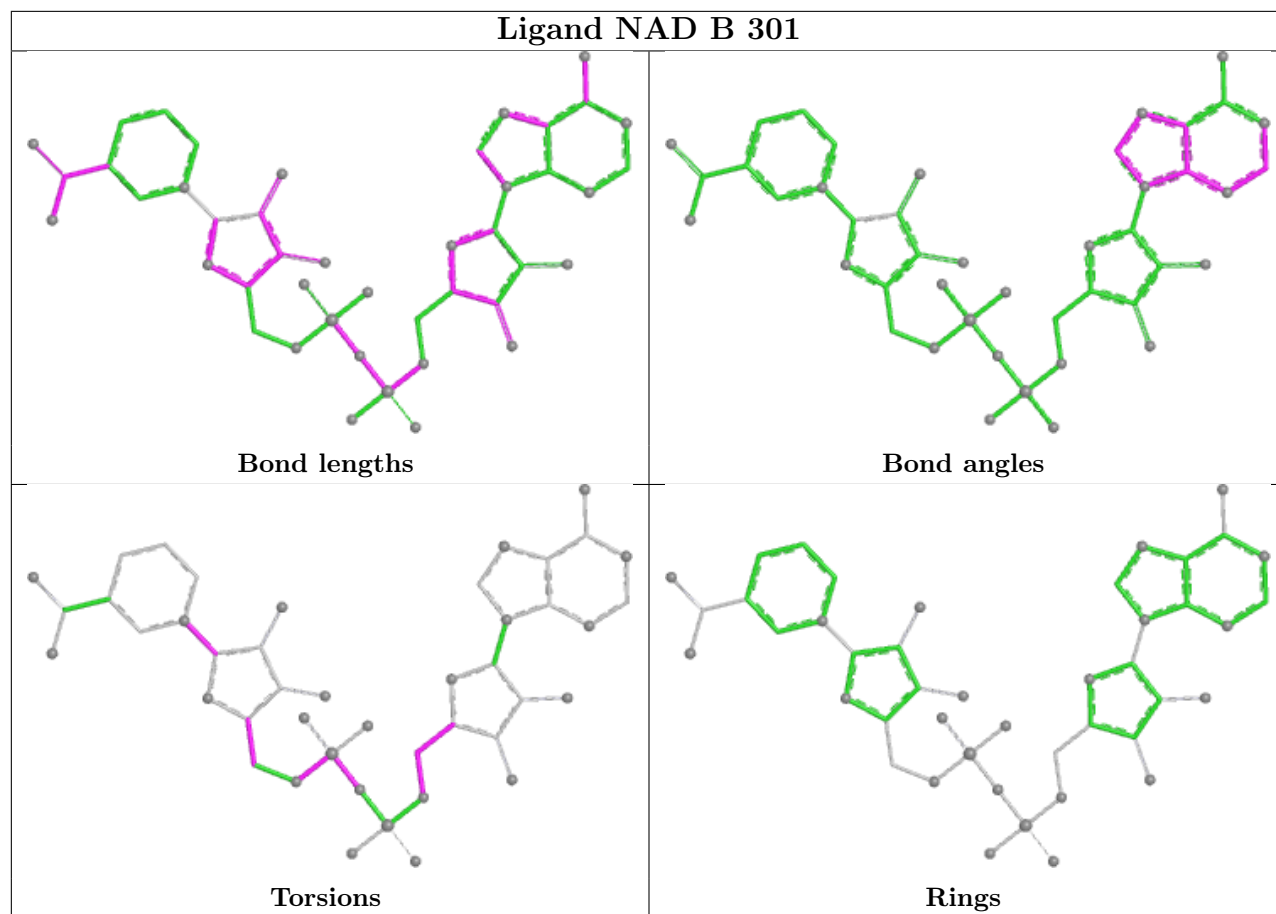
Mol	Chain	Res	Type	Atoms
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2	B	301	NAD	PA-O3-PN-O1N
2	A	301	NAD	PA-O3-PN-O2N
2	D	402	NAD	PA-O3-PN-O1N
2	E	301	NAD	PA-O3-PN-O2N
3	C	401	CAA	P1A-O3A-P2A-O4A
2	B	301	NAD	O4B-C4B-C5B-O5B
2	A	301	NAD	O4B-C4B-C5B-O5B
3	D	401	CAA	C3P-C2P-S1P-C1
2	D	402	NAD	O4B-C4B-C5B-O5B
2	A	301	NAD	PA-O3-PN-O1N
2	E	301	NAD	PA-O3-PN-O1N
3	D	401	CAA	P1A-O3A-P2A-O5A
3	F	401	CAA	P1A-O3A-P2A-O5A

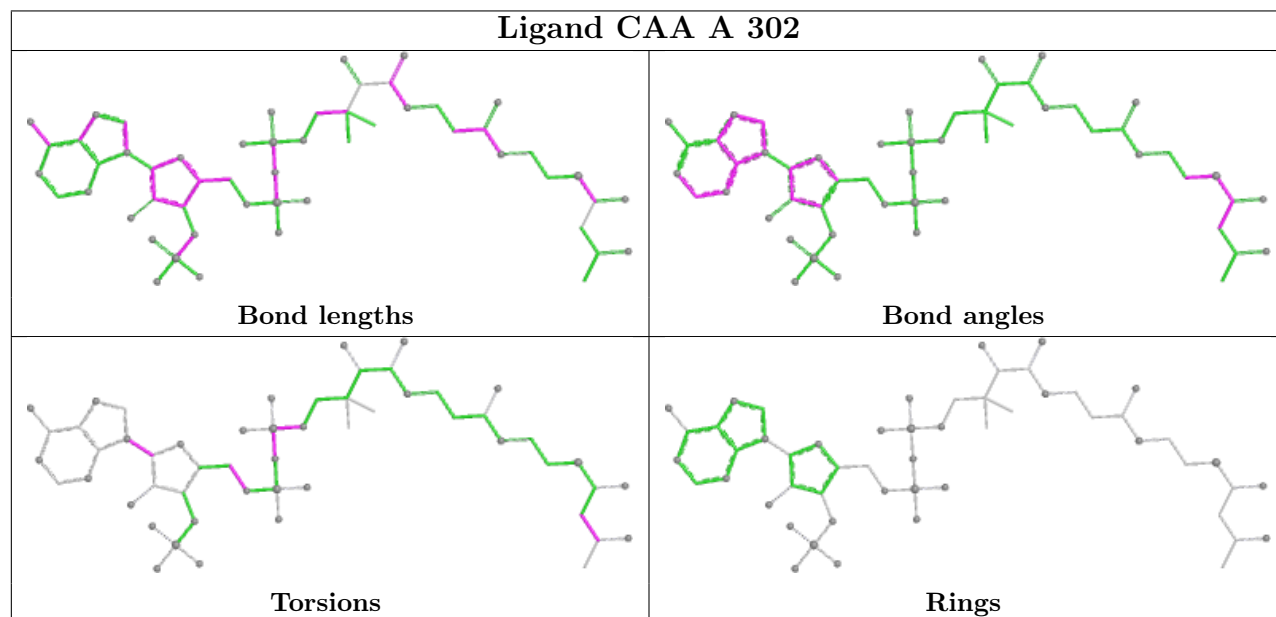
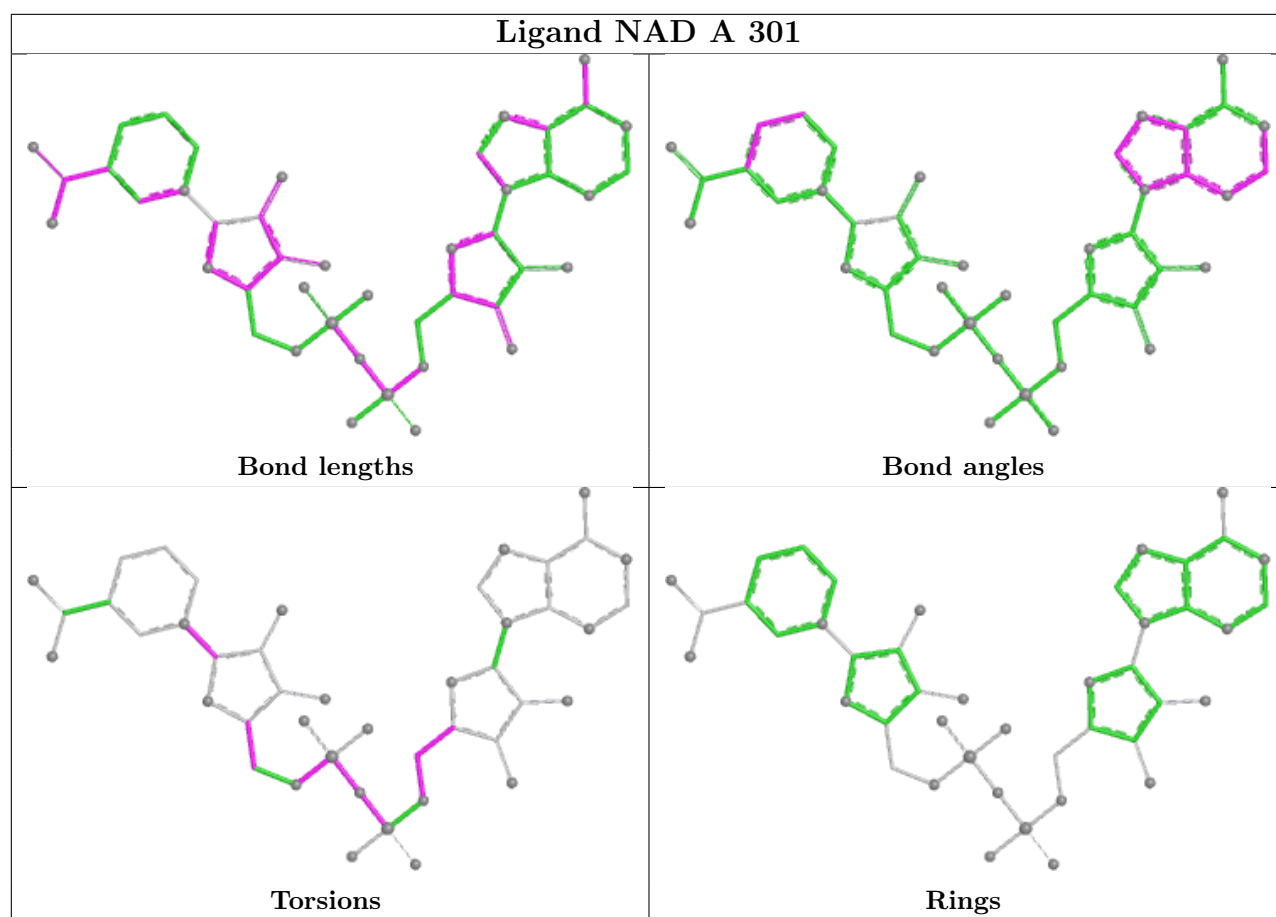
There are no ring outliers.

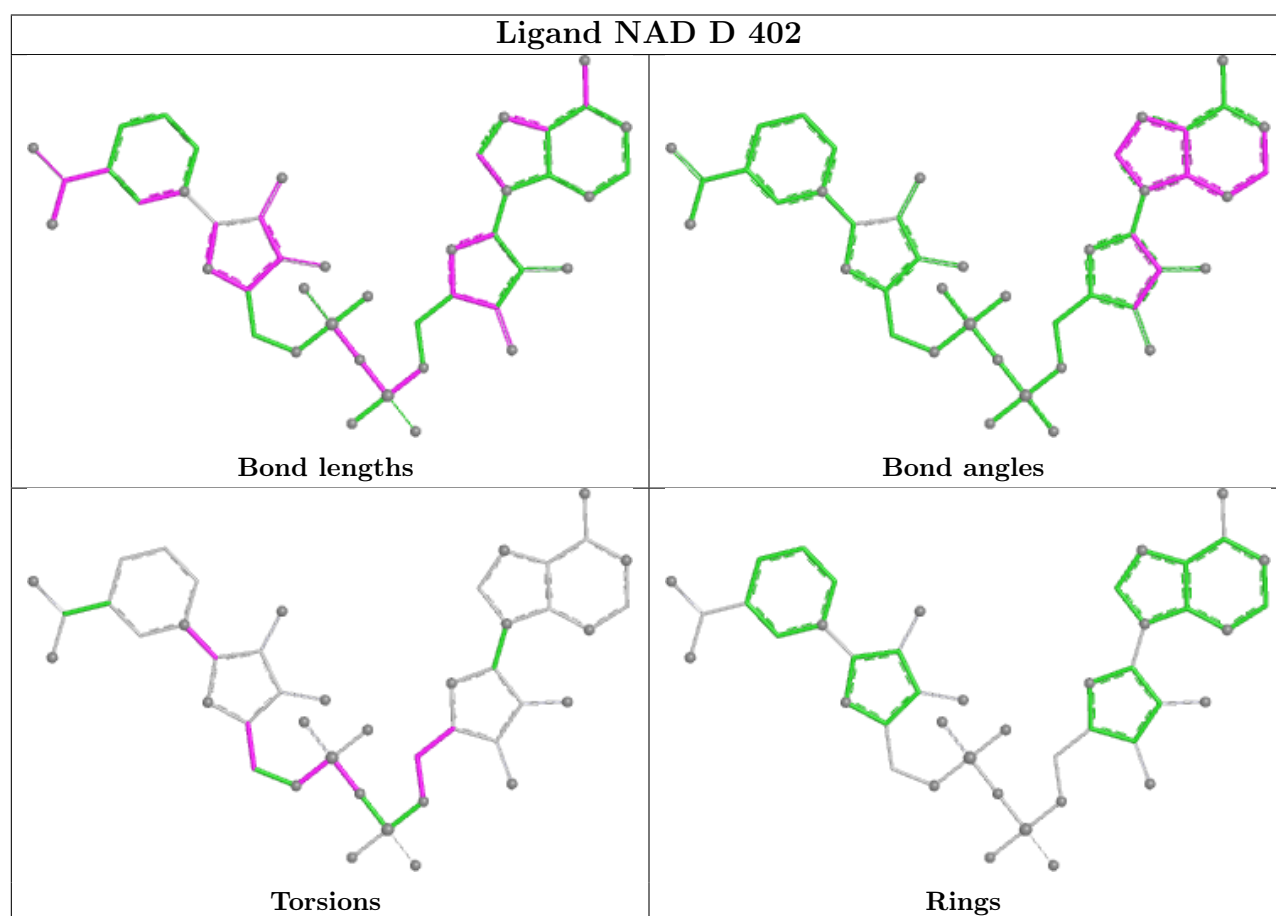
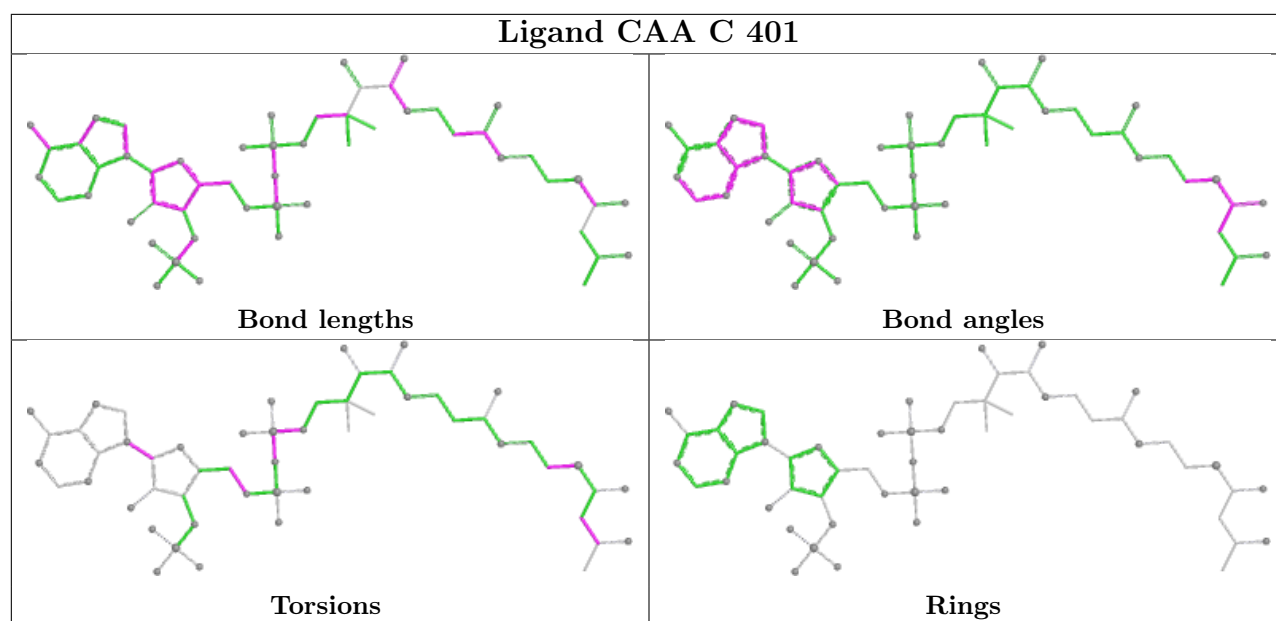
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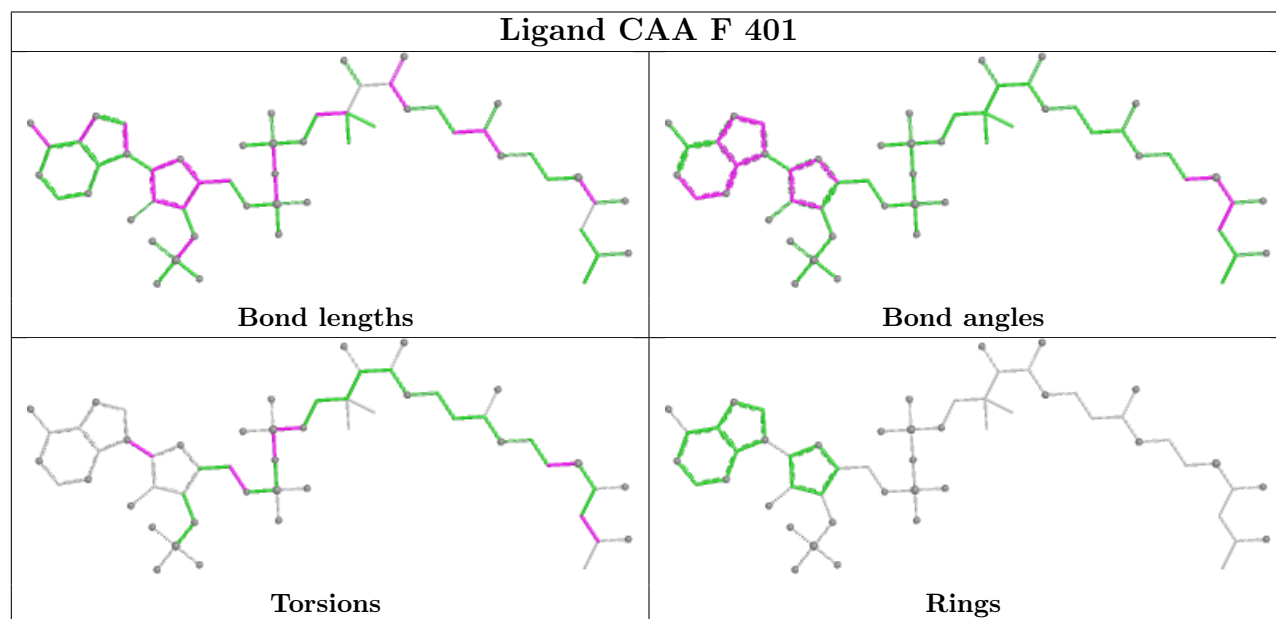
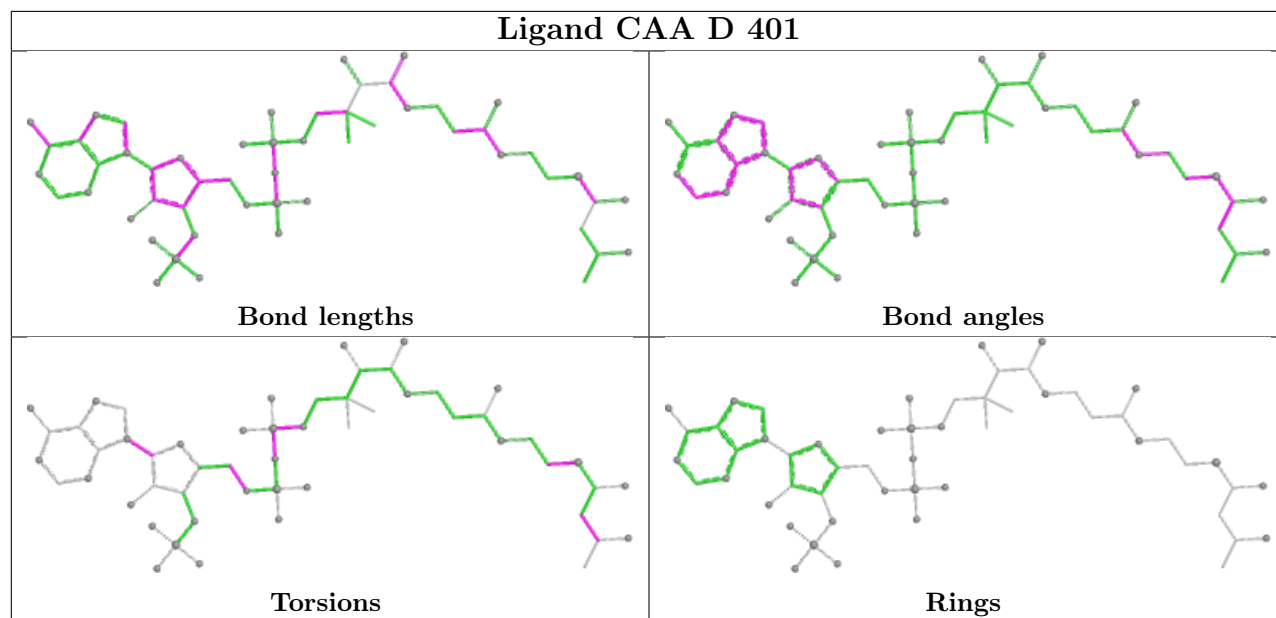
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NAD	2	0
2	A	301	NAD	3	0
3	A	302	CAA	4	0
3	C	401	CAA	2	0
2	D	402	NAD	2	0
3	D	401	CAA	2	0
3	F	401	CAA	1	0
2	E	301	NAD	2	0

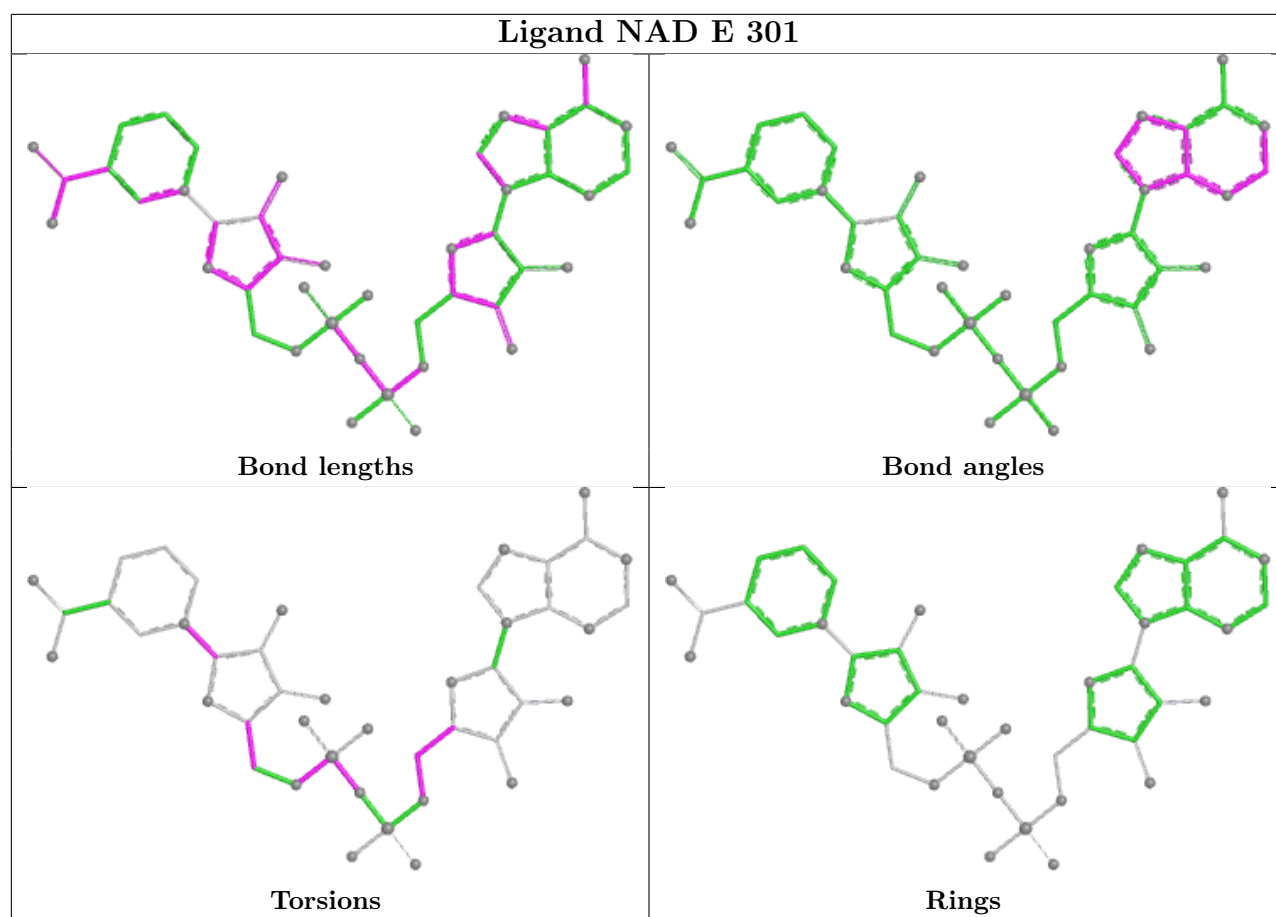
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	289/290 (99%)	-0.25	2 (0%) 84 70	30, 87, 135, 150	0
1	B	289/290 (99%)	-0.28	3 (1%) 79 63	32, 78, 131, 148	0
1	C	289/290 (99%)	0.27	24 (8%) 17 13	29, 106, 185, 201	0
1	D	289/290 (99%)	-0.03	4 (1%) 73 55	36, 89, 146, 162	0
1	E	289/290 (99%)	-0.03	4 (1%) 73 55	35, 85, 129, 164	0
1	F	289/290 (99%)	0.15	7 (2%) 59 40	49, 110, 174, 191	0
All	All	1734/1740 (99%)	-0.03	44 (2%) 58 39	29, 89, 166, 201	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	85	VAL	6.1
1	C	69	ILE	4.8
1	C	29	LEU	3.8
1	E	205	SER	3.6
1	C	106	CYS	3.1
1	E	71	PRO	3.1
1	D	53	ALA	3.0
1	C	51	LEU	2.9
1	D	69	ILE	2.9
1	C	20	ALA	2.9
1	C	65	ILE	2.8
1	F	41	LEU	2.8
1	C	27	VAL	2.7
1	C	70	THR	2.7
1	C	66	VAL	2.7
1	C	44	ILE	2.6
1	B	71	PRO	2.6
1	D	40	GLY	2.6
1	C	83	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	41	LEU	2.5
1	D	71	PRO	2.5
1	C	111	ILE	2.4
1	C	68	ALA	2.4
1	F	44	ILE	2.4
1	C	163	ILE	2.3
1	F	118	SER	2.3
1	B	65	ILE	2.3
1	C	28	ALA	2.3
1	E	70	THR	2.3
1	E	177	VAL	2.3
1	C	64	ALA	2.2
1	A	159	THR	2.2
1	C	5	VAL	2.2
1	A	71	PRO	2.2
1	F	6	ILE	2.2
1	C	47	GLY	2.1
1	F	66	VAL	2.1
1	B	69	ILE	2.1
1	C	166	ILE	2.1
1	F	32	ILE	2.1
1	C	77	LEU	2.1
1	C	62	ALA	2.1
1	F	71	PRO	2.1
1	C	160	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

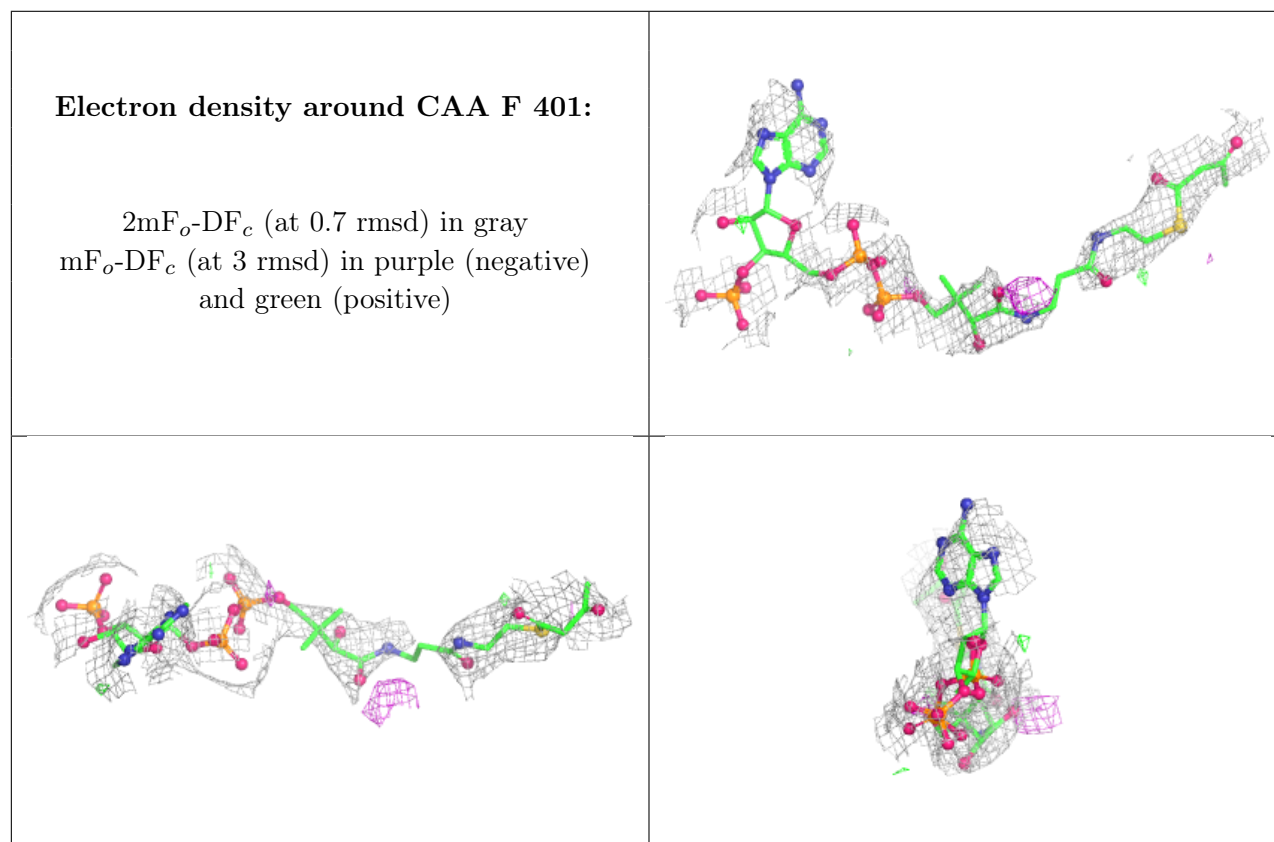
There are no oligosaccharides in this entry.

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.

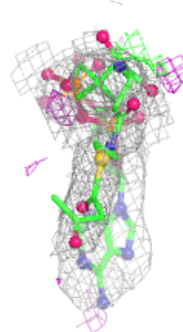
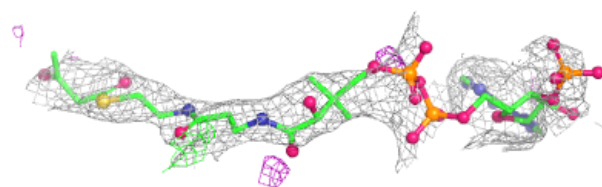
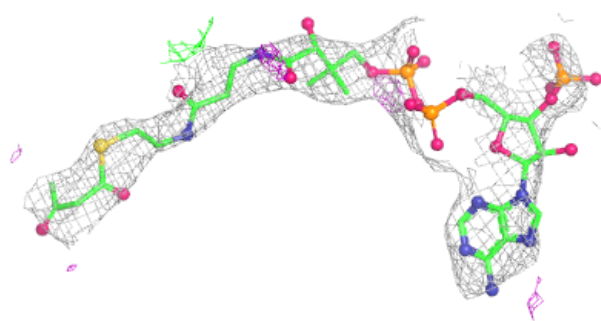
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CAA	F	401	54/54	0.80	0.10	61,122,139,144	0
3	CAA	A	302	54/54	0.81	0.10	69,126,160,168	0
2	NAD	D	402	44/44	0.81	0.10	84,104,126,136	0
3	CAA	D	401	54/54	0.85	0.09	51,121,157,171	0
2	NAD	B	301	44/44	0.88	0.09	68,86,99,113	0
3	CAA	C	401	54/54	0.89	0.09	56,135,162,172	0
2	NAD	A	301	44/44	0.90	0.07	61,83,99,103	0
2	NAD	E	301	44/44	0.91	0.08	53,80,92,104	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.

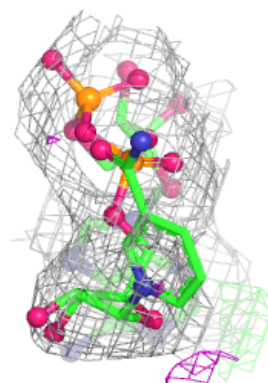
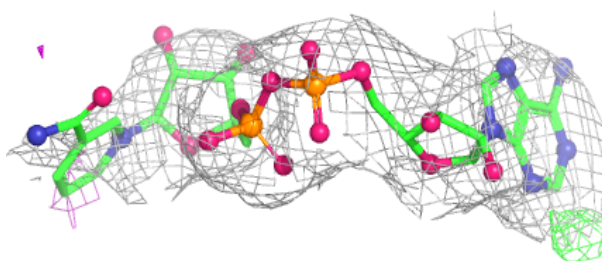
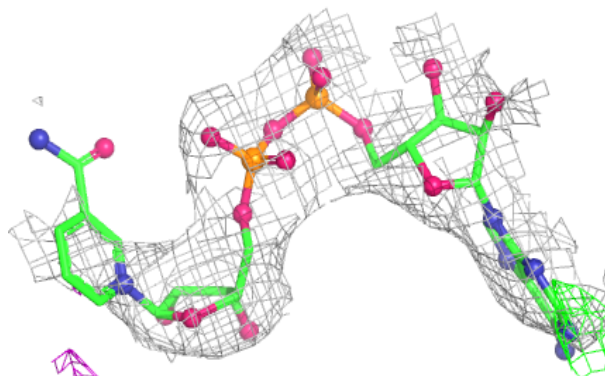


Electron density around CAA A 302:

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

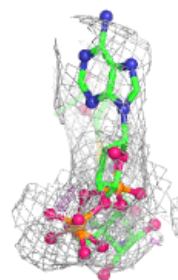
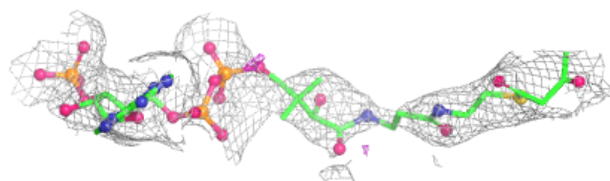
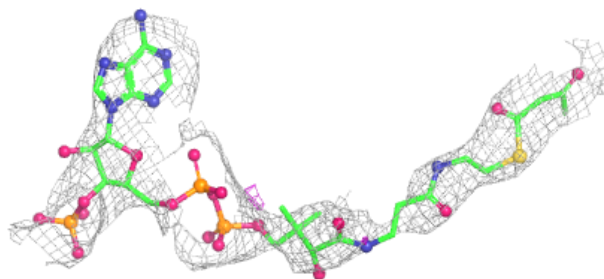
**Electron density around NAD D 402:**

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

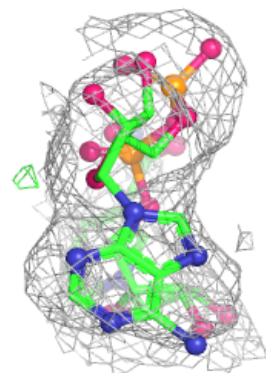
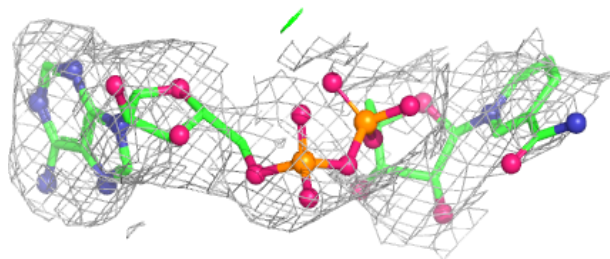
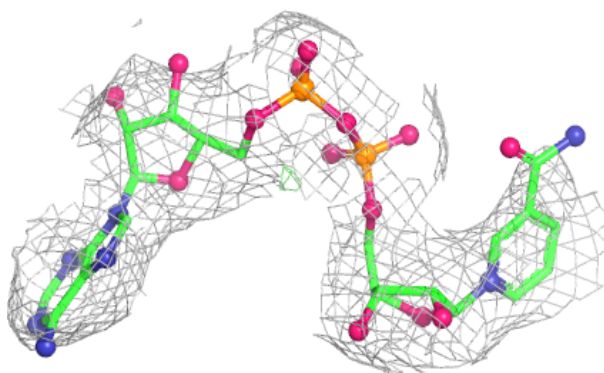


Electron density around CAA D 401:

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

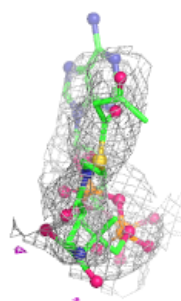
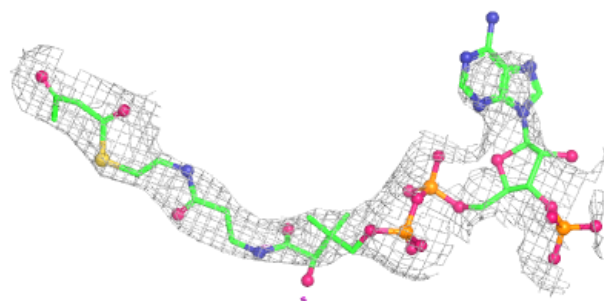
**Electron density around NAD B 301:**

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

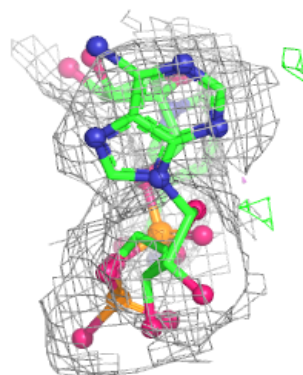
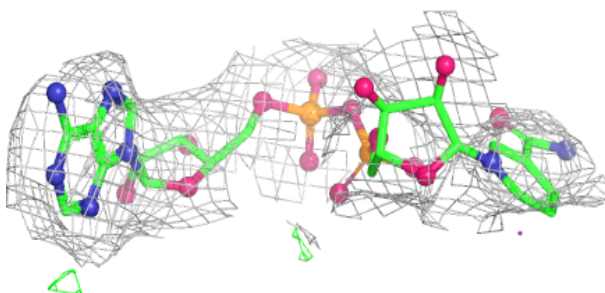
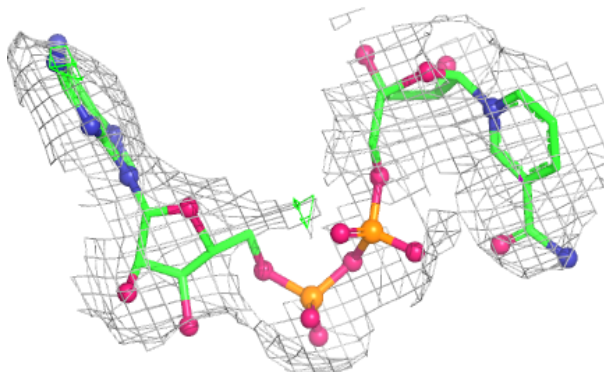


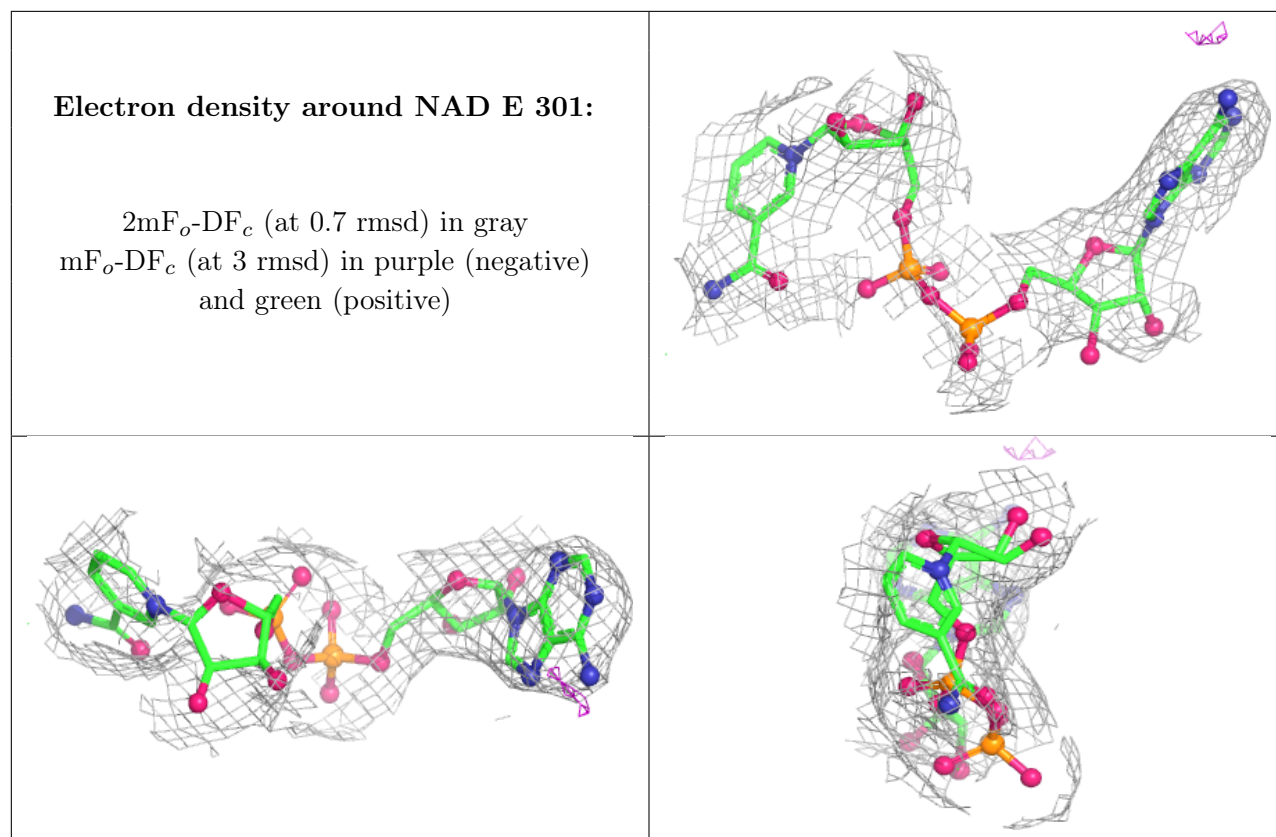
Electron density around CAA C 401:

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

**Electron density around NAD A 301:**

$2mF_o-DF_c$ (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.