



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:26 AM UTC

PDB ID : 5K4Q / pdb_00005k4q
Title : Three-dimensional structure of L-threonine 3-dehydrogenase from Trypanosoma brucei bound to NAD⁺ refined to 2.3 angstroms
Authors : Adjogatse, E.K.; Cooper, J.B.; Erskine, P.T.
Deposited on : 2016-05-21
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

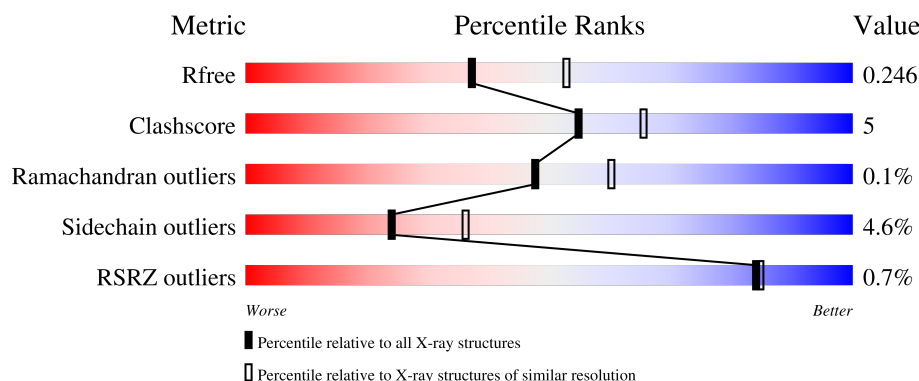
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	320	% 89% 10% .
1	B	320	89% 9% .
1	C	320	% 89% 9% .
1	D	320	% 84% 14% .
1	E	320	% 84% 15% .

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Mol	Chain	Length	Quality of chain
1	F	320	% 83% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	1402	-	-	X	-
3	GOL	C	3402	-	X	X	-
3	GOL	E	5402	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16257 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.

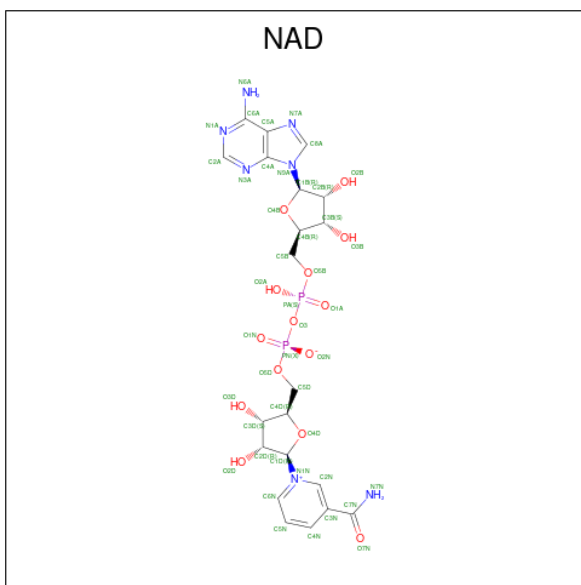
- Molecule 1 is a protein called L-threonine 3-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2501	1595	416	471	19			
1	B	319	Total	C	N	O	S	0	1	0
			2502	1595	417	472	18			
1	C	319	Total	C	N	O	S	0	0	0
			2493	1590	415	470	18			
1	D	320	Total	C	N	O	S	0	0	0
			2501	1595	416	471	19			
1	E	319	Total	C	N	O	S	0	1	0
			2502	1596	417	471	18			
1	F	319	Total	C	N	O	S	0	2	0
			2505	1600	417	470	18			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1002	MET	-	initiating methionine	UNP Q7YW97
B	2002	MET	-	initiating methionine	UNP Q7YW97
C	3002	MET	-	initiating methionine	UNP Q7YW97
D	4002	MET	-	initiating methionine	UNP Q7YW97
E	5002	MET	-	initiating methionine	UNP Q7YW97
F	6002	MET	-	initiating methionine	UNP Q7YW97

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



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

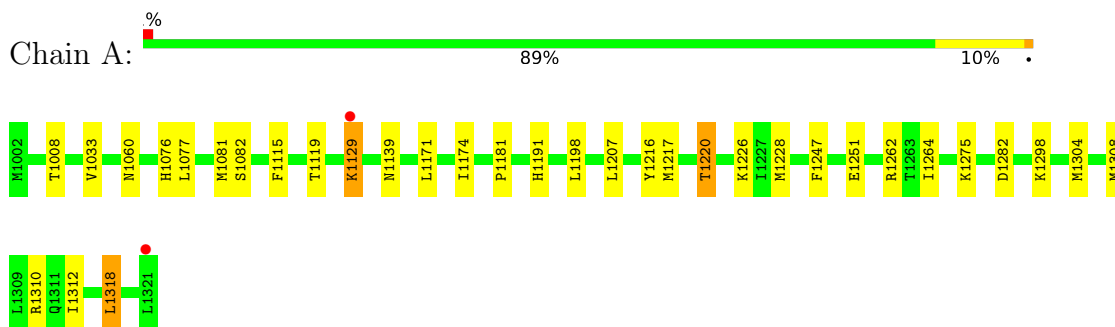
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	161	Total	O	0	0
			161	161		
5	B	168	Total	O	0	0
			168	168		
5	C	174	Total	O	0	0
			174	174		
5	D	143	Total	O	0	0
			143	143		
5	E	131	Total	O	0	0
			131	131		
5	F	151	Total	O	0	0
			151	151		

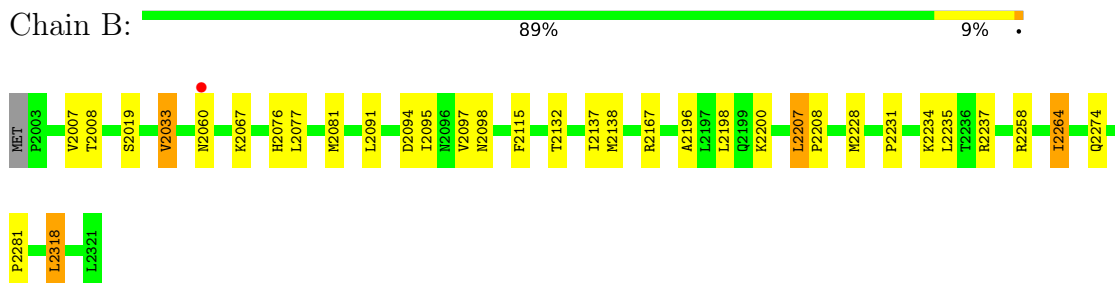
3 Residue-property plots [i](#)

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.

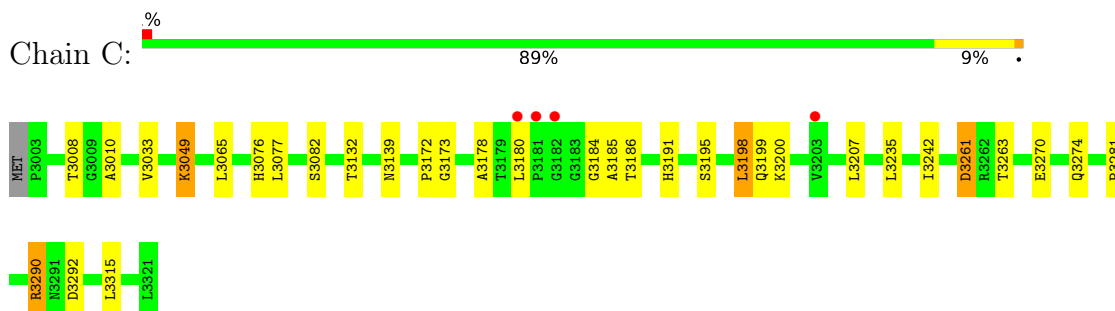
- Molecule 1: L-threonine 3-dehydrogenase



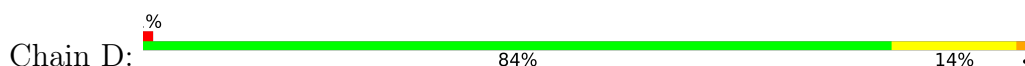
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- Molecule 1: L-threonine 3-dehydrogenase

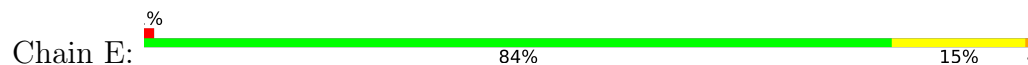


- Molecule 1: L-threonine 3-dehydrogenase

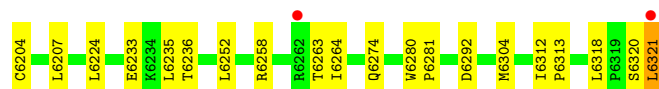
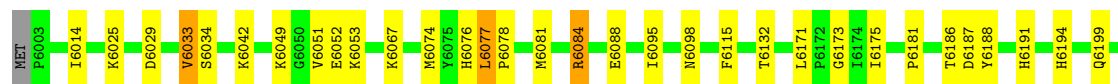
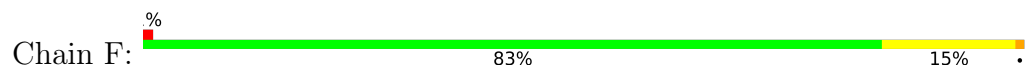




• Molecule 1: L-threonine 3-dehydrogenase



• Molecule 1: L-threonine 3-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.63Å 277.72Å 56.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.30 48.14 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.14-2.30) 99.2 (48.14-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.174 , 0.244 0.180 , 0.246	Depositor DCC
R_{free} test set	4653 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16257	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.63 % 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 1.0728e-03. 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: 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	0.98	0/2557	1.10	4/3469 (0.1%)
1	B	1.02	0/2558	1.07	5/3470 (0.1%)
1	C	0.95	0/2549	1.08	3/3458 (0.1%)
1	D	1.00	1/2557 (0.0%)	1.07	6/3469 (0.2%)
1	E	0.94	1/2558 (0.0%)	1.04	8/3469 (0.2%)
1	F	1.01	0/2567	1.05	6/3480 (0.2%)
All	All	0.98	2/15346 (0.0%)	1.07	32/20815 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4312	ILE	CA-CB	7.11	1.58	1.54
1	E	5212	LEU	CA-C	-5.03	1.47	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1077	LEU	CA-C-N	-13.06	106.70	119.76
1	A	1077	LEU	C-N-CA	-13.06	106.70	119.76
1	B	2077	LEU	CA-C-N	-12.06	107.69	119.76
1	B	2077	LEU	C-N-CA	-12.06	107.69	119.76
1	E	5077	LEU	CA-C-N	-10.05	109.71	119.76
1	E	5077	LEU	C-N-CA	-10.05	109.71	119.76
1	A	1264	ILE	CB-CA-C	-8.14	99.55	111.68
1	F	6025	LYS	N-CA-C	6.84	118.81	111.36
1	C	3077	LEU	CA-C-N	-6.66	112.91	119.90
1	C	3077	LEU	C-N-CA	-6.66	112.91	119.90
1	F	6204	CYS	CA-C-N	6.37	126.49	119.87
1	F	6204	CYS	C-N-CA	6.37	126.49	119.87
1	B	2207	LEU	CA-C-N	6.27	126.18	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2207	LEU	C-N-CA	6.27	126.18	119.28
1	E	5271	GLY	CA-C-N	5.62	125.73	119.32
1	E	5271	GLY	C-N-CA	5.62	125.73	119.32
1	E	5005	VAL	N-CA-C	5.62	116.04	108.17
1	C	3292	ASP	N-CA-C	5.56	117.02	111.07
1	E	5217	MET	CA-C-N	-5.48	112.97	119.05
1	E	5217	MET	C-N-CA	-5.48	112.97	119.05
1	F	6077	LEU	N-CA-C	5.44	121.84	109.81
1	D	4171	LEU	CA-C-N	5.35	126.53	119.84
1	D	4171	LEU	C-N-CA	5.35	126.53	119.84
1	E	5093	MET	N-CA-C	5.26	116.70	111.07
1	B	2097	VAL	CB-CA-C	-5.22	105.64	111.80
1	D	4077	LEU	CA-C-N	-5.21	114.43	119.90
1	D	4077	LEU	C-N-CA	-5.21	114.43	119.90
1	D	4207	LEU	CA-C-N	5.20	125.50	119.47
1	D	4207	LEU	C-N-CA	5.20	125.50	119.47
1	F	6095	ILE	CB-CA-C	-5.20	105.21	112.02
1	F	6098	ASN	N-CA-C	5.08	116.89	111.36
1	A	1282	ASP	N-CA-C	-5.02	105.90	112.23

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	2501	0	2512	20	0
1	B	2502	0	2511	19	0
1	C	2493	0	2504	21	0
1	D	2501	0	2512	27	0
1	E	2502	0	2516	32	0
1	F	2505	0	2530	27	0
2	A	44	0	26	2	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	44	0	26	0	0
2	F	44	0	26	1	0
3	A	6	0	8	4	0
3	B	6	0	8	1	0
3	C	6	0	8	7	0
3	D	6	0	8	3	0
3	E	6	0	8	4	0
3	F	6	0	8	1	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
4	F	5	0	0	0	0
5	A	161	0	0	3	0
5	B	168	0	0	2	0
5	C	174	0	0	1	0
5	D	143	0	0	3	0
5	E	131	0	0	7	0
5	F	151	0	0	3	0
All	All	16257	0	15289	148	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 5.

All (148) 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:E:5210:GLU:HG3	5:E:5502:HOH:O	1.52	1.08
1:E:5175:ILE:HD11	1:E:5214:MET:HE3	1.44	0.99
1:E:5175:ILE:HD11	1:E:5214:MET:CE	2.01	0.89
1:D:4181:PRO:HB2	1:D:4191:HIS:CE1	2.11	0.84
1:E:5179:THR:OG1	5:E:5501:HOH:O	1.93	0.84
1:E:5175:ILE:CD1	1:E:5214:MET:HE3	2.11	0.81
1:D:4233:GLU:OE2	5:D:4501:HOH:O	2.06	0.73
1:A:1217:MET:HA	1:A:1220:THR:HG23	1.70	0.72
1:C:3184:GLY:CA	3:C:3402:GOL:H12	2.21	0.70
1:F:6074:MET:HE2	1:F:6076:HIS:HB2	1.73	0.70
1:E:5185:ALA:H	3:E:5402:GOL:H12	1.58	0.68
1:E:5214:MET:HE2	1:E:5247:PHE:CZ	2.28	0.68
1:C:3184:GLY:HA2	3:C:3402:GOL:H12	1.75	0.67
1:D:4207:LEU:H	1:D:4274:GLN:NE2	1.92	0.67
1:C:3082:SER:OG	3:C:3402:GOL:H31	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2264:ILE:HD12	5:B:2593:HOH:O	1.96	0.66
1:D:4082:SER:H	3:D:4402:GOL:H11	1.62	0.65
1:B:2258:ARG:NH1	5:B:2503:HOH:O	2.30	0.65
1:D:4182:GLY:O	1:D:4191:HIS:HE1	1.81	0.63
1:E:5101:ARG:CZ	5:E:5505:HOH:O	2.46	0.63
1:D:4002:MET:HB2	1:D:4003:PRO:HD2	1.81	0.62
1:C:3184:GLY:HA2	3:C:3402:GOL:C1	2.30	0.61
1:A:1181:PRO:HB2	1:A:1191:HIS:CE1	2.36	0.60
1:D:4257:GLU:OE1	5:D:4502:HOH:O	2.15	0.60
1:F:6084:ARG:HD2	1:F:6088:GLU:OE1	2.03	0.59
1:A:1082:SER:HB3	3:A:1402:GOL:O2	2.03	0.58
1:C:3198:LEU:HB3	1:C:3200:LYS:HG3	1.85	0.58
1:F:6033:VAL:CG2	1:F:6051:VAL:HG22	2.33	0.58
1:E:5210:GLU:CG	5:E:5502:HOH:O	2.27	0.57
1:C:3172:PRO:HD3	1:C:3242:ILE:O	2.05	0.57
1:D:4187:ASP:HB2	5:D:4594:HOH:O	2.05	0.57
1:B:2007:VAL:HB	1:B:2033:VAL:HG22	1.87	0.57
1:B:2198:LEU:HD21	1:B:2318:LEU:HD13	1.86	0.56
1:E:5101:ARG:NE	5:E:5505:HOH:O	2.39	0.56
1:A:1129:LYS:HD2	1:A:1129:LYS:H	1.71	0.56
1:B:2081:MET:HB3	3:B:2402:GOL:H12	1.88	0.55
1:C:3184:GLY:HA3	3:C:3402:GOL:H12	1.87	0.55
1:F:6194:HIS:CD2	1:F:6312:ILE:HD13	2.42	0.55
1:E:5184:GLY:O	1:E:5187:ASP:HB2	2.06	0.54
1:B:2091:LEU:HD11	1:B:2095:ILE:HD11	1.89	0.54
1:A:1082:SER:CB	3:A:1402:GOL:O2	2.55	0.54
1:E:5210:GLU:CD	5:E:5502:HOH:O	2.49	0.52
1:C:3207:LEU:H	1:C:3274:GLN:NE2	2.06	0.52
1:B:2132:THR:OG1	1:B:2281:PRO:HB3	2.09	0.52
1:F:6033:VAL:HG22	1:F:6051:VAL:HG22	1.91	0.52
1:F:6181:PRO:HB2	1:F:6191:HIS:NE2	2.26	0.51
1:E:5207:LEU:H	1:E:5274:GLN:NE2	2.09	0.51
1:A:1198:LEU:HD21	1:A:1318:LEU:HD13	1.93	0.51
1:B:2198:LEU:CD2	1:B:2318:LEU:HD13	2.41	0.51
1:C:3185:ALA:HB3	3:C:3402:GOL:H32	1.92	0.51
1:D:4216:TYR:CD1	1:D:4304:MET:HG3	2.46	0.51
1:B:2196:ALA:HA	1:B:2264:ILE:HD13	1.93	0.50
1:D:4309:LEU:HB3	1:D:4321:LEU:HD11	1.94	0.50
1:C:3173:GLY:HA3	1:C:3186:THR:HG21	1.93	0.50
1:F:6187:ASP:HB2	5:F:6560:HOH:O	2.11	0.50
1:E:5176:SER:OG	1:E:5217:MET:HE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3290:ARG:HH11	1:C:3290:ARG:CG	2.25	0.49
1:E:5214:MET:HE2	1:E:5247:PHE:HZ	1.77	0.49
1:E:5180:LEU:HD23	1:E:5316:HIS:CD2	2.47	0.49
1:E:5045:LEU:HA	1:E:5048:LEU:HD12	1.94	0.49
1:B:2008:THR:OG1	1:B:2076:HIS:HA	2.12	0.49
1:F:6280:TRP:HB3	1:F:6281:PRO:HD2	1.94	0.49
1:F:6081:MET:HE2	3:F:6402:GOL:H32	1.95	0.48
1:C:3270:GLU:HG3	1:C:3274:GLN:CB	2.43	0.48
1:D:4081:MET:HE2	3:D:4402:GOL:H31	1.95	0.48
1:F:6115:PHE:CZ	1:F:6224:LEU:CD2	2.97	0.48
1:D:4217:MET:N	1:D:4218:PRO:CD	2.77	0.48
1:A:1082:SER:CB	3:A:1402:GOL:HO2	2.27	0.47
1:F:6188:TYR:CD1	1:F:6188:TYR:C	2.93	0.47
1:F:6187:ASP:CB	5:F:6560:HOH:O	2.63	0.47
1:C:3290:ARG:NH2	5:C:3509:HOH:O	2.47	0.46
1:F:6132:THR:OG1	1:F:6281:PRO:HB3	2.15	0.46
1:D:4082:SER:N	3:D:4402:GOL:H11	2.28	0.46
1:F:6320:SER:O	1:F:6321:LEU:C	2.58	0.46
1:B:2207:LEU:HB3	1:B:2208:PRO:HD2	1.97	0.46
1:F:6074:MET:CE	1:F:6076:HIS:HB2	2.42	0.46
1:A:1008:THR:OG1	1:A:1076:HIS:HA	2.16	0.46
1:A:1081:MET:HE1	5:A:1516:HOH:O	2.15	0.46
1:B:2115:PHE:HA	1:B:2167:ARG:O	2.16	0.46
1:E:5185:ALA:HB3	3:E:5402:GOL:O2	2.16	0.46
1:B:2115:PHE:CD1	1:B:2115:PHE:C	2.95	0.45
1:C:3132:THR:OG1	1:C:3281:PRO:HB3	2.16	0.45
1:E:5269:VAL:O	1:E:5269:VAL:CG2	2.64	0.45
1:A:1174:ILE:HD12	1:A:1220:THR:HG21	1.98	0.45
1:B:2094:ASP:O	1:B:2098:ASN:HB2	2.16	0.45
1:E:5280:TRP:HH2	3:E:5402:GOL:H31	1.82	0.45
3:A:1402:GOL:C3	5:A:1571:HOH:O	2.65	0.45
1:A:1207:LEU:HD23	1:A:1207:LEU:HA	1.85	0.45
1:F:6207:LEU:H	1:F:6274:GLN:NE2	2.15	0.45
1:D:4205:PRO:HA	1:D:4269:VAL:O	2.17	0.44
1:F:6181:PRO:HB2	1:F:6191:HIS:CD2	2.51	0.44
1:A:1129:LYS:H	1:A:1129:LYS:CD	2.29	0.44
1:B:2115:PHE:HB2	1:B:2228:MET:SD	2.57	0.44
1:E:5139:ASN:O	1:E:5139:ASN:CG	2.60	0.44
1:F:6258:ARG:NH1	5:F:6511:HOH:O	2.48	0.44
1:B:2207:LEU:H	1:B:2274:GLN:NE2	2.16	0.44
1:A:1198:LEU:HG	1:A:1318:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4260:THR:HG22	1:D:4321:LEU:CD2	2.48	0.44
1:F:6033:VAL:O	1:F:6051:VAL:HA	2.18	0.44
1:E:5173:GLY:HA3	1:E:5186:THR:HG21	2.00	0.44
1:D:4203:VAL:HG23	1:D:4203:VAL:O	2.18	0.43
1:E:5185:ALA:N	3:E:5402:GOL:H12	2.29	0.43
1:B:2137:ILE:C	1:B:2138:MET:HG3	2.44	0.43
1:D:4008:THR:OG1	1:D:4076:HIS:HA	2.18	0.43
1:D:4262:ARG:HA	1:D:4262:ARG:HE	1.83	0.43
1:E:5210:GLU:OE1	5:E:5502:HOH:O	2.21	0.43
1:A:1216:TYR:CD1	1:A:1304:MET:HG3	2.54	0.43
1:D:4033:VAL:HG22	1:D:4051:VAL:HB	2.00	0.43
1:A:1308:MET:HE3	1:A:1312:ILE:HD11	2.01	0.43
1:C:3008:THR:OG1	1:C:3076:HIS:HA	2.19	0.43
1:E:5135:ASP:CG	1:E:5237:ARG:HH22	2.26	0.43
1:F:6312:ILE:HB	1:F:6313:PRO:HD3	2.01	0.43
1:F:6175:ILE:HG21	1:F:6304:MET:SD	2.58	0.43
1:C:3270:GLU:HG3	1:C:3274:GLN:HB3	2.00	0.42
1:D:4258:ARG:NH1	1:D:4302:ASP:OD2	2.52	0.42
1:D:4312:ILE:HB	1:D:4313:PRO:HD3	2.01	0.42
1:E:5207:LEU:HG	1:E:5274:GLN:HG2	2.00	0.42
1:C:3010:ALA:CB	1:C:3033:VAL:HG13	2.50	0.42
1:F:6077:LEU:N	1:F:6078:PRO:HD3	2.34	0.42
1:F:6171:LEU:HB2	2:F:6401:NAD:C5N	2.49	0.42
1:A:1139:ASN:O	1:A:1139:ASN:CG	2.62	0.42
1:F:6236:THR:OG1	1:F:6292:ASP:OD2	2.31	0.42
1:E:5312:ILE:N	1:E:5313:PRO:CD	2.83	0.42
1:F:6173:GLY:HA3	1:F:6186:THR:HG21	2.02	0.42
1:E:5222:ASN:O	1:E:5226:LYS:HB2	2.19	0.42
1:A:1181:PRO:HG2	1:A:1191:HIS:CD2	2.54	0.42
2:A:1401:NAD:H2A	5:A:1583:HOH:O	2.19	0.42
1:D:4033:VAL:O	1:D:4051:VAL:HA	2.20	0.42
1:C:3178:ALA:HA	1:C:3315:LEU:HD13	2.02	0.41
1:C:3139:ASN:O	1:C:3139:ASN:CG	2.63	0.41
1:A:1247:PHE:HA	1:A:1251:GLU:OE2	2.20	0.41
1:C:3049:LYS:O	1:C:3049:LYS:HE2	2.20	0.41
1:D:4081:MET:HE3	2:D:4401:NAD:H2D	2.03	0.41
1:A:1115:PHE:HB2	1:A:1228:MET:SD	2.61	0.41
1:B:2019:SER:OG	1:B:2033:VAL:HG21	2.20	0.41
1:E:5032:LEU:HD11	1:E:5052:GLU:HG2	2.03	0.41
1:E:5280:TRP:HB3	1:E:5281:PRO:HD2	2.01	0.41
1:A:1171:LEU:HB2	2:A:1401:NAD:C5N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5115:PHE:CD1	1:E:5115:PHE:C	2.98	0.41
1:F:6034:SER:HA	1:F:6052:GLU:O	2.20	0.41
1:D:4260:THR:HG22	1:D:4321:LEU:HD22	2.02	0.41
1:E:5176:SER:OG	1:E:5217:MET:HB2	2.20	0.41
1:C:3082:SER:OG	3:C:3402:GOL:C3	2.66	0.40
1:D:4159:ARG:HA	1:D:4164:VAL:O	2.21	0.40
1:D:4173:GLY:HA3	1:D:4186:THR:HG21	2.03	0.40
1:B:2231:PRO:HD2	1:B:2234:LYS:HE3	2.03	0.40
1:F:6233:GLU:CD	1:F:6233:GLU:H	2.29	0.40
1:D:4132:THR:OG1	1:D:4281:PRO:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	318/320 (99%)	312 (98%)	6 (2%)	0	100	100
1	B	318/320 (99%)	311 (98%)	7 (2%)	0	100	100
1	C	317/320 (99%)	308 (97%)	8 (2%)	1 (0%)	36	46
1	D	318/320 (99%)	309 (97%)	9 (3%)	0	100	100
1	E	318/320 (99%)	304 (96%)	13 (4%)	1 (0%)	36	46
1	F	319/320 (100%)	313 (98%)	6 (2%)	0	100	100
All	All	1908/1920 (99%)	1857 (97%)	49 (3%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3261	ASP
1	E	5320	SER

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	277/277 (100%)	266 (96%)	11 (4%)	28	42
1	B	277/277 (100%)	269 (97%)	8 (3%)	37	55
1	C	276/277 (100%)	265 (96%)	11 (4%)	28	42
1	D	277/277 (100%)	262 (95%)	15 (5%)	20	29
1	E	277/277 (100%)	261 (94%)	16 (6%)	18	26
1	F	278/277 (100%)	263 (95%)	15 (5%)	20	29
All	All	1662/1662 (100%)	1586 (95%)	76 (5%)	24	36

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1033	VAL
1	A	1060	ASN
1	A	1119	THR
1	A	1129	LYS
1	A	1220	THR
1	A	1226	LYS
1	A	1262	ARG
1	A	1275	LYS
1	A	1298	LYS
1	A	1310	ARG
1	A	1318	LEU
1	B	2033	VAL
1	B	2060	ASN
1	B	2067	LYS
1	B	2200	LYS
1	B	2235	LEU
1	B	2237	ARG
1	B	2264	ILE
1	B	2318	LEU
1	C	3049	LYS
1	C	3065	LEU
1	C	3180	LEU

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Mol	Chain	Res	Type
1	C	3191	HIS
1	C	3195	SER
1	C	3198	LEU
1	C	3199	GLN
1	C	3235	LEU
1	C	3261	ASP
1	C	3263	THR
1	C	3290	ARG
1	D	4030	SER
1	D	4033	VAL
1	D	4042	LYS
1	D	4049	LYS
1	D	4051	VAL
1	D	4057	LEU
1	D	4059	SER
1	D	4064	LYS
1	D	4119	THR
1	D	4200	LYS
1	D	4222	ASN
1	D	4235	LEU
1	D	4261	ASP
1	D	4262	ARG
1	D	4264	ILE
1	E	5011	LEU
1	E	5014	ILE
1	E	5025	LYS
1	E	5033	VAL
1	E	5059	SER
1	E	5067	LYS
1	E	5109	LYS
1	E	5119	THR
1	E	5129	LYS
1	E	5179	THR
1	E	5222	ASN
1	E	5235	LEU
1	E	5258	ARG
1	E	5263	THR
1	E	5269	VAL
1	E	5275	LYS
1	F	6014	ILE
1	F	6029	ASP
1	F	6033	VAL

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Mol	Chain	Res	Type
1	F	6042	LYS
1	F	6049	LYS
1	F	6053	LYS
1	F	6067	LYS
1	F	6084	ARG
1	F	6199	GLN
1	F	6235	LEU
1	F	6252	LEU
1	F	6263	THR
1	F	6264	ILE
1	F	6318	LEU
1	F	6321	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1191	HIS
1	A	1222	ASN
1	A	1296	GLN
1	B	2013	GLN
1	B	2274	GLN
1	B	2278	ASN
1	B	2288	ASN
1	C	3013	GLN
1	C	3199	GLN
1	C	3274	GLN
1	C	3278	ASN
1	C	3311	GLN
1	D	4191	HIS
1	D	4274	GLN
1	E	5278	ASN
1	F	6199	GLN
1	F	6274	GLN
1	F	6278	ASN
1	F	6311	GLN

5.3.3 RNA ⓘ

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](#)

17 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	GOL	E	5402	-	5,5,5	0.20	0	5,5,5	1.32	0
4	SO4	B	2403	-	4,4,4	0.55	0	6,6,6	0.24	0
2	NAD	D	4401	-	46,48,48	1.99	8 (17%)	64,73,73	1.86	13 (20%)
2	NAD	F	6401	-	46,48,48	2.07	6 (13%)	64,73,73	1.76	12 (18%)
2	NAD	A	1401	-	46,48,48	2.11	10 (21%)	64,73,73	1.81	12 (18%)
3	GOL	B	2402	-	5,5,5	0.93	0	5,5,5	2.08	3 (60%)
4	SO4	D	4404	-	4,4,4	0.51	0	6,6,6	0.19	0
3	GOL	F	6402	-	5,5,5	0.32	0	5,5,5	1.09	0
4	SO4	C	3403	-	4,4,4	0.46	0	6,6,6	0.12	0
4	SO4	F	6403	-	4,4,4	0.48	0	6,6,6	0.15	0
3	GOL	A	1402	-	5,5,5	0.74	0	5,5,5	0.88	0
3	GOL	C	3402	-	5,5,5	0.94	0	5,5,5	2.17	2 (40%)
4	SO4	D	4403	-	4,4,4	0.47	0	6,6,6	0.29	0
2	NAD	B	2401	-	46,48,48	2.02	10 (21%)	64,73,73	1.71	12 (18%)
3	GOL	D	4402	-	5,5,5	0.80	0	5,5,5	1.54	1 (20%)
2	NAD	E	5401	-	46,48,48	1.91	8 (17%)	64,73,73	1.80	15 (23%)
2	NAD	C	3401	-	46,48,48	1.65	7 (15%)	64,73,73	1.66	10 (15%)

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
3	GOL	E	5402	-	-	2/4/4/4	-
2	NAD	D	4401	-	-	0/30/62/62	0/5/5/5
2	NAD	F	6401	-	-	3/30/62/62	0/5/5/5
2	NAD	A	1401	-	-	1/30/62/62	0/5/5/5
3	GOL	B	2402	-	-	2/4/4/4	-
3	GOL	F	6402	-	-	4/4/4/4	-
3	GOL	A	1402	-	-	4/4/4/4	-
3	GOL	C	3402	-	-	4/4/4/4	-
2	NAD	B	2401	-	-	2/30/62/62	0/5/5/5
3	GOL	D	4402	-	-	0/4/4/4	-
2	NAD	E	5401	-	-	3/30/62/62	0/5/5/5
2	NAD	C	3401	-	-	4/30/62/62	0/5/5/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	6401	NAD	C2N-N1N	8.28	1.44	1.35
2	A	1401	NAD	C2N-N1N	8.13	1.43	1.35
2	D	4401	NAD	C2N-N1N	7.13	1.42	1.35
2	B	2401	NAD	O7N-C7N	6.98	1.37	1.24
2	F	6401	NAD	O7N-C7N	6.97	1.37	1.24
2	A	1401	NAD	O7N-C7N	6.52	1.36	1.24
2	D	4401	NAD	O7N-C7N	6.51	1.36	1.24
2	B	2401	NAD	PN-O3	6.02	1.66	1.59
2	E	5401	NAD	C2N-N1N	5.89	1.41	1.35
2	E	5401	NAD	O7N-C7N	5.77	1.34	1.24
2	C	3401	NAD	O7N-C7N	5.39	1.34	1.24
2	B	2401	NAD	C2N-N1N	5.07	1.40	1.35
2	C	3401	NAD	O4D-C1D	4.83	1.47	1.40
2	F	6401	NAD	PN-O3	4.66	1.64	1.59
2	D	4401	NAD	O4D-C1D	4.31	1.46	1.40
2	E	5401	NAD	O4D-C1D	4.20	1.46	1.40
2	E	5401	NAD	C3N-C7N	4.10	1.56	1.50
2	A	1401	NAD	PA-O3	4.08	1.63	1.59
2	C	3401	NAD	PN-O3	3.63	1.63	1.59
2	D	4401	NAD	C5A-N7A	-3.55	1.32	1.39
2	A	1401	NAD	C5A-N7A	-3.47	1.32	1.39
2	C	3401	NAD	C2N-N1N	3.47	1.38	1.35
2	B	2401	NAD	C6N-N1N	3.39	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2401	NAD	O4D-C1D	3.25	1.45	1.40
2	A	1401	NAD	C3N-C7N	3.04	1.55	1.50
2	D	4401	NAD	C8A-N9A	-3.00	1.32	1.37
2	B	2401	NAD	C5A-N7A	-2.80	1.34	1.39
2	E	5401	NAD	C6N-N1N	2.73	1.41	1.35
2	C	3401	NAD	C5A-N7A	-2.69	1.34	1.39
2	A	1401	NAD	C5D-C4D	2.68	1.59	1.51
2	D	4401	NAD	C4A-N9A	-2.63	1.32	1.37
2	F	6401	NAD	O4B-C1B	2.61	1.48	1.42
2	A	1401	NAD	C1B-N9A	2.52	1.53	1.46
2	E	5401	NAD	C3B-C4B	2.40	1.59	1.53
2	F	6401	NAD	C5A-N7A	-2.40	1.34	1.39
2	B	2401	NAD	C4A-N9A	-2.39	1.32	1.37
2	E	5401	NAD	C5A-N7A	-2.34	1.34	1.39
2	B	2401	NAD	O4B-C1B	2.31	1.47	1.42
2	D	4401	NAD	C2N-C3N	2.29	1.42	1.39
2	D	4401	NAD	O4B-C1B	-2.28	1.36	1.42
2	C	3401	NAD	C8A-N9A	-2.17	1.33	1.37
2	F	6401	NAD	C8A-N7A	2.14	1.35	1.31
2	A	1401	NAD	O4B-C1B	2.11	1.46	1.42
2	E	5401	NAD	PA-O3	-2.09	1.57	1.59
2	B	2401	NAD	C1B-N9A	2.08	1.52	1.46
2	A	1401	NAD	C6N-N1N	2.07	1.40	1.35
2	A	1401	NAD	PN-O2N	-2.06	1.45	1.55
2	B	2401	NAD	C3B-C4B	2.03	1.58	1.53
2	C	3401	NAD	C1B-N9A	2.03	1.51	1.46

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4401	NAD	C6N-N1N-C2N	-7.62	115.39	121.88
2	E	5401	NAD	N3A-C2A-N1A	-5.96	119.56	128.58
2	A	1401	NAD	O4B-C1B-N9A	5.78	119.20	108.09
2	A	1401	NAD	N3A-C2A-N1A	-5.21	120.69	128.58
2	F	6401	NAD	C5A-C4A-N3A	-5.19	119.57	126.72
2	C	3401	NAD	C6N-N1N-C2N	-4.91	117.70	121.88
2	F	6401	NAD	N3A-C2A-N1A	-4.87	121.21	128.58
2	D	4401	NAD	C5A-C4A-N3A	-4.76	120.17	126.72
2	A	1401	NAD	C5A-C4A-N3A	-4.60	120.39	126.72
2	F	6401	NAD	C6N-N1N-C2N	-4.48	118.07	121.88
2	B	2401	NAD	C3N-C7N-N7N	-4.44	112.26	117.74
2	C	3401	NAD	C5A-C4A-N3A	-4.43	120.61	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5401	NAD	C5A-C4A-N3A	-4.37	120.70	126.72
2	C	3401	NAD	N3A-C2A-N1A	-4.26	122.13	128.58
2	E	5401	NAD	C2A-N3A-C4A	4.22	122.13	111.83
2	B	2401	NAD	N3A-C2A-N1A	-4.17	122.28	128.58
2	B	2401	NAD	C5A-C4A-N3A	-4.13	121.03	126.72
2	B	2401	NAD	O7N-C7N-C3N	4.01	124.50	119.60
2	B	2401	NAD	N9A-C8A-N7A	-3.94	108.34	113.94
2	F	6401	NAD	N3A-C4A-N9A	3.79	133.61	127.17
2	E	5401	NAD	N9A-C8A-N7A	-3.69	108.70	113.94
2	A	1401	NAD	C2A-N3A-C4A	3.63	120.70	111.83
2	D	4401	NAD	C4A-C5A-N7A	-3.59	106.48	110.58
2	F	6401	NAD	C2A-N3A-C4A	3.52	120.44	111.83
2	E	5401	NAD	C6N-N1N-C2N	-3.46	118.93	121.88
2	F	6401	NAD	O4B-C1B-N9A	3.41	114.64	108.09
2	D	4401	NAD	N9A-C8A-N7A	-3.36	109.17	113.94
3	C	3402	GOL	O2-C2-C3	-3.33	95.41	109.18
2	C	3401	NAD	N3A-C4A-N9A	3.32	132.81	127.17
2	E	5401	NAD	N3A-C4A-N9A	3.32	132.81	127.17
2	C	3401	NAD	N9A-C8A-N7A	-3.22	109.36	113.94
2	D	4401	NAD	C5A-N7A-C8A	3.21	108.49	103.45
2	C	3401	NAD	C2A-N3A-C4A	3.13	119.47	111.83
2	B	2401	NAD	C2A-N3A-C4A	3.11	119.44	111.83
2	E	5401	NAD	C4A-N9A-C8A	3.09	108.98	105.74
2	F	6401	NAD	C5B-C4B-C3B	-3.09	104.10	115.21
2	B	2401	NAD	C5A-N7A-C8A	2.99	108.16	103.45
2	F	6401	NAD	C5N-C4N-C3N	-2.97	117.44	120.36
2	A	1401	NAD	C6N-N1N-C2N	-2.97	119.35	121.88
2	A	1401	NAD	N3A-C4A-N9A	2.95	132.18	127.17
2	B	2401	NAD	O4B-C1B-N9A	2.94	113.74	108.09
2	D	4401	NAD	N3A-C4A-N9A	2.94	132.17	127.17
2	A	1401	NAD	N9A-C8A-N7A	-2.91	109.81	113.94
3	C	3402	GOL	O1-C1-C2	2.90	123.42	110.38
2	B	2401	NAD	C4A-N9A-C8A	2.87	108.75	105.74
2	B	2401	NAD	N3A-C4A-N9A	2.86	132.03	127.17
2	D	4401	NAD	C5N-C4N-C3N	-2.81	117.61	120.36
2	C	3401	NAD	C4A-N9A-C8A	2.78	108.66	105.74
2	E	5401	NAD	O4B-C1B-N9A	2.78	113.42	108.09
2	C	3401	NAD	C5A-N7A-C8A	2.75	107.77	103.45
2	D	4401	NAD	N3A-C2A-N1A	-2.71	124.49	128.58
2	E	5401	NAD	C5A-N7A-C8A	2.70	107.70	103.45
2	D	4401	NAD	C2A-N3A-C4A	2.68	118.37	111.83
2	C	3401	NAD	O4B-C1B-N9A	2.66	113.20	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5401	NAD	O7N-C7N-C3N	2.62	122.80	119.60
2	C	3401	NAD	C4A-C5A-N7A	-2.59	107.62	110.58
2	A	1401	NAD	O2N-PN-O3	2.53	114.11	107.27
3	B	2402	GOL	O3-C3-C2	-2.50	99.11	110.38
2	F	6401	NAD	C4B-O4B-C1B	-2.50	103.95	109.47
2	D	4401	NAD	O7N-C7N-C3N	2.49	122.64	119.60
3	B	2402	GOL	O2-C2-C1	2.44	119.30	109.18
2	A	1401	NAD	C4D-O4D-C1D	-2.44	107.69	109.92
2	F	6401	NAD	C6N-C5N-C4N	2.43	122.95	119.45
2	B	2401	NAD	C4A-C5A-N7A	-2.41	107.83	110.58
3	B	2402	GOL	O2-C2-C3	-2.41	99.21	109.18
2	A	1401	NAD	O7N-C7N-C3N	2.38	122.51	119.60
2	D	4401	NAD	C4A-N9A-C8A	2.38	108.23	105.74
2	D	4401	NAD	C6N-C5N-C4N	2.34	122.83	119.45
2	B	2401	NAD	C2N-C3N-C4N	2.33	120.97	118.26
2	F	6401	NAD	O4D-C4D-C5D	-2.33	101.86	109.33
2	A	1401	NAD	C5A-N7A-C8A	2.33	107.11	103.45
2	D	4401	NAD	O4B-C4B-C5B	-2.29	101.99	109.33
2	E	5401	NAD	C6N-C5N-C4N	2.22	122.65	119.45
2	F	6401	NAD	N9A-C8A-N7A	-2.16	110.87	113.94
3	D	4402	GOL	O3-C3-C2	2.14	120.00	110.38
2	E	5401	NAD	C4A-C5A-N7A	-2.13	108.15	110.58
2	E	5401	NAD	C4D-O4D-C1D	-2.11	107.99	109.92
2	E	5401	NAD	C4A-N9A-C1B	-2.08	121.77	126.63
2	E	5401	NAD	O2N-PN-O1N	2.06	122.03	112.44
2	A	1401	NAD	O4B-C4B-C3B	2.03	109.18	105.15

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2401	NAD	C5D-O5D-PN-O1N
2	C	3401	NAD	C5D-O5D-PN-O3
2	C	3401	NAD	C5D-O5D-PN-O1N
2	E	5401	NAD	C5D-O5D-PN-O1N
2	F	6401	NAD	C5D-O5D-PN-O3
2	F	6401	NAD	C5D-O5D-PN-O1N
3	A	1402	GOL	C1-C2-C3-O3
3	B	2402	GOL	C1-C2-C3-O3
3	B	2402	GOL	O2-C2-C3-O3
3	C	3402	GOL	O1-C1-C2-O2
3	C	3402	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	E	5402	GOL	O1-C1-C2-C3
3	F	6402	GOL	O1-C1-C2-C3
3	F	6402	GOL	C1-C2-C3-O3
3	A	1402	GOL	O2-C2-C3-O3
3	A	1402	GOL	O1-C1-C2-C3
3	C	3402	GOL	O1-C1-C2-C3
3	C	3402	GOL	O2-C2-C3-O3
3	E	5402	GOL	O1-C1-C2-O2
3	F	6402	GOL	O1-C1-C2-O2
3	F	6402	GOL	O2-C2-C3-O3
3	A	1402	GOL	O1-C1-C2-O2
2	B	2401	NAD	C5D-O5D-PN-O3
2	C	3401	NAD	C5D-O5D-PN-O2N
2	E	5401	NAD	C5D-O5D-PN-O3
2	F	6401	NAD	C5D-O5D-PN-O2N
2	E	5401	NAD	O4B-C4B-C5B-O5B
2	A	1401	NAD	PN-O3-PA-O2A
2	C	3401	NAD	O4B-C4B-C5B-O5B

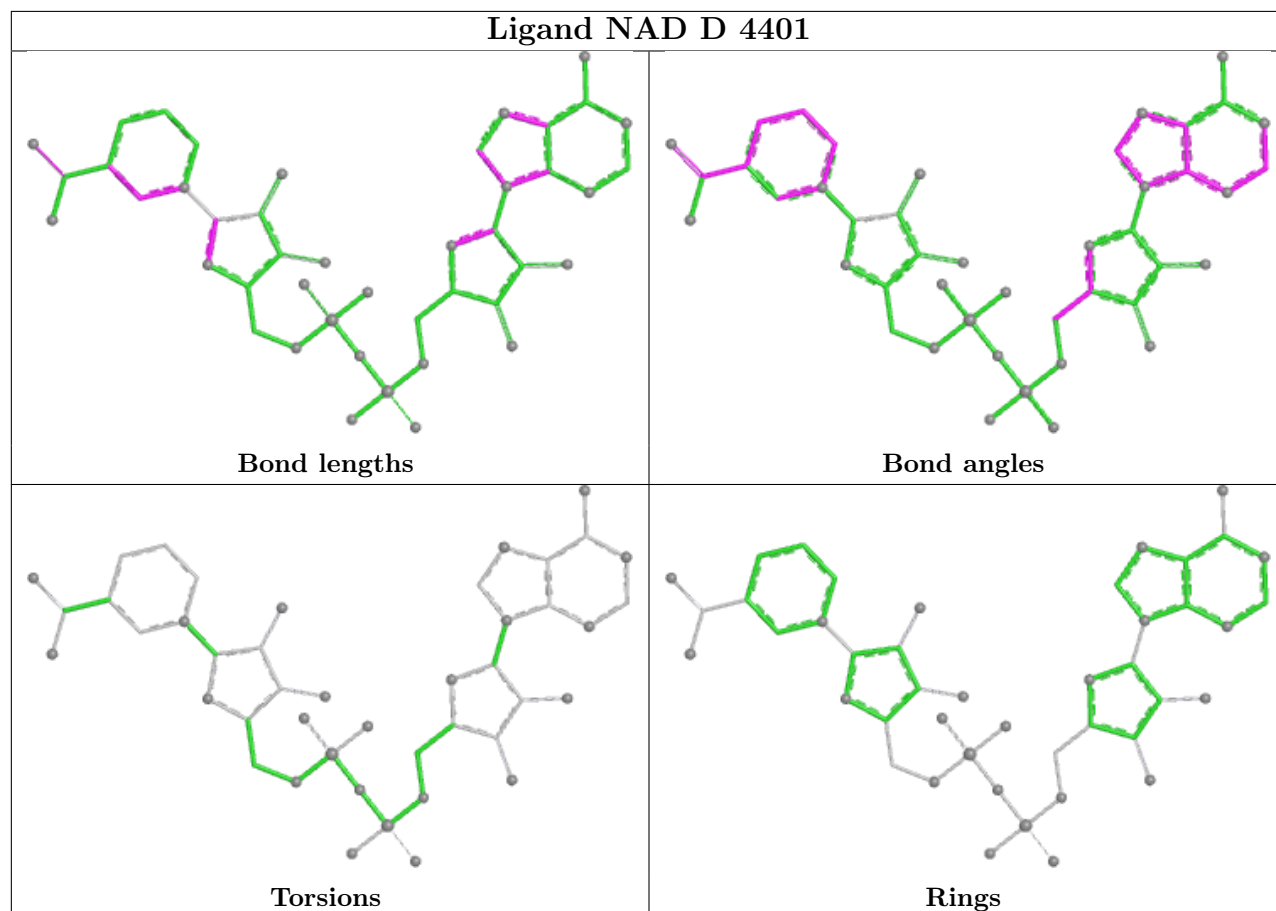
There are no ring outliers.

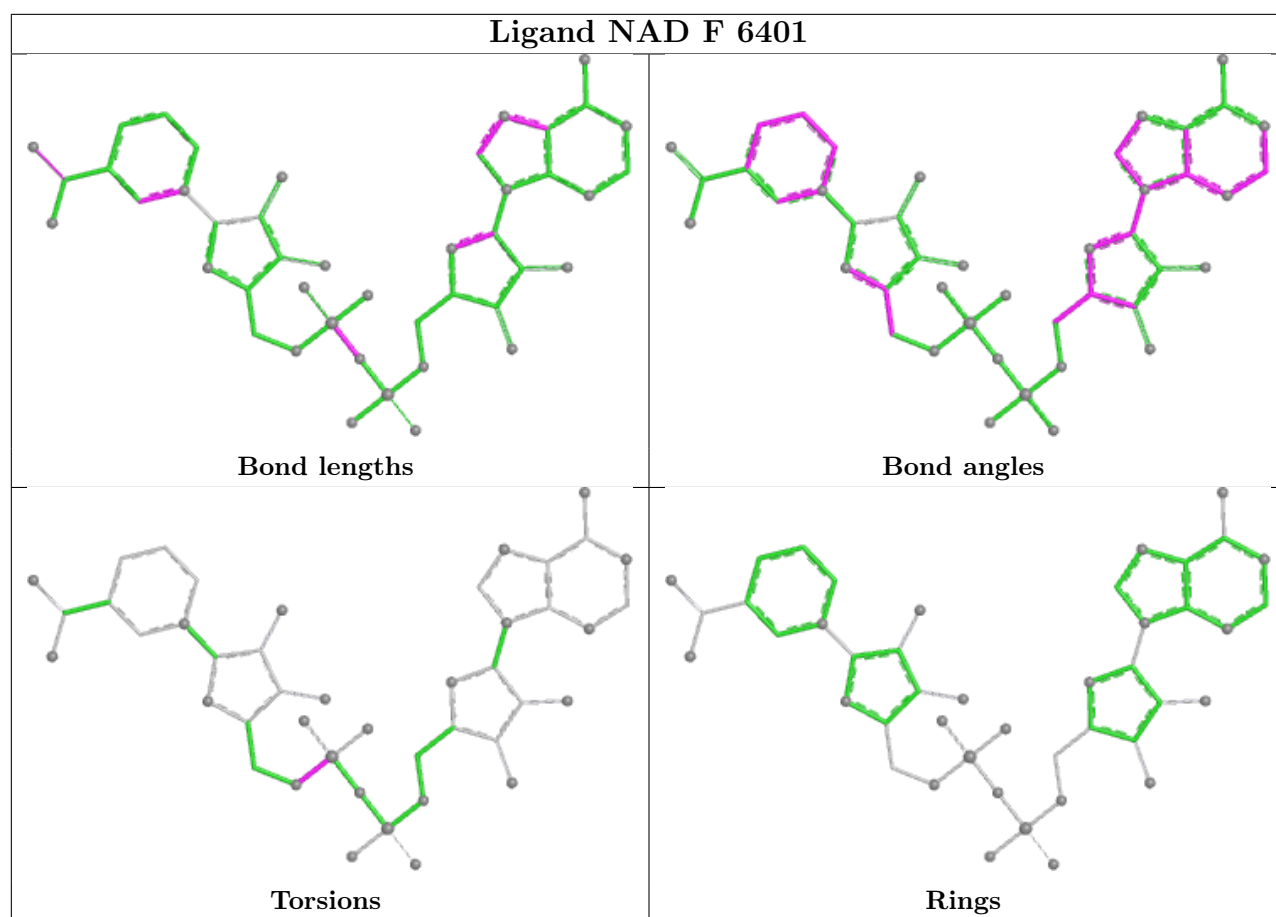
9 monomers are involved in 24 short contacts:

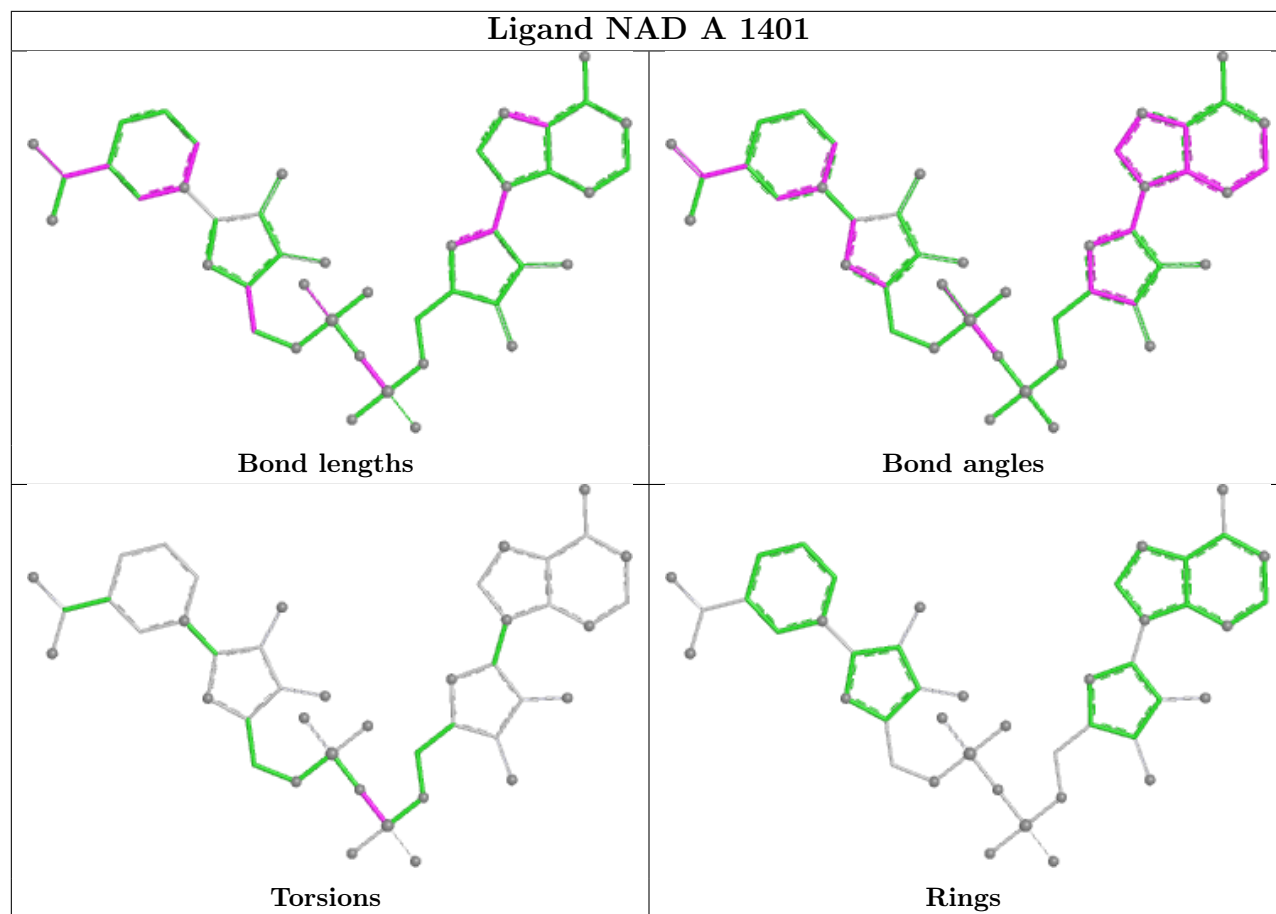
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5402	GOL	4	0
2	D	4401	NAD	1	0
2	F	6401	NAD	1	0
2	A	1401	NAD	2	0
3	B	2402	GOL	1	0
3	F	6402	GOL	1	0
3	A	1402	GOL	4	0
3	C	3402	GOL	7	0
3	D	4402	GOL	3	0

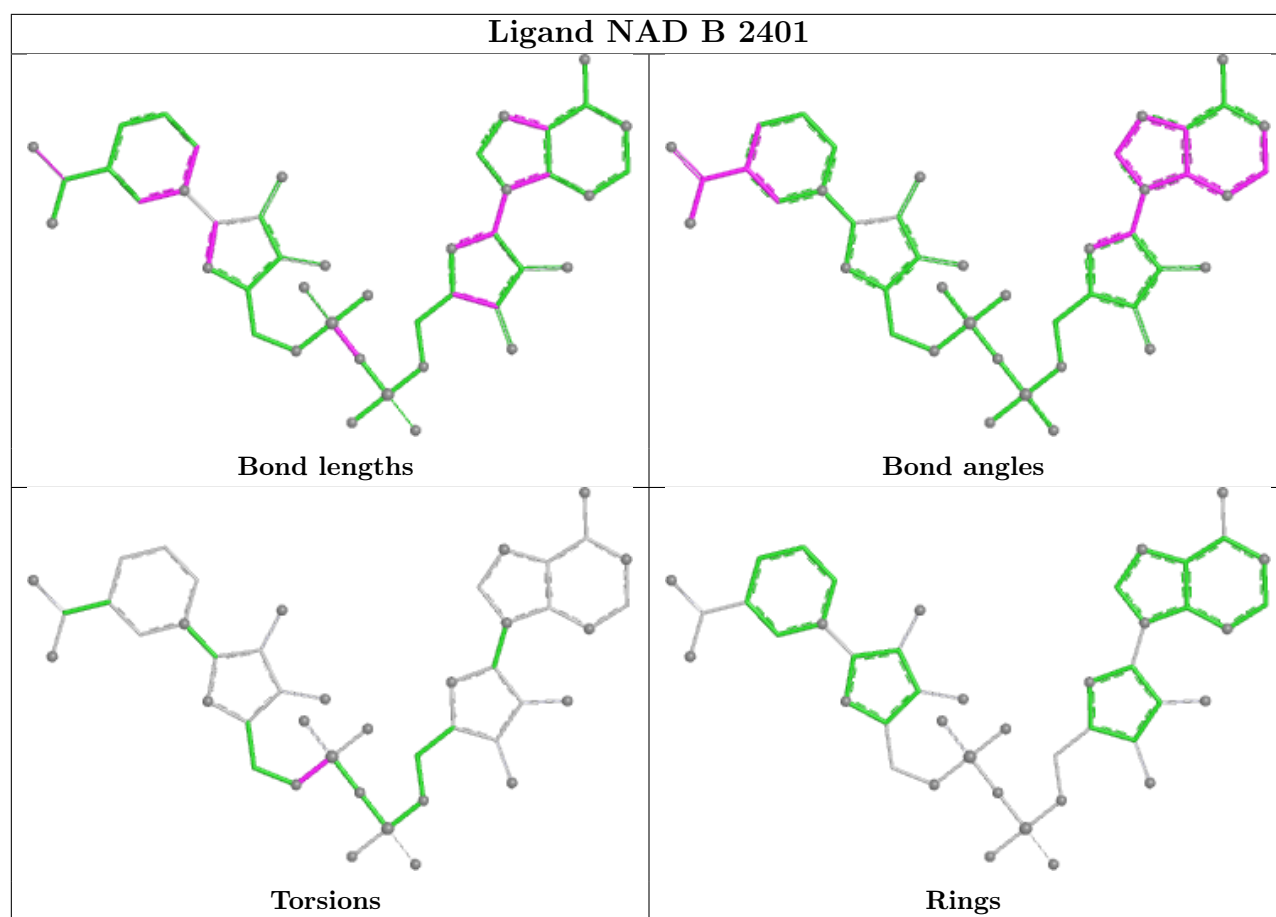
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

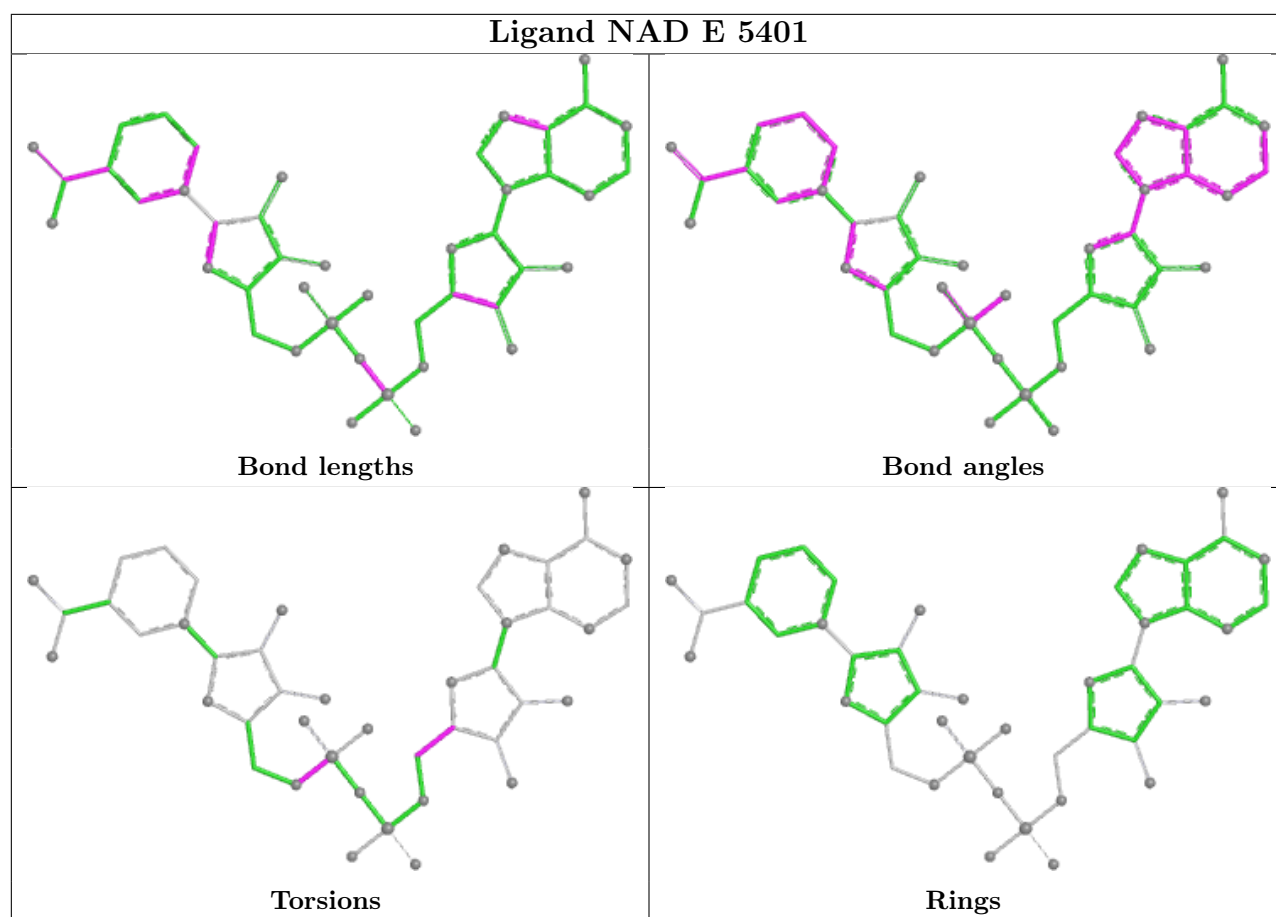
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

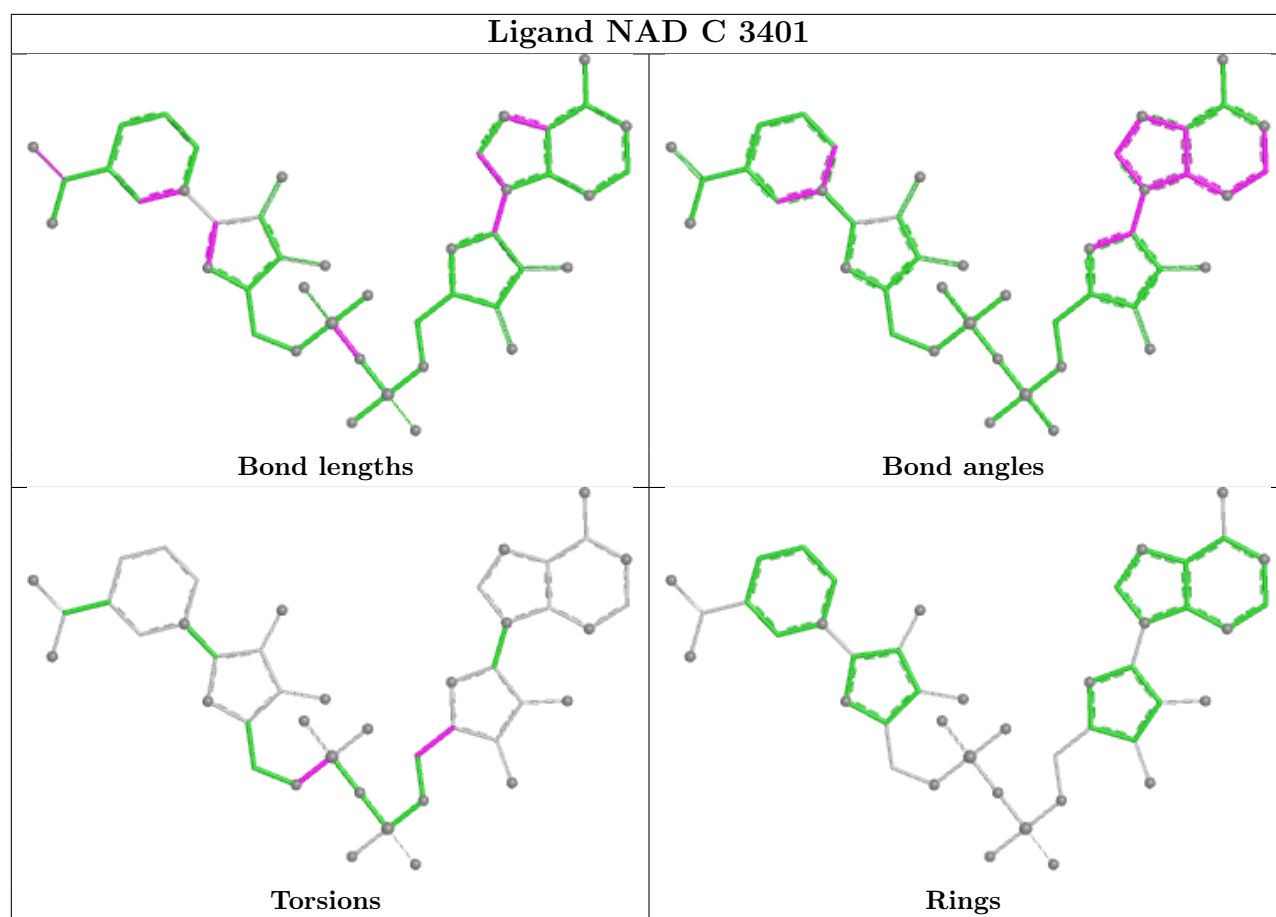












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	320/320 (100%)	-0.37	2 (0%) 85 86	7, 19, 39, 66	4 (1%)
1	B	319/320 (99%)	-0.41	1 (0%) 90 90	8, 20, 38, 55	2 (0%)
1	C	319/320 (99%)	-0.33	4 (1%) 75 76	10, 20, 46, 70	0
1	D	320/320 (100%)	-0.35	2 (0%) 85 86	10, 20, 45, 71	0
1	E	319/320 (99%)	-0.24	2 (0%) 85 86	8, 23, 50, 65	1 (0%)
1	F	319/320 (99%)	-0.38	2 (0%) 85 86	9, 20, 43, 67	2 (0%)
All	All	1916/1920 (99%)	-0.35	13 (0%) 84 85	7, 20, 44, 71	9 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1129	LYS	5.3
1	A	1321	LEU	3.7
1	D	4181	PRO	3.1
1	F	6321	LEU	3.1
1	E	5321	LEU	2.7
1	C	3181	PRO	2.7
1	C	3182	GLY	2.5
1	B	2060	ASN	2.5
1	C	3203	VAL	2.3
1	C	3180	LEU	2.1
1	E	5181	PRO	2.1
1	F	6262	ARG	2.0
1	D	4264	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

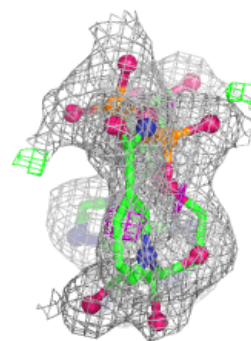
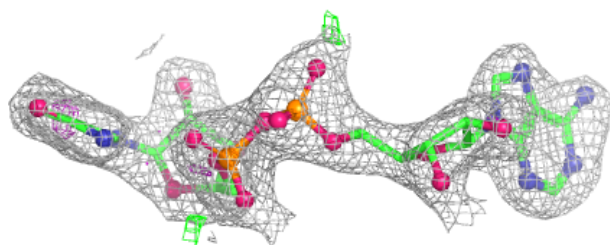
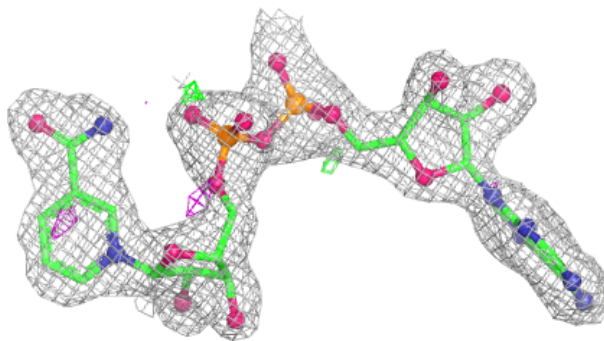
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	F	6403	5/5	0.71	0.12	83,84,86,86	0
3	GOL	B	2402	6/6	0.75	0.18	27,31,32,39	0
4	SO4	C	3403	5/5	0.76	0.12	83,88,88,88	0
3	GOL	D	4402	6/6	0.80	0.15	25,30,35,36	0
4	SO4	D	4404	5/5	0.83	0.17	63,64,68,75	0
3	GOL	A	1402	6/6	0.83	0.16	23,31,34,35	0
3	GOL	C	3402	6/6	0.85	0.13	27,29,30,34	0
4	SO4	B	2403	5/5	0.86	0.17	59,59,63,65	0
3	GOL	E	5402	6/6	0.87	0.13	31,35,35,36	0
3	GOL	F	6402	6/6	0.90	0.12	31,33,37,40	0
4	SO4	D	4403	5/5	0.91	0.11	57,58,65,68	0
2	NAD	B	2401	44/44	0.97	0.06	17,23,26,27	0
2	NAD	C	3401	44/44	0.97	0.05	16,18,19,22	0
2	NAD	E	5401	44/44	0.97	0.06	18,21,25,26	0
2	NAD	F	6401	44/44	0.97	0.05	10,17,19,20	0
2	NAD	A	1401	44/44	0.97	0.06	17,20,24,27	0
2	NAD	D	4401	44/44	0.98	0.04	10,15,16,18	0

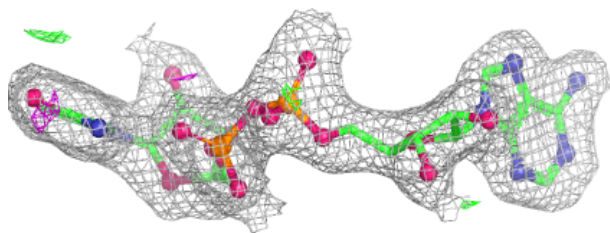
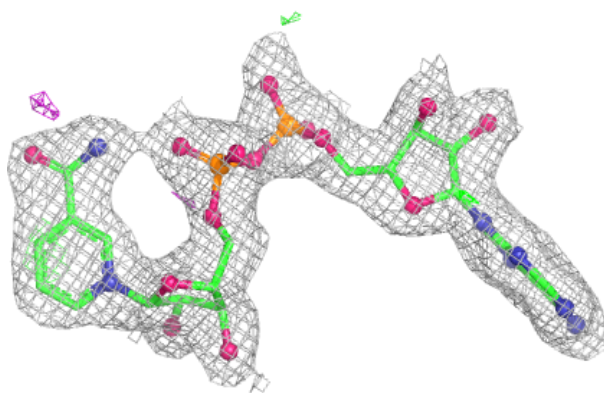
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 2401:

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

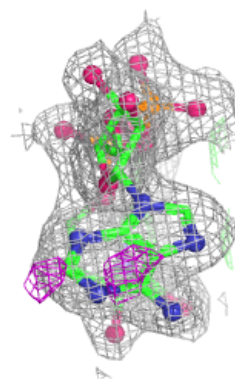
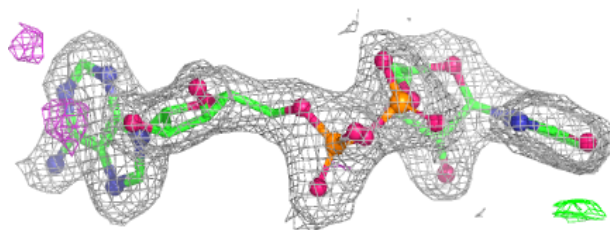
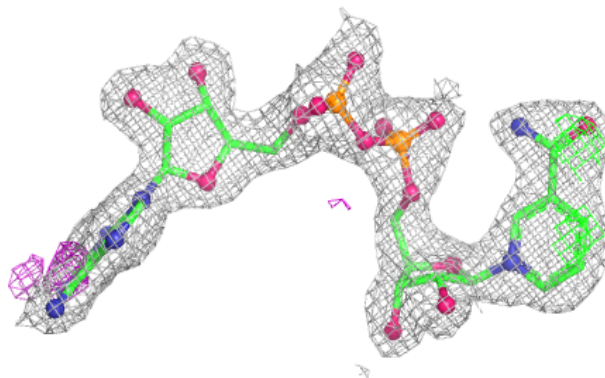
**Electron density around NAD C 3401:**

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

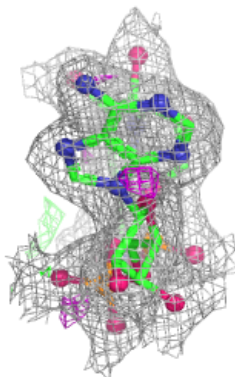
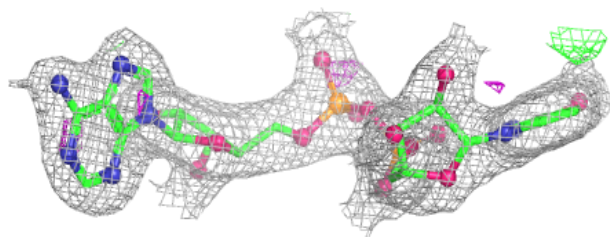
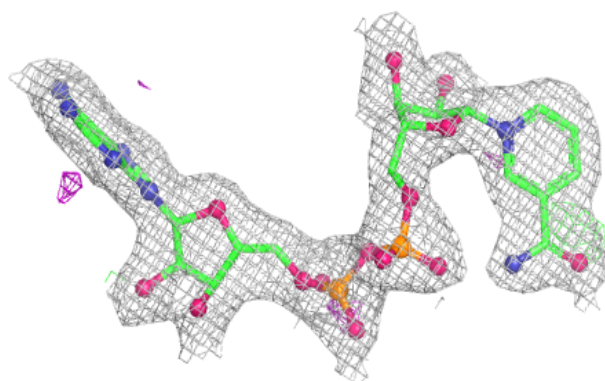


Electron density around NAD E 5401:

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

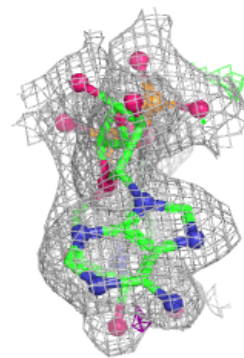
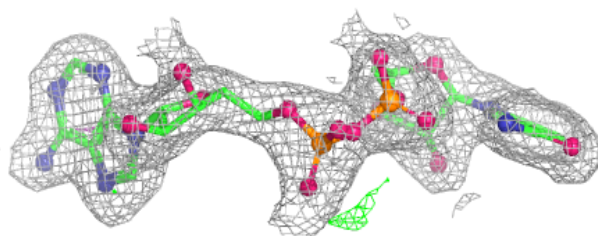
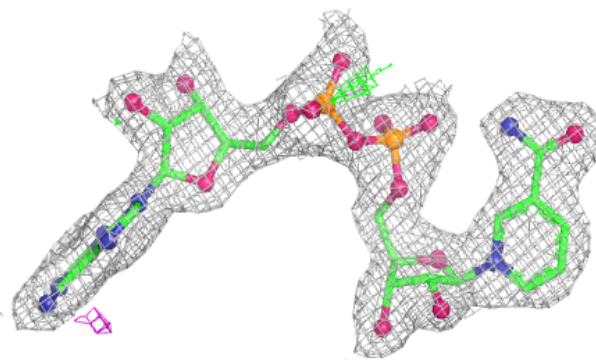
**Electron density around NAD F 6401:**

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

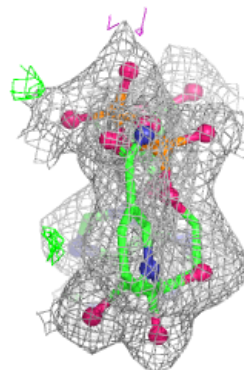
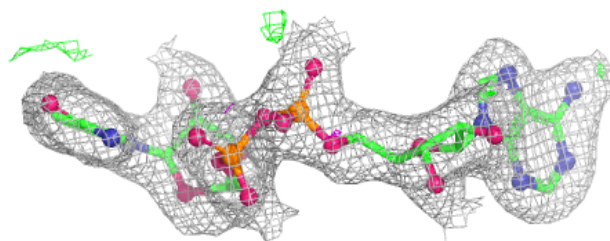
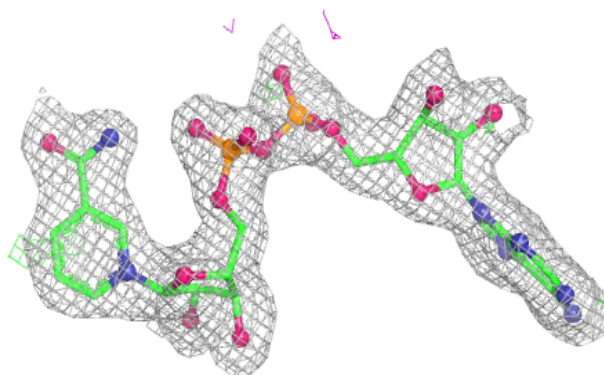


Electron density around NAD A 1401:

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

**Electron density around NAD D 4401:**

$2mF_o-DF_c$ (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.