



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 01:12 am BST

PDB ID : 1D1S  
Title : WILD-TYPE HUMAN SIGMA (CLASS IV) ALCOHOL DEHYDROGENASE  
Authors : Xie, P.T.; Hurley, T.D.  
Deposited on : 1999-09-21  
Resolution : 2.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

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

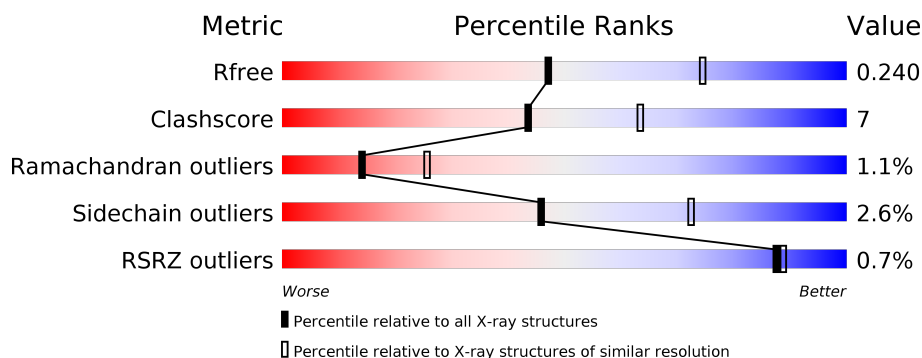
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	373	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; left: 0; top: -5px;">%</span> <span style="position: absolute; left: 82%; top: -5px;">82%</span> <span style="position: absolute; left: 98%; top: -5px;">16%</span> <span style="position: absolute; left: 100%; top: -5px;">•</span> </div> </div>
1	B	373	<div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; left: 84%; top: -5px;">84%</span> <span style="position: absolute; left: 98%; top: -5px;">15%</span> <span style="position: absolute; left: 100%; top: -5px;">•</span> </div> </div>
1	C	373	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; left: 0; top: -5px;">2%</span> <span style="position: absolute; left: 79%; top: -5px;">79%</span> <span style="position: absolute; left: 98%; top: -5px;">20%</span> <span style="position: absolute; left: 100%; top: -5px;">•</span> </div> </div>
1	D	373	<div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; left: 87%; top: -5px;">87%</span> <span style="position: absolute; left: 98%; top: -5px;">12%</span> <span style="position: absolute; left: 100%; top: -5px;">•</span> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	B	506	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11836 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 ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			
1	B	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			
1	C	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			
1	D	373	Total	C	N	O	S	0	0	0
			2789	1772	468	526	23			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

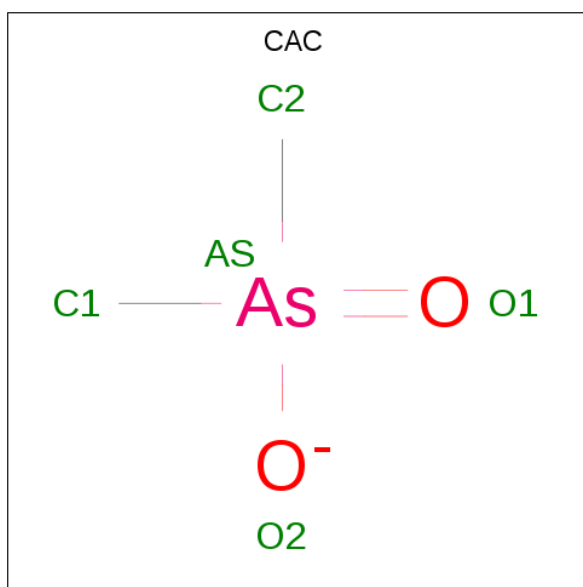
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Zn	0	0
			5	5		
2	A	6	Total	Zn	0	0
			6	6		
2	D	5	Total	Zn	0	0
			5	5		
2	C	3	Total	Zn	0	0
			3	3		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



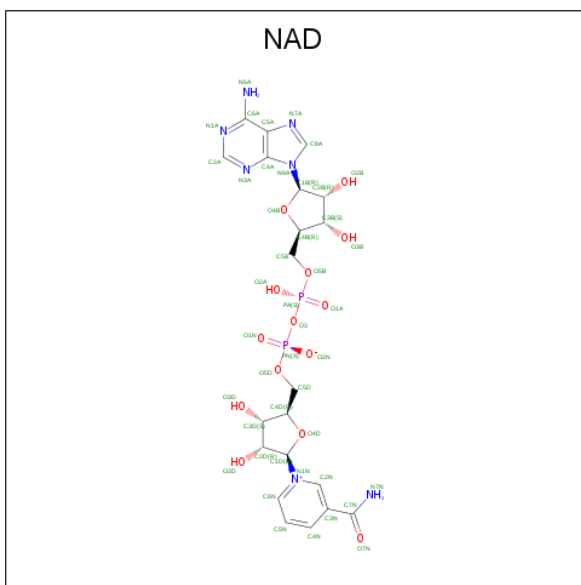
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



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

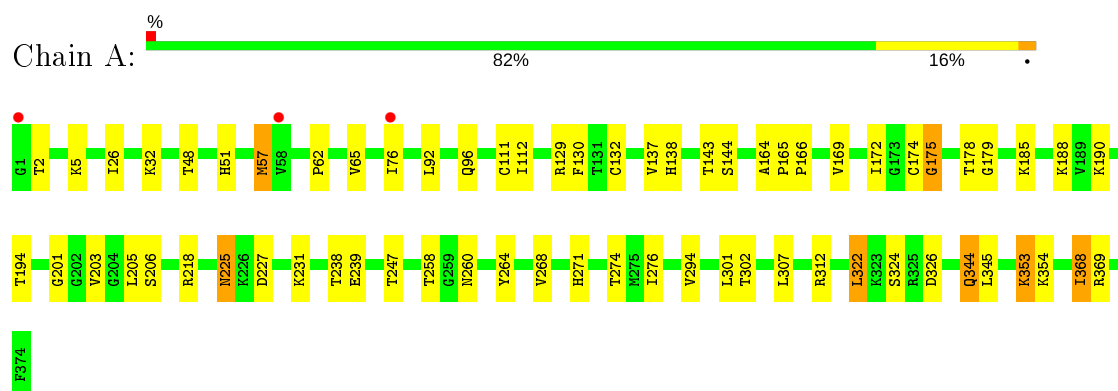
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	91	Total O 91 91	0	0
6	B	124	Total O 124 124	0	0
6	C	58	Total O 58 58	0	0
6	D	135	Total O 135 135	0	0

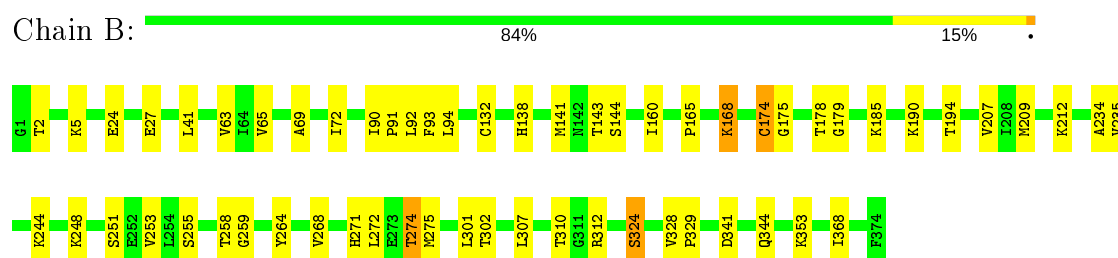
### 3 Residue-property plots [i](#)

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

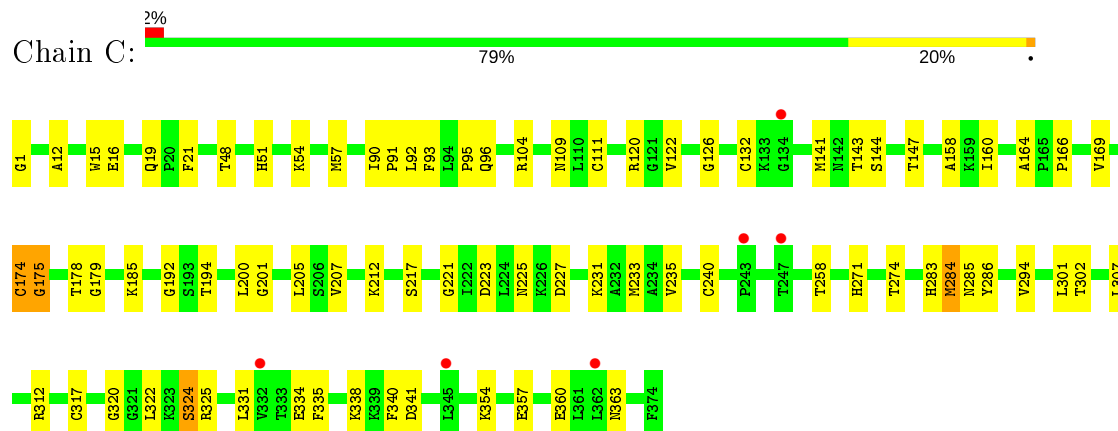
#### • Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN



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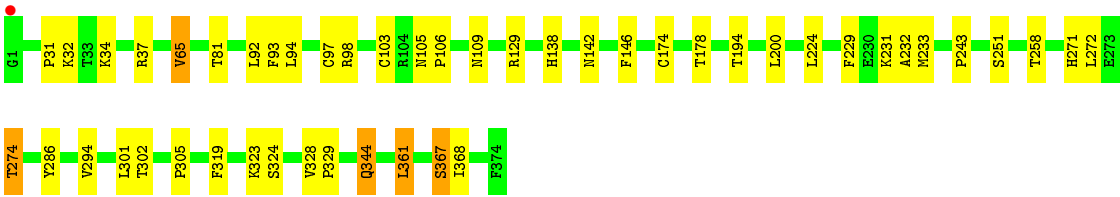
#### • Molecule 1: ALCOHOL DEHYDROGENASE CLASS IV SIGMA CHAIN



Chain D: 

87%

12%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.40 Å 90.90 Å 121.10 Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.4 (50.00-2.50) 87.9 (49.90-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.51 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.217 , 0.268 0.199 , 0.240	Depositor DCC
$R_{free}$ test set	4166 reflections (7.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11836	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.46	0/2840	0.71	2/3839 (0.1%)
1	B	0.50	0/2840	0.73	1/3839 (0.0%)
1	C	0.41	0/2840	0.66	0/3839
1	D	0.49	0/2840	0.73	1/3839 (0.0%)
All	All	0.47	0/11360	0.71	4/15356 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	LEU	CA-CB-CG	6.10	129.34	115.30
1	B	368	ILE	N-CA-C	-5.57	95.97	111.00
1	D	323	LYS	N-CA-C	-5.22	96.89	111.00
1	A	368	ILE	N-CA-C	-5.20	96.95	111.00

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	2789	0	2858	41	0
1	B	2789	0	2858	32	0
1	C	2789	0	2858	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2789	0	2858	32	0
2	A	6	0	0	0	0
2	B	5	0	0	0	0
2	C	3	0	0	0	0
2	D	5	0	0	0	0
3	A	16	0	12	1	0
3	B	8	0	6	2	0
3	C	8	0	6	0	0
3	D	20	0	15	2	0
4	A	5	0	0	0	0
4	B	20	0	0	1	0
5	A	44	0	26	3	0
5	B	44	0	26	2	0
5	C	44	0	26	2	0
5	D	44	0	26	2	0
6	A	91	0	0	3	0
6	B	124	0	0	2	0
6	C	58	0	0	4	0
6	D	135	0	0	5	0
All	All	11836	0	11575	154	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 7.

All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASP:HB3	1:B:344:GLN:NE2	1.92	0.85
1:A:130:PHE:HB2	1:A:137:VAL:HG23	1.64	0.79
1:C:301:LEU:HB2	1:D:305:PRO:HG3	1.65	0.78
1:B:271:HIS:HB2	1:B:274:THR:OG1	1.84	0.77
1:B:41:LEU:HD11	1:B:72:ILE:HG12	1.69	0.74
1:C:307:LEU:O	1:C:312:ARG:HD2	1.89	0.72
1:D:231:LYS:HE2	1:D:344:GLN:NE2	2.04	0.72
1:C:178:THR:HG21	5:C:3377:NAD:C4N	2.21	0.71
1:B:24:GLU:HG2	1:B:132:CYS:SG	2.32	0.70
1:C:283:HIS:HD2	1:C:286:TYR:H	1.41	0.68
1:D:92:LEU:HD13	1:D:324:SER:HB2	1.77	0.66
1:C:192:GLY:HA2	1:C:217:SER:OG	1.97	0.64
1:D:344:GLN:HB2	6:D:882:HOH:O	1.98	0.63
1:B:92:LEU:HD13	1:B:324:SER:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PHE:CB	1:A:137:VAL:HG23	2.30	0.61
1:C:301:LEU:HD12	1:C:302:THR:N	2.16	0.60
1:D:142:ASN:ND2	6:D:982:HOH:O	2.36	0.59
1:C:109:ASN:HA	6:C:959:HOH:O	2.03	0.58
1:C:301:LEU:HD12	1:C:302:THR:H	1.68	0.58
1:C:301:LEU:CB	1:D:305:PRO:HG3	2.34	0.57
1:C:120:ARG:HG3	6:C:960:HOH:O	2.05	0.57
1:C:164:ALA:O	1:C:166:PRO:HD3	2.05	0.56
1:A:271:HIS:HB2	1:A:274:THR:OG1	2.06	0.56
1:B:212:LYS:HD2	6:B:797:HOH:O	2.04	0.55
1:D:286:TYR:O	1:D:286:TYR:HD1	1.89	0.55
1:C:231:LYS:O	1:C:235:VAL:HG23	2.06	0.55
1:A:172:ILE:O	1:A:172:ILE:HG22	2.07	0.55
1:A:276:ILE:HD11	1:A:301:LEU:HD11	1.88	0.55
1:B:63:VAL:HG23	1:B:138:HIS:O	2.06	0.55
1:B:41:LEU:HD11	1:B:72:ILE:CG1	2.35	0.55
1:B:174:CYS:SG	5:B:2377:NAD:H5N	2.47	0.54
1:D:105:ASN:OD1	1:D:106:PRO:HD2	2.08	0.54
1:C:283:HIS:CD2	1:C:285:ASN:H	2.25	0.54
1:B:90:ILE:HG13	1:B:160:ILE:HD13	1.90	0.54
1:B:301:LEU:HD12	1:B:302:THR:N	2.23	0.54
1:C:174:CYS:SG	1:C:175:GLY:N	2.80	0.54
1:B:178:THR:HG21	5:B:2377:NAD:C4N	2.38	0.53
1:B:194:THR:HG21	1:B:258:THR:HG21	1.89	0.53
1:C:15:TRP:HZ2	1:C:132:CYS:HG	1.55	0.53
1:A:48:THR:O	1:A:51:HIS:HB2	2.08	0.53
1:C:317:CYS:SG	1:C:320:GLY:HA2	2.49	0.52
1:C:91:PRO:HB2	1:C:143:THR:HG22	1.90	0.52
1:C:194:THR:HG21	1:C:258:THR:HG21	1.90	0.52
1:C:354:LYS:HZ1	1:C:357:GLU:HB2	1.75	0.52
1:D:231:LYS:HE2	1:D:344:GLN:HE21	1.71	0.52
1:D:272:LEU:HB3	1:D:301:LEU:HD13	1.92	0.52
1:C:51:HIS:HB3	1:C:57:MET:HB2	1.92	0.52
1:A:92:LEU:HD13	1:A:324:SER:HB2	1.92	0.51
1:C:95:PRO:HG2	1:C:111:CYS:HB3	1.92	0.51
1:A:225:ASN:ND2	1:A:227:ASP:H	2.07	0.51
1:C:335:PHE:HB2	1:C:340:PHE:CE2	2.46	0.51
1:A:26:ILE:HG22	1:A:132:CYS:HB2	1.91	0.51
1:C:200:LEU:HD12	1:C:223:ASP:HB2	1.93	0.51
1:C:271:HIS:HB2	1:C:274:THR:OG1	2.10	0.51
1:D:92:LEU:HA	6:D:778:HOH:O	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLY:HA3	1:A:206:SER:HB2	1.93	0.50
1:C:54:LYS:NZ	1:C:363:ASN:OD1	2.43	0.50
1:D:229:PHE:O	1:D:233:MET:HG2	2.12	0.50
1:A:194:THR:HG21	1:A:258:THR:HG21	1.94	0.50
1:A:201:GLY:O	1:A:205:LEU:HG	2.12	0.50
1:A:5:LYS:HD2	1:A:5:LYS:N	2.27	0.50
1:A:76:ILE:O	1:A:76:ILE:HG13	2.13	0.49
1:B:209:MET:HG2	1:B:235:VAL:HG22	1.93	0.49
1:C:354:LYS:HA	1:C:354:LYS:HE2	1.94	0.49
1:C:179:GLY:O	1:C:207:VAL:HA	2.11	0.49
1:C:120:ARG:O	1:C:122:VAL:HG13	2.12	0.49
1:A:294:VAL:HG23	5:A:1377:NAD:H2N	1.94	0.49
1:A:178:THR:HG21	5:A:1377:NAD:C4N	2.43	0.49
1:B:143:THR:O	1:B:144:SER:HB2	2.13	0.49
1:B:190:LYS:HG2	1:B:264:TYR:OH	2.13	0.49
1:C:357:GLU:O	1:C:360:GLU:HB3	2.12	0.49
1:D:361:LEU:HB3	1:D:367:SER:HB2	1.95	0.49
1:A:301:LEU:HA	6:A:720:HOH:O	2.13	0.48
1:D:178:THR:HG21	5:D:4377:NAD:C4N	2.43	0.48
1:C:16:GLU:HB2	1:C:19:GLN:OE1	2.13	0.48
1:C:1:GLY:N	6:C:677:HOH:O	2.43	0.48
1:D:286:TYR:CD1	1:D:286:TYR:O	2.66	0.48
1:B:93:PHE:CZ	3:B:506:ACT:H2	2.49	0.48
1:D:200:LEU:HD13	1:D:232:ALA:HB2	1.95	0.48
1:A:185:LYS:HD2	1:A:322:LEU:HD23	1.96	0.47
1:A:62:PRO:CG	1:A:137:VAL:HG12	2.44	0.47
1:D:328:VAL:HB	1:D:329:PRO:HD3	1.96	0.47
1:B:248:LYS:HG3	1:B:253:VAL:HG23	1.97	0.47
1:B:94:LEU:HB3	1:B:324:SER:HG	1.80	0.47
1:D:31:PRO:HD3	1:D:37:ARG:HB2	1.97	0.47
1:C:334:GLU:HB3	1:C:340:PHE:HE1	1.80	0.46
1:B:24:GLU:HG3	6:B:896:HOH:O	2.14	0.46
1:B:307:LEU:O	1:B:312:ARG:HD2	2.16	0.46
1:B:69:ALA:O	1:B:91:PRO:HD2	2.15	0.46
1:B:93:PHE:CE2	3:B:506:ACT:H2	2.50	0.46
1:C:331:LEU:O	1:C:340:PHE:HZ	1.98	0.46
1:D:34:LYS:HD3	3:D:509:ACT:H1	1.98	0.46
1:A:231:LYS:HE2	1:A:344:GLN:HG3	1.97	0.46
1:C:201:GLY:O	1:C:205:LEU:HG	2.15	0.46
1:A:32:LYS:HD2	1:A:129:ARG:NH2	2.30	0.46
1:A:260:ASN:HB3	4:B:555:CAC:C2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:GLN:HB3	1:C:325:ARG:HD3	1.96	0.46
1:C:354:LYS:NZ	1:C:357:GLU:HB2	2.31	0.46
1:D:271:HIS:HB2	1:D:274:THR:OG1	2.17	0.45
1:D:224:LEU:HD23	1:D:243:PRO:HD2	1.98	0.45
1:A:51:HIS:HB3	1:A:57:MET:HB2	1.97	0.45
1:A:353:LYS:HE2	1:A:353:LYS:HB2	1.84	0.45
1:D:65:VAL:HG22	6:D:688:HOH:O	2.17	0.44
1:A:175:GLY:HA2	1:A:203:VAL:HG22	1.98	0.44
1:C:334:GLU:HB3	1:C:340:PHE:CE1	2.52	0.44
1:D:65:VAL:HG23	1:D:146:PHE:CD1	2.53	0.44
1:A:132:CYS:HA	6:A:741:HOH:O	2.18	0.44
1:B:93:PHE:HB2	1:B:141:MET:HB3	2.00	0.44
1:A:294:VAL:HG23	5:A:1377:NAD:H1D	1.99	0.43
1:C:12:ALA:HB1	1:C:21:PHE:CD2	2.52	0.43
1:C:185:LYS:HD2	1:C:322:LEU:HD23	1.99	0.43
1:A:164:ALA:HA	1:A:165:PRO:HD3	1.92	0.43
1:C:96:GLN:HB3	1:C:325:ARG:CD	2.48	0.43
1:A:188:LYS:NZ	6:A:1006:HOH:O	2.52	0.43
1:A:165:PRO:O	1:A:169:VAL:HG22	2.18	0.43
1:B:301:LEU:HD12	1:B:302:THR:H	1.82	0.43
1:A:111:CYS:SG	1:A:112:ILE:N	2.92	0.43
1:B:165:PRO:HB2	1:B:168:LYS:HG3	2.01	0.43
1:C:225:ASN:OD1	1:C:227:ASP:HB2	2.19	0.43
1:C:164:ALA:HB1	1:C:169:VAL:HG11	2.01	0.42
1:D:138:HIS:CE1	6:D:867:HOH:O	2.71	0.42
1:C:48:THR:HG21	1:C:141:MET:CE	2.49	0.42
1:D:294:VAL:HG23	5:D:4377:NAD:H1D	2.00	0.42
1:A:143:THR:O	1:A:144:SER:HB2	2.19	0.42
1:A:238:THR:O	1:A:239:GLU:HB3	2.19	0.42
1:A:345:LEU:O	1:A:369:ARG:HB2	2.20	0.42
1:C:284:MET:HG2	6:C:970:HOH:O	2.20	0.42
1:D:93:PHE:CZ	3:D:511:ACT:CH3	3.02	0.42
1:B:179:GLY:O	1:B:207:VAL:HA	2.19	0.42
1:C:122:VAL:HG21	1:C:126:GLY:HA2	2.02	0.42
1:D:194:THR:HG21	1:D:258:THR:HG21	2.02	0.42
1:D:98:ARG:HA	1:D:103:CYS:HB3	2.01	0.42
1:B:234:ALA:HA	1:D:81:THR:HG21	2.02	0.41
1:A:302:THR:HA	1:B:301:LEU:O	2.20	0.41
1:C:221:GLY:O	1:C:240:CYS:HA	2.20	0.41
1:A:138:HIS:HE1	3:A:513:ACT:OXT	2.03	0.41
1:A:164:ALA:O	1:A:166:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LYS:HG3	1:A:264:TYR:OH	2.20	0.41
1:B:255:SER:O	1:B:259:GLY:N	2.54	0.41
1:A:62:PRO:HG2	1:A:137:VAL:HG12	2.01	0.41
1:A:307:LEU:O	1:A:312:ARG:HD2	2.20	0.41
1:C:92:LEU:HD13	1:C:324:SER:HB2	2.03	0.41
1:C:143:THR:O	1:C:144:SER:HB2	2.21	0.41
1:B:328:VAL:HB	1:B:329:PRO:HD3	2.03	0.40
1:D:32:LYS:HD2	1:D:129:ARG:NH2	2.36	0.40
1:C:301:LEU:O	1:D:302:THR:HA	2.21	0.40
1:D:94:LEU:HD22	1:D:319:PHE:HB3	2.03	0.40
1:C:48:THR:HG21	1:C:141:MET:HE1	2.03	0.40
1:C:294:VAL:HG23	5:C:3377:NAD:H1D	2.03	0.40
1:A:96:GLN:NE2	1:A:326:ASP:OD1	2.54	0.40
1:B:272:LEU:O	1:B:275:MET:HB2	2.21	0.40
1:C:93:PHE:HB2	1:C:141:MET:HB3	2.04	0.40
1:C:92:LEU:HD21	1:C:158:ALA:HB2	2.02	0.40
1:C:90:ILE:HG13	1:C:160:ILE:HD13	2.02	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	371/373 (100%)	340 (92%)	27 (7%)	4 (1%)	14	26
1	B	371/373 (100%)	341 (92%)	26 (7%)	4 (1%)	14	26
1	C	371/373 (100%)	331 (89%)	36 (10%)	4 (1%)	14	26
1	D	371/373 (100%)	345 (93%)	22 (6%)	4 (1%)	14	26
All	All	1484/1492 (100%)	1357 (91%)	111 (8%)	16 (1%)	14	26

All (16) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	C	338	LYS
1	A	174	CYS
1	A	175	GLY
1	B	174	CYS
1	B	324	SER
1	C	174	CYS
1	C	175	GLY
1	C	324	SER
1	D	174	CYS
1	D	109	ASN
1	B	65	VAL
1	B	175	GLY
1	A	368	ILE
1	A	65	VAL
1	D	368	ILE
1	D	65	VAL

### 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	312/312 (100%)	303 (97%)	9 (3%)	42	69
1	B	312/312 (100%)	301 (96%)	11 (4%)	36	62
1	C	312/312 (100%)	306 (98%)	6 (2%)	57	80
1	D	312/312 (100%)	306 (98%)	6 (2%)	57	80
All	All	1248/1248 (100%)	1216 (97%)	32 (3%)	46	72

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	57	MET
1	A	218	ARG
1	A	225	ASN
1	A	247	THR
1	A	268	VAL

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Mol	Chain	Res	Type
1	A	344	GLN
1	A	353	LYS
1	A	354	LYS
1	B	2	THR
1	B	5	LYS
1	B	27	GLU
1	B	168	LYS
1	B	185	LYS
1	B	244	LYS
1	B	251	SER
1	B	268	VAL
1	B	274	THR
1	B	310	THR
1	B	353	LYS
1	C	104	ARG
1	C	147	THR
1	C	212	LYS
1	C	233	MET
1	C	284	MET
1	C	341	ASP
1	D	97	CYS
1	D	251	SER
1	D	274	THR
1	D	344	GLN
1	D	361	LEU
1	D	367	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	225	ASN
1	A	261	ASN
1	A	344	GLN
1	B	17	GLN
1	B	344	GLN
1	C	51	HIS
1	C	260	ASN
1	C	283	HIS
1	C	344	GLN
1	D	17	GLN
1	D	19	GLN

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Mol	Chain	Res	Type
1	D	138	HIS
1	D	344	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 19 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ACT	D	512	2	1,3,3	1.19	0	0,3,3	0.00	-
4	CAC	B	553	2	0,4,4	0.00	-	0,6,6	0.00	-
5	NAD	B	2377	2	42,48,48	1.97	6 (14%)	50,73,73	1.93	11 (22%)
5	NAD	A	1377	2	42,48,48	1.96	5 (11%)	50,73,73	1.66	9 (18%)
3	ACT	D	508	-	1,3,3	2.52	1 (100%)	0,3,3	0.00	-
3	ACT	B	506	2	1,3,3	0.05	0	0,3,3	0.00	-
4	CAC	B	555	-	0,4,4	0.00	-	0,6,6	0.00	-
5	NAD	D	4377	2	42,48,48	2.13	8 (19%)	50,73,73	2.05	9 (18%)
3	ACT	D	514	2	1,3,3	0.90	0	0,3,3	0.00	-
3	ACT	C	510	2	1,3,3	2.75	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ACT	B	507	2	1,3,3	2.07	1 (100%)	0,3,3	0.00	-
3	ACT	A	504	2	1,3,3	2.04	1 (100%)	0,3,3	0.00	-
3	ACT	D	511	2	1,3,3	0.84	0	0,3,3	0.00	-
4	CAC	B	552	2	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	B	551	2	0,4,4	0.00	-	0,6,6	0.00	-
3	ACT	A	501	2	1,3,3	2.29	1 (100%)	0,3,3	0.00	-
5	NAD	C	3377	2	42,48,48	1.99	8 (19%)	50,73,73	1.73	10 (20%)
3	ACT	D	509	2	1,3,3	0.90	0	0,3,3	0.00	-
3	ACT	A	502	2	1,3,3	5.64	1 (100%)	0,3,3	0.00	-
3	ACT	C	505	2	1,3,3	1.99	0	0,3,3	0.00	-
4	CAC	A	554	-	0,4,4	0.00	-	0,6,6	0.00	-
3	ACT	A	513	2	1,3,3	5.98	1 (100%)	0,3,3	0.00	-

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
5	NAD	C	3377	2	-	9/26/62/62	0/5/5/5
5	NAD	B	2377	2	-	9/26/62/62	0/5/5/5
5	NAD	A	1377	2	-	5/26/62/62	0/5/5/5
5	NAD	D	4377	2	-	7/26/62/62	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	4377	NAD	C3N-C7N	-9.99	1.35	1.50
5	A	1377	NAD	C3N-C7N	-8.99	1.37	1.50
5	C	3377	NAD	C3N-C7N	-7.79	1.38	1.50
5	B	2377	NAD	C3N-C7N	-7.75	1.38	1.50
3	A	513	ACT	CH3-C	5.98	1.56	1.48
3	A	502	ACT	CH3-C	5.64	1.55	1.48
5	C	3377	NAD	C2A-N3A	5.08	1.40	1.32
5	B	2377	NAD	C2A-N3A	4.98	1.40	1.32
5	A	1377	NAD	C2A-N3A	4.44	1.39	1.32
5	B	2377	NAD	C4A-N3A	4.11	1.41	1.35
5	A	1377	NAD	C8A-N7A	4.03	1.41	1.34
5	C	3377	NAD	C2A-N1A	3.98	1.41	1.33
5	D	4377	NAD	C2A-N3A	3.62	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2377	NAD	C2A-N1A	3.56	1.40	1.33
5	D	4377	NAD	C8A-N7A	3.54	1.41	1.34
5	A	1377	NAD	C2A-N1A	3.38	1.40	1.33
5	D	4377	NAD	C2N-C3N	-3.38	1.33	1.39
5	C	3377	NAD	C2N-C3N	-3.29	1.33	1.39
5	C	3377	NAD	O4D-C1D	3.23	1.45	1.41
5	B	2377	NAD	C2N-C3N	-3.10	1.34	1.39
5	C	3377	NAD	C4A-N3A	3.00	1.39	1.35
5	B	2377	NAD	C8A-N7A	2.97	1.40	1.34
5	D	4377	NAD	O4D-C1D	2.91	1.45	1.41
3	C	510	ACT	CH3-C	2.75	1.52	1.48
5	D	4377	NAD	O4B-C4B	-2.68	1.39	1.45
5	A	1377	NAD	C4A-N3A	2.67	1.39	1.35
5	D	4377	NAD	C4N-C3N	-2.57	1.34	1.39
3	D	508	ACT	CH3-C	2.52	1.52	1.48
5	D	4377	NAD	C2A-N1A	2.38	1.38	1.33
5	C	3377	NAD	C8A-N7A	2.36	1.38	1.34
3	A	501	ACT	CH3-C	2.29	1.51	1.48
5	C	3377	NAD	C4N-C3N	-2.20	1.35	1.39
3	B	507	ACT	CH3-C	2.07	1.51	1.48
3	A	504	ACT	CH3-C	2.04	1.51	1.48

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	4377	NAD	O7N-C7N-N7N	-8.64	110.31	122.58
5	B	2377	NAD	O7N-C7N-N7N	-6.06	113.97	122.58
5	A	1377	NAD	O7N-C7N-N7N	-6.06	113.97	122.58
5	D	4377	NAD	N3A-C2A-N1A	-5.75	119.70	128.68
5	B	2377	NAD	N3A-C2A-N1A	-5.24	120.48	128.68
5	C	3377	NAD	O7N-C7N-N7N	-5.01	115.46	122.58
5	B	2377	NAD	C4A-C5A-N7A	4.96	114.57	109.40
5	C	3377	NAD	N3A-C2A-N1A	-4.56	121.55	128.68
5	A	1377	NAD	N3A-C2A-N1A	-4.22	122.08	128.68
5	A	1377	NAD	O4B-C1B-C2B	-4.07	100.98	106.93
5	C	3377	NAD	O4B-C1B-C2B	-4.00	101.08	106.93
5	D	4377	NAD	C3D-C2D-C1D	-3.84	95.19	100.98
5	C	3377	NAD	O5D-C5D-C4D	3.73	121.81	108.99
5	B	2377	NAD	N6A-C6A-N1A	3.50	125.84	118.57
5	C	3377	NAD	O4D-C1D-C2D	-3.37	102.00	106.93
5	B	2377	NAD	C2B-C3B-C4B	-3.13	96.56	102.64
5	D	4377	NAD	O4B-C4B-C3B	3.06	111.17	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2377	NAD	C3N-C2N-N1N	2.89	123.25	120.43
5	D	4377	NAD	C2A-N1A-C6A	2.86	123.64	118.75
5	B	2377	NAD	O4B-C1B-C2B	-2.83	102.79	106.93
5	D	4377	NAD	O5D-C5D-C4D	2.80	118.63	108.99
5	B	2377	NAD	C5A-C6A-N6A	-2.78	116.13	120.35
5	A	1377	NAD	C3B-C2B-C1B	2.77	105.15	100.98
5	D	4377	NAD	C4A-C5A-N7A	2.72	112.24	109.40
5	A	1377	NAD	C2B-C3B-C4B	-2.72	97.35	102.64
5	A	1377	NAD	O4B-C4B-C3B	2.71	110.48	105.11
5	B	2377	NAD	O4B-C4B-C3B	2.62	110.30	105.11
5	C	3377	NAD	C2N-N1N-C1D	-2.62	113.31	119.14
5	B	2377	NAD	C6N-N1N-C2N	-2.58	119.62	121.97
5	C	3377	NAD	C3N-C2N-N1N	2.53	122.90	120.43
5	A	1377	NAD	O4D-C1D-C2D	-2.51	103.25	106.93
5	D	4377	NAD	C2N-N1N-C1D	-2.47	113.65	119.14
5	A	1377	NAD	O5B-C5B-C4B	-2.42	100.65	108.99
5	D	4377	NAD	O7N-C7N-C3N	2.22	122.29	119.63
5	A	1377	NAD	C6N-N1N-C2N	-2.21	119.96	121.97
5	C	3377	NAD	O4B-C4B-C3B	2.16	109.38	105.11
5	C	3377	NAD	C2B-C3B-C4B	-2.10	98.56	102.64
5	B	2377	NAD	O5D-PN-O1N	-2.09	100.92	109.07
5	C	3377	NAD	C6N-N1N-C2N	-2.04	120.11	121.97

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2377	NAD	O4D-C1D-N1N-C2N
5	B	2377	NAD	O4D-C1D-N1N-C6N
5	B	2377	NAD	C2D-C1D-N1N-C2N
5	A	1377	NAD	O4D-C1D-N1N-C2N
5	A	1377	NAD	O4D-C1D-N1N-C6N
5	A	1377	NAD	C2D-C1D-N1N-C2N
5	A	1377	NAD	C2D-C1D-N1N-C6N
5	D	4377	NAD	O4D-C1D-N1N-C2N
5	D	4377	NAD	O4D-C1D-N1N-C6N
5	D	4377	NAD	C2D-C1D-N1N-C2N
5	D	4377	NAD	C2D-C1D-N1N-C6N
5	C	3377	NAD	O4D-C1D-N1N-C2N
5	C	3377	NAD	O4D-C1D-N1N-C6N
5	C	3377	NAD	C2D-C1D-N1N-C2N
5	C	3377	NAD	C2D-C1D-N1N-C6N

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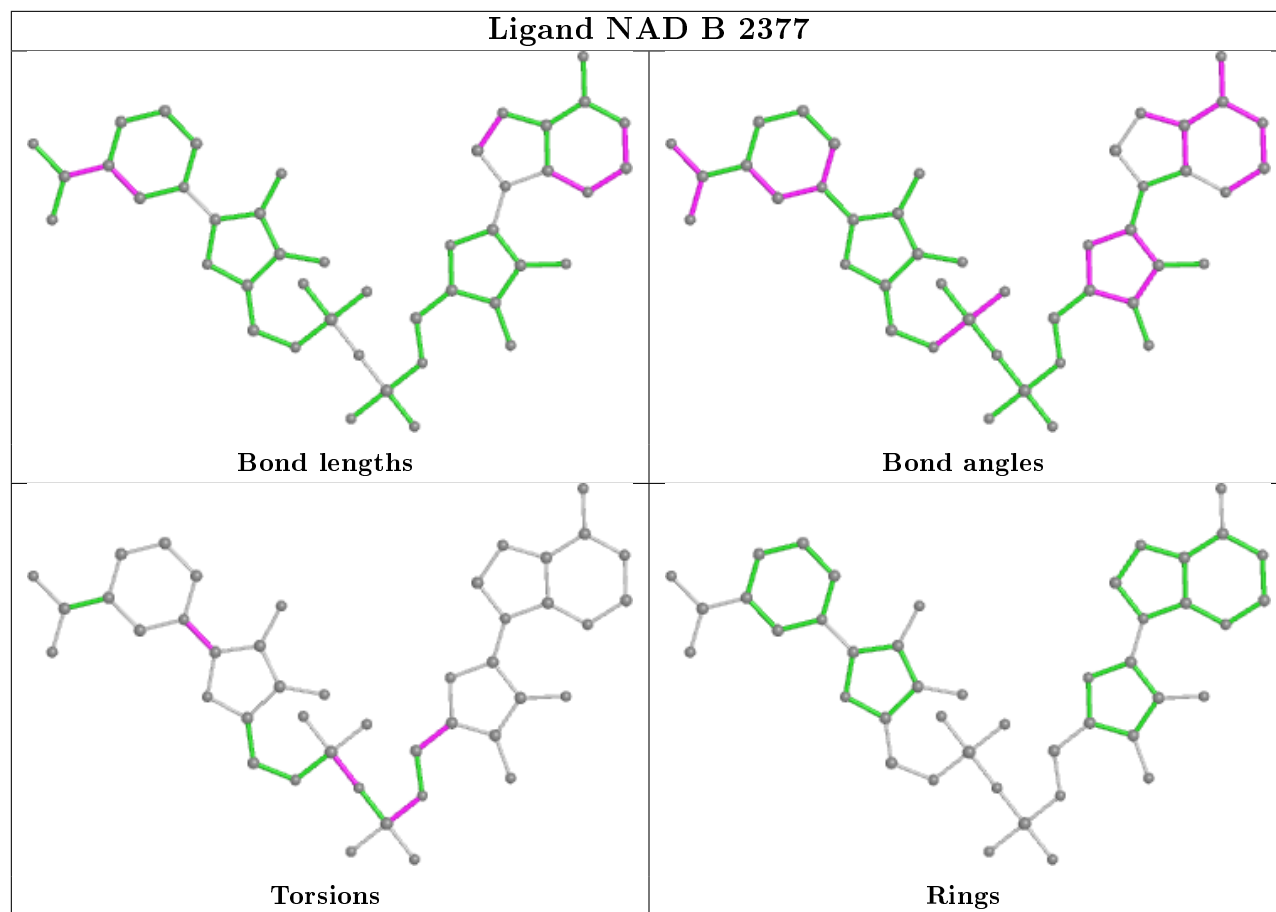
Mol	Chain	Res	Type	Atoms
5	B	2377	NAD	O4B-C4B-C5B-O5B
5	B	2377	NAD	C3B-C4B-C5B-O5B
5	C	3377	NAD	O4D-C4D-C5D-O5D
5	B	2377	NAD	C5B-O5B-PA-O2A
5	C	3377	NAD	C5D-O5D-PN-O2N
5	C	3377	NAD	O4B-C4B-C5B-O5B
5	B	2377	NAD	PA-O3-PN-O2N
5	D	4377	NAD	PN-O3-PA-O2A
5	A	1377	NAD	O4B-C4B-C5B-O5B
5	B	2377	NAD	C5B-O5B-PA-O3
5	B	2377	NAD	C2D-C1D-N1N-C6N
5	C	3377	NAD	C5D-O5D-PN-O3
5	D	4377	NAD	C4N-C3N-C7N-N7N
5	C	3377	NAD	C5B-O5B-PA-O2A
5	D	4377	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

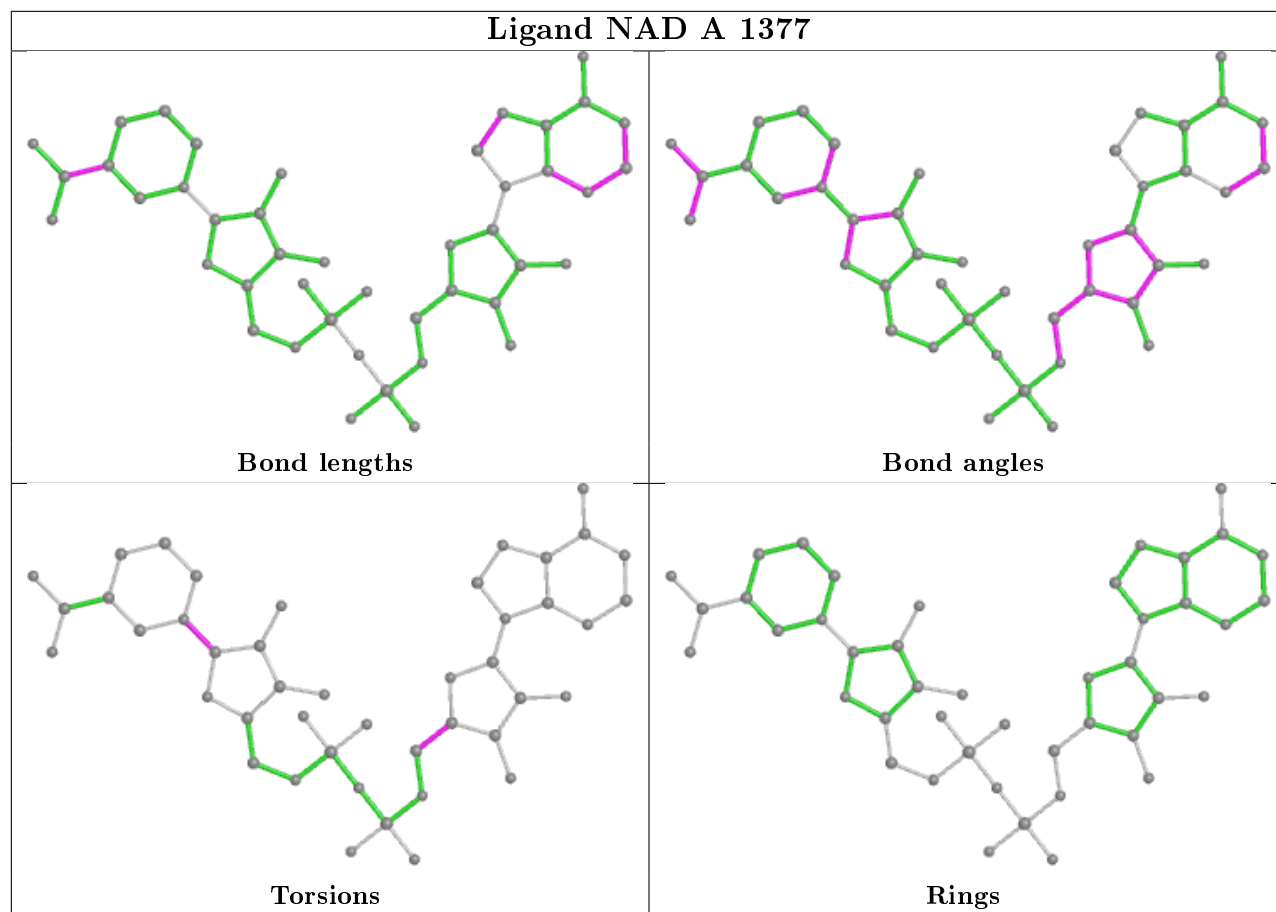
9 monomers are involved in 15 short contacts:

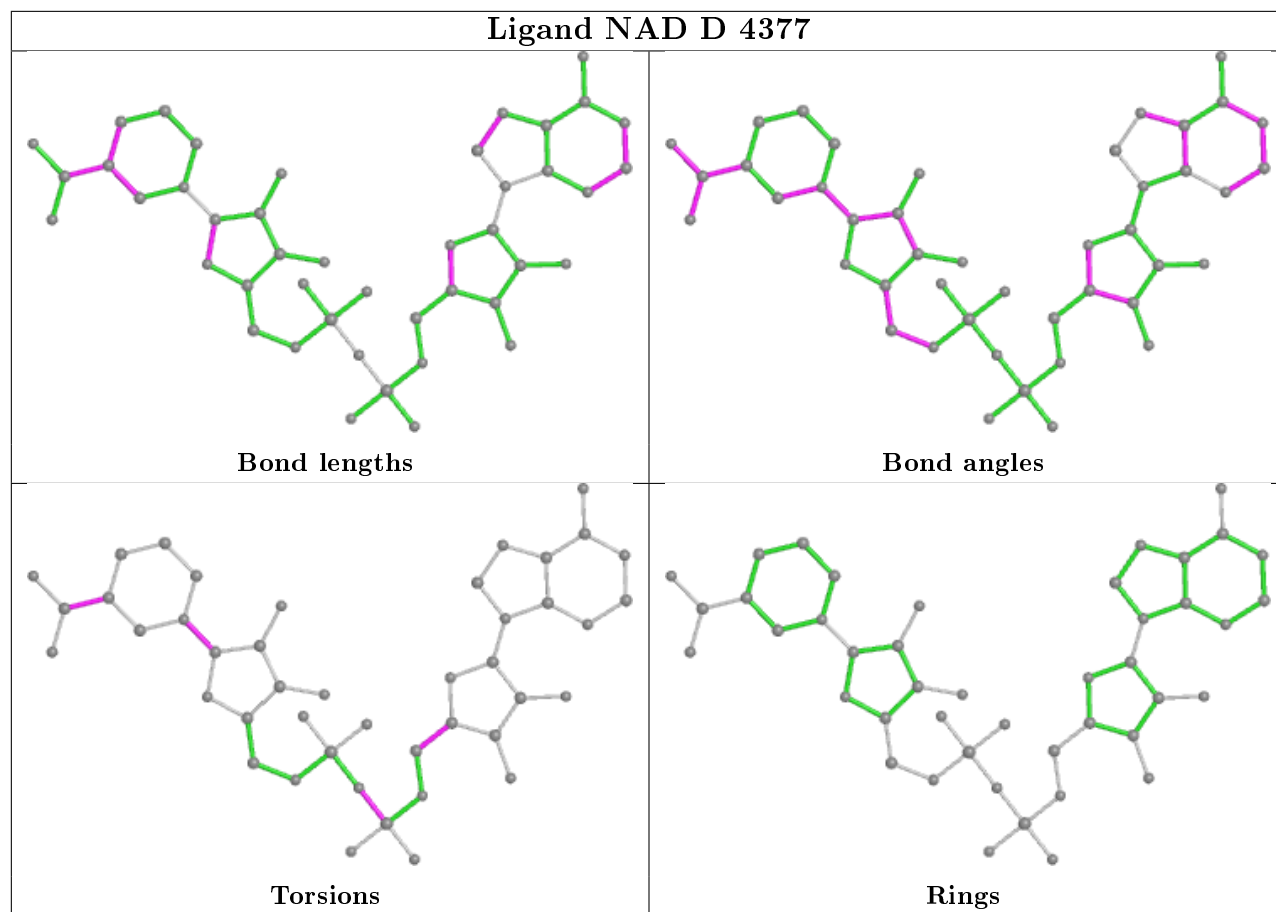
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2377	NAD	2	0
5	A	1377	NAD	3	0
3	B	506	ACT	2	0
4	B	555	CAC	1	0
5	D	4377	NAD	2	0
3	D	511	ACT	1	0
5	C	3377	NAD	2	0
3	D	509	ACT	1	0
3	A	513	ACT	1	0

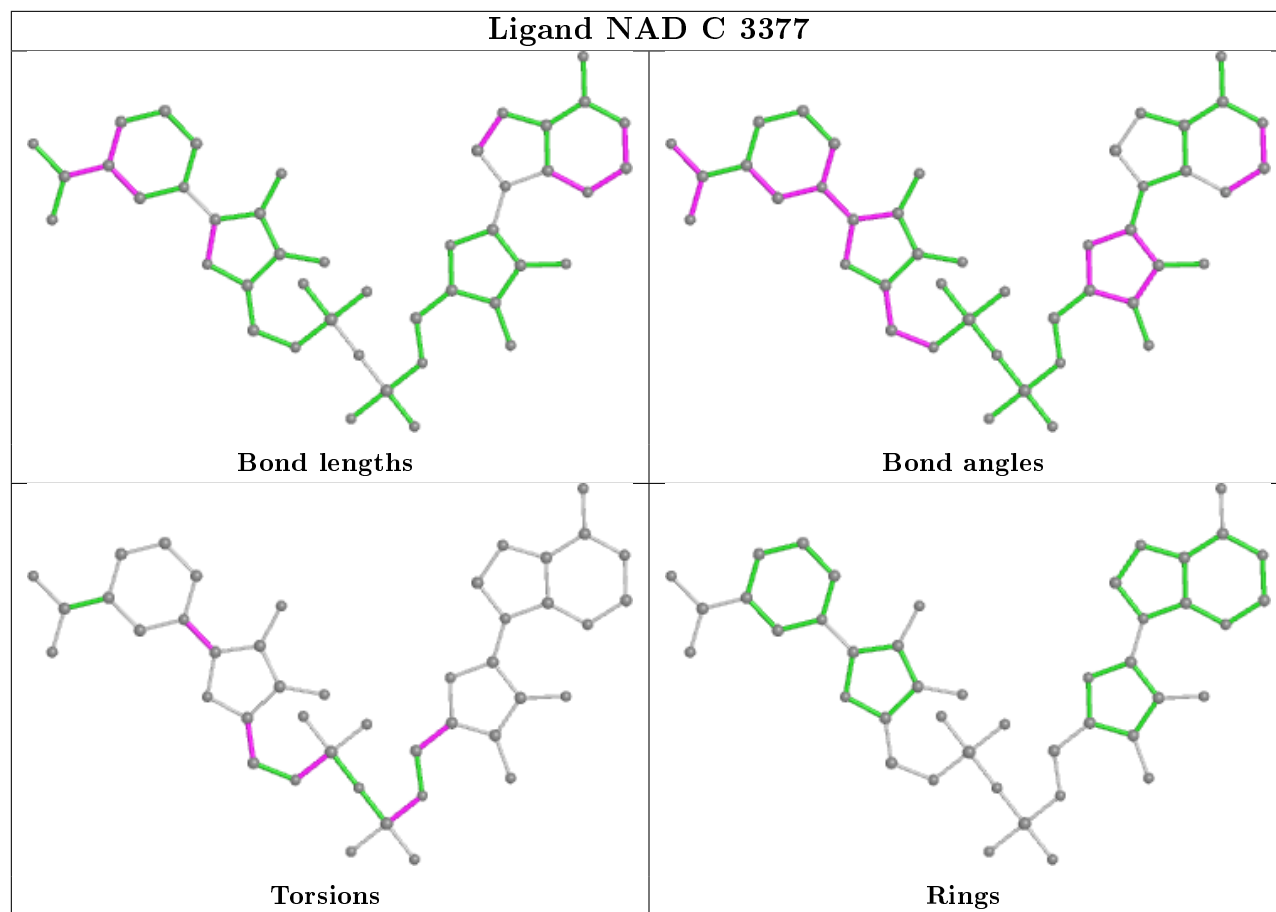
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	373/373 (100%)	-0.15	3 (0%) 86 87	11, 35, 57, 66	0
1	B	373/373 (100%)	-0.35	0 100 100	14, 31, 47, 61	0
1	C	373/373 (100%)	0.18	6 (1%) 72 74	23, 51, 67, 77	0
1	D	373/373 (100%)	-0.40	1 (0%) 94 94	9, 27, 45, 55	0
All	All	1492/1492 (100%)	-0.18	10 (0%) 87 89	9, 34, 61, 77	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	362	LEU	4.1
1	C	134	GLY	2.7
1	A	76	ILE	2.5
1	D	1	GLY	2.5
1	A	58	VAL	2.4
1	C	243	PRO	2.4
1	C	247	THR	2.3
1	A	1	GLY	2.2
1	C	332	VAL	2.1
1	C	345	LEU	2.1

### 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	D	410	1/1	0.89	0.15	41,41,41,41	1
3	ACT	D	514	4/4	0.90	0.36	52,52,52,53	4
3	ACT	A	513	4/4	0.90	0.32	52,53,53,54	4
3	ACT	D	512	4/4	0.91	0.22	25,26,28,31	0
3	ACT	A	502	4/4	0.93	0.27	46,47,47,47	4
2	ZN	C	376	1/1	0.93	0.08	50,50,50,50	0
2	ZN	A	402	1/1	0.94	0.13	40,40,40,40	1
3	ACT	A	501	4/4	0.94	0.26	42,45,45,46	0
4	CAC	B	555	5/5	0.95	0.23	76,78,80,80	0
5	NAD	C	3377	44/44	0.95	0.14	20,48,53,55	0
3	ACT	B	507	4/4	0.96	0.18	20,28,30,31	0
3	ACT	D	509	4/4	0.96	0.15	13,13,14,16	0
2	ZN	C	407	1/1	0.96	0.06	61,61,61,61	0
3	ACT	C	505	4/4	0.96	0.15	39,41,42,43	0
4	CAC	A	554	5/5	0.96	0.14	76,77,78,81	0
3	ACT	D	508	4/4	0.96	0.18	18,21,22,23	0
5	NAD	D	4377	44/44	0.97	0.11	18,24,29,32	0
2	ZN	A	401	1/1	0.97	0.08	40,40,40,40	0
3	ACT	B	506	4/4	0.97	0.16	17,27,29,32	0
5	NAD	A	1377	44/44	0.97	0.12	19,25,30,33	0
2	ZN	D	409	1/1	0.97	0.10	42,42,42,42	0
3	ACT	D	511	4/4	0.97	0.17	34,34,34,36	0
2	ZN	B	405	1/1	0.97	0.07	48,48,48,48	0
3	ACT	A	504	4/4	0.98	0.14	20,20,21,23	0
3	ACT	C	510	4/4	0.98	0.08	29,32,33,36	0
5	NAD	B	2377	44/44	0.98	0.13	11,25,31,36	0
4	CAC	B	552	5/5	0.98	0.11	47,49,52,52	0
2	ZN	D	411	1/1	0.98	0.04	53,53,53,53	0
2	ZN	B	406	1/1	0.98	0.05	43,43,43,43	0
2	ZN	A	403	1/1	0.98	0.12	48,48,48,48	0
2	ZN	A	376	1/1	0.98	0.07	33,33,33,33	0
4	CAC	B	553	5/5	0.99	0.09	45,46,50,55	0
2	ZN	D	376	1/1	0.99	0.10	28,28,28,28	0
2	ZN	A	375	1/1	0.99	0.06	42,42,42,42	0
2	ZN	B	404	1/1	0.99	0.09	27,27,27,27	0
2	ZN	C	375	1/1	0.99	0.09	35,35,35,35	0
2	ZN	D	375	1/1	0.99	0.08	25,25,25,25	0

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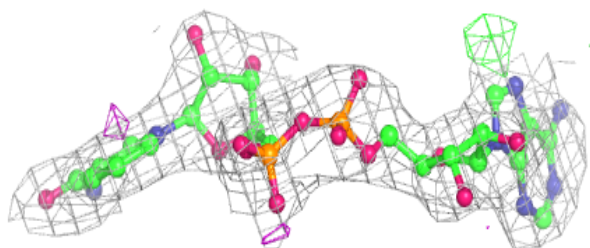
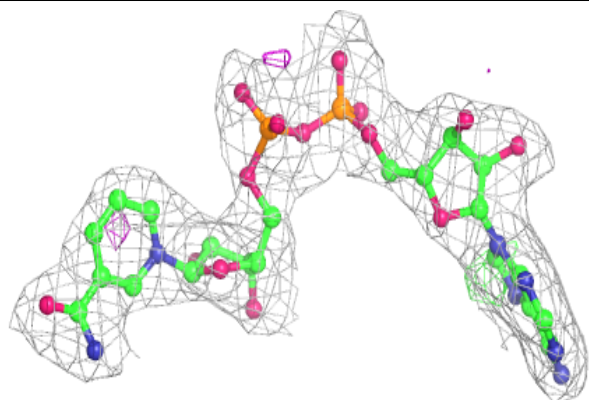
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	408	1/1	0.99	0.06	37,37,37,37	0
2	ZN	B	376	1/1	0.99	0.10	24,24,24,24	0
4	CAC	B	551	5/5	0.99	0.10	16,31,35,38	0
2	ZN	B	375	1/1	0.99	0.10	24,24,24,24	0

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

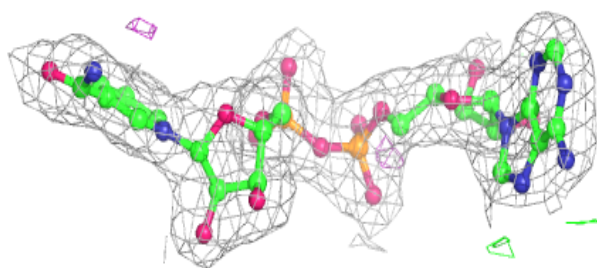
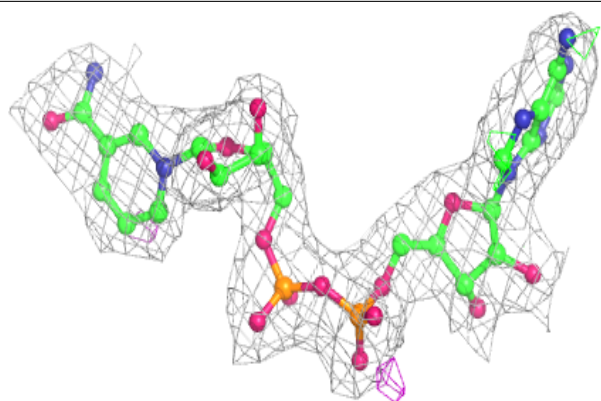
**Electron density around NAD C 3377:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

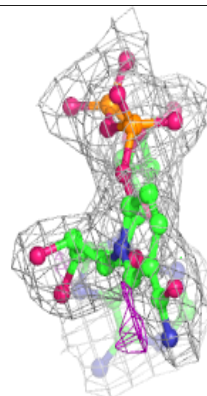
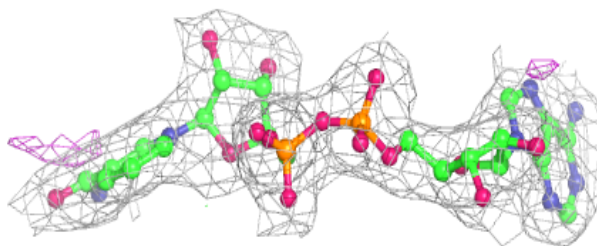
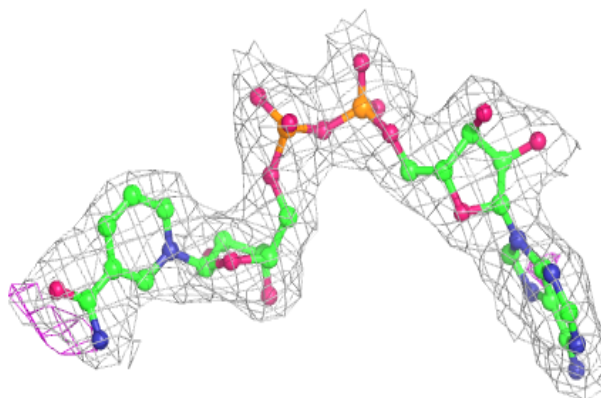


**Electron density around NAD D 4377:**

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

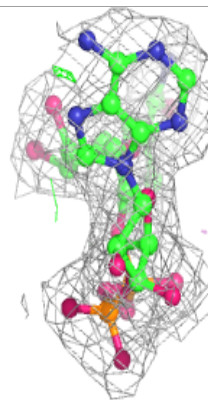
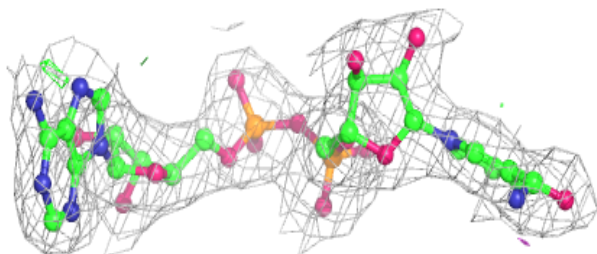
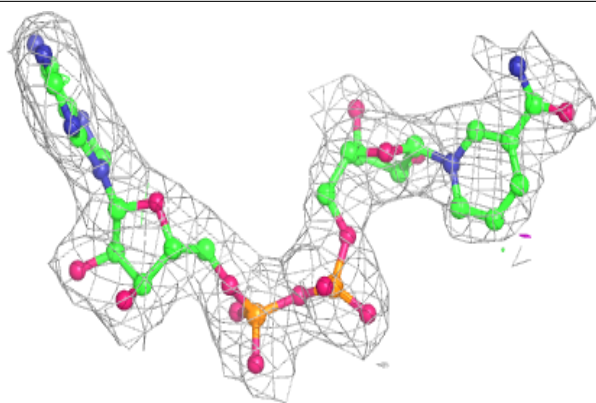
**Electron density around NAD A 1377:**

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



**Electron density around NAD B 2377:**

$2mF_o-DF_c$  (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.