



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:02 PM GMT

PDB ID : 2OXI  
Title : REFINED CRYSTAL STRUCTURE OF CU-SUBSTITUTED ALCOHOL  
DEHYDROGENASE AT 2.1 ANGSTROMS RESOLUTION  
Authors : Al-Karadaghi, S.; Cedergren-Zeppezauer, E.S.  
Deposited on : 1993-11-08  
Resolution : 2.10 Å (reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

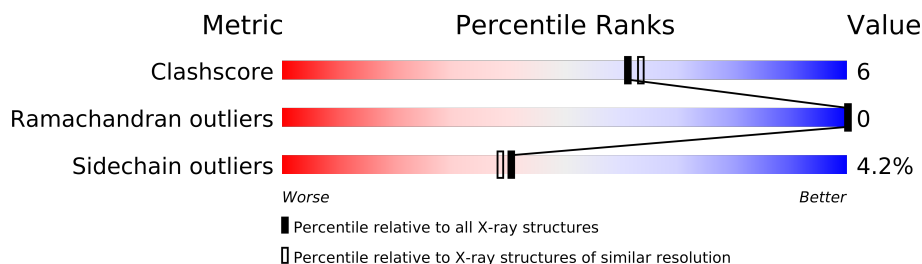
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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))
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	
1	B	374	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6125 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	89	3	0
			2791	1772	472	521	26			
1	B	374	Total	C	N	O	S	64	2	0
			2789	1771	472	521	25			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

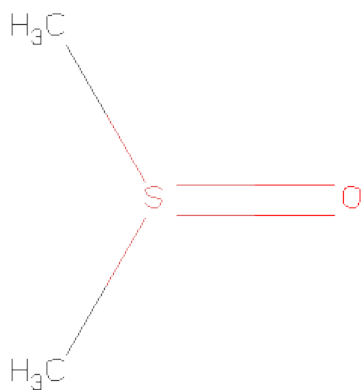
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	222	Total 222	O 222	0	0
6	B	223	Total 223	O 223	0	0

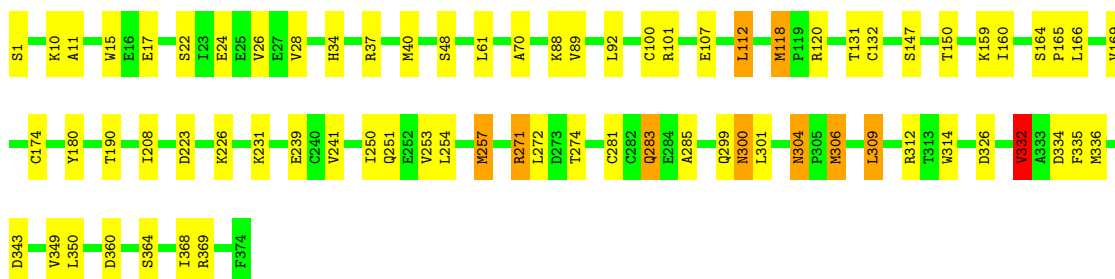
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

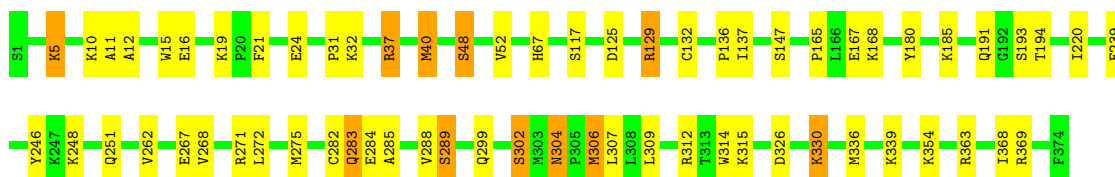
#### • Molecule 1: ALCOHOL DEHYDROGENASE

Chain A: 



#### • Molecule 1: ALCOHOL DEHYDROGENASE

Chain B: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.40Å 180.60Å 50.80Å 90.00° 108.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.97	1/2855 (0.0%)	1.62	36/3858 (0.9%)
1	B	1.01	4/2849 (0.1%)	1.62	34/3850 (0.9%)
All	All	0.99	5/5704 (0.1%)	1.62	70/7708 (0.9%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	SER	CA-CB	-6.27	1.43	1.52
1	B	284	GLU	CD-OE2	-5.62	1.19	1.25
1	B	48	SER	CA-CB	-5.49	1.44	1.52
1	B	302	SER	CA-CB	-5.38	1.44	1.52
1	A	190	THR	C-O	-5.07	1.13	1.23

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	MET	CG-SD-CE	-18.33	70.87	100.20
1	B	15	TRP	CD1-CG-CD2	11.12	115.20	106.30
1	B	40	MET	CG-SD-CE	-10.01	84.19	100.20
1	A	306	MET	CG-SD-CE	9.94	116.10	100.20
1	A	15	TRP	CD1-CG-CD2	9.17	113.64	106.30
1	A	118	MET	CA-CB-CG	9.05	128.69	113.30
1	B	246	TYR	CB-CG-CD2	-8.88	115.67	121.00
1	B	314	TRP	CD1-CG-CD2	8.80	113.34	106.30
1	B	15	TRP	CG-CD1-NE1	-8.43	101.67	110.10
1	A	1	SER	CA-C-N	7.77	134.29	117.20
1	B	15	TRP	CE2-CD2-CG	-7.69	101.14	107.30
1	A	37	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	B	180	TYR	CB-CG-CD1	-7.51	116.50	121.00
1	B	369	ARG	NE-CZ-NH1	7.41	124.01	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	VAL	CG1-CB-CG2	-7.37	99.11	110.90
1	A	314	TRP	CD1-CG-CD2	7.28	112.12	106.30
1	A	15	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	A	1	SER	CA-C-O	-7.17	105.03	120.10
1	B	167	GLU	CA-CB-CG	7.13	129.10	113.40
1	B	193	SER	N-CA-CB	-7.12	99.83	110.50
1	A	112	LEU	CB-CG-CD1	-6.87	99.32	111.00
1	A	312	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	B	314	TRP	CE2-CD2-CG	-6.69	101.95	107.30
1	B	129	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	B	363	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	15	TRP	CB-CG-CD1	-6.55	118.49	127.00
1	B	314	TRP	CG-CD1-NE1	-6.54	103.56	110.10
1	B	5	LYS	CB-CG-CD	-6.31	95.20	111.60
1	B	330	LYS	N-CA-CB	-6.27	99.31	110.60
1	A	271	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	271	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	101	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	28	VAL	CA-CB-CG1	-6.02	101.86	110.90
1	A	309	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	120	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	107	GLU	CA-C-N	5.76	127.72	116.20
1	A	314	TRP	CE2-CD2-CG	-5.72	102.73	107.30
1	B	15	TRP	CG-CD2-CE3	5.70	139.03	133.90
1	B	67	HIS	CA-C-N	5.68	129.69	117.20
1	B	168	LYS	CB-CG-CD	-5.64	96.92	111.60
1	A	1	SER	CA-CB-OG	-5.60	96.07	111.20
1	A	301	LEU	CA-CB-CG	5.60	128.18	115.30
1	B	363	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	257	MET	CG-SD-CE	5.58	109.14	100.20
1	B	180	TYR	CD1-CG-CD2	5.58	124.03	117.90
1	A	332	VAL	CA-CB-CG2	-5.57	102.55	110.90
1	A	314	TRP	CG-CD1-NE1	-5.55	104.55	110.10
1	B	125	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	368	ILE	N-CA-C	-5.52	96.09	111.00
1	A	368	ILE	N-CA-C	-5.49	96.17	111.00
1	A	101	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	37	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	223	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	117	SER	CB-CA-C	-5.39	99.85	110.10
1	B	246	TYR	CD1-CG-CD2	5.35	123.79	117.90
1	A	326	ASP	CB-CG-OD1	5.30	123.07	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	220	ILE	CA-C-N	5.29	126.79	116.20
1	A	364	SER	O-C-N	-5.28	114.22	123.20
1	A	15	TRP	CG-CD1-NE1	-5.26	104.84	110.10
1	B	268	VAL	CG1-CB-CG2	-5.21	102.57	110.90
1	B	251	GLN	CA-CB-CG	5.21	124.85	113.40
1	B	15	TRP	CD1-NE1-CE2	5.19	113.67	109.00
1	A	226	LYS	CA-CB-CG	5.18	124.81	113.40
1	A	300	ASN	CB-CG-ND2	5.11	128.97	116.70
1	A	180	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	A	369	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	271	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	17	GLU	CA-CB-CG	5.03	124.47	113.40
1	A	334	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2791	0	2851	36	0
1	B	2789	0	2850	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	44	0	26	1	0
4	B	44	0	26	0	0
5	A	4	0	6	6	0
5	B	4	0	6	6	0
6	A	222	0	0	2	0
6	B	223	0	0	0	0
All	All	6125	0	5765	64	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (64) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:48:SER:OG	5:B:378:DMS:H11	1.59	1.01
1:B:48:SER:OG	5:B:378:DMS:C1	2.13	0.94
1:A:48:SER:HB3	5:A:378:DMS:H12	1.48	0.92
1:B:48:SER:CB	5:B:378:DMS:H12	2.04	0.87
1:B:48:SER:HB3	5:B:378:DMS:H12	1.57	0.85
1:A:48:SER:CB	5:A:378:DMS:H12	2.16	0.75
1:A:251:GLN:HA	1:A:281[B]:CYS:SG	2.27	0.75
1:B:48:SER:OG	5:B:378:DMS:H12	1.93	0.68
1:A:283:GLN:HE22	1:A:285:ALA:HB3	1.64	0.63
1:B:165:PRO:HD3	1:B:336:MET:HE1	1.83	0.61
1:A:160:ILE:HB	1:A:332:VAL:HG11	1.82	0.60
1:B:48:SER:CB	5:B:378:DMS:C1	2.70	0.59
1:A:100:CYS:HB2	1:A:112:LEU:HD12	1.86	0.58
1:A:40:MET:CE	1:A:150:THR:HG22	2.35	0.57
1:A:283:GLN:NE2	1:A:285:ALA:H	2.05	0.54
1:A:26:VAL:HG12	1:A:132:CYS:HB2	1.90	0.54
1:B:304:ASN:HD22	1:B:306:MET:H	1.56	0.54
1:A:48:SER:CB	5:A:378:DMS:C1	2.84	0.53
1:B:282[B]:CYS:SG	1:B:288:VAL:O	2.66	0.53
1:A:48:SER:OG	5:A:378:DMS:H11	2.09	0.52
1:A:254:LEU:HD12	1:A:281[B]:CYS:SG	2.49	0.52
1:B:31:PRO:HD3	1:B:37:ARG:HB2	1.91	0.52
1:B:283:GLN:HE22	1:B:285:ALA:HB3	1.75	0.52
1:B:272:LEU:HD11	1:B:299:GLN:HE21	1.74	0.52
1:A:34:HIS:HE1	6:A:542:HOH:O	1.93	0.52
1:A:48:SER:HB3	5:A:378:DMS:C1	2.31	0.51
1:A:165:PRO:HD3	1:A:336:MET:HE1	1.91	0.51
1:A:336:MET:HA	1:A:336:MET:HE2	1.92	0.50
1:A:166:LEU:HA	1:A:169:VAL:HG22	1.92	0.50
1:B:283:GLN:NE2	1:B:285:ALA:H	2.09	0.50
1:B:132:CYS:HB3	1:B:137:ILE:HD11	1.94	0.50
1:A:304:ASN:ND2	1:A:306:MET:H	2.10	0.49
1:B:194:THR:HG22	1:B:262:VAL:HG12	1.96	0.48
1:A:253:VAL:O	1:A:257:MET:HG3	2.12	0.48
1:B:304:ASN:ND2	1:B:306:MET:H	2.12	0.48
1:A:89:VAL:HG12	1:A:159:LYS:HA	1.96	0.47
1:A:241:VAL:HG21	1:A:250:ILE:HD11	1.97	0.46
1:B:326:ASP:O	1:B:330:LYS:HE2	2.16	0.46
1:A:48:SER:OG	5:A:378:DMS:C1	2.64	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:174:CYS:SG	4:A:377:NAD:H5N	2.57	0.45
1:A:92:LEU:HA	6:A:443:HOH:O	2.16	0.45
1:A:304:ASN:HD22	1:A:306:MET:H	1.65	0.45
1:A:165:PRO:HG2	1:A:335:PHE:HE2	1.82	0.45
1:A:40:MET:HE3	1:A:150:THR:HG22	2.00	0.44
1:B:16:GLU:HG3	1:B:19:LYS:HG2	1.98	0.44
1:A:283:GLN:HE22	1:A:285:ALA:H	1.64	0.44
1:B:267:GLU:HG3	1:B:275:MET:HA	2.00	0.44
1:B:16:GLU:HG3	1:B:19:LYS:CG	2.48	0.43
1:A:70:ALA:HB1	1:A:166:LEU:HD22	2.00	0.42
1:B:32:LYS:HD2	1:B:129:ARG:NH2	2.33	0.42
1:B:272:LEU:HD11	1:B:299:GLN:HB3	2.02	0.42
1:A:271:ARG:HB2	1:A:274:THR:OG1	2.20	0.42
1:A:272:LEU:HD11	1:A:299:GLN:HB3	2.00	0.42
1:A:88:LYS:HE2	1:A:166:LEU:HG	2.02	0.42
1:B:12:ALA:HB1	1:B:21:PHE:HB3	2.01	0.41
1:A:11:ALA:HA	1:A:147:SER:HA	2.01	0.41
1:A:208:ILE:HG21	1:A:208:ILE:HD13	1.92	0.41
1:B:10:LYS:HA	1:B:24:GLU:O	2.21	0.41
1:A:349:VAL:O	1:A:350:LEU:HD23	2.21	0.41
1:B:307:LEU:O	1:B:312:ARG:HD2	2.22	0.40
1:B:282[B]:CYS:SG	1:B:289:SER:HB2	2.61	0.40
1:B:11:ALA:HA	1:B:147:SER:HA	2.02	0.40
1:B:40:MET:HE2	1:B:40:MET:HB2	1.78	0.40
1:A:10:LYS:HA	1:A:24:GLU:O	2.22	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	375/374 (100%)	359 (96%)	16 (4%)	0	100	100
1	B	374/374 (100%)	358 (96%)	16 (4%)	0	100	100
All	All	749/748 (100%)	717 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	311/308 (101%)	298 (96%)	13 (4%)	40	38
1	B	310/308 (101%)	297 (96%)	13 (4%)	40	38
All	All	621/616 (101%)	595 (96%)	26 (4%)	40	38

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	61	LEU
1	A	118	MET
1	A	131	THR
1	A	164	SER
1	A	231	LYS
1	A	239	GLU
1	A	283	GLN
1	A	300	ASN
1	A	304	ASN
1	A	309	LEU
1	A	332	VAL
1	A	343	ASP
1	B	5	LYS
1	B	136	PRO
1	B	185	LYS
1	B	191	GLN
1	B	239	GLU
1	B	248	LYS
1	B	283	GLN
1	B	302	SER
1	B	304	ASN
1	B	309	LEU
1	B	315	LYS
1	B	339	LYS
1	B	354	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	304	ASN
1	B	283	GLN
1	B	299	GLN
1	B	300	ASN
1	B	304	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z  > 2$
4	NAD	A	377	-	48,48,48	0.98	3 (6%)	73,73,73	1.84	15 (20%)
5	DMS	A	378	-	3,3,3	0.08	0	3,3,3	1.09	0
4	NAD	B	377	-	48,48,48	1.04	3 (6%)	73,73,73	1.83	12 (16%)
5	DMS	B	378	-	3,3,3	0.48	0	3,3,3	2.35	2 (66%)

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
4	NAD	A	377	-	-	0/30/62/62	0/3/5/5
5	DMS	A	378	-	-	0/0/0/0	0/0/0/0
4	NAD	B	377	-	-	0/30/62/62	0/3/5/5
5	DMS	B	378	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	377	NAD	C2N-N1N	3.01	1.39	1.35
4	B	377	NAD	C4A-N9A	-2.99	1.33	1.37
4	A	377	NAD	O4D-C1D	2.58	1.45	1.41
4	B	377	NAD	O4D-C1D	2.38	1.45	1.41
4	B	377	NAD	C2N-N1N	2.22	1.38	1.35
4	A	377	NAD	O4B-C1B	2.15	1.44	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	377	NAD	N3A-C4A-N9A	7.19	138.41	125.43
4	A	377	NAD	N3A-C4A-N9A	6.74	137.61	125.43
4	B	377	NAD	N3A-C2A-N1A	-6.65	123.15	128.71
4	A	377	NAD	N3A-C2A-N1A	-6.14	123.57	128.71
4	A	377	NAD	O4B-C1B-N9A	4.87	112.97	108.44
4	A	377	NAD	C4A-C5A-N7A	4.44	113.33	109.52
4	B	377	NAD	C5A-C4A-N3A	-4.18	116.61	125.70
4	B	377	NAD	O7N-C7N-C3N	-3.70	115.41	119.58
4	B	377	NAD	C6A-C5A-C4A	3.57	123.80	117.25
4	A	377	NAD	C5A-C4A-N3A	-3.45	118.18	125.70
4	A	377	NAD	C6A-C5A-C4A	3.43	123.55	117.25
5	B	378	DMS	O-S-C2	3.01	123.25	106.62
4	B	377	NAD	C4A-C5A-N7A	2.96	112.06	109.52
4	B	377	NAD	O4B-C4B-C5B	-2.95	98.82	109.36
4	B	377	NAD	C2N-C3N-C4N	2.87	121.57	118.31
4	A	377	NAD	C2N-C3N-C4N	2.78	121.45	118.31
4	B	377	NAD	C4D-O4D-C1D	-2.65	106.87	109.75
4	A	377	NAD	N6A-C6A-N1A	2.45	124.17	119.36
5	B	378	DMS	C2-S-C1	-2.42	85.14	98.56
4	A	377	NAD	O3D-C3D-C4D	-2.38	104.08	111.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	377	NAD	C5A-C4A-N9A	-2.33	103.81	107.16
4	A	377	NAD	O4D-C1D-N1N	2.32	110.32	107.95
4	A	377	NAD	O5B-C5B-C4B	-2.29	100.52	108.94
4	A	377	NAD	C6A-C5A-N7A	-2.29	122.58	131.34
4	B	377	NAD	C2A-N3A-C4A	2.14	120.11	114.01
4	B	377	NAD	O4D-C4D-C5D	-2.05	102.03	109.36
4	A	377	NAD	C4B-O4B-C1B	-2.04	107.53	109.75
4	A	377	NAD	C6N-N1N-C2N	-2.04	119.74	122.04
4	B	377	NAD	C3N-C7N-N7N	2.03	120.08	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.