



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2017 – 08:38 PM EST

PDB ID : 1HDX  
Title : THREE-DIMENSIONAL STRUCTURES OF THREE HUMAN ALCOHOL DEHYDROGENASE VARIANTS: CORRELATIONS WITH THEIR FUNCTIONAL DIFFERENCES  
Authors : Hurley, T.D.; Amzel, L.M.  
Deposited on : unknown  
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

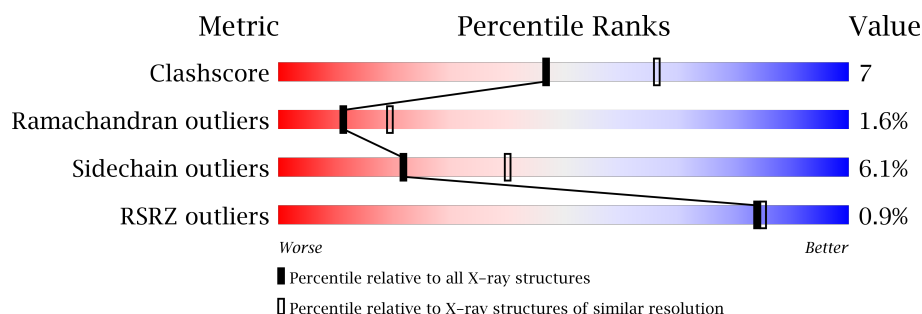
# 1 Overall quality at a glance

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))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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. 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	374	 79% 19% .
1	B	374	 75% 22% ..

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
4	CXL	A	378	-	-	-	X
4	CXL	B	378	-	-	X	X



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.

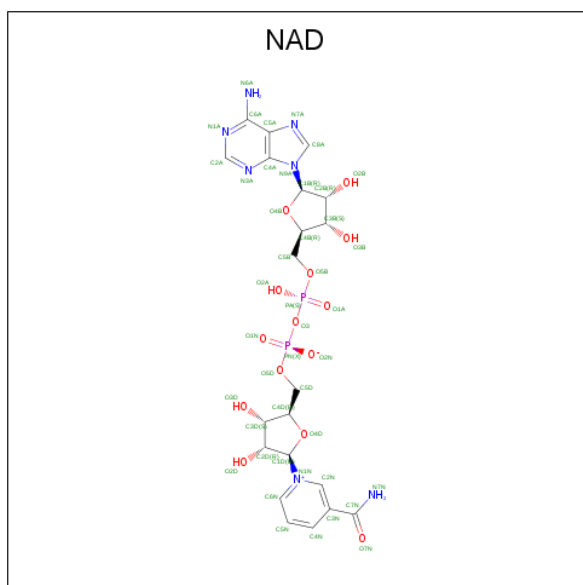
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total 2781	C 1770	N 473	O 516	S 22	0	0	0
1	B	374	Total 2781	C 1770	N 473	O 516	S 22	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula:  $\text{Zn}$ ).

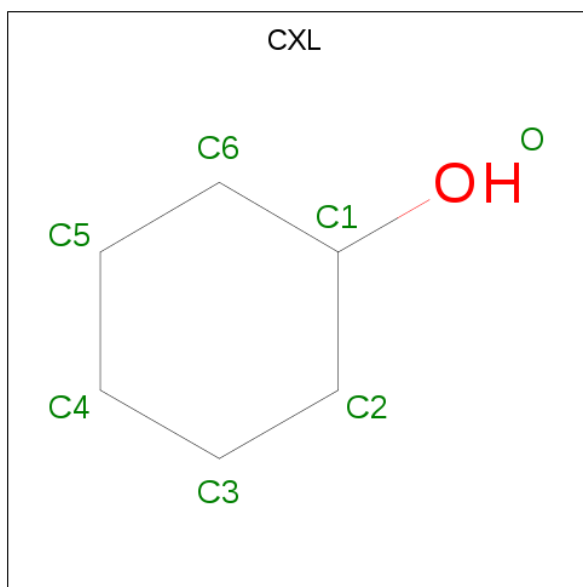
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$ ).



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

- Molecule 4 is CYCLOHEXANOL (three-letter code: CXL) (formula:  $C_6H_{12}O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	6	1		
4	B	1	Total	C	O	0	0
			7	6	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula:  $Cl$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

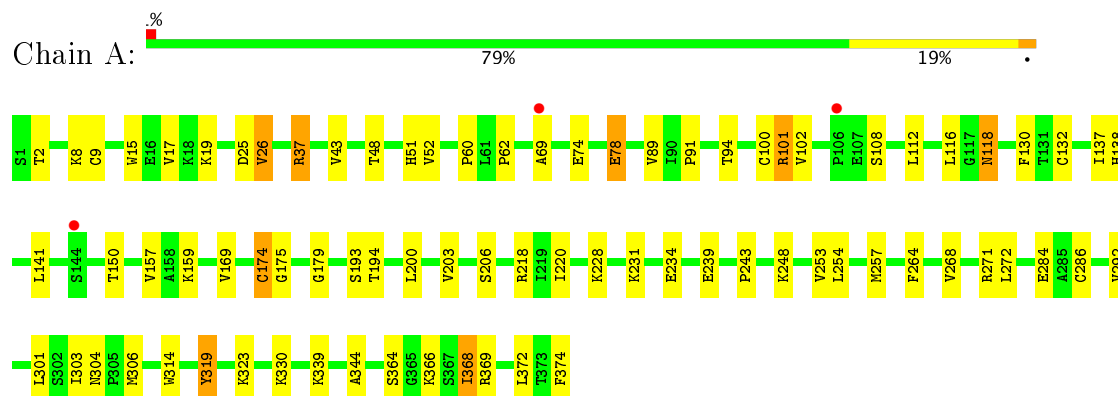
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	63	Total	O	0	0
			63	63		
6	B	47	Total	O	0	0
			47	47		

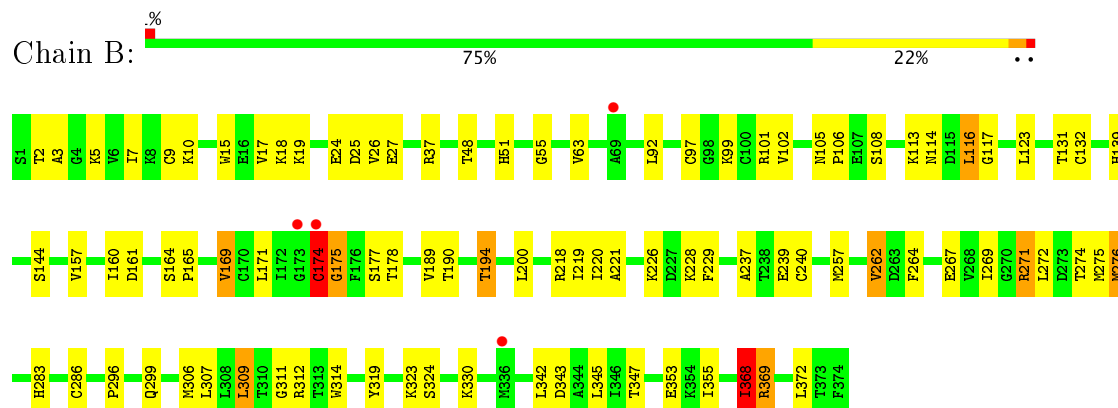
### 3 Residue-property plots [i](#)

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



#### • Molecule 1: ALCOHOL DEHYDROGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.58Å 44.94Å 94.30Å 92.29° 103.37° 68.97°	Depositor
Resolution (Å)	7.00 – 2.50 28.15 – 2.37	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.50) 65.6 (28.15-2.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.21 (at 2.36Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.179 , (Not available) 0.162 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 81.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5779	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% 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

### 5.1 Standard geometry

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

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	0.77	1/2833 (0.0%)	1.40	18/3833 (0.5%)
1	B	0.73	1/2833 (0.0%)	1.36	13/3833 (0.3%)
All	All	0.75	2/5666 (0.0%)	1.38	31/7666 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	VAL	CA-CB	5.08	1.65	1.54
1	B	63	VAL	CA-CB	5.07	1.65	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	ARG	NE-CZ-NH1	9.25	124.93	120.30
1	A	37	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	314	TRP	CD1-CG-CD2	8.61	113.18	106.30
1	A	37	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	A	319	TYR	CB-CG-CD2	-7.82	116.31	121.00
1	A	314	TRP	CE2-CD2-CG	-7.72	101.12	107.30
1	B	368	ILE	N-CA-C	-7.56	90.58	111.00
1	B	15	TRP	CD1-CG-CD2	7.00	111.90	106.30
1	B	314	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	B	15	TRP	CE2-CD2-CG	-6.94	101.75	107.30
1	B	314	TRP	CD1-CG-CD2	6.88	111.81	106.30
1	A	15	TRP	CE2-CD2-CG	-6.79	101.87	107.30
1	A	15	TRP	CD1-CG-CD2	6.79	111.73	106.30
1	B	169	VAL	CG1-CB-CG2	-6.52	100.47	110.90
1	A	257	MET	CA-CB-CG	6.24	123.91	113.30
1	A	101	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	368	ILE	N-CA-C	-5.96	94.91	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	323	LYS	N-CA-C	-5.83	95.27	111.00
1	B	271	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	101	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	369	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	271	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	218	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	52	VAL	CG1-CB-CG2	-5.42	102.23	110.90
1	B	314	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	B	194	THR	CA-CB-CG2	5.32	119.84	112.40
1	B	101	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	319	TYR	CB-CG-CD1	5.09	124.06	121.00
1	A	314	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	B	323	LYS	N-CA-C	-5.04	97.38	111.00

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	2781	0	2856	35	0
1	B	2781	0	2856	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	26	3	0
3	B	44	0	26	1	0
4	A	7	0	12	0	0
4	B	7	0	12	7	0
5	B	1	0	0	0	0
6	A	63	0	0	1	0
6	B	47	0	0	2	0
All	All	5779	0	5788	81	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 (81) 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:116:LEU:HB3	4:B:378:CXL:H41	1.42	0.99
1:B:116:LEU:CD2	4:B:378:CXL:H62	1.93	0.98
1:B:116:LEU:HD22	4:B:378:CXL:H62	1.51	0.92
1:A:116:LEU:HD23	1:A:141:LEU:HD22	1.53	0.88
1:A:8:LYS:HE2	1:A:25:ASP:HB3	1.60	0.82
1:B:272:LEU:HD11	1:B:299:GLN:HB3	1.61	0.81
1:B:116:LEU:HD23	4:B:378:CXL:H62	1.66	0.77
1:B:178:THR:HG21	3:B:377:NAD:C4N	2.18	0.73
1:A:231:LYS:HD2	1:A:344:ALA:HB1	1.71	0.72
1:B:26:VAL:HG12	1:B:132:CYS:HB2	1.72	0.72
1:B:194:THR:HG22	1:B:262:VAL:HG12	1.72	0.71
1:B:116:LEU:CB	4:B:378:CXL:H41	2.23	0.66
1:B:116:LEU:HB3	4:B:378:CXL:C4	2.25	0.61
1:A:175:GLY:HA2	1:A:203:VAL:HG22	1.85	0.58
1:A:108:SER:OG	1:B:286:CYS:HB3	2.04	0.58
1:A:26:VAL:HG12	1:A:132:CYS:HB2	1.85	0.58
1:A:89:VAL:HG12	1:A:159:LYS:HA	1.86	0.57
1:A:200:LEU:O	1:A:228:LYS:HE2	2.07	0.55
1:A:193:SER:HG	1:A:264:PHE:HE2	1.54	0.55
1:B:102:VAL:HG13	1:B:108:SER:HB2	1.89	0.55
1:B:200:LEU:O	1:B:228:LYS:HD2	2.08	0.54
1:B:92:LEU:HD13	1:B:324:SER:HB2	1.90	0.54
1:B:307:LEU:O	1:B:312:ARG:HD2	2.08	0.53
1:B:272:LEU:HD23	1:B:275:MET:CE	2.40	0.52
1:A:69:ALA:O	1:A:91:PRO:HD2	2.10	0.52
1:B:369:ARG:HA	6:B:605:HOH:O	2.11	0.51
1:B:296:PRO:HB2	1:B:299:GLN:NE2	2.27	0.50
1:B:7:ILE:O	1:B:27:GLU:HA	2.13	0.49
1:A:272:LEU:HD22	1:A:301:LEU:HG	1.93	0.48
1:B:345:LEU:O	1:B:368:ILE:HB	2.14	0.48
1:B:17:VAL:HG12	1:B:18:LYS:HG3	1.96	0.48
1:A:268:VAL:HG12	3:A:377:NAD:H52N	1.96	0.47
1:B:174:CYS:SG	1:B:175:GLY:N	2.87	0.47
1:B:10:LYS:HA	1:B:24:GLU:O	2.15	0.47
1:A:100:CYS:HB2	1:A:112:LEU:HD12	1.97	0.47
1:A:94:THR:OG1	1:A:116:LEU:HD11	2.14	0.47
1:B:19:LYS:HA	1:B:19:LYS:HD3	1.68	0.47
1:A:248:LYS:HG3	1:A:253:VAL:HG23	1.96	0.46
1:B:171:LEU:HD12	1:B:342:LEU:HB3	1.97	0.46
1:A:130:PHE:HB2	1:A:137:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:PHE:CD1	1:B:240:CYS:HB3	2.51	0.45
1:A:364:SER:HB2	1:A:366:LYS:HD3	1.97	0.45
1:B:200:LEU:HD11	1:B:221:ALA:HB1	1.97	0.45
1:A:43:VAL:HG13	1:A:374:PHE:HE1	1.80	0.45
1:B:226:LYS:HG2	1:B:229:PHE:CE2	2.51	0.45
1:B:55:GLY:HA2	6:B:604:HOH:O	2.16	0.45
1:B:5:LYS:HD3	1:B:5:LYS:HA	1.80	0.45
1:A:48:THR:O	1:A:51:HIS:HB2	2.17	0.45
1:A:102:VAL:HG13	1:A:108:SER:HB3	1.99	0.45
1:B:306:MET:SD	1:B:309:LEU:HD22	2.57	0.45
1:B:9:CYS:O	1:B:25:ASP:HA	2.16	0.45
1:A:9:CYS:O	1:A:25:ASP:HA	2.16	0.44
1:A:292:VAL:O	3:A:377:NAD:H2N	2.17	0.44
1:A:62:PRO:O	1:A:138:HIS:HB2	2.18	0.43
1:B:116:LEU:HD22	4:B:378:CXL:C6	2.37	0.43
1:B:218:ARG:HH22	1:B:257:MET:HG2	1.84	0.43
1:A:179:GLY:HA3	1:A:206:SER:HB2	2.01	0.43
1:B:347:THR:HG21	1:B:368:ILE:HG12	2.01	0.43
1:B:105:ASN:HA	1:B:106:PRO:HD3	1.89	0.43
1:B:139:HIS:HA	1:B:144:SER:OG	2.18	0.43
1:A:60:PRO:HD3	6:A:404:HOH:O	2.18	0.43
1:A:118:ASN:HD22	1:A:118:ASN:HA	1.71	0.42
1:A:78:GLU:HG3	1:A:78:GLU:H	1.70	0.42
1:B:220:ILE:HG12	1:B:239:GLU:HG3	2.02	0.42
1:B:219:ILE:HB	1:B:237:ALA:HA	2.01	0.42
1:A:304:ASN:OD1	1:A:306:MET:HB2	2.20	0.41
1:B:161:ASP:HB3	1:B:164:SER:OG	2.20	0.41
1:A:174:CYS:SG	3:A:377:NAD:H5N	2.60	0.41
1:B:355:ILE:HG13	1:B:372:LEU:HD11	2.02	0.41
1:B:276:MET:CE	1:B:276:MET:HA	2.50	0.41
1:A:19:LYS:HA	1:A:19:LYS:HD3	1.88	0.41
1:A:220:ILE:HG21	1:A:254:LEU:HD21	2.03	0.41
1:B:123:LEU:HA	1:B:123:LEU:HD23	1.93	0.41
1:B:48:THR:HA	1:B:51:HIS:CD2	2.56	0.41
1:A:286:CYS:HB3	1:B:108:SER:HB3	2.03	0.40
1:B:114:ASN:HB2	1:B:116:LEU:HD12	2.02	0.40
1:B:189:VAL:HA	1:B:264:PHE:CE2	2.56	0.40
1:A:43:VAL:HG22	1:A:372:LEU:HB2	2.04	0.40
1:A:37:ARG:HD2	1:A:74:GLU:OE1	2.22	0.40
1:A:43:VAL:HG12	1:A:69:ALA:HB2	2.03	0.40
1:B:164:SER:HA	1:B:165:PRO:HD2	1.89	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/374 (100%)	346 (93%)	24 (6%)	2 (0%)	32	53
1	B	372/374 (100%)	338 (91%)	24 (6%)	10 (3%)	6	9
All	All	744/748 (100%)	684 (92%)	48 (6%)	12 (2%)	11	19

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	CYS
1	A	284	GLU
1	B	3	ALA
1	B	97	CYS
1	B	117	GLY
1	B	169	VAL
1	B	175	GLY
1	B	311	GLY
1	B	368	ILE
1	A	368	ILE
1	B	269	ILE
1	B	160	ILE

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/305 (100%)	288 (94%)	17 (6%)	25	45
1	B	305/305 (100%)	285 (93%)	20 (7%)	19	36
All	All	610/610 (100%)	573 (94%)	37 (6%)	22	40

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	17	VAL
1	A	78	GLU
1	A	101	ARG
1	A	118	ASN
1	A	150	THR
1	A	157	VAL
1	A	169	VAL
1	A	174	CYS
1	A	194	THR
1	A	234	GLU
1	A	239	GLU
1	A	243	PRO
1	A	303	ILE
1	A	319	TYR
1	A	330	LYS
1	A	339	LYS
1	B	2	THR
1	B	99	LYS
1	B	113	LYS
1	B	116	LEU
1	B	131	THR
1	B	157	VAL
1	B	174	CYS
1	B	177	SER
1	B	190	THR
1	B	262	VAL
1	B	267	GLU
1	B	271	ARG
1	B	274	THR
1	B	276	MET
1	B	283	HIS
1	B	309	LEU
1	B	319	TYR
1	B	330	LYS

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Mol	Chain	Res	Type
1	B	343	ASP
1	B	353	GLU

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	118	ASN
1	A	138	HIS
1	A	283	HIS
1	A	348	HIS
1	B	244	GLN
1	B	300	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 5 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	$\# Z  > 2$
3	NAD	A	377	-	41,48,48	2.06	7 (17%)	43,73,73	1.87	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CXL	A	378	-	7,7,7	1.29	1 (14%)	8,8,8	0.99	1 (12%)
3	NAD	B	377	-	41,48,48	1.95	5 (12%)	43,73,73	1.74	8 (18%)
4	CXL	B	378	-	7,7,7	1.29	1 (14%)	8,8,8	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	377	-	-	0/22/62/62	0/5/5/5
4	CXL	A	378	-	-	0/0/8/8	0/1/1/1
3	NAD	B	377	-	-	0/22/62/62	0/5/5/5
4	CXL	B	378	-	-	0/0/8/8	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	377	NAD	C3N-C7N	-10.58	1.34	1.50
3	B	377	NAD	C3N-C7N	-10.09	1.34	1.50
3	A	377	NAD	C2N-C3N	-3.46	1.33	1.39
3	B	377	NAD	C4N-C3N	-3.04	1.34	1.39
3	B	377	NAD	C2N-C3N	-2.98	1.34	1.39
3	B	377	NAD	C5N-C4N	-2.84	1.33	1.38
3	A	377	NAD	C5N-C4N	-2.79	1.33	1.38
3	A	377	NAD	C4N-C3N	-2.72	1.34	1.39
3	B	377	NAD	C5A-N7A	-2.46	1.31	1.39
3	A	377	NAD	C4A-N3A	-2.36	1.32	1.35
3	A	377	NAD	C5A-N7A	-2.10	1.32	1.39
3	A	377	NAD	C3D-C4D	-2.06	1.47	1.53
4	A	378	CXL	C6-C1	2.41	1.57	1.51
4	B	378	CXL	C6-C1	2.53	1.57	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	377	NAD	N3A-C2A-N1A	-7.36	122.45	128.86
3	B	377	NAD	N3A-C2A-N1A	-6.14	123.51	128.86
3	B	377	NAD	O7N-C7N-N7N	-4.39	116.34	122.58
3	A	377	NAD	O7N-C7N-N7N	-3.31	117.88	122.58
3	A	377	NAD	O2D-C2D-C3D	-3.05	102.06	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	377	NAD	O2D-C2D-C3D	-2.87	102.65	111.83
3	B	377	NAD	O3D-C3D-C4D	-2.44	103.95	111.09
3	B	377	NAD	C5D-C4D-C3D	-2.36	106.30	115.29
3	B	377	NAD	O3B-C3B-C4B	-2.28	104.42	111.09
3	A	377	NAD	O3D-C3D-C4D	-2.25	104.51	111.09
3	A	377	NAD	C4B-O4B-C1B	-2.10	107.54	109.77
3	B	377	NAD	C4B-O4B-C1B	2.02	111.92	109.77
3	A	377	NAD	C2A-N1A-C6A	2.03	122.32	118.77
4	A	378	CXL	C5-C4-C3	2.04	117.60	111.21
3	A	377	NAD	C2N-C3N-C4N	2.18	120.74	118.26
3	A	377	NAD	C4D-O4D-C1D	2.98	112.94	109.77
3	B	377	NAD	C3N-C7N-N7N	3.57	121.85	117.77
3	A	377	NAD	C3N-C7N-N7N	4.17	122.54	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	377	NAD	3	0
3	B	377	NAD	1	0
4	B	378	CXL	7	0

## 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	374/374 (100%)	-0.63	3 (0%) 86 86	8, 25, 43, 58	0
1	B	374/374 (100%)	-0.45	4 (1%) 80 81	9, 32, 54, 69	0
All	All	748/748 (100%)	-0.54	7 (0%) 84 85	8, 28, 49, 69	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	69	ALA	3.3
1	B	336	MET	2.6
1	B	174	CYS	2.5
1	A	144	SER	2.3
1	A	69	ALA	2.2
1	B	173	GLY	2.2
1	A	106	PRO	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CXL	B	378	7/7	0.77	1.01	26.45	48,49,50,50	0
4	CXL	A	378	7/7	0.84	0.46	6.99	32,33,41,42	0
3	NAD	A	377	44/44	0.97	0.13	-0.24	2,17,26,31	0
3	NAD	B	377	44/44	0.97	0.10	-0.89	14,21,30,40	0
2	ZN	B	375	1/1	1.00	0.03	-2.56	31,31,31,31	0
2	ZN	A	376	1/1	0.97	0.10	-2.60	37,37,37,37	1
2	ZN	B	376	1/1	0.94	0.07	-3.41	38,38,38,38	1
2	ZN	A	375	1/1	0.99	0.01	-3.58	29,29,29,29	0
5	CL	B	601	1/1	0.99	0.27	-	47,47,47,47	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.