



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:39 am GMT

PDB ID : 1HF3  
Title : ATOMIC X-RAY STRUCTURE OF LIVER ALCOHOL DEHYDROGENASE CONTAINING CADMIUM AND A HYDROXIDE ADDUCT TO NADH  
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Deposited on : 2000-11-27  
Resolution : 1.95 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 : trunk28620  
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) : recalc28949

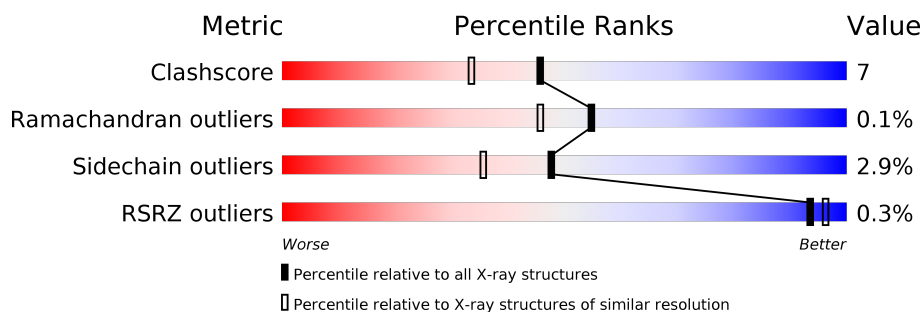
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	<div> <div>78%</div> <div>19%</div> <div>.</div> </div>
1	B	374	<div> <div>77%</div> <div>20%</div> <div>..</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MRD	A	403	-	-	-	X
4	MRD	B	403	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6284 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.

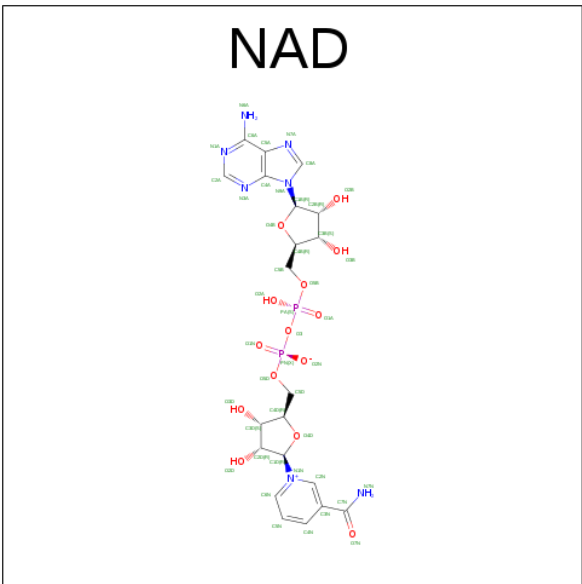
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE E CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	40	0
			2953	1885	488	555	25			
1	B	374	Total	C	N	O	S	1	31	0
			2932	1872	488	546	26			

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

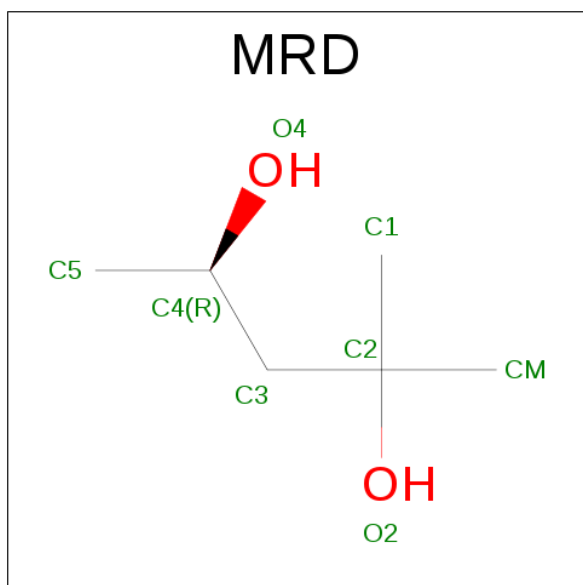
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cd	0	0
			2	2		
2	A	2	Total	Cd	0	0
			2	2		

- Molecule 3 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
3	A	1	Total	C	N	O	P	
			54	26	12	14	2	
3	B	1	Total	C	N	O	P	
			54	26	12	14	2	

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O		
			8	6	2	0	0
4	B	1	Total	C	O		
			8	6	2	0	0


- Molecule 5 is water.

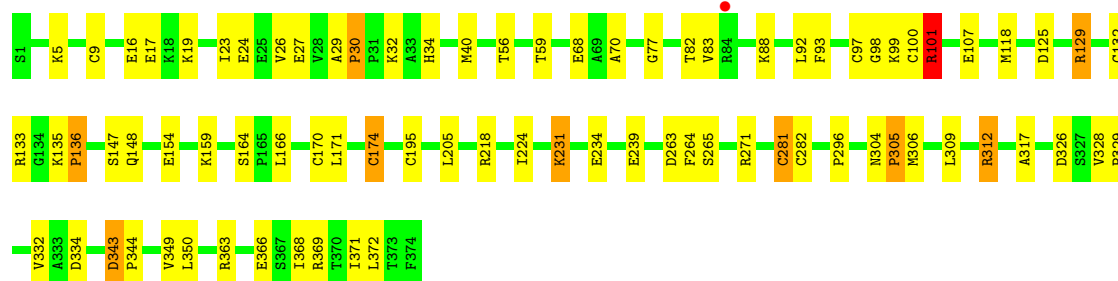
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	118	Total	O		
			118	118	0	2
5	B	153	Total	O		
			153	153	0	2

### 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.

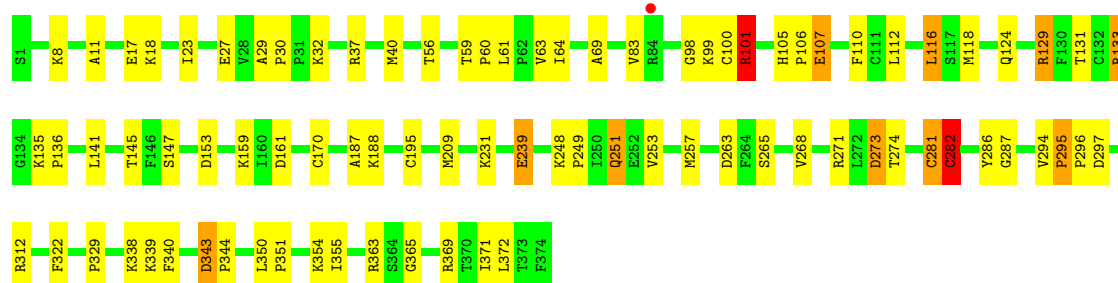
#### • Molecule 1: ALCOHOL DEHYDROGENASE E CHAIN

Chain A: 



#### • Molecule 1: ALCOHOL DEHYDROGENASE E CHAIN

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.90Å 179.00Å 50.50Å 90.00° 107.50° 90.00°	Depositor
Resolution (Å)	15.00 – 1.95 19.98 – 1.96	Depositor EDS
% Data completeness (in resolution range)	86.6 (15.00-1.95) 82.7 (19.98-1.96)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.98 (at 1.96Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.164 , 0.214 0.152 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.811	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6284	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: MRD, NAD, CD

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	0.72	0/3165	1.56	35/4271 (0.8%)
1	B	5.16	4/3102 (0.1%)	1.94	49/4187 (1.2%)
All	All	3.67	4/6267 (0.1%)	1.75	84/8458 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107[A]	GLU	CD-OE2	200.90	3.46	1.25
1	B	107[B]	GLU	CD-OE2	200.90	3.46	1.25
1	B	106[A]	PRO	N-CD	5.16	1.55	1.47
1	B	106[B]	PRO	N-CD	5.16	1.55	1.47

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107[A]	GLU	CG-CD-OE2	-40.62	37.06	118.30
1	B	107[B]	GLU	CG-CD-OE2	-40.62	37.06	118.30
1	B	133	ARG	CD-NE-CZ	34.19	171.47	123.60
1	A	101	ARG	NE-CZ-NH1	16.84	128.72	120.30
1	B	363	ARG	NE-CZ-NH1	-15.13	112.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ARG	CD-NE-CZ	13.34	142.28	123.60
1	B	133	ARG	CA-CB-CG	11.99	139.78	113.40
1	B	101	ARG	CD-NE-CZ	11.94	140.32	123.60
1	B	101	ARG	NE-CZ-NH2	-10.95	114.83	120.30
1	A	101	ARG	NE-CZ-NH2	-10.84	114.88	120.30
1	A	133	ARG	NE-CZ-NH2	10.54	125.57	120.30
1	B	161	ASP	CB-CG-OD2	-9.90	109.39	118.30
1	B	369	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	B	129	ARG	NE-CZ-NH1	-9.16	115.72	120.30
1	A	343	ASP	CB-CG-OD1	9.10	126.49	118.30
1	B	263	ASP	CB-CG-OD1	-8.55	110.60	118.30
1	B	363	ARG	NH1-CZ-NH2	8.10	128.31	119.40
1	A	271	ARG	NE-CZ-NH1	-7.97	116.31	120.30
1	A	312	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	B	101	ARG	CA-CB-CG	7.54	129.99	113.40
1	A	218	ARG	CD-NE-CZ	7.48	134.07	123.60
1	B	99	LYS	CA-C-N	7.47	133.64	117.20
1	B	161	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	281	CYS	N-CA-CB	-7.04	97.94	110.60
1	B	37	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	133	ARG	NH1-CZ-NH2	-6.95	111.76	119.40
1	A	343	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	B	239	GLU	OE1-CD-OE2	6.88	131.55	123.30
1	A	27[A]	GLU	OE1-CD-OE2	6.84	131.51	123.30
1	A	27[B]	GLU	OE1-CD-OE2	6.84	131.51	123.30
1	A	125	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	363	ARG	CA-CB-CG	6.34	127.35	113.40
1	A	265	SER	N-CA-CB	6.31	119.96	110.50
1	B	99	LYS	CA-C-O	-6.21	107.06	120.10
1	B	312	ARG	NE-CZ-NH1	-6.21	117.20	120.30
1	A	99[A]	LYS	CA-C-O	-6.16	107.16	120.10
1	A	99[B]	LYS	CA-C-O	-6.16	107.16	120.10
1	A	312	ARG	CD-NE-CZ	6.08	132.11	123.60
1	B	297	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	B	343	ASP	CB-CG-OD1	6.03	123.72	118.30
1	B	106[A]	PRO	N-CA-CB	5.94	110.42	103.30
1	B	106[B]	PRO	N-CA-CB	5.94	110.42	103.30
1	B	98	GLY	CA-C-O	5.84	131.11	120.60
1	B	369	ARG	NH1-CZ-NH2	5.81	125.79	119.40
1	B	265	SER	N-CA-CB	5.79	119.19	110.50
1	A	369	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	A	135	LYS	C-N-CD	5.73	140.44	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	CYS	CA-CB-SG	-5.73	103.69	114.00
1	B	322	PHE	CB-CG-CD1	-5.67	116.83	120.80
1	A	136[A]	PRO	N-CA-CB	5.67	110.10	103.30
1	A	136[B]	PRO	N-CA-CB	5.67	110.10	103.30
1	B	105	HIS	CA-C-O	5.64	131.95	120.10
1	B	136[A]	PRO	N-CA-CB	5.62	110.04	103.30
1	B	136[B]	PRO	N-CA-CB	5.62	110.04	103.30
1	B	273[A]	ASP	CB-CG-OD1	5.55	123.29	118.30
1	B	273[B]	ASP	CB-CG-OD1	5.55	123.29	118.30
1	B	282[A]	CYS	CB-CA-C	5.52	121.45	110.40
1	B	282[B]	CYS	CB-CA-C	5.52	121.45	110.40
1	A	305	PRO	O-C-N	-5.50	113.89	122.70
1	B	312	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	98	GLY	CA-C-O	5.46	130.43	120.60
1	A	263	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	B	294	VAL	C-N-CD	5.38	139.69	128.40
1	A	24	GLU	CB-CA-C	-5.30	99.80	110.40
1	B	268	VAL	CA-CB-CG2	5.27	118.81	110.90
1	B	312	ARG	NH1-CZ-NH2	5.26	125.19	119.40
1	B	295[A]	PRO	N-CA-CB	5.26	109.61	103.30
1	B	295[B]	PRO	N-CA-CB	5.26	109.61	103.30
1	B	195	CYS	CA-CB-SG	5.25	123.45	114.00
1	A	30	PRO	N-CA-CB	5.23	109.57	103.30
1	A	93	PHE	CB-CG-CD1	-5.22	117.14	120.80
1	A	363	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	317	ALA	N-CA-CB	5.16	117.33	110.10
1	B	281	CYS	CA-CB-SG	-5.15	104.73	114.00
1	A	326	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	135	LYS	C-N-CD	5.11	139.12	128.40
1	B	118	MET	CA-CB-CG	5.10	121.97	113.30
1	B	135	LYS	CA-C-O	5.05	130.71	120.10
1	A	34	HIS	CA-CB-CG	-5.03	105.05	113.60
1	B	106[A]	PRO	CA-N-CD	-5.02	104.47	111.50
1	B	106[B]	PRO	CA-N-CD	-5.02	104.47	111.50
1	B	101	ARG	NH1-CZ-NH2	5.02	124.92	119.40
1	A	129	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	A	334	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	59	THR	Mainchain
1	B	295[A]	PRO	Mainchain
1	B	329	PRO	Mainchain
1	B	354	LYS	Mainchain

## 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	2953	0	3012	35	0
1	B	2932	0	2997	45	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	54	0	10	1	0
3	B	54	0	10	0	0
4	A	8	0	14	1	0
4	B	8	0	14	4	0
5	A	118	0	0	6	0
5	B	153	0	0	12	0
All	All	6284	0	6057	89	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 (89) 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)
4:A:403:MRD:H1C3	5:A:2024[A]:HOH:O	1.07	1.25
4:B:403:MRD:H1C3	5:B:2020[B]:HOH:O	1.08	1.25
4:B:403:MRD:C1	5:B:2020[B]:HOH:O	1.64	1.11
1:B:116:LEU:HD12	1:B:141:LEU:HD22	1.40	1.04
1:B:107[A]:GLU:OE2	1:B:107[A]:GLU:HG3	1.69	0.92
1:B:251:GLN:H	1:B:251:GLN:HE21	1.36	0.73
1:B:40[B]:MET:HE1	1:B:69:ALA:HB1	1.76	0.67
1:A:170:CYS:SG	1:A:371:ILE:HD12	2.34	0.67
1:B:116:LEU:CD1	1:B:141:LEU:HD22	2.23	0.66
1:B:107[A]:GLU:OE2	1:B:107[A]:GLU:CG	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:LYS:HA	5:B:2133:HOH:O	1.96	0.65
1:B:239:GLU:OE1	5:B:2093:HOH:O	2.13	0.65
1:B:40[B]:MET:CE	1:B:69:ALA:HB1	2.28	0.63
1:A:68[B]:GLU:OE1	1:A:174:CYS:HB3	2.01	0.61
1:B:131[A]:THR:HG23	5:B:2061:HOH:O	2.02	0.59
1:A:56:THR:HG23	1:A:296[B]:PRO:HA	1.86	0.58
1:B:248:LYS:HB2	1:B:249:PRO:HD2	1.86	0.57
1:B:56:THR:HG23	1:B:296:PRO:HA	1.85	0.57
1:A:101:ARG:HD2	1:B:286:TYR:OH	2.04	0.57
1:A:224:ILE:HG23	3:A:402[A]:NAD:C2A	2.35	0.56
4:B:403:MRD:H1C2	5:B:2020[B]:HOH:O	1.60	0.55
1:A:171:LEU:HD21	1:A:371:ILE:HD11	1.89	0.53
1:A:231:LYS:HE3	1:A:344:PRO:O	2.07	0.53
1:A:32[A]:LYS:HE3	1:A:129:ARG:CZ	2.40	0.52
1:B:40[A]:MET:CE	1:B:145:THR:HA	2.40	0.52
1:A:328:VAL:N	1:A:329:PRO:CD	2.73	0.52
1:B:27[A]:GLU:HB2	1:B:131[A]:THR:OG1	2.10	0.51
1:B:100:CYS:HB2	1:B:112:LEU:HD12	1.92	0.51
1:A:343:ASP:N	1:A:344:PRO:CD	2.73	0.51
1:B:209[A]:MET:HE1	1:B:340:PHE:HB2	1.91	0.51
1:B:40[A]:MET:HE1	1:B:145:THR:HA	1.91	0.51
1:B:17[A]:GLU:OE2	1:B:18:LYS:NZ	2.44	0.51
1:A:40[B]:MET:HG3	1:A:147:SER:O	2.10	0.50
1:A:16[A]:GLU:HG3	1:A:19:LYS:HG3	1.93	0.50
1:B:23:ILE:HD11	1:B:355:ILE:HG22	1.93	0.50
1:B:17[A]:GLU:CD	1:B:18:LYS:NZ	2.65	0.50
1:B:83:VAL:HG12	1:B:159:LYS:HB2	1.92	0.49
4:B:403:MRD:H5C2	5:B:2152:HOH:O	2.12	0.49
1:A:92:LEU:HA	5:A:2060:HOH:O	2.12	0.49
1:B:282[B]:CYS:HB3	1:B:287:GLY:HA3	1.95	0.49
1:B:101:ARG:NH1	1:B:112:LEU:CD1	2.76	0.48
1:B:8[A]:LYS:HG2	1:B:27[A]:GLU:HG3	1.96	0.47
1:A:29:ALA:HB1	1:A:30:PRO:HD2	1.96	0.47
1:B:11:ALA:HA	1:B:147:SER:HA	1.96	0.47
1:A:16[A]:GLU:HG3	1:A:19:LYS:CG	2.45	0.47
1:A:306:MET:SD	1:A:309[A]:LEU:HD12	2.55	0.47
1:A:70:ALA:HB1	1:A:166[A]:LEU:HD22	1.98	0.46
1:A:26:VAL:HG12	1:A:132:CYS:HB2	1.98	0.46
1:A:82:THR:OG1	1:A:154:GLU:OE2	2.31	0.46
1:B:153:ASP:HB3	5:B:2069:HOH:O	2.15	0.46
1:A:136[A]:PRO:HB3	5:A:2053:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ALA:O	1:B:188[B]:LYS:HB2	2.17	0.45
1:B:61:LEU:HD22	1:B:63:VAL:HG12	1.97	0.45
1:B:29:ALA:HB1	1:B:30:PRO:HD2	1.97	0.45
1:B:350:LEU:O	1:B:372:LEU:HA	2.16	0.45
1:B:365:GLY:HA2	5:B:2145:HOH:O	2.17	0.44
1:A:83:VAL:HG12	1:A:159:LYS:HB2	1.98	0.44
1:B:63:VAL:HG22	1:B:64:ILE:N	2.34	0.43
1:A:88:LYS:HD3	1:A:166[B]:LEU:HD21	2.01	0.43
1:B:32:LYS:HE3	1:B:129:ARG:CZ	2.50	0.42
1:B:124:GLN:HG2	1:B:153:ASP:OD2	2.20	0.42
1:A:234[B]:GLU:OE2	1:A:344:PRO:HB3	2.20	0.42
1:A:282[A]:CYS:SG	1:A:312:ARG:HD3	2.60	0.42
1:A:350:LEU:O	1:A:372:LEU:HA	2.20	0.42
1:B:271:ARG:HB2	1:B:274:THR:OG1	2.19	0.42
1:B:170:CYS:SG	1:B:371:ILE:HD12	2.60	0.42
1:B:110:PHE:HE1	1:B:116:LEU:HD23	1.84	0.41
1:A:304:ASN:HA	1:A:305:PRO:HD2	1.85	0.41
1:A:205:LEU:HD11	1:A:368:ILE:HD12	2.02	0.41
1:A:9:CYS:HB2	1:A:148:GLN:OE1	2.20	0.41
1:B:59:THR:HA	1:B:60:PRO:HD3	1.88	0.41
1:B:350:LEU:HB3	1:B:351:PRO:HD2	2.01	0.41
1:A:5:LYS:HE2	5:A:2002:HOH:O	2.19	0.41
1:B:253:VAL:O	1:B:257:MET:HG3	2.21	0.41
1:A:195:CYS:HA	1:A:264:PHE:O	2.21	0.40
1:B:248:LYS:HE2	1:B:248:LYS:HB3	1.95	0.40
1:B:343:ASP:N	1:B:344:PRO:CD	2.84	0.40
1:A:328:VAL:O	1:A:332:VAL:HG23	2.21	0.40
1:B:271:ARG:HB3	1:B:273[B]:ASP:OD1	2.22	0.40
1:B:343:ASP:HB2	1:B:344:PRO:HD3	2.04	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	412/374 (110%)	393 (95%)	18 (4%)	1 (0%)	51	41
1	B	403/374 (108%)	385 (96%)	18 (4%)	0	100	100
All	All	815/748 (109%)	778 (96%)	36 (4%)	1 (0%)	55	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	CYS

### 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	348/308 (113%)	336 (97%)	12 (3%)	42	29
1	B	339/308 (110%)	330 (97%)	9 (3%)	50	39
All	All	687/616 (112%)	666 (97%)	21 (3%)	48	32

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23[A]	ILE
1	A	23[B]	ILE
1	A	97	CYS
1	A	101	ARG
1	A	107	GLU
1	A	118	MET
1	A	164[A]	SER
1	A	164[B]	SER
1	A	231	LYS
1	A	239	GLU
1	A	281	CYS
1	A	349	VAL
1	B	101	ARG
1	B	116	LEU
1	B	133	ARG

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Mol	Chain	Res	Type
1	B	231	LYS
1	B	251	GLN
1	B	281	CYS
1	B	282[A]	CYS
1	B	282[B]	CYS
1	B	339	LYS

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

Mol	Chain	Res	Type
1	A	244	GLN
1	A	348	HIS
1	B	244	GLN
1	B	251	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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	402[A]	-	41,48,48	2.39	17 (41%)	43,73,73	2.98	20 (46%)
3	NAD	A	402[B]	-	41,48,48	2.45	17 (41%)	43,73,73	2.92	21 (48%)
4	MRD	A	403	-	7,7,7	0.71	0	9,10,10	1.64	2 (22%)
3	NAD	B	402[A]	-	41,48,48	2.38	16 (39%)	43,73,73	2.97	17 (39%)
3	NAD	B	402[B]	-	41,48,48	2.36	16 (39%)	43,73,73	3.01	17 (39%)
4	MRD	B	403	-	7,7,7	0.30	0	9,10,10	2.24	4 (44%)

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	402[A]	-	-	0/22/62/62	0/5/5/5
3	NAD	A	402[B]	-	-	0/22/62/62	0/5/5/5
4	MRD	A	403	-	-	0/5/5/5	0/0/0/0
3	NAD	B	402[A]	-	-	0/22/62/62	0/5/5/5
3	NAD	B	402[B]	-	-	0/22/62/62	0/5/5/5
4	MRD	B	403	-	-	0/5/5/5	0/0/0/0

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402[B]	NAD	C6N-C5N	-3.32	1.31	1.38
3	B	402[A]	NAD	C6N-C5N	-3.32	1.31	1.38
3	B	402[B]	NAD	O3D-C3D	-3.26	1.35	1.43
3	B	402[A]	NAD	O3D-C3D	-3.26	1.35	1.43
3	B	402[B]	NAD	O2B-C2B	-3.23	1.35	1.43
3	B	402[A]	NAD	O2B-C2B	-3.23	1.35	1.43
3	A	402[A]	NAD	O2B-C2B	-3.21	1.35	1.43
3	A	402[B]	NAD	O2B-C2B	-3.21	1.35	1.43
3	B	402[B]	NAD	O2D-C2D	-2.86	1.36	1.43
3	B	402[A]	NAD	O2D-C2D	-2.86	1.36	1.43
3	A	402[A]	NAD	O2D-C2D	-2.40	1.37	1.43
3	A	402[B]	NAD	O2D-C2D	-2.40	1.37	1.43
3	B	402[B]	NAD	PN-O1N	-2.33	1.42	1.50
3	B	402[A]	NAD	PN-O1N	-2.33	1.42	1.50
3	A	402[A]	NAD	PN-O1N	-2.28	1.42	1.50
3	A	402[B]	NAD	PN-O1N	-2.28	1.42	1.50
3	A	402[A]	NAD	C6N-C5N	-2.21	1.33	1.38
3	A	402[B]	NAD	C6N-C5N	-2.21	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[A]	NAD	C3N-C7N	-2.08	1.47	1.50
3	A	402[B]	NAD	C3N-C7N	-2.08	1.47	1.50
3	A	402[A]	NAD	C2D-C1D	2.10	1.57	1.53
3	A	402[B]	NAD	C2D-C1D	2.10	1.57	1.53
3	A	402[A]	NAD	C6N-N1N	2.18	1.41	1.35
3	A	402[B]	NAD	C6N-N1N	2.18	1.41	1.35
3	A	402[A]	NAD	C3D-C4D	2.19	1.58	1.53
3	A	402[B]	NAD	C3D-C4D	2.19	1.58	1.53
3	B	402[B]	NAD	C4N-C3N	2.41	1.43	1.39
3	B	402[A]	NAD	C4N-C3N	2.41	1.43	1.39
3	B	402[B]	NAD	C3N-C7N	2.75	1.54	1.50
3	B	402[A]	NAD	C3N-C7N	2.75	1.54	1.50
3	B	402[B]	NAD	C3B-C4B	2.77	1.60	1.53
3	B	402[A]	NAD	C3B-C4B	2.77	1.60	1.53
3	A	402[A]	NAD	O3B-C3B	2.79	1.49	1.43
3	A	402[B]	NAD	O3B-C3B	2.79	1.49	1.43
3	B	402[B]	NAD	C2B-C1B	2.80	1.58	1.53
3	B	402[A]	NAD	C2B-C1B	2.80	1.58	1.53
3	B	402[B]	NAD	O3B-C3B	2.81	1.49	1.43
3	B	402[A]	NAD	O3B-C3B	2.81	1.49	1.43
3	A	402[A]	NAD	C3B-C4B	2.85	1.60	1.53
3	A	402[B]	NAD	C3B-C4B	2.85	1.60	1.53
3	A	402[A]	NAD	C4A-N3A	2.86	1.39	1.35
3	A	402[A]	NAD	O7N-C7N	2.88	1.30	1.24
3	A	402[B]	NAD	O7N-C7N	2.88	1.30	1.24
3	A	402[A]	NAD	O4D-C4D	2.94	1.51	1.45
3	A	402[B]	NAD	O4D-C4D	2.94	1.51	1.45
3	B	402[B]	NAD	C4A-N3A	3.05	1.40	1.35
3	A	402[B]	NAD	C4A-N3A	3.08	1.40	1.35
3	B	402[A]	NAD	C4A-N3A	3.14	1.40	1.35
3	B	402[B]	NAD	C2D-C1D	3.28	1.58	1.53
3	B	402[A]	NAD	C2D-C1D	3.28	1.58	1.53
3	A	402[A]	NAD	C5N-C4N	3.33	1.45	1.38
3	A	402[B]	NAD	C5N-C4N	3.33	1.45	1.38
3	B	402[B]	NAD	C2A-N3A	3.73	1.38	1.32
3	A	402[A]	NAD	C2A-N3A	3.74	1.38	1.32
3	B	402[B]	NAD	O4D-C4D	3.92	1.53	1.45
3	B	402[A]	NAD	O4D-C4D	3.92	1.53	1.45
3	B	402[B]	NAD	C6N-N1N	4.27	1.46	1.35
3	B	402[A]	NAD	C6N-N1N	4.27	1.46	1.35
3	B	402[A]	NAD	C2A-N3A	4.28	1.39	1.32
3	A	402[A]	NAD	C7N-N7N	4.80	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[B]	NAD	C7N-N7N	4.80	1.42	1.33
3	A	402[B]	NAD	C2A-N3A	4.91	1.40	1.32
3	B	402[B]	NAD	C5N-C4N	6.96	1.52	1.38
3	B	402[A]	NAD	C5N-C4N	6.96	1.52	1.38
3	A	402[A]	NAD	C4N-C3N	8.21	1.52	1.39
3	A	402[B]	NAD	C4N-C3N	8.21	1.52	1.39

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402[B]	NAD	C5N-C4N-C3N	-10.24	108.31	120.35
3	B	402[A]	NAD	C5N-C4N-C3N	-10.24	108.31	120.35
3	A	402[A]	NAD	N3A-C2A-N1A	-8.22	121.70	128.86
3	A	402[A]	NAD	C5N-C4N-C3N	-7.67	111.33	120.35
3	A	402[B]	NAD	C5N-C4N-C3N	-7.67	111.33	120.35
3	B	402[B]	NAD	N3A-C2A-N1A	-7.61	122.23	128.86
3	B	402[A]	NAD	N3A-C2A-N1A	-7.44	122.38	128.86
3	A	402[B]	NAD	N3A-C2A-N1A	-7.39	122.42	128.86
3	A	402[A]	NAD	O7N-C7N-N7N	-5.78	114.36	122.58
3	A	402[B]	NAD	O7N-C7N-N7N	-5.78	114.36	122.58
3	A	402[A]	NAD	C4B-O4B-C1B	-4.47	105.02	109.77
3	A	402[B]	NAD	C4B-O4B-C1B	-4.47	105.02	109.77
4	B	403	MRD	CM-C2-C1	-4.34	100.73	110.42
3	A	402[A]	NAD	C3N-C2N-N1N	-4.30	116.09	120.43
3	A	402[B]	NAD	C3N-C2N-N1N	-4.30	116.09	120.43
3	B	402[B]	NAD	O7N-C7N-C3N	-3.46	115.58	119.62
3	B	402[A]	NAD	O7N-C7N-C3N	-3.46	115.58	119.62
4	A	403	MRD	C5-C4-C3	-3.27	95.87	112.11
3	B	402[B]	NAD	C3N-C2N-N1N	-3.10	117.30	120.43
3	B	402[A]	NAD	C3N-C2N-N1N	-3.10	117.30	120.43
3	A	402[B]	NAD	C5A-C6A-N1A	-2.84	111.11	119.70
3	A	402[A]	NAD	C5A-C6A-N1A	-2.78	111.29	119.70
3	B	402[B]	NAD	C5A-C6A-N1A	-2.77	111.33	119.70
3	B	402[A]	NAD	C5A-C6A-N1A	-2.72	111.48	119.70
3	A	402[A]	NAD	O3D-C3D-C4D	-2.67	103.30	111.09
3	A	402[B]	NAD	O3D-C3D-C4D	-2.67	103.30	111.09
4	A	403	MRD	O4-C4-C5	-2.45	98.25	109.46
3	B	402[B]	NAD	O4D-C4D-C3D	-2.36	100.48	105.17
3	B	402[A]	NAD	O4D-C4D-C3D	-2.36	100.48	105.17
3	B	402[B]	NAD	O5B-C5B-C4B	-2.22	101.12	109.00
3	B	402[A]	NAD	O5B-C5B-C4B	-2.22	101.12	109.00
3	A	402[A]	NAD	O4B-C4B-C5B	-2.19	102.00	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402[B]	NAD	O4B-C4B-C5B	-2.19	102.00	109.40
3	B	402[B]	NAD	C5N-C6N-N1N	-2.13	117.14	120.40
3	B	402[A]	NAD	C5N-C6N-N1N	-2.13	117.14	120.40
3	B	402[B]	NAD	O4B-C4B-C5B	-2.09	102.34	109.40
3	B	402[A]	NAD	O4B-C4B-C5B	-2.09	102.34	109.40
3	A	402[A]	NAD	O4D-C4D-C5D	-2.08	102.39	109.40
3	A	402[B]	NAD	O4D-C4D-C5D	-2.08	102.39	109.40
3	A	402[A]	NAD	C4D-O4D-C1D	-2.07	107.57	109.77
3	A	402[B]	NAD	C4D-O4D-C1D	-2.07	107.57	109.77
3	A	402[A]	NAD	O3B-C3B-C4B	-2.06	105.08	111.09
3	A	402[B]	NAD	O3B-C3B-C4B	-2.06	105.08	111.09
3	A	402[A]	NAD	O2B-C2B-C3B	2.04	118.35	111.83
3	A	402[B]	NAD	O2B-C2B-C3B	2.04	118.35	111.83
3	B	402[B]	NAD	O3D-C3D-C4D	2.08	117.16	111.09
3	B	402[A]	NAD	O3D-C3D-C4D	2.08	117.16	111.09
3	A	402[B]	NAD	C5A-C6A-N6A	2.26	125.07	120.47
4	B	403	MRD	O4-C4-C3	2.26	121.64	111.28
3	A	402[A]	NAD	O2N-PN-O1N	2.27	124.01	112.28
3	A	402[B]	NAD	O2N-PN-O1N	2.27	124.01	112.28
3	B	402[B]	NAD	O2B-C2B-C3B	2.32	119.27	111.83
3	B	402[A]	NAD	O2B-C2B-C3B	2.32	119.27	111.83
4	B	403	MRD	C1-C2-C3	2.41	122.05	110.08
3	A	402[B]	NAD	N6A-C6A-N1A	2.55	123.81	118.77
3	B	402[B]	NAD	O2N-PN-O1N	2.68	126.14	112.28
3	B	402[A]	NAD	O2N-PN-O1N	2.68	126.14	112.28
3	A	402[A]	NAD	O7N-C7N-C3N	2.81	122.91	119.62
3	A	402[B]	NAD	O7N-C7N-C3N	2.81	122.91	119.62
3	B	402[B]	NAD	O2A-PA-O1A	2.90	127.27	112.28
3	B	402[A]	NAD	O2A-PA-O1A	2.90	127.27	112.28
4	B	403	MRD	O2-C2-CM	3.28	119.37	108.00
3	A	402[A]	NAD	C5A-C6A-N6A	3.42	127.44	120.47
3	B	402[A]	NAD	C5A-C6A-N6A	3.45	127.51	120.47
3	A	402[A]	NAD	C6N-C5N-C4N	3.53	124.77	119.44
3	A	402[B]	NAD	C6N-C5N-C4N	3.53	124.77	119.44
3	A	402[A]	NAD	O2A-PA-O1A	3.80	131.95	112.28
3	A	402[B]	NAD	O2A-PA-O1A	3.80	131.95	112.28
3	A	402[A]	NAD	C3N-C7N-N7N	3.98	122.32	117.77
3	A	402[B]	NAD	C3N-C7N-N7N	3.98	122.32	117.77
3	B	402[B]	NAD	C5A-C6A-N6A	4.41	129.46	120.47
3	B	402[B]	NAD	C3N-C7N-N7N	4.75	123.20	117.77
3	B	402[A]	NAD	C3N-C7N-N7N	4.75	123.20	117.77
3	A	402[A]	NAD	C2N-C3N-C4N	4.96	123.92	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402[B]	NAD	C2N-C3N-C4N	4.96	123.92	118.26
3	B	402[A]	NAD	C2A-N1A-C6A	5.34	128.12	118.77
3	A	402[A]	NAD	C2A-N1A-C6A	5.50	128.39	118.77
3	B	402[B]	NAD	C2A-N1A-C6A	5.57	128.51	118.77
3	A	402[B]	NAD	C2A-N1A-C6A	5.60	128.57	118.77
3	B	402[B]	NAD	C2N-C3N-C4N	6.66	125.86	118.26
3	B	402[A]	NAD	C2N-C3N-C4N	6.66	125.86	118.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402[A]	NAD	1	0
4	A	403	MRD	1	0
4	B	403	MRD	4	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%)	-0.32	1 (0%) 93 96	18, 31, 46, 65	0
1	B	374/374 (100%)	-0.41	1 (0%) 93 96	17, 26, 41, 56	0
All	All	748/748 (100%)	-0.37	2 (0%) 93 96	17, 29, 44, 65	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	ARG	3.0
1	B	84	ARG	2.6

### 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(Å <sup>2</sup> )	Q<0.9
4	MRD	A	403	8/8	0.87	0.22	9.35	17,19,19,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MRD	B	403	8/8	0.80	0.18	3.91	37,40,43,44	0
3	NAD	B	402[B]	44/44	0.98	0.06	-1.15	15,19,22,24	10
2	CD	B	401	1/1	1.00	0.03	-1.43	25,25,25,25	0
3	NAD	B	402[A]	44/44	0.98	0.06	-1.45	15,19,22,24	10
3	NAD	A	402[A]	44/44	0.99	0.06	-1.62	17,22,25,25	10
3	NAD	A	402[B]	44/44	0.99	0.06	-1.71	17,21,23,25	10
2	CD	A	401	1/1	1.00	0.02	-2.46	29,29,29,29	0
2	CD	A	400	1/1	1.00	0.03	-2.49	28,28,28,28	0
2	CD	B	400	1/1	1.00	0.02	-2.60	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.