



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:44 PM GMT

PDB ID : 4PT0  
Title : NAD<sup>+</sup> complex structure of Aldehyde Dehydrogenase from *Bacillus cereus*  
Authors : Ngo, H.P.T.; Hong, S.H.; Oh, D.K.; Kang, L.W.  
Deposited on : 2014-03-10  
Resolution : 2.60 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

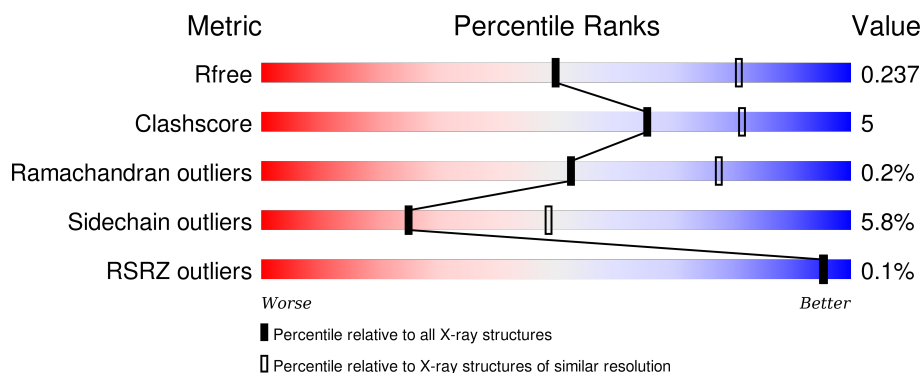
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*




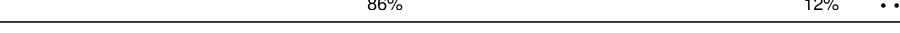
The reported resolution of this entry is 2.60 Å.

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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	494	 85% 13% ..
1	B	494	 84% 14% ..
1	C	494	 83% 14% ..
1	D	494	 86% 12% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	A	502	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15847 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3791	2414	630	733	14			
1	B	488	Total	C	N	O	S	0	1	0
			3771	2402	626	728	15			
1	C	489	Total	C	N	O	S	0	0	0
			3776	2406	627	729	14			
1	D	491	Total	C	N	O	S	0	1	0
			3794	2416	630	733	15			

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



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

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

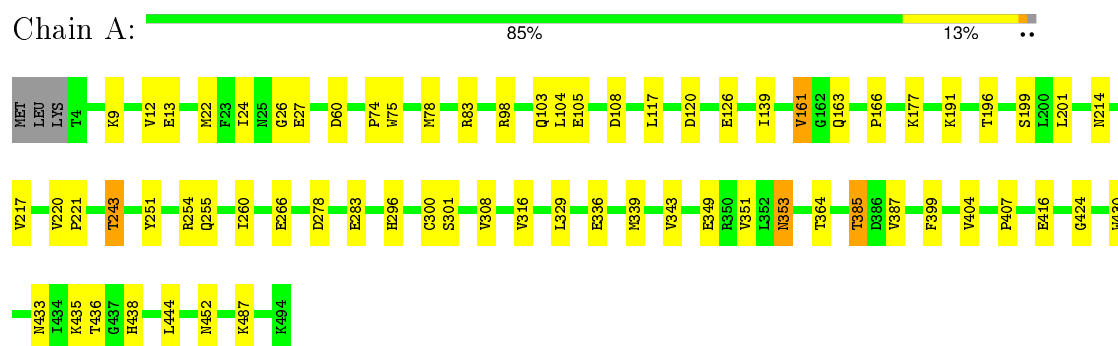
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	141	Total	O	0	0
			141	141		
4	B	143	Total	O	0	0
			143	143		
4	C	126	Total	O	0	0
			126	126		
4	D	126	Total	O	0	0
			126	126		

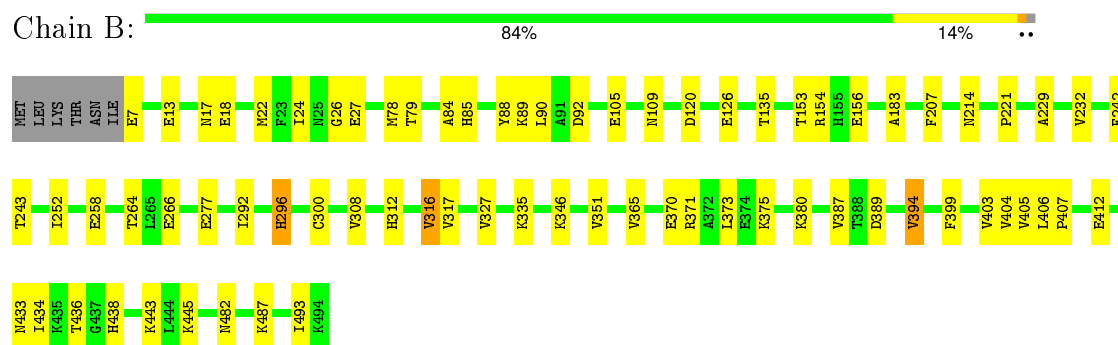
### 3 Residue-property plots

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.

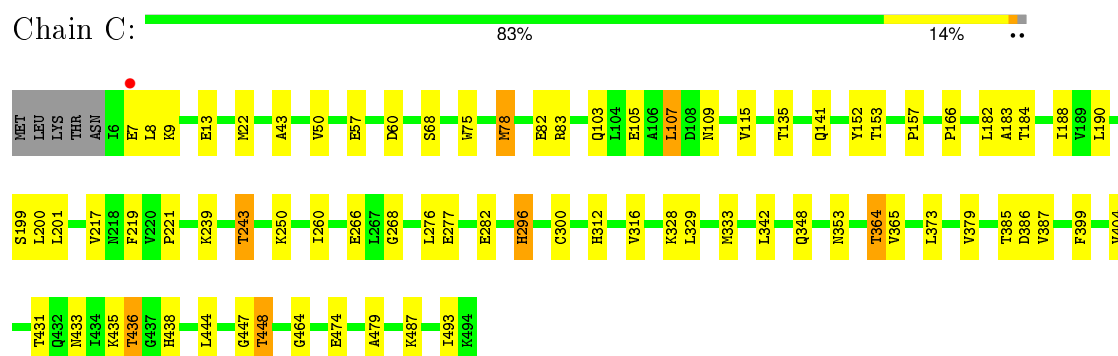
#### • Molecule 1: Aldehyde dehydrogenase



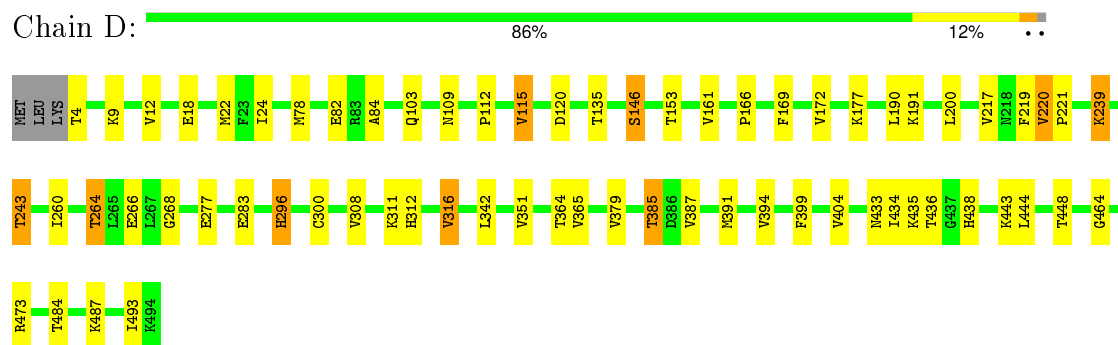
#### • Molecule 1: Aldehyde dehydrogenase



#### • Molecule 1: Aldehyde dehydrogenase



## ● Molecule 1: Aldehyde dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.22Å 93.25Å 145.15Å 90.00° 97.86° 90.00°	Depositor
Resolution (Å)	47.93 – 2.60 47.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.93-2.60) 99.4 (47.93-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	35.35 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.166 , 0.233 0.172 , 0.237	Depositor DCC
$R_{free}$ test set	3414 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 29.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 67300 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15847	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, NAD

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	0.75	0/3870	0.81	1/5250 (0.0%)
1	B	0.73	2/3853 (0.1%)	0.82	2/5226 (0.0%)
1	C	0.74	0/3855	0.83	0/5229
1	D	0.70	0/3876	0.78	0/5258
All	All	0.73	2/15454 (0.0%)	0.81	3/20963 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	GLU	CG-CD	5.17	1.59	1.51
1	B	88	TYR	CG-CD2	5.10	1.45	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	278	ASP	CB-CG-OD1	6.30	123.97	118.30
1	B	78	MET	CG-SD-CE	-5.02	92.17	100.20

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	3791	0	3740	42	0
1	B	3771	0	3721	39	0
1	C	3776	0	3727	44	0
1	D	3794	0	3745	42	0
2	A	44	0	26	2	0
2	B	44	0	26	4	0
2	C	44	0	26	1	0
2	D	44	0	26	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	141	0	0	2	0
4	B	143	0	0	0	0
4	C	126	0	0	5	0
4	D	126	0	0	0	0
All	All	15847	0	15037	151	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (151) 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:D:300[A]:CYS:SG	2:D:501:NAD:C7N	2.54	0.95
1:B:300[B]:CYS:SG	2:B:501:NAD:C7N	2.58	0.91
1:D:364:THR:HB	1:D:385:THR:HG22	1.56	0.87
1:D:243:THR:HB	1:D:266:GLU:HB2	1.61	0.82
1:C:243:THR:HB	1:C:266:GLU:HB2	1.64	0.80
1:D:300[A]:CYS:HG	2:D:501:NAD:C7N	1.96	0.79
1:A:9:LYS:H	1:A:103:GLN:HE22	1.34	0.75
1:C:300:CYS:SG	2:C:501:NAD:C7N	2.74	0.75
1:D:9:LYS:H	1:D:103:GLN:HE22	1.38	0.72
1:B:22:MET:HE3	1:B:24:ILE:HD11	1.71	0.71
1:A:300:CYS:SG	2:A:501:NAD:C7N	2.78	0.71
1:D:433:ASN:HD22	1:D:436:THR:H	1.41	0.67
1:A:438:HIS:HE1	1:C:438:HIS:HE1	1.43	0.67
1:A:300:CYS:HG	2:A:501:NAD:C7N	2.08	0.66
1:B:300[B]:CYS:SG	2:B:501:NAD:N7N	2.69	0.65
1:A:201:LEU:HD11	1:A:221:PRO:HG3	1.80	0.62
1:A:433:ASN:HD22	1:A:436:THR:H	1.47	0.62
1:A:22:MET:HG2	1:A:221:PRO:HD2	1.83	0.61
1:C:22:MET:HG2	1:C:221:PRO:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:THR:HG21	1:C:386:ASP:OD2	2.01	0.61
1:C:260:ILE:O	1:C:260:ILE:HG22	2.02	0.59
1:B:433:ASN:HD22	1:B:436:THR:H	1.50	0.59
1:B:438:HIS:HE1	1:D:438:HIS:HE1	1.48	0.59
1:B:264:THR:HG21	1:B:482:ASN:CG	2.24	0.58
1:C:364:THR:CG2	1:C:386:ASP:OD2	2.52	0.58
1:A:166:PRO:HD3	1:A:243:THR:HG23	1.86	0.58
1:C:433:ASN:HB3	1:C:436:THR:HG23	1.85	0.58
1:C:276:LEU:HD12	1:C:431:THR:HB	1.86	0.57
1:B:258:GLU:O	1:C:250:LYS:HE2	2.04	0.57
1:D:300[A]:CYS:SG	2:D:501:NAD:N7N	2.77	0.57
1:A:26:GLY:HA3	1:A:214:ASN:ND2	2.20	0.56
1:A:251:TYR:O	1:A:255:GLN:HG2	2.06	0.55
1:A:22:MET:HG2	1:A:221:PRO:CD	2.37	0.55
1:D:239:LYS:HZ1	1:D:264:THR:CG2	2.20	0.55
1:C:436:THR:HG21	4:C:701:HOH:O	2.05	0.55
1:C:277:GLU:O	1:C:312:HIS:HE1	1.89	0.55
1:D:22:MET:HG2	1:D:221:PRO:HD2	1.89	0.55
1:B:300[B]:CYS:SG	2:B:501:NAD:C3N	2.95	0.54
1:B:438:HIS:HD2	1:C:152:TYR:OH	1.89	0.54
1:A:201:LEU:HD11	1:A:221:PRO:CG	2.38	0.54
1:A:9:LYS:H	1:A:103:GLN:NE2	2.04	0.54
1:A:9:LYS:HB2	1:A:12:VAL:HG13	1.90	0.54
1:B:487:LYS:NZ	1:C:444:LEU:O	2.41	0.53
1:C:448:THR:HG23	4:C:691:HOH:O	2.07	0.53
1:B:300[B]:CYS:SG	2:B:501:NAD:C2N	2.97	0.53
1:B:22:MET:HG2	1:B:221:PRO:HD2	1.90	0.53
1:A:349:GLU:O	1:A:353:ASN:HB2	2.09	0.53
1:A:243:THR:HB	1:A:266:GLU:HB2	1.91	0.53
1:A:22:MET:CE	1:A:24:ILE:HD11	2.39	0.52
1:B:389:ASP:HA	1:B:394:VAL:HG21	1.89	0.52
1:A:329:LEU:HD21	1:A:339:MET:HE2	1.92	0.52
1:C:435:LYS:HG3	1:D:493:ILE:HA	1.91	0.52
1:D:300[A]:CYS:SG	2:D:501:NAD:O7N	2.67	0.52
1:D:277:GLU:O	1:D:312:HIS:HE1	1.93	0.52
1:B:22:MET:CE	1:B:24:ILE:HD11	2.41	0.51
1:A:353:ASN:ND2	4:A:688:HOH:O	2.44	0.51
1:A:438:HIS:CE1	1:C:438:HIS:HE1	2.24	0.51
1:D:342:LEU:HD22	1:D:379:VAL:HG13	1.93	0.51
1:D:260:ILE:O	1:D:260:ILE:HG22	2.10	0.51
1:A:74:PRO:O	1:A:78:MET:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:VAL:HG11	1:A:404:VAL:HG13	1.92	0.51
1:C:199:SER:HB2	4:C:638:HOH:O	2.10	0.51
1:D:296:HIS:N	1:D:296:HIS:CD2	2.79	0.51
1:D:387:VAL:HG11	1:D:404:VAL:HG13	1.93	0.51
1:C:78:MET:HG3	1:C:82:GLU:HB2	1.94	0.50
1:D:78:MET:HG2	1:D:82:GLU:HB2	1.93	0.50
1:D:84:ALA:HB2	1:D:135:THR:OG1	2.12	0.50
1:D:239:LYS:HZ1	1:D:264:THR:HG23	1.76	0.49
1:D:169:PHE:HB3	1:D:172:VAL:CG1	2.41	0.49
1:C:153:THR:HA	1:C:487:LYS:O	2.12	0.49
1:A:254:ARG:HD2	4:A:678:HOH:O	2.12	0.49
1:C:342:LEU:HD12	1:C:348:GLN:HA	1.95	0.49
1:B:317:VAL:HG22	1:B:405:VAL:HG11	1.95	0.49
1:C:493:ILE:HA	1:D:435:LYS:HG3	1.95	0.49
1:C:22:MET:CG	1:C:221:PRO:HD2	2.42	0.49
1:C:448:THR:CG2	4:C:691:HOH:O	2.61	0.49
1:C:8:LEU:HA	1:C:103:GLN:HE22	1.78	0.49
1:A:438:HIS:HE1	1:C:438:HIS:CE1	2.28	0.49
1:C:201:LEU:HD11	1:C:221:PRO:HG3	1.95	0.48
1:A:26:GLY:HA3	1:A:214:ASN:HD22	1.77	0.48
1:D:153:THR:HA	1:D:487:LYS:O	2.13	0.48
1:A:260:ILE:HG22	1:A:260:ILE:O	2.14	0.48
1:B:242:PHE:CD1	1:B:252:ILE:CD1	2.97	0.47
1:D:190:LEU:HD23	1:D:190:LEU:C	2.34	0.47
1:D:22:MET:CE	1:D:24:ILE:HD11	2.44	0.47
1:D:22:MET:HE3	1:D:220:VAL:HG12	1.96	0.47
1:C:107:LEU:HD13	1:C:333:MET:HG3	1.96	0.47
1:C:433:ASN:HD22	1:C:436:THR:H	1.62	0.47
1:B:370:GLU:OE2	1:B:380:LYS:NZ	2.47	0.47
1:D:217:VAL:CG1	1:D:219:PHE:CZ	2.97	0.46
1:B:264:THR:HG21	1:B:482:ASN:ND2	2.31	0.46
1:D:217:VAL:HG13	1:D:219:PHE:CE1	2.51	0.46
1:C:447:GLY:HA3	1:C:464:GLY:O	2.16	0.46
1:C:268:GLY:HA2	1:C:300:CYS:SG	2.56	0.46
1:B:387:VAL:HG21	1:B:404:VAL:CG1	2.46	0.45
1:A:487:LYS:NZ	1:D:444:LEU:O	2.43	0.45
1:A:75:TRP:CH2	1:A:83:ARG:HD2	2.51	0.45
1:B:135:THR:HG22	1:B:183:ALA:HA	1.98	0.45
1:B:229:ALA:HA	1:B:232:VAL:HG12	1.99	0.45
1:C:182:LEU:HD21	1:C:188:ILE:HD12	1.97	0.45
1:A:444:LEU:O	1:D:487:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:CZ	1:A:117:LEU:HD11	2.46	0.45
1:D:464:GLY:HA3	1:D:473:ARG:HD3	1.98	0.45
1:B:258:GLU:O	1:C:250:LYS:CE	2.65	0.44
1:B:387:VAL:HG21	1:B:404:VAL:HG13	2.00	0.44
1:D:268:GLY:HA2	1:D:300[A]:CYS:SG	2.57	0.44
1:A:105:GLU:OE2	1:A:199:SER:HB2	2.18	0.44
1:B:153:THR:HA	1:B:487:LYS:O	2.18	0.43
1:B:154:ARG:NH2	1:B:156:GLU:OE2	2.47	0.43
1:D:190:LEU:HD22	1:D:200:LEU:CD2	2.48	0.43
1:C:474:GLU:HA	1:C:479:ALA:HB2	2.00	0.43
1:B:292:ILE:HG21	1:B:403:VAL:HB	2.00	0.43
1:C:190:LEU:HD12	1:C:200:LEU:HD21	1.99	0.43
1:A:108:ASP:OD2	1:A:196:THR:HA	2.18	0.43
1:B:277:GLU:O	1:B:312:HIS:HE1	2.01	0.43
1:C:157:PRO:HB3	1:C:184:THR:O	2.19	0.43
1:B:296:HIS:N	1:B:296:HIS:CD2	2.86	0.43
1:D:308:VAL:HG11	1:D:316:VAL:HG13	2.00	0.43
1:A:435:LYS:HG2	1:B:493:ILE:HA	2.00	0.43
1:A:22:MET:HE1	1:A:24:ILE:CD1	2.48	0.42
1:C:190:LEU:HD12	1:C:200:LEU:CD2	2.50	0.42
1:D:22:MET:CE	1:D:220:VAL:HG12	2.48	0.42
1:C:75:TRP:CH2	1:C:83:ARG:HD2	2.54	0.42
1:B:243:THR:HA	1:B:266:GLU:O	2.19	0.42
1:C:9:LYS:H	1:C:103:GLN:HE22	1.68	0.42
1:D:177:LYS:HZ1	1:D:243:THR:HG22	1.84	0.42
1:A:308:VAL:O	1:A:407:PRO:HA	2.20	0.42
1:B:26:GLY:HA3	1:B:214:ASN:ND2	2.34	0.42
1:A:191:LYS:HG3	1:A:220:VAL:O	2.20	0.42
1:C:296:HIS:CD2	1:C:296:HIS:N	2.88	0.42
1:D:190:LEU:HD22	1:D:200:LEU:HD21	2.02	0.41
1:C:217:VAL:HG13	1:C:219:PHE:CZ	2.55	0.41
1:A:161:VAL:HG23	1:A:163:GLN:HG3	2.02	0.41
1:B:105:GLU:O	1:B:109:ASN:HB3	2.20	0.41
1:A:139:ILE:HD12	1:C:141:GLN:HG2	2.03	0.41
1:C:43:ALA:HB2	4:C:717:HOH:O	2.21	0.41
1:B:79:THR:HG22	1:D:146:SER:HB2	2.02	0.41
1:B:90:LEU:HD21	1:B:207:PHE:CZ	2.56	0.41
1:D:433:ASN:HD21	1:D:435:LYS:HB2	1.85	0.40
1:A:177:LYS:NZ	1:A:243:THR:HG22	2.36	0.40
1:B:84:ALA:HB2	1:B:135:THR:OG1	2.22	0.40
1:B:308:VAL:HG21	1:B:316:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:MET:HB2	1:D:394:VAL:HG13	2.02	0.40
1:A:364:THR:HB	1:A:385:THR:HG22	2.03	0.40
1:B:406:LEU:HA	1:B:407:PRO:HD3	1.97	0.40
1:A:430:TRP:CE3	1:A:452:ASN:HA	2.57	0.40
1:B:434:ILE:HA	1:D:434:ILE:HB	2.03	0.40
1:B:85:HIS:CE1	1:B:89:LYS:HD2	2.56	0.40
1:A:308:VAL:HG11	1:A:316:VAL:HG13	2.04	0.40
1:D:112:PRO:HB2	1:D:115:VAL:HG13	2.03	0.40
1:C:135:THR:HG22	1:C:183:ALA:HA	2.03	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	489/494 (99%)	471 (96%)	17 (4%)	1 (0%)	52	77
1	B	487/494 (99%)	473 (97%)	14 (3%)	0	100	100
1	C	487/494 (99%)	467 (96%)	18 (4%)	2 (0%)	39	65
1	D	490/494 (99%)	474 (97%)	15 (3%)	1 (0%)	52	77
All	All	1953/1976 (99%)	1885 (96%)	64 (3%)	4 (0%)	52	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	78	MET
1	C	166	PRO
1	A	424	GLY
1	D	166	PRO

### 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	398/401 (99%)	379 (95%)	19 (5%)	31	58
1	B	396/401 (99%)	375 (95%)	21 (5%)	28	53
1	C	396/401 (99%)	368 (93%)	28 (7%)	18	36
1	D	399/401 (100%)	375 (94%)	24 (6%)	24	47
All	All	1589/1604 (99%)	1497 (94%)	92 (6%)	25	49

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	27	GLU
1	A	60	ASP
1	A	104	LEU
1	A	120	ASP
1	A	126	GLU
1	A	161	VAL
1	A	217	VAL
1	A	243	THR
1	A	283	GLU
1	A	296	HIS
1	A	301	SER
1	A	336	GLU
1	A	343	VAL
1	A	351	VAL
1	A	353	ASN
1	A	385	THR
1	A	399	PHE
1	A	416	GLU
1	B	7	GLU
1	B	13	GLU
1	B	17	ASN
1	B	18	GLU
1	B	27	GLU

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Mol	Chain	Res	Type
1	B	120	ASP
1	B	296	HIS
1	B	316	VAL
1	B	327	VAL
1	B	335	LYS
1	B	346	LYS
1	B	351	VAL
1	B	365	VAL
1	B	371	ARG
1	B	373	LEU
1	B	375	LYS
1	B	394	VAL
1	B	399	PHE
1	B	412	GLU
1	B	443	LYS
1	B	445	LYS
1	C	7	GLU
1	C	13	GLU
1	C	50	VAL
1	C	57	GLU
1	C	60	ASP
1	C	68	SER
1	C	105	GLU
1	C	107	LEU
1	C	109	ASN
1	C	115	VAL
1	C	239	LYS
1	C	243	THR
1	C	282	GLU
1	C	296	HIS
1	C	316	VAL
1	C	328	LYS
1	C	329	LEU
1	C	353	ASN
1	C	364	THR
1	C	365	VAL
1	C	373	LEU
1	C	379	VAL
1	C	385	THR
1	C	387	VAL
1	C	399	PHE
1	C	404	VAL

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Mol	Chain	Res	Type
1	C	436	THR
1	C	448	THR
1	D	4	THR
1	D	12	VAL
1	D	18	GLU
1	D	109	ASN
1	D	115	VAL
1	D	120	ASP
1	D	146	SER
1	D	161	VAL
1	D	191	LYS
1	D	220	VAL
1	D	239	LYS
1	D	243	THR
1	D	264	THR
1	D	283	GLU
1	D	296	HIS
1	D	311	LYS
1	D	316	VAL
1	D	351	VAL
1	D	365	VAL
1	D	385	THR
1	D	399	PHE
1	D	443	LYS
1	D	448	THR
1	D	484	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	103	GLN
1	A	114	GLN
1	A	214	ASN
1	A	262	HIS
1	A	325	ASN
1	A	326	ASN
1	A	353	ASN
1	A	432	GLN
1	A	433	ASN
1	A	438	HIS
1	A	442	ASN

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Mol	Chain	Res	Type
1	B	214	ASN
1	B	312	HIS
1	B	325	ASN
1	B	326	ASN
1	B	357	GLN
1	B	433	ASN
1	B	438	HIS
1	B	442	ASN
1	B	482	ASN
1	C	103	GLN
1	C	214	ASN
1	C	233	ASN
1	C	255	GLN
1	C	290	GLN
1	C	312	HIS
1	C	325	ASN
1	C	326	ASN
1	C	353	ASN
1	C	432	GLN
1	C	433	ASN
1	C	438	HIS
1	C	442	ASN
1	D	103	GLN
1	D	214	ASN
1	D	312	HIS
1	D	325	ASN
1	D	326	ASN
1	D	432	GLN
1	D	433	ASN
1	D	438	HIS
1	D	442	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 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$
2	NAD	A	501	-	38,48,48	0.81	2 (5%)	47,73,73	1.47	4 (8%)
2	NAD	B	501	-	38,48,48	0.93	2 (5%)	47,73,73	1.72	9 (19%)
2	NAD	C	501	-	38,48,48	0.90	1 (2%)	47,73,73	2.08	7 (14%)
2	NAD	D	501	-	38,48,48	0.94	3 (7%)	47,73,73	1.68	4 (8%)

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
2	NAD	A	501	-	-	0/22/62/62	0/5/5/5
2	NAD	B	501	-	-	0/22/62/62	0/5/5/5
2	NAD	C	501	-	-	0/22/62/62	0/5/5/5
2	NAD	D	501	-	-	0/22/62/62	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAD	O4B-C1B	2.08	1.43	1.41
2	A	501	NAD	O4D-C1D	2.21	1.44	1.41
2	A	501	NAD	C5A-C4A	2.23	1.45	1.40
2	D	501	NAD	O4D-C1D	2.61	1.44	1.41
2	B	501	NAD	O4D-C1D	2.62	1.44	1.41
2	B	501	NAD	C5A-C4A	2.67	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NAD	C5A-C4A	2.94	1.47	1.40
2	D	501	NAD	C5A-C4A	3.08	1.47	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	N3A-C2A-N1A	-9.37	121.72	128.89
2	D	501	NAD	N3A-C2A-N1A	-7.73	122.97	128.89
2	B	501	NAD	N3A-C2A-N1A	-7.26	123.34	128.89
2	A	501	NAD	N3A-C2A-N1A	-6.32	124.06	128.89
2	A	501	NAD	PN-O3-PA	-3.98	121.56	132.73
2	B	501	NAD	C1B-N9A-C4A	-3.73	121.32	126.94
2	D	501	NAD	PN-O3-PA	-3.46	123.00	132.73
2	B	501	NAD	PN-O3-PA	-3.28	123.51	132.73
2	C	501	NAD	O3-PN-O5D	-3.07	94.80	102.94
2	C	501	NAD	O3-PA-O5B	-3.01	94.96	102.94
2	A	501	NAD	C4A-C5A-N7A	-2.74	106.96	109.48
2	C	501	NAD	C1B-N9A-C4A	-2.55	123.09	126.94
2	B	501	NAD	O5B-PA-O1A	-2.54	99.75	109.62
2	B	501	NAD	O3-PN-O5D	-2.51	96.28	102.94
2	B	501	NAD	C4A-C5A-N7A	-2.36	107.31	109.48
2	B	501	NAD	O7N-C7N-N7N	-2.28	119.38	122.59
2	C	501	NAD	PN-O3-PA	-2.01	127.08	132.73
2	B	501	NAD	C2B-C3B-C4B	-2.01	98.49	102.61
2	A	501	NAD	O2N-PN-O5D	2.00	118.56	108.46
2	D	501	NAD	O2A-PA-O3	2.07	114.49	105.09
2	B	501	NAD	O4B-C1B-N9A	2.39	113.11	108.10
2	C	501	NAD	C3N-C2N-N1N	2.50	123.24	120.36
2	D	501	NAD	C2N-C3N-C4N	2.87	121.49	118.29
2	C	501	NAD	O4D-C1D-N1N	6.86	115.67	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAD	2	0
2	B	501	NAD	4	0
2	C	501	NAD	1	0
2	D	501	NAD	4	0

## 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 [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	491/494 (99%)	-0.60	0 100 100	6, 12, 24, 40	0
1	B	488/494 (98%)	-0.64	0 100 100	5, 12, 24, 40	0
1	C	489/494 (98%)	-0.59	1 (0%) 95 95	6, 12, 24, 49	0
1	D	491/494 (99%)	-0.51	0 100 100	6, 14, 29, 44	0
All	All	1959/1976 (99%)	-0.58	1 (0%) 95 95	5, 13, 25, 49	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	GLU	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 [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
3	NA	A	502	1/1	0.92	0.14	2.14	14,14,14,14	0
2	NAD	B	501	44/44	0.95	0.14	0.73	16,25,42,47	0
3	NA	B	502	1/1	0.81	0.14	0.67	15,15,15,15	0
2	NAD	D	501	44/44	0.95	0.14	0.46	15,25,38,40	0
2	NAD	A	501	44/44	0.96	0.12	0.09	15,19,28,28	0
2	NAD	C	501	44/44	0.96	0.11	-0.21	17,23,28,31	0
3	NA	D	502	1/1	0.95	0.08	-2.35	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.