Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:04 am GMT

PDB ID	:	1AD3
Title	:	CLASS 3 ALDEHYDE DEHYDROGENASE COMPLEX WITH NICOTINA MIDE-ADENINE-DINUCLEOTIDE
Authors	:	Liu, Z.-J.; Rose, J.; Wang, B.C.
Deposited on	:	1996-06-25
Resolution	:	2.60 Å(reported)

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949
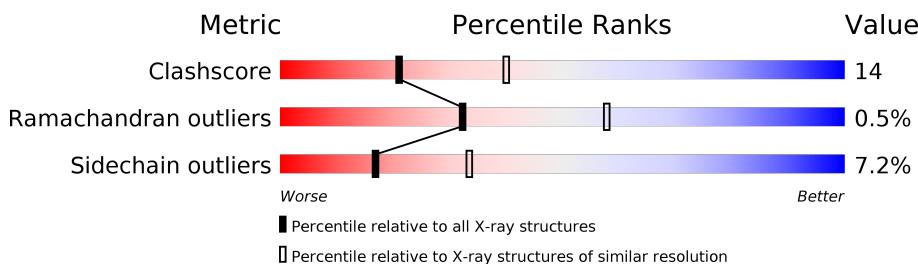
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.
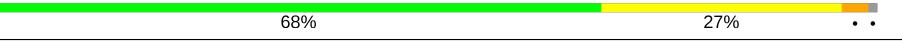
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		14
Ramachandran outliers		0.5%
Sidechain outliers		7.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (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 >=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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	452	68% 27% • •
1	B	452	67% 27% • •

2 Entry composition (i)
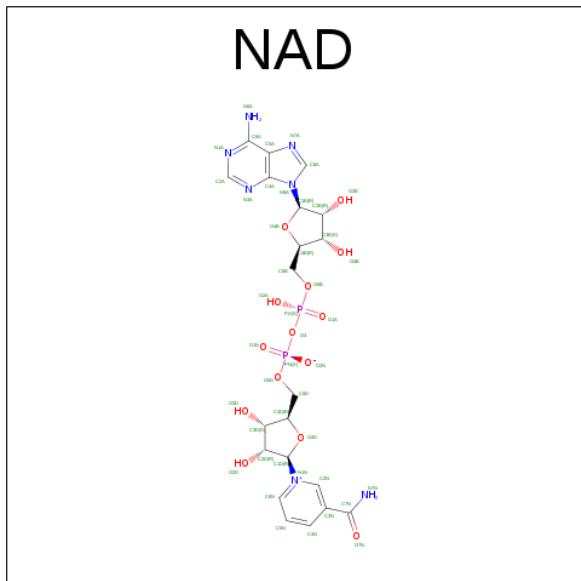
There are 3 unique types of molecules in this entry. The entry contains 8854 atoms, of which 1538 are hydrogens and 0 are deuteriums.

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 (CLASS 3).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	446	Total	C	H	N	O	S	0	0	0
			4245	2199	769	598	661	18			
1	B	446	Total	C	H	N	O	S	0	0	0
			4245	2199	769	598	661	18			

- 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		

- Molecule 3 is water.
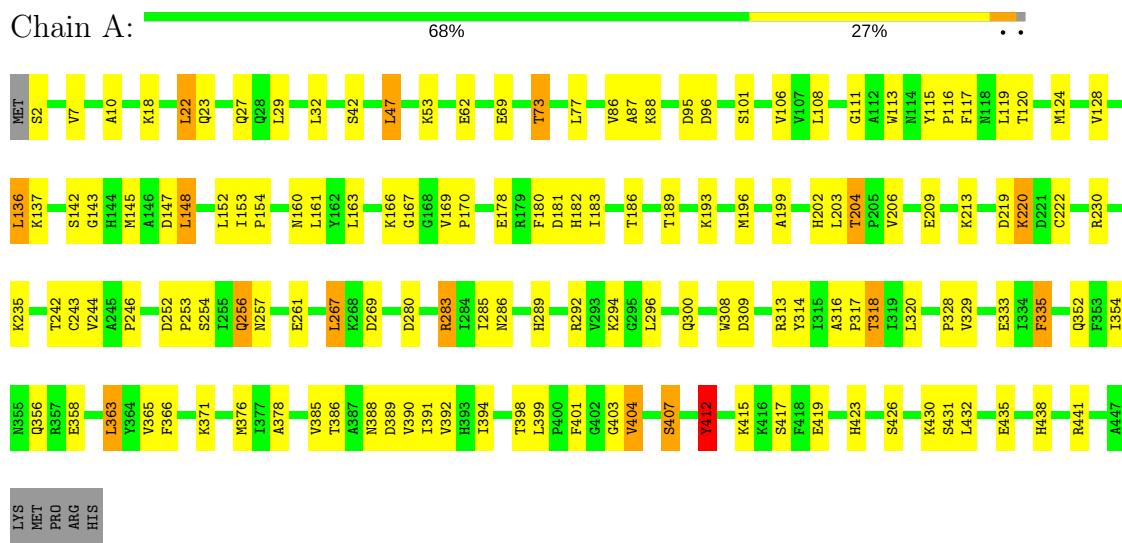
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	127	Total O 127 127	0	0
3	B	149	Total O 149 149	0	0

3 Residue-property plots ⓘ
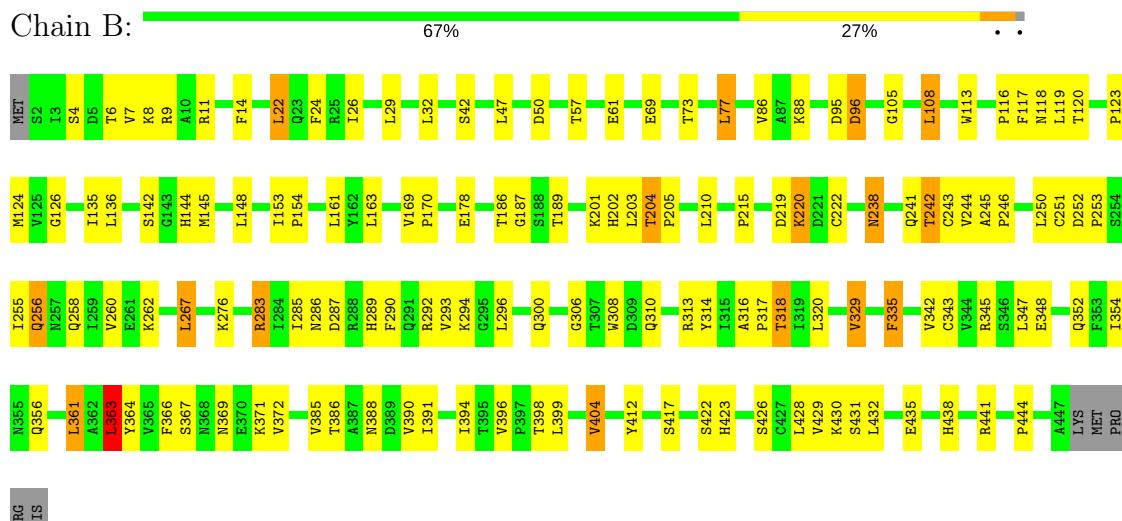
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: ALDEHYDE DEHYDROGENASE (CLASS 3)

• Molecule 1: ALDEHYDE DEHYDROGENASE (CLASS 3)

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.95Å 170.95Å 47.16Å 90.00° 110.25° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	80.0 (8.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.177 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8854	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.40	0/3547	0.67	3/4809 (0.1%)
1	B	0.38	0/3547	0.67	1/4809 (0.0%)
All	All	0.39	0/7094	0.67	4/9618 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	363	LEU	CA-CB-CG	7.11	131.66	115.30
1	B	363	LEU	CA-CB-CG	5.89	128.85	115.30
1	A	412	TYR	N-CA-C	5.71	126.42	111.00
1	A	136	LEU	CA-CB-CG	5.30	127.50	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3476	769	3477	105	0
1	B	3476	769	3477	108	0
2	A	44	0	26	2	0
2	B	44	0	26	0	0
3	A	127	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	149	0	0	8	0
All	All	7316	1538	7006	193	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 14.

All (193) 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:242:THR:HG23	1:B:245:ALA:HB2	1.36	1.06
1:B:390:VAL:HG12	1:B:391:ILE:HG13	1.46	0.94
1:A:300:GLN:HG2	1:A:320:LEU:HD13	1.55	0.88
1:B:300:GLN:HG2	1:B:320:LEU:HD13	1.55	0.88
1:B:296:LEU:HB3	1:B:329:VAL:HG13	1.64	0.80
1:B:347:LEU:HD22	1:B:372:VAL:HG13	1.67	0.76
1:A:189:THR:HG23	1:B:203:LEU:HD11	1.71	0.72
1:A:352:GLN:O	1:A:356:GLN:HG2	1.89	0.71
1:B:292:ARG:HH22	1:B:335:PHE:H	1.40	0.69
1:B:352:GLN:O	1:B:356:GLN:HG2	1.93	0.69
1:B:153:ILE:HB	1:B:154:PRO:HD3	1.76	0.68
1:A:431:SER:HA	1:B:388:ASN:HD22	1.58	0.68
1:A:220:LYS:H	1:A:220:LYS:HE2	1.57	0.68
1:A:431:SER:HA	1:B:388:ASN:ND2	2.12	0.65
1:A:202:HIS:HB2	1:A:204:THR:HG22	1.80	0.64
1:B:215:PRO:HG2	1:B:363:LEU:HD22	1.78	0.64
1:B:113:TRP:O	1:B:116:PRO:HD3	1.98	0.64
1:B:123:PRO:HG3	1:B:412:TYR:CE2	2.33	0.64
1:A:388:ASN:HD22	1:B:431:SER:HA	1.64	0.63
1:A:148:LEU:HD22	1:A:152:LEU:HG	1.81	0.63
1:A:244:VAL:HG21	1:A:394:ILE:HG13	1.81	0.61
1:A:289:HIS:HA	1:A:292:ARG:HG2	1.82	0.61
1:A:394:ILE:HD12	1:A:401:PHE:CD1	2.35	0.61
1:A:253:PRO:O	1:A:256:GLN:HB2	2.01	0.61
1:A:69:GLU:O	1:A:73:THR:HG23	2.02	0.60
1:B:220:LYS:H	1:B:220:LYS:HE2	1.67	0.60
1:B:256:GLN:O	1:B:260:VAL:HG23	2.01	0.60
1:B:246:PRO:HD3	1:B:390:VAL:HG11	1.83	0.60
1:B:438:HIS:O	1:B:441:ARG:HG2	2.02	0.59
1:A:292:ARG:HH22	1:A:335:PHE:H	1.51	0.59
1:A:183:ILE:HB	1:A:206:VAL:HG12	1.86	0.58
1:A:88:LYS:HE2	1:A:95:ASP:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:HIS:HB2	1:B:204:THR:HG22	1.85	0.57
1:B:287:ASP:HB3	3:B:724:HOH:O	2.04	0.57
1:A:294:LYS:HD2	1:A:308:TRP:CE2	2.40	0.57
1:B:366:PHE:HA	1:B:388:ASN:OD1	2.04	0.56
1:B:283:ARG:NH1	1:B:313:ARG:HH12	2.04	0.56
1:A:289:HIS:HD2	1:A:292:ARG:HD3	1.70	0.56
1:A:389:ASP:HB2	1:B:430:LYS:HD3	1.87	0.56
1:B:246:PRO:HD3	1:B:390:VAL:CG1	2.35	0.56
1:A:398:THR:O	1:B:86:VAL:HG11	2.04	0.56
1:B:88:LYS:HE2	1:B:95:ASP:O	2.06	0.56
1:A:371:LYS:HB2	1:A:371:LYS:HZ2	1.71	0.55
1:A:399:LEU:HD22	1:B:426:SER:HB3	1.88	0.55
1:A:412:TYR:O	1:A:417:SER:HB2	2.07	0.54
1:B:316:ALA:O	1:B:318:THR:HG22	2.07	0.54
1:B:7:VAL:HG21	1:B:178:GLU:HG3	1.88	0.54
1:B:371:LYS:HZ2	1:B:371:LYS:HB2	1.72	0.54
1:B:96:ASP:HA	3:B:604:HOH:O	2.07	0.54
1:B:285:ILE:HG23	1:B:286:ASN:N	2.23	0.53
1:B:347:LEU:CD2	1:B:372:VAL:HG13	2.38	0.53
1:A:7:VAL:HG21	1:A:178:GLU:HG3	1.89	0.53
1:B:390:VAL:CG1	1:B:391:ILE:HG13	2.31	0.53
1:A:166:LYS:HA	3:A:658:HOH:O	2.07	0.53
1:A:199:ALA:HB3	3:A:678:HOH:O	2.09	0.53
1:A:285:ILE:HG23	1:A:286:ASN:N	2.24	0.53
1:A:388:ASN:HB2	1:B:430:LYS:O	2.09	0.52
1:A:47:LEU:HD13	1:A:145:MET:HE2	1.91	0.52
1:A:86:VAL:HG12	1:A:87:ALA:N	2.24	0.52
1:A:113:TRP:O	1:A:116:PRO:HD3	2.09	0.52
1:A:220:LYS:HD2	1:A:252:ASP:HB3	1.91	0.52
1:A:193:LYS:HE3	1:B:201:LYS:O	2.09	0.52
1:B:253:PRO:HD3	1:B:343:CYS:HB3	1.91	0.52
1:B:289:HIS:HA	1:B:292:ARG:HG2	1.90	0.52
1:B:11:ARG:HG3	1:B:11:ARG:HH11	1.74	0.52
1:A:189:THR:HG23	1:B:203:LEU:CD1	2.38	0.52
1:A:329:VAL:HG23	3:A:654:HOH:O	2.09	0.52
1:B:126:GLY:HA3	1:B:417:SER:OG	2.09	0.52
1:B:253:PRO:O	1:B:256:GLN:HB2	2.09	0.52
1:B:69:GLU:HA	3:B:721:HOH:O	2.09	0.52
1:A:220:LYS:HE2	1:A:220:LYS:N	2.26	0.51
1:A:292:ARG:O	1:A:296:LEU:HG	2.11	0.51
1:B:57:THR:O	1:B:61:GLU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:THR:HG21	1:A:392:VAL:HG12	1.93	0.51
1:B:294:LYS:HD2	1:B:308:TRP:CE2	2.46	0.51
1:A:309:ASP:HB3	1:A:314:TYR:HB3	1.92	0.50
1:A:283:ARG:HD3	1:A:313:ARG:NH1	2.27	0.50
1:B:354:ILE:HD13	1:B:363:LEU:HD21	1.94	0.50
1:B:256:GLN:HG3	1:B:343:CYS:SG	2.52	0.50
1:A:153:ILE:HB	1:A:154:PRO:HD3	1.93	0.50
1:A:300:GLN:HG3	3:A:704:HOH:O	2.12	0.50
1:A:18:LYS:HD2	1:A:161:LEU:HD11	1.92	0.50
1:A:213:LYS:HD3	3:A:665:HOH:O	2.11	0.50
1:A:117:PHE:HB2	1:A:145:MET:HE3	1.93	0.50
1:A:388:ASN:ND2	1:B:431:SER:HA	2.26	0.50
1:A:111:GLY:HA3	1:A:120:THR:HG22	1.93	0.49
1:A:386:THR:HG23	1:B:428:LEU:HD22	1.93	0.49
1:B:430:LYS:C	1:B:432:LEU:N	2.64	0.49
1:A:86:VAL:HG11	1:B:398:THR:O	2.12	0.49
1:A:62:GLU:HG2	1:A:115:TYR:HD1	1.77	0.49
1:A:438:HIS:O	1:A:441:ARG:HG2	2.13	0.49
1:A:390:VAL:CG1	1:A:391:ILE:HG13	2.43	0.48
1:A:285:ILE:HG23	1:A:286:ASN:OD1	2.13	0.48
1:A:328:PRO:HG2	3:A:654:HOH:O	2.13	0.48
1:A:196:MET:HA	3:A:678:HOH:O	2.13	0.48
1:B:283:ARG:HD3	1:B:313:ARG:NH1	2.29	0.48
1:A:296:LEU:O	1:A:329:VAL:HG22	2.14	0.48
1:B:283:ARG:HH11	1:B:313:ARG:HH12	1.59	0.48
1:A:235:LYS:HD3	1:A:246:PRO:O	2.13	0.48
1:A:415:LYS:O	1:A:419:GLU:HG3	2.14	0.48
1:A:426:SER:HB3	1:B:399:LEU:HD22	1.96	0.48
1:B:205:PRO:HA	3:B:696:HOH:O	2.13	0.48
1:A:10:ALA:HB2	1:A:163:LEU:HD12	1.96	0.47
1:B:289:HIS:O	1:B:293:VAL:HG23	2.14	0.47
1:B:4:SER:O	1:B:8:LYS:HG3	2.14	0.47
1:A:390:VAL:HG12	1:A:391:ILE:HG13	1.96	0.47
1:B:117:PHE:HB2	1:B:145:MET:CE	2.45	0.47
1:A:219:ASP:O	1:A:222:CYS:HB3	2.14	0.47
1:B:14:PHE:CZ	1:B:105:GLY:HA2	2.50	0.47
1:B:250:LEU:HD23	1:B:342:VAL:HB	1.96	0.46
1:B:286:ASN:C	1:B:313:ARG:HD3	2.35	0.46
1:A:430:LYS:C	1:A:432:LEU:N	2.69	0.46
1:A:47:LEU:HG	1:A:53:LYS:HD2	1.98	0.46
1:B:220:LYS:N	1:B:220:LYS:HE2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:VAL:HG11	1:B:394:ILE:CD1	2.46	0.45
1:B:6:THR:HG23	1:B:9:ARG:HH12	1.81	0.45
1:A:23:GLN:O	1:A:27:GLN:HG3	2.15	0.45
1:B:251:CYS:O	1:B:343:CYS:HA	2.16	0.45
1:B:385:VAL:HG12	1:B:386:THR:N	2.31	0.45
1:B:11:ARG:HG3	1:B:11:ARG:NH1	2.31	0.45
1:A:404:VAL:HG22	1:B:423:HIS:NE2	2.31	0.45
1:B:124:MET:SD	1:B:136:LEU:HD21	2.57	0.45
1:B:300:GLN:CG	1:B:320:LEU:HD13	2.37	0.45
1:B:119:LEU:HD13	1:B:186:THR:HG21	1.98	0.45
1:B:219:ASP:HB3	1:B:367:SER:HB2	1.99	0.45
1:B:187:GLY:O	1:B:210:LEU:HA	2.17	0.44
1:A:119:LEU:HD22	1:A:186:THR:HG21	1.99	0.44
1:A:333:GLU:OE1	2:A:600:NAD:H6N	2.17	0.44
1:B:169:VAL:HB	1:B:170:PRO:HD3	1.99	0.44
1:A:423:HIS:NE2	1:B:404:VAL:HG22	2.33	0.44
1:B:316:ALA:O	1:B:318:THR:N	2.50	0.44
1:A:209:GLU:HB3	3:A:705:HOH:O	2.17	0.44
1:A:366:PHE:HA	1:A:388:ASN:OD1	2.18	0.44
1:B:361:LEU:HB2	3:B:630:HOH:O	2.18	0.44
1:A:403:GLY:HA3	1:A:407:SER:HB2	1.99	0.44
1:A:106:VAL:HG12	1:A:180:PHE:HD1	1.82	0.43
1:A:124:MET:SD	1:A:136:LEU:HD21	2.58	0.43
1:A:254:SER:HB2	3:A:711:HOH:O	2.19	0.43
1:A:257:ASN:O	1:A:261:GLU:HG2	2.19	0.43
1:B:283:ARG:HH11	1:B:313:ARG:NH1	2.16	0.43
1:A:390:VAL:O	1:A:391:ILE:HB	2.19	0.43
1:B:135:ILE:HA	1:B:163:LEU:O	2.19	0.43
1:B:108:LEU:HD23	1:B:135:ILE:O	2.19	0.43
1:B:22:LEU:O	1:B:26:ILE:HG12	2.18	0.43
1:B:73:THR:O	1:B:77:LEU:HB2	2.19	0.43
1:B:24:PHE:CZ	1:B:161:LEU:HD12	2.54	0.43
1:A:22:LEU:HA	1:A:22:LEU:HD22	1.88	0.43
1:A:289:HIS:HA	1:A:292:ARG:CG	2.48	0.43
1:A:300:GLN:CG	1:A:320:LEU:HD13	2.39	0.42
1:B:96:ASP:HB2	1:B:429:VAL:HB	2.01	0.42
1:A:196:MET:HG3	3:A:678:HOH:O	2.19	0.42
1:A:366:PHE:CD2	1:A:388:ASN:HA	2.55	0.42
1:A:230:ARG:HG2	1:B:441:ARG:NH2	2.35	0.42
1:B:50:ASP:OD2	1:B:144:HIS:HB2	2.19	0.42
1:A:47:LEU:HD13	1:A:145:MET:CE	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:SER:CA	1:B:388:ASN:HD22	2.30	0.42
1:B:430:LYS:C	1:B:432:LEU:H	2.21	0.42
1:B:219:ASP:O	1:B:222:CYS:HB3	2.20	0.42
1:B:267:LEU:HD12	1:B:267:LEU:HA	1.80	0.42
1:A:124:MET:O	1:A:128:VAL:HG23	2.20	0.42
1:A:285:ILE:HG23	1:A:286:ASN:H	1.85	0.42
1:B:306:GLY:N	1:B:318:THR:HB	2.34	0.42
1:A:394:ILE:HG22	1:A:394:ILE:O	2.20	0.42
1:A:169:VAL:HB	1:A:170:PRO:HD3	2.01	0.42
1:A:378:ALA:HB2	3:B:676:HOH:O	2.18	0.42
1:A:86:VAL:CG1	1:A:87:ALA:N	2.82	0.42
1:B:258:GLN:O	1:B:262:LYS:HG2	2.19	0.41
1:B:438:HIS:HB3	1:B:441:ARG:HD3	2.01	0.41
1:A:101:SER:HA	1:A:423:HIS:O	2.20	0.41
1:A:203:LEU:HD11	1:B:189:THR:HG23	2.02	0.41
1:A:280:ASP:OD2	1:B:444:PRO:HA	2.20	0.41
1:B:255:ILE:HA	1:B:258:GLN:NE2	2.36	0.41
1:A:137:LYS:HE2	1:A:167:GLY:O	2.21	0.41
1:A:169:VAL:HG22	2:A:600:NAD:C8A	2.50	0.41
1:A:316:ALA:O	1:A:318:THR:HG22	2.21	0.41
1:B:238:ASN:ND2	3:B:619:HOH:O	2.54	0.41
1:B:422:SER:HB2	3:B:671:HOH:O	2.20	0.41
1:A:354:ILE:HD12	1:A:376:MET:HE2	2.02	0.41
1:B:241:GLN:HE22	1:B:285:ILE:H	1.68	0.41
1:B:364:TYR:CE1	1:B:390:VAL:HA	2.55	0.41
1:B:69:GLU:O	1:B:73:THR:HG23	2.20	0.41
1:B:396:VAL:HB	1:B:399:LEU:HD12	2.03	0.41
1:A:2:SER:N	3:A:614:HOH:O	2.53	0.41
1:B:220:LYS:HD2	1:B:252:ASP:HB3	2.03	0.41
1:B:276:LYS:HE2	1:B:314:TYR:CD2	2.56	0.41
1:A:358:GLU:HG2	3:A:725:HOH:O	2.20	0.40
1:A:385:VAL:HG12	1:A:386:THR:N	2.35	0.40
1:B:290:PHE:CZ	1:B:310:GLN:HA	2.56	0.40
1:B:369:ASN:ND2	1:B:372:VAL:HG23	2.37	0.40
1:A:10:ALA:HA	1:A:160:ASN:O	2.22	0.40
1:A:181:ASP:O	1:A:182:HIS:HB2	2.22	0.40
1:A:267:LEU:HD12	1:A:267:LEU:HA	1.96	0.40
1:B:120:THR:O	1:B:123:PRO:HD2	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	444/452 (98%)	411 (93%)	30 (7%)	3 (1%)	25	49
1	B	444/452 (98%)	407 (92%)	36 (8%)	1 (0%)	51	76
All	All	888/904 (98%)	818 (92%)	66 (7%)	4 (0%)	32	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	GLY
1	A	412	TYR
1	A	317	PRO
1	B	317	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	382/388 (98%)	355 (93%)	27 (7%)	17	34
1	B	382/388 (98%)	354 (93%)	28 (7%)	16	33
All	All	764/776 (98%)	709 (93%)	55 (7%)	17	33

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	29	LEU

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Mol	Chain	Res	Type
1	A	32	LEU
1	A	42	SER
1	A	47	LEU
1	A	73	THR
1	A	77	LEU
1	A	96	ASP
1	A	108	LEU
1	A	142	SER
1	A	147	ASP
1	A	148	LEU
1	A	204	THR
1	A	220	LYS
1	A	242	THR
1	A	243	CYS
1	A	256	GLN
1	A	267	LEU
1	A	269	ASP
1	A	283	ARG
1	A	318	THR
1	A	335	PHE
1	A	363	LEU
1	A	365	VAL
1	A	404	VAL
1	A	407	SER
1	A	435	GLU
1	B	22	LEU
1	B	29	LEU
1	B	32	LEU
1	B	42	SER
1	B	47	LEU
1	B	77	LEU
1	B	96	ASP
1	B	108	LEU
1	B	118	ASN
1	B	142	SER
1	B	148	LEU
1	B	204	THR
1	B	220	LYS
1	B	238	ASN
1	B	242	THR
1	B	243	CYS
1	B	256	GLN

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Mol	Chain	Res	Type
1	B	267	LEU
1	B	283	ARG
1	B	318	THR
1	B	329	VAL
1	B	335	PHE
1	B	345	ARG
1	B	348	GLU
1	B	361	LEU
1	B	363	LEU
1	B	404	VAL
1	B	435	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	65	HIS
1	A	155	GLN
1	A	241	GLN
1	A	291	GLN
1	A	369	ASN
1	A	406	ASN
1	A	423	HIS
1	B	27	GLN
1	B	39	ASN
1	B	65	HIS
1	B	118	ASN
1	B	122	GLN
1	B	155	GLN
1	B	238	ASN
1	B	241	GLN
1	B	258	GLN
1	B	291	GLN
1	B	423	HIS
1	B	438	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	600	-	41,48,48	1.38	4 (9%)	43,73,73	2.19	16 (37%)
2	NAD	B	600	-	41,48,48	1.25	4 (9%)	43,73,73	2.27	17 (39%)

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	600	-	-	0/22/62/62	0/5/5/5
2	NAD	B	600	-	-	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	B	600	NAD	C3N-C7N	2.41	1.54	1.50
2	A	600	NAD	C6N-N1N	2.65	1.42	1.35
2	A	600	NAD	O4D-C1D	2.91	1.45	1.41
2	B	600	NAD	O4B-C1B	3.28	1.45	1.41
2	B	600	NAD	O4D-C1D	3.29	1.45	1.41
2	A	600	NAD	C3N-C7N	3.33	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	NAD	C6N-N1N	3.35	1.44	1.35
2	A	600	NAD	O4B-C1B	4.50	1.47	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	NAD	N3A-C2A-N1A	-6.66	123.06	128.86
2	A	600	NAD	C5N-C6N-N1N	-5.55	111.87	120.40
2	B	600	NAD	C5N-C6N-N1N	-5.55	111.87	120.40
2	A	600	NAD	N3A-C2A-N1A	-5.08	124.43	128.86
2	A	600	NAD	C3N-C7N-N7N	-3.96	113.25	117.77
2	A	600	NAD	C4N-C3N-C7N	-3.56	111.60	121.07
2	B	600	NAD	C3N-C2N-N1N	-3.42	116.98	120.43
2	B	600	NAD	C4N-C3N-C7N	-3.15	112.70	121.07
2	A	600	NAD	C5N-C4N-C3N	-3.01	116.80	120.35
2	B	600	NAD	O4B-C4B-C5B	-2.89	99.63	109.40
2	A	600	NAD	O4B-C4B-C5B	-2.65	100.45	109.40
2	A	600	NAD	C4D-O4D-C1D	-2.47	107.14	109.77
2	B	600	NAD	C3N-C7N-N7N	-2.35	115.09	117.77
2	A	600	NAD	C3N-C2N-N1N	-2.34	118.08	120.43
2	A	600	NAD	C5B-C4B-C3B	-2.09	107.31	115.29
2	B	600	NAD	O7N-C7N-C3N	-2.04	117.24	119.62
2	B	600	NAD	C1B-N9A-C4A	2.03	130.14	126.64
2	B	600	NAD	O2N-PN-O1N	2.04	122.84	112.28
2	B	600	NAD	O3B-C3B-C2B	2.05	118.40	111.83
2	B	600	NAD	O2B-C2B-C3B	2.25	119.04	111.83
2	B	600	NAD	C2N-C3N-C7N	2.28	125.97	119.34
2	A	600	NAD	C2N-C3N-C4N	2.45	121.05	118.26
2	B	600	NAD	C2N-C3N-C4N	2.52	121.13	118.26
2	A	600	NAD	O2N-PN-O1N	2.60	125.75	112.28
2	A	600	NAD	N6A-C6A-N1A	2.68	124.08	118.77
2	B	600	NAD	C4A-C5A-N7A	2.70	112.02	109.41
2	A	600	NAD	O2B-C2B-C3B	2.73	120.58	111.83
2	A	600	NAD	C2N-C3N-C7N	2.74	127.30	119.34
2	B	600	NAD	O7N-C7N-N7N	3.36	127.36	122.58
2	A	600	NAD	O7N-C7N-N7N	3.40	127.42	122.58
2	B	600	NAD	N6A-C6A-N1A	3.55	125.80	118.77
2	B	600	NAD	C6N-C5N-C4N	3.55	124.80	119.44
2	A	600	NAD	C6N-C5N-C4N	4.86	126.77	119.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	NAD	2	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.