



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 01:22 pm GMT

PDB ID : 4X2Q
Title : Crystal Structure of Human Aldehyde Dehydrogenase, ALDH1a2
Authors : Stenkamp, R.E.; Le Trong, I.; Amory, J.K.; Paik, J.; Goldstein, A.S.
Deposited on : 2014-11-26
Resolution : 2.94 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

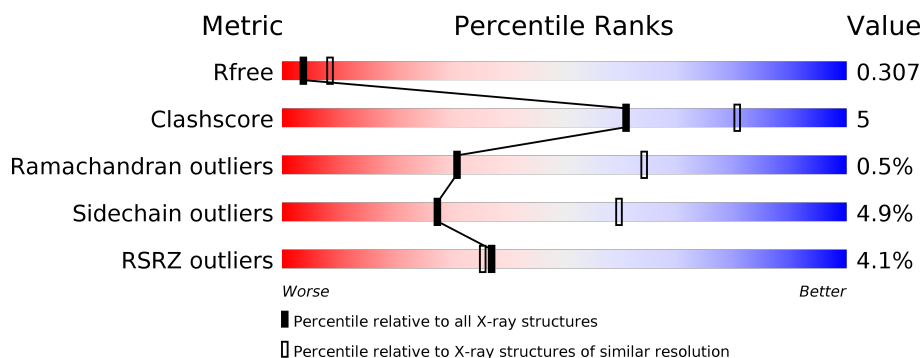
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	111664	2506 (2.98-2.90)
Clashscore	122126	2745 (2.98-2.90)
Ramachandran outliers	120053	2675 (2.98-2.90)
Sidechain outliers	120020	2677 (2.98-2.90)
RSRZ outliers	108989	2445 (2.98-2.90)

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 $\leq 5\%$. 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	504	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>6%</div> </div> </div>
1	B	504	<div> <div></div> <div> <div></div> <div>79%</div> <div>14%</div> <div>6%</div> </div> </div>
1	C	504	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>6%</div> </div> </div>
1	D	504	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>6%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14765 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 Retinal dehydrogenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3657	2333	623	685	16			
1	B	472	Total	C	N	O	S	0	0	0
			3658	2333	623	686	16			
1	C	474	Total	C	N	O	S	0	0	0
			3671	2340	626	689	16			
1	D	474	Total	C	N	O	S	0	0	0
			3671	2340	626	689	16			

There are 24 discrepancies between the modelled and reference sequences:

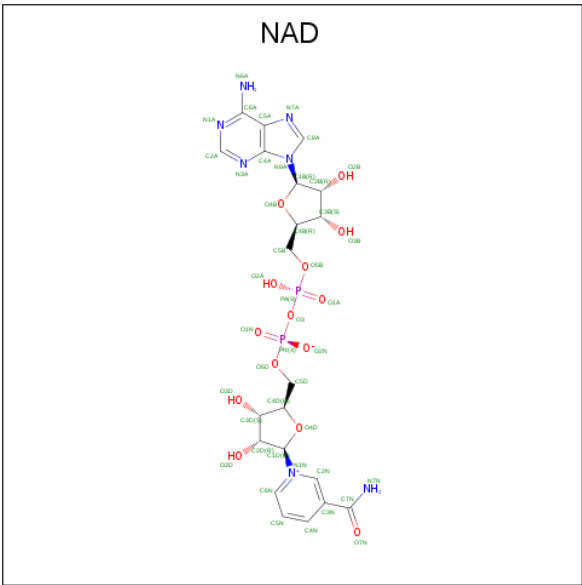
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP O94788
A	-2	HIS	-	expression tag	UNP O94788
A	-1	HIS	-	expression tag	UNP O94788
A	0	HIS	-	expression tag	UNP O94788
A	1	HIS	-	expression tag	UNP O94788
A	2	HIS	-	expression tag	UNP O94788
B	-3	HIS	-	expression tag	UNP O94788
B	-2	HIS	-	expression tag	UNP O94788
B	-1	HIS	-	expression tag	UNP O94788
B	0	HIS	-	expression tag	UNP O94788
B	1	HIS	-	expression tag	UNP O94788
B	2	HIS	-	expression tag	UNP O94788
C	-3	HIS	-	expression tag	UNP O94788
C	-2	HIS	-	expression tag	UNP O94788
C	-1	HIS	-	expression tag	UNP O94788
C	0	HIS	-	expression tag	UNP O94788
C	1	HIS	-	expression tag	UNP O94788
C	2	HIS	-	expression tag	UNP O94788
D	-3	HIS	-	expression tag	UNP O94788
D	-2	HIS	-	expression tag	UNP O94788
D	-1	HIS	-	expression tag	UNP O94788

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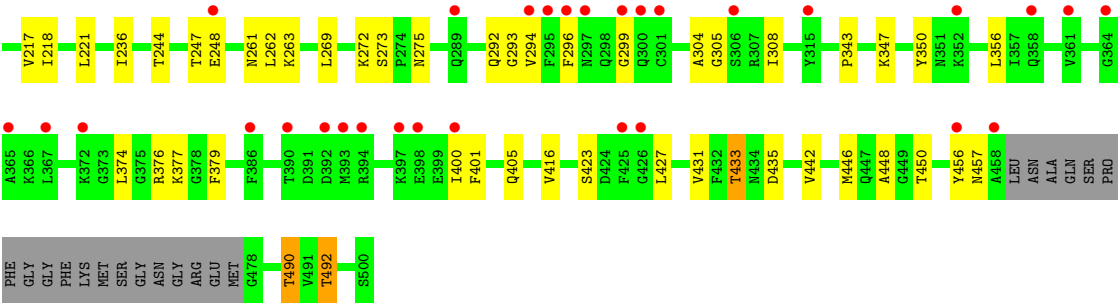
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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP O94788
D	1	HIS	-	expression tag	UNP O94788
D	2	HIS	-	expression tag	UNP O94788

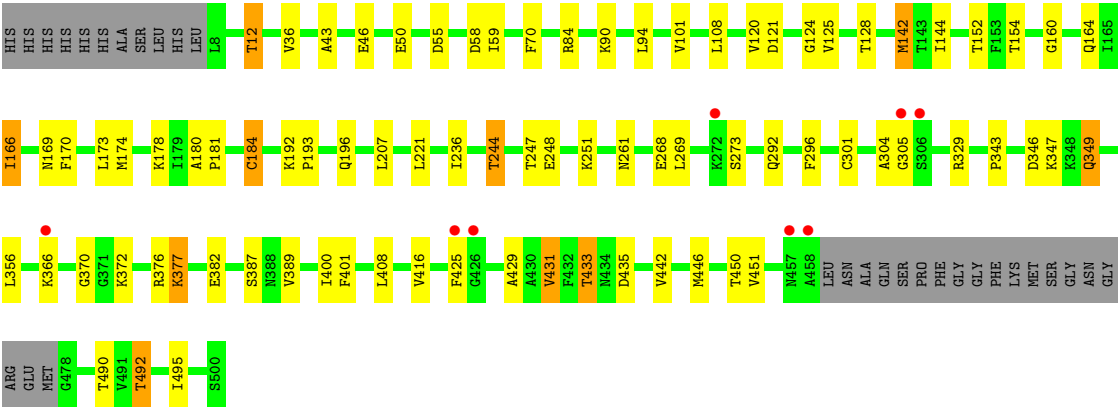
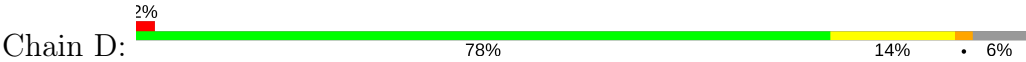
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		



● Molecule 1: Retinal dehydrogenase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.60Å 140.51Å 164.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.94 46.00 – 2.94	Depositor EDS
% Data completeness (in resolution range)	89.0 (50.00-2.94) 89.1 (46.00-2.94)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.266 , 0.313 0.265 , 0.307	Depositor DCC
R_{free} test set	1911 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14765	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4579e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [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	0.34	0/3734	0.46	0/5054
1	B	0.35	0/3735	0.49	1/5056 (0.0%)
1	C	0.35	0/3748	0.47	0/5074
1	D	0.35	0/3748	0.49	1/5074 (0.0%)
All	All	0.35	0/14965	0.48	2/20258 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	LEU	CA-CB-CG	5.17	127.18	115.30
1	D	108	LEU	CA-CB-CG	5.05	126.92	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	3657	0	3644	34	0
1	B	3658	0	3644	38	0
1	C	3671	0	3655	34	0
1	D	3671	0	3655	47	0
2	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
All	All	14765	0	14646	145	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 (145) 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:A:152:THR:HG22	1:A:492:THR:HB	1.49	0.91
1:C:152:THR:HG22	1:C:492:THR:HB	1.50	0.90
1:D:152:THR:HG22	1:D:492:THR:HB	1.53	0.89
1:B:272:LYS:HE2	1:B:423:SER:HB2	1.56	0.86
1:B:59:ILE:HD13	1:B:221:LEU:HD22	1.62	0.81
1:B:12:THR:HG21	1:B:101:VAL:HG12	1.64	0.79
1:D:376:ARG:O	1:D:377:LYS:HB2	1.82	0.78
1:C:59:ILE:HD13	1:C:221:LEU:HD22	1.71	0.72
1:C:356:LEU:HD23	1:C:400:ILE:HG13	1.71	0.72
1:B:142:MET:HA	1:C:142:MET:HA	1.73	0.71
1:B:301:CYS:SG	1:B:304:ALA:HB2	2.32	0.69
1:D:36:VAL:CG1	1:D:50:GLU:HB3	2.22	0.69
1:D:12:THR:HG21	1:D:101:VAL:HG12	1.75	0.69
1:B:152:THR:HG22	1:B:492:THR:HB	1.78	0.66
1:A:43:ALA:HA	1:A:343:PRO:HG3	1.80	0.64
1:C:350:TYR:HB2	1:C:379:PHE:HB3	1.84	0.60
1:A:273:SER:HB3	1:A:305:GLY:HA3	1.84	0.60
1:A:41:ASN:HB3	1:A:46:GLU:HG2	1.84	0.59
1:D:154:THR:HG22	1:D:490:THR:HG22	1.85	0.58
1:A:152:THR:CG2	1:A:492:THR:HB	2.29	0.58
1:B:36:VAL:CG1	1:B:50:GLU:HB3	2.33	0.58
1:A:59:ILE:HD13	1:A:221:LEU:HD22	1.86	0.58
1:D:36:VAL:HG11	1:D:50:GLU:HB3	1.84	0.58
1:B:423:SER:HB3	1:B:427:LEU:HD11	1.85	0.58
1:A:17:ILE:HG21	1:A:199:LEU:HD22	1.86	0.57
1:A:433:THR:HG22	1:A:435:ASP:H	1.69	0.56
1:B:431:VAL:HG11	1:B:442:VAL:HG11	1.87	0.56
1:B:94:LEU:HB3	1:B:207:LEU:HD22	1.87	0.56
1:D:372:LYS:O	1:D:382:GLU:HG2	2.06	0.56
1:C:292:GLN:O	1:C:296:PHE:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:THR:HG22	1:A:492:THR:CB	2.31	0.55
1:B:170:PHE:HB3	1:B:173:LEU:HB2	1.89	0.55
1:C:43:ALA:HA	1:C:343:PRO:HG3	1.90	0.54
1:D:43:ALA:HA	1:D:343:PRO:HG3	1.90	0.54
1:A:251:LYS:HG2	1:B:262:LEU:HD21	1.89	0.53
1:B:244:THR:HB	1:B:268:GLU:HB3	1.90	0.53
1:C:217:VAL:HG12	1:C:218:ILE:HG13	1.89	0.53
1:A:217:VAL:HG12	1:A:218:ILE:HG13	1.92	0.52
1:C:490:THR:HG23	1:D:450:THR:HG22	1.92	0.52
1:D:346:ASP:HB3	1:D:349:GLN:H	1.75	0.52
1:A:94:LEU:HB3	1:A:207:LEU:HD22	1.92	0.52
1:A:294:VAL:HG11	1:A:405:GLN:HB3	1.93	0.51
1:D:247:THR:HG22	1:D:269:LEU:HD13	1.92	0.51
1:B:55:ASP:H	1:B:58:ASP:HB2	1.76	0.51
1:D:59:ILE:HD13	1:D:221:LEU:HD22	1.92	0.51
1:A:247:THR:HG22	1:A:269:LEU:HB3	1.93	0.51
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.46	0.51
1:B:409:ARG:O	1:B:419:ARG:NH2	2.44	0.51
1:C:273:SER:HB3	1:C:305:GLY:HA3	1.93	0.50
1:D:170:PHE:HB3	1:D:173:LEU:HB2	1.93	0.50
1:B:372:LYS:O	1:B:382:GLU:HG2	2.12	0.50
1:D:174:MET:O	1:D:178:LYS:HG3	2.11	0.50
1:A:275:ASN:HB2	1:A:308:ILE:HG12	1.92	0.50
1:B:154:THR:HG22	1:B:490:THR:HB	1.94	0.50
1:B:36:VAL:HG11	1:B:50:GLU:HB3	1.93	0.49
1:D:429:ALA:HB2	1:D:446:MET:HG2	1.93	0.49
1:B:247:THR:HG22	1:B:269:LEU:HB3	1.94	0.49
1:D:376:ARG:O	1:D:377:LYS:CB	2.58	0.49
1:C:152:THR:CG2	1:C:492:THR:HB	2.33	0.49
1:D:431:VAL:HG11	1:D:442:VAL:HG11	1.95	0.48
1:D:366:LYS:HB3	1:D:387:SER:HB3	1.94	0.48
1:C:170:PHE:HB3	1:C:173:LEU:HB2	1.96	0.48
1:C:433:THR:HG22	1:C:435:ASP:H	1.78	0.48
1:D:180:ALA:HB3	1:D:181:PRO:HD3	1.96	0.48
1:D:166:ILE:HD11	1:D:193:PRO:HA	1.96	0.48
1:A:86:ARG:HE	1:A:86:ARG:HA	1.79	0.47
1:B:247:THR:HA	1:B:269:LEU:HD22	1.96	0.47
1:B:435:ASP:HB3	1:B:438:LYS:HB2	1.95	0.47
1:C:294:VAL:O	1:C:299:GLY:HA2	2.15	0.47
1:A:240:LYS:HG3	1:A:264:ARG:HB2	1.97	0.47
1:D:433:THR:HG22	1:D:435:ASP:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:PHE:CZ	1:B:160:GLY:HA2	2.50	0.47
1:A:247:THR:HA	1:A:269:LEU:HD22	1.97	0.47
1:B:172:LEU:HD13	1:B:200:SER:HB2	1.97	0.47
1:C:128:THR:HG21	1:C:177:TRP:HE1	1.79	0.46
1:D:70:PHE:CZ	1:D:160:GLY:HA2	2.50	0.46
1:A:262:LEU:HD21	1:B:251:LYS:HG2	1.97	0.46
1:C:293:GLY:HA3	1:C:456:TYR:HD2	1.79	0.46
1:D:244:THR:HB	1:D:268:GLU:HB3	1.96	0.46
1:C:427:LEU:HB3	1:C:448:ALA:HA	1.96	0.46
1:C:236:ILE:HD12	1:C:261:ASN:HB3	1.98	0.46
1:C:294:VAL:HG11	1:C:405:GLN:HB3	1.97	0.46
1:D:273:SER:HB3	1:D:305:GLY:HA3	1.98	0.46
1:C:121:ASP:O	1:C:125:VAL:HG23	2.15	0.45
1:D:236:ILE:HD12	1:D:261:ASN:HB3	1.97	0.45
1:B:273:SER:O	1:B:305:GLY:HA3	2.15	0.45
1:D:429:ALA:HB3	1:D:451:VAL:HG22	1.99	0.45
1:C:275:ASN:HB2	1:C:308:ILE:HG12	1.99	0.45
1:C:293:GLY:O	1:C:304:ALA:HB1	2.17	0.45
1:B:84:ARG:NH1	1:B:184:CYS:O	2.49	0.45
1:C:168:TRP:HD1	1:C:196:GLN:HE21	1.65	0.44
1:D:429:ALA:CB	1:D:446:MET:HG2	2.47	0.44
1:D:169:ASN:H	1:D:169:ASN:HD22	1.65	0.44
1:A:117:ALA:HA	1:A:121:ASP:HB2	1.99	0.44
1:B:232:ILE:HG23	1:B:238:ILE:HD13	1.99	0.44
1:D:301:CYS:SG	1:D:304:ALA:HB2	2.57	0.44
1:A:435:ASP:HB3	1:A:438:LYS:HB2	1.99	0.44
1:C:247:THR:HA	1:C:269:LEU:HD22	2.00	0.44
1:C:262:LEU:HD21	1:D:251:LYS:HG2	1.99	0.44
1:A:389:VAL:HB	1:A:408:LEU:HG	2.00	0.43
1:D:164:GLN:HB3	1:D:178:LYS:HD3	2.00	0.43
1:D:55:ASP:H	1:D:58:ASP:HB2	1.83	0.43
1:A:154:THR:HG22	1:A:490:THR:HG22	2.00	0.43
1:B:400:ILE:HD12	1:B:400:ILE:H	1.82	0.43
1:A:142:MET:HA	1:D:142:MET:HA	2.00	0.43
1:A:272:LYS:HE2	1:A:427:LEU:HD11	2.00	0.43
1:D:84:ARG:NH1	1:D:184:CYS:O	2.51	0.43
1:D:247:THR:HA	1:D:269:LEU:HD22	1.99	0.43
1:C:442:VAL:O	1:C:446:MET:HG2	2.19	0.43
1:D:292:GLN:O	1:D:296:PHE:HB2	2.19	0.43
1:D:124:GLY:O	1:D:128:THR:HG23	2.19	0.43
1:A:128:THR:HG21	1:A:177:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:SER:HB3	1:D:305:GLY:CA	2.49	0.43
1:A:409:ARG:O	1:A:419:ARG:NH2	2.51	0.42
1:B:294:VAL:O	1:B:299:GLY:HA2	2.19	0.42
1:D:389:VAL:HB	1:D:408:LEU:HG	2.01	0.42
1:C:272:LYS:HD3	1:C:423:SER:HB2	2.00	0.42
1:D:120:VAL:HG11	1:D:296:PHE:HZ	1.84	0.42
1:C:36:VAL:CG1	1:C:50:GLU:HB3	2.50	0.42
1:D:236:ILE:O	1:D:236:ILE:HG13	2.19	0.42
1:A:350:TYR:HB2	1:A:379:PHE:HB3	2.02	0.42
1:B:391:ASP:OD2	1:B:419:ARG:HD2	2.19	0.42
1:D:370:GLY:HA2	1:D:382:GLU:HG3	2.02	0.42
1:B:429:ALA:HB3	1:B:451:VAL:HG22	2.02	0.42
1:D:166:ILE:CG2	1:D:178:LYS:HD2	2.50	0.42
1:D:121:ASP:O	1:D:125:VAL:HG23	2.20	0.42
1:B:95:VAL:HG13	1:B:102:LEU:HD13	2.02	0.41
1:C:128:THR:HG21	1:C:177:TRP:NE1	2.35	0.41
1:A:15:LEU:HD13	1:A:104:THR:HB	2.00	0.41
1:B:232:ILE:HG22	1:B:241:ILE:HD12	2.03	0.41
1:A:331:VAL:HG22	1:A:341:GLN:HB3	2.02	0.41
1:C:167:PRO:HD3	1:C:244:THR:HG23	2.03	0.41
1:B:440:LEU:HD13	1:D:495:ILE:HG22	2.01	0.41
1:B:144:ILE:HG23	1:C:140:HIS:CE1	2.55	0.41
1:D:94:LEU:HB3	1:D:207:LEU:HD22	2.03	0.41
1:A:301:CYS:SG	1:A:304:ALA:HB3	2.61	0.41
1:A:104:THR:HG23	1:A:335:PHE:HE1	1.85	0.41
1:D:400:ILE:HD12	1:D:400:ILE:H	1.85	0.41
1:B:431:VAL:CG1	1:B:442:VAL:HG11	2.50	0.40
1:C:112:LYS:HE2	1:C:116:GLN:HB3	2.02	0.40
1:C:124:GLY:O	1:C:128:THR:HG23	2.21	0.40
1:A:179:ILE:HD13	1:A:189:VAL:HG11	2.04	0.40
1:B:179:ILE:CD1	1:B:189:VAL:HG11	2.51	0.40
1:B:433:THR:HG22	1:B:435:ASP:H	1.85	0.40
1:C:400:ILE:H	1:C:400:ILE:HD12	1.87	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	468/504 (93%)	445 (95%)	18 (4%)	5 (1%)	16	45
1	B	468/504 (93%)	443 (95%)	24 (5%)	1 (0%)	49	79
1	C	470/504 (93%)	447 (95%)	22 (5%)	1 (0%)	49	79
1	D	470/504 (93%)	449 (96%)	19 (4%)	2 (0%)	36	68
All	All	1876/2016 (93%)	1784 (95%)	83 (4%)	9 (0%)	31	64

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	377	LYS
1	A	377	LYS
1	A	422	ASN
1	A	425	PHE
1	C	377	LYS
1	A	13	PRO
1	B	377	LYS
1	D	425	PHE
1	A	167	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	387/412 (94%)	371 (96%)	16 (4%)	33	66
1	B	387/412 (94%)	368 (95%)	19 (5%)	27	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	388/412 (94%)	367 (95%)	21 (5%)	24	56
1	D	388/412 (94%)	368 (95%)	20 (5%)	25	57
All	All	1550/1648 (94%)	1474 (95%)	76 (5%)	27	60

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	86	ARG
1	A	90	LYS
1	A	122	LEU
1	A	166	ILE
1	A	192	LYS
1	A	196	GLN
1	A	330	VAL
1	A	347	LYS
1	A	401	PHE
1	A	416	VAL
1	A	431	VAL
1	A	450	THR
1	A	456	TYR
1	A	479	GLU
1	A	492	THR
1	B	12	THR
1	B	46	GLU
1	B	86	ARG
1	B	90	LYS
1	B	122	LEU
1	B	144	ILE
1	B	166	ILE
1	B	192	LYS
1	B	196	GLN
1	B	244	THR
1	B	347	LYS
1	B	401	PHE
1	B	416	VAL
1	B	425	PHE
1	B	427	LEU
1	B	433	THR
1	B	441	THR
1	B	479	GLU

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Mol	Chain	Res	Type
1	B	490	THR
1	C	46	GLU
1	C	86	ARG
1	C	90	LYS
1	C	109	ASN
1	C	122	LEU
1	C	166	ILE
1	C	192	LYS
1	C	196	GLN
1	C	248	GLU
1	C	263	LYS
1	C	347	LYS
1	C	374	LEU
1	C	376	ARG
1	C	401	PHE
1	C	416	VAL
1	C	431	VAL
1	C	433	THR
1	C	450	THR
1	C	457	ASN
1	C	490	THR
1	C	492	THR
1	D	12	THR
1	D	46	GLU
1	D	90	LYS
1	D	142	MET
1	D	144	ILE
1	D	166	ILE
1	D	184	CYS
1	D	192	LYS
1	D	196	GLN
1	D	244	THR
1	D	248	GLU
1	D	329	ARG
1	D	347	LYS
1	D	349	GLN
1	D	356	LEU
1	D	401	PHE
1	D	416	VAL
1	D	431	VAL
1	D	433	THR
1	D	492	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	5001	-	25,29,48	0.86	0	25,45,73	1.78	2 (8%)
2	NAD	B	601	-	25,29,48	0.82	0	25,45,73	1.85	2 (8%)
2	NAD	C	601	-	25,29,48	0.84	1 (4%)	25,45,73	1.82	3 (12%)
2	NAD	D	601	-	25,29,48	0.85	0	25,45,73	1.80	2 (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	5001	-	-	0/12/32/62	0/3/3/5
2	NAD	B	601	-	-	0/12/32/62	0/3/3/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	C	601	-	-	0/12/32/62	0/3/3/5
2	NAD	D	601	-	-	0/12/32/62	0/3/3/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAD	C8A-N9A	-2.02	1.34	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAD	N3A-C2A-N1A	-7.61	122.35	128.86
2	D	601	NAD	N3A-C2A-N1A	-7.45	122.48	128.86
2	A	5001	NAD	N3A-C2A-N1A	-7.35	122.57	128.86
2	C	601	NAD	N3A-C2A-N1A	-7.06	122.82	128.86
2	C	601	NAD	PA-O3-PN	-3.30	121.53	132.63
2	B	601	NAD	PA-O3-PN	-2.83	123.10	132.63
2	D	601	NAD	PA-O3-PN	-2.72	123.49	132.63
2	A	5001	NAD	PA-O3-PN	-2.55	124.05	132.63
2	C	601	NAD	C4A-C5A-N7A	-2.02	107.46	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

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, 95th 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 ²)	Q<0.9
1	A	472/504 (93%)	0.44	37 (7%) 13 11	41, 83, 127, 146	0
1	B	472/504 (93%)	0.04	2 (0%) 92 92	33, 53, 91, 119	0
1	C	474/504 (94%)	0.39	31 (6%) 19 16	39, 80, 146, 194	0
1	D	474/504 (94%)	0.03	8 (1%) 70 71	33, 54, 91, 112	0
All	All	1892/2016 (93%)	0.23	78 (4%) 37 35	33, 67, 122, 194	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	392	ASP	4.5
1	A	300	GLN	4.3
1	A	409	ARG	4.0
1	A	367	LEU	4.0
1	A	291	HIS	4.0
1	D	457	ASN	4.0
1	C	299	GLY	3.9
1	A	362	ALA	3.7
1	C	361	VAL	3.6
1	A	295	PHE	3.6
1	A	400	ILE	3.6
1	A	296	PHE	3.6
1	A	327	LYS	3.6
1	C	392	ASP	3.5
1	A	222	PRO	3.4
1	C	365	ALA	3.4
1	C	394	ARG	3.4
1	A	298	GLN	3.4
1	A	425	PHE	3.3
1	A	279	ALA	3.3
1	C	372	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	304	ALA	3.2
1	C	301	CYS	3.1
1	A	374	LEU	3.1
1	A	375	GLY	3.1
1	C	295	PHE	3.1
1	C	386	PHE	3.1
1	C	358	GLN	3.1
1	C	248	GLU	3.1
1	C	425	PHE	3.1
1	A	292	GLN	3.0
1	C	297	ASN	3.0
1	C	296	PHE	3.0
1	A	294	VAL	3.0
1	C	367	LEU	2.9
1	A	302	CYS	2.9
1	D	458	ALA	2.9
1	B	303	THR	2.9
1	C	400	ILE	2.9
1	C	294	VAL	2.8
1	A	325	ARG	2.7
1	A	299	GLY	2.7
1	D	366	LYS	2.7
1	D	306	SER	2.6
1	A	119	TYR	2.6
1	C	36	VAL	2.6
1	A	386	PHE	2.6
1	A	280	ASP	2.6
1	C	426	GLY	2.6
1	D	426	GLY	2.5
1	C	300	GLN	2.5
1	C	397	LYS	2.5
1	C	456	TYR	2.4
1	A	359	SER	2.4
1	C	398	GLU	2.4
1	A	356	LEU	2.4
1	C	352	LYS	2.4
1	C	390	THR	2.3
1	C	458	ALA	2.3
1	C	306	SER	2.3
1	A	305	GLY	2.3
1	A	289	GLN	2.3
1	C	289	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	297	ASN	2.2
1	A	384	THR	2.2
1	D	305	GLY	2.2
1	D	272	LYS	2.2
1	C	364	GLY	2.1
1	A	198	PRO	2.1
1	A	339	THR	2.1
1	A	293	GLY	2.1
1	A	306	SER	2.1
1	D	425	PHE	2.1
1	A	426	GLY	2.1
1	C	315	TYR	2.0
1	C	393	MET	2.0
1	A	326	ALA	2.0
1	A	304	ALA	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. The B-factors column lists the minimum, median, 95th 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	B-factors(\AA^2)	Q<0.9
2	NAD	C	601	27/44	0.90	0.25	27,29,30,30	27
2	NAD	A	5001	27/44	0.90	0.18	84,85,86,86	5
2	NAD	D	601	27/44	0.93	0.22	48,49,50,50	4
2	NAD	B	601	27/44	0.93	0.21	50,51,52,53	5

6.5 Other polymers [i](#)

There are no such residues in this entry.