



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 02:49 PM EST

PDB ID : 3HUD
Title : THE STRUCTURE OF HUMAN BETA 1 BETA 1 ALCOHOL DEHYDROGENASE: CATALYTIC EFFECTS OF NON-ACTIVE-SITE SUBSTITUTIONS
Authors : Hurley, T.D.; Bosron, W.F.; Hamilton, J.A.; Amzel, L.M.
Deposited on : unknown
Resolution : 3.20 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (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) : rb-20030345

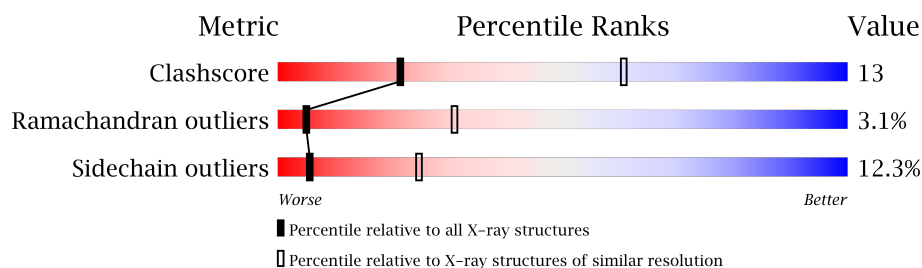
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	 60% 33% 6%
1	B	374	 59% 34% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5654 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.

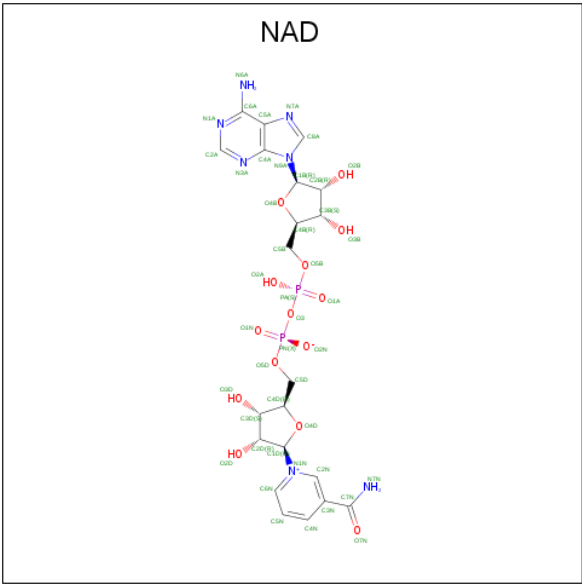
- Molecule 1 is a protein called ALCOHOL DEHYDROGENASE.

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

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



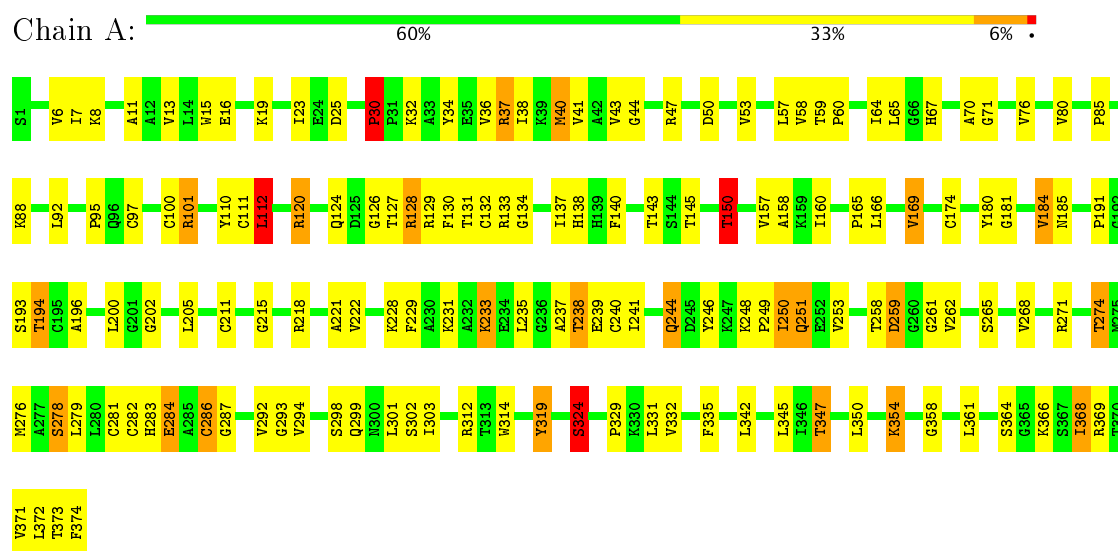
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

3 Residue-property plots

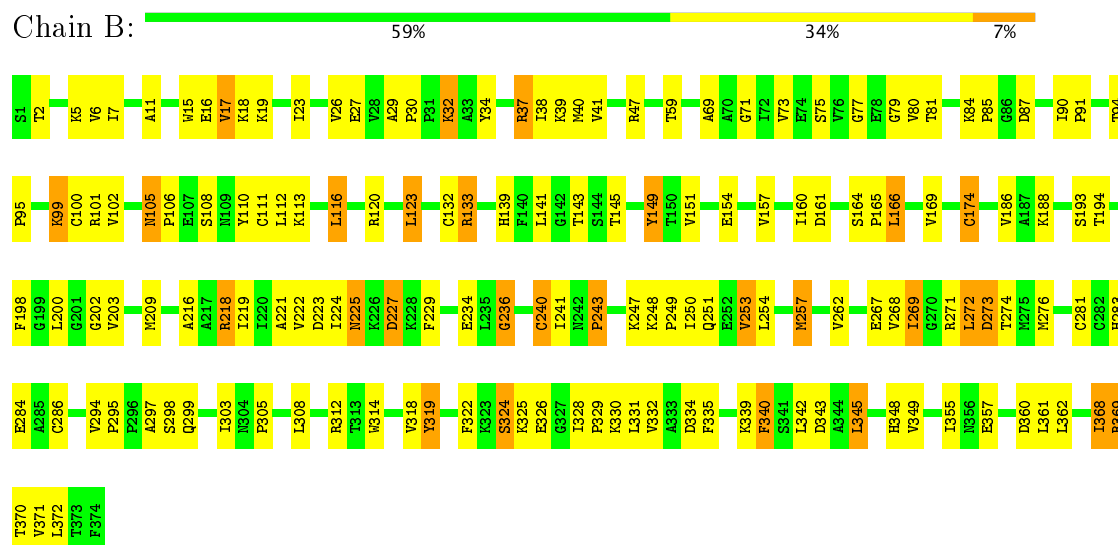
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



• Molecule 1: ALCOHOL DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.59 Å 45.05 Å 93.86 Å 91.93° 102.50° 68.82°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5654	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.79	0/2833	1.58	32/3833 (0.8%)
1	B	0.81	0/2833	1.62	30/3833 (0.8%)
All	All	0.80	0/5666	1.60	62/7666 (0.8%)

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ARG	NE-CZ-NH1	11.63	126.12	120.30
1	B	120	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	A	47	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	B	120	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B	47	ARG	NE-CZ-NH2	7.89	124.25	120.30
1	A	368	ILE	N-CA-C	-7.83	89.85	111.00
1	B	218	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	180	TYR	CB-CG-CD2	-7.52	116.49	121.00
1	B	139	HIS	CA-CB-CG	7.29	126.00	113.60
1	B	314	TRP	CD1-CG-CD2	7.25	112.10	106.30
1	B	105	ASN	CB-CA-C	-7.06	96.28	110.40
1	A	101	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	B	368	ILE	N-CA-C	-6.92	92.32	111.00
1	B	15	TRP	CE2-CD2-CG	-6.91	101.78	107.30
1	A	319	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	B	15	TRP	CD1-CG-CD2	6.78	111.73	106.30
1	A	15	TRP	CD1-CG-CD2	6.65	111.62	106.30
1	B	314	TRP	CE2-CD2-CG	-6.58	102.04	107.30
1	A	15	TRP	CE2-CD2-CG	-6.56	102.05	107.30
1	A	128	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	B	369	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	37	ARG	NE-CZ-NH1	6.38	123.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	B	133	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	133	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	B	357	GLU	CA-CB-CG	6.04	126.69	113.40
1	A	129	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	314	TRP	CE2-CD2-CG	-5.85	102.62	107.30
1	B	369	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	371	VAL	CG1-CB-CG2	-5.78	101.65	110.90
1	A	347	THR	CA-CB-CG2	-5.67	104.46	112.40
1	A	222	VAL	CG1-CB-CG2	-5.63	101.90	110.90
1	A	312	ARG	CB-CG-CD	-5.58	97.10	111.60
1	B	116	LEU	CA-CB-CG	5.56	128.09	115.30
1	B	312	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	259	ASP	CA-C-N	-5.47	105.26	116.20
1	A	369	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	253	VAL	CG1-CB-CG2	-5.44	102.19	110.90
1	B	149	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	A	88	LYS	CA-CB-CG	-5.40	101.52	113.40
1	B	99	LYS	CA-CB-CG	5.39	125.26	113.40
1	B	209	MET	CG-SD-CE	5.38	108.81	100.20
1	B	243	PRO	CA-C-N	5.37	129.02	117.20
1	A	32	LYS	CB-CG-CD	-5.36	97.67	111.60
1	B	15	TRP	CB-CG-CD1	-5.29	120.12	127.00
1	A	127	THR	N-CA-C	5.29	125.29	111.00
1	B	123	LEU	N-CA-C	-5.27	96.78	111.00
1	B	17	VAL	CB-CA-C	-5.23	101.46	111.40
1	A	30	PRO	N-CA-C	5.22	125.68	112.10
1	A	150	THR	CA-CB-CG2	-5.22	105.09	112.40
1	A	184	VAL	CA-CB-CG2	-5.18	103.13	110.90
1	B	257	MET	CA-CB-CG	5.17	122.09	113.30
1	A	250	ILE	CA-C-N	5.15	128.53	117.20
1	A	58	VAL	CG1-CB-CG2	-5.11	102.73	110.90
1	B	101	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	314	TRP	CD1-CG-CD2	5.10	110.38	106.30
1	A	133	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	238	THR	N-CA-C	-5.08	97.28	111.00
1	B	188	LYS	CA-CB-CG	5.07	124.55	113.40
1	A	15	TRP	CA-CB-CG	5.04	123.28	113.70
1	A	193	SER	N-CA-C	5.04	124.61	111.00
1	A	211	CYS	CA-CB-SG	5.03	123.05	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2781	0	2856	75	0
1	B	2781	0	2856	80	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	44	0	26	5	0
3	B	44	0	26	4	0
All	All	5654	0	5764	154	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 13.

All (154) 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:92:LEU:HD13	1:A:324:SER:HB2	1.25	1.14
1:B:269:ILE:HD12	1:B:274:THR:HG21	1.49	0.95
1:A:174:CYS:SG	3:A:377:NAD:H5N	2.14	0.87
1:B:174:CYS:SG	3:B:377:NAD:H5N	2.19	0.82
1:B:143:THR:HG22	1:B:145:THR:HG23	1.65	0.77
1:A:282:CYS:HB2	1:A:287:GLY:HA3	1.69	0.75
1:A:120:ARG:HH12	1:A:126:GLY:HA2	1.53	0.72
1:A:43:VAL:HG23	1:A:374:PHE:HE2	1.56	0.70
1:A:292:VAL:O	3:A:377:NAD:H2N	1.92	0.69
1:B:355:ILE:HA	1:B:372:LEU:HD21	1.75	0.68
1:A:92:LEU:HD13	1:A:324:SER:CB	2.15	0.67
1:B:80:VAL:HG22	1:B:154:GLU:HG3	1.77	0.67
1:A:233:LYS:HA	1:A:237:ALA:HB3	1.77	0.66
1:B:348:HIS:CD2	1:B:361:LEU:HD21	2.30	0.66
1:A:7:ILE:HG13	1:A:37:ARG:NH1	2.11	0.66
1:B:348:HIS:HB2	1:B:370:THR:HG23	1.77	0.65
1:A:350:LEU:HD23	1:A:354:LYS:HB3	1.78	0.65
1:B:110:TYR:HE1	1:B:116:LEU:HD22	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:CYS:SG	1:B:133:ARG:HD2	2.37	0.64
1:B:221:ALA:HB3	1:B:240:CYS:HB3	1.79	0.64
1:A:345:LEU:O	1:A:368:ILE:HB	1.98	0.63
1:B:95:PRO:HG3	1:B:113:LYS:HB2	1.81	0.62
1:A:70:ALA:HB1	1:A:166:LEU:HD22	1.82	0.61
1:B:100:CYS:HB2	1:B:112:LEU:HD22	1.82	0.61
1:B:194:THR:HG22	1:B:262:VAL:HG23	1.83	0.61
1:A:11:ALA:O	1:A:23:ILE:HA	2.01	0.61
1:A:97:CYS:HB3	1:A:111:CYS:SG	2.42	0.59
1:A:6:VAL:HG22	1:A:30:PRO:HD2	1.86	0.58
1:A:92:LEU:HD21	1:A:158:ALA:HB2	1.86	0.58
1:A:194:THR:HG23	1:A:218:ARG:HB2	1.85	0.58
1:A:143:THR:O	1:A:150:THR:HG21	2.04	0.57
1:A:229:PHE:CD1	1:A:240:CYS:HB3	2.40	0.56
1:B:26:VAL:HG12	1:B:132:CYS:HB2	1.87	0.56
1:B:161:ASP:HB3	1:B:164:SER:HG	1.71	0.56
1:B:69:ALA:O	1:B:90:ILE:HG23	2.06	0.56
1:A:258:THR:HG21	1:A:262:VAL:HA	1.88	0.56
1:B:37:ARG:HG2	1:B:151:VAL:HG22	1.88	0.55
1:B:95:PRO:HG2	1:B:111:CYS:HB3	1.89	0.55
1:B:248:LYS:HG2	1:B:253:VAL:HG23	1.88	0.54
1:A:160:ILE:HG21	1:A:332:VAL:HG21	1.91	0.53
1:B:73:VAL:HB	1:B:85:PRO:HA	1.89	0.53
1:B:200:LEU:HD21	1:B:221:ALA:HB1	1.91	0.53
1:A:246:TYR:CE2	1:A:253:VAL:HG11	2.43	0.53
1:A:120:ARG:NH1	1:A:126:GLY:HA2	2.24	0.52
1:B:342:LEU:HA	1:B:345:LEU:HD12	1.92	0.52
1:A:43:VAL:HG21	1:A:145:THR:O	2.10	0.52
1:A:38:ILE:HD11	1:A:157:VAL:HG21	1.92	0.51
1:B:219:ILE:HD12	1:B:236:GLY:O	2.10	0.51
1:B:116:LEU:HD11	1:B:318:VAL:HG11	1.93	0.51
1:B:161:ASP:HB3	1:B:164:SER:OG	2.11	0.51
1:B:5:LYS:HA	1:B:30:PRO:HG3	1.92	0.51
1:A:364:SER:HB2	1:A:366:LYS:HE2	1.92	0.51
1:B:174:CYS:SG	3:B:377:NAD:C5N	2.97	0.51
1:A:174:CYS:SG	3:A:377:NAD:C5N	2.94	0.50
1:B:271:ARG:HB3	1:B:273:ASP:OD1	2.10	0.50
1:A:249:PRO:HB2	1:A:251:GLN:OE1	2.12	0.50
1:B:222:VAL:HG22	1:B:241:ILE:HG12	1.92	0.50
1:B:250:ILE:O	1:B:254:LEU:HD12	2.11	0.50
1:A:100:CYS:SG	1:A:112:LEU:HD22	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:HH11	1:B:283:HIS:CD2	2.29	0.50
1:B:11:ALA:O	1:B:23:ILE:HA	2.10	0.50
1:B:91:PRO:HB2	1:B:143:THR:HG23	1.94	0.50
1:B:34:TYR:CE1	1:B:79:GLY:HA3	2.47	0.50
1:A:181:GLY:O	1:A:185:ASN:HB2	2.12	0.49
1:A:294:VAL:HB	3:A:377:NAD:O2D	2.11	0.49
1:B:16:GLU:HG2	1:B:17:VAL:H	1.76	0.49
1:A:200:LEU:HD21	1:A:221:ALA:HB1	1.94	0.49
1:A:194:THR:HG21	1:A:258:THR:HG23	1.94	0.49
1:B:271:ARG:HB2	1:B:274:THR:OG1	2.12	0.49
1:B:41:VAL:HG11	1:B:166:LEU:HD12	1.94	0.49
1:A:268:VAL:HG22	1:A:292:VAL:HB	1.93	0.49
1:B:32:LYS:O	1:B:77:GLY:HA3	2.13	0.49
1:A:347:THR:HG21	1:A:368:ILE:HG12	1.94	0.49
1:B:250:ILE:HA	1:B:253:VAL:HB	1.95	0.49
1:A:40:MET:HB3	1:A:374:PHE:CD2	2.48	0.49
1:B:164:SER:HB3	1:B:169:VAL:HG21	1.94	0.48
1:A:65:LEU:HA	1:A:140:PHE:CB	2.43	0.48
1:B:102:VAL:HG13	1:B:108:SER:HB2	1.96	0.48
1:B:73:VAL:HG23	1:B:87:ASP:O	2.14	0.48
1:B:203:VAL:HG12	3:B:377:NAD:O2N	2.14	0.47
1:B:223:ASP:OD1	3:B:377:NAD:H1B	2.13	0.47
1:A:248:LYS:HG3	1:A:253:VAL:HG22	1.96	0.47
1:A:6:VAL:HG22	1:A:30:PRO:CD	2.43	0.47
1:A:100:CYS:HB2	1:A:112:LEU:HD23	1.97	0.47
1:B:334:ASP:HB3	1:B:339:LYS:HG2	1.96	0.47
1:A:128:ARG:HD2	1:A:138:HIS:HA	1.96	0.47
1:B:91:PRO:HA	1:B:157:VAL:HG23	1.96	0.47
1:B:94:THR:HG1	1:B:319:TYR:HD2	1.61	0.47
1:A:16:GLU:HB2	1:A:19:LYS:HB2	1.97	0.46
1:B:39:LYS:HG3	1:B:149:TYR:CZ	2.51	0.46
1:A:218:ARG:HA	1:A:238:THR:HG21	1.98	0.46
1:A:7:ILE:HD12	1:A:37:ARG:HD2	1.97	0.46
1:B:331:LEU:HD23	1:B:340:PHE:CZ	2.50	0.46
1:B:7:ILE:O	1:B:27:GLU:HA	2.16	0.46
1:A:271:ARG:HG3	1:A:274:THR:OG1	2.15	0.46
1:B:16:GLU:HB3	1:B:19:LYS:CG	2.46	0.46
1:A:276:MET:HG2	1:A:301:LEU:HD22	1.98	0.46
1:B:345:LEU:O	1:B:368:ILE:HB	2.16	0.45
1:A:358:GLY:HA2	1:A:361:LEU:HD12	1.99	0.45
1:B:16:GLU:HG2	1:B:17:VAL:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:HIS:HB3	1:A:286:CYS:SG	2.57	0.45
1:B:335:PHE:HB2	1:B:340:PHE:HE1	1.81	0.45
1:A:160:ILE:CG2	1:A:332:VAL:HG21	2.47	0.44
1:B:193:SER:H	1:B:216:ALA:HA	1.82	0.44
1:A:241:ILE:HD12	1:A:250:ILE:HD11	1.98	0.44
1:A:41:VAL:HG23	1:A:71:GLY:HA2	1.99	0.44
1:B:328:ILE:O	1:B:332:VAL:HG23	2.17	0.44
1:B:34:TYR:HA	1:B:80:VAL:HG23	2.00	0.44
1:B:37:ARG:CG	1:B:151:VAL:HG22	2.48	0.44
1:A:43:VAL:HG12	1:A:44:GLY:N	2.33	0.43
1:A:293:GLY:HA2	3:A:377:NAD:H1D	2.00	0.43
1:B:272:LEU:HD21	1:B:299:GLN:O	2.18	0.43
1:B:319:TYR:O	1:B:322:PHE:HB2	2.19	0.43
1:B:326:GLU:O	1:B:329:PRO:HD2	2.18	0.43
1:B:39:LYS:O	1:B:71:GLY:HA3	2.19	0.43
1:B:91:PRO:HG3	1:B:145:THR:HG21	2.00	0.43
1:A:41:VAL:HG21	1:A:166:LEU:CD1	2.49	0.43
1:A:60:PRO:HB2	1:A:138:HIS:CE1	2.54	0.43
1:B:34:TYR:HE1	1:B:79:GLY:HA3	1.83	0.42
1:A:274:THR:O	1:A:278:SER:HB3	2.19	0.42
1:B:6:VAL:HG22	1:B:29:ALA:HA	2.01	0.42
1:A:65:LEU:HA	1:A:140:PHE:HB3	2.00	0.42
1:A:200:LEU:O	1:A:228:LYS:HE2	2.20	0.42
1:B:17:VAL:O	1:B:19:LYS:HE3	2.19	0.42
1:B:34:TYR:O	1:B:154:GLU:HB2	2.20	0.42
1:B:349:VAL:HA	1:B:371:VAL:O	2.19	0.42
1:A:132:CYS:HB2	1:A:137:ILE:HD11	2.01	0.42
1:B:369:ARG:HA	1:B:369:ARG:HD3	1.72	0.42
1:B:223:ASP:HB3	1:B:229:PHE:HE1	1.85	0.42
1:A:130:PHE:HB2	1:A:137:ILE:HB	2.01	0.42
1:A:165:PRO:CG	1:A:335:PHE:HE2	2.33	0.42
1:A:248:LYS:HE2	1:A:248:LYS:HB3	1.79	0.41
1:A:169:VAL:HG21	1:A:332:VAL:HG13	2.02	0.41
1:A:244:GLN:HE21	1:A:244:GLN:HB2	1.74	0.41
1:A:261:GLY:HA2	1:A:281:CYS:O	2.19	0.41
1:B:294:VAL:HA	1:B:295:PRO:HD2	1.94	0.41
1:B:335:PHE:HB2	1:B:340:PHE:CE1	2.55	0.41
1:A:191:PRO:HA	1:A:215:GLY:O	2.20	0.41
1:B:198:PHE:O	1:B:269:ILE:HG13	2.20	0.41
1:A:50:ASP:HA	1:A:53:VAL:HG12	2.02	0.41
1:B:224:ILE:HG13	1:B:225:ASN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:TYR:HA	1:A:80:VAL:HG22	2.02	0.41
1:B:254:LEU:HA	1:B:257:MET:HE3	2.03	0.41
1:A:36:VAL:HG11	1:A:157:VAL:HG11	2.03	0.41
1:A:76:VAL:HB	1:A:80:VAL:HB	2.02	0.41
1:B:105:ASN:HA	1:B:106:PRO:HD3	1.85	0.41
1:A:283:HIS:O	1:A:287:GLY:N	2.51	0.41
1:A:8:LYS:HE3	1:A:25:ASP:HB3	2.01	0.41
1:B:194:THR:HG23	1:B:218:ARG:HB2	2.03	0.41
1:B:123:LEU:HA	1:B:123:LEU:HD23	1.79	0.40
1:B:164:SER:HA	1:B:165:PRO:HD2	1.96	0.40
1:A:196:ALA:HB2	1:A:262:VAL:HG11	2.02	0.40
1:A:231:LYS:O	1:A:235:LEU:HG	2.21	0.40
1:B:241:ILE:HD11	1:B:250:ILE:HD11	2.03	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	372/374 (100%)	317 (85%)	44 (12%)	11 (3%)	5	32
1	B	372/374 (100%)	311 (84%)	49 (13%)	12 (3%)	5	30
All	All	744/748 (100%)	628 (84%)	93 (12%)	23 (3%)	5	31

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	CYS
1	B	284	GLU
1	B	286	CYS
1	A	124	GLN
1	A	284	GLU

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Mol	Chain	Res	Type
1	A	298	SER
1	B	18	LYS
1	B	202	GLY
1	B	324	SER
1	A	67	HIS
1	A	324	SER
1	B	297	ALA
1	A	112	LEU
1	A	259	ASP
1	B	166	LEU
1	A	30	PRO
1	A	202	GLY
1	A	286	CYS
1	B	32	LYS
1	B	227	ASP
1	B	236	GLY
1	A	134	GLY
1	B	269	ILE

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	305/305 (100%)	269 (88%)	36 (12%)	6	27
1	B	305/305 (100%)	266 (87%)	39 (13%)	5	23
All	All	610/610 (100%)	535 (88%)	75 (12%)	5	25

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	30	PRO
1	A	40	MET
1	A	57	LEU
1	A	59	THR

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Mol	Chain	Res	Type
1	A	64	ILE
1	A	85	PRO
1	A	95	PRO
1	A	112	LEU
1	A	120	ARG
1	A	131	THR
1	A	150	THR
1	A	169	VAL
1	A	184	VAL
1	A	194	THR
1	A	205	LEU
1	A	233	LYS
1	A	239	GLU
1	A	244	GLN
1	A	251	GLN
1	A	265	SER
1	A	274	THR
1	A	278	SER
1	A	279	LEU
1	A	284	GLU
1	A	299	GLN
1	A	302	SER
1	A	303	ILE
1	A	319	TYR
1	A	324	SER
1	A	329	PRO
1	A	331	LEU
1	A	342	LEU
1	A	354	LYS
1	A	372	LEU
1	A	373	THR
1	B	2	THR
1	B	37	ARG
1	B	38	ILE
1	B	40	MET
1	B	59	THR
1	B	75	SER
1	B	81	THR
1	B	84	LYS
1	B	99	LYS
1	B	141	LEU
1	B	160	ILE

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Mol	Chain	Res	Type
1	B	186	VAL
1	B	225	ASN
1	B	227	ASP
1	B	234	GLU
1	B	240	CYS
1	B	243	PRO
1	B	247	LYS
1	B	249	PRO
1	B	251	GLN
1	B	267	GLU
1	B	268	VAL
1	B	272	LEU
1	B	273	ASP
1	B	276	MET
1	B	281	CYS
1	B	298	SER
1	B	303	ILE
1	B	305	PRO
1	B	308	LEU
1	B	319	TYR
1	B	324	SER
1	B	325	LYS
1	B	330	LYS
1	B	340	PHE
1	B	343	ASP
1	B	345	LEU
1	B	360	ASP
1	B	362	LEU

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	185	ASN
1	A	244	GLN
1	A	283	HIS
1	B	118	ASN
1	B	225	ASN

5.3.3 RNA ⓘ

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAD	A	377	-	41,48,48	1.51	5 (12%)	43,73,73	1.56	5 (11%)
3	NAD	B	377	-	41,48,48	1.48	8 (19%)	43,73,73	1.75	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	377	-	-	0/22/62/62	0/5/5/5
3	NAD	B	377	-	-	0/22/62/62	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	377	NAD	C3N-C7N	-5.84	1.41	1.50
3	B	377	NAD	C3N-C7N	-4.42	1.43	1.50
3	A	377	NAD	C4A-N3A	-4.29	1.29	1.35
3	B	377	NAD	C4A-N3A	-3.23	1.30	1.35
3	A	377	NAD	C5A-C4A	-3.03	1.33	1.40
3	B	377	NAD	C5A-C4A	-2.89	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	377	NAD	C5A-N7A	-2.78	1.30	1.39
3	B	377	NAD	C5A-N7A	-2.61	1.30	1.39
3	B	377	NAD	C2B-C1B	-2.33	1.49	1.53
3	A	377	NAD	O4D-C4D	-2.18	1.40	1.45
3	B	377	NAD	C2D-C1D	2.11	1.57	1.53
3	B	377	NAD	PN-O5D	2.44	1.69	1.59
3	B	377	NAD	O4D-C1D	2.62	1.44	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	377	NAD	O7N-C7N-N7N	-5.73	114.44	122.58
3	B	377	NAD	O7N-C7N-N7N	-5.25	115.11	122.58
3	B	377	NAD	N3A-C2A-N1A	-3.44	125.86	128.86
3	A	377	NAD	C4B-O4B-C1B	-2.96	106.62	109.77
3	A	377	NAD	N3A-C2A-N1A	-2.36	126.80	128.86
3	B	377	NAD	O2D-C2D-C3D	-2.02	105.35	111.83
3	A	377	NAD	C3N-C7N-N7N	2.65	120.80	117.77
3	B	377	NAD	C4D-O4D-C1D	2.65	112.59	109.77
3	A	377	NAD	O7N-C7N-C3N	3.57	123.80	119.62
3	B	377	NAD	C3N-C7N-N7N	4.40	122.80	117.77
3	B	377	NAD	O5D-C5D-C4D	4.66	125.54	109.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	377	NAD	5	0
3	B	377	NAD	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 ⓘ

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.