



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 12:12 PM EST

PDB ID : 1BMD
Title : DETERMINANTS OF PROTEIN THERMOSTABILITY OBSERVED IN THE 1.9 ANGSTROMS CRYSTAL STRUCTURE OF MALATE DEHYDROGENASE FROM THE THERMOPHILIC BACTERIUM THERMUS FLAVUS
Authors : Kelly, C.A.; Birktoft, J.J.
Deposited on : unknown
Resolution : 1.90 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

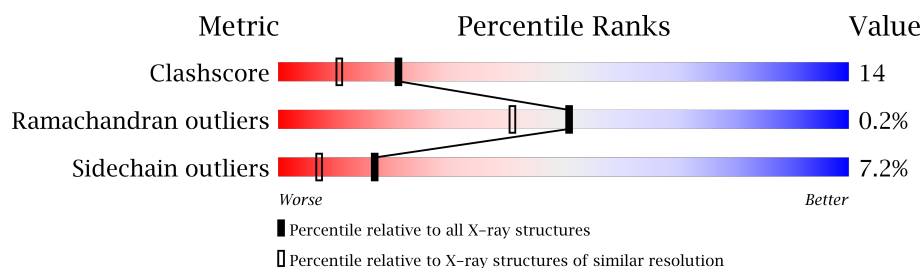
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	327	 67% 27% 5% .
1	B	327	 72% 23% . .

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5366 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.

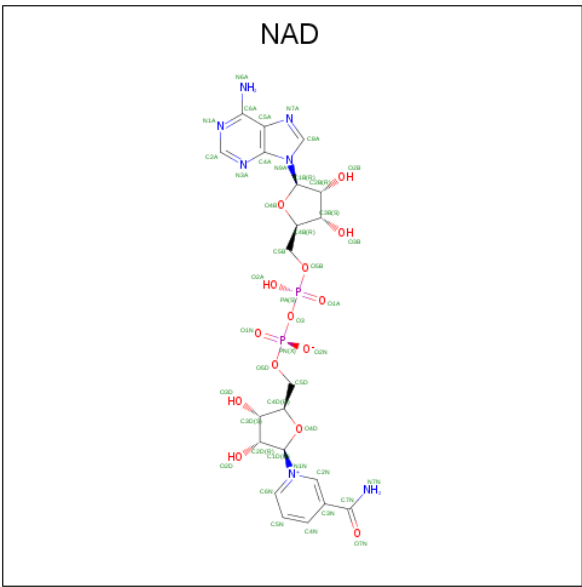
- Molecule 1 is a protein called MALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	1	0
			2493	1577	436	467	13			
1	B	327	Total	C	N	O	S	0	2	0
			2497	1579	436	469	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ASP	LYS	CONFLICT	UNP P10584
B	74	ASP	LYS	CONFLICT	UNP P10584

- 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
			44	21	7	14	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	125	Total	O	0	0
			125	125		
3	B	163	Total	O	0	0
			163	163		

3 Residue-property plots [i](#)

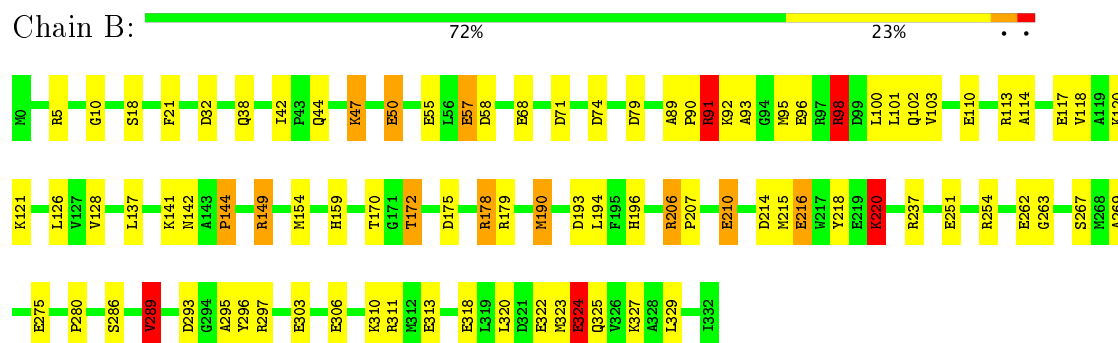
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: MALATE DEHYDROGENASE



• Molecule 1: MALATE DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.51Å 87.59Å 118.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.154 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5366	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: 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	1.07	22/2531 (0.9%)	1.54	39/3427 (1.1%)
1	B	1.09	18/2531 (0.7%)	1.58	31/3426 (0.9%)
All	All	1.08	40/5062 (0.8%)	1.56	70/6853 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	262	GLU	CD-OE2	8.55	1.35	1.25
1	B	96	GLU	CD-OE1	8.22	1.34	1.25
1	A	324	GLU	CD-OE2	8.20	1.34	1.25
1	A	96	GLU	CD-OE1	7.94	1.34	1.25
1	B	324	GLU	CD-OE1	7.92	1.34	1.25
1	B	210	GLU	CD-OE1	7.56	1.33	1.25
1	B	313	GLU	CD-OE1	7.54	1.33	1.25
1	B	306	GLU	CD-OE2	7.36	1.33	1.25
1	B	68	GLU	CD-OE1	7.29	1.33	1.25
1	A	262	GLU	CD-OE1	7.15	1.33	1.25
1	A	216	GLU	CD-OE1	7.08	1.33	1.25
1	B	251	GLU	CD-OE2	-6.90	1.18	1.25
1	A	306	GLU	CD-OE1	6.80	1.33	1.25
1	A	281	GLU	CD-OE1	6.73	1.33	1.25
1	A	50	GLU	CD-OE1	6.66	1.32	1.25
1	A	210	GLU	CD-OE1	6.57	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	GLU	CD-OE1	6.55	1.32	1.25
1	B	117	GLU	CD-OE2	6.41	1.32	1.25
1	B	50	GLU	CD-OE2	6.34	1.32	1.25
1	A	313	GLU	CD-OE2	6.33	1.32	1.25
1	B	216	GLU	CD-OE1	6.32	1.32	1.25
1	A	110	GLU	CD-OE1	6.23	1.32	1.25
1	A	198	GLU	CD-OE1	6.11	1.32	1.25
1	A	303	GLU	CD-OE2	6.09	1.32	1.25
1	A	68	GLU	CD-OE1	6.06	1.32	1.25
1	A	300	GLU	CD-OE2	6.03	1.32	1.25
1	B	303	GLU	CD-OE2	6.01	1.32	1.25
1	A	117	GLU	CD-OE2	5.88	1.32	1.25
1	B	318	GLU	CD-OE1	-5.76	1.19	1.25
1	B	322	GLU	CD-OE2	5.70	1.31	1.25
1	B	57	GLU	CD-OE2	-5.64	1.19	1.25
1	A	55	GLU	CD-OE1	5.63	1.31	1.25
1	B	110	GLU	CD-OE1	5.62	1.31	1.25
1	B	55	GLU	CD-OE1	5.56	1.31	1.25
1	A	55	GLU	CD-OE2	-5.38	1.19	1.25
1	B	275	GLU	CD-OE1	5.34	1.31	1.25
1	A	251	GLU	CD-OE2	-5.33	1.19	1.25
1	A	41	GLU	CD-OE1	-5.30	1.19	1.25
1	A	318	GLU	CD-OE1	5.18	1.31	1.25
1	A	322	GLU	CD-OE1	5.03	1.31	1.25

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ARG	NE-CZ-NH1	12.66	126.63	120.30
1	B	96	GLU	N-CA-CB	-10.69	91.36	110.60
1	B	178	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	B	193	ASP	CB-CG-OD2	-10.54	108.81	118.30
1	B	193	ASP	CB-CG-OD1	9.93	127.23	118.30
1	A	297	ARG	NE-CZ-NH1	-9.80	115.40	120.30
1	A	237	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	B	74	ASP	CB-CG-OD2	9.39	126.75	118.30
1	A	214	ASP	CB-CG-OD2	-9.13	110.08	118.30
1	A	5	ARG	NE-CZ-NH2	8.85	124.73	120.30
1	B	74	ASP	CB-CG-OD1	-8.79	110.39	118.30
1	B	71	ASP	CB-CG-OD2	-8.78	110.40	118.30
1	A	72	ASP	CB-CG-OD2	-8.14	110.98	118.30
1	A	71	ASP	CB-CG-OD1	7.92	125.42	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	311	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	122	ASP	CB-CG-OD2	7.74	125.26	118.30
1	A	193	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	B	79	ASP	CB-CG-OD2	7.27	124.84	118.30
1	B	71	ASP	CB-CG-OD1	7.22	124.80	118.30
1	B	58	ASP	CB-CG-OD1	7.21	124.79	118.30
1	B	98	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	B	32	ASP	CB-CG-OD1	7.13	124.72	118.30
1	A	214	ASP	CB-CG-OD1	7.12	124.71	118.30
1	A	97	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	71	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	A	200	ASP	CB-CG-OD1	-6.87	112.12	118.30
1	A	72	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	175	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	B	220	LYS	N-CA-CB	6.60	122.48	110.60
1	B	293	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	264	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	5	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	A	264	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	297	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	B	254	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	A	321	ASP	CB-CG-OD2	6.18	123.87	118.30
1	A	237	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	206	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	98	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	215	MET	CB-CA-C	-5.98	98.45	110.40
1	A	73	PRO	N-CA-CB	5.94	110.43	103.30
1	A	149	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	A	74	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	56	LEU	CB-CG-CD2	-5.86	101.03	111.00
1	A	74	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	A	152	THR	CA-CB-CG2	-5.77	104.33	112.40
1	B	190	MET	CA-CB-CG	-5.75	103.53	113.30
1	A	35	VAL	CG1-CB-CG2	-5.67	101.82	110.90
1	B	214	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	21	PHE	CB-CG-CD2	5.65	124.75	120.80
1	A	122	ASP	CB-CG-OD1	-5.63	113.23	118.30
1	A	193	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	289	VAL	N-CA-CB	-5.57	99.26	111.50
1	A	190	MET	CG-SD-CE	-5.55	91.32	100.20
1	B	190	MET	CG-SD-CE	-5.55	91.33	100.20
1	B	79	ASP	CB-CG-OD1	-5.54	113.31	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	TYR	CB-CG-CD1	5.53	124.32	121.00
1	A	58	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	293	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	255	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	178	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	B	91	ARG	N-CA-CB	5.30	120.14	110.60
1	B	144	PRO	C-N-CA	-5.28	111.20	122.30
1	B	206	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	B	237	ARG	CB-CA-C	-5.27	99.87	110.40
1	A	210	GLU	CA-CB-CG	-5.18	102.01	113.40
1	B	293	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	B	323	MET	CG-SD-CE	-5.10	92.04	100.20
1	A	158	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	A	161	ARG	NE-CZ-NH1	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	HIS	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2493	0	2520	73	0
1	B	2497	0	2520	66	0
2	A	44	0	26	6	0
2	B	44	0	26	3	0
3	A	125	0	0	3	0
3	B	163	0	0	10	0
All	All	5366	0	5092	139	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 (139) 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:98:ARG:H	1:A:98:ARG:HD2	1.20	1.05
1:A:89:ALA:H	1:A:104:ASN:HD21	1.13	0.95
1:A:105:GLY:O	1:A:109:THR:HG23	1.74	0.88
1:B:47:LYS:O	1:B:47:LYS:HE2	1.74	0.87
1:B:92:LYS:HG2	1:B:93:ALA:N	1.92	0.83
1:A:306:GLU:HA	1:A:309:ARG:HD2	1.60	0.83
1:A:98:ARG:O	1:A:102:GLN:HG2	1.80	0.81
1:A:121:LYS:HD2	1:A:121:LYS:N	1.95	0.79
1:B:295:ALA:HA	3:B:494:HOH:O	1.83	0.79
1:A:89:ALA:H	1:A:104:ASN:ND2	1.81	0.78
1:A:97:ARG:HB3	1:A:98:ARG:CZ	2.15	0.76
1:B:126:LEU:HD11	1:B:154:MET:HB2	1.66	0.76
1:B:5:ARG:HD3	1:B:38:GLN:HE22	1.48	0.76
1:B:92:LYS:HE2	1:B:93:ALA:O	1.86	0.75
1:A:98:ARG:H	1:A:98:ARG:CD	1.99	0.74
1:B:92:LYS:HB3	1:B:95:MET:SD	2.28	0.73
1:B:206:ARG:HD2	1:B:210:GLU:OE1	1.87	0.73
1:B:190:MET:HG3	1:B:190:MET:O	1.87	0.72
1:A:326:VAL:HG13	1:A:331:LEU:HB2	1.71	0.71
1:A:89:ALA:HB2	1:A:103:VAL:HG22	1.71	0.71
1:B:190:MET:HE2	3:B:474:HOH:O	1.89	0.71
1:A:140:TYR:CE1	1:A:141:LYS:HD2	2.25	0.70
1:B:10:GLY:HA2	2:B:334:NAD:H1B	1.74	0.70
1:A:92:LYS:HG2	1:A:95:MET:CE	2.21	0.70
1:B:89:ALA:HB2	1:B:103:VAL:HG12	1.73	0.70
1:A:92:LYS:HG2	1:A:95:MET:HB2	1.73	0.68
2:B:334:NAD:H52N	3:B:491:HOH:O	1.92	0.68
1:B:5:ARG:HD3	1:B:38:GLN:NE2	2.09	0.68
1:B:47:LYS:HE3	1:B:50:GLU:CD	2.14	0.68
1:A:98:ARG:N	1:A:98:ARG:HD2	2.02	0.66
1:A:92:LYS:HG2	1:A:95:MET:SD	2.35	0.66
1:A:14:GLN:NE2	2:A:334:NAD:O2A	2.28	0.66
1:B:159:HIS:HD2	1:B:267:SER:OG	1.79	0.66
1:B:92:LYS:O	1:B:95:MET:HB3	1.94	0.66
1:A:92:LYS:O	1:A:95:MET:HB3	1.95	0.66
1:B:170:THR:OG1	1:B:172:THR:HG23	1.95	0.66
1:B:128:VAL:O	2:B:334:NAD:H2N	1.96	0.65
1:A:306:GLU:N	1:A:306:GLU:OE1	2.32	0.63
1:A:306:GLU:HA	1:A:309:ARG:CD	2.28	0.63
1:B:47:LYS:C	1:B:47:LYS:HE2	2.18	0.63
1:A:92:LYS:HG2	1:A:95:MET:CB	2.28	0.63
1:B:91:ARG:HG3	1:B:91:ARG:HH11	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLN:HG2	1:B:329:LEU:HD13	1.80	0.62
1:B:137:LEU:CD1	1:B:141:LYS:HD2	2.32	0.60
1:A:269:ALA:HA	1:A:286:SER:HA	1.84	0.59
1:B:269:ALA:HA	1:B:286:SER:HA	1.84	0.59
1:B:280:PRO:HG2	1:B:320:LEU:HD11	1.84	0.59
1:B:142:ASN:O	1:B:144:PRO:HD3	2.03	0.59
1:B:47:LYS:NZ	1:B:50:GLU:OE1	2.33	0.59
1:A:187:SER:O	1:A:190:MET:HG2	2.02	0.58
1:A:102:GLN:HE22	1:A:329:LEU:HD21	1.67	0.58
1:A:304:ILE:HB	1:A:309:ARG:HH21	1.69	0.58
1:A:92:LYS:HG2	1:A:95:MET:HE3	1.86	0.58
1:A:99:ASP:O	1:A:103:VAL:HG12	2.04	0.58
1:B:47:LYS:HE2	1:B:47:LYS:CA	2.34	0.57
1:A:304:ILE:O	1:A:309:ARG:NH2	2.39	0.55
1:A:102:GLN:OE1	1:A:329:LEU:HD22	2.05	0.55
1:A:89:ALA:CB	1:A:103:VAL:HG22	2.38	0.54
1:B:206:ARG:HG3	1:B:207:PRO:N	2.23	0.54
1:B:289:VAL:HG13	1:B:296:TYR:HB2	1.90	0.54
1:B:47:LYS:HA	1:B:47:LYS:CE	2.38	0.54
1:A:168:LYS:NZ	1:B:57:GLU:OE2	2.41	0.53
1:A:130:ASN:ND2	2:A:334:NAD:O2D	2.37	0.53
1:B:149:ARG:HD2	3:B:450:HOH:O	2.07	0.53
1:A:98:ARG:HA	1:A:101:LEU:HB2	1.90	0.53
1:A:169:LYS:NZ	1:A:217:TRP:CD1	2.78	0.52
1:A:102:GLN:HE22	1:A:329:LEU:CD2	2.23	0.52
1:B:91:ARG:NH1	1:B:91:ARG:HG3	2.23	0.51
1:A:219:GLU:HG2	1:A:220:LYS:HE3	1.92	0.51
1:A:93:ALA:C	1:A:95:MET:H	2.13	0.51
1:A:130:ASN:HB2	2:A:334:NAD:O2D	2.12	0.50
1:B:170:THR:O	1:B:172:THR:HG22	2.11	0.50
1:B:18:SER:O	3:B:425:HOH:O	2.20	0.50
1:B:216:GLU:O	1:B:220:LYS:HD2	2.12	0.50
1:B:178:ARG:HH22	1:B:263:GLY:HA3	1.77	0.50
1:B:47:LYS:CA	1:B:47:LYS:CE	2.89	0.50
1:A:2:ALA:HB1	1:A:3:PRO:HD2	1.95	0.49
1:A:16:GLY:O	1:A:20:LEU:HG	2.12	0.49
1:A:306:GLU:HA	1:A:309:ARG:CG	2.43	0.49
1:B:196:HIS:HD2	3:B:471:HOH:O	1.96	0.49
1:A:320:LEU:HA	1:A:320:LEU:HD23	1.49	0.48
1:A:126:LEU:HD11	1:A:154:MET:HB2	1.95	0.48
1:B:91:ARG:CG	1:B:91:ARG:HH11	2.24	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HB3	1:A:98:ARG:NH1	2.28	0.48
1:A:10:GLY:HA2	2:A:334:NAD:H1B	1.95	0.47
1:A:92:LYS:HD3	1:A:95:MET:HE1	1.96	0.47
1:B:113:ARG:NH1	1:B:144:PRO:HG3	2.29	0.47
1:A:306:GLU:HA	1:A:309:ARG:HG2	1.97	0.47
1:B:149:ARG:HD3	1:B:296:TYR:OH	2.15	0.47
1:A:326:VAL:HG12	1:A:332:ILE:HG12	1.97	0.47
1:A:100:LEU:HD12	1:A:100:LEU:HA	1.73	0.46
1:B:5:ARG:HH11	1:B:38:GLN:NE2	2.14	0.46
1:A:252:HIS:HD2	3:A:354:HOH:O	1.97	0.46
1:A:178:ARG:HH22	1:A:263:GLY:HA3	1.80	0.46
1:A:163:LYS:NZ	3:A:370:HOH:O	2.30	0.45
1:A:92:LYS:HD3	1:A:95:MET:CE	2.47	0.45
1:A:106:LYS:HD2	1:A:106:LYS:N	2.28	0.45
1:B:89:ALA:HB1	1:B:90:PRO:HD2	1.99	0.45
1:B:142:ASN:C	1:B:144:PRO:HD3	2.37	0.45
1:B:159:HIS:CD2	1:B:267:SER:OG	2.66	0.45
1:A:97:ARG:O	1:A:100:LEU:HB3	2.17	0.45
1:B:159:HIS:HE1	3:B:354:HOH:O	2.00	0.44
1:B:89:ALA:CB	1:B:90:PRO:HD2	2.42	0.44
1:B:92:LYS:HG2	1:B:93:ALA:H	1.78	0.44
1:B:137:LEU:HD12	1:B:141:LYS:HD2	1.96	0.44
1:A:121:LYS:H	1:A:121:LYS:HD2	1.77	0.44
1:A:287:PHE:HB3	1:A:288:PRO:HD2	1.99	0.44
1:A:42:ILE:HD13	1:A:42:ILE:HG21	1.65	0.43
1:A:178:ARG:NH2	1:A:263:GLY:HA3	2.33	0.43
1:A:100:LEU:HD23	3:A:436:HOH:O	2.18	0.43
1:A:101:LEU:HD12	1:A:101:LEU:HA	1.82	0.43
1:A:140:TYR:CD1	1:A:148:PRO:HB3	2.53	0.43
1:A:309:ARG:O	1:A:313:GLU:HG2	2.18	0.43
1:B:89:ALA:HB2	1:B:103:VAL:CG1	2.45	0.42
1:B:324:GLU:HG2	1:B:325:GLN:N	2.34	0.42
1:B:114:ALA:O	1:B:118:VAL:HG22	2.20	0.42
1:A:92:LYS:CG	1:A:95:MET:CE	2.95	0.42
1:B:175:ASP:N	1:B:175:ASP:OD1	2.42	0.42
1:A:128:VAL:O	2:A:334:NAD:H2N	2.19	0.42
1:B:98:ARG:CZ	1:B:98:ARG:HB3	2.49	0.42
1:A:124:LYS:HB3	1:A:256:TRP:CH2	2.54	0.42
1:B:196:HIS:CD2	3:B:471:HOH:O	2.72	0.42
1:A:279:ILE:HD13	1:A:285:TYR:CE1	2.54	0.42
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:HD11	1:B:141:LYS:HD2	2.00	0.41
1:B:178:ARG:NH2	1:B:263:GLY:HA3	2.35	0.41
1:A:190:MET:HB2	1:A:190:MET:HE3	1.87	0.41
1:A:326:VAL:CG1	1:A:331:LEU:HB2	2.45	0.41
1:B:42:ILE:HD13	1:B:42:ILE:HG21	1.80	0.41
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.87	0.41
1:B:100:LEU:HD12	1:B:100:LEU:HA	1.79	0.41
1:B:141:LYS:HZ2	1:B:141:LYS:HG2	1.80	0.41
1:B:179:ARG:HD3	3:B:451:HOH:O	2.21	0.41
1:A:114:ALA:O	1:A:118:VAL:HG22	2.21	0.40
1:A:186:HIS:CD2	2:A:334:NAD:C7N	3.05	0.40
1:B:47:LYS:HA	1:B:47:LYS:HE2	2.02	0.40
1:A:97:ARG:O	1:A:100:LEU:N	2.54	0.40
1:B:120:LYS:HE3	3:B:487:HOH:O	2.20	0.40
1:B:216:GLU:OE2	1:B:220:LYS:HE2	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	326/327 (100%)	321 (98%)	4 (1%)	1 (0%)	44	34
1	B	327/327 (100%)	325 (99%)	2 (1%)	0	100	100
All	All	653/654 (100%)	646 (99%)	6 (1%)	1 (0%)	51	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	ARG

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	251/252 (100%)	229 (91%)	22 (9%)	12	4
1	B	250/252 (99%)	236 (94%)	14 (6%)	25	13
All	All	501/504 (99%)	465 (93%)	36 (7%)	17	7

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	91	ARG
1	A	92	LYS
1	A	98	ARG
1	A	101	LEU
1	A	103	VAL
1	A	106	LYS
1	A	109	THR
1	A	121	LYS
1	A	140	TYR
1	A	141	LYS
1	A	149	ARG
1	A	168	LYS
1	A	190	MET
1	A	194	LEU
1	A	209	LEU
1	A	219	GLU
1	A	220	LYS
1	A	262	GLU
1	A	292	LYS
1	A	306	GLU
1	A	317	GLN
1	B	44	GLN
1	B	47	LYS
1	B	91	ARG
1	B	98	ARG
1	B	101	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	121	LYS
1	B	149	ARG
1	B	172	THR
1	B	220	LYS
1	B	289	VAL
1	B	297	ARG
1	B	310	LYS
1	B	324	GLU
1	B	327	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	130	ASN
1	A	165	GLN
1	A	252	HIS
1	A	273	GLN
1	B	38	GLN
1	B	44	GLN
1	B	102	GLN
1	B	111	GLN
1	B	147	ASN
1	B	159	HIS
1	B	235	GLN
1	B	273	GLN

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

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	334	-	41,48,48	0.76	0	43,73,73	1.85	10 (23%)
2	NAD	B	334	-	41,48,48	0.74	0	43,73,73	1.90	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
2	NAD	A	334	-	-	0/22/62/62	0/5/5/5
2	NAD	B	334	-	-	0/22/62/62	0/5/5/5

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	334	NAD	C4B-O4B-C1B	-6.32	103.04	109.77
2	B	334	NAD	O7N-C7N-C3N	-6.12	112.47	119.62
2	A	334	NAD	O7N-C7N-C3N	-5.88	112.75	119.62
2	A	334	NAD	C4D-O4D-C1D	-4.64	104.83	109.77
2	A	334	NAD	C4B-O4B-C1B	-3.72	105.81	109.77
2	A	334	NAD	C1B-N9A-C4A	-3.14	121.21	126.64
2	A	334	NAD	C3N-C2N-N1N	-3.07	117.34	120.43
2	A	334	NAD	N3A-C2A-N1A	-2.86	126.37	128.86
2	B	334	NAD	C4D-O4D-C1D	-2.76	106.83	109.77
2	A	334	NAD	O3D-C3D-C2D	-2.70	103.19	111.83
2	A	334	NAD	O4D-C4D-C3D	-2.12	100.95	105.17
2	B	334	NAD	O7N-C7N-N7N	2.49	126.12	122.58
2	A	334	NAD	C4A-C5A-N7A	2.95	112.26	109.41
2	B	334	NAD	C3N-C7N-N7N	3.17	121.39	117.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	334	NAD	O7N-C7N-N7N	3.32	127.30	122.58
2	B	334	NAD	C4A-C5A-N7A	4.14	113.41	109.41

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
2	A	334	NAD	6	0
2	B	334	NAD	3	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.