



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 05:43 AM GMT

PDB ID : 2P5U  
Title : Crystal structure of Thermus thermophilus HB8 UDP-glucose 4-epimerase complex with NAD  
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Deposited on : 2007-03-16  
Resolution : 2.37 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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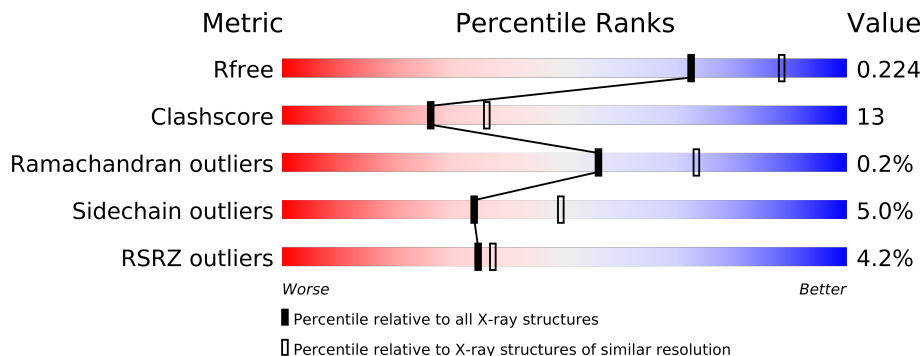
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.37 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))
$R_{free}$	66092	2963 (2.40-2.36)
Clashscore	79885	3668 (2.40-2.36)
Ramachandran outliers	78287	3600 (2.40-2.36)
Sidechain outliers	78261	3602 (2.40-2.36)
RSRZ outliers	66119	2966 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	311	
1	B	311	
1	C	311	
1	D	311	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAD	B	1118	-	X
2	NAD	C	1118	-	X
2	NAD	D	1118	-	X

## 2 Entry composition i

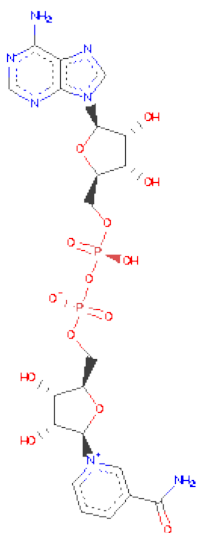
There are 3 unique types of molecules in this entry. The entry contains 10139 atoms, of which 0 are hydrogen and 0 are deuterium.

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 UDP-glucose 4-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2388	1520	424	439	5			
1	B	311	Total	C	N	O	S	0	0	0
			2388	1520	424	439	5			
1	C	311	Total	C	N	O	S	0	0	0
			2388	1520	424	439	5			
1	D	311	Total	C	N	O	S	0	0	0
			2388	1520	424	439	5			

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



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

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

- Molecule 3 is water.

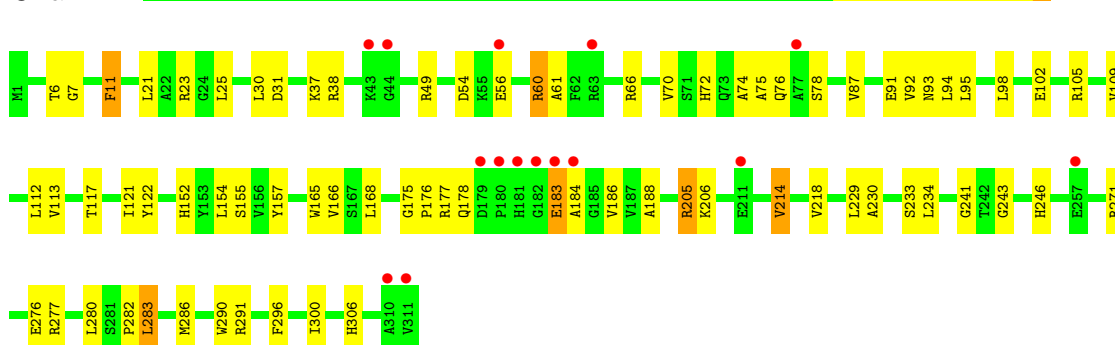
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total	O	0	0
			112	112		
3	B	99	Total	O	0	0
			99	99		
3	C	78	Total	O	0	0
			78	78		
3	D	122	Total	O	0	0
			122	122		

### 3 Residue-property plots

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

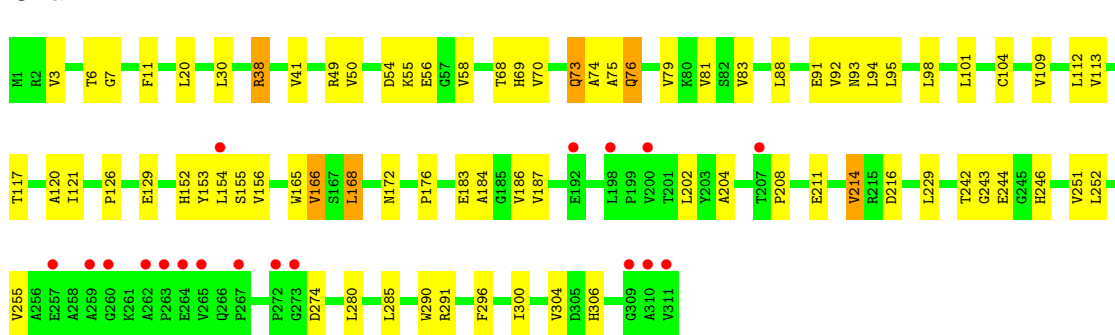
#### • Molecule 1: UDP-glucose 4-epimerase

Chain A:



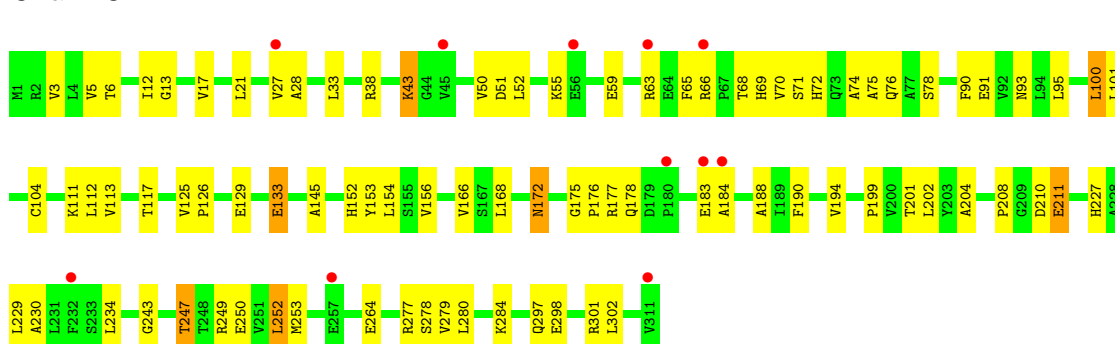
#### • Molecule 1: UDP-glucose 4-epimerase

Chain B:



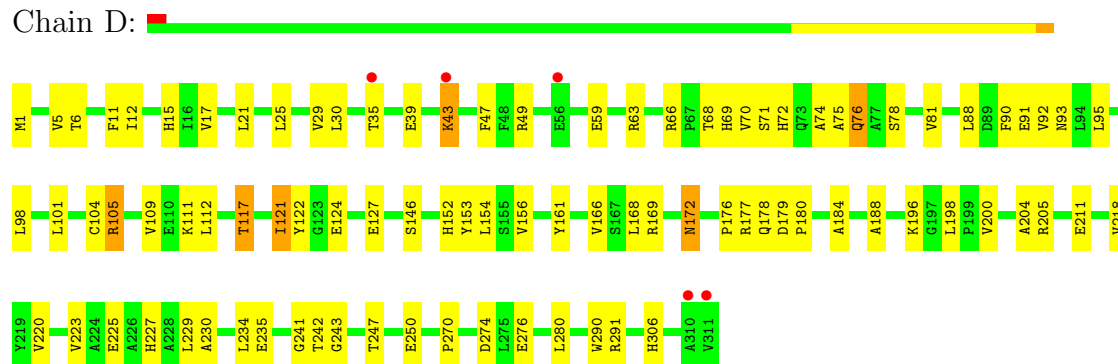
#### • Molecule 1: UDP-glucose 4-epimerase

Chain C:



● Molecule 1: UDP-glucose 4-epimerase

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	250.92Å 250.92Å 121.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.85 – 2.37 49.85 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.85-2.37) 99.8 (49.85-2.37)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	14.57 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.235 , 0.261 0.226 , 0.224	Depositor DCC
$R_{free}$ test set	4519 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 19.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 90065 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.38	0/2446	0.60	0/3320
1	B	0.36	0/2446	0.56	0/3320
1	C	0.35	0/2446	0.57	0/3320
1	D	0.39	0/2446	0.60	0/3320
All	All	0.37	0/9784	0.58	0/13280

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2370	65	0
1	B	2388	0	2370	62	0
1	C	2388	0	2370	69	0
1	D	2388	0	2370	68	0
2	A	44	0	26	3	0
2	B	44	0	25	3	0
2	C	44	0	25	1	0
2	D	44	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	112	0	0	2	0
3	B	99	0	0	5	0
3	C	78	0	0	3	0
3	D	122	0	0	7	0
All	All	10139	0	9581	256	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (256) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:218:VAL:HG11	1:D:241:GLY:HA2	1.52	0.91
1:C:247:THR:HG22	1:C:250:GLU:H	1.42	0.84
1:B:216:ASP:OD1	1:B:242:THR:HG22	1.76	0.84
1:A:76:GLN:HB2	1:A:92:VAL:HG21	1.59	0.84
1:B:76:GLN:HE22	1:B:81:VAL:HB	1.43	0.84
1:A:183:GLU:HA	1:A:271:ARG:HH12	1.42	0.84
1:A:76:GLN:HE22	1:A:78:SER:HB3	1.44	0.82
1:B:291:ARG:HH21	1:B:291:ARG:HG3	1.46	0.81
1:D:76:GLN:HB2	1:D:92:VAL:HG11	1.64	0.80
1:D:218:VAL:HG12	1:D:242:THR:HG23	1.65	0.79
1:C:230:ALA:HA	1:C:234:LEU:HB2	1.64	0.78
1:A:54:ASP:OD2	1:A:56:GLU:HG2	1.83	0.77
1:B:76:GLN:HB3	1:B:92:VAL:HG11	1.67	0.76
1:A:152:HIS:HE1	1:D:152:HIS:HE1	1.32	0.76
1:B:76:GLN:O	1:B:76:GLN:HG3	1.86	0.75
1:B:242:THR:HG23	1:B:244:GLU:H	1.53	0.73
1:A:152:HIS:CE1	1:D:152:HIS:HE1	2.07	0.71
1:C:297:GLN:HG2	1:C:301:ARG:HH22	1.54	0.71
1:D:63:ARG:HA	1:D:66:ARG:NH2	2.05	0.71
1:A:117:THR:HG23	1:A:121:ILE:HG23	1.73	0.70
1:A:178:GLN:HG3	1:A:188:ALA:HB2	1.72	0.70
1:D:172:ASN:HB3	1:D:184:ALA:HB2	1.75	0.69
1:C:12:ILE:HD11	2:C:1118:NAD:H71N	1.58	0.69
1:D:290:TRP:O	1:D:291:ARG:HG3	1.95	0.67
1:C:297:GLN:HG2	1:C:301:ARG:NH2	2.10	0.66
1:B:290:TRP:O	1:B:291:ARG:HG3	1.95	0.65
1:B:172:ASN:HB3	1:B:184:ALA:HB2	1.78	0.65
1:A:11:PHE:HB3	2:A:1118:NAD:O2N	1.97	0.65
1:A:113:VAL:HA	1:A:166:VAL:HG13	1.77	0.65
1:D:291:ARG:HG3	1:D:291:ARG:HH11	1.63	0.63
1:B:291:ARG:NH2	1:B:291:ARG:HG3	2.12	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:43:LYS:HA	1:C:43:LYS:NZ	2.14	0.63
1:B:154:LEU:HD13	1:B:165:TRP:CE3	2.33	0.63
1:C:75:ALA:HB1	1:C:93:ASN:OD1	2.00	0.62
1:C:76:GLN:NE2	1:C:78:SER:H	1.98	0.61
1:A:154:LEU:HD13	1:A:165:TRP:CD2	2.34	0.61
1:C:76:GLN:HE22	1:C:78:SER:HB3	1.65	0.60
1:A:218:VAL:HG21	1:A:241:GLY:HA2	1.83	0.60
1:A:154:LEU:HD13	1:A:165:TRP:CE3	2.36	0.60
1:D:127:GLU:HG3	3:D:1129:HOH:O	2.02	0.59
1:A:183:GLU:HA	1:A:271:ARG:NH1	2.16	0.59
1:A:102:GLU:OE1	1:A:105:ARG:HD3	2.03	0.59
1:C:125:VAL:CG1	1:C:278:SER:HA	2.33	0.59
1:C:91:GLU:O	1:C:95:LEU:HB3	2.02	0.58
1:D:39:GLU:HG3	3:D:1214:HOH:O	2.03	0.58
1:D:218:VAL:CG1	1:D:241:GLY:HA2	2.31	0.58
1:B:242:THR:HG23	1:B:244:GLU:N	2.17	0.58
1:D:88:LEU:O	1:D:92:VAL:HG12	2.04	0.58
1:C:125:VAL:HG12	1:C:277:ARG:O	2.03	0.58
1:D:29:VAL:HG23	1:D:47:PHE:HD1	1.68	0.57
1:C:43:LYS:HA	1:C:43:LYS:HZ3	1.68	0.57
1:C:126:PRO:HG2	1:C:129:GLU:CD	2.25	0.57
1:B:41:VAL:HB	3:B:1158:HOH:O	2.04	0.57
1:A:152:HIS:HE1	1:D:152:HIS:CE1	2.19	0.57
1:C:74:ALA:O	1:C:75:ALA:HB2	2.05	0.57
1:C:211:GLU:O	1:C:247:THR:HG23	2.04	0.57
1:A:218:VAL:CG2	1:A:241:GLY:HA2	2.35	0.57
1:B:154:LEU:HD13	1:B:165:TRP:CD2	2.39	0.57
1:C:6:THR:O	1:C:74:ALA:HB2	2.04	0.56
1:B:211:GLU:H	1:B:211:GLU:CD	2.08	0.56
1:B:176:PRO:HB3	1:B:306:HIS:HB2	1.87	0.56
1:B:300:ILE:O	1:B:304:VAL:HG23	2.05	0.56
1:B:113:VAL:HA	1:B:166:VAL:HG13	1.87	0.56
1:B:75:ALA:HB1	1:B:93:ASN:OD1	2.05	0.56
1:B:76:GLN:HE22	1:B:81:VAL:CB	2.16	0.56
1:C:3:VAL:HB	1:C:27:VAL:HG12	1.88	0.56
1:B:154:LEU:HD12	1:B:155:SER:N	2.21	0.55
1:A:76:GLN:HB2	1:A:92:VAL:CG2	2.35	0.55
1:C:172:ASN:HB3	1:C:184:ALA:HB2	1.87	0.55
1:C:243:GLY:HA2	1:C:280:LEU:O	2.06	0.55
1:D:105:ARG:HD3	1:D:161:TYR:CG	2.42	0.55
1:C:113:VAL:HA	1:C:166:VAL:HG13	1.89	0.54
1:D:15:HIS:HE1	1:D:176:PRO:O	1.91	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:251:VAL:O	1:B:255:VAL:HG23	2.07	0.54
1:D:121:ILE:HD13	1:D:169:ARG:CZ	2.38	0.53
1:A:178:GLN:CG	1:A:188:ALA:HB2	2.39	0.53
1:D:291:ARG:HG3	1:D:291:ARG:NH1	2.21	0.53
1:C:176:PRO:O	1:C:177:ARG:HB2	2.08	0.53
1:C:153:TYR:HA	1:C:156:VAL:HG22	1.91	0.53
1:D:93:ASN:HB2	1:D:146:SER:OG	2.08	0.53
1:C:175:GLY:O	1:C:178:GLN:HG2	2.09	0.53
1:D:243:GLY:HA2	1:D:280:LEU:O	2.09	0.53
1:A:6:THR:OG1	1:A:72:HIS:HD2	1.92	0.53
1:C:70:VAL:HG23	1:C:112:LEU:HG	1.89	0.53
1:A:175:GLY:H	1:A:178:GLN:NE2	2.07	0.53
1:C:125:VAL:HG11	1:C:278:SER:HA	1.91	0.53
1:B:74:ALA:O	1:B:75:ALA:HB2	2.09	0.53
1:A:176:PRO:O	1:A:177:ARG:HB2	2.08	0.53
1:A:246:HIS:HD2	3:A:1128:HOH:O	1.91	0.52
1:D:5:VAL:HG11	1:D:17:VAL:HG22	1.89	0.52
1:D:176:PRO:O	1:D:177:ARG:HB2	2.10	0.52
1:B:152:HIS:HE1	1:C:152:HIS:NE2	2.07	0.52
1:A:291:ARG:HH11	1:A:291:ARG:HG3	1.74	0.52
1:A:205:ARG:HD3	1:A:276:GLU:HB3	1.91	0.52
1:D:70:VAL:HG12	1:D:109:VAL:HG11	1.92	0.52
1:D:71:SER:OG	1:D:227:HIS:HE1	1.93	0.52
1:D:127:GLU:OE1	3:D:1151:HOH:O	2.19	0.51
1:D:71:SER:OG	1:D:227:HIS:CE1	2.63	0.51
1:B:55:LYS:HE2	3:B:1151:HOH:O	2.09	0.51
1:B:38:ARG:CZ	3:B:1158:HOH:O	2.57	0.51
1:B:126:PRO:HG2	1:B:129:GLU:CD	2.31	0.51
1:A:91:GLU:O	1:A:95:LEU:HB3	2.10	0.51
1:B:113:VAL:HG22	1:B:166:VAL:CG1	2.40	0.51
1:D:91:GLU:O	1:D:95:LEU:HB3	2.10	0.51
1:A:243:GLY:HA2	1:A:280:LEU:O	2.10	0.51
1:D:204:ALA:HB3	1:D:270:PRO:HD3	1.93	0.50
1:D:12:ILE:HD11	2:D:1118:NAD:H71N	1.76	0.50
1:C:247:THR:HG23	1:C:249:ARG:H	1.75	0.50
1:C:199:PRO:HB3	1:C:264:GLU:HG3	1.94	0.50
1:D:112:LEU:HD23	1:D:112:LEU:C	2.32	0.50
1:D:124:GLU:HG3	3:D:1189:HOH:O	2.12	0.50
1:C:5:VAL:HG11	1:C:17:VAL:HG22	1.93	0.50
1:B:38:ARG:HD3	1:B:49:ARG:NH2	2.27	0.50
1:A:291:ARG:HG3	1:A:291:ARG:NH1	2.27	0.50
1:A:112:LEU:C	1:A:112:LEU:HD23	2.33	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:205:ARG:HD2	1:A:206:LYS:HD2	1.94	0.49
1:C:183:GLU:HB2	3:C:1145:HOH:O	2.13	0.49
1:A:7:GLY:HA2	1:A:31:ASP:OD2	2.12	0.49
1:A:290:TRP:O	1:A:291:ARG:HG3	2.13	0.49
1:D:70:VAL:HG11	1:D:104:CYS:SG	2.53	0.49
1:D:218:VAL:HG11	1:D:241:GLY:CA	2.35	0.48
1:B:6:THR:HG1	1:B:73:GLN:H	1.61	0.48
1:D:153:TYR:HA	1:D:156:VAL:HG22	1.96	0.48
1:A:183:GLU:HG2	1:A:271:ARG:NH1	2.29	0.48
1:D:121:ILE:HD11	1:D:122:TYR:CZ	2.48	0.48
1:D:63:ARG:HA	1:D:66:ARG:HH21	1.77	0.48
1:B:246:HIS:HD2	3:B:1131:HOH:O	1.96	0.48
1:C:68:THR:OG1	1:C:69:HIS:HD2	1.97	0.48
1:A:11:PHE:HB3	2:A:1118:NAD:PN	2.53	0.48
1:C:112:LEU:C	1:C:112:LEU:HD23	2.33	0.48
1:B:153:TYR:HA	1:B:156:VAL:HG22	1.96	0.48
1:A:113:VAL:HG22	1:A:166:VAL:CG1	2.44	0.48
1:A:184:ALA:C	1:A:186:VAL:H	2.18	0.48
1:B:70:VAL:HG11	1:B:104:CYS:SG	2.54	0.47
1:C:190:PHE:O	1:C:194:VAL:HG23	2.14	0.47
1:C:63:ARG:HG3	1:C:66:ARG:NH2	2.29	0.47
1:C:6:THR:OG1	1:C:72:HIS:HA	2.15	0.47
1:C:125:VAL:HG11	1:C:279:VAL:H	1.80	0.47
1:D:117:THR:O	1:D:121:ILE:HG12	2.14	0.47
1:A:70:VAL:HG12	1:A:109:VAL:HG11	1.96	0.47
1:C:247:THR:CG2	1:C:249:ARG:H	2.28	0.47
1:C:55:LYS:O	1:C:59:GLU:HG2	2.15	0.47
1:C:71:SER:OG	1:C:227:HIS:CE1	2.68	0.47
1:D:59:GLU:O	1:D:63:ARG:HG3	2.14	0.47
1:A:154:LEU:HD12	1:A:155:SER:N	2.31	0.46
1:B:38:ARG:CG	1:B:38:ARG:HH11	2.29	0.46
1:A:30:LEU:C	1:A:30:LEU:HD23	2.35	0.46
1:D:74:ALA:O	1:D:75:ALA:HB2	2.15	0.46
1:D:166:VAL:HG22	1:D:235:GLU:HA	1.97	0.46
1:B:79:VAL:O	1:B:83:VAL:HG23	2.15	0.46
1:D:68:THR:OG1	1:D:69:HIS:HD2	1.97	0.46
1:D:205:ARG:HD2	3:D:1145:HOH:O	2.15	0.46
1:B:30:LEU:HG	1:B:50:VAL:HG22	1.97	0.46
1:D:247:THR:OG1	1:D:250:GLU:HG2	2.16	0.46
1:B:3:VAL:HA	1:B:69:HIS:O	2.15	0.46
1:C:6:THR:HG21	1:C:100:LEU:HD11	1.96	0.46
1:B:68:THR:OG1	1:B:69:HIS:HD2	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:283:LEU:CD1	1:A:286:MET:HE3	2.46	0.46
1:A:70:VAL:HG13	1:A:112:LEU:HG	1.98	0.46
1:B:166:VAL:HG22	1:B:168:LEU:HD13	1.97	0.45
1:C:13:GLY:O	1:C:17:VAL:HG23	2.16	0.45
1:D:230:ALA:HA	1:D:234:LEU:HB2	1.98	0.45
1:C:21:LEU:HD13	1:C:27:VAL:HG22	1.98	0.45
1:D:196:LYS:HB3	1:D:198:LEU:HD13	1.98	0.45
1:A:74:ALA:O	1:A:75:ALA:HB2	2.16	0.45
1:A:92:VAL:HG23	1:A:93:ASN:N	2.31	0.45
1:B:3:VAL:HG11	1:B:20:LEU:HD13	1.99	0.45
1:B:183:GLU:HB2	2:B:1118:NAD:H71N	1.81	0.45
1:A:205:ARG:HG3	1:A:206:LYS:HG3	1.99	0.45
1:A:75:ALA:HB1	1:A:93:ASN:OD1	2.16	0.45
1:C:168:LEU:N	1:C:168:LEU:HD22	2.32	0.45
1:A:205:ARG:HG3	1:A:206:LYS:N	2.32	0.45
1:D:112:LEU:HD22	1:D:154:LEU:HD21	1.98	0.45
1:D:30:LEU:HD23	1:D:30:LEU:C	2.37	0.45
1:C:76:GLN:HE22	1:C:78:SER:H	1.61	0.44
1:A:98:LEU:HD22	1:D:90:PHE:CG	2.52	0.44
1:D:43:LYS:N	1:D:43:LYS:HD2	2.32	0.44
1:B:243:GLY:HA2	1:B:280:LEU:O	2.17	0.44
1:B:94:LEU:HA	1:B:94:LEU:HD23	1.77	0.44
1:D:179:ASP:HB2	1:D:180:PRO:HD2	1.99	0.44
1:D:78:SER:HB3	1:D:81:VAL:HB	1.99	0.44
1:A:11:PHE:CE2	1:A:178:GLN:HB3	2.53	0.44
1:D:220:VAL:O	1:D:223:VAL:HG22	2.18	0.44
1:B:70:VAL:HG12	1:B:109:VAL:HG11	2.00	0.44
1:B:296:PHE:O	1:B:300:ILE:HD13	2.17	0.44
1:A:113:VAL:HG22	1:A:166:VAL:HG11	2.00	0.44
1:B:202:LEU:HA	3:B:1198:HOH:O	2.17	0.44
1:B:117:THR:HG23	1:B:121:ILE:HG23	2.00	0.44
1:A:283:LEU:HD13	1:A:286:MET:CE	2.48	0.43
1:D:176:PRO:HB3	1:D:306:HIS:HB2	2.00	0.43
1:A:60:ARG:HG3	1:A:61:ALA:N	2.32	0.43
1:D:166:VAL:HG11	1:D:230:ALA:HB1	2.01	0.43
1:D:205:ARG:NH2	1:D:276:GLU:OE2	2.51	0.43
1:B:98:LEU:HD22	1:C:90:PHE:CG	2.52	0.43
1:B:204:ALA:HB2	1:B:208:PRO:HA	2.01	0.43
1:D:35:THR:HG22	2:D:1118:NAD:H2B	2.00	0.43
1:C:38:ARG:HA	1:C:38:ARG:HD2	1.91	0.43
1:A:23:ARG:HB2	1:A:25:LEU:HD23	2.01	0.43
1:A:87:VAL:HG22	1:D:98:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:88:LEU:O	1:B:92:VAL:HG12	2.18	0.43
1:D:111:LYS:HG2	1:D:112:LEU:N	2.34	0.43
1:A:49:ARG:HG2	1:A:49:ARG:HH11	1.84	0.43
1:B:75:ALA:HB3	2:B:1118:NAD:O3D	2.19	0.42
1:B:7:GLY:N	1:B:74:ALA:HB2	2.35	0.42
1:B:117:THR:CG2	1:B:120:ALA:HB3	2.49	0.42
1:C:50:VAL:HG12	1:C:51:ASP:N	2.34	0.42
1:C:133:GLU:HG3	1:C:284:LYS:HD2	2.01	0.42
1:C:211:GLU:OE2	1:C:249:ARG:HD2	2.20	0.42
1:A:214:VAL:HA	1:A:246:HIS:O	2.19	0.42
1:A:296:PHE:O	1:A:300:ILE:HD13	2.20	0.42
1:C:252:LEU:HD13	1:C:253:MET:CE	2.49	0.42
1:A:176:PRO:HB3	1:A:306:HIS:HB2	2.02	0.42
1:C:227:HIS:HD2	3:C:1126:HOH:O	2.02	0.42
1:D:1:MET:HG3	1:D:69:HIS:CD2	2.55	0.42
1:D:6:THR:OG1	1:D:72:HIS:HD2	2.03	0.42
1:C:113:VAL:HG22	1:C:166:VAL:CG1	2.50	0.42
1:B:54:ASP:O	1:B:58:VAL:HG23	2.19	0.42
1:C:33:LEU:HD12	1:C:33:LEU:N	2.34	0.42
1:C:101:LEU:HD21	1:C:154:LEU:CD1	2.50	0.42
1:A:121:ILE:HD11	1:A:122:TYR:CE2	2.55	0.42
1:A:105:ARG:HD2	1:A:157:TYR:CE1	2.54	0.42
1:A:214:VAL:HG13	1:A:277:ARG:HA	2.02	0.42
1:A:283:LEU:HD12	1:A:286:MET:HE3	2.02	0.42
1:C:298:GLU:O	1:C:302:LEU:HD13	2.20	0.42
1:C:210:ASP:HB2	3:C:1175:HOH:O	2.18	0.41
1:C:71:SER:OG	1:C:227:HIS:HE1	2.02	0.41
1:D:105:ARG:NH2	3:D:1187:HOH:O	2.53	0.41
1:D:227:HIS:HD2	3:D:1121:HOH:O	2.03	0.41
1:D:75:ALA:HB3	2:D:1118:NAD:O3D	2.20	0.41
1:A:282:PRO:HG2	1:A:286:MET:CE	2.49	0.41
1:B:112:LEU:HD23	1:B:112:LEU:C	2.40	0.41
1:C:204:ALA:HB2	1:C:208:PRO:HA	2.01	0.41
1:B:91:GLU:O	1:B:95:LEU:HB3	2.20	0.41
1:A:75:ALA:HB3	2:A:1118:NAD:H3D	2.02	0.41
1:D:92:VAL:HG13	1:D:93:ASN:N	2.35	0.41
1:C:111:LYS:HG2	1:C:112:LEU:N	2.35	0.41
1:D:178:GLN:HG3	1:D:188:ALA:HB2	2.03	0.41
1:B:166:VAL:CG2	1:B:168:LEU:HD13	2.51	0.41
1:B:11:PHE:HB3	2:B:1118:NAD:PN	2.61	0.41
1:C:178:GLN:HG3	1:C:188:ALA:HB2	2.02	0.41
1:B:76:GLN:HB3	1:B:92:VAL:CG1	2.43	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:21:LEU:HA	1:C:21:LEU:HD12	1.91	0.40
1:C:172:ASN:CB	1:C:184:ALA:HB2	2.50	0.40
1:C:70:VAL:HG21	1:C:104:CYS:SG	2.61	0.40
1:B:156:VAL:HG11	1:C:145:ALA:HB2	2.03	0.40
1:B:252:LEU:C	1:B:252:LEU:HD13	2.41	0.40
1:C:100:LEU:O	1:C:100:LEU:HD23	2.21	0.40
1:C:5:VAL:O	1:C:5:VAL:HG13	2.21	0.40
1:B:214:VAL:HG23	1:B:246:HIS:H	1.86	0.40
1:D:49:ARG:HH11	1:D:49:ARG:HG2	1.86	0.40
1:A:230:ALA:HA	1:A:234:LEU:HB2	2.03	0.40
1:B:186:VAL:HG13	1:B:187:VAL:N	2.36	0.40
1:D:29:VAL:CG2	1:D:47:PHE:HD1	2.34	0.40
1:C:117:THR:O	1:C:117:THR:HG23	2.21	0.40
1:C:28:ALA:HB2	1:C:65:PHE:CE1	2.56	0.40
1:A:233:SER:HB2	3:A:1222:HOH:O	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	309/311 (99%)	297 (96%)	11 (4%)	1 (0%)	50	66
1	B	309/311 (99%)	300 (97%)	9 (3%)	0	100	100
1	C	309/311 (99%)	298 (96%)	11 (4%)	0	100	100
1	D	309/311 (99%)	299 (97%)	9 (3%)	1 (0%)	50	66
All	All	1236/1244 (99%)	1194 (97%)	40 (3%)	2 (0%)	56	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	11	PHE
1	A	11	PHE

### 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	244/244 (100%)	232 (95%)	12 (5%)	35	50
1	B	244/244 (100%)	233 (96%)	11 (4%)	38	55
1	C	244/244 (100%)	233 (96%)	11 (4%)	38	55
1	D	244/244 (100%)	229 (94%)	15 (6%)	26	37
All	All	976/976 (100%)	927 (95%)	49 (5%)	34	49

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	37	LYS
1	A	38	ARG
1	A	60	ARG
1	A	66	ARG
1	A	94	LEU
1	A	168	LEU
1	A	183	GLU
1	A	205	ARG
1	A	214	VAL
1	A	229	LEU
1	A	283	LEU
1	B	38	ARG
1	B	56	GLU
1	B	73	GLN
1	B	76	GLN
1	B	101	LEU
1	B	166	VAL
1	B	168	LEU
1	B	214	VAL
1	B	229	LEU
1	B	274	ASP
1	B	285	LEU
1	C	43	LYS
1	C	52	LEU
1	C	100	LEU

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Mol	Chain	Res	Type
1	C	133	GLU
1	C	172	ASN
1	C	201	THR
1	C	202	LEU
1	C	211	GLU
1	C	229	LEU
1	C	247	THR
1	C	252	LEU
1	D	21	LEU
1	D	25	LEU
1	D	43	LYS
1	D	76	GLN
1	D	101	LEU
1	D	105	ARG
1	D	117	THR
1	D	121	ILE
1	D	168	LEU
1	D	172	ASN
1	D	200	VAL
1	D	211	GLU
1	D	225	GLU
1	D	229	LEU
1	D	274	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	72	HIS
1	A	76	GLN
1	A	106	GLN
1	A	152	HIS
1	A	172	ASN
1	A	178	GLN
1	A	239	ASN
1	A	246	HIS
1	B	15	HIS
1	B	69	HIS
1	B	72	HIS
1	B	76	GLN
1	B	152	HIS
1	B	239	ASN

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Mol	Chain	Res	Type
1	B	246	HIS
1	B	266	GLN
1	C	69	HIS
1	C	76	GLN
1	C	172	ASN
1	C	227	HIS
1	C	239	ASN
1	C	297	GLN
1	D	15	HIS
1	D	69	HIS
1	D	72	HIS
1	D	106	GLN
1	D	152	HIS
1	D	172	ASN
1	D	227	HIS
1	D	239	ASN
1	D	288	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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	1118	-	48,48,48	1.55	7 (14%)	73,73,73	2.81	21 (28%)
2	NAD	B	1118	-	48,48,48	1.56	8 (16%)	73,73,73	2.96	22 (30%)
2	NAD	C	1118	-	48,48,48	1.49	5 (10%)	73,73,73	2.71	25 (34%)
2	NAD	D	1118	-	48,48,48	1.53	5 (10%)	73,73,73	2.71	18 (24%)

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	1118	-	-	0/30/62/62	0/3/5/5
2	NAD	B	1118	-	-	0/30/62/62	0/3/5/5
2	NAD	C	1118	-	-	0/30/62/62	0/3/5/5
2	NAD	D	1118	-	-	0/30/62/62	0/3/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1118	NAD	C2N-N1N	6.77	1.44	1.35
2	B	1118	NAD	C2N-N1N	6.69	1.43	1.35
2	D	1118	NAD	C2N-N1N	6.56	1.43	1.35
2	A	1118	NAD	C2N-N1N	6.49	1.43	1.35
2	D	1118	NAD	PA-O3	3.74	1.66	1.59
2	A	1118	NAD	PA-O3	3.62	1.66	1.59
2	B	1118	NAD	C4A-N9A	-3.37	1.32	1.37
2	A	1118	NAD	O4B-C1B	3.20	1.46	1.41
2	C	1118	NAD	C4A-N9A	-3.15	1.33	1.37
2	A	1118	NAD	C4A-N9A	-3.12	1.33	1.37
2	D	1118	NAD	C4A-N9A	-3.08	1.33	1.37
2	D	1118	NAD	O4B-C1B	2.77	1.45	1.41
2	B	1118	NAD	PA-O3	2.54	1.64	1.59
2	B	1118	NAD	C6N-N1N	2.48	1.42	1.35
2	C	1118	NAD	C6N-N1N	2.39	1.42	1.35
2	B	1118	NAD	O4D-C1D	2.32	1.44	1.41
2	C	1118	NAD	C3N-C7N	2.29	1.54	1.50
2	B	1118	NAD	O4B-C1B	2.27	1.44	1.41
2	A	1118	NAD	C6N-N1N	2.24	1.41	1.35
2	D	1118	NAD	C6N-N1N	2.22	1.41	1.35
2	B	1118	NAD	C5D-C4D	2.13	1.58	1.51
2	B	1118	NAD	PN-O3	2.03	1.64	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1118	NAD	O4D-C1D	2.03	1.44	1.41
2	A	1118	NAD	C3N-C7N	2.00	1.54	1.50
2	C	1118	NAD	O4B-C1B	2.00	1.44	1.41

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1118	NAD	O4D-C1D-N1N	11.53	119.75	107.95
2	A	1118	NAD	O4B-C1B-N9A	10.85	118.53	108.44
2	D	1118	NAD	N3A-C2A-N1A	-10.11	120.25	128.71
2	A	1118	NAD	N3A-C2A-N1A	-10.01	120.34	128.71
2	B	1118	NAD	N3A-C2A-N1A	-9.92	120.42	128.71
2	D	1118	NAD	O4B-C1B-N9A	9.91	117.66	108.44
2	C	1118	NAD	N3A-C2A-N1A	-9.79	120.52	128.71
2	B	1118	NAD	O4B-C1B-N9A	8.32	116.17	108.44
2	C	1118	NAD	O4B-C1B-N9A	8.26	116.12	108.44
2	C	1118	NAD	O4D-C1D-N1N	7.78	115.91	107.95
2	D	1118	NAD	C4D-O4D-C1D	7.15	117.51	109.75
2	A	1118	NAD	C2D-C1D-N1N	6.24	124.43	113.86
2	B	1118	NAD	C4D-O4D-C1D	6.16	116.44	109.75
2	A	1118	NAD	N3A-C4A-N9A	6.06	136.37	125.43
2	D	1118	NAD	N3A-C4A-N9A	6.00	136.26	125.43
2	B	1118	NAD	N3A-C4A-N9A	5.99	136.24	125.43
2	C	1118	NAD	N3A-C4A-N9A	5.96	136.19	125.43
2	C	1118	NAD	C4D-O4D-C1D	5.95	116.21	109.75
2	B	1118	NAD	O4D-C4D-C5D	5.81	130.08	109.36
2	A	1118	NAD	C4D-O4D-C1D	5.72	115.96	109.75
2	D	1118	NAD	C2D-C1D-N1N	5.58	123.31	113.86
2	A	1118	NAD	C4B-O4B-C1B	5.15	115.34	109.75
2	A	1118	NAD	O4D-C1D-C2D	-4.74	99.50	106.77
2	A	1118	NAD	O5D-C5D-C4D	4.64	125.95	108.94
2	C	1118	NAD	C2D-C1D-N1N	4.52	121.51	113.86
2	B	1118	NAD	C2D-C1D-N1N	4.52	121.51	113.86
2	D	1118	NAD	PN-O5D-C5D	4.42	135.51	120.24
2	C	1118	NAD	C4B-O4B-C1B	4.33	114.45	109.75
2	B	1118	NAD	PN-O5D-C5D	4.21	134.81	120.24
2	D	1118	NAD	C4B-O4B-C1B	4.15	114.26	109.75
2	C	1118	NAD	O4D-C4D-C5D	4.14	124.13	109.36
2	D	1118	NAD	C3D-C2D-C1D	4.13	107.36	100.91
2	A	1118	NAD	O4D-C4D-C3D	-4.05	96.96	105.17
2	B	1118	NAD	O4D-C1D-C2D	-3.89	100.81	106.77
2	C	1118	NAD	C4A-C5A-N7A	3.87	112.83	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1118	NAD	O4D-C4D-C5D	3.86	123.15	109.36
2	A	1118	NAD	O4D-C1D-N1N	3.83	111.87	107.95
2	A	1118	NAD	O4D-C4D-C5D	3.80	122.93	109.36
2	B	1118	NAD	O4D-C4D-C3D	-3.79	97.48	105.17
2	B	1118	NAD	C4A-C5A-N7A	3.65	112.64	109.52
2	C	1118	NAD	O4D-C1D-C2D	-3.63	101.21	106.77
2	D	1118	NAD	O4D-C1D-C2D	-3.62	101.22	106.77
2	A	1118	NAD	C4A-C5A-N7A	3.61	112.61	109.52
2	B	1118	NAD	C3D-C2D-C1D	3.55	106.46	100.91
2	A	1118	NAD	C5A-C4A-N3A	-3.51	118.06	125.70
2	B	1118	NAD	C4B-O4B-C1B	3.45	113.50	109.75
2	D	1118	NAD	C5A-C4A-N3A	-3.45	118.20	125.70
2	B	1118	NAD	O5D-C5D-C4D	3.37	121.31	108.94
2	C	1118	NAD	C5A-C4A-N3A	-3.35	118.41	125.70
2	D	1118	NAD	C3N-C7N-N7N	-3.33	113.99	117.77
2	B	1118	NAD	C5A-C4A-N3A	-3.28	118.56	125.70
2	A	1118	NAD	O4B-C1B-C2B	-3.27	101.76	106.77
2	C	1118	NAD	C3D-C2D-C1D	3.23	105.96	100.91
2	C	1118	NAD	PN-O5D-C5D	3.15	131.14	120.24
2	D	1118	NAD	C4A-C5A-N7A	3.02	112.11	109.52
2	B	1118	NAD	C6N-N1N-C2N	-3.00	118.65	122.04
2	C	1118	NAD	O4B-C1B-C2B	-2.93	102.27	106.77
2	C	1118	NAD	O5D-C5D-C4D	2.89	119.56	108.94
2	D	1118	NAD	O4B-C1B-C2B	-2.75	102.56	106.77
2	C	1118	NAD	O7N-C7N-C3N	2.69	122.61	119.58
2	C	1118	NAD	C3N-C7N-N7N	-2.68	114.73	117.77
2	D	1118	NAD	C2A-N3A-C4A	2.67	121.61	114.01
2	A	1118	NAD	C6N-N1N-C2N	-2.66	119.03	122.04
2	B	1118	NAD	C2N-N1N-C1D	2.62	125.81	119.33
2	A	1118	NAD	C2A-N3A-C4A	2.60	121.42	114.01
2	C	1118	NAD	O4B-C4B-C5B	2.57	118.54	109.36
2	C	1118	NAD	O4D-C4D-C3D	-2.55	100.00	105.17
2	C	1118	NAD	C6N-N1N-C2N	-2.48	119.23	122.04
2	C	1118	NAD	C2A-N3A-C4A	2.44	120.96	114.01
2	B	1118	NAD	C2A-N3A-C4A	2.44	120.95	114.01
2	B	1118	NAD	O4B-C4B-C5B	2.44	118.06	109.36
2	B	1118	NAD	O4B-C1B-C2B	-2.43	103.05	106.77
2	C	1118	NAD	C2N-N1N-C1D	2.39	125.27	119.33
2	A	1118	NAD	C6A-C5A-C4A	2.39	121.63	117.25
2	C	1118	NAD	C2B-C1B-N9A	2.32	119.22	113.27
2	A	1118	NAD	O3-PN-O1N	-2.30	103.33	108.83
2	D	1118	NAD	C2N-N1N-C1D	2.30	125.04	119.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1118	NAD	C6A-C5A-C4A	2.28	121.43	117.25
2	C	1118	NAD	C6A-C5A-C4A	2.26	121.40	117.25
2	D	1118	NAD	O7N-C7N-C3N	2.25	122.11	119.58
2	A	1118	NAD	C3D-C2D-C1D	2.24	104.41	100.91
2	A	1118	NAD	C2N-N1N-C1D	2.22	124.83	119.33
2	D	1118	NAD	C6A-C5A-C4A	2.14	121.17	117.25
2	A	1118	NAD	O4B-C4B-C3B	-2.12	100.88	105.17
2	C	1118	NAD	C1B-N9A-C4A	-2.05	123.10	126.64
2	B	1118	NAD	C1B-N9A-C4A	-2.03	123.12	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	311/311 (100%)	0.04	15 (4%)	29 31	9, 21, 42, 80	0
1	B	311/311 (100%)	0.14	18 (5%)	22 24	13, 24, 65, 89	0
1	C	311/311 (100%)	0.16	11 (3%)	42 44	14, 28, 50, 67	0
1	D	311/311 (100%)	-0.16	5 (1%)	68 71	8, 21, 40, 60	0
All	All	1244/1244 (100%)	0.05	49 (3%)	35 40	8, 23, 51, 89	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	311	VAL	13.7
1	A	184	ALA	12.5
1	A	311	VAL	11.2
1	C	311	VAL	11.0
1	A	310	ALA	8.1
1	D	311	VAL	8.0
1	B	310	ALA	6.1
1	B	262	ALA	5.6
1	A	180	PRO	5.3
1	A	181	HIS	4.5
1	C	180	PRO	4.1
1	A	44	GLY	3.9
1	B	265	VAL	3.8
1	B	259	ALA	3.6
1	B	198	LEU	3.2
1	B	272	PRO	3.1
1	B	267	PRO	3.1
1	C	63	ARG	3.0
1	A	77	ALA	3.0
1	C	184	ALA	2.9
1	D	310	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	200	VAL	2.9
1	A	183	GLU	2.8
1	A	179	ASP	2.7
1	C	66	ARG	2.7
1	B	263	PRO	2.5
1	B	264	GLU	2.5
1	C	183	GLU	2.5
1	B	207	THR	2.4
1	D	43	LYS	2.4
1	C	257	GLU	2.3
1	B	309	GLY	2.3
1	A	211	GLU	2.3
1	A	63	ARG	2.3
1	A	43	LYS	2.2
1	B	273	GLY	2.2
1	D	56	GLU	2.2
1	D	35	THR	2.2
1	C	56	GLU	2.2
1	B	154	LEU	2.2
1	B	260	GLY	2.1
1	A	182	GLY	2.1
1	C	27	VAL	2.1
1	B	257	GLU	2.1
1	A	56	GLU	2.1
1	C	45	VAL	2.1
1	A	257	GLU	2.1
1	B	192	GLU	2.1
1	C	232	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron



density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAD	B	1118	44/44	0.47	10.38	51,102,136,141	0
2	NAD	D	1118	44/44	0.47	10.10	52,98,136,140	0
2	NAD	C	1118	44/44	0.44	4.95	80,112,144,149	0
2	NAD	A	1118	44/44	0.39	1.99	56,96,130,134	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.