



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 01:14 AM GMT

PDB ID : 1IE3  
Title : CRYSTAL STRUCTURE OF R153C E. COLI MALATE DEHYDROGENASE  
Authors : Bell, J.K.; Yennawar, H.P.; Wright, S.K.; Thompson, J.R.; Viola, R.E.; Banaszak, L.J.  
Deposited on : 2001-04-05  
Resolution : 2.50 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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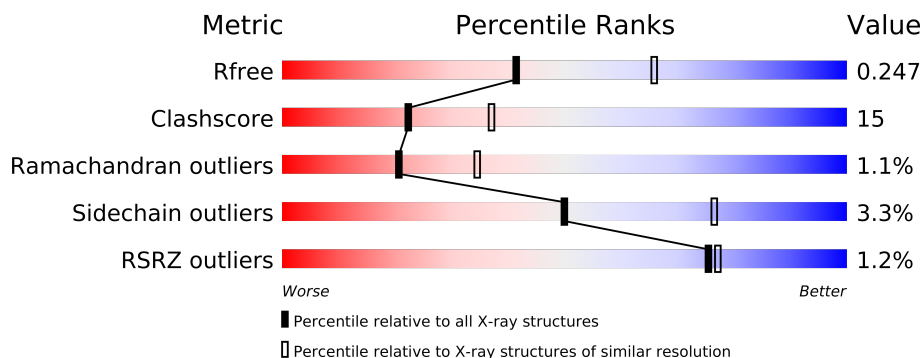
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	312	
1	B	312	
1	C	312	
1	D	312	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	PYR	C	317	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9416 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 MALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	40	0	0
			2267	1435	384	440	8			
1	B	312	Total	C	N	O	S	0	0	0
			2267	1435	384	440	8			
1	C	312	Total	C	N	O	S	29	0	0
			2267	1435	384	440	8			
1	D	312	Total	C	N	O	S	26	0	0
			2267	1435	384	440	8			

There are 8 discrepancies between the modelled and reference sequences:

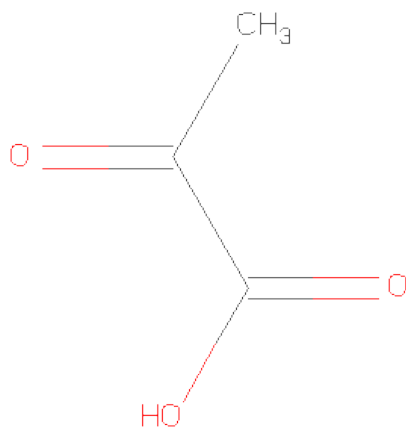
Chain	Residue	Modelled	Actual	Comment	Reference
A	153	CYS	ARG	ENGINEERED	UNP P61889
A	307	GLN	GLU	SEE REMARK 999	UNP P61889
B	153	CYS	ARG	ENGINEERED	UNP P61889
B	307	GLN	GLU	SEE REMARK 999	UNP P61889
C	153	CYS	ARG	ENGINEERED	UNP P61889
C	307	GLN	GLU	SEE REMARK 999	UNP P61889
D	153	CYS	ARG	ENGINEERED	UNP P61889
D	307	GLN	GLU	SEE REMARK 999	UNP P61889

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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		
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 PYRUVIC ACID (three-letter code: PYR) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		

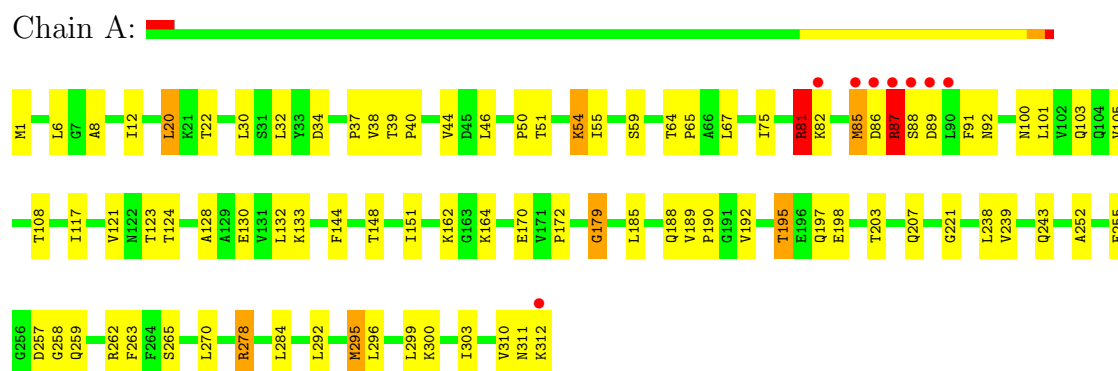
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	56	Total	O	0	0
			56	56		
4	C	35	Total	O	0	0
			35	35		
4	D	25	Total	O	0	0
			25	25		

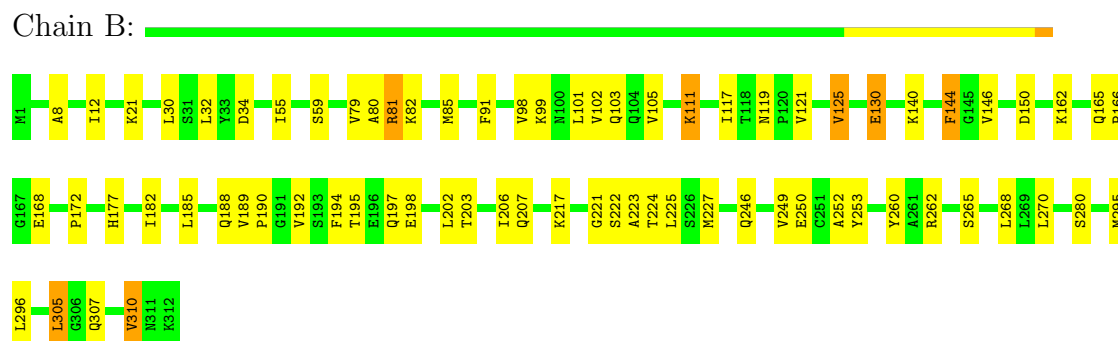
### 3 Residue-property plots

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.

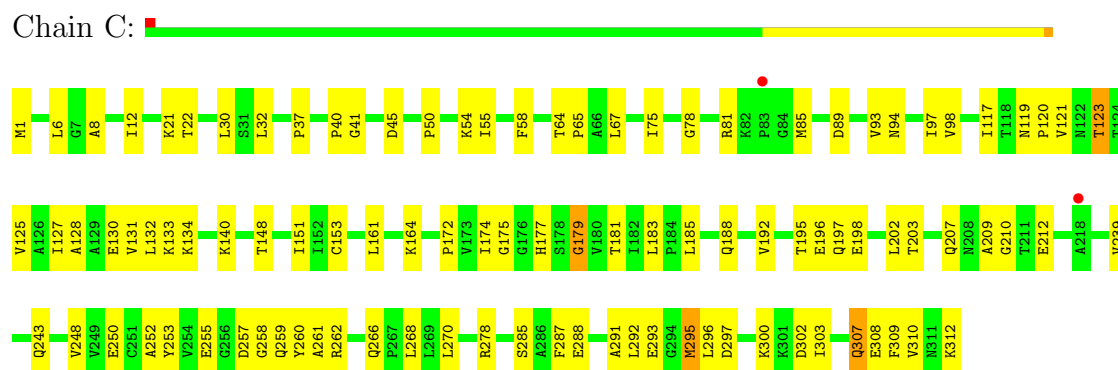
#### • Molecule 1: MALATE DEHYDROGENASE



#### • Molecule 1: MALATE DEHYDROGENASE

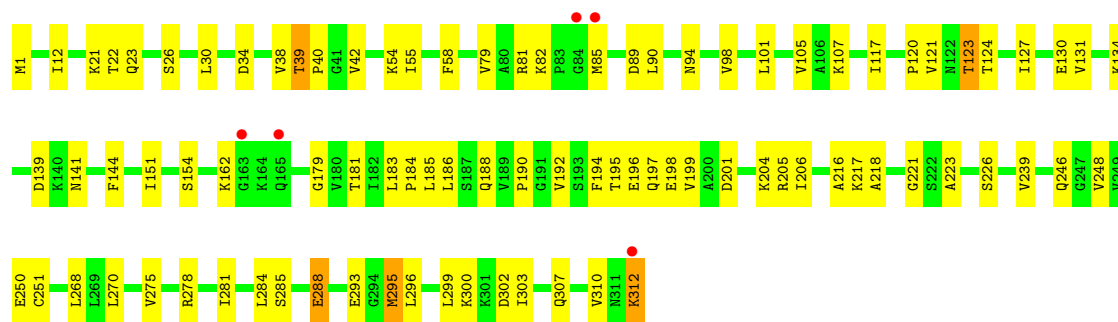


#### • Molecule 1: MALATE DEHYDROGENASE



#### • Molecule 1: MALATE DEHYDROGENASE

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.41Å 52.85Å 169.91Å 90.00° 101.76° 90.00°	Depositor
Resolution (Å)	39.70 – 2.50 39.70 – 2.10	Depositor EDS
% Data completeness (in resolution range)	86.8 (39.70-2.50) 86.0 (39.70-2.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.10Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.186 , 0.252 0.184 , 0.247	Depositor DCC
$R_{free}$ test set	3927 reflections (10.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.6	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	2 of 64878 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: PYR, 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	0.56	1/2295 (0.0%)	0.70	4/3108 (0.1%)
1	B	0.38	0/2295	0.63	0/3108
1	C	0.45	1/2295 (0.0%)	0.61	0/3108
1	D	0.36	0/2295	0.62	1/3108 (0.0%)
All	All	0.45	2/9180 (0.0%)	0.64	5/12432 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	PRO	N-CD	-18.04	1.22	1.47
1	C	312	LYS	C-OXT	13.71	1.49	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	A	87	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	A	81	ARG	NE-CZ-NH2	6.55	123.58	120.30
1	D	295	MET	CG-SD-CE	6.10	109.96	100.20
1	A	50	PRO	N-CD-CG	5.48	111.42	103.20

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	2267	0	2351	76	0
1	B	2267	0	2351	57	0
1	C	2267	0	2351	76	0
1	D	2267	0	2351	70	0
2	A	44	0	26	3	0
2	B	44	0	26	3	0
2	C	44	0	26	3	0
2	D	44	0	26	3	0
3	C	6	0	3	2	0
4	A	50	0	0	0	0
4	B	56	0	0	5	0
4	C	35	0	0	2	0
4	D	25	0	0	2	0
All	All	9416	0	9511	276	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 15.

All (276) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:195:THR:HG22	1:B:197:GLN:H	1.25	0.98
1:A:54:LYS:H	1:A:54:LYS:HD2	1.32	0.94
1:C:195:THR:HG22	1:C:197:GLN:H	1.31	0.94
1:A:81:ARG:HE	1:A:221:GLY:HA2	1.41	0.85
1:C:148:THR:HA	1:C:151:ILE:HD13	1.60	0.84
1:D:162:LYS:HG3	1:D:192:VAL:HG11	1.60	0.83
1:A:195:THR:HG22	1:A:198:GLU:H	1.44	0.81
1:B:130:GLU:HB3	1:B:310:VAL:HG11	1.64	0.80
1:A:12:ILE:HD12	2:A:313:NAD:H51N	1.62	0.80
1:A:54:LYS:CD	1:A:54:LYS:H	1.95	0.79
1:C:293:GLU:HA	1:C:296:LEU:HD23	1.66	0.78
1:B:12:ILE:HD12	2:B:314:NAD:H51N	1.66	0.78
1:B:260:TYR:HB3	1:B:296:LEU:HD11	1.66	0.77
1:D:181:THR:HA	1:D:295:MET:HG3	1.67	0.77
1:C:303:ILE:O	1:C:307:GLN:HG2	1.86	0.75
1:A:91:PHE:HE2	1:A:123:THR:HG21	1.51	0.74
1:C:125:VAL:HG11	1:C:253:TYR:CE2	2.21	0.74
1:D:12:ILE:HD12	2:D:316:NAD:H51N	1.70	0.72
1:B:117:ILE:O	2:B:314:NAD:H2N	1.89	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:121:VAL:O	1:C:125:VAL:HG12	1.90	0.72
1:B:195:THR:HB	1:B:198:GLU:HG3	1.70	0.71
1:D:195:THR:HG22	1:D:197:GLN:H	1.56	0.71
1:C:37:PRO:O	1:C:40:PRO:HD2	1.90	0.71
1:B:172:PRO:HG2	1:B:185:LEU:HB2	1.72	0.70
1:A:30:LEU:HD23	1:A:55:ILE:HD12	1.73	0.69
1:D:201:ASP:O	1:D:204:LYS:HG2	1.93	0.69
1:B:121:VAL:O	1:B:125:VAL:HG13	1.93	0.69
1:D:185:LEU:HD22	1:D:288:GLU:HG2	1.75	0.68
1:D:151:ILE:HD11	1:D:251:CYS:HB2	1.74	0.68
1:A:54:LYS:HD2	1:A:54:LYS:N	2.08	0.68
1:C:164:LYS:HE3	1:C:192:VAL:HG22	1.73	0.68
1:C:195:THR:HB	1:C:198:GLU:HG3	1.76	0.68
1:C:151:ILE:HD12	1:C:151:ILE:N	2.09	0.68
1:D:303:ILE:HG22	1:D:307:GLN:HE21	1.59	0.68
1:B:130:GLU:CB	1:B:310:VAL:HG11	2.24	0.67
1:B:310:VAL:HG22	1:B:310:VAL:O	1.93	0.67
1:C:292:LEU:O	1:C:295:MET:HG3	1.95	0.67
1:C:210:GLY:H	3:C:317:PYR:H33	1.59	0.66
1:B:81:ARG:HH21	1:B:221:GLY:HA2	1.61	0.66
1:D:312:LYS:HD3	1:D:312:LYS:OXT	1.96	0.66
1:C:12:ILE:HD12	2:C:315:NAD:H51N	1.78	0.65
1:C:278:ARG:HG3	1:C:278:ARG:HH11	1.61	0.65
1:D:144:PHE:CE2	1:D:275:VAL:HG13	2.32	0.65
1:D:281:ILE:HD11	1:D:284:LEU:HD11	1.79	0.65
1:A:81:ARG:NE	1:A:221:GLY:HA2	2.11	0.64
1:C:195:THR:HG22	1:C:197:GLN:N	2.10	0.64
1:C:85:MET:HB3	1:C:89:ASP:HB2	1.80	0.64
1:A:64:THR:HB	1:A:65:PRO:HD3	1.80	0.64
1:D:82:LYS:HB2	1:D:85:MET:HE2	1.79	0.64
1:B:222:SER:O	1:B:224:THR:HG23	1.97	0.63
1:C:203:THR:HG22	1:C:207:GLN:NE2	2.14	0.62
1:C:179:GLY:O	1:C:207:GLN:HG2	1.99	0.62
1:D:101:LEU:O	1:D:105:VAL:HG23	2.00	0.62
1:B:165:GLN:HB2	1:B:168:GLU:HG2	1.82	0.61
1:B:185:LEU:HD13	1:B:188:GLN:NE2	2.16	0.61
1:C:125:VAL:HG11	1:C:253:TYR:HE2	1.64	0.61
1:C:278:ARG:HG3	1:C:278:ARG:NH1	2.16	0.61
1:C:151:ILE:HD12	1:C:151:ILE:H	1.65	0.60
1:C:123:THR:HB	1:C:302:ASP:O	2.01	0.60
1:C:130:GLU:HA	1:C:133:LYS:HD2	1.84	0.60
1:C:239:VAL:O	1:C:243:GLN:HG3	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:257:ASP:O	1:A:257:ASP:OD1	2.21	0.59
1:B:30:LEU:HD23	1:B:55:ILE:HD12	1.82	0.59
1:C:285:SER:OG	1:C:288:GLU:HG3	2.02	0.59
1:D:82:LYS:HD2	1:D:85:MET:HE1	1.86	0.58
1:D:127:ILE:O	1:D:131:VAL:HG23	2.03	0.58
1:C:287:PHE:O	1:C:291:ALA:HB2	2.03	0.58
1:C:41:GLY:HA2	1:D:216:ALA:HB1	1.86	0.58
1:A:252:ALA:O	1:A:265:SER:HA	2.03	0.58
1:B:130:GLU:HG2	1:B:310:VAL:CG1	2.33	0.57
1:C:6:LEU:HD12	1:C:75:ILE:HG12	1.86	0.57
1:D:285:SER:H	1:D:288:GLU:HB2	1.69	0.57
1:C:250:GLU:HG3	4:C:429:HOH:O	2.04	0.56
1:C:174:ILE:HG22	1:C:266:GLN:HA	1.88	0.56
1:C:307:GLN:HE21	1:C:307:GLN:HA	1.71	0.56
1:B:101:LEU:O	1:B:105:VAL:HG23	2.05	0.56
1:A:30:LEU:O	1:A:55:ILE:HA	2.06	0.56
1:A:151:ILE:HD12	1:A:151:ILE:N	2.22	0.55
1:A:117:ILE:O	2:A:313:NAD:H2N	2.06	0.55
1:C:260:TYR:HB3	1:C:296:LEU:HD11	1.87	0.55
1:C:127:ILE:O	1:C:131:VAL:HG23	2.06	0.55
1:D:117:ILE:O	2:D:316:NAD:H2N	2.07	0.55
1:C:117:ILE:O	2:C:315:NAD:H2N	2.07	0.55
1:C:172:PRO:HG2	1:C:185:LEU:HB2	1.88	0.55
1:A:37:PRO:O	1:A:40:PRO:HD2	2.06	0.55
1:D:39:THR:HB	1:D:40:PRO:CD	2.37	0.55
1:C:21:LYS:HD3	1:C:21:LYS:O	2.07	0.54
1:D:79:VAL:HG13	1:D:82:LYS:HE2	1.87	0.54
1:A:91:PHE:CE2	1:A:123:THR:HG21	2.39	0.54
1:A:128:ALA:O	1:A:132:LEU:HG	2.07	0.54
1:A:100:ASN:O	1:A:103:GLN:HB3	2.07	0.54
1:B:146:VAL:HA	4:B:385:HOH:O	2.07	0.54
1:A:296:LEU:O	1:A:300:LYS:HG3	2.08	0.53
1:B:270:LEU:HD22	1:B:270:LEU:N	2.23	0.53
1:C:125:VAL:HG11	1:C:253:TYR:CD2	2.43	0.53
1:C:252:ALA:HB3	1:C:268:LEU:HD12	1.90	0.53
1:B:82:LYS:HB2	1:B:85:MET:CE	2.38	0.53
1:A:86:ASP:O	1:A:89:ASP:N	2.42	0.53
1:D:22:THR:HG23	1:D:23:GLN:HG3	1.90	0.53
1:A:257:ASP:O	1:A:259:GLN:N	2.40	0.53
1:C:161:LEU:HD23	1:C:202:LEU:HD11	1.91	0.53
1:D:34:ASP:HB3	1:D:39:THR:OG1	2.08	0.53
1:C:120:PRO:HG2	1:C:123:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:151:ILE:HD12	1:A:151:ILE:H	1.75	0.52
1:A:292:LEU:O	1:A:295:MET:HG3	2.09	0.52
1:D:38:VAL:HG12	1:D:42:VAL:HG23	1.90	0.52
1:C:185:LEU:HD13	1:C:188:GLN:NE2	2.25	0.52
1:D:284:LEU:N	1:D:284:LEU:HD12	2.24	0.52
1:A:185:LEU:HD13	1:A:188:GLN:NE2	2.24	0.52
1:C:1:MET:SD	1:C:239:VAL:HG13	2.49	0.52
1:B:195:THR:HG22	1:B:197:GLN:N	2.09	0.51
1:B:130:GLU:HG2	1:B:310:VAL:HG13	1.91	0.51
1:C:128:ALA:O	1:C:132:LEU:HG	2.10	0.51
1:B:12:ILE:HD13	1:B:227:MET:HG2	1.91	0.51
1:D:94:ASN:O	1:D:98:VAL:HG23	2.10	0.51
1:A:40:PRO:O	1:A:44:VAL:HG23	2.11	0.51
1:A:170:GLU:HA	1:A:170:GLU:OE1	2.10	0.51
1:C:119:ASN:OD1	1:C:121:VAL:HG23	2.10	0.50
1:B:21:LYS:O	1:B:21:LYS:HD3	2.12	0.50
1:C:127:ILE:HG23	1:C:310:VAL:HG22	1.93	0.50
1:C:125:VAL:CG1	1:C:253:TYR:HE2	2.23	0.50
1:C:209:ALA:O	1:C:212:GLU:HB3	2.11	0.50
1:C:292:LEU:O	1:C:296:LEU:HD22	2.13	0.49
1:C:293:GLU:HA	1:C:296:LEU:CD2	2.38	0.49
1:B:34:ASP:O	1:B:59:SER:HA	2.12	0.49
1:D:123:THR:HB	1:D:302:ASP:O	2.12	0.49
1:A:88:SER:O	1:A:92:ASN:ND2	2.46	0.49
1:C:255:GLU:OE2	1:C:262:ARG:NH1	2.46	0.49
1:D:201:ASP:HB3	1:D:204:LYS:HE2	1.95	0.49
1:B:30:LEU:O	1:B:55:ILE:HA	2.12	0.49
1:B:125:VAL:HG11	1:B:253:TYR:HD2	1.78	0.49
1:A:86:ASP:O	1:A:87:ARG:C	2.52	0.49
1:D:186:LEU:HD12	1:D:199:VAL:HG13	1.95	0.48
1:B:182:ILE:HB	1:B:207:GLN:HG2	1.95	0.48
1:D:217:LYS:HD3	1:D:221:GLY:HA3	1.95	0.48
1:A:89:ASP:HA	1:A:92:ASN:HD22	1.78	0.48
1:A:130:GLU:HA	1:A:133:LYS:NZ	2.28	0.48
1:B:194:PHE:HA	1:B:198:GLU:OE1	2.12	0.48
1:A:81:ARG:HE	1:A:221:GLY:CA	2.21	0.48
1:D:278:ARG:HH11	1:D:278:ARG:HG3	1.78	0.48
1:C:248:VAL:HG12	1:C:270:LEU:HD12	1.96	0.48
1:C:260:TYR:O	1:C:261:ALA:HB2	2.13	0.48
1:C:6:LEU:HD21	1:C:67:LEU:HD21	1.96	0.48
1:D:246:GLN:HA	4:D:469:HOH:O	2.14	0.48
1:C:175:GLY:HA3	1:C:181:THR:O	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1:MET:HG2	1:D:239:VAL:HG13	1.94	0.48
1:C:260:TYR:CE2	1:C:292:LEU:HD21	2.48	0.48
1:C:296:LEU:O	1:C:300:LYS:HG3	2.13	0.48
1:C:195:THR:HG22	1:C:196:GLU:N	2.28	0.48
1:D:195:THR:HG22	1:D:196:GLU:N	2.29	0.47
1:C:58:PHE:CE2	1:C:65:PRO:HB2	2.50	0.47
3:C:317:PYR:H31	4:C:456:HOH:O	2.14	0.47
1:D:90:LEU:O	1:D:94:ASN:ND2	2.47	0.47
1:A:311:ASN:O	1:A:312:LYS:HB2	2.14	0.47
1:C:30:LEU:O	1:C:55:ILE:HA	2.15	0.47
1:A:162:LYS:HE2	1:A:162:LYS:HA	1.96	0.47
1:D:82:LYS:HB2	1:D:85:MET:CE	2.44	0.47
1:A:295:MET:HE2	1:A:296:LEU:HD12	1.95	0.47
1:D:127:ILE:HG23	1:D:310:VAL:HG22	1.96	0.47
1:D:188:GLN:O	1:D:190:PRO:HD3	2.15	0.47
1:B:252:ALA:O	1:B:265:SER:HA	2.15	0.47
1:A:195:THR:HG23	1:A:197:GLN:H	1.79	0.47
1:B:119:ASN:OD1	1:B:121:VAL:HG23	2.14	0.46
1:B:82:LYS:HB2	1:B:85:MET:HE1	1.97	0.46
1:B:111:LYS:HD2	1:B:111:LYS:N	2.30	0.46
1:D:127:ILE:HG23	1:D:310:VAL:CG2	2.45	0.46
1:A:130:GLU:HA	1:A:133:LYS:HZ3	1.80	0.46
1:D:204:LYS:HG3	1:D:205:ARG:N	2.31	0.46
1:B:162:LYS:HG3	1:B:192:VAL:CG1	2.45	0.46
1:D:293:GLU:C	1:D:295:MET:H	2.18	0.46
1:D:39:THR:HG21	1:D:58:PHE:O	2.16	0.46
1:A:172:PRO:HG2	1:A:185:LEU:HB2	1.97	0.46
1:D:144:PHE:HE2	1:D:275:VAL:HG13	1.77	0.46
1:A:188:GLN:O	1:A:190:PRO:HD3	2.16	0.46
1:B:98:VAL:O	1:B:102:VAL:HG23	2.15	0.46
1:B:165:GLN:O	1:B:168:GLU:HG2	2.16	0.45
1:B:99:LYS:O	1:B:103:GLN:HG3	2.16	0.45
2:B:314:NAD:H6N	4:B:397:HOH:O	2.15	0.45
1:A:310:VAL:O	1:A:312:LYS:HD2	2.16	0.45
1:D:194:PHE:CD1	1:D:194:PHE:N	2.84	0.45
1:A:82:LYS:H	1:A:85:MET:CE	2.30	0.45
1:C:151:ILE:N	1:C:151:ILE:CD1	2.78	0.45
1:B:162:LYS:HG3	1:B:192:VAL:HG11	1.99	0.45
1:B:8:ALA:CB	1:B:32:LEU:HB3	2.47	0.45
1:D:130:GLU:O	1:D:134:LYS:HG2	2.16	0.45
1:D:30:LEU:O	1:D:55:ILE:HA	2.16	0.45
1:C:195:THR:CG2	1:C:196:GLU:N	2.79	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:85:MET:HB3	1:D:89:ASP:HB2	1.97	0.45
1:C:41:GLY:HA3	1:D:217:LYS:HG3	1.98	0.45
1:A:179:GLY:O	1:A:207:GLN:HB3	2.16	0.45
1:B:140:LYS:HG2	4:B:373:HOH:O	2.16	0.45
1:A:257:ASP:C	1:A:259:GLN:H	2.20	0.45
1:A:1:MET:HG2	1:A:239:VAL:HG13	1.99	0.45
1:A:203:THR:O	1:A:207:GLN:HG3	2.16	0.45
1:A:270:LEU:HD12	1:A:270:LEU:N	2.32	0.45
1:D:268:LEU:HD13	1:D:275:VAL:CG1	2.47	0.45
1:B:250:GLU:HG3	4:B:390:HOH:O	2.17	0.45
1:C:151:ILE:H	1:C:151:ILE:CD1	2.28	0.44
1:A:311:ASN:N	1:A:311:ASN:HD22	2.13	0.44
1:D:21:LYS:O	1:D:21:LYS:HD3	2.18	0.44
1:B:195:THR:C	1:B:197:GLN:N	2.69	0.44
1:B:262:ARG:NH2	1:B:307:GLN:HE22	2.14	0.44
1:D:195:THR:O	1:D:199:VAL:HG23	2.18	0.44
1:B:249:VAL:HA	1:B:268:LEU:O	2.18	0.44
1:D:284:LEU:HD12	1:D:284:LEU:H	1.82	0.44
1:D:216:ALA:C	1:D:218:ALA:H	2.21	0.44
1:A:82:LYS:N	1:A:85:MET:SD	2.90	0.44
1:D:195:THR:HB	1:D:198:GLU:HG3	1.98	0.44
1:B:203:THR:HG22	1:B:207:GLN:NE2	2.33	0.44
1:A:164:LYS:HE3	1:A:192:VAL:HG13	2.00	0.44
1:C:257:ASP:OD1	1:C:259:GLN:NE2	2.51	0.44
1:B:130:GLU:HG2	1:B:310:VAL:HG11	1.99	0.43
1:A:151:ILE:H	1:A:151:ILE:CD1	2.30	0.43
1:D:293:GLU:O	1:D:295:MET:N	2.47	0.43
1:B:80:ALA:HB3	4:B:403:HOH:O	2.19	0.43
1:C:260:TYR:O	1:C:296:LEU:HD12	2.19	0.43
1:D:107:LYS:HD3	1:D:107:LYS:O	2.18	0.43
1:C:22:THR:O	1:C:22:THR:HG22	2.19	0.43
1:A:255:GLU:OE2	1:A:262:ARG:NH1	2.51	0.43
1:D:296:LEU:O	1:D:300:LYS:HG3	2.18	0.43
1:A:195:THR:CG2	1:A:198:GLU:HG3	2.49	0.43
1:A:311:ASN:N	1:A:311:ASN:ND2	2.66	0.43
2:A:313:NAD:H2D	2:A:313:NAD:H6N	1.86	0.43
1:A:148:THR:HA	1:A:151:ILE:HD13	1.99	0.43
1:A:299:LEU:O	1:A:303:ILE:HG13	2.18	0.43
1:B:150:ASP:OD2	1:B:177:HIS:ND1	2.47	0.43
1:A:195:THR:HG22	1:A:198:GLU:N	2.22	0.43
1:A:262:ARG:HG2	1:A:263:PHE:CE1	2.53	0.42
1:A:6:LEU:HD12	1:A:75:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:64:THR:N	1:C:65:PRO:HD2	2.35	0.42
1:A:67:LEU:HB2	1:A:108:THR:HG21	2.00	0.42
1:A:144:PHE:N	1:A:144:PHE:CD1	2.87	0.42
1:A:38:VAL:HG13	1:B:217:LYS:HG2	2.01	0.42
1:C:45:ASP:O	1:D:226:SER:HB3	2.19	0.42
1:B:202:LEU:O	1:B:206:ILE:HG13	2.19	0.42
1:A:130:GLU:CD	1:A:133:LYS:HZ1	2.22	0.42
1:D:248:VAL:HG12	1:D:270:LEU:HD23	2.02	0.42
1:C:78:GLY:HA2	1:C:97:ILE:HD13	2.01	0.42
1:D:250:GLU:HG3	4:D:464:HOH:O	2.20	0.42
1:B:144:PHE:CD1	1:B:144:PHE:N	2.88	0.42
1:A:46:LEU:HD21	1:B:225:LEU:HD13	2.01	0.42
1:D:141:ASN:HA	1:D:275:VAL:CG2	2.50	0.42
1:A:8:ALA:CB	1:A:32:LEU:HB3	2.50	0.42
1:B:177:HIS:O	1:B:177:HIS:CG	2.73	0.42
1:C:78:GLY:HA2	1:C:97:ILE:CD1	2.50	0.42
1:C:94:ASN:O	1:C:98:VAL:HG23	2.20	0.42
1:A:22:THR:HA	1:A:51:THR:HG21	2.01	0.42
1:A:101:LEU:O	1:A:105:VAL:HG23	2.20	0.42
1:C:292:LEU:O	1:C:296:LEU:CD2	2.68	0.41
1:A:239:VAL:O	1:A:243:GLN:HG3	2.19	0.41
1:D:130:GLU:HB3	1:D:310:VAL:HG11	2.02	0.41
1:D:183:LEU:HA	1:D:184:PRO:HD2	1.99	0.41
1:C:89:ASP:O	1:C:93:VAL:HG23	2.20	0.41
1:B:79:VAL:CG1	1:B:82:LYS:HG3	2.51	0.41
1:A:189:VAL:HG12	1:A:192:VAL:HG22	2.02	0.41
1:D:127:ILE:HA	1:D:310:VAL:HG21	2.02	0.41
1:D:120:PRO:HG2	1:D:123:THR:HG23	2.03	0.41
1:A:121:VAL:HA	1:A:124:THR:OG1	2.20	0.41
1:B:246:GLN:HG2	1:D:26:SER:OG	2.20	0.41
1:A:164:LYS:HE3	1:A:192:VAL:CG1	2.50	0.41
1:A:278:ARG:HG3	1:A:278:ARG:HH11	1.85	0.41
1:A:195:THR:HG22	1:A:198:GLU:HG3	2.02	0.41
1:A:185:LEU:HD22	1:A:284:LEU:HD22	2.03	0.41
1:D:121:VAL:HA	1:D:124:THR:OG1	2.20	0.41
1:A:130:GLU:HB2	1:A:310:VAL:HG21	2.03	0.41
1:D:154:SER:OG	1:D:206:ILE:HD13	2.21	0.41
1:A:20:LEU:HD12	1:A:20:LEU:HA	1.93	0.41
1:A:34:ASP:HB3	1:A:39:THR:OG1	2.21	0.41
1:D:139:ASP:OD1	1:D:141:ASN:HB2	2.21	0.41
1:D:144:PHE:CD1	1:D:144:PHE:N	2.89	0.40
2:D:316:NAD:H2D	2:D:316:NAD:H6N	1.87	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:41:GLY:HA2	1:D:216:ALA:CB	2.50	0.40
1:B:189:VAL:HA	1:B:190:PRO:HD2	1.95	0.40
1:B:91:PHE:CZ	1:B:305:LEU:HD12	2.56	0.40
1:C:177:HIS:NE2	2:C:315:NAD:O7N	2.54	0.40
1:C:8:ALA:HB1	1:C:32:LEU:HG	2.04	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	310/312 (99%)	295 (95%)	12 (4%)	3 (1%)	22	38
1	B	310/312 (99%)	298 (96%)	10 (3%)	2 (1%)	33	55
1	C	310/312 (99%)	289 (93%)	15 (5%)	6 (2%)	12	19
1	D	310/312 (99%)	285 (92%)	22 (7%)	3 (1%)	22	38
All	All	1240/1248 (99%)	1167 (94%)	59 (5%)	14 (1%)	21	34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ARG
1	A	179	GLY
1	A	258	GLY
1	C	179	GLY
1	D	179	GLY
1	B	223	ALA
1	C	309	PHE
1	C	134	LYS
1	C	140	LYS
1	C	258	GLY
1	C	308	GLU
1	D	39	THR
1	D	223	ALA

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Mol	Chain	Res	Type
1	B	310	VAL

### 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	241/241 (100%)	233 (97%)	8 (3%)	50	76
1	B	241/241 (100%)	232 (96%)	9 (4%)	45	72
1	C	241/241 (100%)	232 (96%)	9 (4%)	45	72
1	D	241/241 (100%)	235 (98%)	6 (2%)	60	85
All	All	964/964 (100%)	932 (97%)	32 (3%)	50	76

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	54	LYS
1	A	59	SER
1	A	81	ARG
1	A	85	MET
1	A	195	THR
1	A	238	LEU
1	A	295	MET
1	B	81	ARG
1	B	111	LYS
1	B	125	VAL
1	B	130	GLU
1	B	144	PHE
1	B	166	PRO
1	B	280	SER
1	B	295	MET
1	B	305	LEU
1	C	50	PRO
1	C	54	LYS
1	C	81	ARG
1	C	123	THR

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Mol	Chain	Res	Type
1	C	153	CYS
1	C	183	LEU
1	C	295	MET
1	C	297	ASP
1	C	307	GLN
1	D	54	LYS
1	D	81	ARG
1	D	123	THR
1	D	288	GLU
1	D	299	LEU
1	D	312	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	311	ASN
1	B	259	GLN
1	C	207	GLN
1	C	229	GLN
1	C	246	GLN
1	C	259	GLN
1	D	307	GLN

### 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 ⓘ

5 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	313	-	48,48,48	2.07	8 (16%)	73,73,73	1.55	11 (15%)
2	NAD	B	314	-	48,48,48	2.00	10 (20%)	73,73,73	1.55	10 (13%)
2	NAD	C	315	-	48,48,48	2.01	9 (18%)	73,73,73	1.54	11 (15%)
3	PYR	C	317	-	5,5,5	2.03	2 (40%)	6,6,6	1.22	1 (16%)
2	NAD	D	316	-	48,48,48	2.03	9 (18%)	73,73,73	1.57	10 (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	313	-	-	0/30/62/62	0/3/5/5
2	NAD	B	314	-	-	0/30/62/62	0/3/5/5
2	NAD	C	315	-	-	0/30/62/62	0/3/5/5
3	PYR	C	317	-	-	0/4/4/4	0/0/0/0
2	NAD	D	316	-	-	0/30/62/62	0/3/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	313	NAD	C2N-C3N	7.83	1.49	1.38
2	C	315	NAD	C4N-C3N	7.77	1.52	1.39
2	D	316	NAD	C4N-C3N	7.63	1.52	1.39
2	B	314	NAD	C4N-C3N	7.57	1.52	1.39
2	A	313	NAD	C4N-C3N	7.51	1.52	1.39
2	D	316	NAD	C2N-C3N	7.36	1.49	1.38
2	B	314	NAD	C2N-C3N	7.06	1.48	1.38
2	C	315	NAD	C2N-C3N	7.04	1.48	1.38
2	D	316	NAD	C5N-C4N	4.79	1.50	1.39
2	C	315	NAD	C5N-C4N	4.72	1.50	1.39
2	B	314	NAD	C5N-C4N	4.71	1.49	1.39
2	A	313	NAD	C5N-C4N	4.59	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	313	NAD	C2N-N1N	3.52	1.39	1.35
3	C	317	PYR	C2-C1	-3.49	1.45	1.53
2	B	314	NAD	C2N-N1N	3.40	1.39	1.35
2	D	316	NAD	C2N-N1N	3.31	1.39	1.35
2	C	315	NAD	PA-O3	-3.30	1.53	1.59
2	D	316	NAD	C6N-N1N	3.23	1.44	1.35
2	C	315	NAD	C6N-N1N	3.18	1.44	1.35
2	A	313	NAD	C6N-N1N	3.16	1.44	1.35
2	B	314	NAD	C6N-N1N	3.13	1.44	1.35
2	A	313	NAD	PA-O3	-3.11	1.54	1.59
2	C	315	NAD	C2N-N1N	3.01	1.39	1.35
2	B	314	NAD	C6N-C5N	-2.64	1.32	1.38
2	A	313	NAD	C6N-C5N	-2.48	1.32	1.38
2	D	316	NAD	C6N-C5N	-2.44	1.32	1.38
2	D	316	NAD	C2A-N1A	2.39	1.38	1.33
2	A	313	NAD	C2A-N1A	2.33	1.38	1.33
2	D	316	NAD	PN-O3	2.32	1.65	1.60
2	B	314	NAD	PA-O3	-2.32	1.55	1.59
2	C	315	NAD	C6N-C5N	-2.30	1.33	1.38
2	C	315	NAD	C2A-N1A	2.21	1.38	1.33
2	B	314	NAD	PN-O3	2.17	1.64	1.60
2	B	314	NAD	C2A-N1A	2.08	1.38	1.33
2	D	316	NAD	PA-O3	-2.04	1.56	1.59
2	B	314	NAD	C2D-C1D	-2.02	1.50	1.53
2	C	315	NAD	C2D-C1D	-2.01	1.50	1.53
3	C	317	PYR	C3-C2	-2.00	1.45	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	315	NAD	C5N-C4N-C3N	-6.00	112.53	120.32
2	D	316	NAD	C5N-C4N-C3N	-5.95	112.59	120.32
2	A	313	NAD	C5N-C4N-C3N	-5.90	112.66	120.32
2	B	314	NAD	C5N-C4N-C3N	-5.71	112.91	120.32
2	B	314	NAD	C3N-C7N-N7N	5.46	123.98	117.77
2	A	313	NAD	C3N-C7N-N7N	5.20	123.69	117.77
2	C	315	NAD	C3N-C7N-N7N	4.93	123.38	117.77
2	D	316	NAD	C3N-C7N-N7N	4.77	123.20	117.77
2	D	316	NAD	O4B-C1B-C2B	-3.97	100.69	106.77
2	A	313	NAD	C6N-C5N-C4N	3.93	125.69	119.44
2	D	316	NAD	C6N-C5N-C4N	3.90	125.64	119.44
2	C	315	NAD	C6N-C5N-C4N	3.84	125.55	119.44

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	314	NAD	C6N-C5N-C4N	3.80	125.47	119.44
2	D	316	NAD	C4B-O4B-C1B	-3.74	105.69	109.75
2	C	315	NAD	C4B-O4B-C1B	-3.43	106.02	109.75
2	A	313	NAD	C6N-N1N-C2N	-3.25	118.37	122.04
2	A	313	NAD	C4B-O4B-C1B	-3.19	106.29	109.75
2	B	314	NAD	O4B-C1B-C2B	-3.17	101.91	106.77
2	C	315	NAD	O4B-C1B-C2B	-3.16	101.92	106.77
2	B	314	NAD	C4B-O4B-C1B	-3.14	106.33	109.75
2	D	316	NAD	C6N-N1N-C2N	-3.14	118.49	122.04
2	C	315	NAD	C6N-N1N-C2N	-3.11	118.52	122.04
2	B	314	NAD	C6N-N1N-C2N	-3.05	118.59	122.04
2	A	313	NAD	O4B-C1B-C2B	-3.00	102.17	106.77
2	B	314	NAD	O7N-C7N-C3N	-2.80	116.42	119.58
2	A	313	NAD	O7N-C7N-C3N	-2.50	116.76	119.58
2	D	316	NAD	C5A-C6A-N6A	2.48	126.32	120.72
2	B	314	NAD	C5A-C6A-N6A	2.43	126.21	120.72
2	A	313	NAD	O2N-PN-O5D	2.40	118.12	108.19
2	D	316	NAD	O2N-PN-O5D	2.39	118.08	108.19
2	A	313	NAD	O4D-C1D-N1N	2.37	110.37	107.95
2	C	315	NAD	O2N-PN-O5D	2.34	117.85	108.19
2	A	313	NAD	C5A-C6A-N6A	2.32	125.97	120.72
2	C	315	NAD	C5A-C6A-N6A	2.31	125.94	120.72
2	D	316	NAD	O7N-C7N-C3N	-2.26	117.03	119.58
2	C	315	NAD	O7N-C7N-C3N	-2.24	117.05	119.58
2	B	314	NAD	O2N-PN-O5D	2.23	117.41	108.19
3	C	317	PYR	O2-C1-C2	2.22	119.27	114.37
2	A	313	NAD	O7N-C7N-N7N	-2.11	119.55	122.59
2	C	315	NAD	O7N-C7N-N7N	-2.10	119.56	122.59
2	D	316	NAD	N3A-C2A-N1A	2.08	130.44	128.71
2	B	314	NAD	O7N-C7N-N7N	-2.07	119.60	122.59
2	C	315	NAD	C4A-C5A-N7A	2.02	111.25	109.52

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	310/312 (99%)	-0.54	8 (2%) 53 55	18, 36, 61, 101	7 (2%)
1	B	312/312 (100%)	-0.58	0 100 100	17, 34, 60, 95	1 (0%)
1	C	311/312 (99%)	-0.48	2 (0%) 86 88	23, 48, 74, 101	7 (2%)
1	D	312/312 (100%)	-0.42	5 (1%) 68 71	23, 46, 83, 101	9 (2%)
All	All	1245/1248 (99%)	-0.51	15 (1%) 75 77	17, 41, 74, 101	24 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	84	GLY	4.4
1	A	85	MET	4.3
1	A	86	ASP	4.1
1	A	88	SER	4.0
1	D	312	LYS	3.6
1	C	83	PRO	3.6
1	A	82	LYS	3.5
1	A	90	LEU	3.5
1	A	87	ARG	3.4
1	D	85	MET	2.9
1	D	165	GLN	2.8
1	D	163	GLY	2.6
1	A	89	ASP	2.6
1	C	218	ALA	2.4
1	A	312	LYS	2.3

### 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
3	PYR	C	317	6/6	0.32	9.32	91,100,101,101	0
2	NAD	B	314	44/44	0.13	0.09	24,43,61,68	8
2	NAD	D	316	44/44	0.12	0.04	20,49,63,77	9
2	NAD	A	313	44/44	0.12	0.01	25,37,49,61	8
2	NAD	C	315	44/44	0.11	-0.31	12,49,69,82	9

### 6.5 Other polymers ⓘ

There are no such residues in this entry.