



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:42 PM GMT

PDB ID : 3RU9  
Title : Specific recognition of N-acetylated substrates and domain flexibility in WbgU:  
a UDP-GalNAc 4-epimerase  
Authors : Bhatt, V.S.; Guan, W; Wang, P.G.  
Deposited on : 2011-05-04  
Resolution : 2.21 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](mailto: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.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

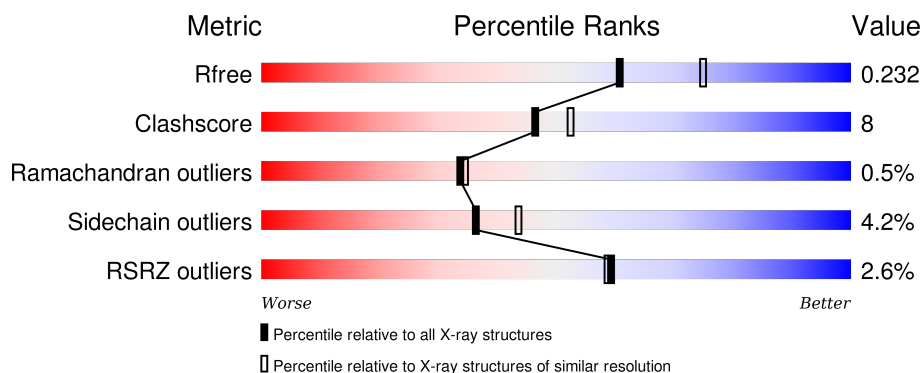
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.21 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))
$R_{free}$	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	351	<div> <div>4%</div> <div>79%</div> <div>14%</div> <div>• •</div> </div>
1	B	351	<div> <div>4%</div> <div>79%</div> <div>15%</div> <div>• •</div> </div>
1	C	351	<div> <div>%</div> <div>77%</div> <div>16%</div> <div>• •</div> </div>
1	D	351	<div> <div>%</div> <div>78%</div> <div>16%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	346	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11333 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 WbgU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2681	1712	459	502	8			
1	B	336	Total	C	N	O	S	0	0	0
			2681	1712	459	502	8			
1	C	336	Total	C	N	O	S	0	0	0
			2681	1712	459	502	8			
1	D	336	Total	C	N	O	S	0	0	0
			2681	1712	459	502	8			

There are 24 discrepancies between the modelled and reference sequences:

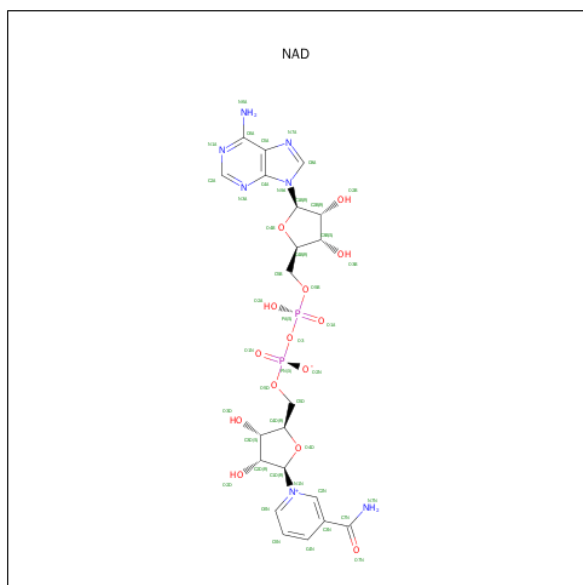
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9

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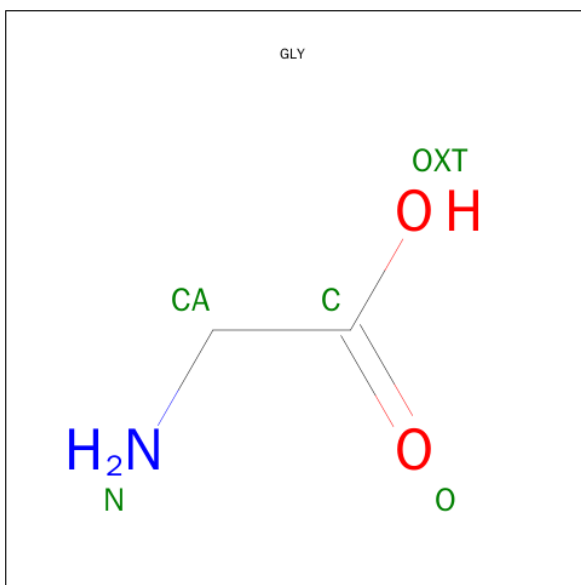
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9

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



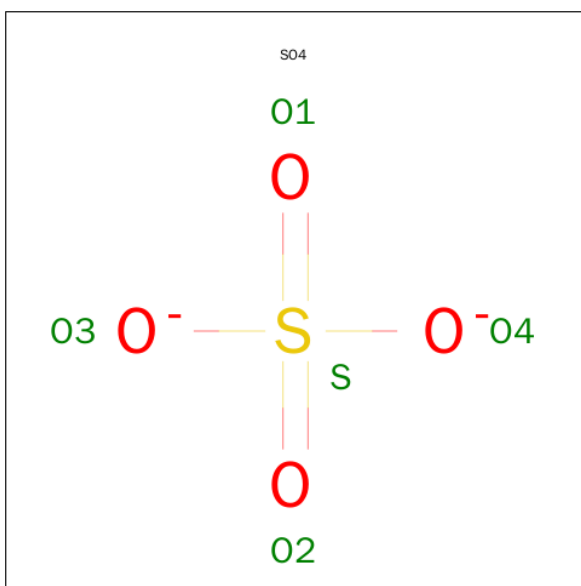
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula:  $C_2H_5NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			5	2	1	2		
3	D	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 4 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
5	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
5	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
5	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

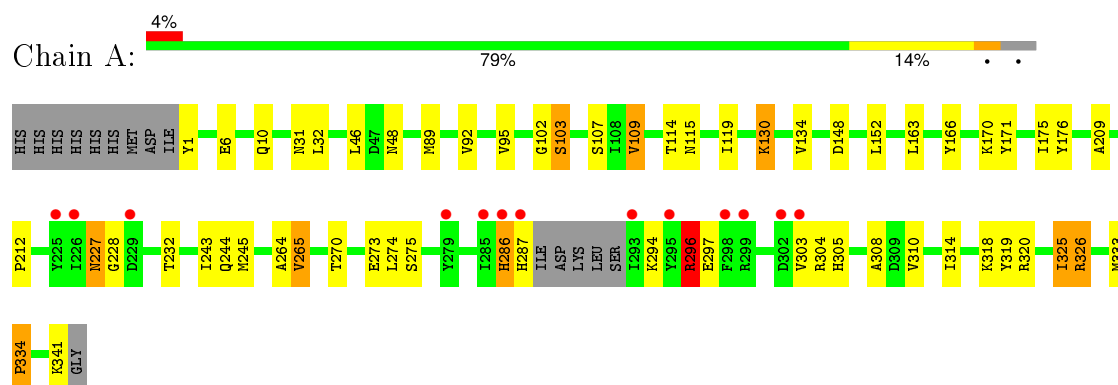
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	83	Total	O	0	0
			83	83		
6	B	71	Total	O	0	0
			71	71		
6	C	77	Total	O	0	0
			77	77		
6	D	82	Total	O	0	0
			82	82		

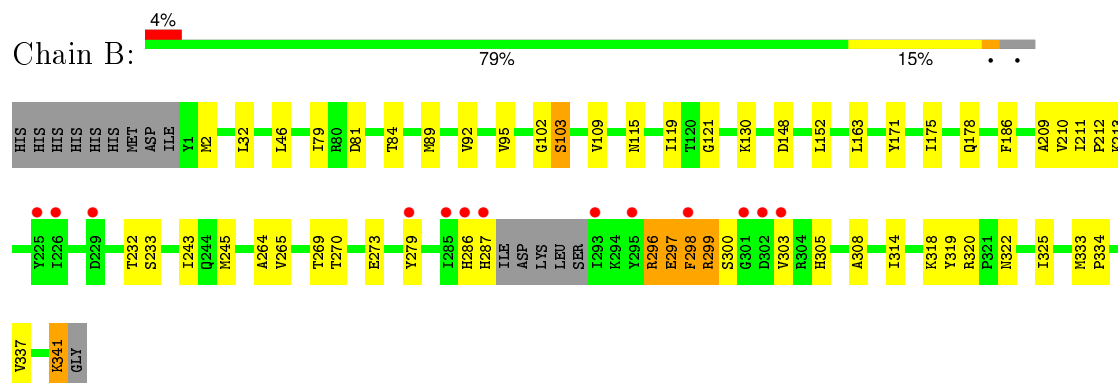
### 3 Residue-property plots

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.

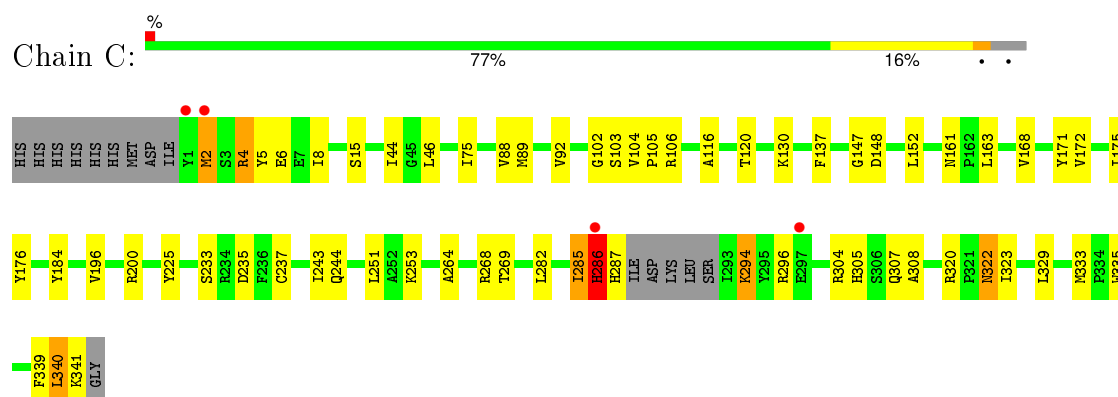
#### • Molecule 1: WbgU



#### • Molecule 1: WbgU

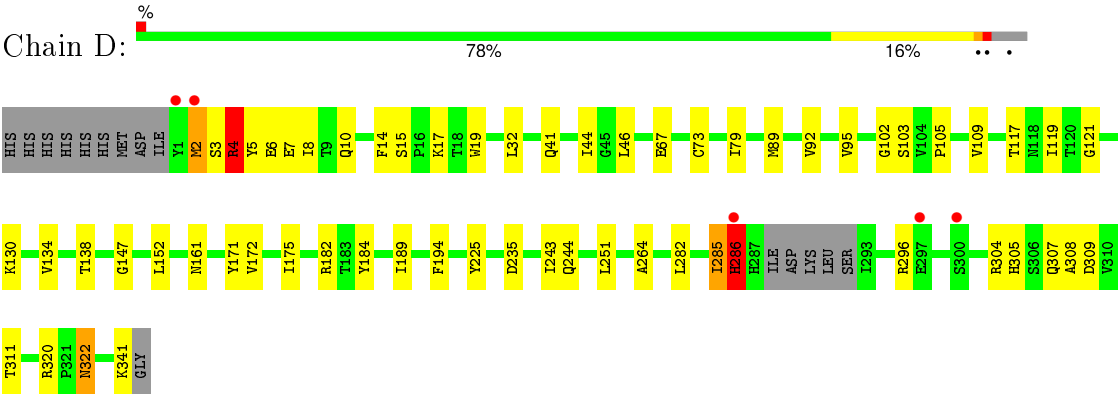


#### • Molecule 1: WbgU





● Molecule 1: WbgU



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.41Å 77.41Å 224.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.80 – 2.21 29.34 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.80-2.21) 99.9 (29.34-2.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.181 , 0.232 0.184 , 0.232	Depositor DCC
$R_{free}$ test set	3800 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 18.3	EDS
Estimated twinning fraction	0.032 for -h,-k,l 0.478 for h,-h-k,-l 0.035 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 75420 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11333	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, SO4, 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	0.95	1/2739 (0.0%)	0.86	1/3717 (0.0%)
1	B	0.94	2/2739 (0.1%)	0.85	0/3717
1	C	0.94	3/2739 (0.1%)	0.85	1/3717 (0.0%)
1	D	0.93	1/2739 (0.0%)	0.86	2/3717 (0.1%)
All	All	0.94	7/10956 (0.1%)	0.85	4/14868 (0.0%)

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	C	0	1
1	D	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	5	TYR	CD1-CE1	-5.69	1.30	1.39
1	B	265	VAL	CB-CG1	-5.69	1.41	1.52
1	A	265	VAL	CB-CG1	-5.42	1.41	1.52
1	C	137	PHE	CE1-CZ	5.19	1.47	1.37
1	C	5	TYR	CD2-CE2	-5.18	1.31	1.39
1	D	109	VAL	CB-CG1	-5.16	1.42	1.52
1	B	186	PHE	CE1-CZ	5.04	1.47	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	152	LEU	CA-CB-CG	7.20	131.87	115.30
1	C	152	LEU	CA-CB-CG	6.44	130.11	115.30
1	A	109	VAL	CG1-CB-CG2	5.94	120.40	110.90
1	D	4	ARG	NE-CZ-NH1	5.33	122.97	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	285	ILE	Peptide
1	D	285	ILE	Peptide

## 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	2681	0	2658	44	0
1	B	2681	0	2658	44	0
1	C	2681	0	2658	40	0
1	D	2681	0	2658	39	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0
3	C	5	0	2	0	0
3	D	5	0	2	0	0
4	A	10	0	0	3	0
5	A	25	0	0	0	0
5	B	25	0	0	1	0
5	C	25	0	0	0	0
5	D	25	0	0	0	0
6	A	83	0	0	1	0
6	B	71	0	0	2	0
6	C	77	0	0	0	0
6	D	82	0	0	1	0
All	All	11333	0	10740	165	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 8.

All (165) 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:B:296:ARG:HG3	1:B:297:GLU:N	1.52	1.05
1:A:296:ARG:HD3	1:A:297:GLU:H	1.20	1.04
1:B:296:ARG:CG	1:B:297:GLU:H	1.74	1.00
1:C:89:MET:HE3	1:C:89:MET:HA	1.47	0.93
1:B:296:ARG:HG3	1:B:297:GLU:H	0.79	0.92
1:B:296:ARG:HD2	1:B:297:GLU:HB2	1.52	0.90
1:A:326:ARG:HG2	1:A:326:ARG:HH11	1.33	0.90
1:D:19:TRP:HE1	1:D:41:GLN:HE21	1.31	0.79
1:A:318:LYS:HE3	4:A:345:SO4:O1	1.84	0.77
1:A:244:GLN:HE22	1:A:320:ARG:H	1.29	0.76
1:C:285:ILE:O	1:C:286:HIS:HB2	1.84	0.76
1:A:296:ARG:CD	1:A:297:GLU:H	1.99	0.75
1:B:171:TYR:CZ	1:B:175:ILE:HD11	2.22	0.74
1:B:296:ARG:CG	1:B:297:GLU:N	2.34	0.73
1:C:8:ILE:CG2	1:C:251:LEU:HD22	2.19	0.72
1:B:171:TYR:CE2	1:B:175:ILE:HD11	2.26	0.71
1:C:244:GLN:HE22	1:C:320:ARG:H	1.37	0.71
1:A:102:GLY:O	1:A:103:SER:HB3	1.89	0.70
1:B:210:VAL:HG13	1:B:211:ILE:N	2.06	0.69
1:D:2:MET:SD	1:D:322:ASN:ND2	2.66	0.69
1:D:244:GLN:HE22	1:D:320:ARG:H	1.40	0.69
1:A:171:TYR:CE2	1:A:175:ILE:HD11	2.28	0.68
1:D:102:GLY:O	1:D:103:SER:HB3	1.92	0.68
1:D:2:MET:O	1:D:6:GLU:HG3	1.94	0.68
1:A:89:MET:HE1	1:A:95:VAL:HG22	1.76	0.68
1:C:8:ILE:HG23	1:C:251:LEU:HD22	1.74	0.67
1:A:89:MET:CE	1:A:92:VAL:HG11	2.24	0.67
1:B:89:MET:CE	1:B:92:VAL:HG11	2.25	0.67
4:A:346:SO4:O3	1:B:318:LYS:HE2	1.96	0.66
1:D:8:ILE:HG23	1:D:251:LEU:HD22	1.76	0.65
1:B:2:MET:SD	1:B:322:ASN:OD1	2.55	0.65
1:D:285:ILE:O	1:D:286:HIS:HB2	1.93	0.65
1:B:102:GLY:O	1:B:103:SER:HB3	1.96	0.64
1:C:147:GLY:HA3	1:C:161:ASN:O	1.97	0.64
1:A:244:GLN:NE2	1:A:320:ARG:H	1.96	0.64
1:B:148:ASP:HB3	1:B:163:LEU:HD21	1.81	0.62
1:B:152:LEU:HD11	1:B:305:HIS:HB3	1.80	0.62
1:C:225:TYR:HB3	1:C:296:ARG:HE	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:HD3	1:A:297:GLU:N	2.05	0.61
1:B:337:VAL:O	1:B:341:LYS:HB2	1.99	0.61
1:B:341:LYS:NZ	1:B:341:LYS:HB3	2.16	0.60
1:D:8:ILE:CG2	1:D:251:LEU:HD22	2.32	0.60
1:C:106:ARG:NH1	1:D:14:PHE:O	2.35	0.59
1:C:2:MET:HG3	1:C:322:ASN:OD1	2.03	0.59
1:A:148:ASP:HB3	1:A:163:LEU:HD21	1.84	0.59
1:B:270:THR:OG1	1:B:273:GLU:HG3	2.04	0.58
1:C:2:MET:O	1:C:6:GLU:HG3	2.03	0.58
1:C:44:ILE:HD12	1:C:92:VAL:HG22	1.86	0.58
1:D:147:GLY:HA3	1:D:161:ASN:O	2.04	0.58
1:B:213:LYS:HE2	5:B:344:UNL:O4	2.03	0.58
1:C:339:PHE:HD2	1:C:340:LEU:HD23	1.69	0.57
1:C:102:GLY:O	1:C:103:SER:HB3	2.04	0.57
1:D:103:SER:OG	1:D:105:PRO:HD2	2.04	0.57
1:C:322:ASN:HD22	1:C:323:ILE:HG13	1.69	0.57
1:B:32:LEU:HD23	1:B:243:ILE:HD12	1.87	0.56
1:C:116:ALA:O	1:C:120:THR:HB	2.06	0.55
1:B:210:VAL:CG1	1:B:211:ILE:N	2.70	0.55
1:B:89:MET:HE3	1:B:92:VAL:HB	1.87	0.55
1:C:244:GLN:NE2	1:C:320:ARG:H	2.04	0.55
1:D:225:TYR:HB3	1:D:296:ARG:HE	1.72	0.55
1:D:2:MET:HB3	1:D:5:TYR:HB3	1.88	0.54
1:C:8:ILE:HG23	1:C:251:LEU:CD2	2.38	0.53
1:B:210:VAL:HG13	1:B:211:ILE:HG13	1.91	0.52
1:B:89:MET:HE2	1:B:95:VAL:CG2	2.39	0.52
1:A:270:THR:OG1	1:A:273:GLU:HG3	2.10	0.52
1:D:309:ASP:OD1	1:D:311:THR:HB	2.09	0.52
1:D:119:ILE:HD13	1:D:172:VAL:HG11	1.92	0.51
1:B:115:ASN:OD1	1:B:119:ILE:HD12	2.10	0.51
1:A:152:LEU:HD11	1:A:305:HIS:HB3	1.93	0.51
1:A:326:ARG:CG	1:A:326:ARG:HH11	2.14	0.51
1:D:244:GLN:NE2	1:D:320:ARG:H	2.06	0.51
1:A:333:MET:HB2	1:A:334:PRO:HD3	1.92	0.51
1:A:31:ASN:HB3	1:A:243:ILE:HD11	1.93	0.50
1:A:89:MET:CE	1:A:95:VAL:HG22	2.40	0.50
1:D:89:MET:HE1	1:D:95:VAL:HG22	1.93	0.50
1:C:8:ILE:HG21	1:C:251:LEU:HD22	1.92	0.50
1:A:314:ILE:HG23	1:A:320:ARG:NH1	2.27	0.50
1:B:314:ILE:HG23	1:B:320:ARG:NH1	2.27	0.49
1:A:326:ARG:NH1	1:A:326:ARG:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:MET:HG2	1:B:319:TYR:CE1	2.48	0.49
1:D:4:ARG:HG3	1:D:4:ARG:O	2.13	0.49
1:C:286:HIS:C	1:C:287:HIS:HD1	2.16	0.49
1:C:2:MET:O	1:C:6:GLU:N	2.36	0.49
1:C:171:TYR:CZ	1:C:175:ILE:HD11	2.48	0.48
1:B:89:MET:HE1	1:B:92:VAL:HG11	1.95	0.48
1:A:227:ASN:OD1	1:A:296:ARG:HD2	2.12	0.48
1:D:117:THR:HG22	2:D:343:NAD:H61A	1.79	0.48
1:B:178:GLN:NE2	6:B:376:HOH:O	2.44	0.48
1:A:89:MET:HE2	1:A:134:VAL:HG11	1.95	0.48
1:A:228:GLY:N	1:A:297:GLU:O	2.48	0.47
1:D:89:MET:HE1	1:D:95:VAL:CG2	2.44	0.47
1:A:209:ALA:O	1:A:212:PRO:HD2	2.13	0.47
1:A:6:GLU:O	1:A:10:GLN:HG3	2.14	0.47
1:B:89:MET:HE2	1:B:95:VAL:HG22	1.96	0.47
1:B:233:SER:HA	1:B:269:THR:O	2.15	0.47
1:A:130:LYS:NZ	1:D:67:GLU:OE2	2.41	0.46
1:D:304:ARG:HG3	1:D:305:HIS:CD2	2.51	0.46
1:B:333:MET:HB2	1:B:334:PRO:HD3	1.98	0.46
1:A:245:MET:HG2	1:A:319:TYR:CE1	2.51	0.46
1:D:264:ALA:HB3	1:D:308:ALA:HB3	1.97	0.45
1:C:4:ARG:O	1:C:4:ARG:HG3	2.17	0.45
1:B:89:MET:CE	1:B:92:VAL:CG1	2.93	0.45
1:C:225:TYR:CD1	1:C:294:LYS:HG3	2.52	0.45
1:C:235:ASP:HB2	1:C:307:GLN:HA	1.98	0.45
1:C:329:LEU:O	1:C:333:MET:HG2	2.16	0.45
1:D:130:LYS:HD2	1:D:184:TYR:CG	2.51	0.45
1:C:282:LEU:HD23	1:C:282:LEU:HA	1.84	0.45
1:D:44:ILE:HD12	1:D:92:VAL:CG2	2.48	0.44
1:B:209:ALA:O	1:B:212:PRO:HD2	2.17	0.44
1:A:274:LEU:HD13	1:A:325:ILE:HD11	1.98	0.44
1:C:322:ASN:ND2	1:C:323:ILE:HG13	2.32	0.44
1:A:286:HIS:O	1:A:287:HIS:HB2	2.18	0.44
1:B:300:SER:HA	6:B:389:HOH:O	2.18	0.44
1:B:264:ALA:HB3	1:B:308:ALA:HB3	2.00	0.43
1:A:115:ASN:OD1	1:A:119:ILE:HD12	2.18	0.43
1:C:286:HIS:C	1:C:287:HIS:ND1	2.71	0.43
1:D:235:ASP:HB2	1:D:307:GLN:HA	1.99	0.43
1:D:89:MET:HE1	1:D:134:VAL:HG11	2.00	0.43
1:B:89:MET:CE	1:B:95:VAL:HG22	2.48	0.43
1:C:148:ASP:HB3	1:C:163:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:CD1	1:A:325:ILE:HD11	2.49	0.43
1:A:89:MET:HE3	1:A:89:MET:HA	2.01	0.43
1:D:171:TYR:CZ	1:D:175:ILE:HD11	2.54	0.43
1:A:264:ALA:HB3	1:A:308:ALA:HB3	2.01	0.42
1:C:233:SER:HA	1:C:269:THR:O	2.20	0.42
1:B:286:HIS:O	1:B:287:HIS:HB2	2.20	0.42
4:A:346:SO4:O3	1:B:318:LYS:CE	2.66	0.42
1:D:89:MET:HE2	1:D:92:VAL:HB	2.01	0.42
1:B:81:ASP:OD2	1:B:84:THR:OG1	2.30	0.42
1:A:265:VAL:CG1	1:A:265:VAL:O	2.67	0.42
1:B:297:GLU:HB3	1:B:298:PHE:H	1.74	0.42
1:A:1:TYR:N	6:A:392:HOH:O	2.52	0.42
1:D:102:GLY:O	1:D:103:SER:CB	2.58	0.42
1:B:232:THR:O	1:B:270:THR:HA	2.18	0.42
1:C:304:ARG:HG3	1:C:305:HIS:CD2	2.54	0.42
1:D:79:ILE:HD12	1:D:121:GLY:HA3	2.02	0.42
1:A:89:MET:CE	1:A:92:VAL:CG1	2.96	0.42
1:D:2:MET:HE3	1:D:5:TYR:CD2	2.55	0.42
1:B:245:MET:HG2	1:B:319:TYR:CD1	2.55	0.42
1:A:294:LYS:HB3	1:A:294:LYS:HE2	1.91	0.42
1:A:310:VAL:HG23	1:A:314:ILE:HD11	2.02	0.42
1:B:299:ARG:CG	1:B:300:SER:H	2.33	0.41
1:D:17:LYS:H	1:D:41:GLN:NE2	2.18	0.41
1:A:107:SER:HB3	1:A:166:TYR:HB2	2.02	0.41
1:D:194:PHE:HB2	1:D:264:ALA:HB2	2.02	0.41
1:C:225:TYR:CE1	1:C:294:LYS:HG3	2.56	0.41
1:C:104:VAL:HB	1:C:105:PRO:HD3	2.02	0.41
1:C:196:VAL:HA	1:C:237:CYS:O	2.20	0.41
1:A:171:TYR:CZ	1:A:175:ILE:HD11	2.54	0.41
1:A:265:VAL:O	1:A:265:VAL:HG12	2.20	0.41
1:C:200:ARG:HA	1:C:335:TRP:CH2	2.56	0.41
1:C:130:LYS:HD2	1:C:184:TYR:CG	2.56	0.41
1:C:168:VAL:O	1:C:172:VAL:HG23	2.20	0.41
1:C:264:ALA:HB3	1:C:308:ALA:HB3	2.01	0.41
1:A:232:THR:HG23	1:A:304:ARG:O	2.21	0.41
1:D:138:THR:HA	1:D:189:ILE:O	2.21	0.41
1:A:170:LYS:HA	1:A:170:LYS:HD3	1.90	0.41
1:D:282:LEU:HA	1:D:282:LEU:HD23	1.84	0.41
1:D:8:ILE:HD11	6:D:359:HOH:O	2.19	0.40
1:C:75:ILE:HG13	1:C:88:VAL:HG12	2.02	0.40
1:A:32:LEU:HD23	1:A:243:ILE:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:ARG:HD3	1:C:268:ARG:HH11	1.64	0.40
1:D:67:GLU:CD	1:D:67:GLU:H	2.25	0.40
1:D:32:LEU:HD23	1:D:243:ILE:HD12	2.03	0.40
1:B:79:ILE:HG13	1:B:121:GLY:HA3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	332/351 (95%)	317 (96%)	12 (4%)	3 (1%)	21	18
1	B	332/351 (95%)	319 (96%)	12 (4%)	1 (0%)	46	50
1	C	332/351 (95%)	322 (97%)	9 (3%)	1 (0%)	46	50
1	D	332/351 (95%)	320 (96%)	11 (3%)	1 (0%)	46	50
All	All	1328/1404 (95%)	1278 (96%)	44 (3%)	6 (0%)	34	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	286	HIS
1	D	286	HIS
1	A	103	SER
1	A	296	ARG
1	B	103	SER
1	A	286	HIS

### 5.3.2 Protein sidechains [i](#)

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	290/304 (95%)	276 (95%)	14 (5%)	31	36
1	B	290/304 (95%)	279 (96%)	11 (4%)	40	48
1	C	290/304 (95%)	278 (96%)	12 (4%)	37	45
1	D	290/304 (95%)	278 (96%)	12 (4%)	37	45
All	All	1160/1216 (95%)	1111 (96%)	49 (4%)	36	43

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

Mol	Chain	Res	Type
1	A	46	LEU
1	A	48	ASN
1	A	109	VAL
1	A	114	THR
1	A	130	LYS
1	A	176	TYR
1	A	227	ASN
1	A	275	SER
1	A	296	ARG
1	A	303	VAL
1	A	325	ILE
1	A	326	ARG
1	A	334	PRO
1	A	341	LYS
1	B	46	LEU
1	B	109	VAL
1	B	130	LYS
1	B	279	TYR
1	B	296	ARG
1	B	297	GLU
1	B	298	PHE
1	B	299	ARG
1	B	303	VAL
1	B	325	ILE
1	B	341	LYS
1	C	2	MET
1	C	4	ARG
1	C	15	SER

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Mol	Chain	Res	Type
1	C	46	LEU
1	C	176	TYR
1	C	243	ILE
1	C	253	LYS
1	C	286	HIS
1	C	294	LYS
1	C	322	ASN
1	C	340	LEU
1	C	341	LYS
1	D	2	MET
1	D	3	SER
1	D	4	ARG
1	D	7	GLU
1	D	10	GLN
1	D	15	SER
1	D	46	LEU
1	D	73	CYS
1	D	182	ARG
1	D	286	HIS
1	D	322	ASN
1	D	341	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	173	ASN
1	A	244	GLN
1	B	173	ASN
1	B	246	ASN
1	C	244	GLN
1	C	322	ASN
1	D	10	GLN
1	D	41	GLN
1	D	195	ASN
1	D	244	GLN
1	D	322	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 12 ligands modelled in this entry, 4 are unknown - leaving 8 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$
2	NAD	A	343	-	38,48,48	1.54	7 (18%)	47,73,73	2.09	6 (12%)
4	SO4	A	345	-	4,4,4	0.37	0	6,6,6	0.58	0
4	SO4	A	346	-	4,4,4	0.22	0	6,6,6	0.84	0
2	NAD	B	343	-	38,48,48	1.50	6 (15%)	47,73,73	1.89	4 (8%)
2	NAD	C	343	-	38,48,48	1.17	3 (7%)	47,73,73	1.66	6 (12%)
3	GLY	C	345	-	1,4,4	0.92	0	0,4,4	0.00	-
2	NAD	D	343	-	38,48,48	1.36	5 (13%)	47,73,73	1.81	8 (17%)
3	GLY	D	345	-	1,4,4	0.98	0	0,4,4	0.00	-

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	343	-	-	0/22/62/62	0/5/5/5
4	SO4	A	345	-	-	0/0/0/0	0/0/0/0
4	SO4	A	346	-	-	0/0/0/0	0/0/0/0
2	NAD	B	343	-	-	0/22/62/62	0/5/5/5
2	NAD	C	343	-	-	0/22/62/62	0/5/5/5
3	GLY	C	345	-	-	0/0/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	343	-	-	0/22/62/62	0/5/5/5
3	GLY	D	345	-	-	0/0/2/2	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	343	NAD	O4B-C1B	-3.14	1.37	1.41
2	A	343	NAD	PA-O2A	-2.54	1.44	1.54
2	B	343	NAD	PN-O2N	-2.52	1.44	1.54
2	D	343	NAD	PN-O2N	-2.49	1.44	1.54
2	C	343	NAD	O4B-C1B	-2.47	1.38	1.41
2	C	343	NAD	PN-O2N	-2.44	1.44	1.54
2	A	343	NAD	PA-O1A	-2.14	1.43	1.51
2	D	343	NAD	C5A-N7A	-2.05	1.32	1.39
2	B	343	NAD	PA-O1A	-2.02	1.43	1.51
2	A	343	NAD	O5D-C5D	-2.00	1.36	1.44
2	A	343	NAD	C6N-N1N	2.09	1.41	1.35
2	D	343	NAD	C4N-C3N	2.21	1.43	1.39
2	B	343	NAD	C5B-C4B	2.21	1.58	1.51
2	A	343	NAD	O3B-C3B	2.25	1.48	1.43
2	B	343	NAD	C6N-N1N	2.37	1.41	1.35
2	A	343	NAD	O4D-C1D	2.54	1.44	1.41
2	D	343	NAD	C6N-N1N	3.47	1.44	1.35
2	C	343	NAD	C6N-N1N	3.48	1.44	1.35
2	B	343	NAD	O4D-C1D	4.03	1.46	1.41
2	B	343	NAD	O4B-C1B	4.32	1.46	1.41
2	A	343	NAD	O4B-C1B	6.08	1.48	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	343	NAD	N3A-C2A-N1A	-11.13	120.38	128.89
2	B	343	NAD	N3A-C2A-N1A	-9.47	121.64	128.89
2	D	343	NAD	N3A-C2A-N1A	-9.21	121.84	128.89
2	C	343	NAD	N3A-C2A-N1A	-7.83	122.90	128.89
2	A	343	NAD	C4B-O4B-C1B	-3.44	105.93	109.72
2	B	343	NAD	C4B-O4B-C1B	-3.31	106.08	109.72
2	D	343	NAD	C4A-C5A-N7A	-3.10	106.63	109.48
2	C	343	NAD	C3N-C7N-N7N	-2.86	114.68	117.82
2	D	343	NAD	C4B-O4B-C1B	-2.73	106.72	109.72
2	D	343	NAD	C3N-C7N-N7N	-2.59	114.98	117.82
2	C	343	NAD	O3-PN-O5D	-2.54	96.19	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	343	NAD	C2B-C1B-N9A	-2.53	110.43	114.29
2	C	343	NAD	C4B-O4B-C1B	-2.44	107.04	109.72
2	D	343	NAD	O3-PN-O5D	-2.35	96.71	102.94
2	B	343	NAD	C4A-C5A-N7A	-2.16	107.49	109.48
2	D	343	NAD	O4B-C1B-N9A	-2.15	103.59	108.10
2	A	343	NAD	C2B-C1B-N9A	-2.14	111.03	114.29
2	A	343	NAD	O7N-C7N-C3N	-2.13	117.26	119.59
2	A	343	NAD	O3-PA-O5B	-2.09	97.40	102.94
2	D	343	NAD	C2A-N1A-C6A	2.01	122.37	118.77
2	A	343	NAD	C2N-C3N-C4N	2.23	120.77	118.29
2	C	343	NAD	O7N-C7N-N7N	2.33	125.87	122.59
2	D	343	NAD	C2N-C3N-C4N	2.33	120.89	118.29
2	C	343	NAD	C2N-C3N-C4N	2.34	120.89	118.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	345	SO4	1	0
4	A	346	SO4	2	0
2	D	343	NAD	1	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 ⓘ

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	336/351 (95%)	-0.46	13 (3%) 43 42	14, 26, 82, 100	0
1	B	336/351 (95%)	-0.44	13 (3%) 43 42	14, 26, 81, 105	0
1	C	336/351 (95%)	-0.62	4 (1%) 81 80	17, 27, 50, 75	0
1	D	336/351 (95%)	-0.59	5 (1%) 76 75	17, 27, 51, 77	0
All	All	1344/1404 (95%)	-0.53	35 (2%) 59 59	14, 27, 69, 105	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	MET	8.9
1	C	2	MET	8.0
1	C	1	TYR	6.3
1	A	225	TYR	5.0
1	D	1	TYR	4.5
1	B	225	TYR	4.3
1	B	293	ILE	4.3
1	B	286	HIS	4.3
1	A	286	HIS	3.6
1	B	298	PHE	3.6
1	B	226	ILE	3.6
1	B	287	HIS	3.4
1	A	299	ARG	3.4
1	B	229	ASP	3.3
1	A	293	ILE	3.1
1	A	279	TYR	3.1
1	A	229	ASP	3.1
1	B	295	TYR	3.0
1	B	302	ASP	2.9
1	B	279	TYR	2.8
1	A	287	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	301	GLY	2.7
1	C	286	HIS	2.6
1	D	286	HIS	2.5
1	A	295	TYR	2.5
1	A	303	VAL	2.5
1	B	303	VAL	2.5
1	A	285	ILE	2.5
1	A	298	PHE	2.5
1	B	285	ILE	2.4
1	C	297	GLU	2.4
1	A	226	ILE	2.2
1	D	297	GLU	2.2
1	D	300	SER	2.2
1	A	302	ASP	2.2

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAD	A	343	44/44	0.98	0.09	0.07	12,20,38,44	0
2	NAD	D	343	44/44	0.98	0.09	0.04	15,22,44,46	0
2	NAD	C	343	44/44	0.98	0.09	-0.08	18,23,44,47	0
2	NAD	B	343	44/44	0.98	0.09	-0.40	15,20,39,44	0
5	UNL	D	344	25/-	0.98	0.09	-0.51	30,35,37,41	0
5	UNL	A	344	25/-	0.94	0.13	-0.55	33,66,79,80	0
5	UNL	B	344	25/-	0.94	0.12	-0.64	34,63,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	UNL	C	344	25/-	0.98	0.08	-0.75	28,34,37,38	0
4	SO4	A	346	5/5	1.00	0.09	-0.85	24,25,28,29	0
4	SO4	A	345	5/5	0.99	0.07	-1.18	26,28,29,29	0
3	GLY	D	345	5/5	0.87	0.13	-	49,50,50,51	0
3	GLY	C	345	5/5	0.84	0.14	-	56,56,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.