



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 01:59 PM EDT

PDB ID : 2HCT  
Title : Acidic residues at the active sites of CD38 and ADP-ribosyl cyclase determine NAAPD synthesis and hydrolysis activities  
Authors : Liu, Q.; Kriksunov, I.A.; Hao, Q.; Graeff, R.; Lee, H.C.  
Deposited on : 2006-06-18  
Resolution : 1.95 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

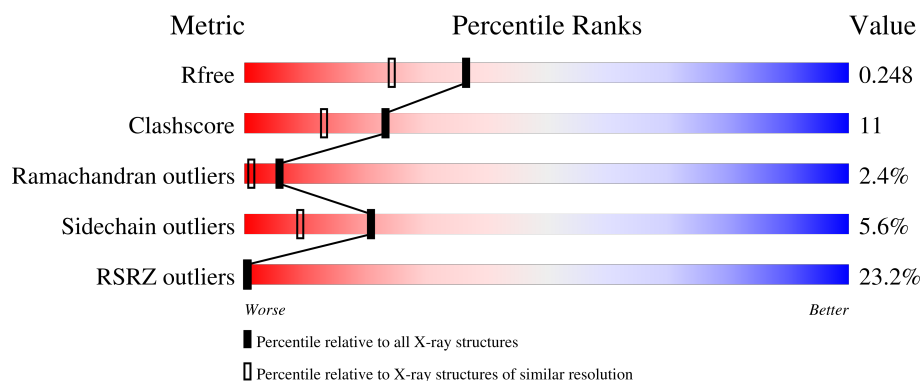
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	262	<div> <div>17%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>
1	B	262	<div> <div>28%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• • •</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4307 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.

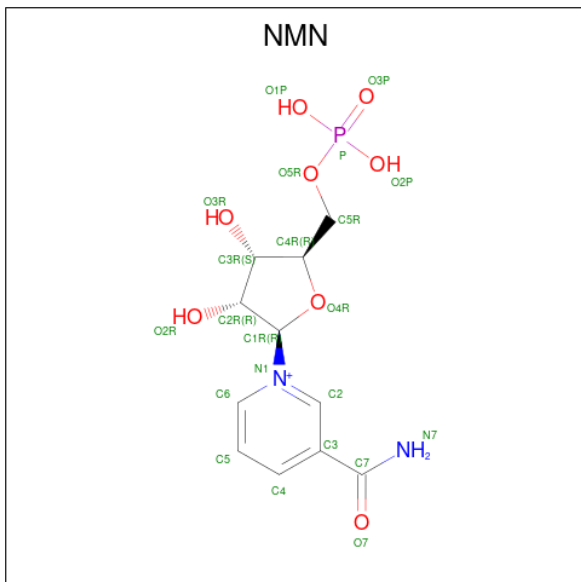
- Molecule 1 is a protein called ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2003	1263	351	373	16			
1	B	252	Total	C	N	O	S	0	0	0
			2003	1263	351	373	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LYS	-	cloning artifact	UNP P28907
A	40	ARG	-	cloning artifact	UNP P28907
A	41	GLU	-	cloning artifact	UNP P28907
A	42	ALA	-	cloning artifact	UNP P28907
A	43	GLU	-	cloning artifact	UNP P28907
A	44	ALA	-	cloning artifact	UNP P28907
A	49	THR	-	engineered mutation	UNP P28907
A	100	ASP	ASN	engineered mutation	UNP P28907
A	164	ASP	ASN	engineered mutation	UNP P28907
A	209	ASP	ASN	engineered mutation	UNP P28907
A	219	ASP	ASN	engineered mutation	UNP P28907
A	226	GLY	GLU	engineered mutation	UNP P28907
B	39	LYS	-	cloning artifact	UNP P28907
B	40	ARG	-	cloning artifact	UNP P28907
B	41	GLU	-	cloning artifact	UNP P28907
B	42	ALA	-	cloning artifact	UNP P28907
B	43	GLU	-	cloning artifact	UNP P28907
B	44	ALA	-	cloning artifact	UNP P28907
B	49	THR	GLN	engineered mutation	UNP P28907
B	100	ASP	ASN	engineered mutation	UNP P28907
B	164	ASP	ASN	engineered mutation	UNP P28907
B	209	ASP	ASN	engineered mutation	UNP P28907
B	219	ASP	ASN	engineered mutation	UNP P28907
B	226	GLY	GLU	engineered mutation	UNP P28907

- Molecule 2 is BETA-NICOTINAMIDE RIBOSE MONOPHOSPHATE (three-letter code: NMN) (formula:  $C_{11}H_{16}N_2O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

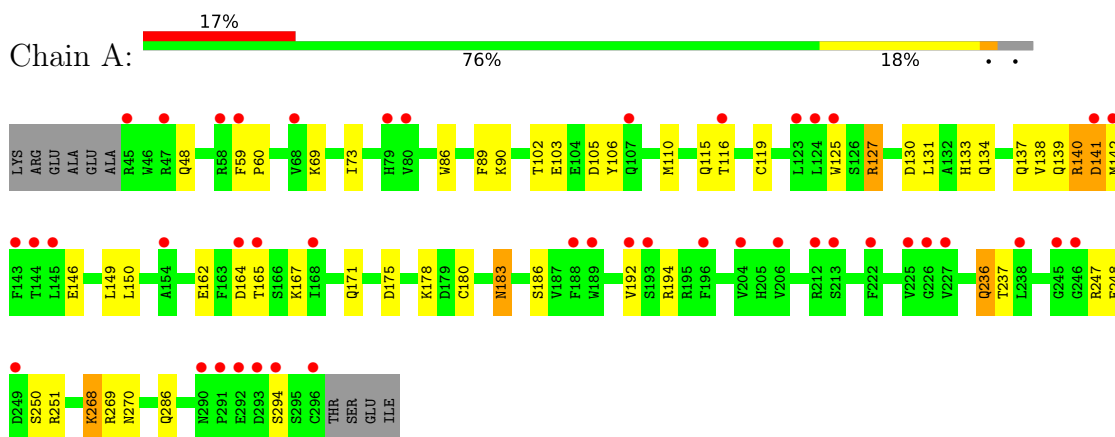
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	115	Total	O	0	0
			115	115		

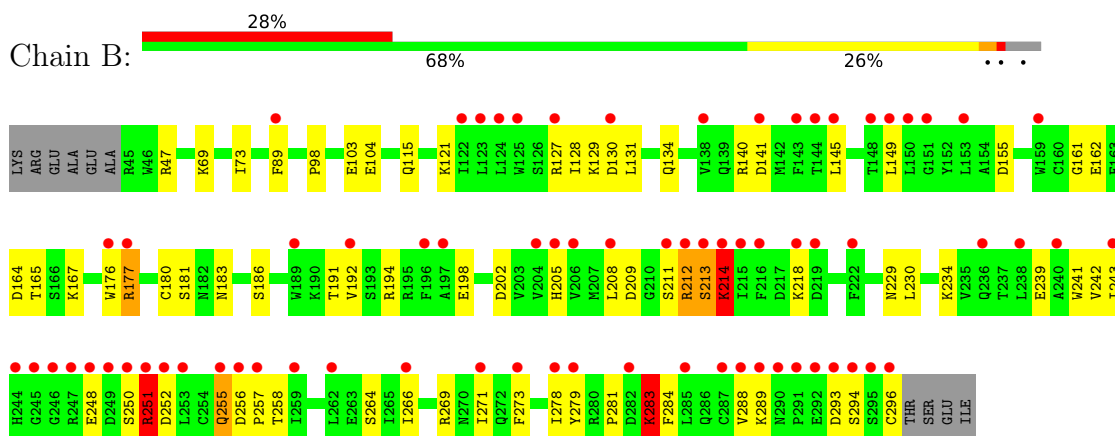
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: ADP-ribosyl cyclase 1



#### • Molecule 1: ADP-ribosyl cyclase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.72Å 52.82Å 65.58Å 106.26° 91.85° 95.25°	Depositor
Resolution (Å)	20.00 – 1.95 30.12 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.95) 96.0 (30.12-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.195 , 0.248 0.197 , 0.248	Depositor DCC
$R_{free}$ test set	1856 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4307	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NMN

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	0.66	0/2053	0.69	0/2778
1	B	0.73	4/2053 (0.2%)	0.66	0/2778
All	All	0.70	4/4106 (0.1%)	0.68	0/5556

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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	296	CYS	C-O	9.61	1.41	1.23
1	B	283	LYS	CE-NZ	8.13	1.69	1.49
1	B	214	LYS	CE-NZ	6.35	1.65	1.49
1	B	283	LYS	CD-CE	6.25	1.66	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	164	ASP	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	2003	0	1914	50	0
1	B	2003	0	1914	41	0
2	A	22	0	14	2	0
2	B	22	0	14	1	0
3	A	142	0	0	9	0
3	B	115	0	0	8	0
All	All	4307	0	3856	89	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 11.

All (89) 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:283:LYS:NZ	1:B:283:LYS:CE	1.69	1.53
1:B:266:ILE:HD11	1:B:273:PHE:HB2	1.26	1.16
1:A:103:GLU:OE1	1:A:194:ARG:NH2	1.77	1.14
1:A:268:LYS:HG2	3:B:409:HOH:O	1.65	0.97
1:A:250:SER:HB2	1:A:251:ARG:NH1	1.81	0.96
1:A:103:GLU:CD	1:A:194:ARG:HH22	1.72	0.92
1:A:115:GLN:HE22	1:A:149:LEU:H	1.16	0.90
1:A:268:LYS:CG	3:B:409:HOH:O	2.22	0.86
1:B:115:GLN:HE22	1:B:149:LEU:H	1.23	0.84
1:A:140:ARG:O	1:A:140:ARG:HG2	1.76	0.83
1:A:268:LYS:HD3	3:A:343:HOH:O	1.79	0.83
1:B:230:LEU:O	1:B:269:ARG:NH1	2.11	0.82
1:A:141:ASP:HB3	3:A:432:HOH:O	1.81	0.78
1:A:250:SER:HB2	1:A:251:ARG:HH12	1.48	0.78
1:A:142:MET:N	3:A:432:HOH:O	2.20	0.74
1:A:165:THR:HG23	1:A:167:LYS:H	1.53	0.74
1:A:162:GLU:HB2	1:A:165:THR:HG22	1.71	0.71
1:A:268:LYS:O	1:A:268:LYS:HD2	1.93	0.69
1:B:176:TRP:CZ3	1:B:181:SER:HB2	2.29	0.67
1:B:279:TYR:O	1:B:281:PRO:HD3	1.97	0.65
1:A:139:GLN:C	1:A:141:ASP:H	2.00	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:HA	3:A:415:HOH:O	1.99	0.63
1:A:110:MET:HE1	1:A:150:LEU:HD13	1.81	0.62
1:B:194:ARG:HG3	1:B:229:ASN:ND2	2.14	0.62
1:B:165:THR:HG23	1:B:167:LYS:H	1.66	0.60
1:B:266:ILE:HD11	1:B:273:PHE:CB	2.16	0.60
1:A:268:LYS:CD	3:A:343:HOH:O	2.44	0.58
1:B:183:ASN:ND2	1:B:186:SER:H	2.02	0.58
1:A:140:ARG:N	3:A:428:HOH:O	2.35	0.57
1:A:268:LYS:CE	3:B:409:HOH:O	2.52	0.57
1:A:268:LYS:O	1:A:268:LYS:CD	2.52	0.57
1:B:162:GLU:HB2	1:B:165:THR:HG22	1.85	0.57
1:A:130:ASP:O	1:A:134:GLN:HG3	2.06	0.56
1:B:69:LYS:HE2	1:B:73:ILE:HD11	1.87	0.56
1:A:133:HIS:O	1:A:137:GLN:HG2	2.07	0.55
1:B:103:GLU:HG2	1:B:191:THR:OG1	2.06	0.55
1:B:180:CYS:HB2	3:B:320:HOH:O	2.06	0.55
1:A:59:PHE:HB3	1:A:60:PRO:HD3	1.88	0.54
1:B:161:GLY:C	1:B:162:GLU:HG3	2.27	0.54
1:A:165:THR:HG21	1:A:167:LYS:HB2	1.89	0.54
1:A:183:ASN:ND2	1:A:186:SER:H	2.06	0.54
1:B:255:GLN:HE21	1:B:255:GLN:HA	1.73	0.53
1:B:194:ARG:O	1:B:198:GLU:HG3	2.09	0.52
1:B:202:ASP:HB3	3:B:324:HOH:O	2.09	0.51
1:B:250:SER:HB2	1:B:251:ARG:HE	1.75	0.51
1:A:138:VAL:HA	3:A:340:HOH:O	2.11	0.51
1:A:102:THR:HG22	1:B:177:ARG:NH2	2.26	0.50
1:A:268:LYS:HE2	3:B:409:HOH:O	2.10	0.50
1:B:129:LYS:NZ	1:B:155:ASP:OD2	2.34	0.50
1:A:139:GLN:C	1:A:141:ASP:N	2.65	0.49
1:B:194:ARG:HB3	1:B:194:ARG:NH1	2.27	0.49
1:B:212:ARG:C	1:B:214:LYS:H	2.16	0.49
1:A:139:GLN:O	1:A:141:ASP:N	2.47	0.48
1:A:115:GLN:NE2	1:A:149:LEU:H	1.98	0.48
1:A:250:SER:CB	1:A:251:ARG:HH12	2.23	0.48
1:A:269:ARG:O	1:A:270:ASN:HB2	2.13	0.48
1:B:284:PHE:O	1:B:288:VAL:HG23	2.14	0.47
1:A:125:TRP:CZ2	2:A:301:NMN:H2RC	2.50	0.47
1:A:236:GLN:HG3	1:A:237:THR:OG1	2.15	0.46
1:A:106:TYR:O	1:A:110:MET:HG2	2.14	0.46
1:B:98:PRO:O	1:B:183:ASN:HA	2.14	0.46
1:A:119:CYS:HB3	3:A:384:HOH:O	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ARG:HD2	3:B:375:HOH:O	2.16	0.46
1:B:250:SER:C	1:B:251:ARG:HG3	2.36	0.46
1:A:180:CYS:HB2	3:A:327:HOH:O	2.17	0.45
1:A:165:THR:CG2	1:A:167:LYS:HB2	2.46	0.45
1:B:183:ASN:HD21	1:B:186:SER:H	1.65	0.45
1:B:211:SER:O	1:B:212:ARG:HB2	2.17	0.45
1:A:110:MET:HE1	1:A:192:VAL:HG12	1.98	0.45
1:B:145:LEU:HD21	1:B:192:VAL:HG23	1.99	0.44
1:B:208:LEU:O	1:B:243:ILE:HG12	2.18	0.44
1:B:241:TRP:HB3	1:B:278:ILE:CD1	2.49	0.43
1:A:115:GLN:HE22	1:A:149:LEU:N	1.99	0.42
1:B:145:LEU:HB3	2:B:302:NMN:O2R	2.19	0.42
1:B:104:GLU:HG3	3:B:380:HOH:O	2.19	0.42
1:A:102:THR:O	1:A:105:ASP:HB2	2.19	0.42
1:A:146:GLU:OE2	2:A:301:NMN:HC2	2.20	0.42
1:B:256:ASP:HA	1:B:257:PRO:HD2	1.84	0.42
1:B:127:ARG:O	1:B:209:ASP:HB2	2.20	0.42
1:A:175:ASP:OD1	1:A:178:LYS:HG3	2.20	0.41
1:A:86:TRP:CE2	1:A:90:LYS:HG3	2.56	0.41
1:A:102:THR:CG2	1:B:177:ARG:HH21	2.34	0.41
1:B:130:ASP:O	1:B:134:GLN:HG3	2.20	0.41
1:A:286:GLN:NE2	1:A:286:GLN:HA	2.36	0.41
1:B:205:HIS:HA	1:B:239:GLU:O	2.21	0.41
1:B:266:ILE:HD12	1:B:271:ILE:O	2.21	0.40
1:B:121:LYS:HB3	1:B:141:ASP:O	2.22	0.40
1:A:48:GLN:OE1	1:A:171:GLN:HB3	2.22	0.40
1:A:69:LYS:O	1:A:73:ILE:HG12	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	250/262 (95%)	234 (94%)	12 (5%)	4 (2%)	9	2
1	B	250/262 (95%)	230 (92%)	12 (5%)	8 (3%)	4	0
All	All	500/524 (95%)	464 (93%)	24 (5%)	12 (2%)	6	1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	GLU
1	B	128	ILE
1	B	212	ARG
1	B	251	ARG
1	B	293	ASP
1	B	294	SER
1	B	252	ASP
1	A	140	ARG
1	A	247	ARG
1	A	294	SER
1	B	213	SER
1	B	248	GLU

### 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	222/240 (92%)	213 (96%)	9 (4%)	30	18
1	B	222/240 (92%)	206 (93%)	16 (7%)	14	4
All	All	444/480 (92%)	419 (94%)	25 (6%)	21	9

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	PHE
1	A	116	THR
1	A	127	ARG
1	A	131	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	141	ASP
1	A	164	ASP
1	A	183	ASN
1	A	236	GLN
1	A	268	LYS
1	B	47	ARG
1	B	89	PHE
1	B	131	LEU
1	B	140	ARG
1	B	177	ARG
1	B	213	SER
1	B	214	LYS
1	B	218	LYS
1	B	234	LYS
1	B	242	VAL
1	B	251	ARG
1	B	255	GLN
1	B	258	THR
1	B	264	SER
1	B	283	LYS
1	B	289	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	183	ASN
1	A	244	HIS
1	A	270	ASN
1	A	286	GLN
1	B	115	GLN
1	B	183	ASN
1	B	205	HIS
1	B	229	ASN
1	B	255	GLN
1	B	270	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NMN	A	301	-	22,23,23	0.95	0	30,34,34	1.50	5 (16%)
2	NMN	B	302	-	22,23,23	0.76	1 (4%)	30,34,34	1.54	3 (10%)

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	NMN	A	301	-	-	4/14/30/30	0/2/2/2
2	NMN	B	302	-	-	2/14/30/30	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	NMN	O4R-C1R	2.08	1.44	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	NMN	C3R-C2R-C1R	4.56	107.84	100.98
2	A	301	NMN	C3R-C2R-C1R	4.41	107.62	100.98
2	B	302	NMN	C6-N1-C2	-4.00	118.33	121.97
2	A	301	NMN	C6-N1-C2	-2.60	119.61	121.97
2	A	301	NMN	O4R-C1R-C2R	-2.35	103.50	106.93
2	B	302	NMN	O4R-C1R-C2R	-2.31	103.55	106.93
2	A	301	NMN	O1P-P-O5R	-2.08	101.19	106.73
2	A	301	NMN	O5R-C5R-C4R	2.07	116.10	108.99

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	302	NMN	C2R-C1R-N1-C2
2	B	302	NMN	C2R-C1R-N1-C6
2	A	301	NMN	C3R-C4R-C5R-O5R
2	A	301	NMN	O4R-C4R-C5R-O5R
2	A	301	NMN	C2R-C1R-N1-C2
2	A	301	NMN	C2R-C1R-N1-C6

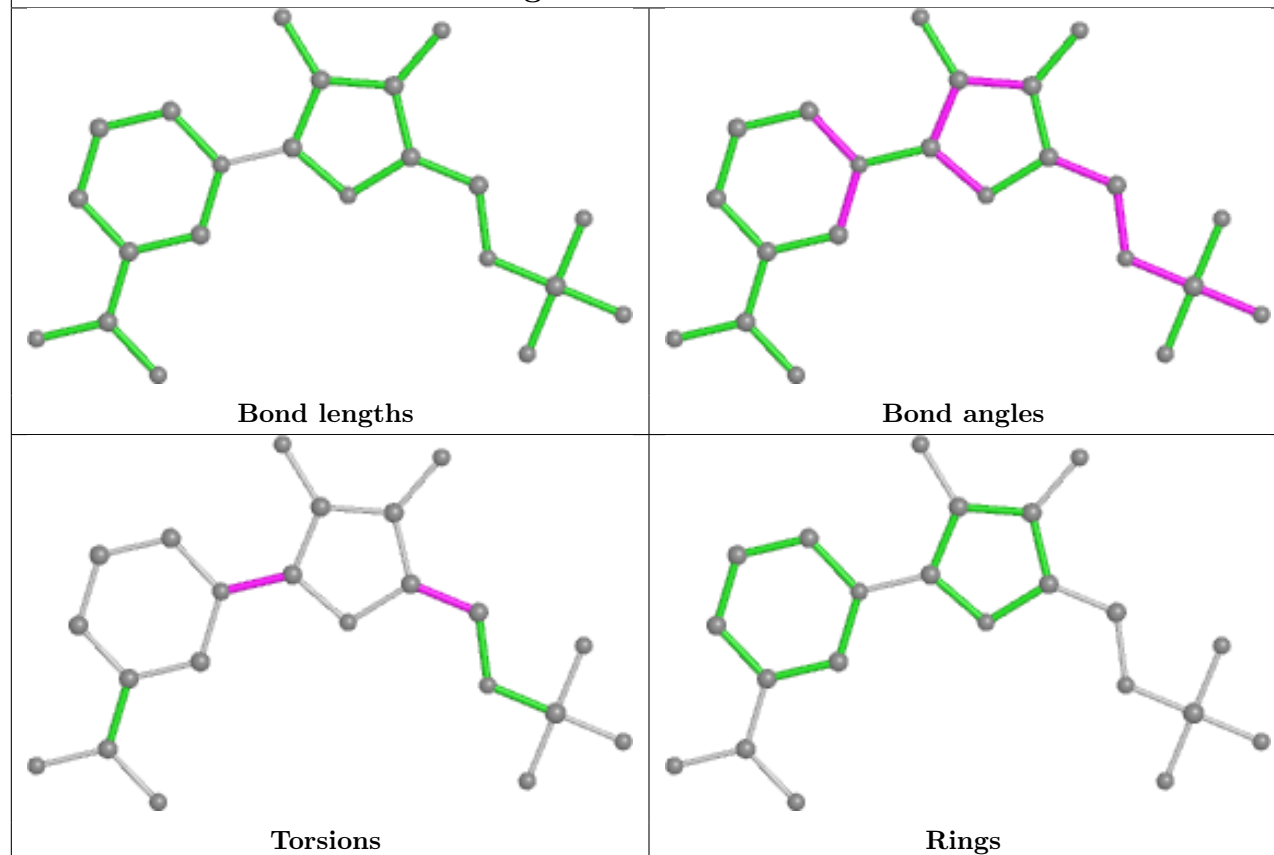
There are no ring outliers.

2 monomers are involved in 3 short contacts:

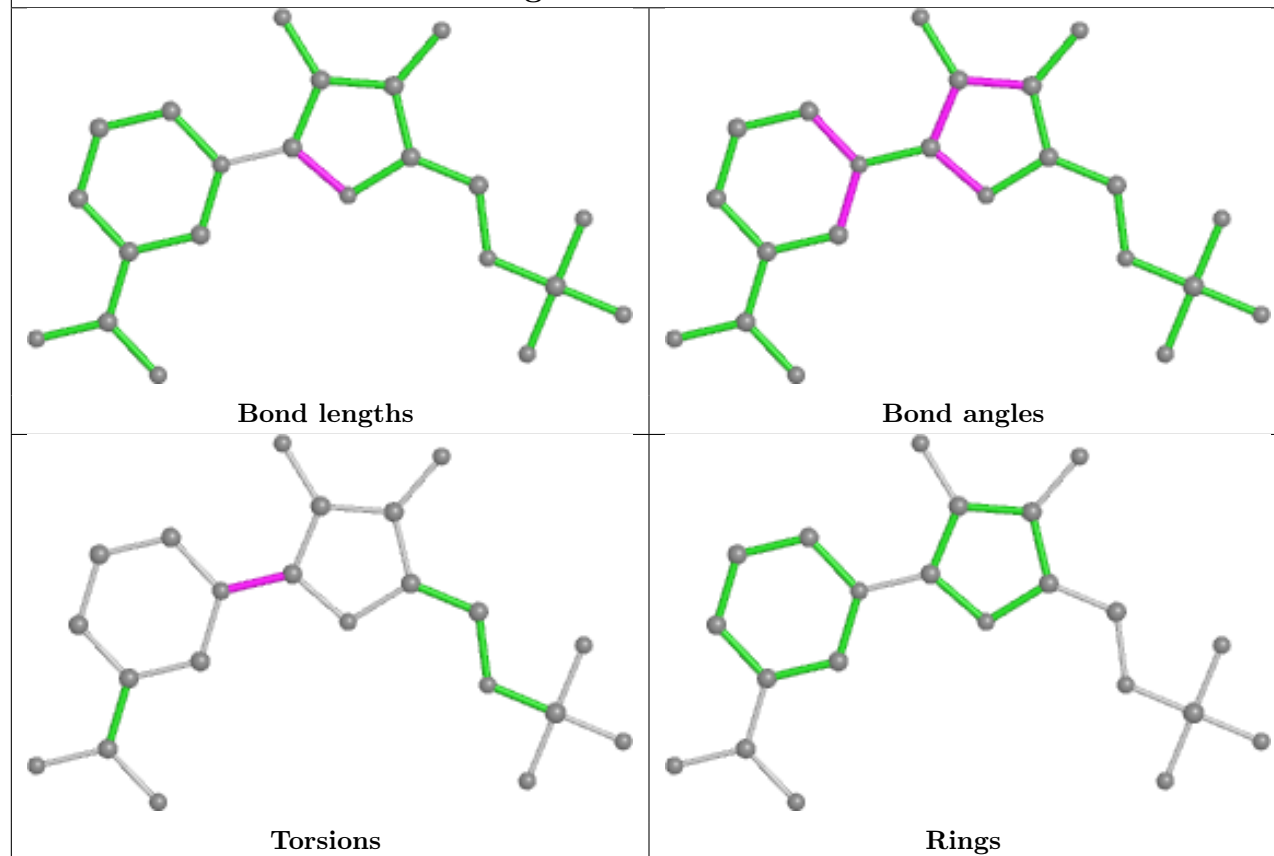
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NMN	2	0
2	B	302	NMN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand NMN A 301



## Ligand NMN B 302



## 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	252/262 (96%)	1.08	44 (17%) <b>1</b> <b>1</b>	35, 42, 56, 62	0
1	B	252/262 (96%)	1.58	73 (28%) <b>0</b> <b>0</b>	31, 44, 60, 70	0
All	All	504/524 (96%)	1.33	117 (23%) <b>0</b> <b>0</b>	31, 43, 58, 70	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	ASP	14.4
1	B	246	GLY	12.8
1	B	213	SER	10.7
1	B	296	CYS	8.5
1	B	211	SER	6.9
1	B	292	GLU	6.6
1	B	212	ARG	6.2
1	B	294	SER	6.1
1	B	124	LEU	6.0
1	B	288	VAL	5.8
1	B	295	SER	5.6
1	A	246	GLY	5.5
1	B	293	ASP	5.2
1	B	216	PHE	5.1
1	A	124	LEU	4.9
1	A	245	GLY	4.9
1	B	215	ILE	4.7
1	A	47	ARG	4.7
1	A	291	PRO	4.7
1	B	250	SER	4.7
1	A	212	ARG	4.7
1	B	123	LEU	4.6
1	B	287	CYS	4.6
1	A	213	SER	4.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	214	LYS	4.5
1	B	282	ASP	4.5
1	B	208	LEU	4.5
1	B	222	PHE	4.3
1	B	257	PRO	4.1
1	B	176	TRP	4.1
1	A	79	HIS	4.1
1	B	145	LEU	4.0
1	B	247	ARG	4.0
1	B	245	GLY	3.9
1	A	123	LEU	3.8
1	B	127	ARG	3.8
1	A	145	LEU	3.8
1	B	259	ILE	3.7
1	B	150	LEU	3.7
1	A	189	TRP	3.6
1	B	206	VAL	3.6
1	B	289	LYS	3.6
1	B	219	ASP	3.5
1	B	253	LEU	3.5
1	B	204	VAL	3.4
1	B	266	ILE	3.4
1	B	279	TYR	3.4
1	A	294	SER	3.4
1	A	293	ASP	3.4
1	B	144	THR	3.3
1	B	256	ASP	3.3
1	A	196	PHE	3.2
1	B	149	LEU	3.2
1	B	238	LEU	3.2
1	A	165	THR	3.2
1	B	218	LYS	3.2
1	A	164	ASP	3.2
1	A	68	VAL	3.1
1	B	138	VAL	3.1
1	A	107	GLN	3.1
1	B	89	PHE	3.0
1	B	125	TRP	3.0
1	B	189	TRP	3.0
1	B	240	ALA	3.0
1	A	144	THR	2.9
1	A	58	ARG	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	122	ILE	2.9
1	B	192	VAL	2.8
1	B	262	LEU	2.8
1	A	206	VAL	2.8
1	A	143	PHE	2.8
1	A	192	VAL	2.8
1	A	227	VAL	2.8
1	B	285	LEU	2.7
1	B	252	ASP	2.7
1	A	193	SER	2.7
1	B	243	ILE	2.6
1	B	255	GLN	2.6
1	B	205	HIS	2.6
1	B	153	LEU	2.6
1	A	238	LEU	2.5
1	B	148	THR	2.5
1	B	278	ILE	2.5
1	B	248	GLU	2.5
1	A	296	CYS	2.5
1	A	141	ASP	2.5
1	B	141	ASP	2.5
1	B	244	HIS	2.5
1	B	143	PHE	2.5
1	A	222	PHE	2.4
1	A	142	MET	2.4
1	B	130	ASP	2.3
1	B	290	ASN	2.3
1	B	196	PHE	2.3
1	A	290	ASN	2.3
1	B	236	GLN	2.3
1	A	168	ILE	2.3
1	B	197	ALA	2.3
1	A	45	ARG	2.3
1	A	226	GLY	2.3
1	A	80	VAL	2.3
1	B	177	ARG	2.3
1	B	249	ASP	2.3
1	A	188	PHE	2.2
1	B	273	PHE	2.2
1	B	151	GLY	2.2
1	A	125	TRP	2.2
1	A	59	PHE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	292	GLU	2.1
1	A	204	VAL	2.1
1	A	116	THR	2.1
1	B	271	ILE	2.1
1	B	251	ARG	2.1
1	A	225	VAL	2.0
1	B	291	PRO	2.0
1	A	154	ALA	2.0
1	B	159	TRP	2.0

## 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

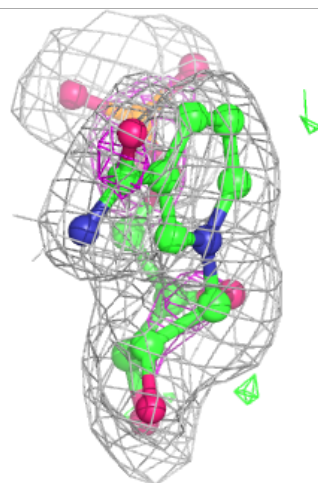
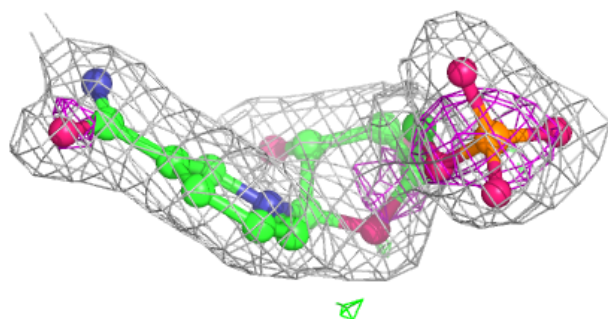
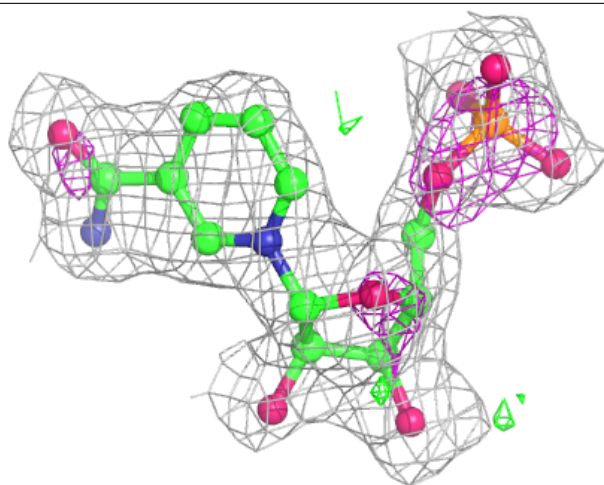
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NMN	B	302	22/22	0.85	0.14	44,53,66,66	0
2	NMN	A	301	22/22	0.86	0.16	45,58,60,61	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

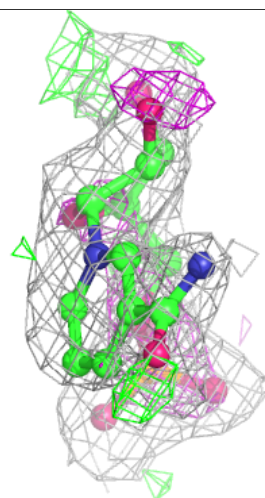
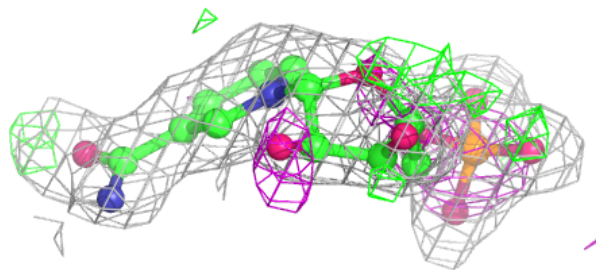
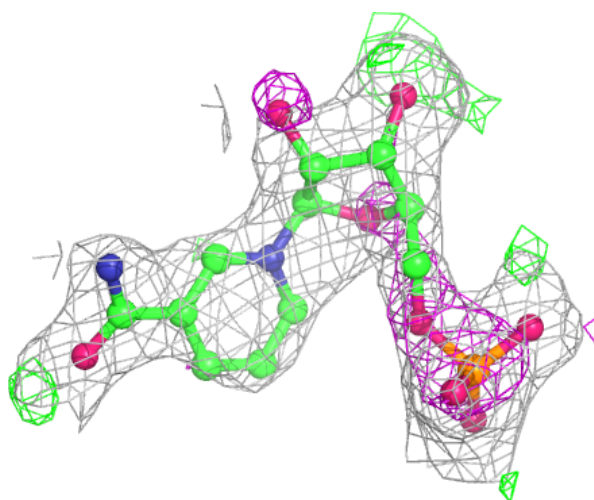
**Electron density around NMN B 302:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around NMN A 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.