Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:16 AM GMT

PDB ID	:	3DZK
Title	:	Crystal structure of human CD38 extracellular domain, NMN complex
Authors	:	Liu, Q.; Kriksunov, I.A.; Jiang, H.; Graeff, R.; Lin, H.; Lee, H.C.; Hao, Q.
Deposited on	:	2008-07-29
Resolution	:	1.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

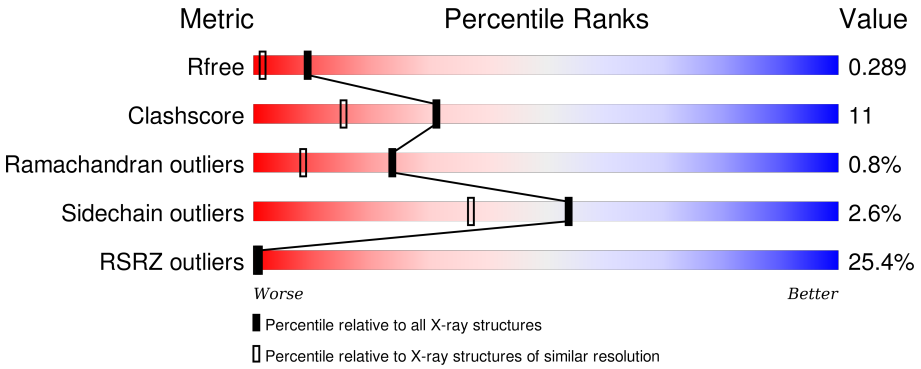
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	5422 (1.84-1.80)
Clashscore	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)
RSRZ outliers	91569	5439 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	22% 78% 17%
1	B	262	27% 76% 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4498 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.

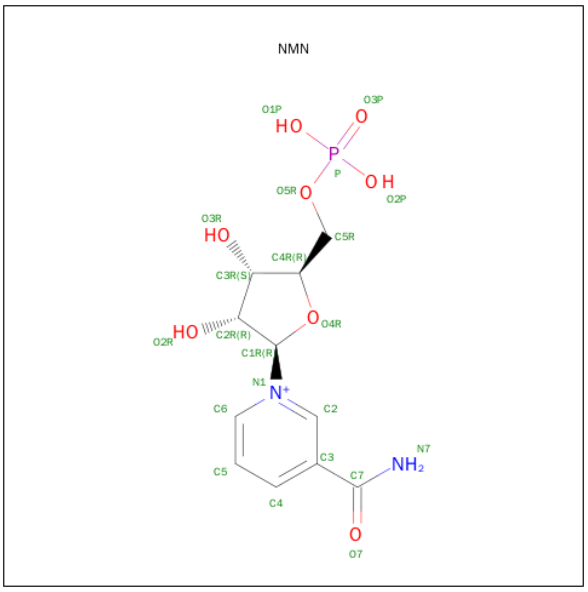
- Molecule 1 is a protein called ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	B	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LYS	-	EXPRESSION TAG	UNP P28907
A	40	ARG	-	EXPRESSION TAG	UNP P28907
A	41	GLU	-	EXPRESSION TAG	UNP P28907
A	42	ALA	-	EXPRESSION TAG	UNP P28907
A	43	GLU	-	EXPRESSION TAG	UNP P28907
A	44	ALA	-	EXPRESSION TAG	UNP P28907
A	49	THR	GLN	ENGINEERED	UNP P28907
A	100	ASP	ASN	ENGINEERED	UNP P28907
A	164	ASP	ASN	ENGINEERED	UNP P28907
A	209	ASP	ASN	ENGINEERED	UNP P28907
A	219	ASP	ASN	ENGINEERED	UNP P28907
B	39	LYS	-	EXPRESSION TAG	UNP P28907
B	40	ARG	-	EXPRESSION TAG	UNP P28907
B	41	GLU	-	EXPRESSION TAG	UNP P28907
B	42	ALA	-	EXPRESSION TAG	UNP P28907
B	43	GLU	-	EXPRESSION TAG	UNP P28907
B	44	ALA	-	EXPRESSION TAG	UNP P28907
B	49	THR	GLN	ENGINEERED	UNP P28907
B	100	ASP	ASN	ENGINEERED	UNP P28907
B	164	ASP	ASN	ENGINEERED	UNP P28907
B	209	ASP	ASN	ENGINEERED	UNP P28907
B	219	ASP	ASN	ENGINEERED	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.

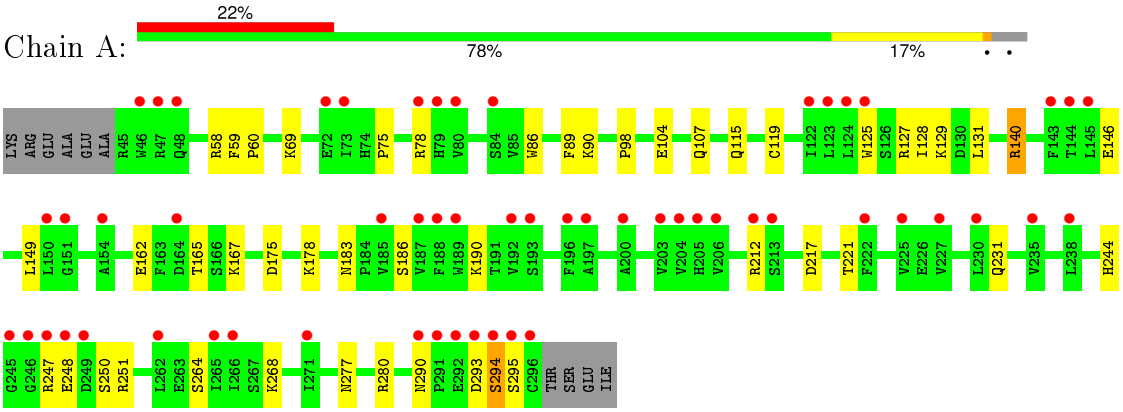
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	174	Total	O	0	0
			174	174		
3	B	180	Total	O	0	0
			180	180		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

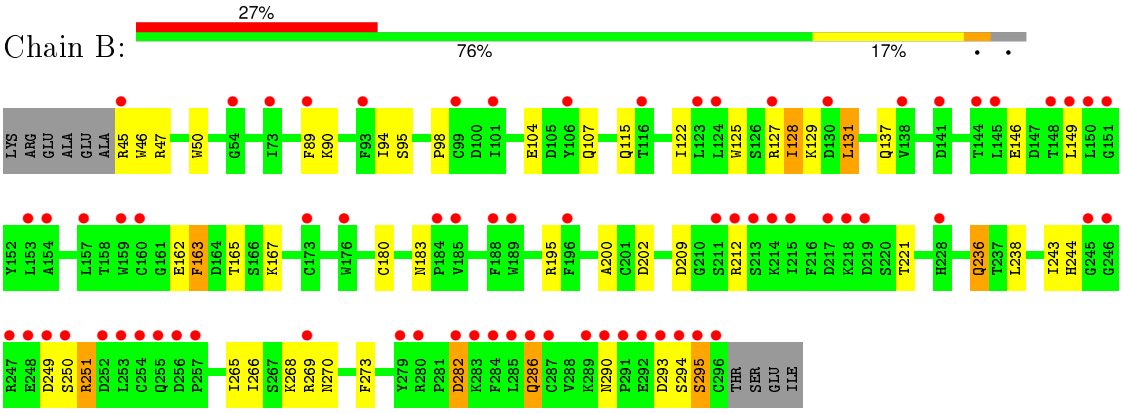
- Molecule 1: ADP-ribosyl cyclase 1

Chain A:



- Molecule 1: ADP-ribosyl cyclase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.89Å 53.20Å 65.60Å 106.20° 91.84° 95.05°	Depositor
Resolution (Å)	20.00 – 1.81 28.25 – 1.81	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.81) 87.5 (28.25-1.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.3.0021	Depositor
R, R_{free}	0.174 , 0.217 0.264 , 0.289	Depositor DCC
R_{free} test set	2383 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 47142 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4498	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.76	0/2101	0.73	0/2846
1	B	0.73	1/2101 (0.0%)	0.67	0/2846
All	All	0.74	1/4202 (0.0%)	0.70	0/5692

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	PHE	CB-CG	-5.07	1.42	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2050	0	1976	37	0
1	B	2050	0	1976	55	0
2	A	22	0	14	2	0
2	B	22	0	14	2	0
3	A	174	0	0	7	0
3	B	180	0	0	7	0
All	All	4498	0	3980	88	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 (88) 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:165:THR:HG23	1:B:167:LYS:H	1.20	1.02
1:A:231:GLN:HG3	3:A:469:HOH:O	1.67	0.93
1:B:137:GLN:HG2	3:B:647:HOH:O	1.70	0.90
1:A:165:THR:HG23	1:A:167:LYS:H	1.38	0.86
1:B:115:GLN:HE22	1:B:149:LEU:H	1.23	0.85
1:A:115:GLN:HE22	1:A:149:LEU:H	1.27	0.82
1:A:268:LYS:HD3	1:B:163:PHE:HE1	1.45	0.81
1:B:195:ARG:HD2	3:B:639:HOH:O	1.81	0.80
1:B:269:ARG:HG3	3:B:642:HOH:O	1.83	0.79
1:B:266:ILE:HD11	1:B:273:PHE:HB2	1.70	0.73
1:A:268:LYS:HD3	1:B:163:PHE:CE1	2.23	0.72
1:B:290:ASN:HB3	1:B:293:ASP:HB2	1.75	0.67
1:A:127:ARG:HB3	1:A:212:ARG:HE	1.59	0.67
1:B:127:ARG:CG	1:B:212:ARG:HH12	2.08	0.66
1:B:244:HIS:CD2	1:B:250:SER:HB3	2.32	0.65
1:B:127:ARG:HG2	1:B:212:ARG:HH12	1.63	0.63
1:A:175:ASP:OD1	1:A:178:LYS:HG3	1.97	0.63
1:B:238:LEU:HB3	1:B:266:ILE:HD13	1.81	0.63
1:B:202:ASP:HB3	3:B:519:HOH:O	1.98	0.62
1:B:221:THR:HG21	2:B:301:NMN:HC6	1.81	0.62
1:B:162:GLU:HB2	1:B:165:THR:HG22	1.82	0.60
1:A:127:ARG:HB3	1:A:212:ARG:NE	2.17	0.60
1:B:266:ILE:HD11	1:B:273:PHE:CB	2.31	0.59
1:A:294:SER:O	1:A:295:SER:OG	2.16	0.59
1:A:119:CYS:HB3	3:A:341:HOH:O	2.03	0.59
1:A:183:ASN:ND2	1:A:186:SER:H	2.01	0.58
1:A:221:THR:HG21	2:A:301:NMN:HC6	1.86	0.58
1:A:248:GLU:HA	1:A:280:ARG:NH2	2.19	0.57
1:B:127:ARG:HB3	1:B:212:ARG:NH1	2.18	0.57
1:A:247:ARG:HG2	1:A:248:GLU:HG3	1.88	0.56
1:A:290:ASN:HB3	3:A:360:HOH:O	2.06	0.56
1:B:244:HIS:HD2	1:B:250:SER:HB3	1.71	0.55
1:A:75:PRO:HA	1:A:78:ARG:HG3	1.89	0.54
1:B:146:GLU:OE2	2:B:301:NMN:HC2	2.07	0.54
1:B:244:HIS:HD2	1:B:250:SER:CB	2.20	0.54
1:B:45:ARG:HG3	1:B:46:TRP:H	1.72	0.54
1:B:127:ARG:HG2	1:B:212:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PHE:HB3	1:A:60:PRO:HD3	1.90	0.53
1:A:125:TRP:CH2	1:A:129:LYS:HB3	2.43	0.53
1:A:127:ARG:NH1	1:A:217:ASP:OD2	2.41	0.53
1:A:140:ARG:NH2	3:A:456:HOH:O	2.43	0.52
1:B:268:LYS:HB3	1:B:269:ARG:HH21	1.74	0.52
1:B:45:ARG:HG3	1:B:46:TRP:N	2.24	0.52
1:B:127:ARG:HB3	1:B:212:ARG:HH12	1.73	0.52
1:A:162:GLU:HB2	1:A:165:THR:HG22	1.91	0.52
1:B:122:ILE:HD12	1:B:200:ALA:HA	1.91	0.51
1:B:251:ARG:H	1:B:251:ARG:HD3	1.74	0.51
1:B:282:ASP:OD2	1:B:282:ASP:N	2.42	0.50
1:A:183:ASN:HD21	1:A:186:SER:H	1.58	0.50
1:B:286:GLN:HE21	1:B:286:GLN:HA	1.75	0.50
1:A:244:HIS:HD2	1:A:250:SER:HB3	1.77	0.50
1:B:125:TRP:CH2	1:B:129:LYS:HB3	2.47	0.49
1:A:244:HIS:HE1	1:A:277:ASN:OD1	1.95	0.49
1:B:90:LYS:HG3	1:B:94:ILE:HG13	1.95	0.48
1:B:209:ASP:OD2	1:B:212:ARG:HG2	2.13	0.48
1:A:264:SER:HG	1:B:163:PHE:HZ	1.56	0.48
1:B:115:GLN:NE2	1:B:149:LEU:H	2.03	0.48
1:B:127:ARG:CB	1:B:212:ARG:HH12	2.26	0.47
1:B:282:ASP:O	1:B:286:GLN:HG2	2.15	0.47
1:B:125:TRP:CZ3	1:B:129:LYS:HB3	2.50	0.47
1:B:265:ILE:O	1:B:269:ARG:HG2	2.15	0.47
1:A:86:TRP:CZ2	1:A:90:LYS:HG3	2.50	0.46
1:B:195:ARG:CD	3:B:639:HOH:O	2.50	0.46
1:B:98:PRO:O	1:B:183:ASN:HA	2.14	0.46
1:B:104:GLU:HA	1:B:107:GLN:HG2	1.99	0.45
1:B:180:CYS:HB2	3:B:491:HOH:O	2.17	0.45
1:B:266:ILE:HD11	1:B:273:PHE:CA	2.47	0.44
1:A:264:SER:OG	1:B:163:PHE:HZ	2.00	0.44
1:A:290:ASN:O	1:A:293:ASP:HB2	2.18	0.43
1:B:94:ILE:HD12	1:B:94:ILE:HG23	1.75	0.43
1:B:131:LEU:HD12	1:B:243:ILE:HG21	2.01	0.43
1:B:50:TRP:CZ2	1:B:98:PRO:HG2	2.53	0.43
1:A:293:ASP:O	1:A:294:SER:HB3	2.19	0.43
1:B:268:LYS:HB3	1:B:269:ARG:NH2	2.34	0.43
1:B:212:ARG:HA	1:B:212:ARG:HD3	1.90	0.43
1:A:104:GLU:HA	1:A:107:GLN:HG2	2.01	0.42
1:B:46:TRP:CD1	1:B:47:ARG:HG3	2.54	0.42
1:A:251:ARG:HD3	1:A:251:ARG:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PRO:O	1:A:183:ASN:HA	2.19	0.42
1:A:244:HIS:CD2	1:A:250:SER:HB3	2.54	0.42
1:A:190:LYS:NZ	3:A:386:HOH:O	2.52	0.42
1:A:231:GLN:CG	3:A:469:HOH:O	2.42	0.42
1:B:94:ILE:O	1:B:95:SER:HB2	2.20	0.42
1:A:69:LYS:HD3	3:A:368:HOH:O	2.18	0.41
1:B:236:GLN:HG3	3:B:570:HOH:O	2.19	0.41
1:B:294:SER:O	1:B:295:SER:C	2.59	0.41
1:B:128:ILE:HB	1:B:209:ASP:HB2	2.01	0.41
1:A:146:GLU:OE2	2:A:301:NMN:HC2	2.22	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	250/262 (95%)	238 (95%)	10 (4%)	2 (1%)	24	8
1	B	250/262 (95%)	240 (96%)	8 (3%)	2 (1%)	24	8
All	All	500/524 (95%)	478 (96%)	18 (4%)	4 (1%)	24	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	295	SER
1	A	294	SER
1	A	128	ILE
1	B	128	ILE

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	233/241 (97%)	229 (98%)	4 (2%)	68 57
1	B	233/241 (97%)	225 (97%)	8 (3%)	44 26
All	All	466/482 (97%)	454 (97%)	12 (3%)	54 37

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	89	PHE
1	A	131	LEU
1	A	140	ARG
1	B	89	PHE
1	B	131	LEU
1	B	236	GLN
1	B	249	ASP
1	B	251	ARG
1	B	270	ASN
1	B	282	ASP
1	B	286	GLN

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

Mol	Chain	Res	Type
1	A	48	GLN
1	A	115	GLN
1	A	134	GLN
1	A	139	GLN
1	A	183	ASN
1	A	244	HIS
1	A	290	ASN
1	B	115	GLN
1	B	134	GLN
1	B	229	ASN

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Mol	Chain	Res	Type
1	B	244	HIS
1	B	270	ASN
1	B	286	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NMN	A	301	-	20,23,23	0.77	1 (5%)	26,34,34	1.83	8 (30%)
2	NMN	B	301	-	20,23,23	0.87	1 (5%)	26,34,34	2.11	9 (34%)

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	-	-	0/10/30/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NMN	B	301	-	-	0/10/30/30	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NMN	C2-C3	2.25	1.42	1.39
2	B	301	NMN	O4R-C1R	2.83	1.44	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	NMN	O7-C7-C3	-4.23	114.97	119.59
2	B	301	NMN	O4R-C1R-N1	-3.92	103.82	108.13
2	A	301	NMN	O2R-C2R-C3R	-2.73	102.96	111.83
2	A	301	NMN	O7-C7-C3	-2.52	116.83	119.59
2	B	301	NMN	C4-C3-C7	-2.37	114.82	121.09
2	A	301	NMN	C4-C3-C7	-2.31	114.98	121.09
2	A	301	NMN	O4R-C1R-N1	-2.22	105.69	108.13
2	B	301	NMN	O2R-C2R-C3R	-2.21	104.64	111.83
2	A	301	NMN	O3R-C3R-C4R	-2.20	104.45	111.05
2	B	301	NMN	O2P-P-O1P	2.05	115.17	107.38
2	B	301	NMN	C5-C6-N1	2.05	124.03	120.47
2	B	301	NMN	C2R-C3R-C4R	2.07	106.87	102.61
2	A	301	NMN	C2-C3-C7	2.11	125.45	119.31
2	B	301	NMN	C2-C3-C7	2.16	125.58	119.31
2	A	301	NMN	O2P-P-O1P	2.19	115.73	107.38
2	A	301	NMN	C3-C7-N7	5.08	123.37	117.82
2	B	301	NMN	C3-C7-N7	5.97	124.35	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

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^{th} 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^2)	Q<0.9
1	A	252/262 (96%)	1.20	57 (22%) 1 1	24, 31, 41, 49	0
1	B	252/262 (96%)	1.46	71 (28%) 1 0	25, 31, 39, 44	0
All	All	504/524 (96%)	1.33	128 (25%) 1 0	24, 31, 40, 49	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	GLY	11.4
1	B	249	ASP	7.5
1	A	292	GLU	7.4
1	B	295	SER	7.3
1	B	245	GLY	7.2
1	A	249	ASP	7.2
1	B	293	ASP	7.1
1	B	294	SER	6.9
1	A	293	ASP	6.9
1	B	247	ARG	6.9
1	B	296	CYS	6.6
1	A	248	GLU	6.3
1	B	248	GLU	5.7
1	B	292	GLU	5.6
1	A	294	SER	5.6
1	B	291	PRO	5.2
1	B	287	CYS	5.1
1	A	47	ARG	4.9
1	B	290	ASN	4.7
1	B	211	SER	4.6
1	A	124	LEU	4.5
1	A	246	GLY	4.5
1	B	213	SER	4.4
1	B	189	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	123	LEU	4.0
1	A	145	LEU	4.0
1	A	296	CYS	3.9
1	A	206	VAL	3.9
1	B	286	GLN	3.8
1	A	73	ILE	3.8
1	A	204	VAL	3.8
1	B	153	LEU	3.8
1	B	250	SER	3.8
1	B	188	PHE	3.7
1	A	227	VAL	3.7
1	A	164	ASP	3.6
1	A	245	GLY	3.6
1	A	189	TRP	3.5
1	B	145	LEU	3.5
1	A	225	VAL	3.5
1	A	222	PHE	3.5
1	B	219	ASP	3.5
1	B	154	ALA	3.4
1	B	159	TRP	3.4
1	B	141	ASP	3.4
1	B	252	ASP	3.4
1	B	285	LEU	3.4
1	B	151	GLY	3.3
1	B	269	ARG	3.3
1	A	295	SER	3.3
1	A	46	TRP	3.3
1	A	78	ARG	3.3
1	B	212	ARG	3.3
1	A	196	PHE	3.2
1	B	127	ARG	3.2
1	B	176	TRP	3.2
1	A	238	LEU	3.1
1	B	280	ARG	3.1
1	A	48	GLN	3.1
1	A	80	VAL	3.1
1	B	150	LEU	3.1
1	B	184	PRO	3.0
1	A	230	LEU	3.0
1	A	247	ARG	3.0
1	A	188	PHE	3.0
1	B	282	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	124	LEU	2.9
1	B	284	PHE	2.9
1	B	160	CYS	2.9
1	B	185	VAL	2.9
1	A	79	HIS	2.8
1	B	149	LEU	2.8
1	A	192	VAL	2.8
1	B	144	THR	2.7
1	B	254	CYS	2.7
1	A	203	VAL	2.7
1	A	212	ARG	2.7
1	B	283	LYS	2.6
1	B	123	LEU	2.6
1	A	205	HIS	2.6
1	A	291	PRO	2.6
1	A	266	ILE	2.6
1	B	279	TYR	2.6
1	B	196	PHE	2.5
1	A	235	VAL	2.5
1	B	214	LYS	2.5
1	A	197	ALA	2.4
1	B	89	PHE	2.4
1	B	93	PHE	2.4
1	A	143	PHE	2.4
1	B	255	GLN	2.4
1	B	116	THR	2.4
1	A	271	ILE	2.4
1	B	54	GLY	2.4
1	B	257	PRO	2.4
1	A	144	THR	2.3
1	B	256	ASP	2.3
1	B	228	HIS	2.3
1	B	253	LEU	2.3
1	A	150	LEU	2.3
1	B	173	CYS	2.3
1	A	151	GLY	2.3
1	A	154	ALA	2.3
1	A	193	SER	2.2
1	B	148	THR	2.2
1	A	122	ILE	2.2
1	A	290	ASN	2.2
1	B	106	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	217	ASP	2.2
1	A	213	SER	2.2
1	A	185	VAL	2.2
1	B	73	ILE	2.2
1	B	101	ILE	2.2
1	A	262	LEU	2.2
1	B	215	ILE	2.2
1	A	200	ALA	2.1
1	B	157	LEU	2.1
1	A	125	TRP	2.1
1	B	99	CYS	2.1
1	B	45	ARG	2.1
1	A	187	VAL	2.1
1	A	84	SER	2.1
1	B	289	LYS	2.1
1	A	72	GLU	2.0
1	A	265	ILE	2.0
1	B	218	LYS	2.0
1	B	138	VAL	2.0
1	B	130	ASP	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 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^{th} 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^2)	Q<0.9
2	NMN	B	301	22/22	0.88	0.13	-0.74	41,45,47,48	0
2	NMN	A	301	22/22	0.93	0.12	-1.90	22,32,42,46	0

6.5 Other polymers (i)

There are no such residues in this entry.