



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:58 AM UTC

PDB ID : 3DZK / pdb_00003dzk
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

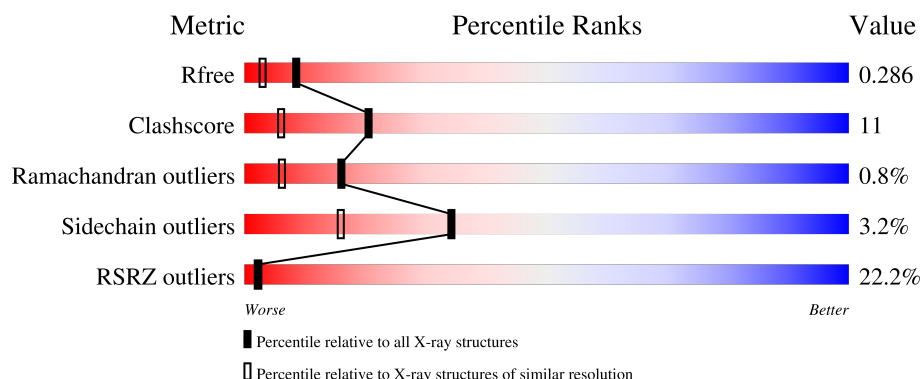
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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}	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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 ≥ 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	18% 77% 16% . .
1	B	262	25% 76% 16% . .

2 Entry composition

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.

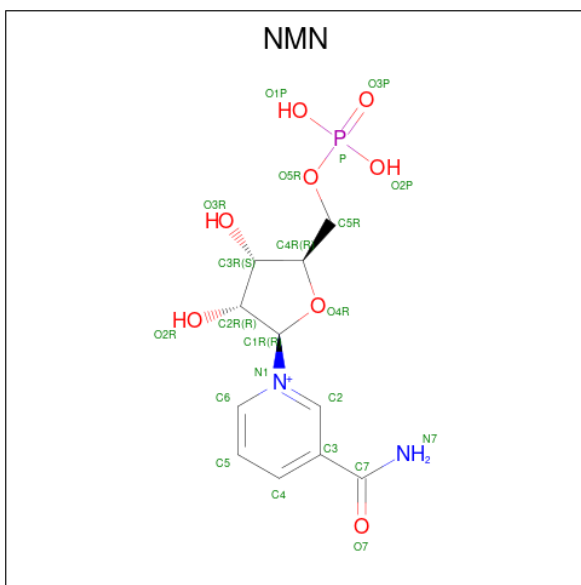
- Molecule 1 is a protein called ADP-ribosyl cyclase 1.

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 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
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 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

- Molecule 2 is BETA-NICOTINAMIDE RIBOSE MONOPHOSPHATE (CCD ID: NMN) (formula: C₁₁H₁₆N₂O₈P).



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

- Molecule 3 is water.

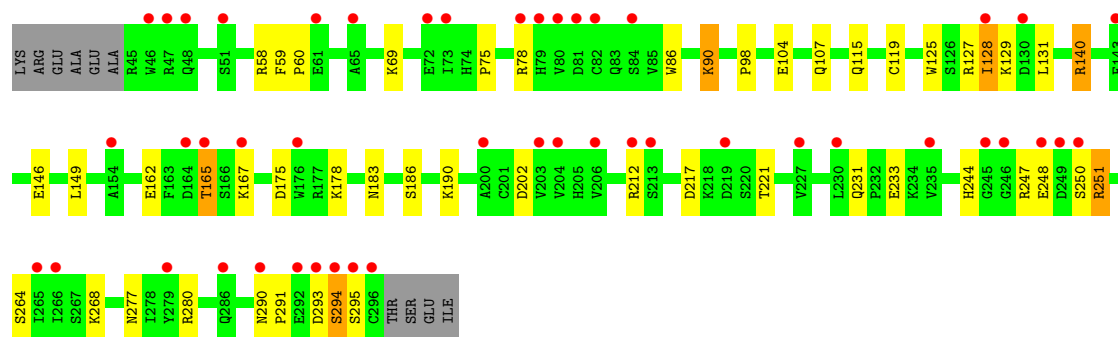
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	174	Total O 174 174	0	0
3	B	180	Total O 180 180	0	0

3 Residue-property plots

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.

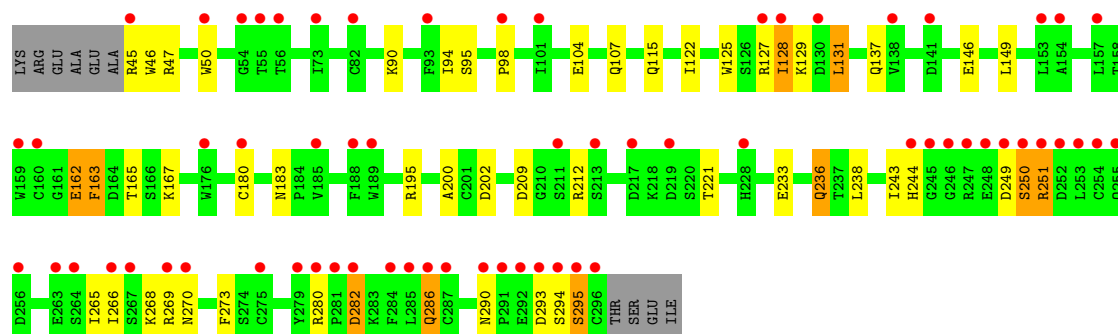
• Molecule 1: ADP-ribosyl cyclase 1

Chain A: 



• Molecule 1: ADP-ribosyl cyclase 1

Chain B: 



4 Data and refinement statistics

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 20.00 – 1.81	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.81) 95.6 (20.00-1.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.3.0021	Depositor
R, R_{free}	0.174 , 0.217 0.263 , 0.286	Depositor DCC
R_{free} test set	2385 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.89	1/2101 (0.0%)	0.95	1/2846 (0.0%)
1	B	0.83	2/2101 (0.1%)	0.88	1/2846 (0.0%)
All	All	0.86	3/4202 (0.1%)	0.92	2/5692 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	PHE	N-CA	-5.35	1.39	1.46
1	A	202	ASP	C-O	-5.27	1.19	1.24
1	B	162	GLU	CA-C	-5.00	1.46	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	SER	N-CA-C	6.53	117.75	108.74
1	A	251	ARG	N-CA-C	5.19	116.80	110.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	91	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 (91) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:45:ARG:HG3	1:B:46:TRP:H	1.72	0.54
1:B:244:HIS:HD2	1:B:250:SER:CB	2.20	0.54
1:A:59:PHE:HB3	1:A:60:PRO:HD3	1.90	0.53
1:B:127:ARG:HG2	1:B:212:ARG:NH1	2.23	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:HD3	1:B:251:ARG:H	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:A:244:HIS:HD2	1:A:250:SER:HB3	1.77	0.50
1:B:286:GLN:HE21	1:B:286:GLN:HA	1.75	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:125:TRP:CZ3	1:B:129:LYS:HB3	2.50	0.47
1:B:282:ASP:O	1:B:286:GLN:HG2	2.15	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:294:SER:O	1:B:295:SER:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:291:PRO:C	1:A:293:ASP:N	2.75	0.43
1:B:50:TRP:CZ2	1:B:98:PRO:HG2	2.53	0.43
1:A:233:GLU:H	1:A:233:GLU:CD	2.26	0.43
1:A:293:ASP:O	1:A:294:SER:HB3	2.19	0.43
1:B:212:ARG:HA	1:B:212:ARG:HD3	1.90	0.43
1:B:268:LYS:HB3	1:B:269:ARG:NH2	2.34	0.43
1:A:104:GLU:HA	1:A:107:GLN:HG2	2.01	0.42
1:A:251:ARG:H	1:A:251:ARG:HD3	1.84	0.42
1:B:46:TRP:CD1	1:B:47:ARG:HG3	2.54	0.42
1:A:98:PRO:O	1:A:183:ASN:HA	2.19	0.42
1:A:190:LYS:NZ	3:A:386:HOH:O	2.52	0.42
1:A:244:HIS:CD2	1:A:250:SER:HB3	2.54	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:128:ILE:HB	1:B:209:ASP:HB2	2.01	0.41
1:A:291:PRO:C	1:A:293:ASP:H	2.29	0.40
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%)	16	6
1	B	250/262 (95%)	240 (96%)	8 (3%)	2 (1%)	16	6
All	All	500/524 (95%)	478 (96%)	18 (4%)	4 (1%)	16	6

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 ⓘ

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%)	227 (97%)	6 (3%)	40	23
1	B	233/241 (97%)	224 (96%)	9 (4%)	28	11
All	All	466/482 (97%)	451 (97%)	15 (3%)	34	16

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ARG
1	A	90	LYS
1	A	128	ILE
1	A	131	LEU
1	A	140	ARG
1	A	165	THR
1	B	131	LEU
1	B	233	GLU
1	B	236	GLN
1	B	249	ASP
1	B	251	ARG
1	B	270	ASN
1	B	280	ARG
1	B	282	ASP
1	B	286	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	74	HIS
1	A	83	GLN
1	A	115	GLN
1	A	134	GLN
1	A	139	GLN
1	A	182	ASN
1	A	183	ASN
1	A	244	HIS
1	A	290	ASN
1	B	83	GLN
1	B	115	GLN
1	B	134	GLN
1	B	236	GLN
1	B	244	HIS
1	B	270	ASN
1	B	286	GLN

5.3.3 RNA [i](#)

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 oligosaccharides 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	B	301	-	21,23,23	0.90	1 (4%)	27,34,34	2.21	10 (37%)
2	NMN	A	301	-	21,23,23	0.83	1 (4%)	27,34,34	2.03	12 (44%)

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	B	301	-	-	3/14/30/30	0/2/2/2
2	NMN	A	301	-	-	3/14/30/30	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NMN	O4R-C1R	2.96	1.44	1.40
2	A	301	NMN	C2-C3	2.14	1.42	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NMN	C3-C7-N7	5.36	124.35	117.74
2	A	301	NMN	C3-C7-N7	4.57	123.37	117.74
2	B	301	NMN	C6-N1-C2	-4.32	118.20	121.88
2	A	301	NMN	C6-N1-C2	-3.88	118.58	121.88
2	B	301	NMN	O7-C7-C3	-3.78	114.97	119.60
2	B	301	NMN	C2-N1-C1R	3.55	126.97	119.13
2	A	301	NMN	C2-N1-C1R	3.45	126.74	119.13
2	A	301	NMN	O2R-C2R-C3R	-2.76	102.96	111.82
2	B	301	NMN	C5-C6-N1	2.67	124.03	120.38
2	A	301	NMN	C6-N1-C1R	-2.58	114.67	119.73
2	B	301	NMN	C6-N1-C1R	-2.52	114.78	119.73
2	A	301	NMN	O3R-C3R-C4R	-2.31	104.45	111.08
2	B	301	NMN	C4-C3-C7	-2.29	114.82	121.06
2	A	301	NMN	O7-C7-C3	-2.26	116.83	119.60
2	B	301	NMN	O2R-C2R-C3R	-2.24	104.64	111.82
2	A	301	NMN	C4-C3-C7	-2.23	114.98	121.06
2	B	301	NMN	C2R-C3R-C4R	2.20	106.87	102.61
2	A	301	NMN	C5-C6-N1	2.18	123.36	120.38
2	B	301	NMN	C2-C3-C7	2.12	125.58	119.46
2	A	301	NMN	O2P-P-O1P	2.12	115.73	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NMN	C2-C3-C7	2.07	125.45	119.46
2	A	301	NMN	C2R-C3R-C4R	2.01	106.50	102.61

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

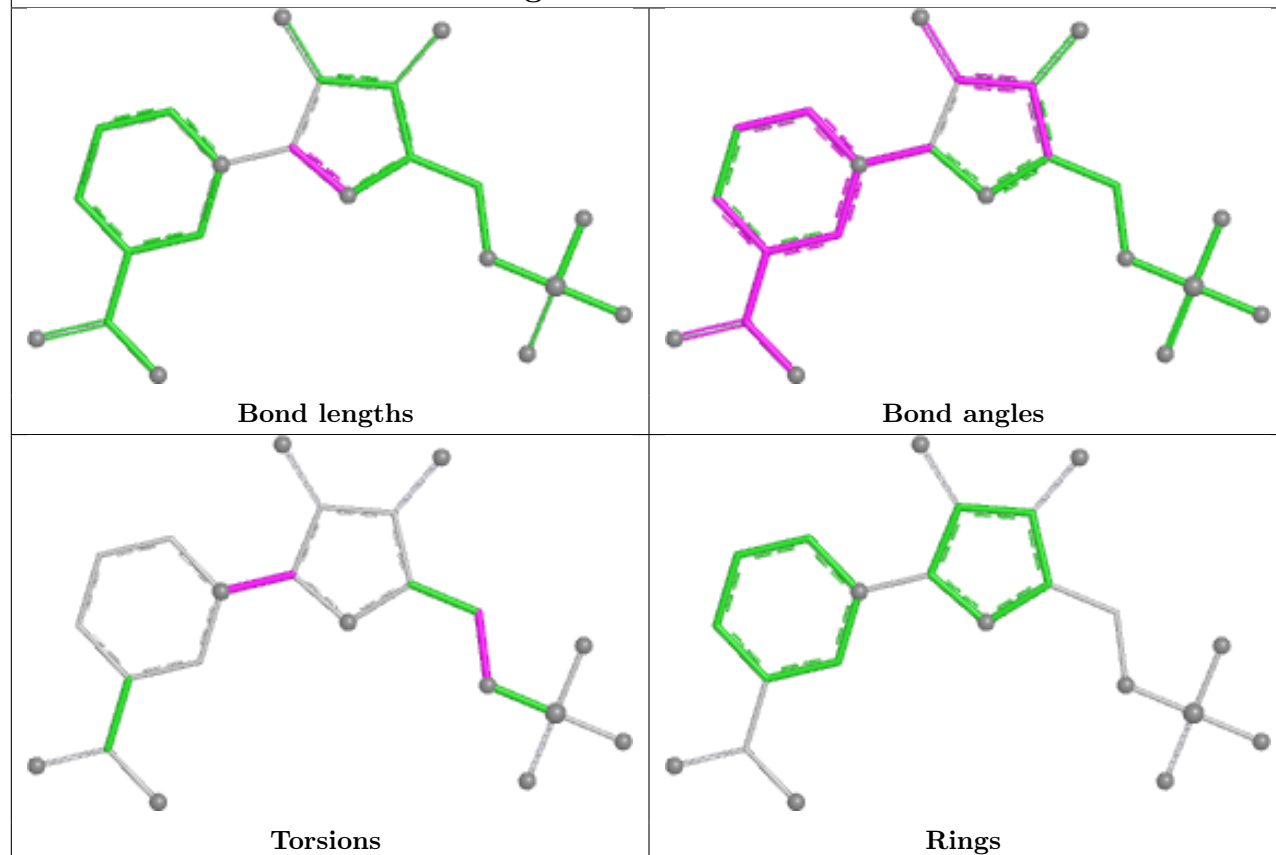
There are no ring outliers.

2 monomers are involved in 4 short contacts:

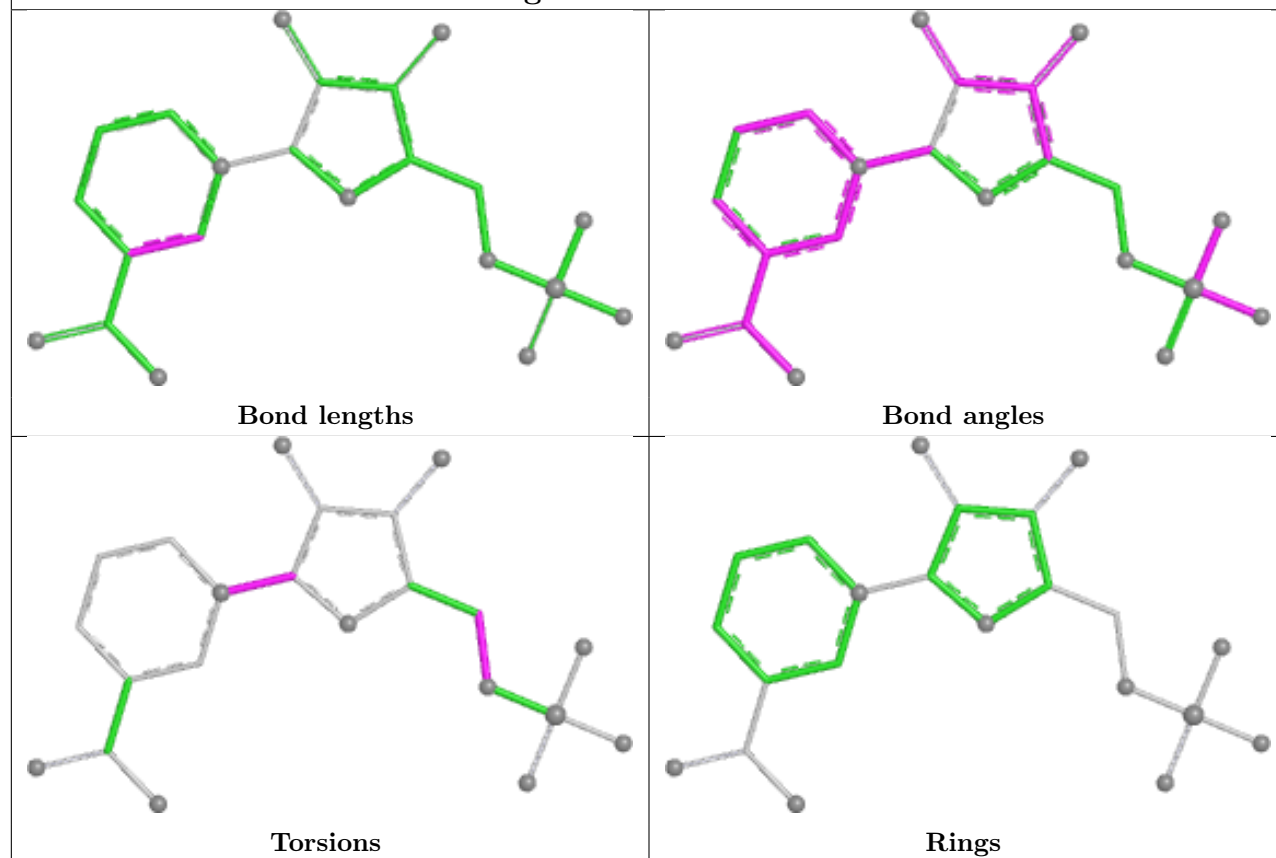
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NMN	2	0
2	A	301	NMN	2	0

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 B 301



Ligand NMN A 301



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, 95th 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%)	1.42	47 (18%) 3 4	24, 31, 41, 49	0
1	B	252/262 (96%)	1.52	65 (25%) 1 2	25, 31, 39, 44	0
All	All	504/524 (96%)	1.47	112 (22%) 2 2	24, 31, 40, 49	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	GLY	7.5
1	B	249	ASP	6.7
1	A	292	GLU	6.5
1	A	294	SER	6.0
1	A	293	ASP	5.7
1	B	294	SER	5.6
1	B	293	ASP	5.3
1	A	248	GLU	5.0
1	B	295	SER	4.8
1	A	249	ASP	4.7
1	A	80	VAL	4.6
1	B	245	GLY	4.6
1	A	164	ASP	4.6
1	B	291	PRO	4.6
1	B	290	ASN	4.4
1	B	248	GLU	4.3
1	B	287	CYS	4.3
1	B	176	TRP	3.9
1	A	296	CYS	3.9
1	B	292	GLU	3.8
1	B	254	CYS	3.8
1	A	73	ILE	3.8
1	B	296	CYS	3.8
1	B	247	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	165	THR	3.7
1	B	141	ASP	3.7
1	A	246	GLY	3.6
1	A	79	HIS	3.6
1	B	286	GLN	3.6
1	B	54	GLY	3.5
1	A	47	ARG	3.5
1	B	250	SER	3.5
1	B	252	ASP	3.1
1	A	84	SER	3.1
1	B	73	ILE	3.0
1	B	127	ARG	3.0
1	B	219	ASP	2.9
1	A	219	ASP	2.8
1	B	282	ASP	2.8
1	A	46	TRP	2.8
1	A	82	CYS	2.8
1	A	48	GLN	2.8
1	B	211	SER	2.8
1	A	51	SER	2.7
1	B	280	ARG	2.7
1	B	284	PHE	2.7
1	A	295	SER	2.7
1	B	267	SER	2.7
1	B	189	TRP	2.7
1	B	253	LEU	2.7
1	A	245	GLY	2.6
1	B	269	ARG	2.6
1	B	266	ILE	2.6
1	B	185	VAL	2.6
1	B	213	SER	2.6
1	B	263	GLU	2.6
1	B	160	CYS	2.6
1	A	143	PHE	2.6
1	B	50	TRP	2.5
1	B	159	TRP	2.5
1	B	138	VAL	2.5
1	B	55	THR	2.5
1	A	130	ASP	2.5
1	A	279	TYR	2.5
1	A	250	SER	2.5
1	A	65	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	244	HIS	2.5
1	B	217	ASP	2.5
1	A	78	ARG	2.4
1	B	279	TYR	2.4
1	B	256	ASP	2.4
1	B	130	ASP	2.4
1	A	235	VAL	2.4
1	B	157	LEU	2.3
1	B	128	ILE	2.3
1	B	154	ALA	2.3
1	B	228	HIS	2.3
1	A	203	VAL	2.3
1	A	227	VAL	2.3
1	B	285	LEU	2.3
1	A	128	ILE	2.3
1	A	212	ARG	2.3
1	A	81	ASP	2.3
1	A	230	LEU	2.3
1	B	98	PRO	2.3
1	A	200	ALA	2.2
1	B	188	PHE	2.2
1	A	265	ILE	2.2
1	A	290	ASN	2.2
1	A	72	GLU	2.2
1	B	153	LEU	2.2
1	A	204	VAL	2.2
1	B	56	THR	2.2
1	B	281	PRO	2.2
1	A	154	ALA	2.2
1	A	167	LYS	2.2
1	B	270	ASN	2.1
1	B	255	GLN	2.1
1	A	206	VAL	2.1
1	B	45	ARG	2.1
1	B	251	ARG	2.1
1	B	275	CYS	2.1
1	B	93	PHE	2.1
1	B	101	ILE	2.1
1	A	61	GLU	2.1
1	A	176	TRP	2.1
1	A	286	GLN	2.1
1	B	180	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	213	SER	2.0
1	B	82	CYS	2.0
1	B	264	SER	2.0
1	A	266	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

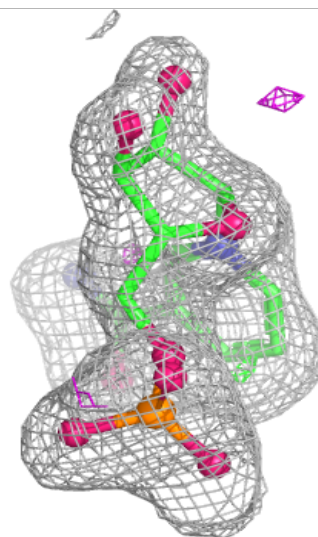
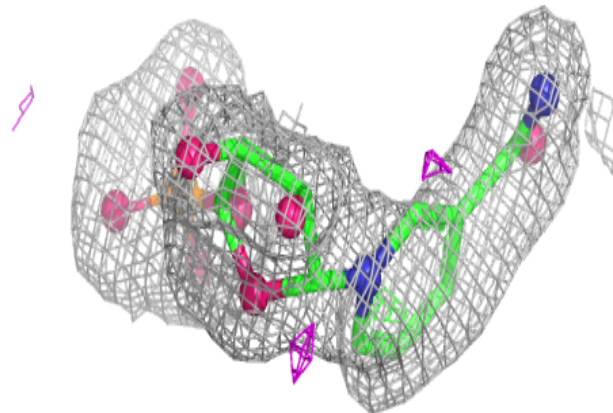
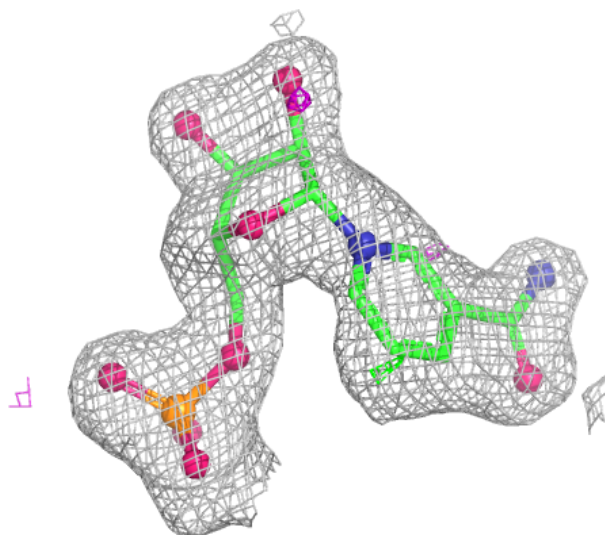
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	301	22/22	0.87	0.12	41,45,47,48	0
2	NMN	A	301	22/22	0.93	0.10	22,32,42,46	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.

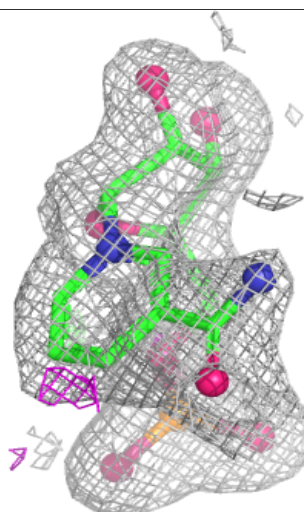
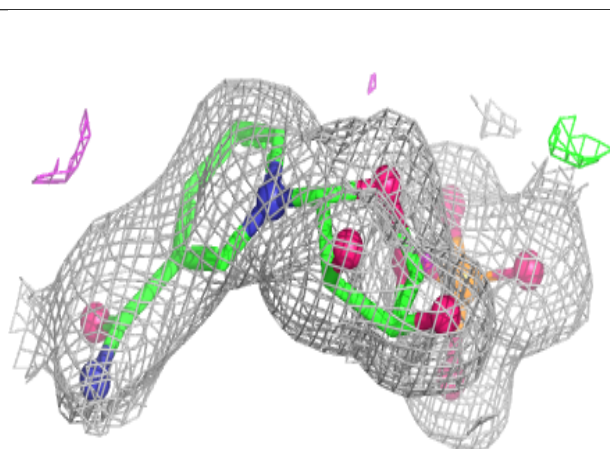
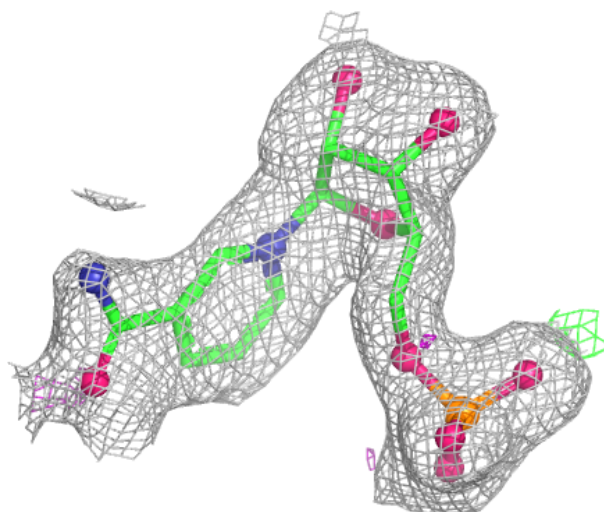
Electron density around NMN B 301:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.