



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 06:59 PM EDT

PDB ID : 3DZJ
Title : Crystal structure of human CD38 extracellular domain E226Q mutant, 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 : 1.90 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 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

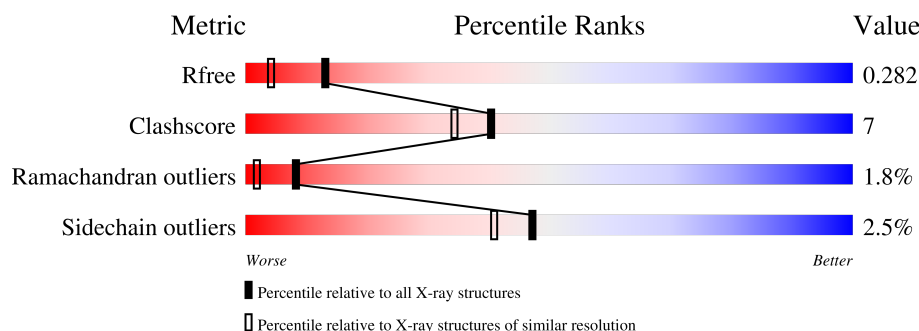
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	262	 81% 15% . .
1	B	262	 79% 16% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4424 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.

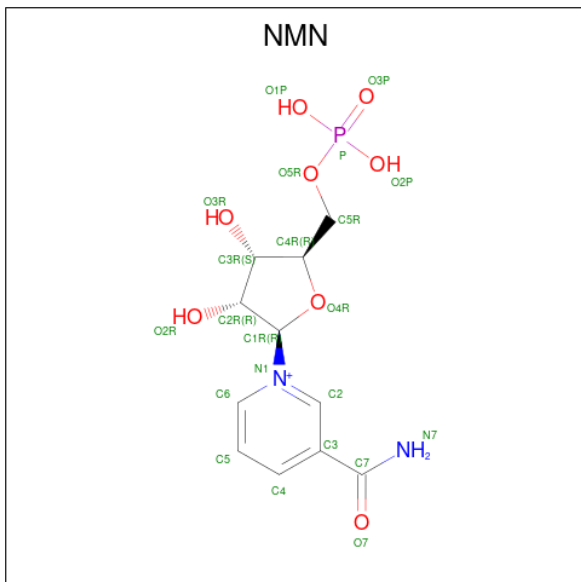
- Molecule 1 is a protein called ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2005	1265	352	372	16			
1	B	252	Total	C	N	O	S	0	0	0
			2005	1265	352	372	16			

There are 24 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	ALA	ASN	engineered mutation	UNP P28907
A	209	ASP	ASN	engineered mutation	UNP P28907
A	219	ASP	ASN	engineered mutation	UNP P28907
A	226	GLN	GLU	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	ALA	ASN	engineered mutation	UNP P28907
B	209	ASP	ASN	engineered mutation	UNP P28907
B	219	ASP	ASN	engineered mutation	UNP P28907
B	226	GLN	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		

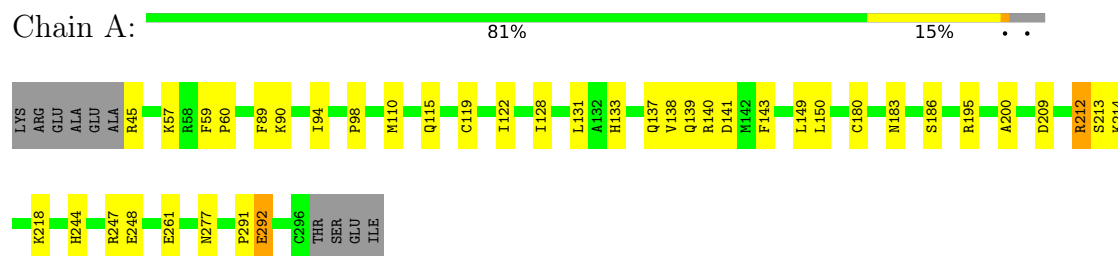
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	200	Total	O	0	0
			200	200		
3	B	170	Total	O	0	0
			170	170		

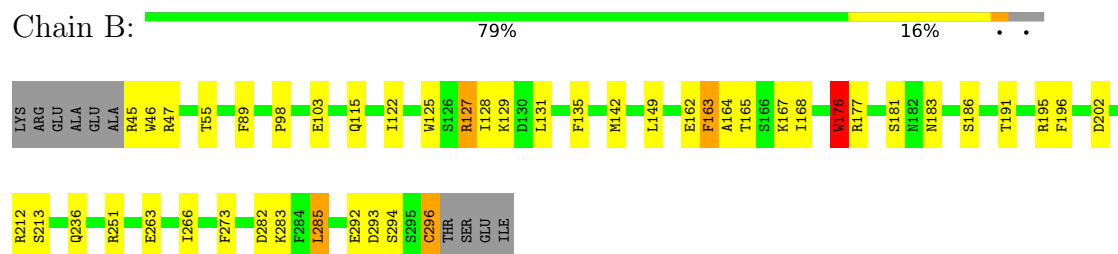
3 Residue-property plots [i](#)

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. 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. 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, α , β , γ	41.86Å 53.23Å 65.67Å 106.11° 91.97° 95.03°	Depositor
Resolution (Å)	20.00 – 1.90 19.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.90) 96.6 (19.98-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.241 0.240 , 0.282	Depositor DCC
R_{free} test set	2061 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4424	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 7.25% 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

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	0.85	0/2055	0.84	0/2781
1	B	0.93	4/2055 (0.2%)	0.82	0/2781
All	All	0.89	4/4110 (0.1%)	0.83	0/5562

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	7.33	1.37	1.23
1	B	283	LYS	C-O	7.25	1.37	1.23
1	B	263	GLU	CD-OE1	5.99	1.32	1.25
1	B	176	TRP	CB-CG	-5.87	1.39	1.50

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	ALA	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	2005	0	1920	30	0
1	B	2005	0	1920	28	0
2	A	22	0	14	0	0
2	B	22	0	14	0	0
3	A	200	0	0	10	0
3	B	170	0	0	4	0
All	All	4424	0	3868	57	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 7.

All (57) 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:A:180:CYS:HB2	3:A:492:HOH:O	1.64	0.97
1:B:165:THR:HG23	1:B:167:LYS:H	1.30	0.95
1:A:115:GLN:HE22	1:A:149:LEU:H	1.24	0.86
1:B:115:GLN:HE22	1:B:149:LEU:H	1.23	0.82
1:A:141:ASP:O	1:A:143:PHE:CE2	2.34	0.80
1:B:176:TRP:CD1	1:B:177:ARG:HG3	2.16	0.80
1:B:162:GLU:HB2	1:B:165:THR:HG22	1.68	0.75
1:B:176:TRP:CZ3	1:B:181:SER:HB2	2.29	0.67
1:A:139:GLN:C	1:A:141:ASP:H	1.96	0.67
1:B:202:ASP:HA	1:B:236:GLN:HG2	1.77	0.66
1:A:45:ARG:HD2	3:A:494:HOH:O	2.00	0.62
1:B:115:GLN:NE2	1:B:149:LEU:H	1.96	0.62
1:B:266:ILE:HD11	1:B:273:PHE:HB2	1.81	0.61
1:B:135:PHE:HE1	1:B:142:MET:HG3	1.67	0.60
1:A:90:LYS:HG2	1:A:94:ILE:HG13	1.83	0.59
1:A:128:ILE:HG13	3:A:341:HOH:O	2.03	0.58
1:B:176:TRP:HD1	1:B:177:ARG:HG3	1.66	0.57
1:A:45:ARG:CD	3:A:494:HOH:O	2.52	0.56
1:B:183:ASN:ND2	1:B:186:SER:H	2.04	0.56
1:A:115:GLN:NE2	1:A:149:LEU:H	2.01	0.55
1:A:244:HIS:HE1	1:A:277:ASN:OD1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLN:O	1:A:141:ASP:N	2.42	0.53
1:A:139:GLN:C	1:A:141:ASP:N	2.61	0.53
1:A:195:ARG:HD3	3:A:359:HOH:O	2.09	0.52
1:B:202:ASP:HB3	3:B:474:HOH:O	2.10	0.52
1:B:128:ILE:O	1:B:128:ILE:HG23	2.10	0.51
1:A:218:LYS:HE3	3:A:453:HOH:O	2.10	0.50
1:A:133:HIS:O	1:A:137:GLN:HG2	2.13	0.48
1:A:195:ARG:CD	3:A:359:HOH:O	2.60	0.48
1:B:125:TRP:CH2	1:B:129:LYS:HB3	2.50	0.47
1:B:212:ARG:O	1:B:213:SER:HB3	2.14	0.47
1:A:138:VAL:O	1:A:140:ARG:N	2.48	0.46
1:B:45:ARG:HG3	1:B:47:ARG:H	1.80	0.46
1:A:98:PRO:O	1:A:183:ASN:HA	2.16	0.46
1:B:103:GLU:HG2	1:B:191:THR:OG1	2.16	0.46
1:A:128:ILE:HG23	1:A:128:ILE:O	2.17	0.45
1:A:183:ASN:ND2	1:A:186:SER:H	2.14	0.45
1:B:122:ILE:HG23	1:B:196:PHE:CE2	2.52	0.45
1:A:128:ILE:HB	1:A:209:ASP:HB2	1.99	0.44
1:A:214:LYS:HE3	3:A:425:HOH:O	2.16	0.44
1:B:47:ARG:NH1	3:B:548:HOH:O	2.49	0.44
1:A:209:ASP:HB3	1:A:212:ARG:HG3	2.00	0.43
1:B:45:ARG:HG3	1:B:46:TRP:N	2.34	0.43
1:B:45:ARG:HB2	3:B:504:HOH:O	2.18	0.43
1:A:122:ILE:HD12	1:A:200:ALA:HA	2.01	0.43
1:A:291:PRO:O	1:A:292:GLU:O	2.36	0.42
1:B:195:ARG:HD3	3:B:550:HOH:O	2.18	0.42
1:B:266:ILE:HD11	1:B:273:PHE:CB	2.47	0.42
1:B:55:THR:HG21	1:B:168:ILE:HG21	2.00	0.42
1:B:98:PRO:O	1:B:183:ASN:HA	2.19	0.42
1:A:119:CYS:HB3	3:A:346:HOH:O	2.20	0.42
1:A:261:GLU:HG3	1:B:163:PHE:HZ	1.85	0.42
1:B:183:ASN:HD21	1:B:186:SER:H	1.69	0.41
1:A:59:PHE:HB3	1:A:60:PRO:HD3	2.03	0.40
1:A:110:MET:HE1	1:A:150:LEU:HD13	2.02	0.40
1:B:285:LEU:HD22	1:B:285:LEU:HA	1.94	0.40
1:A:57:LYS:HG2	3:A:440:HOH:O	2.21	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%)	229 (92%)	16 (6%)	5 (2%)	7	1
1	B	250/262 (95%)	238 (95%)	8 (3%)	4 (2%)	9	2
All	All	500/524 (95%)	467 (93%)	24 (5%)	9 (2%)	8	2

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	ARG
1	A	247	ARG
1	A	248	GLU
1	B	293	ASP
1	B	294	SER
1	A	213	SER
1	A	292	GLU
1	B	127	ARG
1	B	292	GLU

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	222/240 (92%)	220 (99%)	2 (1%)	78	79
1	B	222/240 (92%)	213 (96%)	9 (4%)	30	21
All	All	444/480 (92%)	433 (98%)	11 (2%)	47	41

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	PHE
1	A	131	LEU
1	B	89	PHE
1	B	127	ARG
1	B	131	LEU
1	B	163	PHE
1	B	176	TRP
1	B	251	ARG
1	B	282	ASP
1	B	285	LEU
1	B	296	CYS

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

Mol	Chain	Res	Type
1	A	115	GLN
1	A	134	GLN
1	A	183	ASN
1	A	244	HIS
1	A	270	ASN
1	B	115	GLN
1	B	183	ASN
1	B	270	ASN

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 monosaccharides 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	B	301	-	22,23,23	0.78	0	30,34,34	2.26	7 (23%)
2	NMN	A	301	-	22,23,23	0.90	0	30,34,34	1.70	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NMN	B	301	-	-	2/14/30/30	0/2/2/2
2	NMN	A	301	-	-	3/14/30/30	0/2/2/2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NMN	C3-C7-N7	6.17	125.15	117.75
2	B	301	NMN	O7-C7-C3	-5.99	112.46	119.63
2	B	301	NMN	C3R-C2R-C1R	4.99	108.49	100.98
2	A	301	NMN	C3-C7-N7	4.83	123.54	117.75
2	A	301	NMN	C3R-C2R-C1R	3.99	106.99	100.98
2	B	301	NMN	O4R-C1R-C2R	-3.30	102.10	106.93
2	A	301	NMN	O7-C7-C3	-3.12	115.90	119.63
2	A	301	NMN	O4R-C1R-C2R	-2.98	102.56	106.93
2	B	301	NMN	C6-N1-C2	-2.69	119.52	121.97
2	B	301	NMN	O2P-P-O1P	2.33	116.53	107.64
2	B	301	NMN	O2P-P-O5R	-2.21	100.86	106.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

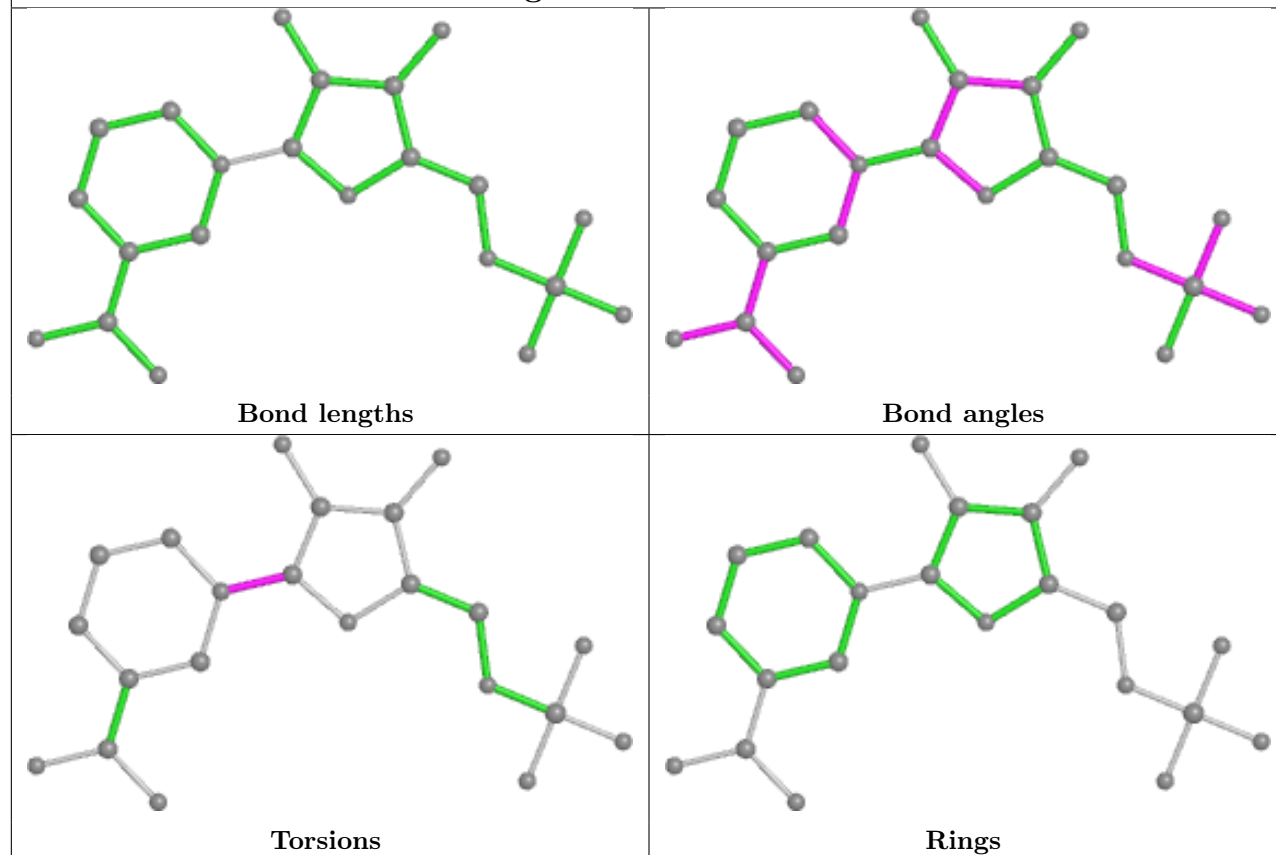
Mol	Chain	Res	Type	Atoms
2	A	301	NMN	C2R-C1R-N1-C2
2	A	301	NMN	C2R-C1R-N1-C6
2	B	301	NMN	C2R-C1R-N1-C2
2	B	301	NMN	C2R-C1R-N1-C6
2	A	301	NMN	C3R-C4R-C5R-O5R

There are no ring outliers.

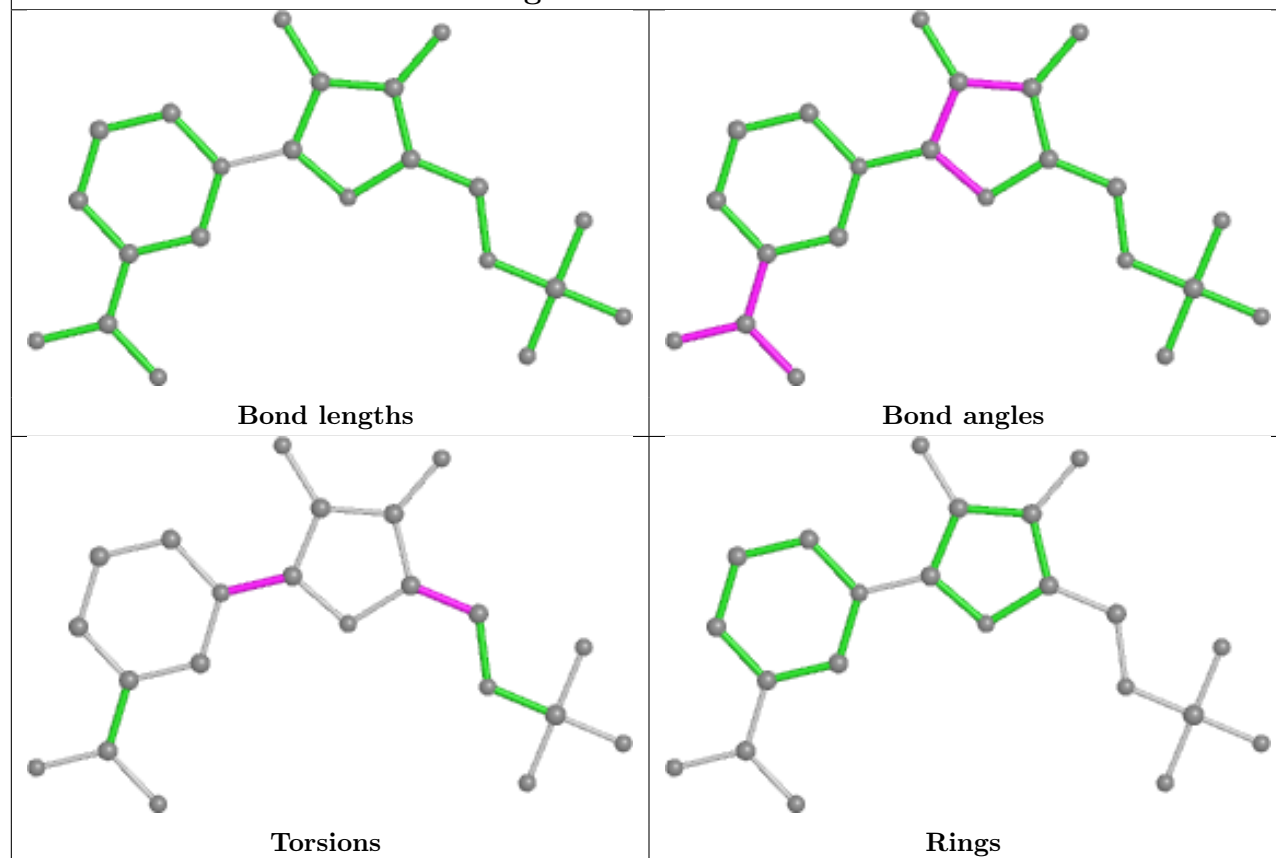
No monomer is involved in short contacts.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

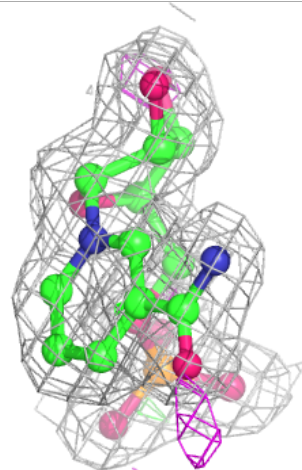
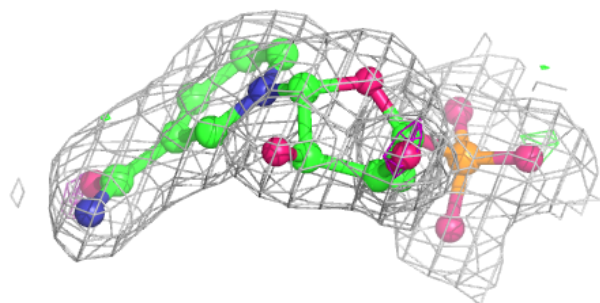
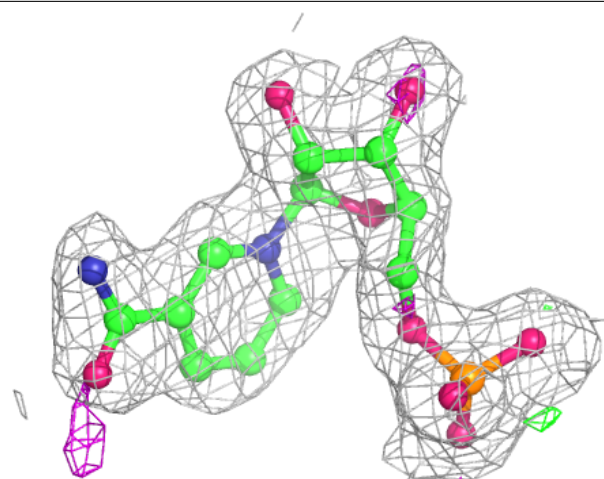
6.4 Ligands

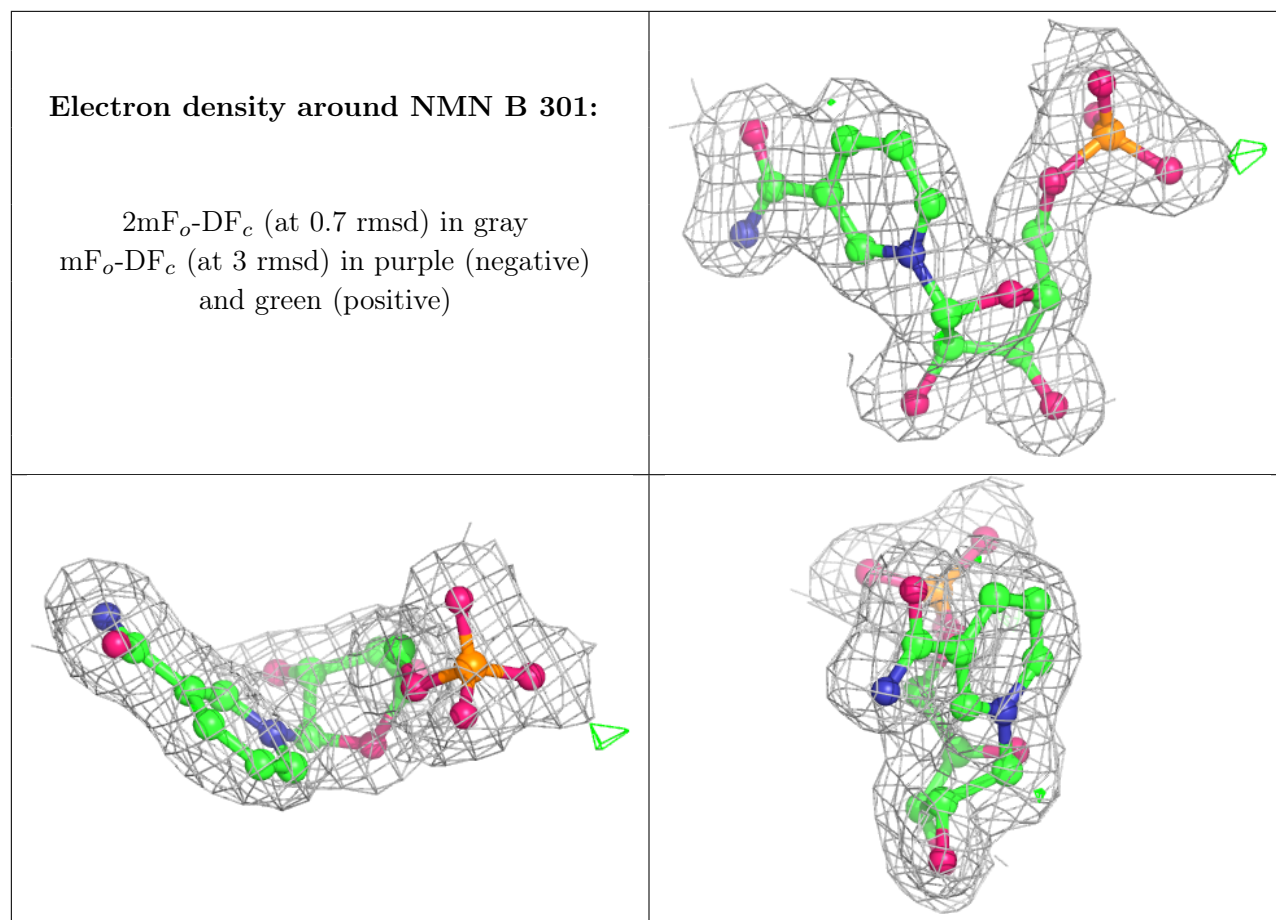
Unable to reproduce the depositors R factor - this section is therefore empty.

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 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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.