



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:27 AM UTC

PDB ID : 1GZU / pdb_00001gzu
Title : Crystal Structure of Human Nicotinamide Mononucleotide Adenylyltransferase
in Complex with NMN
Authors : Werner, E.; Ziegler, M.; Lerner, F.; Schweiger, M.; Heinemann, U.
Deposited on : 2002-06-06
Resolution : 2.90 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 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

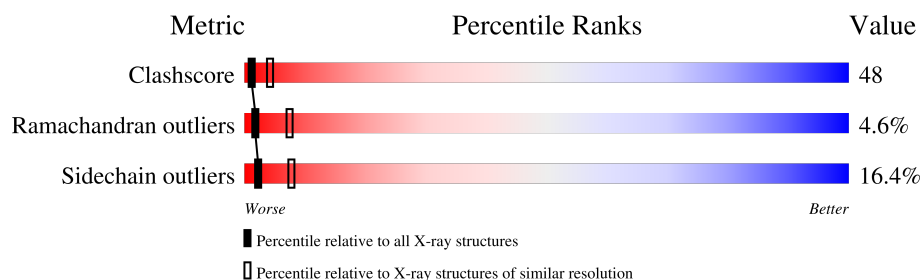
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	290	
1	B	290	
1	C	290	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NMN	A	501	X	-	-	-
2	NMN	B	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NMN	C	501	X	-	-	-

2 Entry composition [i](#)

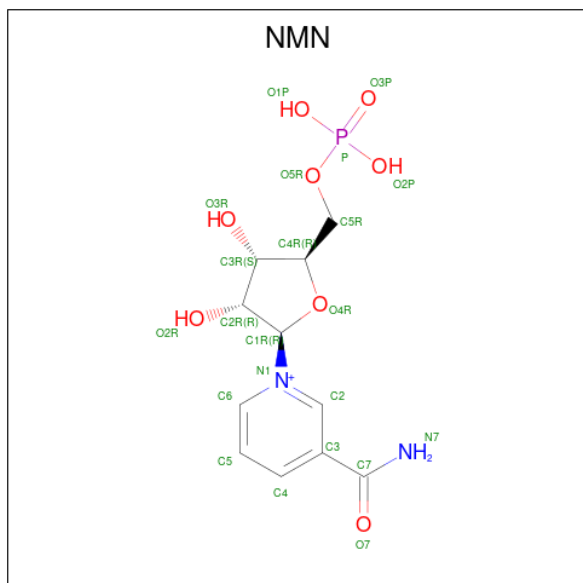
There are 2 unique types of molecules in this entry. The entry contains 5544 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NICOTINAMIDE MONONUCLEOTIDE ADENYLYL TRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	Se	4	0	1
			1826	1168	321	331	3	3			
1	B	228	Total	C	N	O	S	Se	3	0	1
			1826	1168	321	331	3	3			
1	C	228	Total	C	N	O	S	Se	19	0	1
			1826	1168	321	331	3	3			

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



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

S255	T187	ARG	G52	MSE
S256	R188	LYS	D53	ARG
E257	A189	ARG		GLY
S258	G190	LYS	K56	SER
E259	N191	TRP	K57	HIS
D260	D192	THR	K58	HIS
R261	A193	GLU		HIS
N262	Q194	THR	I61	HIS
	K195	GLN	P62	HIS
	F196	ASP	A63	HIS
		SER	Y64	GLY
V265		SER	H65	SER
I266	E199	GLN	R66	GLU
L267	S200	LYS	V67	ASN
A268		LYS	I68	SER
P269	W204	SER	M69	GLU
L270	H211	LEU	K6	
Q271	V212	GLU	T7	
ARG	V213	PRO	E3	
ASN	N214	LYS	E8	
ALA	E215	THR	V9	
GLU	W216	LYS	V10	
ALA	I217	LYS	L11	
LYS	A218		L12	
THR	N219		A13	
	D220		C14	
	I221		G15	
	S222		C15	
	S223		W79	
	T224		V80	
	K225		S81	
	I226		H82	
	R227		D83	
	R228		T84	
	A229		W85	
	L230		E86	
	L230			
	R231		E94	
	R232		T95	
	G233		I96	
	Q234		K97	
	S235			
	I236			
	R237			
	Y238			
	L239			
	V240			
	P241			
	D242			
	L243			
	V244			
	Q245			
	E246			
	Y247			
	I248			
	E249			
	K250			
	H251			
	N252			
	L253			
	Y254			

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	140.80 Å 235.70 Å 89.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	86.0 (20.00-2.90)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.246 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5544	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

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	1.14	9/1860 (0.5%)	1.06	5/2513 (0.2%)
1	B	1.07	7/1860 (0.4%)	1.09	9/2513 (0.4%)
1	C	1.41	10/1860 (0.5%)	1.35	16/2513 (0.6%)
All	All	1.21	26/5580 (0.5%)	1.18	30/7539 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	267	LEU	CB-CG	29.27	2.12	1.53
1	C	78	LYS	CG-CD	28.77	2.38	1.52
1	C	220	ASP	CB-CG	-15.63	1.12	1.52
1	A	260	ASP	CA-CB	10.98	1.73	1.53
1	B	69	MSE	SE-CE	-9.32	1.67	1.95
1	C	150	LYS	CG-CD	-8.65	1.26	1.52
1	A	69	MSE	SE-CE	-8.25	1.70	1.95
1	B	270	LEU	C-N	-7.31	1.23	1.33
1	B	187	THR	CA-C	-6.93	1.44	1.52
1	C	270	LEU	C-N	-6.88	1.23	1.33
1	A	270	LEU	C-N	-6.83	1.23	1.33
1	A	197	ILE	CA-CB	-6.80	1.46	1.54
1	A	210	ILE	CA-CB	-6.29	1.46	1.54
1	C	68	ILE	C-O	6.29	1.31	1.24
1	C	184	ILE	CA-CB	-6.23	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	170	LYS	CB-CG	-6.23	1.33	1.52
1	B	213	VAL	CA-CB	-5.91	1.47	1.54
1	A	212	VAL	CA-CB	-5.81	1.47	1.53
1	B	217	ILE	CA-CB	5.80	1.62	1.54
1	C	102	HIS	ND1-CE1	5.70	1.38	1.32
1	B	251	HIS	ND1-CE1	5.58	1.38	1.32
1	A	184	ILE	CA-CB	-5.30	1.47	1.54
1	A	244	VAL	CA-CB	-5.08	1.48	1.54
1	A	178	VAL	CA-CB	-5.05	1.48	1.54
1	C	213	VAL	CA-CB	-5.05	1.48	1.54
1	B	234	GLN	CD-OE1	5.05	1.33	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	220	ASP	CA-CB-CG	24.30	136.90	112.60
1	C	78	LYS	CB-CG-CD	-23.18	57.98	111.30
1	C	78	LYS	CG-CD-CE	15.89	147.85	111.30
1	C	257	GLU	N-CA-C	-9.46	100.97	111.28
1	C	170	LYS	CA-CB-CG	9.14	132.38	114.10
1	B	257	GLU	N-CA-C	-8.70	101.80	111.28
1	A	257	GLU	N-CA-C	-8.13	102.50	111.36
1	C	188	ARG	N-CA-C	-7.94	102.50	112.90
1	C	51	VAL	CB-CA-C	-7.93	102.56	111.45
1	B	51	VAL	CB-CA-C	-7.46	100.99	111.28
1	A	188	ARG	N-CA-C	-7.37	103.24	112.90
1	C	102	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	B	24	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	C	267	LEU	CA-CB-CG	-6.59	93.23	116.30
1	B	20	ILE	N-CA-C	-6.34	101.37	109.80
1	B	188	ARG	N-CA-C	-6.29	104.66	112.90
1	B	251	HIS	CB-CG-CD2	-6.24	123.08	131.20
1	C	150	LYS	CB-CG-CD	6.24	125.66	111.30
1	C	267	LEU	CB-CG-CD2	5.82	128.16	110.70
1	C	20	ILE	N-CA-C	-5.73	100.73	109.78
1	C	102	HIS	CB-CG-ND1	5.69	131.24	122.70
1	A	253	LEU	N-CA-C	5.61	117.47	111.36
1	C	170	LYS	CB-CG-CD	5.57	124.11	111.30
1	C	243	LEU	N-CA-C	-5.55	104.62	111.33
1	B	251	HIS	CB-CG-ND1	5.53	130.99	122.70
1	A	20	ILE	N-CA-C	-5.43	102.58	109.80
1	B	18	ASN	N-CA-C	-5.40	97.87	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	HIS	CB-CG-ND1	5.39	130.79	122.70
1	A	195	LYS	N-CA-C	-5.24	105.26	110.97
1	C	18	ASN	N-CA-C	-5.02	98.71	109.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	220	ASP	Sidechain

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	1826	0	1858	144	0
1	B	1826	0	1858	152	0
1	C	1826	0	1858	245	0
2	A	22	0	9	2	0
2	B	22	0	8	3	0
2	C	22	0	8	5	0
All	All	5544	0	5599	532	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 48.

All (532) 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:C:250:LYS:O	1:C:251:HIS:ND1	1.60	1.33
1:C:18:ASN:HB3	1:C:19:PRO:CD	1.57	1.32
1:C:27:LEU:HD22	1:C:186:VAL:CG2	1.69	1.21
1:C:168:LEU:HD23	1:C:169:TRP:CD1	1.75	1.20
1:B:58:LYS:HE2	1:B:58:LYS:N	1.59	1.17
1:A:18:ASN:HB3	1:A:19:PRO:CD	1.74	1.15
1:C:58:LYS:H	1:C:58:LYS:HD2	1.03	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:SER:O	1:A:256:SER:HB3	1.48	1.13
1:C:27:LEU:HD22	1:C:186:VAL:HG21	1.17	1.12
1:C:187:THR:HG22	1:C:189:ALA:H	1.08	1.09
1:A:27:LEU:HD22	1:A:186:VAL:HG21	1.27	1.07
1:B:18:ASN:HB3	1:B:19:PRO:CD	1.84	1.07
1:B:58:LYS:HE2	1:B:58:LYS:H	0.93	1.05
1:B:16:SER:HA	1:B:51:VAL:CG2	1.86	1.04
1:C:18:ASN:HB3	1:C:19:PRO:HD2	1.31	1.03
1:C:234:GLN:OE1	1:C:234:GLN:HA	1.59	1.02
1:B:58:LYS:H	1:B:58:LYS:CE	1.72	1.02
1:B:216:TRP:O	1:B:217:ILE:HD13	1.58	1.01
1:C:168:LEU:HD23	1:C:169:TRP:NE1	1.74	1.01
1:A:18:ASN:HB3	1:A:19:PRO:HD3	1.43	1.01
1:C:18:ASN:HB3	1:C:19:PRO:HD3	1.42	1.00
1:C:68:ILE:CG2	1:C:72:LEU:HD11	1.92	1.00
1:C:18:ASN:CB	1:C:19:PRO:CD	2.40	0.99
1:A:217:ILE:HG12	1:A:217:ILE:O	1.62	0.99
1:C:68:ILE:HG22	1:C:72:LEU:CD1	1.93	0.97
1:B:16:SER:HA	1:B:51:VAL:HG23	1.46	0.97
1:C:228:ARG:HA	1:C:231:ARG:NH1	1.77	0.97
1:C:17:PHE:HD2	1:C:20:ILE:HG13	1.26	0.95
1:C:228:ARG:HA	1:C:231:ARG:HH12	1.31	0.95
1:A:27:LEU:HD22	1:A:186:VAL:CG2	1.96	0.94
1:A:27:LEU:CD2	1:A:186:VAL:HG21	1.97	0.94
1:C:26:ARG:HH11	1:C:26:ARG:HG3	1.32	0.92
1:A:250:LYS:HE3	1:A:250:LYS:O	1.69	0.92
1:B:95:THR:OG1	2:B:501:NMN:HC2	1.70	0.91
1:C:187:THR:HG22	1:C:189:ALA:N	1.86	0.91
1:C:16:SER:HA	1:C:51:VAL:HG23	1.52	0.90
1:C:227:ARG:HG3	1:C:227:ARG:HH11	1.37	0.90
1:C:16:SER:HA	1:C:51:VAL:CG2	2.02	0.90
1:B:217:ILE:HG12	1:B:217:ILE:O	1.71	0.90
1:C:58:LYS:H	1:C:58:LYS:CD	1.84	0.90
1:C:17:PHE:C	1:C:18:ASN:O	2.13	0.89
1:C:250:LYS:O	1:C:251:HIS:CG	2.25	0.89
1:C:10:VAL:HG22	1:C:45:LYS:HG3	1.54	0.88
1:C:58:LYS:HD2	1:C:58:LYS:N	1.88	0.88
1:C:268:ALA:O	1:C:270:LEU:N	2.06	0.88
1:A:268:ALA:O	1:A:270:LEU:N	2.07	0.88
1:C:67:VAL:O	1:C:71:GLU:HG3	1.73	0.88
1:C:38:THR:HG23	1:C:40:ARG:H	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LEU:CD2	1:C:186:VAL:CG2	2.52	0.88
1:C:247:TYR:HE1	1:C:253:LEU:HD11	1.39	0.87
1:C:183:LEU:C	1:C:183:LEU:HD12	1.96	0.87
1:C:226:ILE:HG23	1:C:236:ILE:HD11	1.54	0.87
1:B:157:ALA:HB2	1:B:187:THR:HG21	1.57	0.87
1:A:58:LYS:H	1:A:58:LYS:HD2	1.38	0.86
1:B:268:ALA:O	1:B:270:LEU:N	2.09	0.86
1:C:18:ASN:CB	1:C:19:PRO:HD3	2.04	0.86
1:B:18:ASN:HB3	1:B:19:PRO:HD3	1.58	0.84
1:C:168:LEU:CD2	1:C:169:TRP:NE1	2.40	0.84
1:C:183:LEU:HD12	1:C:184:ILE:N	1.91	0.84
1:A:38:THR:HG23	1:A:40:ARG:H	1.41	0.84
1:B:159:LEU:HD23	2:B:501:NMN:H5R1	1.60	0.84
1:C:70:ALA:O	1:C:73:ALA:HB3	1.78	0.83
1:C:10:VAL:HG22	1:C:45:LYS:CG	2.09	0.83
1:B:17:PHE:C	1:B:18:ASN:O	2.14	0.82
1:B:148:VAL:O	1:B:148:VAL:HG12	1.79	0.82
1:A:17:PHE:C	1:A:18:ASN:O	2.16	0.82
1:C:255:SER:O	1:C:256:SER:HB3	1.79	0.81
1:C:228:ARG:CA	1:C:231:ARG:HH12	1.93	0.81
1:A:187:THR:HG22	1:A:189:ALA:H	1.46	0.81
1:C:16:SER:N	2:C:501:NMN:O3P	2.13	0.81
1:A:250:LYS:O	1:A:251:HIS:CG	2.34	0.80
1:B:82:VAL:HG12	1:B:83:ASP:N	1.97	0.80
1:C:68:ILE:HG23	1:C:72:LEU:HD11	1.63	0.80
1:A:268:ALA:HB3	1:A:269:PRO:HD3	1.64	0.80
1:B:38:THR:HG23	1:B:40:ARG:H	1.46	0.80
1:A:18:ASN:O	1:A:19:PRO:C	2.25	0.79
1:A:95:THR:OG1	2:A:501:NMN:HC2	1.82	0.79
1:C:21:THR:HA	1:C:240:VAL:CG1	2.11	0.79
1:B:21:THR:H	1:B:24:HIS:HD2	1.30	0.79
1:B:168:LEU:HD12	1:B:268:ALA:CB	2.13	0.79
1:A:18:ASN:HB3	1:A:19:PRO:HD2	1.62	0.78
1:C:22:ASN:ND2	1:C:239:LEU:C	2.42	0.78
1:C:17:PHE:CD2	1:C:20:ILE:HG13	2.17	0.77
1:B:18:ASN:HB3	1:B:19:PRO:HD2	1.65	0.77
1:C:227:ARG:HG3	1:C:227:ARG:NH1	1.97	0.77
1:A:250:LYS:NZ	1:A:251:HIS:CE1	2.53	0.76
1:C:49:SER:OG	1:C:86:GLU:OE1	2.03	0.76
1:C:53:ASP:OD2	1:C:62:PRO:HA	1.86	0.76
1:B:245:GLN:HE22	1:B:249:GLU:CD	1.94	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LEU:CD2	1:C:169:TRP:HE1	1.99	0.76
1:A:204:TRP:CE3	1:B:232:ARG:HD3	2.21	0.76
1:A:27:LEU:CD2	1:A:186:VAL:CG2	2.63	0.75
1:A:36:ASN:OD1	1:A:43:VAL:HG23	1.86	0.74
1:B:168:LEU:HD12	1:B:268:ALA:HB1	1.69	0.74
1:C:95:THR:OG1	2:C:501:NMN:HC2	1.88	0.74
1:C:68:ILE:C	1:C:72:LEU:HD12	2.11	0.74
1:B:27:LEU:HG	1:B:186:VAL:HG21	1.70	0.74
1:C:68:ILE:HG22	1:C:72:LEU:HD11	1.57	0.73
1:A:217:ILE:O	1:A:217:ILE:CG1	2.37	0.73
1:B:35:MSE:O	1:B:38:THR:HG22	1.89	0.73
1:C:231:ARG:HH11	1:C:231:ARG:HB2	1.53	0.72
1:B:152:LYS:HD3	1:B:182:GLY:HA3	1.71	0.72
1:C:170:LYS:O	1:C:173:ASP:N	2.23	0.71
1:A:82:VAL:HG12	1:A:83:ASP:N	2.05	0.71
1:B:16:SER:HA	1:B:51:VAL:HG21	1.73	0.71
1:A:235:SER:O	1:A:236:ILE:HB	1.89	0.71
1:C:21:THR:HA	1:C:240:VAL:HG12	1.72	0.70
1:C:69:MSE:HG2	1:C:244:VAL:HG13	1.73	0.70
1:B:19:PRO:HG3	1:B:254:TYR:CE2	2.26	0.70
1:C:268:ALA:C	1:C:270:LEU:H	1.97	0.70
1:C:17:PHE:HD2	1:C:20:ILE:CG1	2.04	0.70
1:B:215:GLU:O	1:B:215:GLU:HG2	1.90	0.70
1:C:35:MSE:O	1:C:38:THR:HG22	1.93	0.69
1:B:29:GLU:HA	1:B:29:GLU:OE1	1.92	0.69
1:C:82:VAL:HG12	1:C:83:ASP:H	1.57	0.69
1:C:241:PRO:HB2	1:C:244:VAL:HG23	1.73	0.69
1:B:18:ASN:O	1:B:19:PRO:C	2.35	0.69
1:A:95:THR:N	2:A:501:NMN:O7	2.26	0.68
1:C:6:LYS:O	1:C:7:THR:HB	1.93	0.68
1:C:27:LEU:CD2	1:C:186:VAL:HG21	2.10	0.68
1:B:215:GLU:OE2	1:B:219:ASN:HB2	1.94	0.68
1:C:10:VAL:CG2	1:C:45:LYS:HG2	2.24	0.68
1:C:231:ARG:NH1	1:C:231:ARG:HB2	2.09	0.67
1:A:58:LYS:H	1:A:58:LYS:CD	2.07	0.67
1:B:255:SER:O	1:B:256:SER:HB3	1.93	0.67
1:C:27:LEU:HD22	1:C:186:VAL:HG22	1.71	0.67
1:A:45:LYS:HE3	1:A:47:ILE:HD11	1.76	0.67
1:A:268:ALA:C	1:A:270:LEU:H	2.02	0.67
1:C:168:LEU:HD11	2:C:501:NMN:HC5	1.76	0.67
1:B:26:ARG:HD3	1:B:219:ASN:HD21	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ILE:O	1:C:72:LEU:HD12	1.95	0.67
1:C:67:VAL:O	1:C:71:GLU:CG	2.43	0.67
1:B:56:LYS:HA	1:B:262:ASN:ND2	2.10	0.67
1:C:48:ILE:HG22	1:C:50:PRO:HD3	1.77	0.67
1:A:6:LYS:O	1:A:7:THR:HB	1.94	0.66
1:C:68:ILE:CG2	1:C:72:LEU:CD1	2.60	0.66
1:B:204:TRP:CZ3	1:C:232:ARG:HB3	2.30	0.66
1:C:227:ARG:NE	1:C:259:GLU:OE2	2.25	0.66
1:C:168:LEU:CD2	1:C:169:TRP:CD1	2.69	0.66
1:C:62:PRO:HG3	1:C:261:ARG:NH2	2.11	0.66
1:C:168:LEU:HD23	1:C:169:TRP:HE1	1.58	0.66
1:C:10:VAL:CG2	1:C:45:LYS:CG	2.74	0.66
1:C:34:TYR:HD2	1:C:35:MSE:HG2	1.59	0.66
1:A:55:TYR:CE2	1:A:57:LYS:HB2	2.31	0.65
1:A:232:ARG:HD3	1:C:204:TRP:CE3	2.30	0.65
1:C:26:ARG:HG3	1:C:26:ARG:NH1	2.04	0.65
1:B:268:ALA:HB3	1:B:269:PRO:HD3	1.78	0.65
1:B:168:LEU:CD1	1:B:268:ALA:CB	2.75	0.65
1:C:255:SER:O	1:C:256:SER:CB	2.45	0.65
1:B:168:LEU:CD1	1:B:268:ALA:HB2	2.27	0.64
1:A:148:VAL:HG12	1:A:148:VAL:O	1.96	0.64
1:A:250:LYS:HZ1	1:A:251:HIS:CE1	2.14	0.64
1:C:15:GLY:O	1:C:17:PHE:HD1	1.80	0.64
1:A:250:LYS:O	1:A:250:LYS:CE	2.46	0.64
1:C:21:THR:HA	1:C:240:VAL:HG13	1.79	0.64
1:A:222:SER:OG	1:A:225:LYS:HG2	1.98	0.64
1:B:148:VAL:O	1:B:148:VAL:CG1	2.46	0.63
1:C:187:THR:HG22	1:C:188:ARG:N	2.12	0.63
1:C:65:HIS:ND1	1:C:253:LEU:HD21	2.14	0.63
1:B:82:VAL:CG1	1:B:83:ASP:N	2.61	0.63
1:C:95:THR:HG1	2:C:501:NMN:HC2	1.64	0.63
1:C:18:ASN:O	1:C:19:PRO:C	2.39	0.62
1:C:235:SER:O	1:C:237:ARG:N	2.33	0.62
1:B:255:SER:OG	1:B:256:SER:N	2.30	0.62
1:A:246:GLU:HA	1:A:249:GLU:HG2	1.79	0.62
1:A:268:ALA:HB3	1:A:269:PRO:CD	2.30	0.62
1:C:17:PHE:O	1:C:18:ASN:O	2.16	0.62
1:B:183:LEU:HD12	1:B:183:LEU:C	2.25	0.62
1:C:237:ARG:O	1:C:238:TYR:CB	2.47	0.62
1:B:268:ALA:N	1:B:269:PRO:HD2	2.15	0.62
1:A:88:LEU:HD23	1:A:88:LEU:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLN:HA	1:B:103:GLN:NE2	2.15	0.61
1:C:252:ASN:HD22	1:C:252:ASN:H	1.47	0.61
1:A:246:GLU:HA	1:A:249:GLU:CG	2.31	0.61
1:C:268:ALA:HB3	1:C:269:PRO:HD3	1.81	0.61
1:C:237:ARG:O	1:C:238:TYR:HB2	2.00	0.61
1:A:55:TYR:CD2	1:A:57:LYS:HB2	2.36	0.61
1:B:65:HIS:CE1	1:B:253:LEU:HD21	2.36	0.61
1:C:26:ARG:NH1	1:C:26:ARG:CG	2.64	0.60
1:C:250:LYS:O	1:C:251:HIS:CB	2.46	0.60
1:A:230:LEU:HG	1:A:236:ILE:HD11	1.84	0.60
1:C:152:LYS:HG2	1:C:182:GLY:H	1.66	0.60
1:C:157:ALA:O	1:C:161:GLU:HG3	2.01	0.60
1:B:215:GLU:OE2	1:B:219:ASN:N	2.31	0.60
1:A:207:ARG:HG2	1:A:207:ARG:HH11	1.66	0.60
1:C:17:PHE:HB3	1:C:20:ILE:HD11	1.83	0.60
1:C:165:VAL:CG1	1:C:168:LEU:HB2	2.32	0.60
1:C:228:ARG:N	1:C:231:ARG:HH12	2.00	0.60
1:A:178:VAL:CG1	1:A:206:HIS:HB2	2.32	0.59
1:B:82:VAL:HG12	1:B:83:ASP:H	1.67	0.59
1:C:175:THR:O	1:C:178:VAL:HG12	2.02	0.59
1:A:170:LYS:O	1:A:173:ASP:N	2.34	0.59
1:C:34:TYR:HE2	1:C:35:MSE:SE	2.35	0.59
1:B:168:LEU:HD12	1:B:268:ALA:HB2	1.84	0.59
1:C:82:VAL:HG12	1:C:83:ASP:N	2.16	0.59
1:B:58:LYS:N	1:B:58:LYS:CE	2.46	0.59
1:C:26:ARG:NH1	1:C:30:LEU:HG	2.17	0.59
1:C:51:VAL:O	1:C:66:ARG:NH1	2.27	0.59
1:B:57:LYS:HA	1:B:58:LYS:HE2	1.85	0.59
1:B:83:ASP:C	1:B:83:ASP:OD1	2.44	0.58
1:C:266:ILE:HG13	1:C:268:ALA:H	1.67	0.58
1:A:170:LYS:O	1:A:173:ASP:HB2	2.03	0.58
1:C:242:ASP:O	1:C:243:LEU:C	2.46	0.58
1:A:226:ILE:HG23	1:A:236:ILE:CD1	2.33	0.58
1:A:246:GLU:O	1:A:249:GLU:HG3	2.02	0.58
1:B:174:ILE:O	1:B:178:VAL:HG23	2.02	0.58
1:B:250:LYS:O	1:B:251:HIS:CG	2.57	0.58
1:A:17:PHE:O	1:A:18:ASN:O	2.21	0.58
1:B:57:LYS:C	1:B:58:LYS:HE2	2.25	0.58
1:B:268:ALA:C	1:B:270:LEU:H	2.04	0.58
1:C:152:LYS:NZ	1:C:182:GLY:HA3	2.17	0.58
1:B:204:TRP:CE2	1:B:207:ARG:NH1	2.71	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:VAL:HG23	1:C:215:GLU:OE1	2.03	0.58
1:B:58:LYS:NZ	1:B:266:ILE:HG22	2.19	0.58
1:C:18:ASN:O	1:C:20:ILE:HD12	2.04	0.57
1:B:255:SER:O	1:B:256:SER:CB	2.52	0.57
1:B:268:ALA:H	1:B:269:PRO:HD2	1.70	0.57
1:A:237:ARG:HG3	1:A:238:TYR:CD2	2.39	0.57
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.70	0.57
1:C:237:ARG:HG2	1:C:238:TYR:CZ	2.39	0.57
1:C:34:TYR:CE2	1:C:35:MSE:SE	3.08	0.57
1:B:251:HIS:O	1:B:252:ASN:C	2.48	0.57
1:A:87:SER:C	1:A:88:LEU:HD23	2.30	0.56
1:A:236:ILE:HA	1:A:239:LEU:HD12	1.86	0.56
1:C:226:ILE:HG12	1:C:236:ILE:HG12	1.86	0.56
1:B:27:LEU:HG	1:B:186:VAL:CG2	2.35	0.56
1:C:63:ALA:O	1:C:64:TYR:C	2.47	0.56
1:C:231:ARG:HD2	1:C:256:SER:HB3	1.86	0.56
1:C:268:ALA:N	1:C:269:PRO:HD2	2.21	0.56
1:C:266:ILE:O	1:C:269:PRO:HD2	2.04	0.56
1:C:235:SER:C	1:C:237:ARG:H	2.14	0.56
1:B:22:ASN:ND2	1:B:239:LEU:C	2.63	0.56
1:C:18:ASN:CG	1:C:19:PRO:HD3	2.30	0.56
1:C:22:ASN:ND2	1:C:238:TYR:O	2.38	0.56
1:C:61:ILE:HD12	1:C:253:LEU:HD22	1.87	0.56
1:B:204:TRP:CE3	1:C:232:ARG:HD3	2.41	0.56
1:A:168:LEU:HD12	1:A:268:ALA:CB	2.36	0.55
1:B:58:LYS:H	1:B:58:LYS:CD	2.19	0.55
1:C:268:ALA:N	1:C:269:PRO:CD	2.69	0.55
1:A:250:LYS:NZ	1:A:251:HIS:NE2	2.52	0.55
1:B:21:THR:N	1:B:24:HIS:HD2	2.01	0.55
1:B:82:VAL:CG1	1:B:83:ASP:H	2.19	0.55
1:C:170:LYS:O	1:C:171:SER:C	2.50	0.55
1:A:204:TRP:CG	1:B:232:ARG:NH1	2.76	0.54
1:C:35:MSE:SE	1:C:184:ILE:HD11	2.58	0.54
1:C:68:ILE:HG22	1:C:72:LEU:HD12	1.83	0.54
1:A:191:ASN:O	1:A:192:ASP:C	2.50	0.54
1:A:251:HIS:O	1:A:252:ASN:C	2.51	0.54
1:B:17:PHE:O	1:B:18:ASN:O	2.25	0.54
1:B:57:LYS:CA	1:B:58:LYS:HE2	2.36	0.54
1:B:152:LYS:HD3	1:B:182:GLY:CA	2.35	0.54
1:C:65:HIS:CE1	1:C:253:LEU:HD21	2.42	0.54
1:B:177:ILE:O	1:B:181:TYR:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:TYR:CD2	1:C:35:MSE:N	2.76	0.54
1:C:228:ARG:HA	1:C:231:ARG:CZ	2.36	0.54
1:C:191:ASN:O	1:C:192:ASP:C	2.51	0.54
1:A:157:ALA:O	1:A:161:GLU:HG3	2.08	0.54
1:A:216:TRP:O	1:A:217:ILE:HG23	2.08	0.54
1:A:226:ILE:HG23	1:A:236:ILE:HD11	1.90	0.54
1:C:12:LEU:HD22	1:C:13:ALA:N	2.22	0.54
1:B:21:THR:H	1:B:24:HIS:CD2	2.17	0.53
1:B:250:LYS:O	1:B:251:HIS:CB	2.55	0.53
1:B:268:ALA:N	1:B:269:PRO:CD	2.71	0.53
1:C:7:THR:HG22	1:C:7:THR:O	2.07	0.53
1:C:61:ILE:HD11	1:C:65:HIS:CB	2.38	0.53
1:C:251:HIS:O	1:C:252:ASN:C	2.51	0.53
1:A:207:ARG:HG2	1:A:207:ARG:NH1	2.24	0.53
1:A:228:ARG:HD3	1:A:232:ARG:NH2	2.22	0.53
1:A:237:ARG:HG3	1:A:238:TYR:CE2	2.44	0.53
1:C:38:THR:HG21	1:C:41:TYR:HD2	1.74	0.53
1:A:18:ASN:CB	1:A:19:PRO:HD3	2.29	0.53
1:C:168:LEU:HD23	1:C:169:TRP:HD1	1.61	0.53
1:A:26:ARG:HH11	1:A:26:ARG:HG2	1.74	0.53
1:B:170:LYS:O	1:B:173:ASP:N	2.41	0.53
1:A:190:GLY:HA3	1:A:214:ASN:HD21	1.74	0.52
1:A:204:TRP:CZ3	1:B:232:ARG:HB3	2.44	0.52
1:C:177:ILE:HG22	1:C:178:VAL:N	2.25	0.52
1:A:82:VAL:CG1	1:A:83:ASP:N	2.71	0.52
1:C:244:VAL:O	1:C:245:GLN:C	2.50	0.52
1:C:247:TYR:HE1	1:C:253:LEU:CD1	2.17	0.52
1:C:252:ASN:HD22	1:C:252:ASN:N	2.06	0.52
1:B:173:ASP:O	1:B:177:ILE:HG13	2.09	0.52
1:C:165:VAL:HG12	1:C:168:LEU:HB2	1.91	0.52
1:A:9:VAL:CG1	1:A:10:VAL:N	2.72	0.52
1:B:235:SER:O	1:B:236:ILE:HB	2.09	0.52
1:C:168:LEU:HD21	1:C:169:TRP:HE1	1.75	0.52
1:C:241:PRO:HD2	1:C:244:VAL:HG21	1.91	0.52
1:A:166:PRO:O	1:A:167:ASN:HB2	2.09	0.52
1:B:172:GLU:HG3	1:B:176:GLN:NE2	2.25	0.52
1:C:191:ASN:O	1:C:194:GLN:N	2.42	0.52
1:C:231:ARG:HG3	1:C:255:SER:O	2.10	0.52
1:A:96:LEU:HD12	1:A:96:LEU:O	2.10	0.51
1:B:12:LEU:HD12	1:B:99:LEU:HD23	1.91	0.51
1:C:16:SER:CA	1:C:51:VAL:CG2	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:THR:HG23	1:C:40:ARG:N	2.17	0.51
1:C:221:ILE:CG2	1:C:226:ILE:HD12	2.40	0.51
1:A:18:ASN:CB	1:A:19:PRO:CD	2.62	0.51
1:B:16:SER:CA	1:B:51:VAL:CG2	2.75	0.51
1:B:191:ASN:O	1:B:192:ASP:C	2.53	0.51
1:B:250:LYS:O	1:B:250:LYS:HG2	2.10	0.51
1:B:255:SER:OG	1:B:257:GLU:N	2.44	0.51
1:B:155:CYS:O	1:B:185:CYS:HA	2.11	0.51
1:A:250:LYS:CE	1:A:251:HIS:CE1	2.93	0.51
1:C:247:TYR:CE1	1:C:253:LEU:HD11	2.32	0.51
1:C:152:LYS:HG2	1:C:182:GLY:N	2.26	0.50
1:A:228:ARG:HD3	1:A:232:ARG:CZ	2.41	0.50
1:B:26:ARG:CG	1:B:26:ARG:HH11	2.24	0.50
1:B:204:TRP:CD2	1:B:207:ARG:NH1	2.80	0.50
1:C:237:ARG:HG2	1:C:238:TYR:CE1	2.47	0.50
1:C:16:SER:CB	2:C:501:NMN:O3P	2.60	0.50
1:B:245:GLN:NE2	1:B:249:GLU:CD	2.68	0.50
1:C:221:ILE:HG22	1:C:226:ILE:HD12	1.93	0.50
1:B:38:THR:HG21	1:B:41:TYR:HD2	1.77	0.50
1:B:170:LYS:O	1:B:173:ASP:HB2	2.11	0.50
1:C:32:LYS:HA	1:C:43:VAL:HG21	1.94	0.49
1:A:216:TRP:C	1:A:217:ILE:HG23	2.37	0.49
1:B:204:TRP:CZ2	1:B:207:ARG:NH2	2.80	0.49
1:C:16:SER:HA	1:C:51:VAL:HG21	1.92	0.49
1:A:177:ILE:O	1:A:181:TYR:O	2.29	0.49
1:B:234:GLN:HA	1:B:234:GLN:NE2	2.27	0.49
1:A:82:VAL:HG12	1:A:83:ASP:H	1.74	0.49
1:A:85:TRP:CE2	1:A:101:HIS:CE1	3.00	0.49
1:C:23:MSE:HE3	1:C:221:ILE:C	2.37	0.49
1:A:188:ARG:HD3	1:A:218:ALA:HA	1.95	0.49
1:C:19:PRO:HG3	1:C:254:TYR:CZ	2.48	0.49
1:C:32:LYS:HG3	1:C:43:VAL:HG11	1.95	0.49
1:C:230:LEU:HD21	1:C:236:ILE:HD12	1.95	0.49
1:C:236:ILE:HA	1:C:239:LEU:HD12	1.94	0.49
1:C:216:TRP:O	1:C:217:ILE:HB	2.13	0.48
1:C:245:GLN:O	1:C:248:ILE:HB	2.13	0.48
1:A:178:VAL:HG11	1:A:206:HIS:HB2	1.94	0.48
1:B:221:ILE:CG2	1:B:226:ILE:HD11	2.43	0.48
1:A:85:TRP:CD1	1:A:101:HIS:CE1	3.02	0.48
1:B:226:ILE:HG23	1:B:236:ILE:HD11	1.93	0.48
1:C:234:GLN:OE1	1:C:234:GLN:CA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:PRO:O	1:A:271:GLN:N	2.46	0.48
1:C:152:LYS:HZ2	1:C:182:GLY:HA3	1.78	0.48
1:A:268:ALA:C	1:A:270:LEU:N	2.66	0.48
1:B:83:ASP:OD2	1:B:102:HIS:HE1	1.95	0.48
1:B:166:PRO:O	1:B:167:ASN:HB2	2.12	0.48
1:A:38:THR:CG2	1:A:40:ARG:H	2.17	0.48
1:A:255:SER:O	1:A:256:SER:CB	2.33	0.48
1:B:64:TYR:O	1:B:68:ILE:HG13	2.13	0.48
1:B:198:TYR:CZ	1:C:228:ARG:HD2	2.49	0.48
1:B:266:ILE:HG13	1:B:268:ALA:H	1.79	0.48
1:A:235:SER:C	1:A:237:ARG:H	2.22	0.48
1:B:57:LYS:HA	1:B:58:LYS:CE	2.43	0.48
1:C:222:SER:HG	1:C:225:LYS:H	1.62	0.48
1:B:183:LEU:HD12	1:B:184:ILE:N	2.29	0.47
1:B:216:TRP:O	1:B:217:ILE:CD1	2.46	0.47
1:C:61:ILE:HD11	1:C:65:HIS:HB2	1.95	0.47
1:A:26:ARG:HG2	1:A:26:ARG:NH1	2.28	0.47
1:C:74:THR:O	1:C:75:LYS:C	2.56	0.47
1:C:20:ILE:HD12	1:C:20:ILE:N	2.28	0.47
1:C:100:ARG:O	1:C:101:HIS:C	2.58	0.47
1:C:230:LEU:HD23	1:C:230:LEU:HA	1.66	0.47
1:B:204:TRP:CD2	1:C:232:ARG:HD3	2.50	0.47
1:C:229:ALA:HB1	1:C:234:GLN:HB2	1.96	0.47
1:A:168:LEU:HD12	1:A:268:ALA:HB1	1.96	0.47
1:C:227:ARG:HH11	1:C:227:ARG:CG	2.15	0.47
1:C:258:SER:O	1:C:261:ARG:HB2	2.15	0.47
1:A:83:ASP:OD2	1:A:102:HIS:CE1	2.68	0.47
1:A:170:LYS:O	1:A:171:SER:C	2.58	0.47
1:C:22:ASN:ND2	1:C:239:LEU:CA	2.77	0.47
1:C:211:HIS:N	1:C:211:HIS:CD2	2.82	0.47
1:B:38:THR:HG23	1:B:40:ARG:N	2.23	0.47
1:A:226:ILE:CG2	1:A:236:ILE:HD11	2.45	0.47
1:B:18:ASN:CB	1:B:19:PRO:CD	2.70	0.47
1:B:19:PRO:HD3	1:B:254:TYR:OH	2.16	0.46
1:C:56:LYS:HA	1:C:262:ASN:ND2	2.30	0.46
1:B:26:ARG:HH21	1:B:30:LEU:HD21	1.80	0.46
1:C:155:CYS:SG	1:C:183:LEU:HD11	2.55	0.46
1:C:237:ARG:O	1:C:238:TYR:CG	2.69	0.46
1:B:183:LEU:C	1:B:183:LEU:CD1	2.89	0.46
1:C:158:ASP:O	1:C:159:LEU:C	2.59	0.46
1:A:12:LEU:HD11	1:A:102:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:NH1	1:B:26:ARG:HG2	2.29	0.46
1:C:195:LYS:O	1:C:196:PHE:C	2.59	0.46
1:B:236:ILE:HA	1:B:236:ILE:HD12	1.70	0.46
1:A:152:LYS:HG3	1:A:182:GLY:CA	2.45	0.46
1:A:241:PRO:O	1:A:244:VAL:HB	2.14	0.46
1:B:175:THR:O	1:B:176:GLN:C	2.57	0.46
1:C:247:TYR:CD1	1:C:247:TYR:C	2.93	0.46
1:A:195:LYS:O	1:A:196:PHE:C	2.58	0.46
1:C:172:GLU:O	1:C:172:GLU:HG3	2.16	0.46
1:C:47:ILE:HD13	1:C:102:HIS:CD2	2.51	0.46
1:C:165:VAL:HG11	1:C:168:LEU:HB2	1.97	0.46
1:C:94:GLU:O	1:C:97:LYS:N	2.49	0.45
1:A:232:ARG:HB3	1:C:204:TRP:CZ3	2.51	0.45
1:C:77:SER:HG	1:C:80:VAL:H	1.64	0.45
1:C:228:ARG:O	1:C:232:ARG:HG3	2.16	0.45
1:C:268:ALA:H	1:C:269:PRO:HD2	1.82	0.45
1:B:215:GLU:O	1:B:215:GLU:CG	2.60	0.45
1:C:178:VAL:HG13	1:C:179:ALA:N	2.30	0.45
1:A:187:THR:HG22	1:A:189:ALA:N	2.23	0.45
1:C:23:MSE:O	1:C:24:HIS:C	2.56	0.45
1:C:229:ALA:O	1:C:230:LEU:C	2.59	0.45
1:A:155:CYS:SG	1:A:183:LEU:HD11	2.57	0.45
1:A:172:GLU:O	1:A:172:GLU:HG3	2.17	0.45
1:A:229:ALA:HB1	1:A:234:GLN:HB2	1.98	0.45
1:B:221:ILE:HG21	1:B:226:ILE:HD11	1.98	0.45
1:C:215:GLU:OE2	1:C:219:ASN:HB2	2.16	0.45
1:A:74:THR:O	1:A:75:LYS:C	2.60	0.45
1:B:195:LYS:O	1:B:196:PHE:C	2.59	0.45
1:C:219:ASN:O	1:C:220:ASP:HB3	2.15	0.45
1:B:85:TRP:CD2	1:B:101:HIS:CD2	3.04	0.45
1:B:266:ILE:O	1:B:269:PRO:HD2	2.16	0.45
1:A:82:VAL:CG1	1:A:83:ASP:H	2.29	0.45
1:B:168:LEU:HD11	2:B:501:NMN:HC5	1.99	0.45
1:B:268:ALA:HB3	1:B:269:PRO:CD	2.45	0.45
1:B:154:LEU:HD12	1:B:154:LEU:HA	1.73	0.45
1:A:230:LEU:HG	1:A:236:ILE:CD1	2.48	0.44
1:B:163:PHE:HE1	1:B:169:TRP:CZ3	2.36	0.44
1:B:168:LEU:HA	1:B:268:ALA:HB1	2.00	0.44
1:C:12:LEU:HA	1:C:12:LEU:HD23	1.54	0.44
1:C:175:THR:O	1:C:176:GLN:C	2.61	0.44
1:C:236:ILE:HG23	1:C:240:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:MSE:HE3	1:A:221:ILE:C	2.42	0.44
1:A:67:VAL:HG21	1:A:84:THR:HG22	1.98	0.44
1:A:195:LYS:O	1:A:198:TYR:N	2.50	0.44
1:C:166:PRO:O	1:C:167:ASN:HB2	2.17	0.44
1:C:178:VAL:CG1	1:C:179:ALA:N	2.81	0.44
1:A:178:VAL:CG1	1:A:206:HIS:CB	2.95	0.44
1:A:237:ARG:CG	1:A:238:TYR:CE2	3.01	0.44
1:B:38:THR:HG21	1:B:41:TYR:CD2	2.53	0.44
1:B:100:ARG:O	1:B:101:HIS:C	2.61	0.44
1:B:155:CYS:SG	1:B:159:LEU:HB3	2.58	0.44
1:C:230:LEU:CG	1:C:236:ILE:HD12	2.47	0.44
1:A:148:VAL:O	1:A:148:VAL:CG1	2.65	0.44
1:B:86:GLU:CD	1:B:98:VAL:HG21	2.42	0.44
1:B:228:ARG:HG3	1:B:228:ARG:HH11	1.83	0.44
1:B:204:TRP:CZ2	1:B:207:ARG:CZ	3.01	0.44
1:C:266:ILE:HG13	1:C:267:LEU:N	2.29	0.44
1:A:32:LYS:O	1:A:33:ASP:C	2.60	0.44
1:A:229:ALA:O	1:A:230:LEU:C	2.61	0.44
1:C:31:ALA:O	1:C:34:TYR:HB3	2.18	0.44
1:A:61:ILE:HB	1:A:62:PRO:HD2	2.00	0.43
1:B:103:GLN:NE2	1:B:103:GLN:CA	2.80	0.43
1:C:241:PRO:O	1:C:244:VAL:HB	2.18	0.43
1:B:170:LYS:O	1:B:171:SER:C	2.60	0.43
1:C:155:CYS:O	1:C:185:CYS:HA	2.18	0.43
1:C:177:ILE:O	1:C:181:TYR:O	2.35	0.43
1:C:18:ASN:O	1:C:20:ILE:N	2.52	0.43
1:A:161:GLU:HA	1:A:196:PHE:CZ	2.53	0.43
1:A:235:SER:O	1:A:237:ARG:N	2.48	0.43
1:C:174:ILE:O	1:C:175:THR:C	2.60	0.43
1:B:230:LEU:HA	1:B:230:LEU:HD23	1.69	0.43
1:B:268:ALA:C	1:B:270:LEU:N	2.68	0.43
1:C:237:ARG:HG2	1:C:238:TYR:CE2	2.53	0.43
1:A:32:LYS:HA	1:A:43:VAL:HG21	2.00	0.43
1:A:63:ALA:O	1:A:64:TYR:C	2.61	0.43
1:A:191:ASN:O	1:A:194:GLN:N	2.51	0.43
1:A:244:VAL:O	1:A:245:GLN:C	2.58	0.43
1:C:10:VAL:HG21	1:C:45:LYS:HG2	2.00	0.43
1:C:30:LEU:HD23	1:C:30:LEU:HA	1.77	0.43
1:C:35:MSE:SE	1:C:184:ILE:CD1	3.17	0.43
1:C:221:ILE:CG2	1:C:226:ILE:CD1	2.96	0.43
1:B:6:LYS:O	1:B:7:THR:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:LEU:HD22	1:C:13:ALA:H	1.84	0.43
1:C:165:VAL:HG12	1:C:168:LEU:CB	2.49	0.43
1:A:245:GLN:HE21	1:A:245:GLN:HB3	1.72	0.43
1:B:235:SER:C	1:B:237:ARG:H	2.27	0.43
1:B:237:ARG:O	1:B:238:TYR:HB2	2.19	0.43
1:B:19:PRO:HG3	1:B:254:TYR:CZ	2.54	0.43
1:C:9:VAL:CG1	1:C:10:VAL:N	2.82	0.42
1:C:23:MSE:HE3	1:C:221:ILE:O	2.19	0.42
1:C:27:LEU:CD2	1:C:186:VAL:HG22	2.36	0.42
1:A:18:ASN:O	1:A:20:ILE:N	2.53	0.42
1:A:100:ARG:O	1:A:101:HIS:C	2.61	0.42
1:A:165:VAL:HB	1:A:168:LEU:HD22	2.01	0.42
1:B:269:PRO:C	1:B:270:LEU:HG	2.44	0.42
1:A:85:TRP:NE1	1:A:101:HIS:CE1	2.87	0.42
1:B:16:SER:O	1:B:17:PHE:C	2.62	0.42
1:C:20:ILE:O	1:C:240:VAL:CG1	2.68	0.42
1:C:69:MSE:HE3	1:C:69:MSE:HB2	1.85	0.42
1:C:228:ARG:CA	1:C:231:ARG:NH1	2.59	0.42
1:A:64:TYR:CE2	1:A:68:ILE:HD11	2.55	0.42
1:A:6:LYS:O	1:A:40:ARG:O	2.37	0.42
1:A:84:THR:O	1:A:88:LEU:HG	2.19	0.42
1:C:23:MSE:CE	1:C:221:ILE:N	2.83	0.42
1:C:163:PHE:CZ	1:C:174:ILE:HG23	2.53	0.42
1:C:235:SER:C	1:C:237:ARG:N	2.77	0.42
1:A:165:VAL:HA	1:A:166:PRO:HD3	1.94	0.42
1:A:269:PRO:C	1:A:271:GLN:N	2.77	0.42
1:C:187:THR:CG2	1:C:189:ALA:H	2.01	0.42
1:A:15:GLY:O	1:A:16:SER:C	2.61	0.42
1:A:228:ARG:O	1:A:229:ALA:C	2.62	0.42
1:A:106:LEU:C	1:A:108:ALA:H	2.28	0.41
1:B:92:TRP:CH2	1:B:94:GLU:HA	2.55	0.41
1:A:71:GLU:HG3	1:A:82:VAL:HG21	2.00	0.41
1:C:17:PHE:O	1:C:20:ILE:CD1	2.67	0.41
1:C:236:ILE:HG23	1:C:240:VAL:HG23	2.02	0.41
1:A:204:TRP:CD1	1:A:207:ARG:HD3	2.55	0.41
1:A:250:LYS:O	1:A:251:HIS:CD2	2.73	0.41
1:B:188:ARG:NH2	1:B:220:ASP:OD2	2.51	0.41
1:B:226:ILE:HG23	1:B:236:ILE:CG1	2.51	0.41
1:B:235:SER:O	1:B:237:ARG:N	2.53	0.41
1:C:63:ALA:O	1:C:66:ARG:N	2.54	0.41
1:C:67:VAL:O	1:C:68:ILE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:THR:O	1:A:176:GLN:C	2.63	0.41
1:B:65:HIS:ND1	1:B:247:TYR:OH	2.42	0.41
1:B:103:GLN:HA	1:B:103:GLN:HE21	1.83	0.41
1:A:250:LYS:O	1:A:251:HIS:CB	2.69	0.41
1:B:219:ASN:O	1:B:220:ASP:CB	2.68	0.41
1:C:223:SER:O	1:C:224:THR:C	2.64	0.41
1:A:27:LEU:HA	1:A:27:LEU:HD23	1.51	0.41
1:B:92:TRP:CG	1:B:93:LYS:N	2.88	0.41
1:C:20:ILE:HD12	1:C:20:ILE:H	1.86	0.41
1:C:25:LEU:HD22	1:C:25:LEU:HA	1.73	0.41
1:C:237:ARG:C	1:C:238:TYR:CG	2.97	0.41
1:B:74:THR:O	1:B:75:LYS:C	2.63	0.41
1:B:168:LEU:HG	1:B:169:TRP:CD1	2.56	0.41
1:C:18:ASN:OD1	1:C:254:TYR:CE1	2.74	0.41
1:C:23:MSE:O	1:C:26:ARG:N	2.54	0.41
1:C:168:LEU:O	1:C:168:LEU:HG	2.20	0.41
1:C:228:ARG:O	1:C:229:ALA:C	2.62	0.41
1:A:27:LEU:HD21	1:A:215:GLU:OE2	2.21	0.41
1:C:21:THR:O	1:C:22:ASN:C	2.64	0.40
1:C:53:ASP:OD2	1:C:63:ALA:N	2.49	0.40
1:A:26:ARG:O	1:A:27:LEU:C	2.62	0.40
1:B:195:LYS:HE2	1:B:195:LYS:HB2	1.72	0.40
1:C:82:VAL:CG1	1:C:83:ASP:H	2.31	0.40
1:A:250:LYS:HZ3	1:A:251:HIS:CE1	2.37	0.40
1:B:203:LEU:O	1:B:204:TRP:C	2.62	0.40
1:C:221:ILE:HG22	1:C:221:ILE:O	2.22	0.40
1:A:152:LYS:HG3	1:A:182:GLY:HA3	2.04	0.40
1:A:227:ARG:O	1:A:228:ARG:C	2.63	0.40
1:B:178:VAL:HG23	1:B:178:VAL:H	1.64	0.40
1:A:8:GLU:HB3	1:A:44:VAL:HG23	2.04	0.40
1:B:103:GLN:CA	1:B:103:GLN:HE21	2.35	0.40
1:C:85:TRP:CD2	1:C:85:TRP:C	3.00	0.40
1:C:187:THR:CG2	1:C:188:ARG:N	2.79	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	224/290 (77%)	189 (84%)	25 (11%)	10 (4%)	2	8
1	B	224/290 (77%)	188 (84%)	26 (12%)	10 (4%)	2	8
1	C	224/290 (77%)	184 (82%)	29 (13%)	11 (5%)	1	6
All	All	672/870 (77%)	561 (84%)	80 (12%)	31 (5%)	2	7

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	251	HIS
1	A	265	VAL
1	B	18	ASN
1	B	251	HIS
1	C	18	ASN
1	C	251	HIS
1	A	234	GLN
1	A	256	SER
1	A	269	PRO
1	B	234	GLN
1	B	236	ILE
1	B	256	SER
1	B	265	VAL
1	B	269	PRO
1	C	236	ILE
1	C	256	SER
1	C	265	VAL
1	C	269	PRO
1	A	270	LEU
1	B	252	ASN
1	C	234	GLN
1	C	270	LEU
1	A	236	ILE

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Mol	Chain	Res	Type
1	A	217	ILE
1	A	219	ASN
1	B	7	THR
1	B	217	ILE
1	C	7	THR
1	C	217	ILE
1	C	252	ASN

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	199/253 (79%)	173 (87%)	26 (13%)	4	13
1	B	199/253 (79%)	166 (83%)	33 (17%)	2	7
1	C	199/253 (79%)	160 (80%)	39 (20%)	1	5
All	All	597/759 (79%)	499 (84%)	98 (16%)	2	8

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	45	LYS
1	A	58	LYS
1	A	68	ILE
1	A	69	MSE
1	A	74	THR
1	A	94	GLU
1	A	107	GLU
1	A	148	VAL
1	A	159	LEU
1	A	175	THR
1	A	178	VAL
1	A	186	VAL
1	A	191	ASN
1	A	194	GLN

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Mol	Chain	Res	Type
1	A	195	LYS
1	A	199	GLU
1	A	200	SER
1	A	205	LYS
1	A	217	ILE
1	A	235	SER
1	A	236	ILE
1	A	249	GLU
1	A	256	SER
1	A	260	ASP
1	A	267	LEU
1	B	7	THR
1	B	9	VAL
1	B	12	LEU
1	B	26	ARG
1	B	44	VAL
1	B	45	LYS
1	B	51	VAL
1	B	58	LYS
1	B	61	ILE
1	B	74	THR
1	B	106	LEU
1	B	148	VAL
1	B	175	THR
1	B	176	GLN
1	B	183	LEU
1	B	187	THR
1	B	188	ARG
1	B	191	ASN
1	B	195	LYS
1	B	197	ILE
1	B	199	GLU
1	B	200	SER
1	B	202	VAL
1	B	205	LYS
1	B	217	ILE
1	B	234	GLN
1	B	236	ILE
1	B	240	VAL
1	B	245	GLN
1	B	251	HIS
1	B	253	LEU

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Mol	Chain	Res	Type
1	B	266	ILE
1	B	270	LEU
1	C	7	THR
1	C	9	VAL
1	C	10	VAL
1	C	11	LEU
1	C	12	LEU
1	C	25	LEU
1	C	26	ARG
1	C	27	LEU
1	C	42	THR
1	C	44	VAL
1	C	51	VAL
1	C	58	LYS
1	C	61	ILE
1	C	69	MSE
1	C	77	SER
1	C	150	LYS
1	C	151	VAL
1	C	159	LEU
1	C	165	VAL
1	C	168	LEU
1	C	173	ASP
1	C	174	ILE
1	C	183	LEU
1	C	186	VAL
1	C	188	ARG
1	C	199	GLU
1	C	200	SER
1	C	226	ILE
1	C	231	ARG
1	C	234	GLN
1	C	236	ILE
1	C	240	VAL
1	C	242	ASP
1	C	248	ILE
1	C	257	GLU
1	C	259	GLU
1	C	266	ILE
1	C	267	LEU
1	C	270	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	167	ASN
1	A	206	HIS
1	A	214	ASN
1	A	245	GLN
1	B	18	ASN
1	B	24	HIS
1	B	76	ASN
1	B	102	HIS
1	B	103	GLN
1	B	176	GLN
1	B	180	ASN
1	B	191	ASN
1	B	219	ASN
1	B	234	GLN
1	B	245	GLN
1	C	22	ASN
1	C	89	GLN
1	C	102	HIS
1	C	167	ASN
1	C	176	GLN
1	C	206	HIS
1	C	252	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	501	-	21,23,23	3.66	5 (23%)	27,34,34	3.02	11 (40%)
2	NMN	C	501	-	21,23,23	3.57	5 (23%)	27,34,34	3.32	9 (33%)
2	NMN	B	501	-	21,23,23	3.79	6 (28%)	27,34,34	3.82	10 (37%)

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	501	-	2/2/6/6	7/14/30/30	0/2/2/2
2	NMN	C	501	-	1/1/6/6	3/14/30/30	0/2/2/2
2	NMN	B	501	-	1/1/6/6	7/14/30/30	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NMN	O3R-C3R	-8.99	1.20	1.43
2	A	501	NMN	O3R-C3R	-8.79	1.21	1.43
2	A	501	NMN	C3R-C4R	-8.66	1.31	1.53
2	B	501	NMN	C3R-C4R	-8.56	1.31	1.53
2	C	501	NMN	O2R-C2R	-8.37	1.22	1.43
2	C	501	NMN	C3R-C4R	-8.20	1.32	1.53
2	C	501	NMN	O3R-C3R	-8.09	1.22	1.43
2	B	501	NMN	O2R-C2R	-8.07	1.23	1.43
2	B	501	NMN	C2R-C3R	-8.06	1.31	1.53
2	A	501	NMN	O2R-C2R	-8.00	1.23	1.43
2	C	501	NMN	C2R-C3R	-7.14	1.34	1.53
2	A	501	NMN	C2R-C3R	-6.97	1.34	1.53
2	A	501	NMN	O4R-C1R	3.13	1.45	1.40
2	C	501	NMN	O4R-C1R	2.47	1.44	1.40
2	B	501	NMN	O4R-C1R	2.34	1.44	1.40
2	B	501	NMN	C3-C7	-2.12	1.47	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NMN	C4R-O4R-C1R	-16.74	94.59	109.92
2	C	501	NMN	C4R-O4R-C1R	-13.99	97.11	109.92
2	A	501	NMN	C4R-O4R-C1R	-11.08	99.78	109.92
2	A	501	NMN	O4R-C4R-C5R	4.79	124.68	109.33
2	B	501	NMN	O4R-C4R-C5R	4.40	123.42	109.33
2	B	501	NMN	O4R-C4R-C3R	4.01	113.11	105.15
2	B	501	NMN	O3R-C3R-C4R	3.87	122.19	111.08
2	C	501	NMN	O4R-C4R-C5R	3.67	121.10	109.33
2	C	501	NMN	O2R-C2R-C3R	3.64	123.49	111.82
2	B	501	NMN	O2R-C2R-C3R	3.63	123.45	111.82
2	A	501	NMN	C6-N1-C2	-3.61	118.81	121.88
2	C	501	NMN	O2P-P-O1P	3.60	121.29	107.80
2	B	501	NMN	O2P-P-O1P	3.55	121.10	107.80
2	C	501	NMN	O3R-C3R-C2R	3.47	122.95	111.82
2	C	501	NMN	O3R-C3R-C4R	3.43	120.94	111.08
2	A	501	NMN	O2R-C2R-C3R	3.25	122.24	111.82
2	A	501	NMN	C5-C4-C3	-3.25	117.17	120.36
2	A	501	NMN	O2P-P-O1P	3.22	119.89	107.80
2	B	501	NMN	O3R-C3R-C2R	3.14	121.88	111.82
2	A	501	NMN	C2R-C3R-C4R	3.13	108.66	102.61
2	A	501	NMN	O3R-C3R-C2R	3.08	121.69	111.82
2	A	501	NMN	O3R-C3R-C4R	2.89	119.40	111.08
2	C	501	NMN	C5R-C4R-C3R	2.77	125.18	115.21
2	A	501	NMN	O4R-C4R-C3R	2.60	110.32	105.15
2	A	501	NMN	C5R-C4R-C3R	2.57	124.47	115.21
2	C	501	NMN	C6-N1-C1R	-2.23	115.34	119.73
2	B	501	NMN	C2-C3-C4	2.18	120.80	118.26
2	B	501	NMN	C3-C7-N7	-2.10	115.15	117.74
2	B	501	NMN	C2R-C3R-C4R	2.02	106.51	102.61
2	C	501	NMN	O4R-C4R-C3R	2.02	109.16	105.15

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	NMN	C2R
2	A	501	NMN	C4R
2	B	501	NMN	C2R
2	C	501	NMN	C2R

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NMN	C5R-O5R-P-O2P
2	A	501	NMN	O4R-C1R-N1-C2
2	A	501	NMN	O4R-C1R-N1-C6
2	B	501	NMN	C5R-O5R-P-O3P
2	B	501	NMN	C5R-O5R-P-O1P
2	B	501	NMN	C5R-O5R-P-O2P
2	B	501	NMN	O4R-C1R-N1-C2
2	B	501	NMN	O4R-C1R-N1-C6
2	B	501	NMN	O4R-C4R-C5R-O5R
2	C	501	NMN	C3R-C4R-C5R-O5R
2	A	501	NMN	C3R-C4R-C5R-O5R
2	B	501	NMN	C3R-C4R-C5R-O5R
2	C	501	NMN	O4R-C4R-C5R-O5R
2	A	501	NMN	C5R-O5R-P-O3P
2	C	501	NMN	O4R-C1R-N1-C2
2	A	501	NMN	C5R-O5R-P-O1P
2	A	501	NMN	O4R-C4R-C5R-O5R

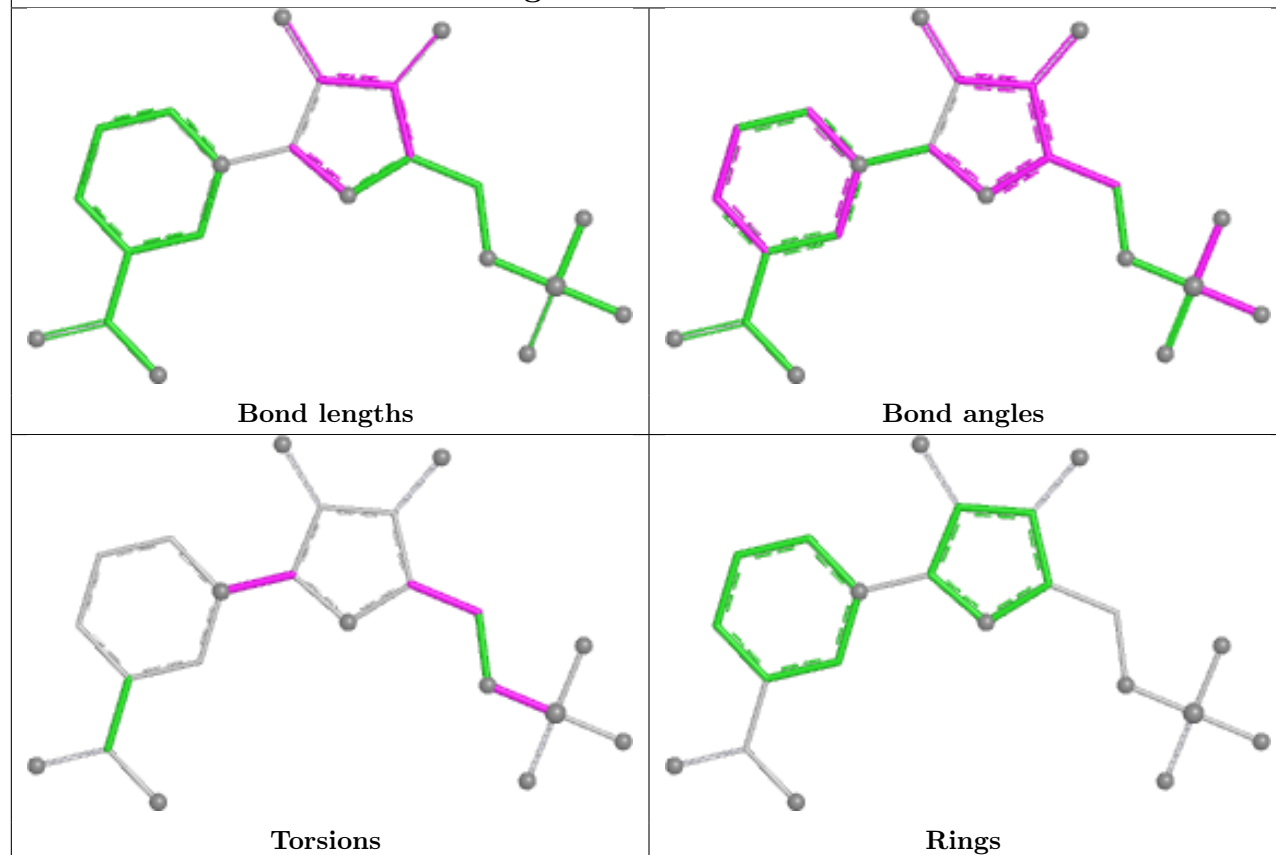
There are no ring outliers.

3 monomers are involved in 10 short contacts:

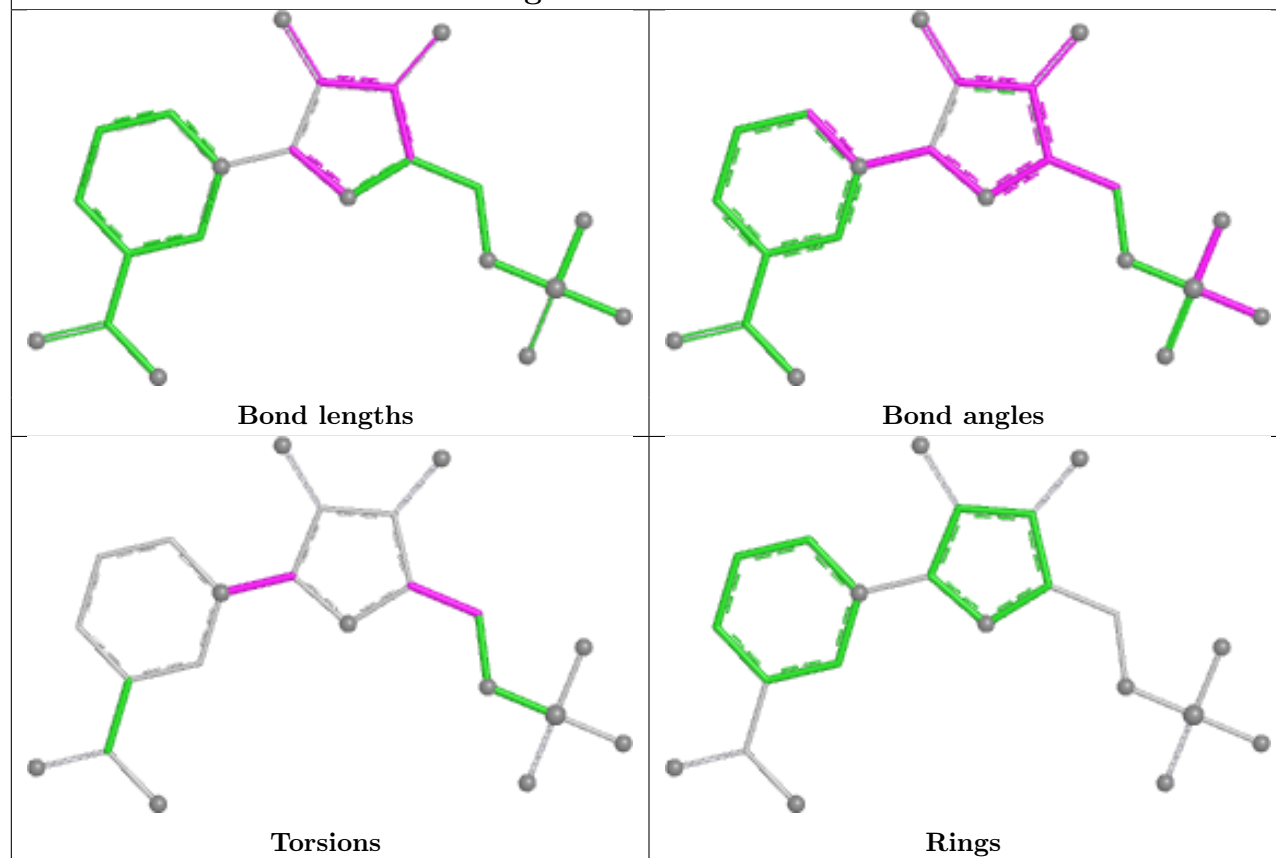
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NMN	2	0
2	C	501	NMN	5	0
2	B	501	NMN	3	0

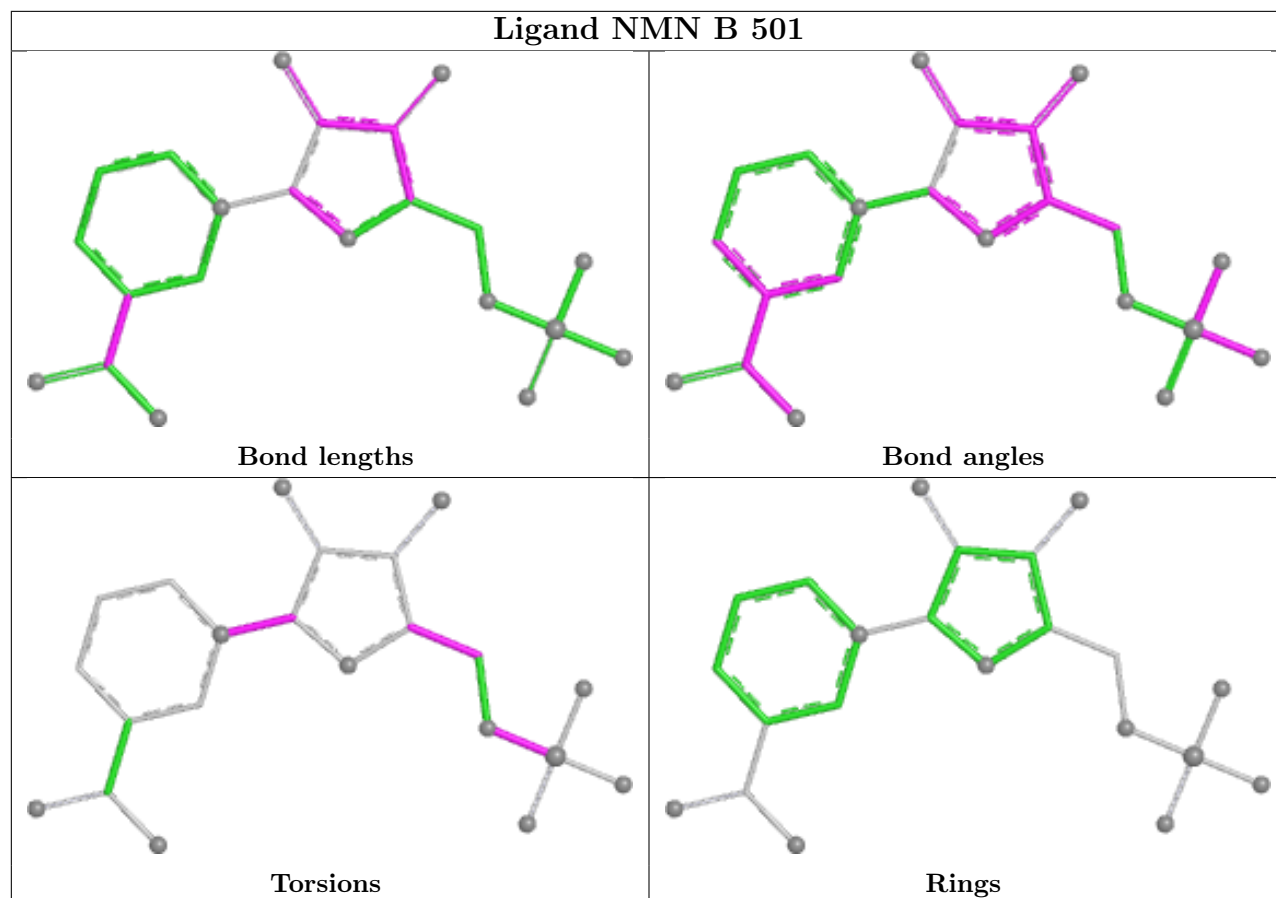
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 501



Ligand NMN C 501





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.