



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:48 AM UTC

PDB ID : 9I5I / pdb_00009i5i
Title : PR1 phage heterodimeric DNA ligase in complex with 21-mer nicked DNA (random sequence)
Authors : Richardson, J.M.; MacNeill, S.A.
Deposited on : 2025-01-28
Resolution : 2.65 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

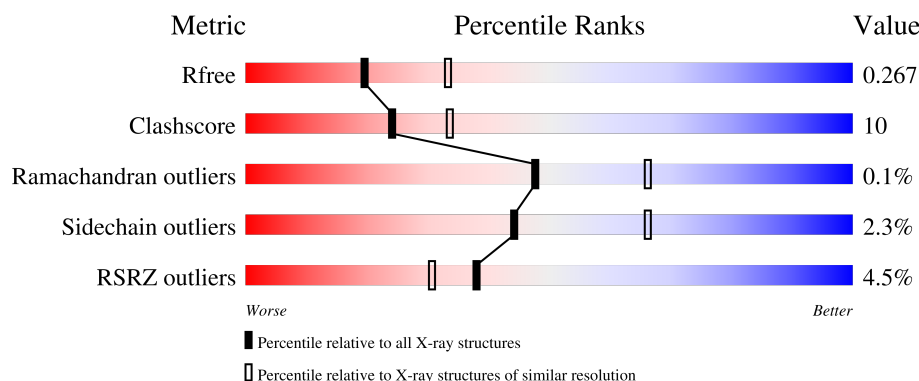
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	339	<div> <div>2%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>
1	E	339	<div> <div>8%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>
2	B	248	<div> <div>6%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>
2	F	248	<div> <div>%</div> <div>53%</div> <div>12%</div> <div>35%</div> </div>
3	C	21	<div> <div>67%</div> <div>33%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	21	 67% 33%
4	D	21	 71% 29%
4	G	21	 86% 14%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18909 atoms, of which 8896 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 DNA ligase (NAD(+)).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	325	Total	C	H	N	O	S	0	0	0
			4984	1597	2449	424	502	12			
1	E	326	Total	C	H	N	O	S	0	0	0
			5040	1615	2482	427	504	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP A0A1S6KUY4
A	-4	ASN	-	expression tag	UNP A0A1S6KUY4
A	-3	SER	-	expression tag	UNP A0A1S6KUY4
A	-2	GLY	-	expression tag	UNP A0A1S6KUY4
A	-1	ASP	-	expression tag	UNP A0A1S6KUY4
A	0	PRO	-	expression tag	UNP A0A1S6KUY4
E	-5	GLY	-	expression tag	UNP A0A1S6KUY4
E	-4	ASN	-	expression tag	UNP A0A1S6KUY4
E	-3	SER	-	expression tag	UNP A0A1S6KUY4
E	-2	GLY	-	expression tag	UNP A0A1S6KUY4
E	-1	ASP	-	expression tag	UNP A0A1S6KUY4
E	0	PRO	-	expression tag	UNP A0A1S6KUY4

- Molecule 2 is a protein called DNA ligase subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	247	Total	C	H	N	O	S	0	0	0
			3690	1174	1827	310	368	11			
2	F	161	Total	C	H	N	O	S	0	0	0
			2501	778	1271	204	238	10			

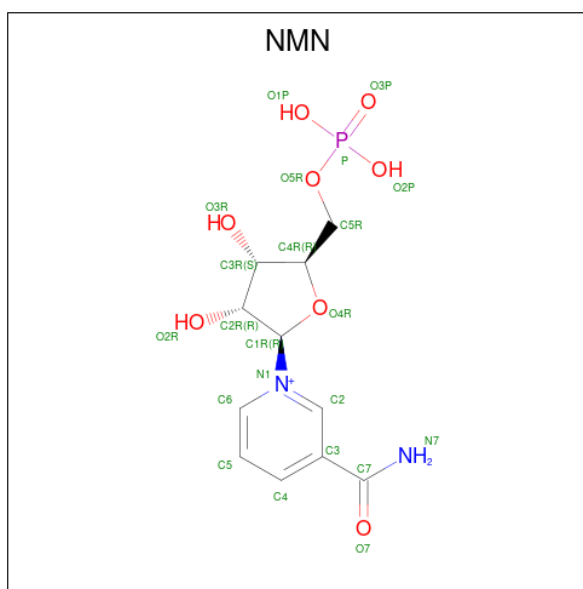
- Molecule 3 is a DNA chain called DNA nicked strand.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	21	Total	C	H	N	O	P	0	0	0
			607	201	187	81	119	19			
3	H	21	Total	C	H	N	O	P	0	0	0
			641	201	221	81	119	19			

- Molecule 4 is a DNA chain called DNA intact strand.

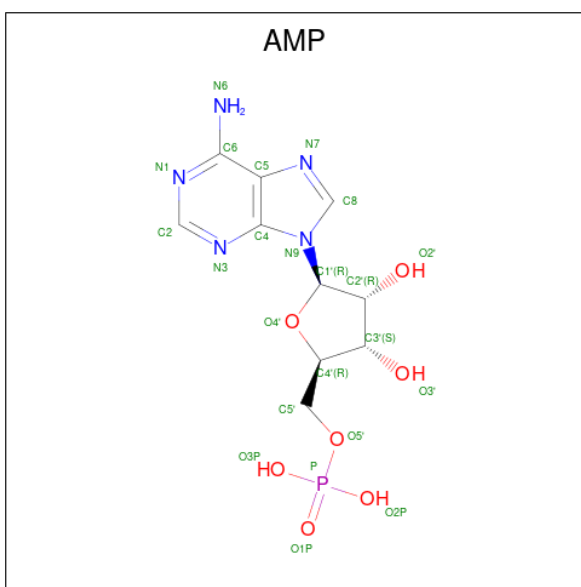
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	21	Total	C	H	N	O	P	0	0	0
			613	205	181	80	127	20			
4	G	21	Total	C	H	N	O	P	0	0	0
			670	205	238	80	127	20			

- Molecule 5 is BETA-NICOTINAMIDE RIBOSE MONOPHOSPHATE (CCD ID: NMN) (formula: $C_{11}H_{16}N_2O_8P$).



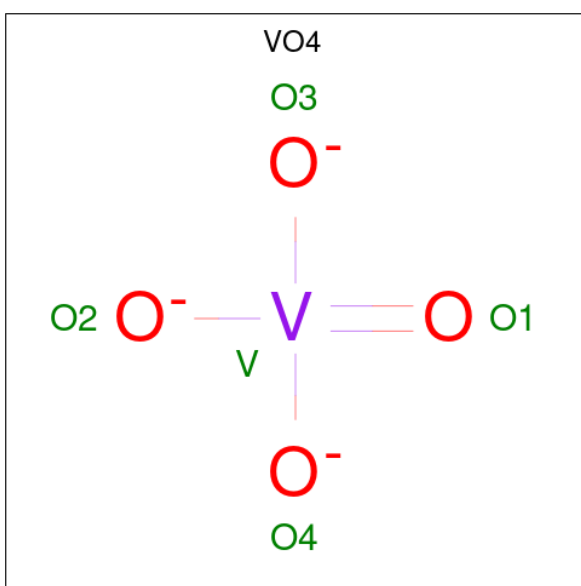
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			36	11	14	2	8	1		
5	E	1	Total	C	H	N	O	P	0	0
			36	11	14	2	8	1		

- Molecule 6 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		
6	E	1	Total	C	N	O	P	0	0	
			23	10	5	7	1			

- Molecule 7 is VANADATE ION (CCD ID: VO4) (formula: O_4V).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O V	0	0
			4	3 1		
7	B	1	Total	O V	0	0
			5	4 1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	O	V	0	0
			4	3	1		
7	G	1	Total	O	V	0	0
			5	4	1		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Zn	0	0
			1	1		
8	F	1	Total	Zn	0	0
			1	1		

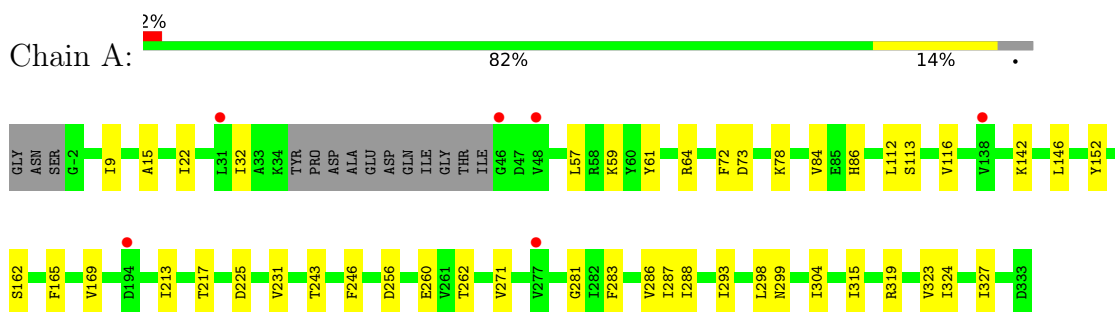
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	5	Total	O	0	0
			5	5		
9	C	1	Total	O	0	0
			1	1		
9	E	1	Total	O	0	0
			1	1		
9	F	2	Total	O	0	0
			2	2		
9	G	1	Total	O	0	0
			1	1		
9	H	3	Total	O	0	0
			3	3		

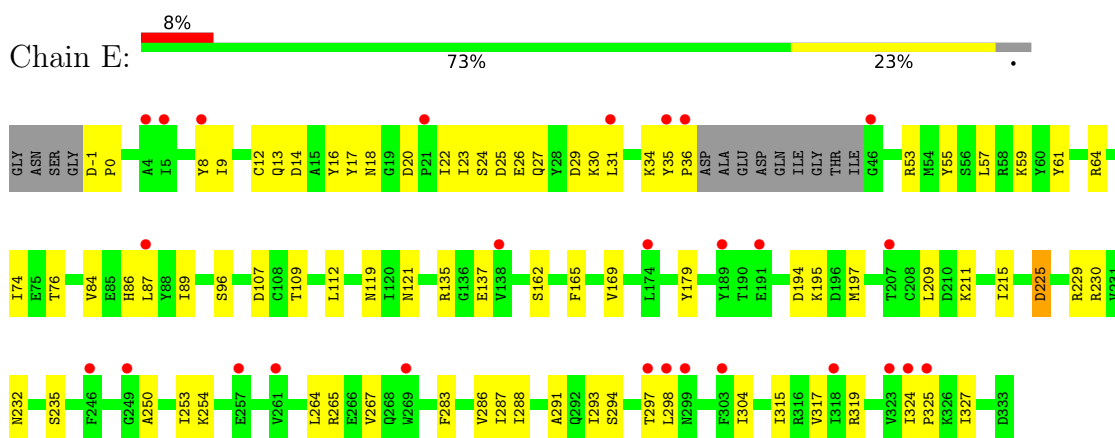
3 Residue-property plots [i](#)

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

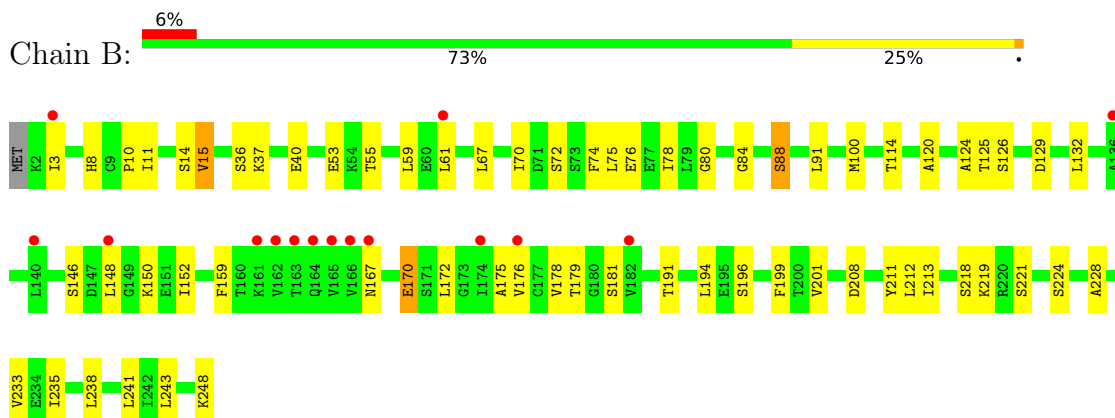
- Molecule 1: DNA ligase (NAD(+))



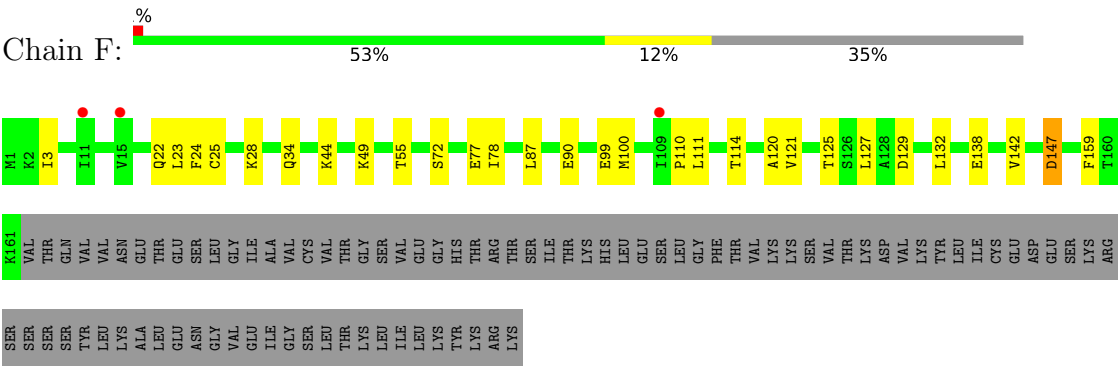
- Molecule 1: DNA ligase (NAD(+))



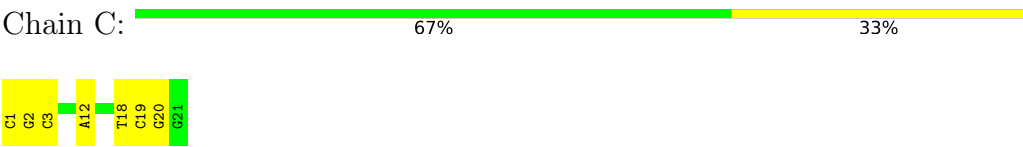
- Molecule 2: DNA ligase subunit B



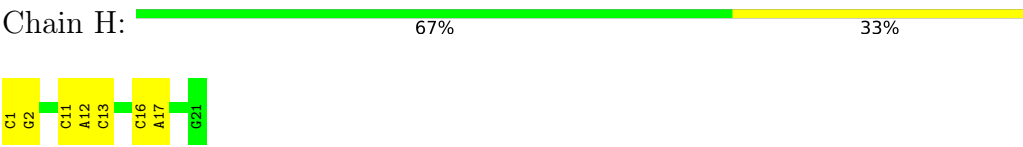
● Molecule 2: DNA ligase subunit B



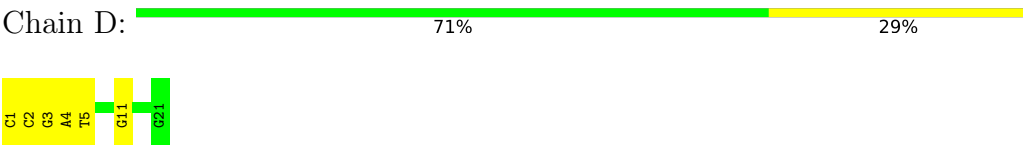
● Molecule 3: DNA nicked strand



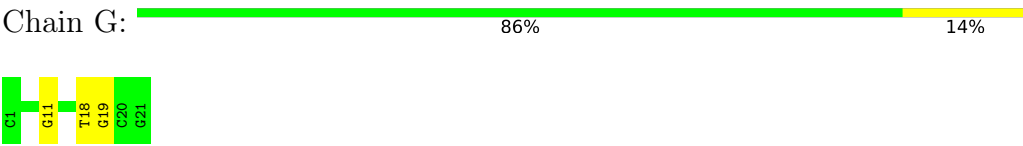
● Molecule 3: DNA nicked strand



● Molecule 4: DNA intact strand



● Molecule 4: DNA intact strand



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.70Å 110.25Å 115.52Å 90.00° 96.91° 90.00°	Depositor
Resolution (Å)	62.67 – 2.65 62.67 – 2.65	Depositor EDS
% Data completeness (in resolution range)	96.6 (62.67-2.65) 96.7 (62.67-2.65)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.219 , 0.264 0.221 , 0.267	Depositor DCC
R_{free} test set	2409 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.1	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	0.94	EDS
Total number of atoms	18909	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: ZN, AMP, VO4, 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	0.12	0/2580	0.30	0/3488
1	E	0.13	0/2605	0.33	0/3521
2	B	0.12	0/1886	0.29	0/2535
2	F	0.12	0/1247	0.28	0/1674
3	C	0.21	0/470	0.49	0/720
3	H	0.21	0/470	0.46	0/720
4	D	0.20	0/484	0.43	0/747
4	G	0.20	0/484	0.48	0/747
All	All	0.14	0/10226	0.35	0/14152

There are no bond length outliers.

There are no bond angle outliers.

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	2535	2449	2485	35	0
1	E	2558	2482	2520	72	0
2	B	1863	1827	1898	53	0
2	F	1230	1271	1271	16	0
3	C	420	187	236	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	420	221	236	6	0
4	D	432	181	238	6	0
4	G	432	238	238	2	0
5	A	22	14	13	0	0
5	E	22	14	13	0	0
6	A	23	12	12	0	0
6	E	23	0	12	5	0
7	A	4	0	0	0	0
7	B	5	0	0	0	0
7	E	4	0	0	0	0
7	G	5	0	0	0	0
8	B	1	0	0	0	0
8	F	1	0	0	0	0
9	A	5	0	0	0	0
9	C	1	0	0	0	0
9	E	1	0	0	0	0
9	F	2	0	0	0	0
9	G	1	0	0	0	0
9	H	3	0	0	0	0
All	All	10013	8896	9172	192	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 10.

All (192) 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:E:9:ILE:HD11	1:E:31:LEU:HD12	1.40	1.04
1:E:9:ILE:HD11	1:E:31:LEU:CD1	1.93	0.98
2:B:124:ALA:HA	2:B:129:ASP:OD2	1.73	0.88
1:E:18:ASN:OD1	1:E:18:ASN:O	1.94	0.85
1:E:9:ILE:CD1	1:E:31:LEU:HD12	2.11	0.81
1:E:23:ILE:HG22	1:E:24:SER:O	1.82	0.80
1:A:298:LEU:HD12	1:A:304:ILE:HG12	1.66	0.78
2:F:77:GLU:HG2	2:F:78:ILE:HD13	1.66	0.78
2:F:138:GLU:O	2:F:142:VAL:HG23	1.85	0.76
1:E:12:CYS:SG	1:E:23:ILE:HD12	2.28	0.73
4:D:1:DC:H2''	4:D:2:DC:H5''	1.70	0.72
1:A:165:PHE:O	1:A:169:VAL:HG23	1.89	0.72
1:E:31:LEU:C	1:E:31:LEU:HD13	2.15	0.71
1:A:271:VAL:O	2:B:37:LYS:NZ	2.22	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:DC:H2''	3:C:20:DG:C8	2.26	0.70
1:A:286:VAL:C	1:A:287:ILE:HD12	2.18	0.69
1:A:281:GLY:H	1:A:298:LEU:HD23	1.58	0.68
2:B:100:MET:HE2	2:B:159:PHE:CD2	2.29	0.67
1:A:78:LYS:HG2	1:A:225:ASP:OD1	1.94	0.67
4:D:3:DG:H2''	4:D:4:DA:OP2	1.94	0.67
1:A:260:GLU:HB2	1:A:286:VAL:HG21	1.77	0.66
2:B:172:LEU:HD23	2:B:199:PHE:CE1	2.31	0.66
1:A:281:GLY:N	1:A:298:LEU:HD23	2.11	0.64
1:E:86:HIS:HD1	1:E:96:SER:HG	1.43	0.64
3:C:20:DG:H2'	3:C:20:DG:OP2	1.98	0.63
2:B:194:LEU:HD21	2:B:238:LEU:HD11	1.79	0.63
1:E:20:ASP:O	1:E:20:ASP:OD1	2.18	0.62
6:E:402:AMP:O1P	3:H:11:DC:H5''	1.99	0.62
2:B:67:LEU:HD11	2:B:91:LEU:HD21	1.81	0.61
1:E:31:LEU:O	1:E:34:LYS:N	2.34	0.61
1:E:267:VAL:HG21	2:F:3:ILE:HD13	1.83	0.61
1:A:260:GLU:CB	1:A:286:VAL:HG21	2.32	0.60
2:B:55:THR:O	2:B:59:LEU:HD12	2.02	0.60
1:E:8:TYR:CE2	1:E:23:ILE:HD11	2.37	0.60
2:B:175:ALA:HB3	2:B:208:ASP:OD2	2.03	0.59
1:E:225:ASP:OD1	1:E:225:ASP:N	2.31	0.59
2:F:125:THR:OG1	2:F:129:ASP:OD2	2.20	0.59
1:E:298:LEU:HD22	1:E:304:ILE:CD1	2.34	0.58
2:B:3:ILE:HD12	2:B:3:ILE:O	2.03	0.58
2:F:49:LYS:N	2:F:90:GLU:OE1	2.35	0.58
1:E:74:ILE:CD1	1:E:232:ASN:OD1	2.51	0.58
1:E:286:VAL:HG23	1:E:288:ILE:CD1	2.34	0.58
2:B:55:THR:HG22	2:B:59:LEU:HD11	1.85	0.57
2:B:243:LEU:O	2:B:248:LYS:HG3	2.03	0.57
1:E:137:GLU:OE2	6:E:402:AMP:H1'	2.05	0.57
2:B:176:VAL:HG11	2:B:194:LEU:HD13	1.87	0.56
1:E:194:ASP:OD1	1:E:195:LYS:N	2.38	0.56
2:B:213:ILE:CD1	2:B:238:LEU:HD12	2.36	0.56
1:E:23:ILE:HG23	1:E:27:GLN:HB2	1.87	0.56
2:B:208:ASP:OD2	2:B:208:ASP:C	2.49	0.56
1:E:8:TYR:CZ	1:E:23:ILE:HD11	2.40	0.56
2:B:125:THR:N	2:B:129:ASP:OD2	2.37	0.56
1:E:20:ASP:OD1	1:E:20:ASP:C	2.47	0.56
1:A:298:LEU:HD22	1:A:327:ILE:HD12	1.88	0.54
1:E:8:TYR:OH	1:E:23:ILE:HD11	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:402:AMP:P	3:H:11:DC:H5''	2.48	0.54
1:E:197:MET:HA	1:E:197:MET:HE2	1.89	0.53
2:F:25:CYS:SG	2:F:34:GLN:NE2	2.80	0.53
2:F:147:ASP:OD1	2:F:147:ASP:N	2.39	0.53
2:B:59:LEU:CD2	2:B:75:LEU:HD23	2.39	0.52
1:E:31:LEU:CD1	1:E:31:LEU:C	2.82	0.52
2:B:148:LEU:O	2:B:152:ILE:HG13	2.09	0.52
1:E:74:ILE:HD11	1:E:232:ASN:OD1	2.09	0.52
1:E:135:ARG:HB3	1:E:179:TYR:CE1	2.44	0.52
1:A:9:ILE:HD12	1:A:32:ILE:HD13	1.92	0.52
1:E:96:SER:H	1:E:109:THR:HG22	1.74	0.52
3:C:2:DG:H2''	3:C:3:DC:H5'	1.92	0.51
1:E:165:PHE:O	1:E:169:VAL:HG23	2.10	0.51
1:E:293:ILE:HG21	1:E:317:VAL:HG11	1.92	0.51
3:H:1:DC:H2'	3:H:2:DG:C8	2.45	0.51
2:B:211:TYR:CG	2:B:241:LEU:HD13	2.46	0.51
1:E:61:TYR:CE1	1:E:254:LYS:HB2	2.46	0.51
2:B:228:ALA:HB1	2:B:233:VAL:HB	1.93	0.51
1:A:323:VAL:HG12	1:A:324:ILE:HD13	1.93	0.50
4:D:4:DA:H1'	4:D:5:DT:H5'	1.92	0.50
4:D:2:DC:H2''	4:D:3:DG:O5'	2.12	0.50
1:E:87:LEU:HD21	1:E:89:ILE:HD12	1.94	0.50
1:E:135:ARG:CB	1:E:179:TYR:CE1	2.95	0.49
1:E:107:ASP:OD1	1:E:109:THR:HG23	2.12	0.49
1:A:146:LEU:CD2	1:A:152:TYR:CE2	2.95	0.49
1:E:53:ARG:HD2	1:E:55:TYR:CZ	2.48	0.48
1:E:283:PHE:CZ	1:E:317:VAL:HG21	2.48	0.48
1:A:64:ARG:NH2	1:A:256:ASP:OD1	2.45	0.48
1:E:324:ILE:CD1	4:G:11:DG:H21	2.26	0.48
2:B:67:LEU:CD1	2:B:91:LEU:HD21	2.43	0.48
1:E:25:ASP:O	1:E:29:ASP:OD2	2.31	0.48
1:A:15:ALA:CB	1:A:22:ILE:HG23	2.44	0.48
1:A:84:VAL:HG11	1:A:112:LEU:HD22	1.96	0.48
1:E:16:TYR:HD2	1:E:17:TYR:CE1	2.31	0.48
6:E:402:AMP:H2'	6:E:402:AMP:N3	2.29	0.48
1:A:293:ILE:HD11	1:A:319:ARG:HG3	1.96	0.47
3:C:1:DC:H2''	3:C:2:DG:C8	2.50	0.47
1:E:31:LEU:HD13	1:E:31:LEU:O	2.15	0.47
2:B:129:ASP:O	2:B:129:ASP:OD1	2.33	0.47
1:E:59:LYS:HG2	1:E:254:LYS:HD2	1.96	0.47
1:E:297:THR:HG23	1:E:297:THR:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:THR:CG2	1:E:209:LEU:HD22	2.45	0.46
1:A:15:ALA:HB1	1:A:22:ILE:HG23	1.97	0.46
1:E:12:CYS:HA	1:E:22:ILE:HD12	1.98	0.46
2:B:55:THR:HG22	2:B:59:LEU:CD1	2.46	0.46
2:B:228:ALA:HB3	2:B:235:ILE:HD11	1.98	0.46
2:F:120:ALA:HB2	2:F:132:LEU:HG	1.97	0.46
1:A:146:LEU:HD22	1:A:152:TYR:CE2	2.51	0.46
2:B:61:LEU:HD11	2:B:70:ILE:HD12	1.98	0.45
2:B:100:MET:HE2	2:B:159:PHE:CG	2.50	0.45
1:E:84:VAL:HG21	1:E:112:LEU:CD1	2.46	0.45
1:E:18:ASN:O	1:E:18:ASN:CG	2.59	0.45
1:E:229:ARG:HD2	1:E:253:ILE:HD11	1.98	0.45
2:B:228:ALA:CB	2:B:235:ILE:HD11	2.46	0.45
4:G:18:DT:H2"	4:G:19:DG:C8	2.50	0.45
2:B:36:SER:O	2:B:40:GLU:OE2	2.34	0.45
2:B:74:PHE:CE1	2:B:78:ILE:HG13	2.52	0.45
2:B:167:ASN:N	2:B:170:GLU:OE1	2.49	0.45
1:A:86:HIS:CE1	1:A:116:VAL:HG11	2.52	0.45
1:E:293:ILE:HG13	1:E:325:PRO:HG3	1.97	0.45
2:B:14:SER:OG	2:B:15:VAL:N	2.49	0.45
1:A:243:THR:HG1	1:A:246:PHE:H	1.65	0.44
1:E:287:ILE:C	1:E:288:ILE:HD12	2.42	0.44
1:A:288:ILE:HG13	1:A:293:ILE:HD12	1.99	0.44
2:B:67:LEU:HD11	2:B:91:LEU:HD11	1.98	0.44
1:E:211:LYS:O	1:E:215:ILE:HG12	2.18	0.44
2:F:127:LEU:CD2	2:F:159:PHE:CZ	3.00	0.44
1:A:262:THR:HG21	1:A:283:PHE:CD2	2.53	0.44
1:A:57:LEU:C	1:A:246:PHE:CD1	2.95	0.44
2:B:3:ILE:HD12	2:B:3:ILE:C	2.43	0.44
2:B:146:SER:O	2:B:150:LYS:HG3	2.17	0.44
2:B:211:TYR:CD1	2:B:241:LEU:HD13	2.53	0.44
2:B:179:THR:HG22	2:B:213:ILE:O	2.18	0.43
2:B:124:ALA:CA	2:B:129:ASP:OD2	2.57	0.43
1:E:324:ILE:CG2	3:H:12:DA:O4'	2.66	0.43
2:B:84:GLY:O	2:B:88:SER:OG	2.26	0.43
1:E:317:VAL:HG22	1:E:327:ILE:HG12	2.00	0.43
2:B:178:VAL:HG22	2:B:213:ILE:HB	2.00	0.43
1:E:14:ASP:O	1:E:18:ASN:HB3	2.18	0.43
1:E:288:ILE:HD12	1:E:288:ILE:N	2.34	0.43
2:F:127:LEU:HD21	2:F:159:PHE:CE1	2.52	0.43
2:B:76:GLU:O	2:B:80:GLY:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:MET:HE2	2:B:159:PHE:CE2	2.54	0.43
2:B:120:ALA:HB2	2:B:132:LEU:HG	2.00	0.43
1:E:9:ILE:O	1:E:13:GLN:HG3	2.18	0.43
1:A:61:TYR:HB3	1:A:64:ARG:HG3	2.01	0.43
2:B:212:LEU:HD11	2:B:224:SER:HB3	2.01	0.43
1:E:291:ALA:HB2	1:E:319:ARG:NH1	2.34	0.42
2:F:55:THR:HG21	2:F:87:LEU:HD21	2.01	0.42
1:A:78:LYS:HZ2	1:A:225:ASP:CG	2.27	0.42
1:E:35:TYR:N	1:E:36:PRO:CD	2.82	0.42
1:E:298:LEU:HB3	1:E:304:ILE:HD11	2.01	0.42
1:A:59:LYS:NZ	3:C:12:DA:OP2	2.47	0.42
1:E:87:LEU:HD21	1:E:89:ILE:CD1	2.49	0.42
1:E:264:LEU:HD23	1:E:265:ARG:N	2.35	0.42
2:B:213:ILE:CD1	2:B:238:LEU:CD1	2.97	0.42
3:C:18:DT:H2''	3:C:19:DC:C6	2.54	0.42
4:D:2:DC:H6	4:D:2:DC:H2'	1.68	0.42
1:E:324:ILE:HG13	1:E:325:PRO:HD2	2.01	0.42
2:B:70:ILE:HD13	2:B:75:LEU:HD21	2.01	0.42
2:F:110:PRO:O	2:F:111:LEU:HB2	2.19	0.42
1:A:213:ILE:O	1:A:217:THR:HG23	2.19	0.42
1:E:64:ARG:NH1	3:H:13:DC:OP1	2.49	0.42
1:E:315:ILE:HD12	1:E:327:ILE:HD13	2.02	0.42
1:E:16:TYR:CD2	1:E:17:TYR:CE1	3.08	0.42
1:E:298:LEU:HD22	1:E:304:ILE:HD13	2.01	0.42
1:A:262:THR:HG23	1:A:315:ILE:HG12	2.02	0.42
1:A:324:ILE:HG13	4:D:11:DG:N2	2.35	0.42
3:C:18:DT:H2''	3:C:19:DC:C5	2.55	0.42
2:F:23:LEU:C	2:F:24:PHE:CD1	2.98	0.42
3:H:16:DC:H2''	3:H:17:DA:C8	2.54	0.42
2:B:126:SER:H	2:B:129:ASP:HB3	1.85	0.42
2:B:10:PRO:C	2:B:11:ILE:HD13	2.44	0.41
1:E:119:ASN:ND2	1:E:121:ASN:OD1	2.53	0.41
1:E:230:ARG:HG3	1:E:250:ALA:HB2	2.02	0.41
2:B:8:HIS:HA	2:B:14:SER:O	2.21	0.41
2:B:67:LEU:CD1	2:B:91:LEU:HD11	2.50	0.41
1:E:179:TYR:C	1:E:179:TYR:CD1	2.99	0.41
2:B:36:SER:C	2:B:40:GLU:OE2	2.64	0.41
2:B:40:GLU:OE1	2:B:53:GLU:HG3	2.20	0.41
2:B:100:MET:CE	2:B:159:PHE:CD2	3.00	0.41
1:E:-1:ASP:N	1:E:0:PRO:HD2	2.36	0.41
1:A:152:TYR:CD1	1:A:152:TYR:C	2.99	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:LYS:HA	2:B:219:LYS:HD2	1.92	0.41
2:F:78:ILE:HD13	2:F:78:ILE:N	2.36	0.41
2:F:100:MET:HG2	2:F:121:VAL:HG12	2.03	0.41
1:A:142:LYS:O	1:A:146:LEU:CD1	2.69	0.41
1:E:27:GLN:O	1:E:30:LYS:HB2	2.21	0.41
1:A:73:ASP:OD1	1:A:73:ASP:N	2.53	0.41
3:C:1:DC:C2'	3:C:2:DG:C8	3.04	0.41
1:A:64:ARG:HH21	1:A:256:ASP:CG	2.29	0.40
1:A:72:PHE:CD2	1:A:231:VAL:HG13	2.57	0.40
1:E:26:GLU:HA	1:E:29:ASP:OD2	2.22	0.40
1:E:57:LEU:HG	6:E:402:AMP:H5'2	2.02	0.40
2:B:191:THR:HG23	2:B:201:VAL:HG11	2.03	0.40
1:E:135:ARG:HB2	1:E:179:TYR:CE1	2.56	0.40
2:F:44:LYS:HD2	2:F:44:LYS:HA	1.86	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	321/339 (95%)	302 (94%)	18 (6%)	1 (0%)	36	52
1	E	322/339 (95%)	305 (95%)	17 (5%)	0	100	100
2	B	245/248 (99%)	232 (95%)	13 (5%)	0	100	100
2	F	159/248 (64%)	151 (95%)	8 (5%)	0	100	100
All	All	1047/1174 (89%)	990 (95%)	56 (5%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	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	277/290 (96%)	275 (99%)	2 (1%)	76	86
1	E	281/290 (97%)	277 (99%)	4 (1%)	59	76
2	B	209/219 (95%)	200 (96%)	9 (4%)	26	44
2	F	140/219 (64%)	134 (96%)	6 (4%)	26	44
All	All	907/1018 (89%)	886 (98%)	21 (2%)	44	66

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	SER
1	A	162	SER
2	B	15	VAL
2	B	72	SER
2	B	88	SER
2	B	114	THR
2	B	170	GLU
2	B	181	SER
2	B	196	SER
2	B	218	SER
2	B	221	SER
1	E	162	SER
1	E	225	ASP
1	E	235	SER
1	E	294	SER
2	F	22	GLN
2	F	28	LYS
2	F	72	SER
2	F	99	GLU
2	F	114	THR
2	F	147	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	167	GLN
2	B	145	HIS
1	E	13	GLN
1	E	50	HIS
1	E	119	ASN
1	E	299	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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
6	AMP	E	402	7	25,25,25	1.44	4 (16%)	37,38,38	1.93	7 (18%)
5	NMN	A	401	-	21,23,23	3.68	10 (47%)	27,34,34	1.57	2 (7%)
7	VO4	E	403	6,3	0,3,4	-	-	-	-	-
7	VO4	B	301	-	0,4,4	-	-	-	-	-
7	VO4	A	403	6,3	0,3,4	-	-	-	-	-
5	NMN	E	401	-	21,23,23	3.66	10 (47%)	27,34,34	1.04	1 (3%)
6	AMP	A	402	7	25,25,25	1.42	4 (16%)	37,38,38	2.03	8 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	VO4	G	101	-	0,4,4	-	-	-		

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
6	AMP	A	402	7	-	4/10/26/26	0/3/3/3
5	NMN	A	401	-	-	4/14/30/30	0/2/2/2
5	NMN	E	401	-	-	2/14/30/30	0/2/2/2
6	AMP	E	402	7	-	5/10/26/26	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	401	NMN	C3R-C4R	-8.68	1.31	1.53
5	A	401	NMN	C3R-C4R	-8.54	1.31	1.53
5	A	401	NMN	O4R-C4R	7.83	1.62	1.45
5	E	401	NMN	O4R-C4R	7.77	1.62	1.45
5	A	401	NMN	O4R-C1R	-7.23	1.31	1.40
5	A	401	NMN	C7-N7	7.09	1.46	1.33
5	E	401	NMN	O4R-C1R	-7.04	1.31	1.40
5	E	401	NMN	C7-N7	6.99	1.45	1.33
6	E	402	AMP	C5-C4	4.93	1.47	1.39
6	A	402	AMP	C5-C4	4.80	1.47	1.39
5	E	401	NMN	O3R-C3R	2.97	1.50	1.43
5	A	401	NMN	O3R-C3R	2.92	1.50	1.43
5	E	401	NMN	O7-C7	-2.87	1.18	1.24
5	A	401	NMN	O7-C7	-2.86	1.18	1.24
6	E	402	AMP	C5-C6	2.78	1.48	1.41
5	A	401	NMN	C3-C7	2.65	1.54	1.50
6	A	402	AMP	C5-C6	2.64	1.48	1.41
5	A	401	NMN	O2R-C2R	-2.63	1.36	1.43
5	E	401	NMN	O2R-C2R	-2.62	1.36	1.43
5	E	401	NMN	C3-C7	2.59	1.54	1.50
6	A	402	AMP	C5-N7	-2.45	1.34	1.39
5	E	401	NMN	C4-C3	-2.41	1.35	1.39
5	A	401	NMN	C4-C3	-2.39	1.35	1.39
6	E	402	AMP	C5-N7	-2.30	1.34	1.39
6	E	402	AMP	C8-N7	2.28	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	402	AMP	C8-N7	2.18	1.35	1.31
5	A	401	NMN	P-O5R	2.05	1.66	1.60
5	E	401	NMN	P-O5R	2.03	1.66	1.60

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	NMN	C4R-O4R-C1R	-6.56	103.92	109.92
6	A	402	AMP	C5-C4-N3	-6.51	117.76	126.72
6	E	402	AMP	C5-C4-N3	-6.26	118.10	126.72
6	A	402	AMP	N3-C4-N9	5.32	136.21	127.17
6	E	402	AMP	N3-C4-N9	4.91	135.52	127.17
6	A	402	AMP	C2-N3-C4	3.99	121.58	111.83
6	E	402	AMP	C2-N3-C4	3.86	121.25	111.83
6	A	402	AMP	N3-C2-N1	-3.55	123.22	128.58
6	E	402	AMP	C4-C5-N7	-3.48	106.61	110.58
6	A	402	AMP	C4-C5-N7	-3.24	106.88	110.58
6	E	402	AMP	N3-C2-N1	-3.19	123.76	128.58
6	E	402	AMP	C5-N7-C8	2.51	107.40	103.45
6	A	402	AMP	C5-N7-C8	2.51	107.39	103.45
6	A	402	AMP	C4-N9-C8	2.25	108.11	105.74
6	A	402	AMP	C1'-N9-C8	-2.19	122.23	127.09
5	E	401	NMN	C6-N1-C2	-2.18	120.03	121.88
6	E	402	AMP	C4-N9-C8	2.10	107.94	105.74
5	A	401	NMN	C3-C7-N7	2.06	120.28	117.74

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	401	NMN	C5R-O5R-P-O1P
5	E	401	NMN	C5R-O5R-P-O2P
6	A	402	AMP	C4'-C5'-O5'-P
6	E	402	AMP	C5'-O5'-P-O2P
6	E	402	AMP	C4'-C5'-O5'-P
6	E	402	AMP	C2'-C1'-N9-C4
5	A	401	NMN	C5R-O5R-P-O3P
6	E	402	AMP	C2'-C1'-N9-C8
5	A	401	NMN	O4R-C4R-C5R-O5R
5	A	401	NMN	C3R-C4R-C5R-O5R
5	A	401	NMN	C5R-O5R-P-O1P
6	A	402	AMP	O4'-C1'-N9-C8

Continued on next page...

Continued from previous page...

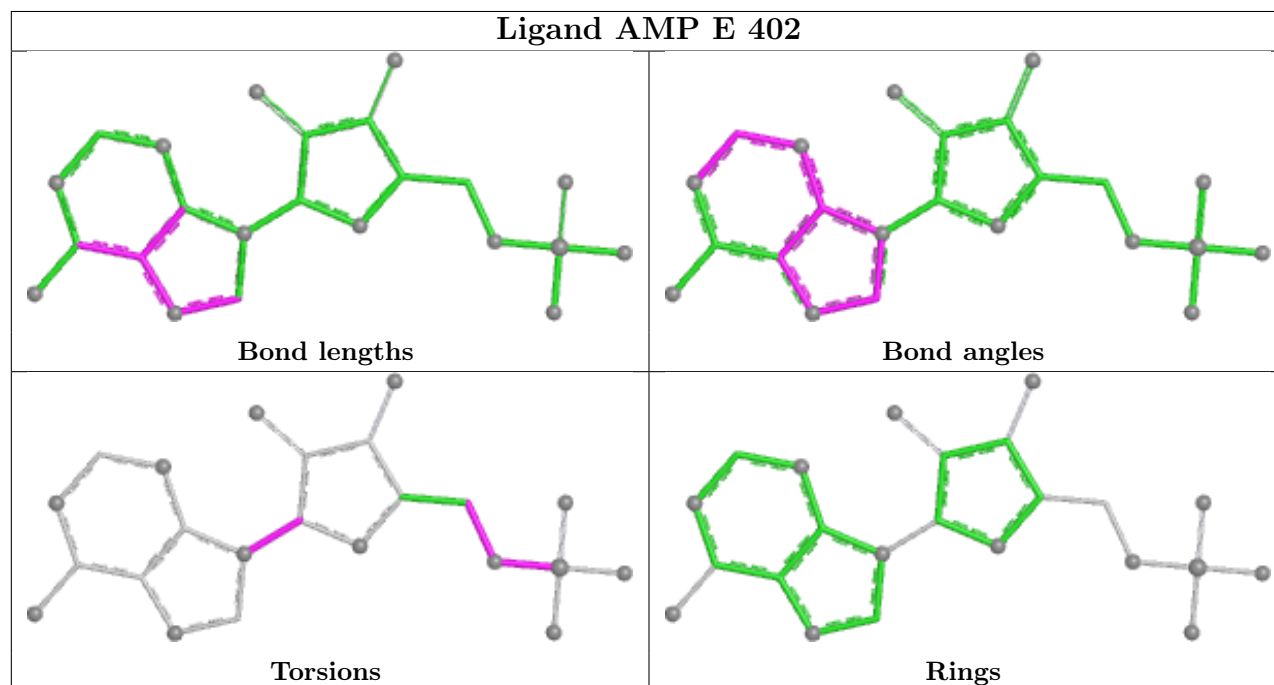
Mol	Chain	Res	Type	Atoms
6	A	402	AMP	C2'-C1'-N9-C8
6	A	402	AMP	C2'-C1'-N9-C4
6	E	402	AMP	O4'-C1'-N9-C8

There are no ring outliers.

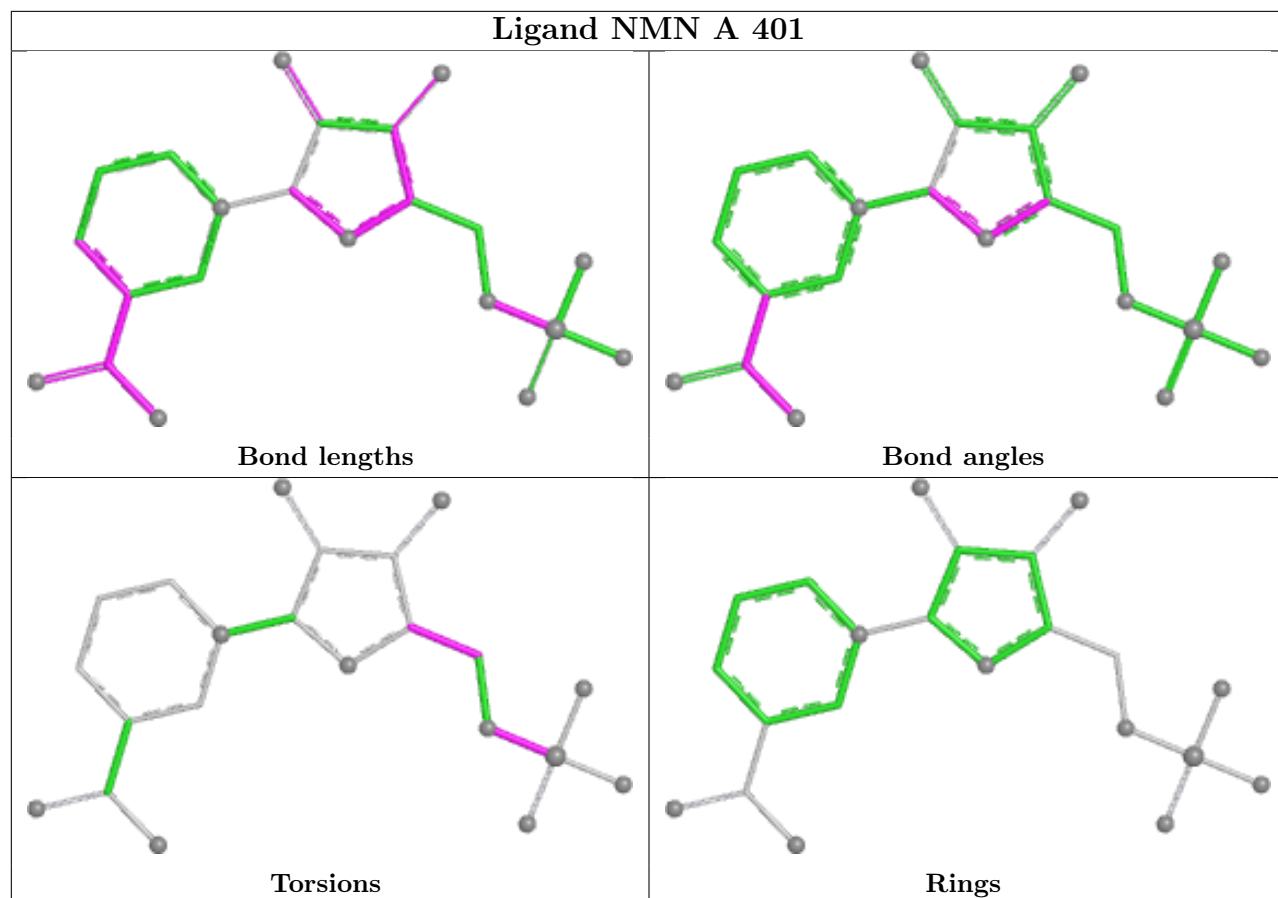
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	402	AMP	5	0

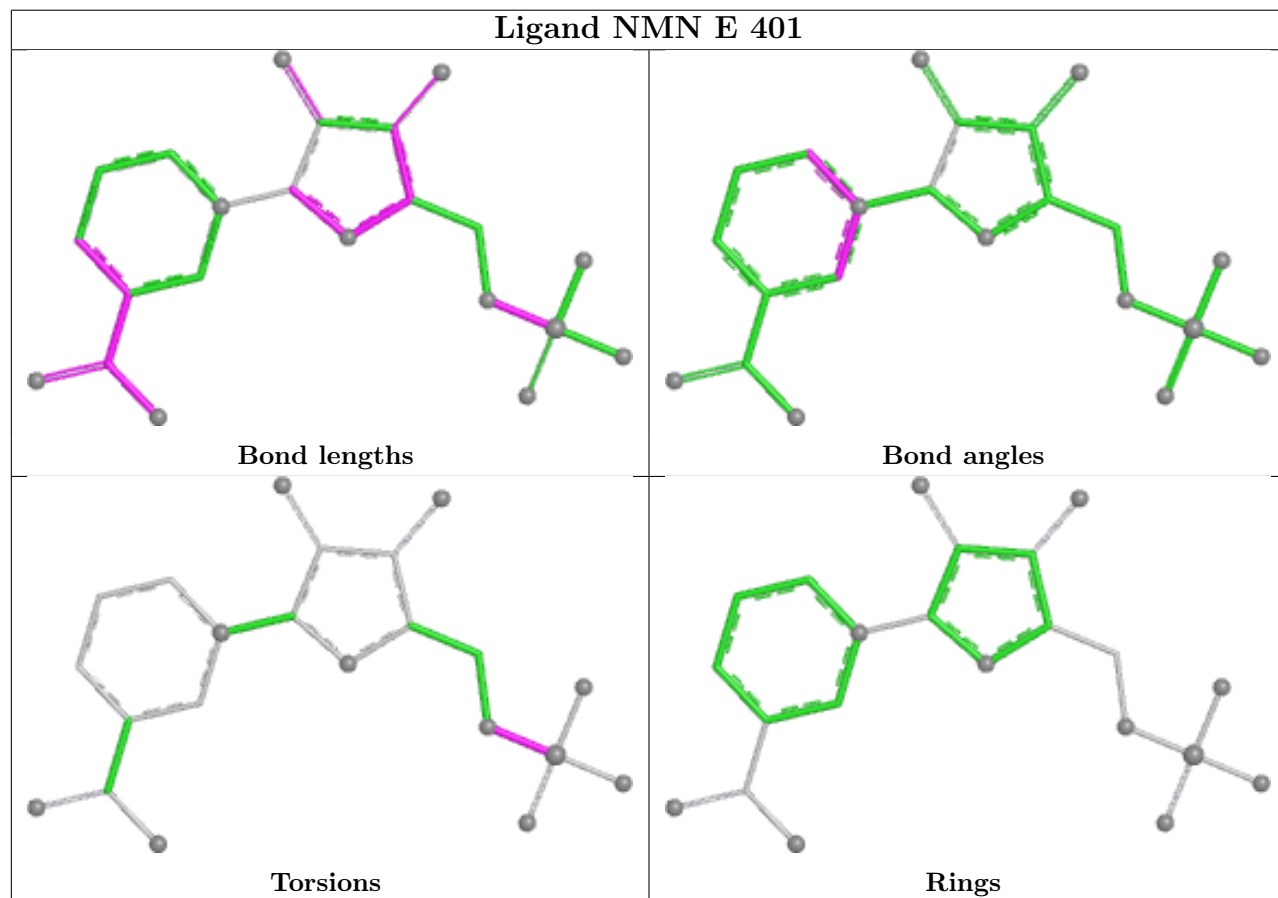
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

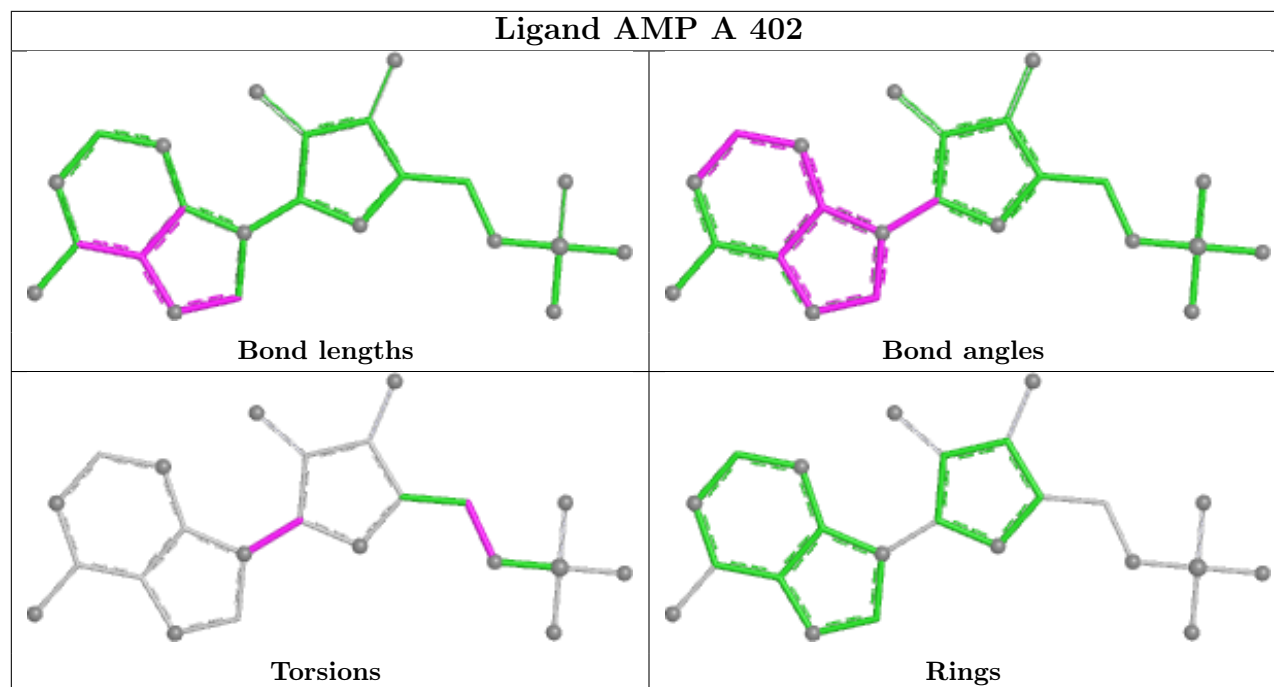


Ligand NMN A 401



Ligand NMN E 401





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	325/339 (95%)	0.48	6 (1%) 67 63	56, 79, 101, 131	0
1	E	326/339 (96%)	0.70	27 (8%) 17 12	58, 92, 126, 144	0
2	B	247/248 (99%)	0.76	15 (6%) 27 20	64, 97, 117, 131	0
2	F	161/248 (64%)	0.35	3 (1%) 66 61	53, 84, 112, 122	0
3	C	21/21 (100%)	0.04	0 100 100	52, 67, 87, 95	0
3	H	21/21 (100%)	0.20	0 100 100	59, 78, 99, 104	0
4	D	21/21 (100%)	0.12	0 100 100	59, 66, 82, 91	0
4	G	21/21 (100%)	0.06	0 100 100	62, 77, 97, 99	0
All	All	1143/1258 (90%)	0.56	51 (4%) 38 31	52, 88, 118, 144	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	46	GLY	4.2
2	B	164	GLN	4.2
2	B	162	VAL	4.2
2	B	3	ILE	3.7
1	E	8	TYR	3.6
1	A	277	VAL	3.3
1	A	46	GLY	3.3
1	E	323	VAL	3.2
1	E	138	VAL	3.1
2	B	161	LYS	3.1
1	A	138	VAL	3.1
2	B	148	LEU	3.1
2	B	167	ASN	3.0
2	B	176	VAL	2.9
1	E	35	TYR	2.9
1	E	324	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	298	LEU	2.9
2	B	163	THR	2.8
1	E	5	ILE	2.8
2	B	136	ALA	2.7
2	B	174	ILE	2.6
2	B	166	VAL	2.6
1	A	48	VAL	2.6
1	E	299	ASN	2.6
1	E	303	PHE	2.6
1	E	31	LEU	2.5
1	E	246	PHE	2.5
1	E	36	PRO	2.5
1	E	318	ILE	2.4
1	E	257	GLU	2.4
1	E	189	TYR	2.3
1	E	249	GLY	2.3
2	B	165	VAL	2.3
1	E	207	THR	2.3
1	E	269	TRP	2.3
2	B	61	LEU	2.3
2	F	15	VAL	2.3
2	F	11	ILE	2.2
1	E	297	THR	2.2
1	E	21	PRO	2.2
1	E	4	ALA	2.2
1	E	174	LEU	2.2
1	A	194	ASP	2.2
1	A	31	LEU	2.1
2	F	109	ILE	2.1
1	E	261	VAL	2.1
1	E	87	LEU	2.1
1	E	325	PRO	2.0
1	E	191	GLU	2.0
2	B	140	LEU	2.0
2	B	182	VAL	2.0

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

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](#)

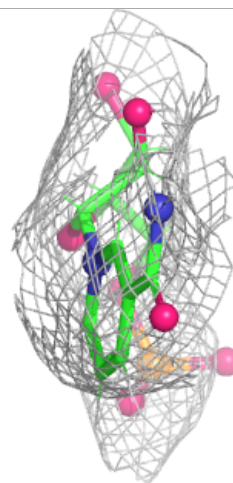
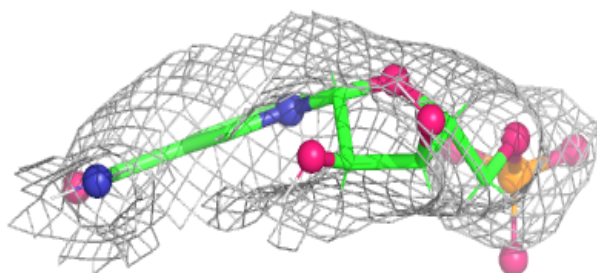
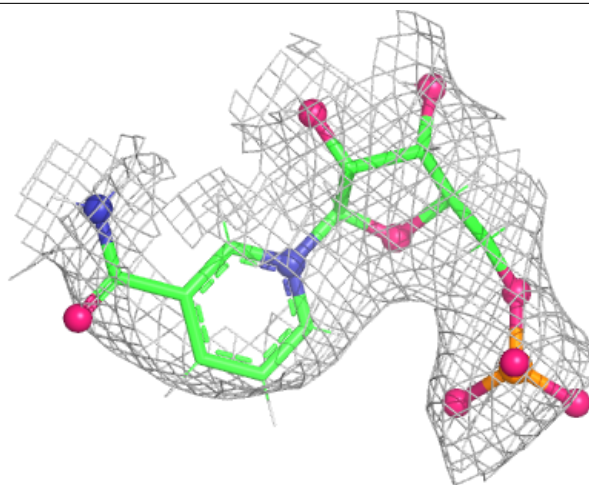
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NMN	E	401	22/22	0.74	0.11	106,127,151,153	0
5	NMN	A	401	22/22	0.81	0.12	62,87,130,150	0
7	VO4	B	301	5/5	0.83	0.07	91,94,103,147	0
7	VO4	E	403	4/5	0.86	0.18	94,97,97,112	0
7	VO4	G	101	5/5	0.87	0.14	62,72,101,132	0
6	AMP	E	402	23/23	0.88	0.14	73,85,90,92	0
6	AMP	A	402	23/23	0.93	0.09	60,72,82,82	0
7	VO4	A	403	4/5	0.96	0.11	79,79,84,105	0
8	ZN	B	302	1/1	0.99	0.03	82,82,82,82	0
8	ZN	F	401	1/1	0.99	0.03	87,87,87,87	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.

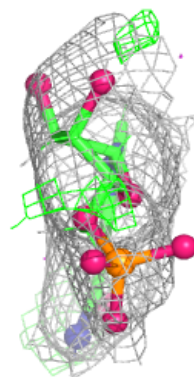
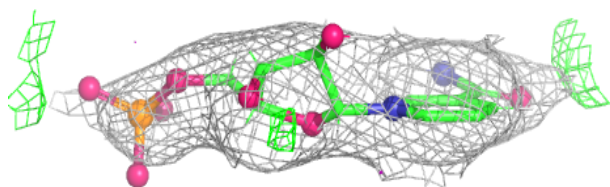
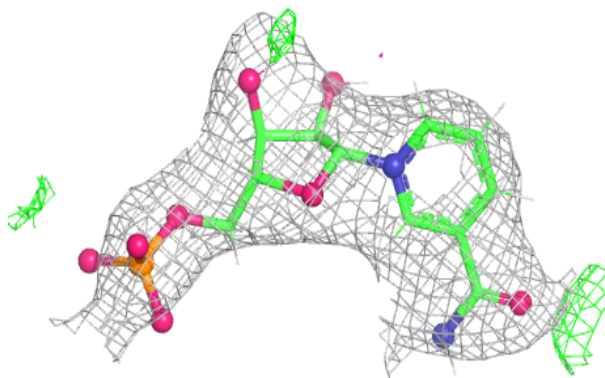
Electron density around NMN E 401:

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

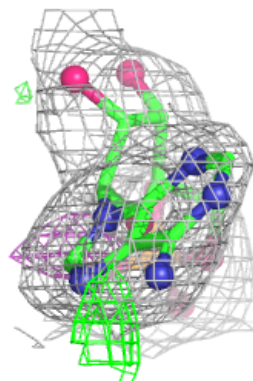
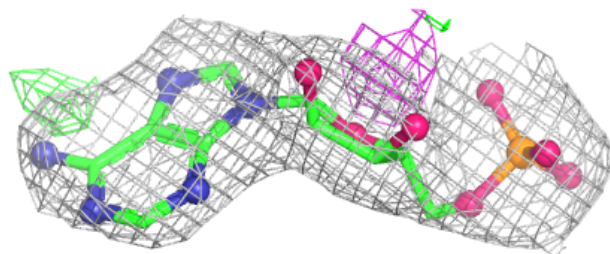
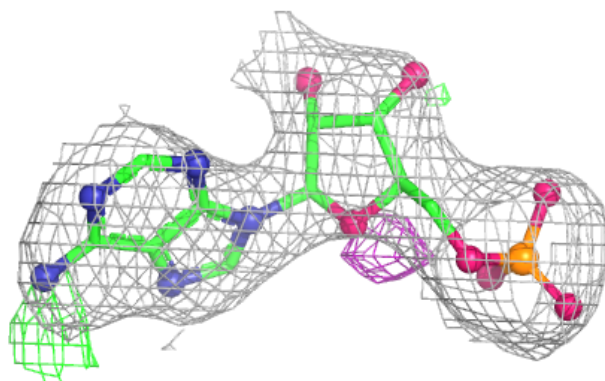


Electron density around NMN A 401:

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

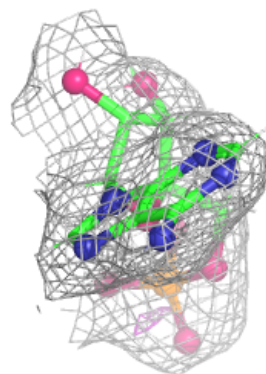
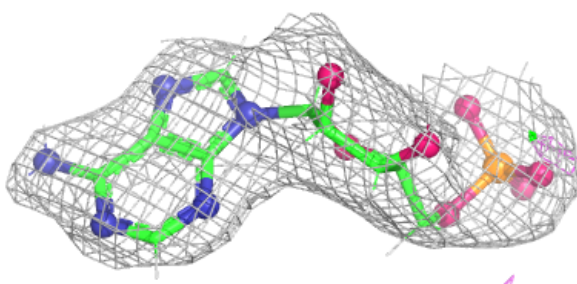
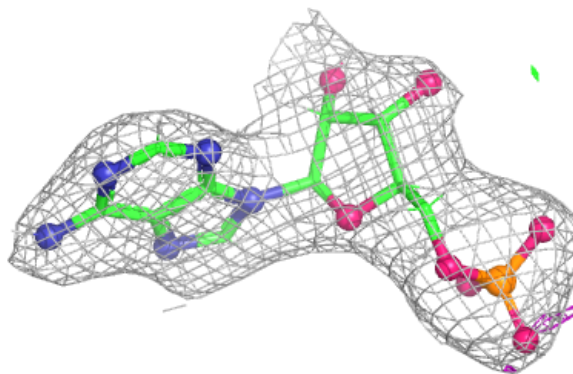
**Electron density around AMP E 402:**

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



Electron density around AMP A 402:

$2mF_o-DF_c$ (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.