Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 02:01 PM EDT

PDB ID	:	6ZYZ
Title	:	Structure of the borneol dehydrogenases of Salvia rosmarinus with NAD+
Authors	:	Dimos, N.; Helmer, C.P.O.; Loll, B.
Deposited on	:	2020-08-03
Resolution	:	2.27 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 (i) 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 (i)) were used in the production of this report:

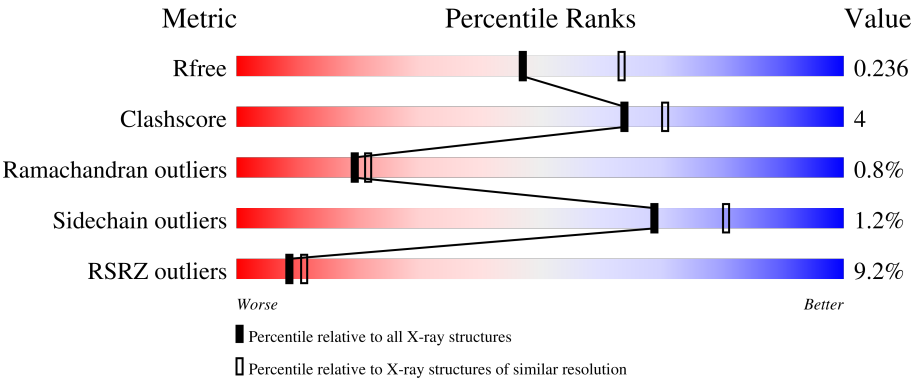
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 <=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	290	6% 80% 8% 11%
1	B	290	8% 77% 11% • 11%
1	C	290	10% 79% 10% • 11%
1	D	290	8% 78% 10% • 11%

2 Entry composition

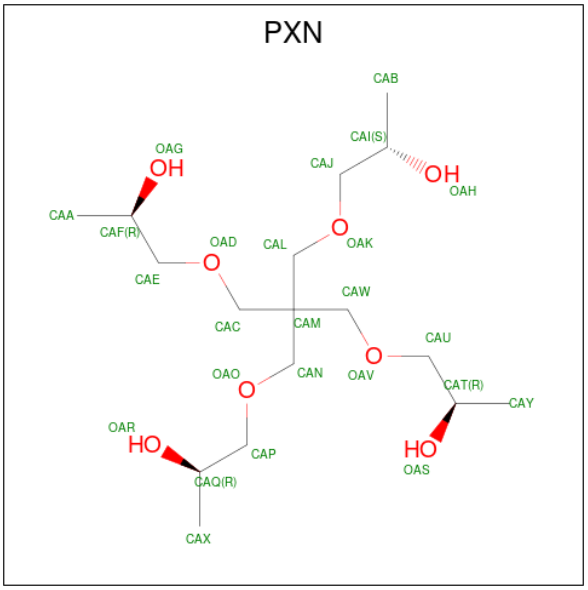
There are 5 unique types of molecules in this entry. The entry contains 8044 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Borneol dehydrogenase from salvia rosmarinus.

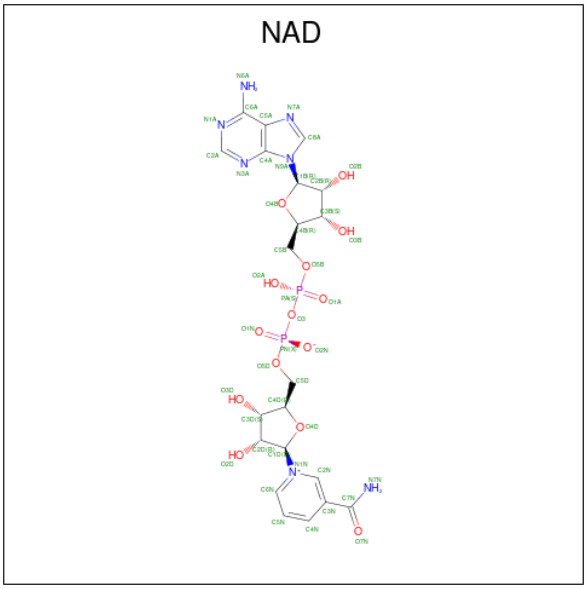
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	1	0
			1903	1199	326	368	10			
1	B	258	Total	C	N	O	S	0	1	0
			1900	1197	328	365	10			
1	C	259	Total	C	N	O	S	0	1	0
			1903	1199	326	368	10			
1	D	259	Total	C	N	O	S	0	3	0
			1915	1205	328	372	10			

- Molecule 2 is (2S)-1-[3-{[(2R)-2-hydroxypropyl]oxy}-2,2-bis({[(2R)-2-hydroxypropyl]oxy}methyl)propoxy]propan-2-ol (three-letter code: PXN) (formula: $C_{17}H_{36}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			25	17	8		
2	D	1	Total	C	O	0	0
			25	17	8		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	68	Total	O	0	0
			68	68		
5	C	31	Total	O	0	0
			31	31		

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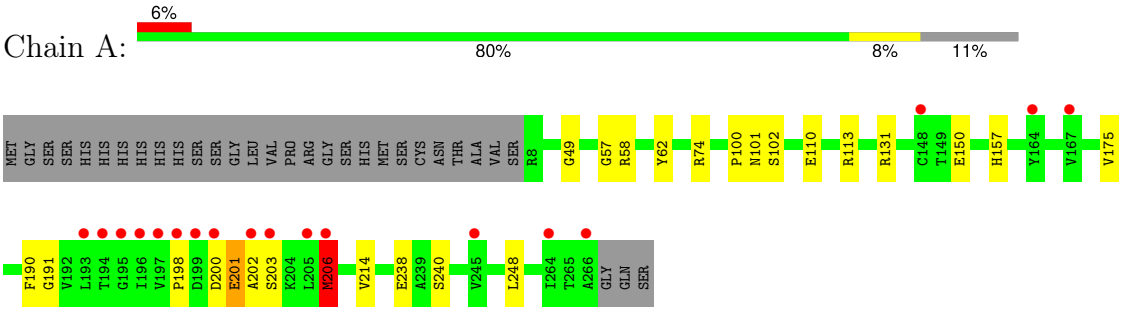
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	27	Total O 27 27	0	0

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.

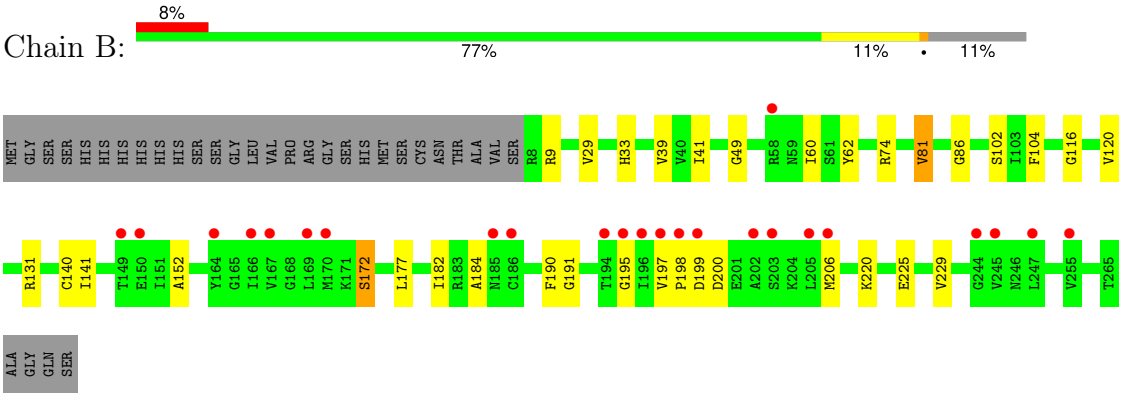
• Molecule 1: Borneol dehydrogenase from salvia rosmarinus

Chain A:



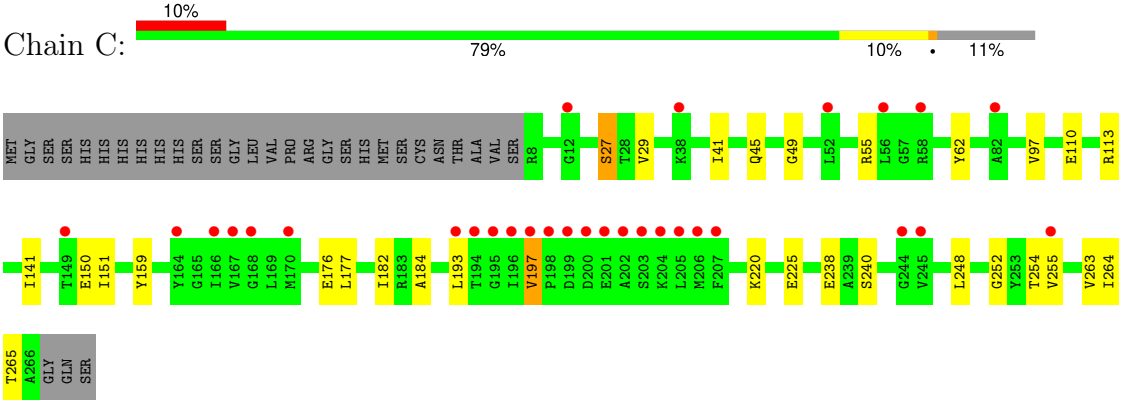
• Molecule 1: Borneol dehydrogenase from salvia rosmarinus

Chain B:



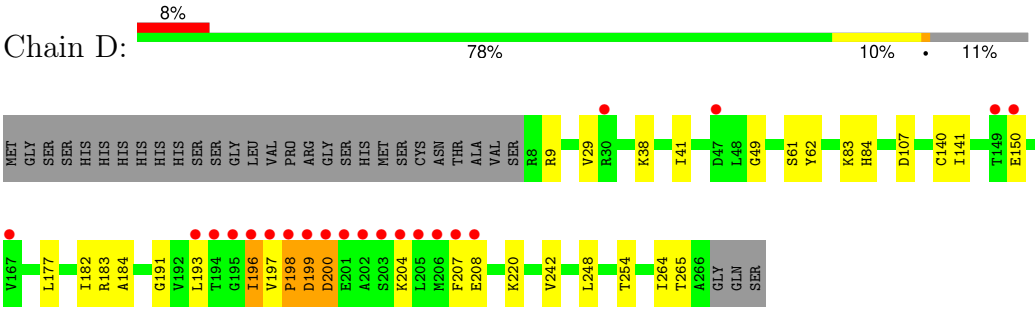
• Molecule 1: Borneol dehydrogenase from salvia rosmarinus

Chain C:



• Molecule 1: Borneol dehydrogenase from salvia rosmarinus

Chain D:


8%
78%
10%
11%
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER CYS ASN THR ALA VAL SER R8 R9 V29 R30 K38 I41 D47 L48 G49 S61 Y62 K83 H84 D107 C140 I141 T149 E150 A161 Y164
V167 L177 I182 R183 A184 G191 V192 L193 T194 G195 I196 V197 P198 D199 D200 E201 A202 S203 K204 L205 M206 F207 E208 K220 V242 L248 T254 I264 T265 A266 GLY GLN SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	196.84Å 196.84Å 65.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.28 – 2.27 47.28 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.28-2.27) 99.7 (47.28-2.27)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.197 , 0.235 0.198 , 0.236	Depositor DCC
R_{free} test set	2100 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8044	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: CL, PXN, NAD

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	0.43	0/1928	0.61	2/2611 (0.1%)
1	B	0.43	1/1925 (0.1%)	0.62	1/2606 (0.0%)
1	C	0.37	0/1928	0.55	0/2611
1	D	0.38	1/1940 (0.1%)	0.55	0/2627
All	All	0.40	2/7721 (0.0%)	0.58	3/10455 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	140	CYS	CB-SG	-5.70	1.72	1.81
1	B	140	CYS	CB-SG	-5.67	1.72	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	206	MET	CA-CB-CG	8.33	127.47	113.30
1	A	206	MET	CA-CB-CG	7.50	126.05	113.30
1	A	206	MET	CG-SD-CE	5.67	109.28	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1903	0	1928	17	0
1	B	1900	0	1930	18	0
1	C	1903	0	1928	18	0
1	D	1915	0	1936	17	1
2	A	25	0	36	4	0
2	D	25	0	36	1	0
3	A	44	0	25	0	0
3	B	44	0	26	1	0
3	C	44	0	25	2	0
3	D	44	0	26	0	0
4	D	1	0	0	1	0
5	A	70	0	0	1	0
5	B	68	0	0	0	0
5	C	31	0	0	0	0
5	D	27	0	0	0	0
All	All	8044	0	7896	66	1

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 4.

All (66) 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:101:ASN:HA	2:A:301:PXN:HAXA	1.65	0.76
1:D:264:ILE:HG13	1:D:265:THR:HG23	1.72	0.72
1:D:193:LEU:HD21	1:D:204:LYS:HG2	1.71	0.71
1:D:150:GLU:HG3	1:D:248:LEU:HD11	1.75	0.67
3:C:301:NAD:H2N	3:C:301:NAD:O1N	1.99	0.62
1:B:9:ARG:NH2	1:C:238:GLU:OE2	2.33	0.61
1:A:202:ALA:O	1:A:206:MET:HG3	2.01	0.60
1:A:110[A]:GLU:OE1	1:A:113:ARG:NH1	2.35	0.60
1:A:238:GLU:OE2	1:D:9:ARG:NH2	2.35	0.60
1:A:150:GLU:HG3	1:A:248:LEU:HD21	1.85	0.58
1:C:176:GLU:HB2	2:D:301:PXN:HAU	1.85	0.58
1:C:151:ILE:HG13	1:C:254:THR:HG22	1.87	0.56
1:A:157:HIS:CE1	1:B:172:SER:HB2	2.42	0.55
1:D:49:GLY:HA3	1:D:62:TYR:CE1	2.41	0.55
1:A:200:ASP:OD1	1:A:201:GLU:N	2.38	0.55
1:C:151:ILE:HG12	1:C:254:THR:HA	1.89	0.54
1:D:177:LEU:HB3	1:D:182:ILE:HB	1.88	0.54
3:B:301:NAD:O1N	3:B:301:NAD:H2N	2.07	0.54
1:D:38:LYS:HD3	1:D:84:HIS:ND1	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:PRO:O	1:D:200:ASP:N	2.42	0.52
1:D:197:VAL:O	1:D:199:ASP:N	2.42	0.51
1:C:27:SER:OG	1:C:225:GLU:OE2	2.29	0.51
1:B:190:PHE:CG	1:B:191:GLY:N	2.79	0.51
1:A:57:GLY:O	5:A:401:HOH:O	2.19	0.50
1:A:240:SER:OG	1:D:220:LYS:HE3	2.12	0.50
1:A:190:PHE:CG	1:A:191:GLY:N	2.80	0.49
1:D:254:THR:O	4:D:303:CL:CL	2.68	0.49
1:B:81:VAL:HG22	1:B:86:GLY:HA2	1.94	0.49
1:D:196:ILE:HG22	1:D:197:VAL:H	1.78	0.48
1:B:177:LEU:HB3	1:B:182:ILE:HB	1.96	0.47
1:C:110[A]:GLU:OE2	1:C:113:ARG:NH1	2.47	0.47
1:B:197:VAL:N	1:B:198:PRO:HD2	2.30	0.46
1:D:141:ILE:O	1:D:184:ALA:HA	2.15	0.46
1:B:198:PRO:O	1:B:200:ASP:N	2.49	0.46
1:B:29:VAL:HG11	1:B:41:ILE:HD11	1.98	0.45
1:C:97:VAL:HA	1:C:159:TYR:CD2	2.52	0.45
1:D:204:LYS:O	1:D:208:GLU:HG3	2.17	0.45
1:A:214:VAL:CG2	1:C:263:VAL:HG21	2.47	0.44
1:A:100:PRO:HB3	2:A:301:PXN:HAAB	1.99	0.44
1:A:175:VAL:HG21	1:B:152:ALA:HB3	1.99	0.44
1:B:74[A]:ARG:HG3	1:B:131:ARG:NH2	2.32	0.43
1:B:141:ILE:O	1:B:184:ALA:HA	2.18	0.43
1:D:207:PHE:HD1	1:D:208:GLU:HG2	1.83	0.43
1:B:225:GLU:O	1:B:229:VAL:HG23	2.19	0.43
2:A:301:PXN:OAH	2:A:301:PXN:HAXB	2.19	0.43
1:C:45:GLN:OE1	3:C:301:NAD:O2B	2.36	0.43
1:B:39:VAL:HB	1:B:60:ILE:HD12	2.00	0.42
1:C:150:GLU:HG3	1:C:248:LEU:HD21	2.01	0.42
1:B:102:SER:OG	1:B:104:PHE:HD1	2.01	0.42
1:C:177:LEU:HB3	1:C:182:ILE:HB	2.01	0.42
1:A:201:GLU:HB3	1:A:203:SER:H	1.84	0.42
1:C:141:ILE:O	1:C:184:ALA:HA	2.20	0.42
1:C:193:LEU:HD12	1:C:197:VAL:HG23	2.01	0.42
1:B:220:LYS:HE3	1:C:240:SER:OG	2.19	0.42
1:C:49:GLY:HA3	1:C:62:TYR:CE1	2.55	0.41
1:C:29:VAL:HG11	1:C:41:ILE:HD11	2.02	0.41
1:C:264:ILE:HG13	1:C:265:THR:HG23	2.03	0.41
1:D:183:ARG:HD2	1:D:242:VAL:O	2.20	0.41
1:D:29:VAL:HG11	1:D:41:ILE:HD11	2.02	0.41
1:A:49:GLY:HA3	1:A:62:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:HG3	1:A:131:ARG:NH2	2.36	0.41
1:C:252:GLY:O	1:C:255:VAL:HG22	2.20	0.41
1:B:116:GLY:HA2	1:B:120:VAL:HB	2.03	0.40
1:A:102:SER:HB2	2:A:301:PXN:HAPA	2.02	0.40
1:B:33:HIS:HB2	1:B:60:ILE:HD11	2.04	0.40
1:B:49:GLY:HA3	1:B:62:TYR:CE1	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:LYS:NZ	1:D:107:ASP:OD2[4_665]	2.17	0.03

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	258/290 (89%)	250 (97%)	7 (3%)	1 (0%)	34 40
1	B	257/290 (89%)	249 (97%)	6 (2%)	2 (1%)	19 22
1	C	258/290 (89%)	251 (97%)	7 (3%)	0	100 100
1	D	260/290 (90%)	251 (96%)	4 (2%)	5 (2%)	8 6
All	All	1033/1160 (89%)	1001 (97%)	24 (2%)	8 (1%)	19 22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	195	GLY
1	B	199	ASP
1	D	191	GLY
1	D	196	ILE

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Mol	Chain	Res	Type
1	D	200	ASP
1	D	199	ASP
1	A	198	PRO
1	D	198	PRO

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	201/226 (89%)	198 (98%)	3 (2%)	65	77
1	B	201/226 (89%)	199 (99%)	2 (1%)	76	86
1	C	201/226 (89%)	197 (98%)	4 (2%)	55	70
1	D	203/226 (90%)	201 (99%)	2 (1%)	76	86
All	All	806/904 (89%)	795 (99%)	11 (1%)	69	79

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

Mol	Chain	Res	Type
1	A	58	ARG
1	A	201	GLU
1	A	206	MET
1	B	81	VAL
1	B	172	SER
1	C	27	SER
1	C	55	ARG
1	C	197	VAL
1	C	220	LYS
1	D	61[A]	SER
1	D	61[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	NAD	B	301	-	42,48,48	4.37	18 (42%)	50,73,73	2.18	6 (12%)
3	NAD	D	302	-	42,48,48	4.28	19 (45%)	50,73,73	2.14	6 (12%)
2	PXN	A	301	-	24,24,24	0.47	0	30,30,30	1.00	3 (10%)
3	NAD	A	302	-	42,48,48	4.32	18 (42%)	50,73,73	2.45	5 (10%)
3	NAD	C	301	-	42,48,48	4.23	19 (45%)	50,73,73	2.30	8 (16%)
2	PXN	D	301	-	24,24,24	0.53	0	30,30,30	0.62	1 (3%)

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
3	NAD	B	301	-	-	4/26/62/62	0/5/5/5
3	NAD	D	302	-	-	8/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PXN	A	301	-	-	13/28/28/28	-
3	NAD	A	302	-	-	9/26/62/62	0/5/5/5
3	NAD	C	301	-	-	5/26/62/62	0/5/5/5
2	PXN	D	301	-	-	8/28/28/28	-

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	NAD	PN-O3	11.24	1.71	1.59
3	B	301	NAD	PN-O3	11.17	1.71	1.59
3	A	302	NAD	PN-O3	10.74	1.71	1.59
3	A	302	NAD	O4D-C1D	-10.46	1.27	1.40
3	B	301	NAD	O4D-C1D	-10.38	1.27	1.40
3	C	301	NAD	O4D-C1D	-10.27	1.27	1.40
3	C	301	NAD	PN-O3	10.14	1.70	1.59
3	D	302	NAD	O4D-C1D	-9.37	1.28	1.40
3	A	302	NAD	C7N-N7N	9.01	1.49	1.33
3	D	302	NAD	C7N-N7N	8.94	1.49	1.33
3	C	301	NAD	C7N-N7N	8.93	1.49	1.33
3	C	301	NAD	C3B-C4B	-8.91	1.30	1.53
3	B	301	NAD	C3B-C4B	-8.85	1.30	1.53
3	B	301	NAD	C7N-N7N	8.79	1.49	1.33
3	D	302	NAD	C3B-C4B	-8.50	1.31	1.53
3	A	302	NAD	C3B-C4B	-8.47	1.31	1.53
3	B	301	NAD	O4D-C4D	8.25	1.63	1.45
3	D	302	NAD	O4D-C4D	8.11	1.63	1.45
3	B	301	NAD	O4B-C4B	7.88	1.62	1.45
3	A	302	NAD	O4B-C4B	7.87	1.62	1.45
3	C	301	NAD	C3D-C4D	-7.86	1.33	1.53
3	A	302	NAD	O4D-C4D	7.81	1.62	1.45
3	C	301	NAD	O4D-C4D	7.80	1.62	1.45
3	D	302	NAD	O4B-C4B	7.74	1.62	1.45
3	B	301	NAD	C3D-C4D	-7.72	1.33	1.53
3	C	301	NAD	O4B-C4B	7.70	1.62	1.45
3	D	302	NAD	C3D-C4D	-7.65	1.33	1.53
3	A	302	NAD	C3D-C4D	-7.23	1.34	1.53
3	C	301	NAD	O4B-C1B	-7.17	1.31	1.40
3	A	302	NAD	O4B-C1B	-7.09	1.31	1.40
3	D	302	NAD	O4B-C1B	-6.73	1.32	1.40
3	B	301	NAD	O4B-C1B	-6.70	1.32	1.40
3	A	302	NAD	PA-O3	6.52	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	NAD	PA-O3	6.38	1.66	1.59
3	D	302	NAD	PA-O3	6.10	1.66	1.59
3	A	302	NAD	O3D-C3D	5.40	1.56	1.43
3	B	301	NAD	C3N-C7N	5.17	1.58	1.50
3	C	301	NAD	C3N-C7N	5.15	1.58	1.50
3	B	301	NAD	O3D-C3D	5.05	1.55	1.43
3	A	302	NAD	C3N-C7N	4.97	1.58	1.50
3	C	301	NAD	PA-O3	4.95	1.64	1.59
3	D	302	NAD	O3D-C3D	4.92	1.55	1.43
3	D	302	NAD	C3N-C7N	4.88	1.57	1.50
3	C	301	NAD	O3D-C3D	4.62	1.54	1.43
3	D	302	NAD	C2N-N1N	3.69	1.39	1.35
3	D	302	NAD	O3B-C3B	3.68	1.52	1.43
3	A	302	NAD	C2N-N1N	3.56	1.38	1.35
3	B	301	NAD	C2N-N1N	3.47	1.38	1.35
3	A	302	NAD	O3B-C3B	3.38	1.51	1.43
3	B	301	NAD	O3B-C3B	3.35	1.51	1.43
3	C	301	NAD	C2N-N1N	3.25	1.38	1.35
3	B	301	NAD	C2A-N1A	3.23	1.39	1.33
3	C	301	NAD	O3B-C3B	3.10	1.50	1.43
3	D	302	NAD	C2A-N1A	3.08	1.39	1.33
3	C	301	NAD	C2A-N1A	3.06	1.39	1.33
3	A	302	NAD	C2A-N1A	3.05	1.39	1.33
3	B	301	NAD	C2A-N3A	2.74	1.36	1.32
3	D	302	NAD	C4A-N3A	2.68	1.39	1.35
3	A	302	NAD	C2A-N3A	2.60	1.36	1.32
3	D	302	NAD	C2A-N3A	2.59	1.36	1.32
3	C	301	NAD	C2A-N3A	2.55	1.36	1.32
3	C	301	NAD	O2B-C2B	-2.53	1.36	1.43
3	A	302	NAD	O2B-C2B	-2.49	1.36	1.43
3	D	302	NAD	O7N-C7N	-2.47	1.19	1.24
3	B	301	NAD	C4A-N3A	2.41	1.38	1.35
3	C	301	NAD	O7N-C7N	-2.36	1.19	1.24
3	B	301	NAD	PA-O5B	2.33	1.68	1.59
3	C	301	NAD	PA-O5B	2.32	1.68	1.59
3	A	302	NAD	PA-O5B	2.30	1.68	1.59
3	D	302	NAD	O2B-C2B	-2.29	1.37	1.43
3	B	301	NAD	O2B-C2B	-2.28	1.37	1.43
3	D	302	NAD	PA-O5B	2.26	1.68	1.59
3	A	302	NAD	O7N-C7N	-2.13	1.20	1.24
3	C	301	NAD	C4A-N3A	2.11	1.38	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	NAD	C1B-N9A-C4A	-9.78	109.46	126.64
3	C	301	NAD	C1B-N9A-C4A	-9.77	109.48	126.64
3	D	302	NAD	C1B-N9A-C4A	-9.65	109.68	126.64
3	A	302	NAD	C4B-O4B-C1B	-9.48	101.24	109.92
3	B	301	NAD	C1B-N9A-C4A	-8.71	111.34	126.64
3	B	301	NAD	C4D-O4D-C1D	-6.93	103.58	109.92
3	D	302	NAD	N3A-C2A-N1A	-6.54	119.80	128.67
3	C	301	NAD	N3A-C2A-N1A	-6.53	119.81	128.67
3	A	302	NAD	C4D-O4D-C1D	-6.41	104.05	109.92
3	C	301	NAD	C4B-O4B-C1B	-6.41	104.06	109.92
3	B	301	NAD	C4B-O4B-C1B	-6.27	104.18	109.92
3	D	302	NAD	C4B-O4B-C1B	-6.17	104.28	109.92
3	C	301	NAD	C4D-O4D-C1D	-5.95	104.48	109.92
3	B	301	NAD	N3A-C2A-N1A	-5.89	120.68	128.67
3	A	302	NAD	N3A-C2A-N1A	-5.69	120.94	128.67
3	A	302	NAD	O4B-C1B-N9A	3.45	113.32	108.75
3	C	301	NAD	O4B-C1B-N9A	3.28	113.09	108.75
3	D	302	NAD	C4D-O4D-C1D	-2.99	107.19	109.92
3	D	302	NAD	O4B-C1B-N9A	2.80	112.46	108.75
2	A	301	PXN	OAV-CAW-CAM	2.60	115.78	108.84
3	B	301	NAD	O4B-C1B-N9A	2.55	112.12	108.75
3	D	302	NAD	C6N-N1N-C2N	-2.50	119.75	121.88
3	C	301	NAD	C3N-C7N-N7N	2.32	120.60	117.74
2	A	301	PXN	OAK-CAL-CAM	2.30	114.97	108.84
3	C	301	NAD	C6N-N1N-C2N	-2.12	120.08	121.88
2	D	301	PXN	OAK-CAL-CAM	2.11	114.46	108.84
3	B	301	NAD	C5B-C4B-C3B	-2.07	107.75	115.21
3	C	301	NAD	O7N-C7N-N7N	-2.05	119.65	122.62
2	A	301	PXN	OAV-CAU-CAT	2.00	115.53	109.34

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	PXN	CAB-CAI-CAJ-OAK
2	A	301	PXN	OAO-CAP-CAQ-OAR
2	A	301	PXN	OAO-CAP-CAQ-CAX
2	A	301	PXN	OAS-CAT-CAU-OAV
3	A	302	NAD	C5B-O5B-PA-O1A
3	A	302	NAD	C5B-O5B-PA-O3
3	A	302	NAD	C5D-O5D-PN-O3
3	B	301	NAD	C5D-O5D-PN-O3
3	C	301	NAD	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
3	C	301	NAD	C5D-O5D-PN-O1N
3	D	302	NAD	PN-O3-PA-O5B
3	D	302	NAD	C5D-O5D-PN-O3
3	D	302	NAD	C5D-O5D-PN-O2N
2	D	301	PXN	CAW-CAM-CAN-OAO
2	D	301	PXN	CAC-CAM-CAN-OAO
2	D	301	PXN	CAL-CAM-CAN-OAO
2	D	301	PXN	CAM-CAC-OAD-CAE
2	A	301	PXN	CAM-CAC-OAD-CAE
2	A	301	PXN	OAD-CAE-CAF-CAA
2	A	301	PXN	CAY-CAT-CAU-OAV
3	A	302	NAD	PN-O3-PA-O5B
3	A	302	NAD	PA-O3-PN-O5D
3	B	301	NAD	PN-O3-PA-O5B
3	C	301	NAD	PN-O3-PA-O5B
2	A	301	PXN	OAD-CAE-CAF-OAG
2	A	301	PXN	OAH-CAI-CAJ-OAK
2	A	301	PXN	CAM-CAN-OAO-CAP
2	A	301	PXN	CAM-CAW-OAV-CAU
2	D	301	PXN	CAM-CAL-OAK-CAJ
3	A	302	NAD	PA-O3-PN-O1N
3	A	302	NAD	C5B-O5B-PA-O2A
3	A	302	NAD	C5D-O5D-PN-O1N
3	B	301	NAD	C5D-O5D-PN-O1N
3	D	302	NAD	C5B-O5B-PA-O2A
3	D	302	NAD	C5D-O5D-PN-O1N
2	D	301	PXN	CAM-CAN-OAO-CAP
3	C	301	NAD	PN-O3-PA-O1A
2	D	301	PXN	CAF-CAE-OAD-CAC
2	D	301	PXN	CAI-CAJ-OAK-CAL
2	A	301	PXN	CAM-CAL-OAK-CAJ
3	D	302	NAD	O4D-C1D-N1N-C6N
2	A	301	PXN	CAF-CAE-OAD-CAC
3	B	301	NAD	C4D-C5D-O5D-PN
3	C	301	NAD	C4D-C5D-O5D-PN
3	A	302	NAD	C4B-C5B-O5B-PA
3	D	302	NAD	C4B-C5B-O5B-PA
3	D	302	NAD	PN-O3-PA-O2A

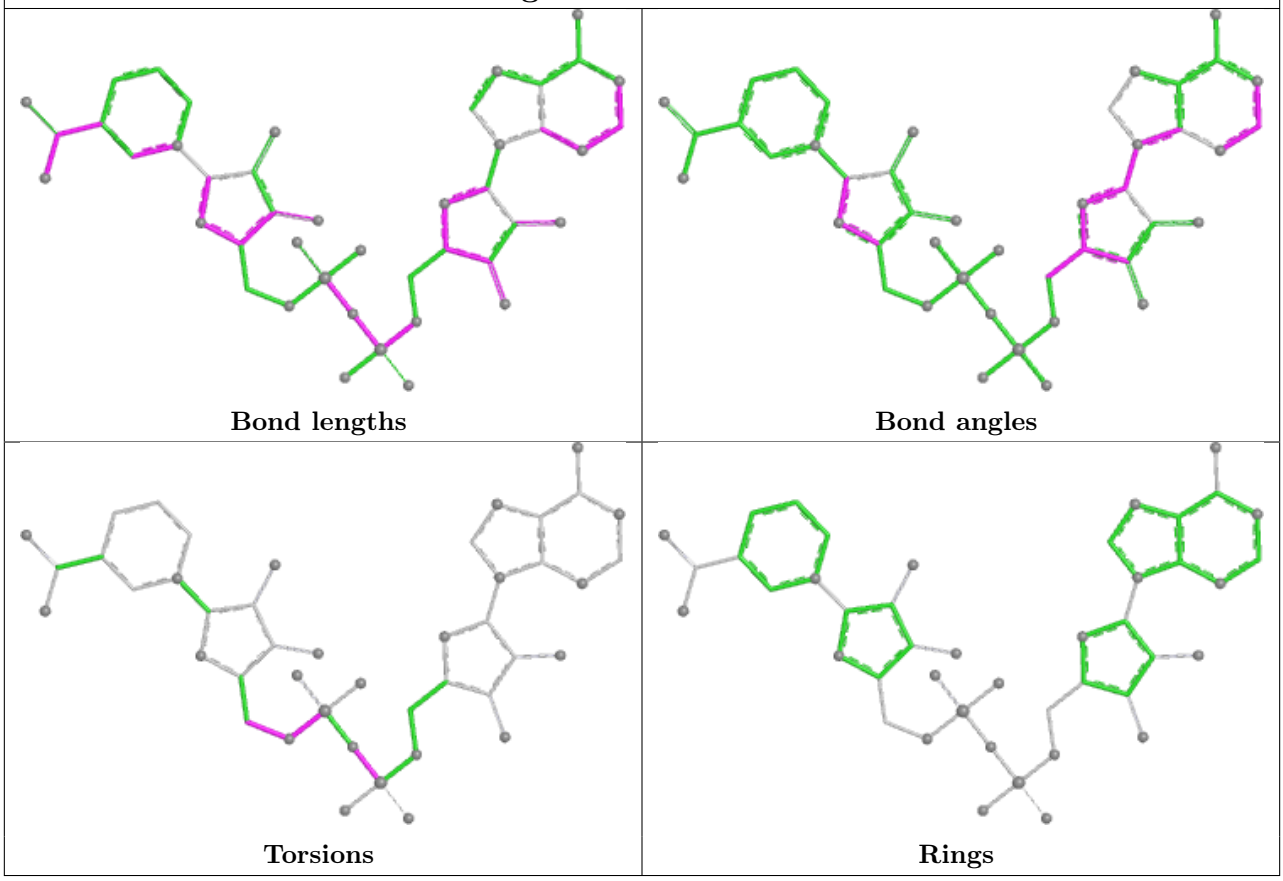
There are no ring outliers.

4 monomers are involved in 8 short contacts:

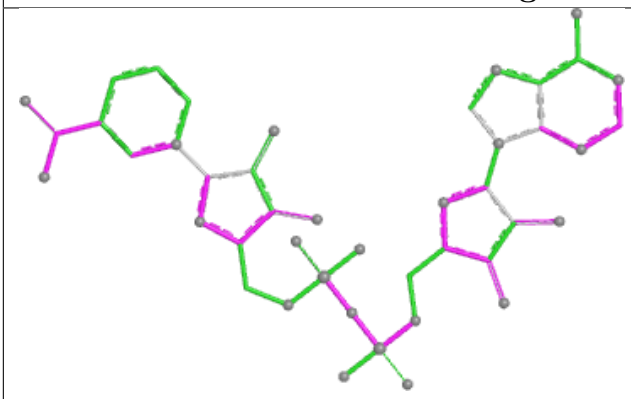
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	NAD	1	0
2	A	301	PXN	4	0
3	C	301	NAD	2	0
2	D	301	PXN	1	0

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 then 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.

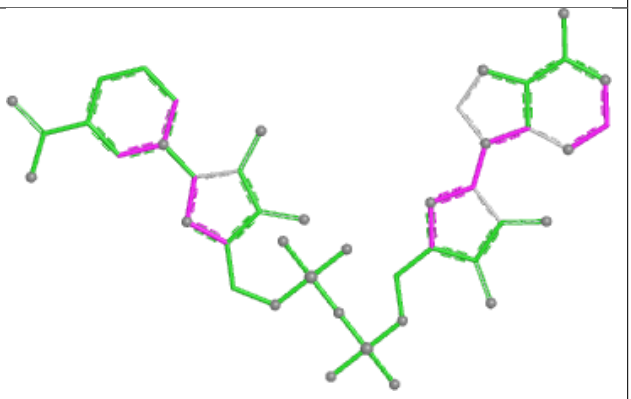
Ligand NAD B 301



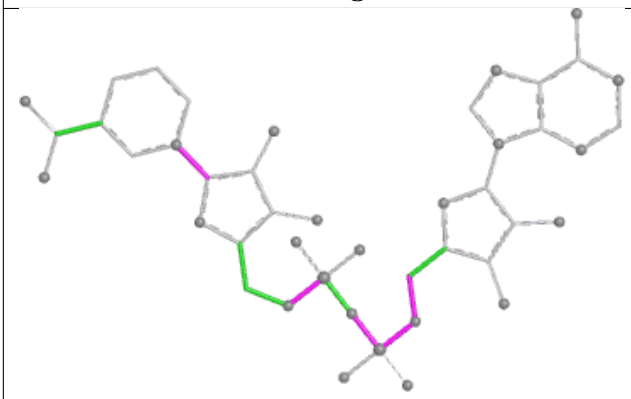
Ligand NAD D 302



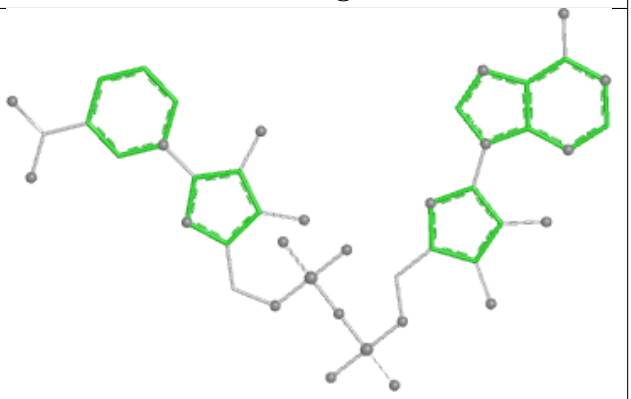
Bond lengths



Bond angles

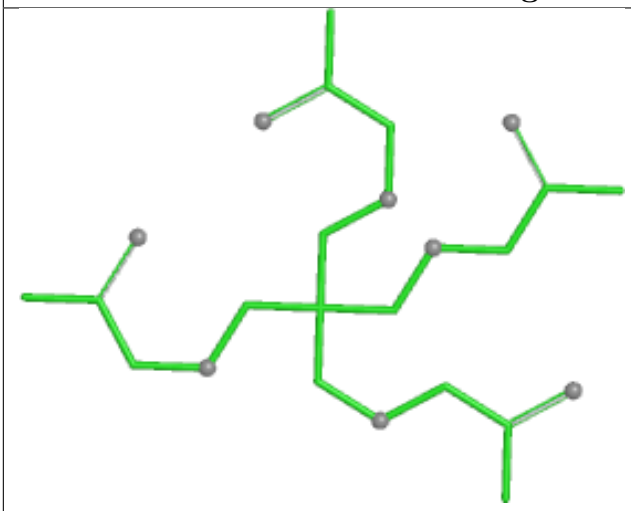


Torsions

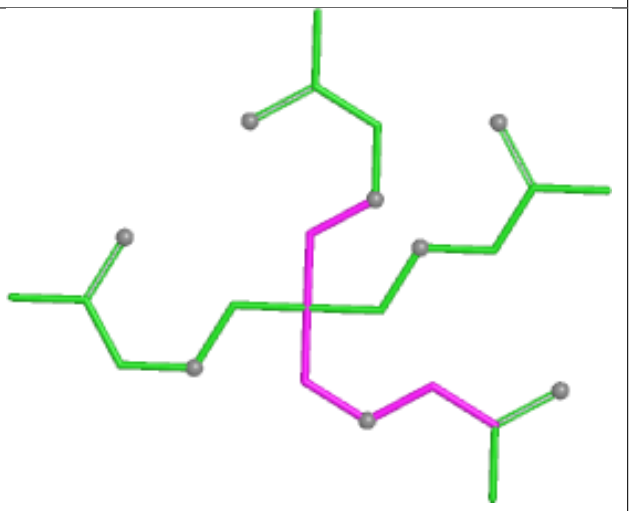


Rings

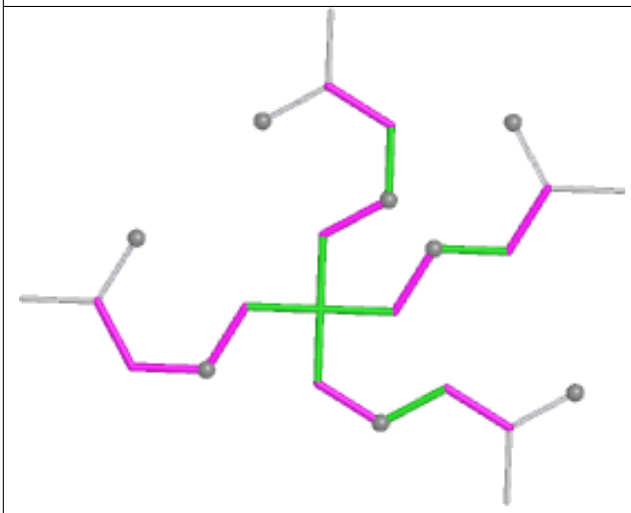
Ligand PXN A 301



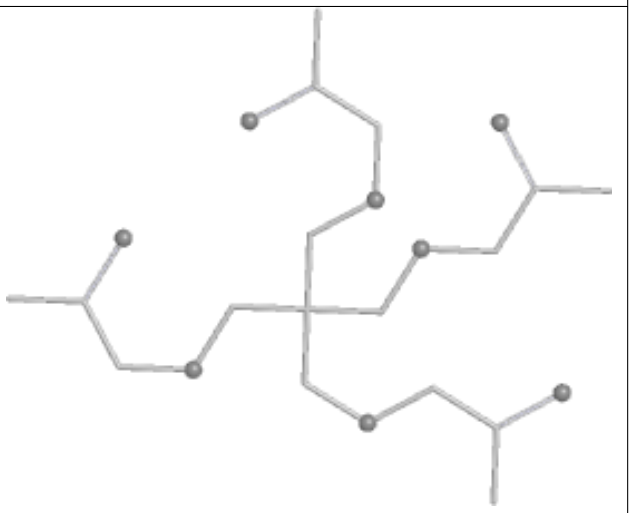
Bond lengths



Bond angles

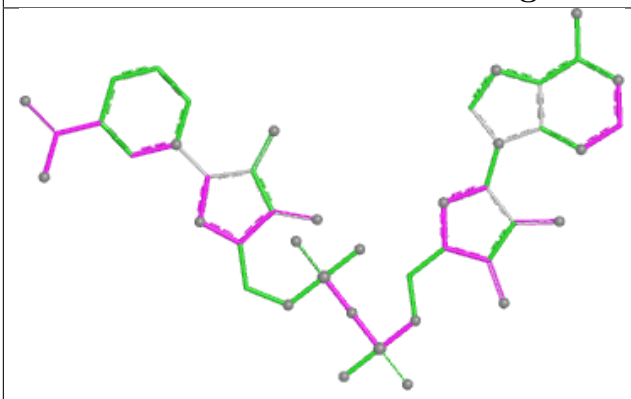


Torsions

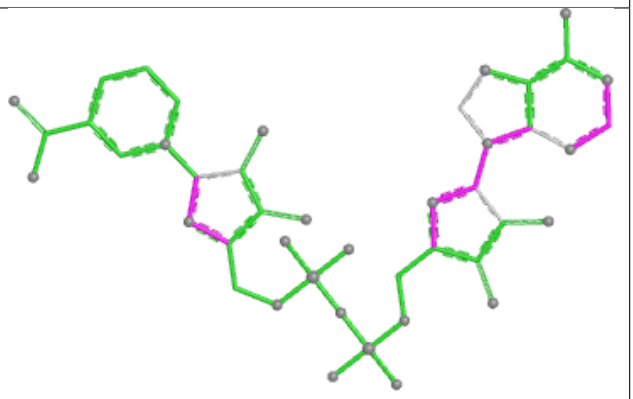


Rings

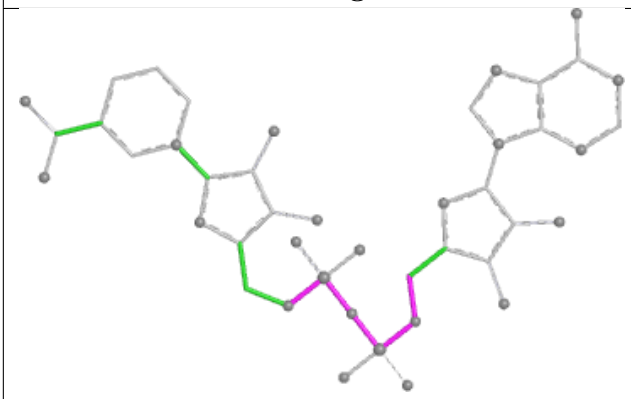
Ligand NAD A 302



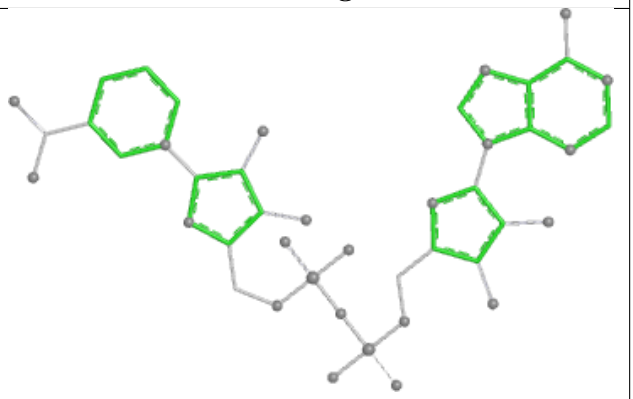
Bond lengths



Bond angles

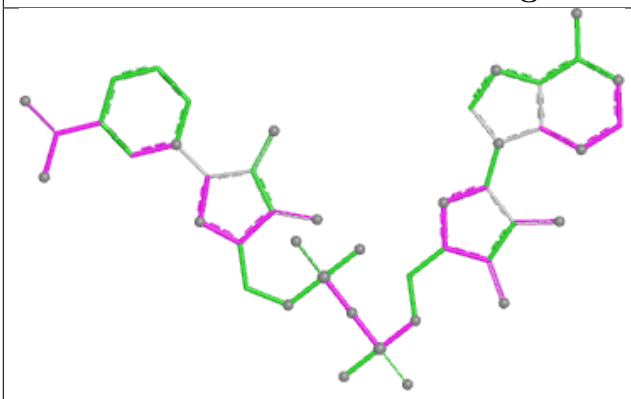


Torsions

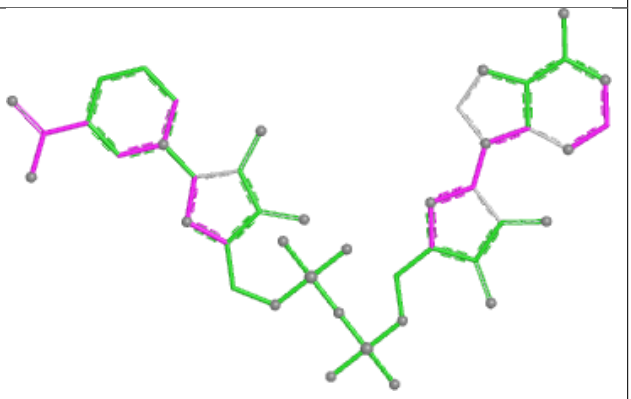


Rings

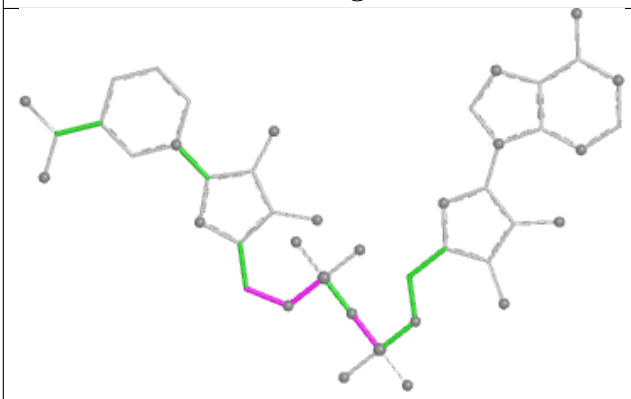
Ligand NAD C 301



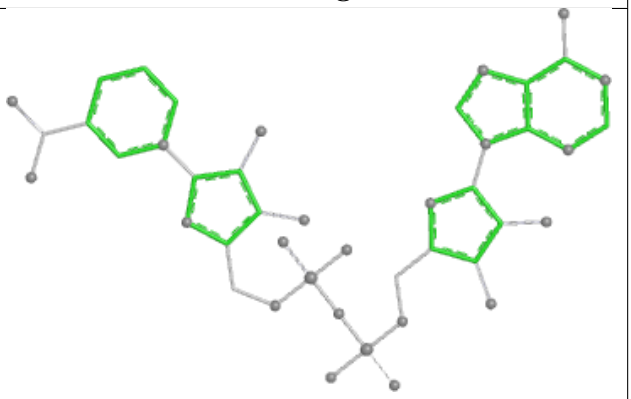
Bond lengths



Bond angles

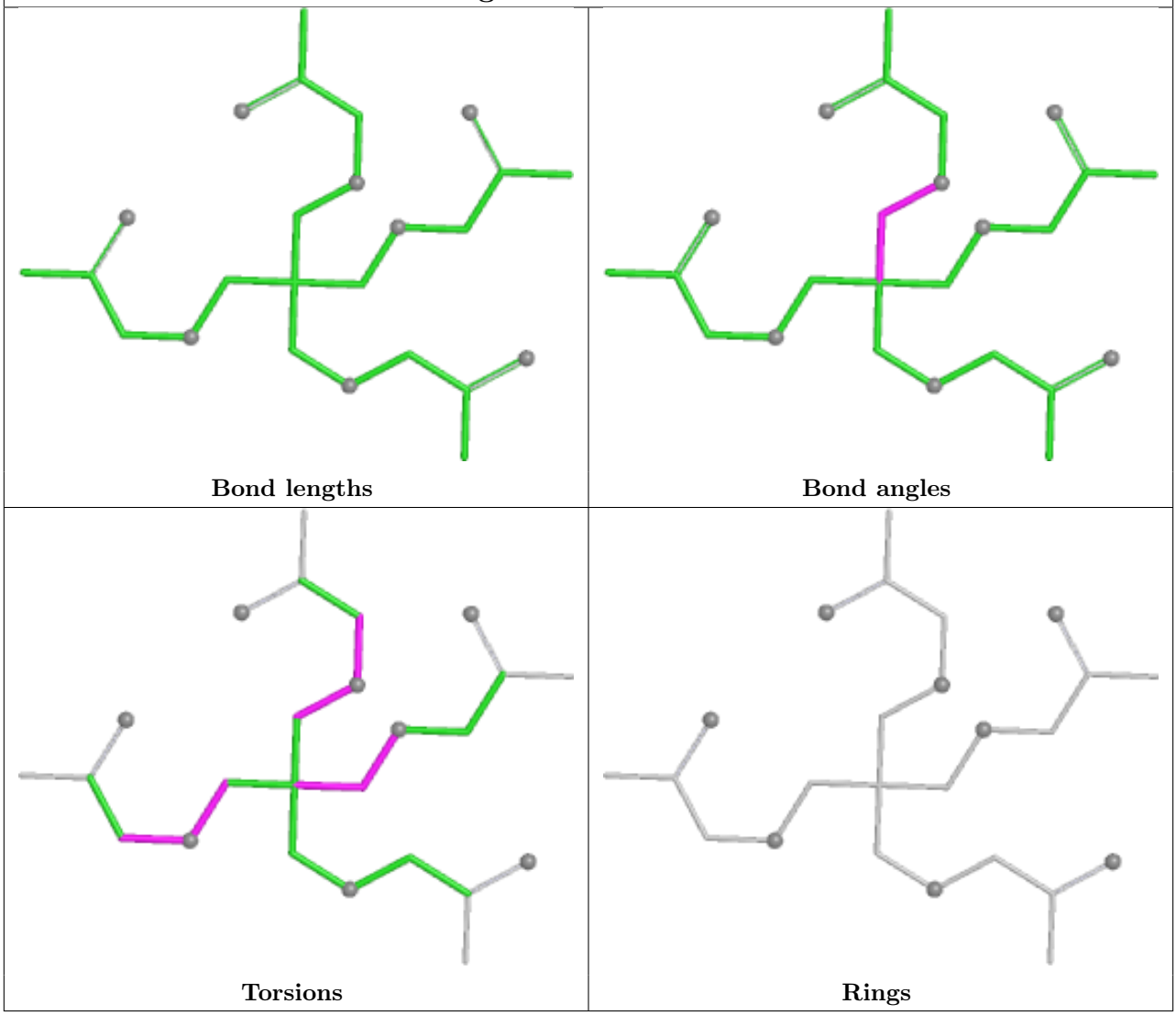


Torsions



Rings

Ligand PXN D 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	259/290 (89%)	0.12	18 (6%) 16 21	31, 40, 71, 122	0
1	B	258/290 (88%)	0.23	24 (9%) 8 11	29, 41, 69, 120	0
1	C	259/290 (89%)	0.50	30 (11%) 4 6	34, 54, 98, 133	0
1	D	259/290 (89%)	0.38	23 (8%) 9 12	34, 54, 94, 136	0
All	All	1035/1160 (89%)	0.30	95 (9%) 9 11	29, 46, 83, 136	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	PRO	9.2
1	D	200	ASP	8.5
1	A	197	VAL	8.3
1	D	197	VAL	8.3
1	C	203	SER	7.5
1	A	199	ASP	7.5
1	A	198	PRO	7.4
1	D	202	ALA	7.4
1	C	202	ALA	7.3
1	B	197	VAL	7.3
1	C	197	VAL	7.2
1	C	196	ILE	6.6
1	A	196	ILE	6.5
1	D	203	SER	6.5
1	C	198	PRO	6.4
1	C	200	ASP	5.9
1	A	202	ALA	5.7
1	D	196	ILE	5.7
1	D	198	PRO	5.4
1	D	205	LEU	5.3
1	D	201	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	D	206	MET	5.3
1	A	195	GLY	5.2
1	C	206	MET	4.9
1	B	195	GLY	4.8
1	C	207	PHE	4.7
1	B	199	ASP	4.7
1	B	196	ILE	4.6
1	D	194	THR	4.5
1	A	200	ASP	4.5
1	D	204	LYS	4.4
1	C	205	LEU	4.4
1	C	204	LYS	4.4
1	C	199	ASP	4.3
1	D	199	ASP	4.2
1	C	167	VAL	4.2
1	B	206	MET	4.0
1	C	56	LEU	3.9
1	A	205	LEU	3.7
1	D	195	GLY	3.6
1	D	207	PHE	3.4
1	D	167	VAL	3.4
1	C	193	LEU	3.2
1	D	193	LEU	3.2
1	A	193	LEU	3.2
1	A	194	THR	3.1
1	B	58	ARG	3.1
1	B	245	VAL	3.0
1	C	168	GLY	3.0
1	A	167	VAL	3.0
1	D	149	THR	2.9
1	B	167	VAL	2.9
1	C	195	GLY	2.8
1	A	203	SER	2.8
1	B	194	THR	2.8
1	B	202	ALA	2.7
1	B	203	SER	2.7
1	A	266	ALA	2.7
1	B	150	GLU	2.7
1	C	58	ARG	2.6
1	D	164	TYR	2.6
1	B	164	TYR	2.6
1	D	47	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	194	THR	2.5
1	C	201	GLU	2.5
1	C	149	THR	2.5
1	C	245	VAL	2.5
1	B	244	GLY	2.4
1	B	247	LEU	2.4
1	B	255	VAL	2.4
1	D	30	ARG	2.4
1	C	170	MET	2.4
1	C	255	VAL	2.4
1	D	208	GLU	2.4
1	B	186	CYS	2.4
1	A	164	TYR	2.3
1	C	52	LEU	2.3
1	D	150	GLU	2.2
1	B	185	ASN	2.2
1	A	148	CYS	2.2
1	D	161	ALA	2.2
1	C	164	TYR	2.2
1	B	166	ILE	2.2
1	B	149	THR	2.1
1	C	82	ALA	2.1
1	A	264	ILE	2.1
1	C	244	GLY	2.1
1	C	38	LYS	2.1
1	C	12	GLY	2.1
1	A	206	MET	2.1
1	C	166	ILE	2.0
1	B	170	MET	2.0
1	A	245	VAL	2.0
1	B	169	LEU	2.0
1	B	205	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

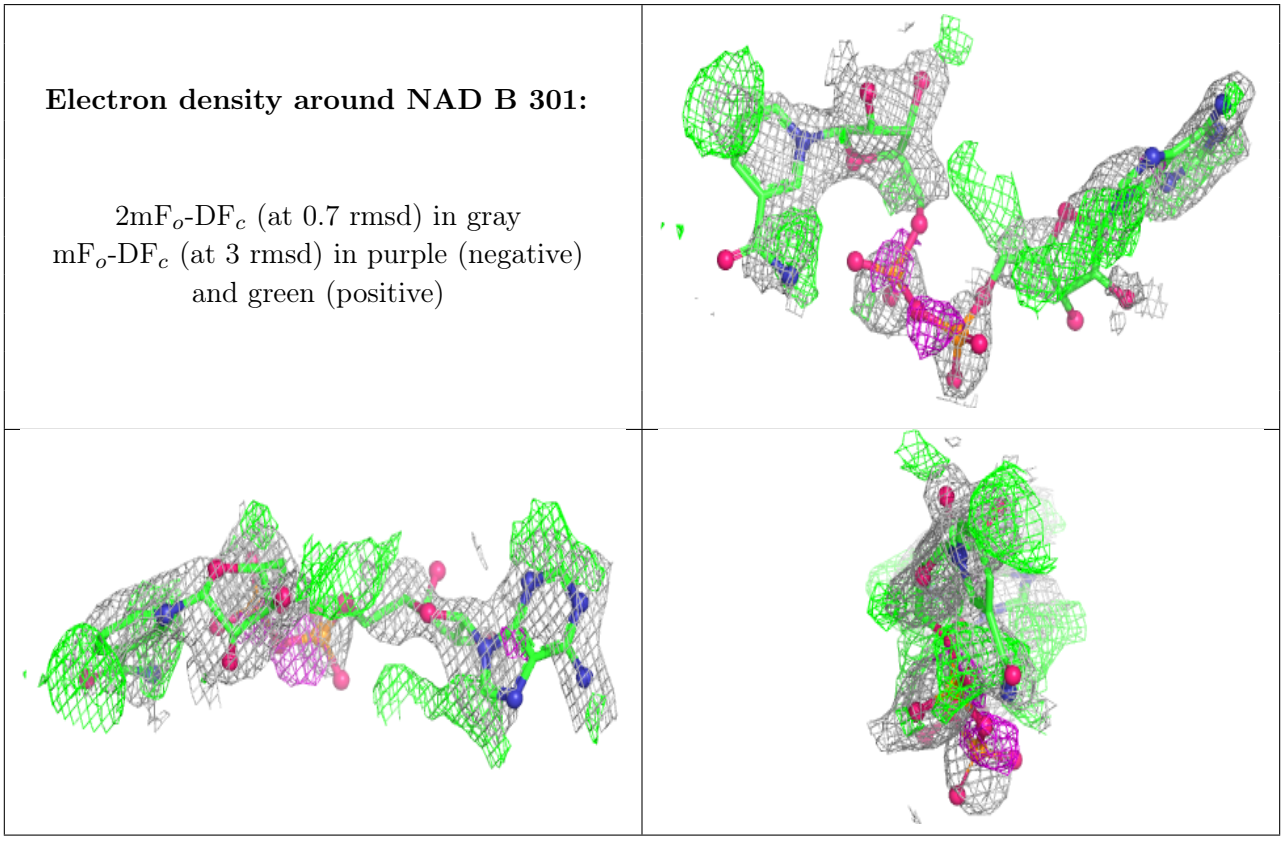
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAD	B	301	44/44	0.60	0.38	34,52,67,71	44
3	NAD	A	302	44/44	0.70	0.32	36,50,63,72	44
3	NAD	C	301	44/44	0.75	0.24	52,65,81,86	44
2	PXN	D	301	25/25	0.77	0.23	57,80,93,99	0
3	NAD	D	302	44/44	0.78	0.25	50,80,98,110	0
2	PXN	A	301	25/25	0.83	0.20	45,71,78,80	0
4	CL	D	303	1/1	0.97	0.22	50,50,50,50	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.

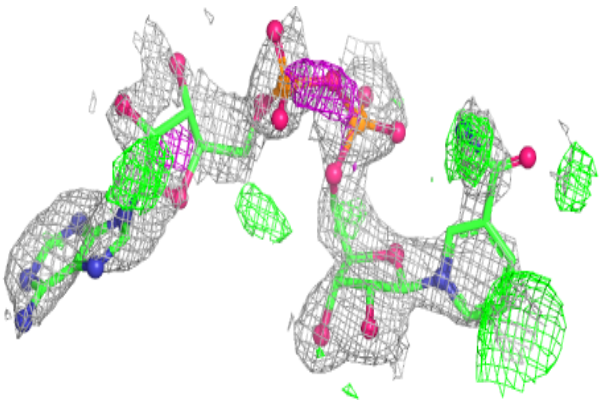
Electron density around NAD B 301:

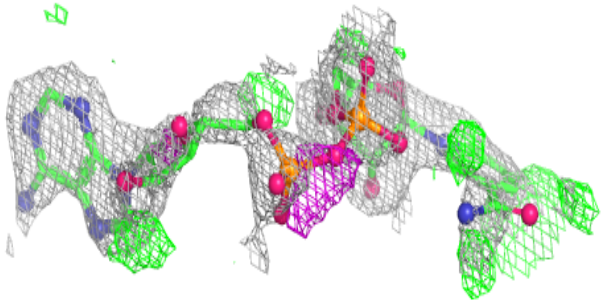
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

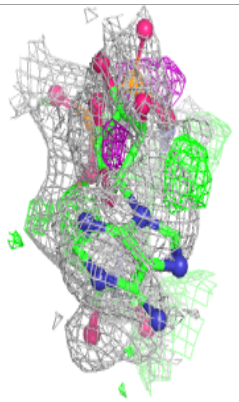


Electron density around NAD A 302:

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

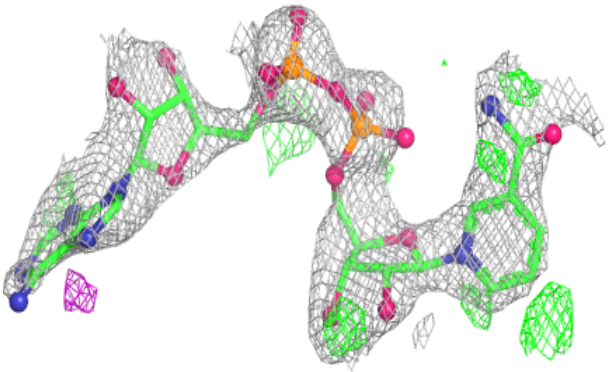


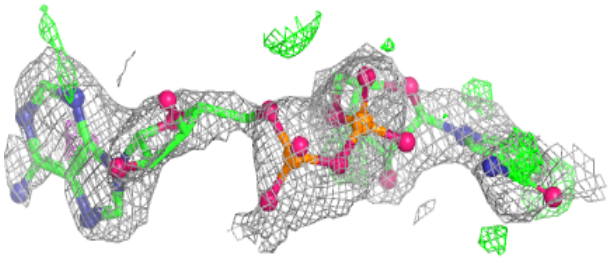


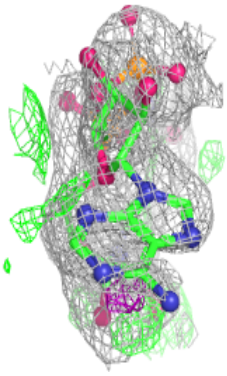


Electron density around NAD C 301:

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

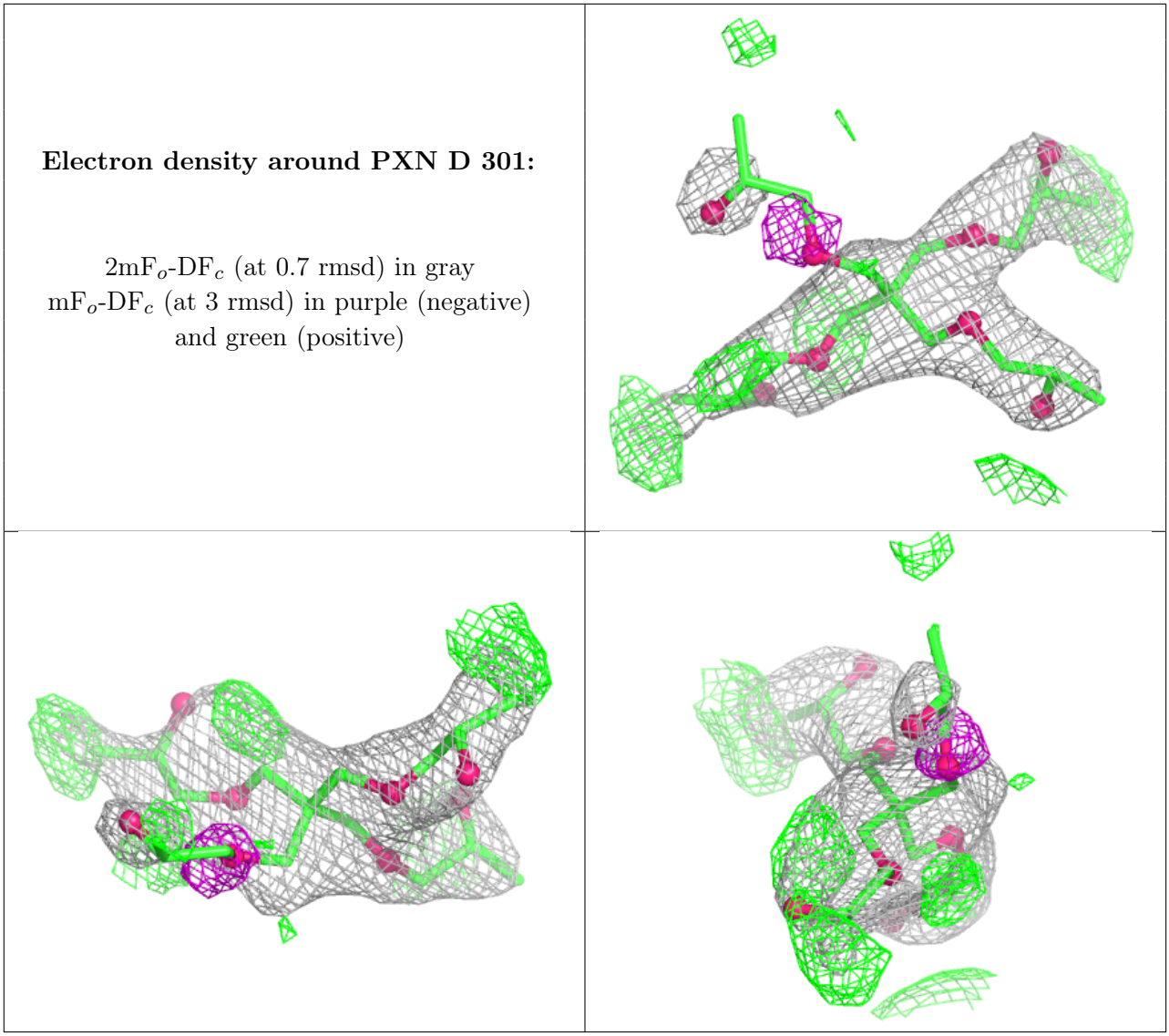






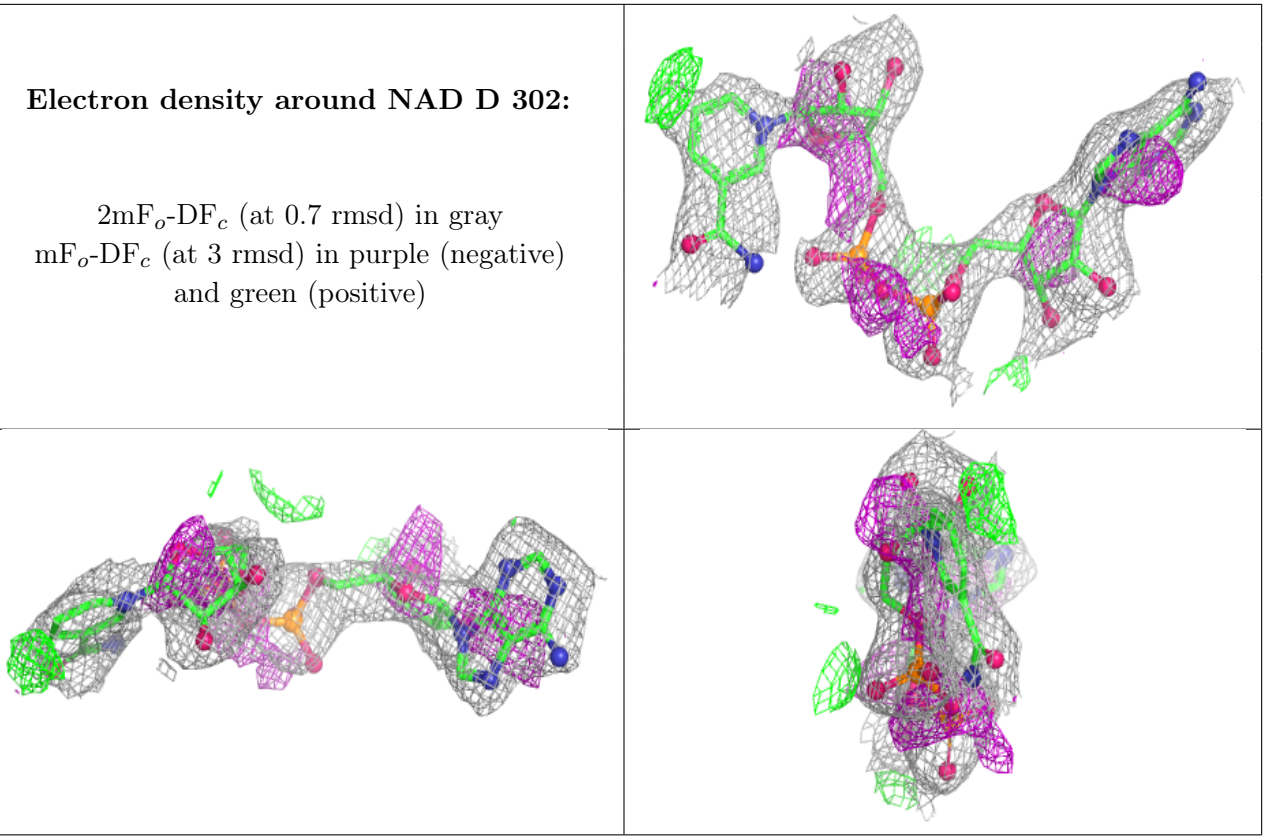
Electron density around PXN D 301:

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



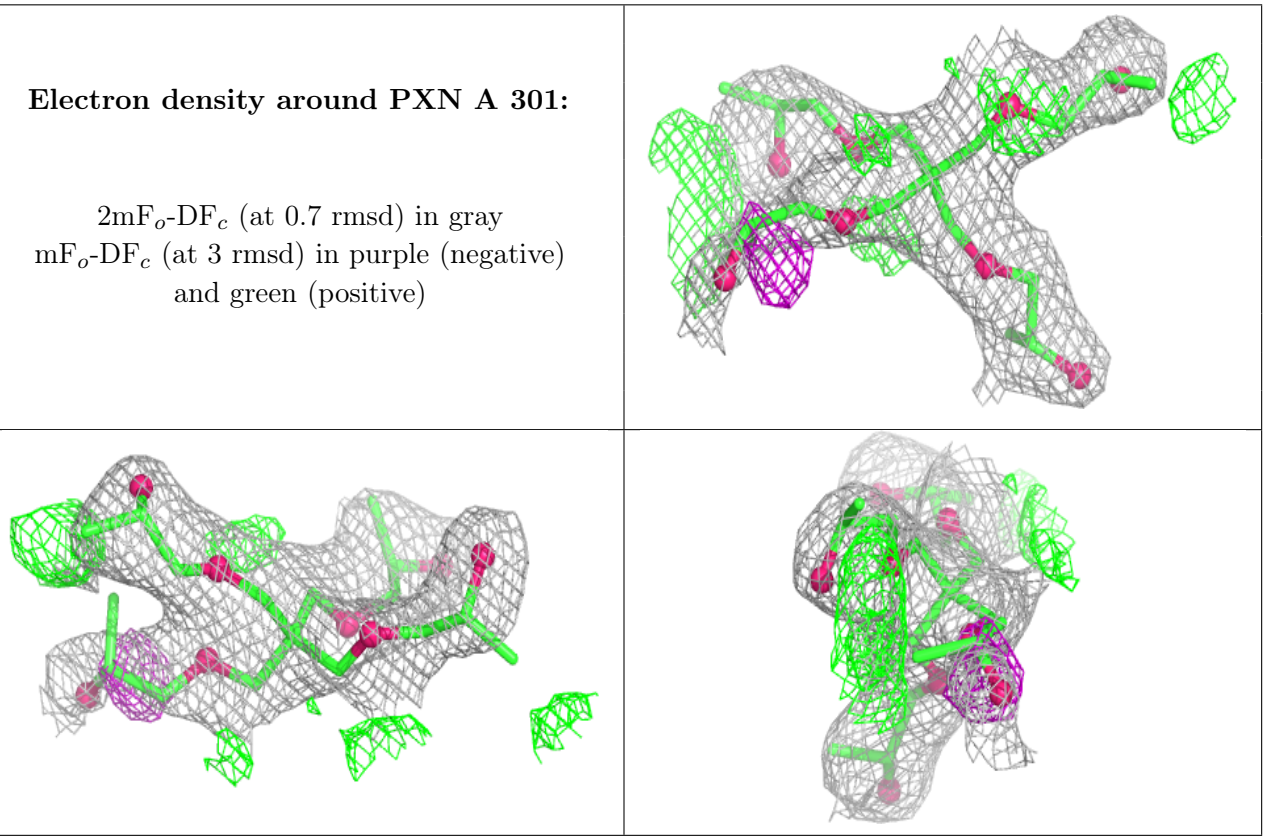
Electron density around NAD D 302:

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



Electron density around PXN A 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.