



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:38 pm BST

PDB ID : 4Q3C
Title : PylD cocrystallized with L-Lysine-Ne-L-lysine and NAD+
Authors : Quitterer, F.; Beck, P.; Bacher, A.; Groll, M.
Deposited on : 2014-04-11
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

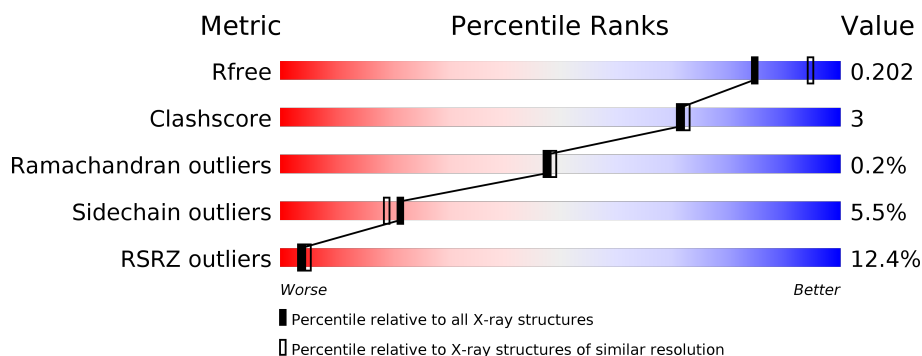
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	260	
1	B	260	
1	C	260	
1	D	260	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	EDO	A	910	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8384 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 PylD, pyrrolysine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			1956	1246	314	385	11			
1	B	259	Total	C	N	O	S	0	0	0
			1956	1246	314	385	11			
1	C	259	Total	C	N	O	S	0	0	0
			1956	1246	314	385	11			
1	D	258	Total	C	N	O	S	0	0	0
			1948	1241	313	384	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q46E80
B	0	SER	-	EXPRESSION TAG	UNP Q46E80
C	0	SER	-	EXPRESSION TAG	UNP Q46E80
D	0	SER	-	EXPRESSION TAG	UNP Q46E80

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

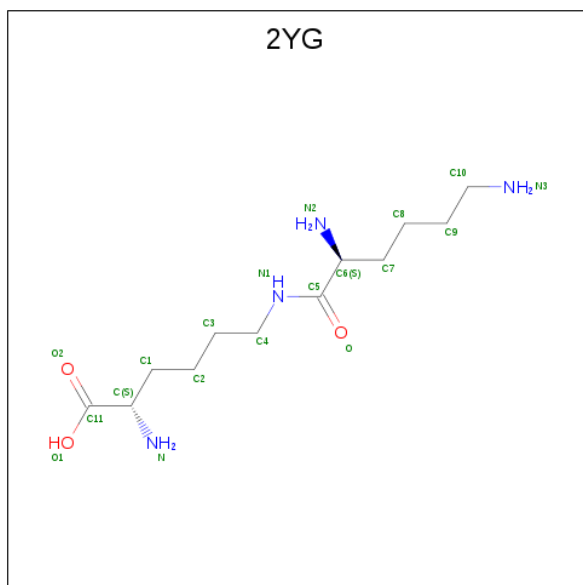
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

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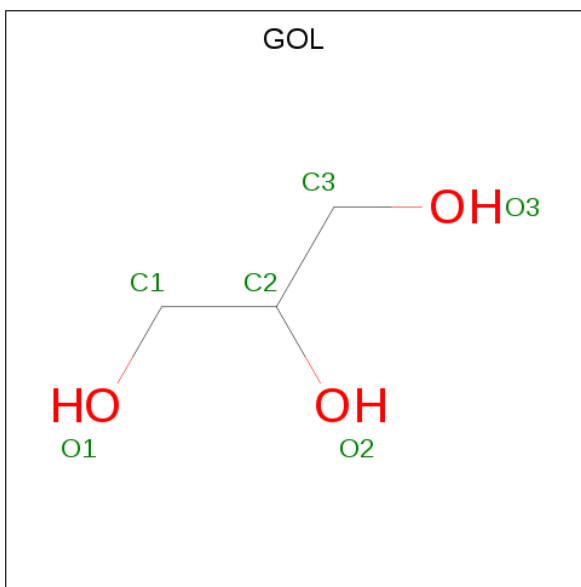
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is N 6 -L-lysyl-L-lysine (three-letter code: 2YG) (formula: $C_{12}H_{26}N_4O_3$).



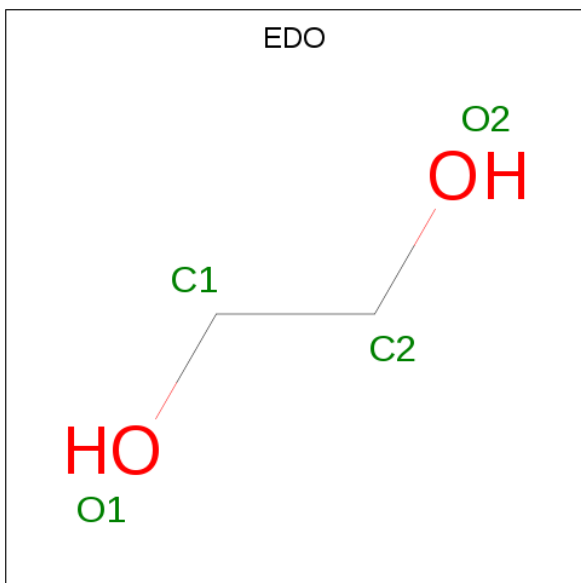
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			19	12	4	3		
5	B	1	Total	C	N	O	0	0
			19	12	4	3		
5	C	1	Total	C	N	O	0	0
			15	9	3	3		
5	D	1	Total	C	N	O	0	0
			15	9	3	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



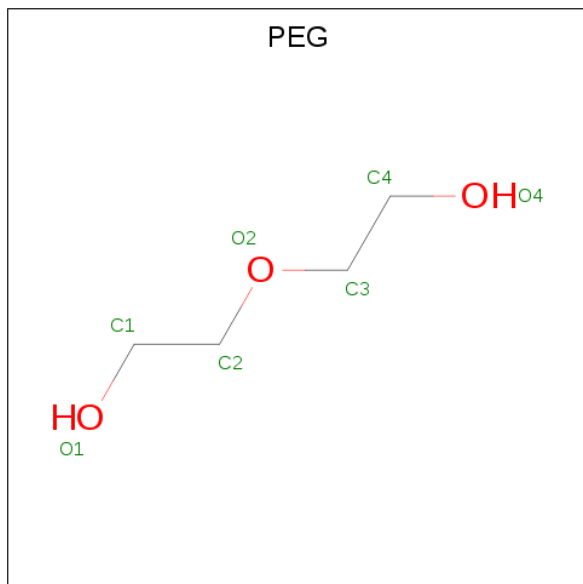
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	4	3		

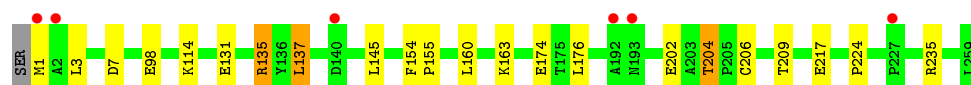
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	133	Total	O	0	0
			133	133		
9	B	111	Total	O	0	0
			111	111		
9	C	16	Total	O	0	0
			16	16		
9	D	13	Total	O	0	0
			13	13		

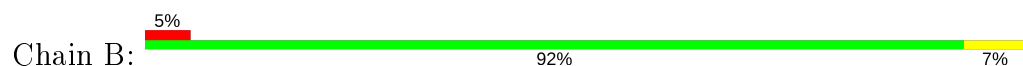
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

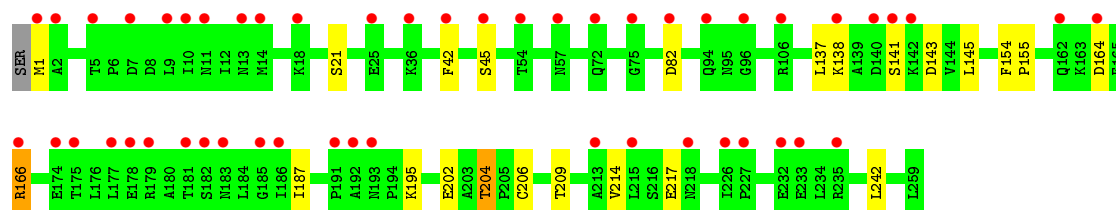
- Molecule 1: PylD, pyrrolysine synthase



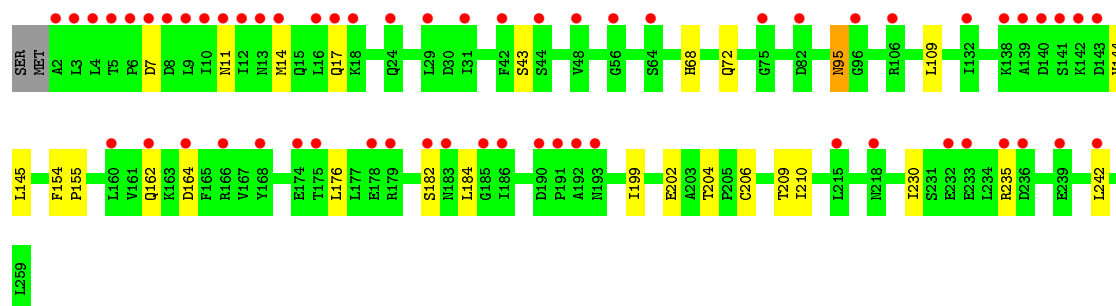
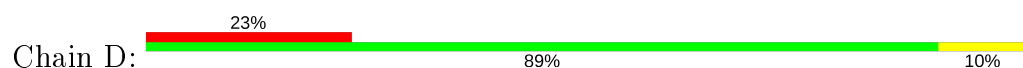
- Molecule 1: PylD, pyrrolysine synthase



- Molecule 1: PylD, pyrrolysine synthase



- Molecule 1: PylD, pyrrolysine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.25Å 259.77Å 48.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10 14.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.00-2.10) 99.9 (14.93-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.169 , 0.198 0.179 , 0.202	Depositor DCC
R_{free} test set	6351 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.987	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8384	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, NAD, 2YG, EDO, NA, PEG

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	0.68	0/1992	0.84	3/2705 (0.1%)
1	B	0.67	0/1992	0.81	1/2705 (0.0%)
1	C	0.34	0/1992	0.58	0/2705
1	D	0.33	0/1984	0.56	0/2695
All	All	0.53	0/7960	0.71	4/10810 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ARG	NE-CZ-NH1	-11.29	114.66	120.30
1	A	135	ARG	NE-CZ-NH2	8.42	124.51	120.30
1	B	166	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	135	ARG	CG-CD-NE	-5.10	101.08	111.80

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	1956	0	1950	16	0
1	B	1956	0	1950	10	0
1	C	1956	0	1950	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1948	0	1938	9	0
2	A	44	0	26	4	0
2	B	44	0	26	7	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	19	0	25	7	0
5	B	19	0	25	8	0
5	C	15	0	15	0	0
5	D	15	0	15	0	0
6	A	18	0	24	0	0
6	B	6	0	8	0	0
7	A	12	0	18	6	0
8	B	7	0	10	0	0
9	A	133	0	0	1	0
9	B	111	0	0	2	0
9	C	16	0	0	0	0
9	D	13	0	0	0	0
All	All	8384	0	8032	56	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 3.

All (56) 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:204:THR:HG21	1:A:209:THR:HG21	1.64	0.79
5:B:904:2YG:H27	5:B:904:2YG:H15	1.48	0.77
2:B:901:NAD:C4N	5:B:904:2YG:H26	2.16	0.75
1:D:204:THR:HG21	1:D:209:THR:HG21	1.70	0.74
1:A:204:THR:HG22	1:A:206:CYS:H	1.50	0.73
5:B:904:2YG:H15	5:B:904:2YG:N3	2.03	0.73
2:A:901:NAD:C4N	5:A:904:2YG:H23	2.21	0.70
1:D:204:THR:HG22	1:D:206:CYS:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLU:OE1	1:A:204:THR:HB	1.99	0.62
1:C:204:THR:HG21	1:C:209:THR:HG21	1.82	0.62
1:C:204:THR:HG22	1:C:206:CYS:H	1.66	0.60
1:A:163:LYS:HD2	7:A:909:EDO:H22	1.84	0.59
1:D:95:ASN:HD22	1:D:95:ASN:N	2.04	0.56
1:A:135:ARG:HB3	7:A:910:EDO:H11	1.89	0.55
1:A:131:GLU:OE1	1:A:135:ARG:HD2	2.07	0.54
2:B:901:NAD:C4N	5:B:904:2YG:C10	2.86	0.53
1:A:163:LYS:HD2	7:A:909:EDO:C2	2.40	0.52
1:B:109:LEU:C	1:B:109:LEU:HD12	2.30	0.52
1:B:2:ALA:HB3	9:B:1111:HOH:O	2.10	0.51
1:A:137:LEU:HD13	7:A:910:EDO:H12	1.93	0.51
2:B:901:NAD:C5N	5:B:904:2YG:H26	2.41	0.50
2:B:901:NAD:C3N	5:B:904:2YG:C10	2.90	0.50
1:B:36:LYS:NZ	9:B:1095:HOH:O	2.45	0.50
9:A:1094:HOH:O	1:B:36:LYS:HE2	2.12	0.49
2:B:901:NAD:C3N	5:B:904:2YG:H25	2.42	0.49
1:A:204:THR:CG2	1:A:206:CYS:H	2.24	0.49
1:D:68:HIS:O	1:D:72:GLN:HG2	2.11	0.49
5:A:904:2YG:H15	5:A:904:2YG:H26	1.94	0.48
1:D:202:GLU:OE1	1:D:204:THR:HB	2.14	0.48
1:A:98:GLU:OE1	1:A:114:LYS:HD3	2.13	0.48
2:A:901:NAD:C2N	5:A:904:2YG:H25	2.43	0.48
1:A:154:PHE:HB3	1:A:155:PRO:HD3	1.96	0.47
2:A:901:NAD:C3N	5:A:904:2YG:H25	2.45	0.46
2:A:901:NAD:C4N	5:A:904:2YG:C9	2.93	0.46
1:A:135:ARG:CB	7:A:910:EDO:H11	2.45	0.46
1:D:154:PHE:HB3	1:D:155:PRO:HD3	1.96	0.46
1:A:137:LEU:CD1	7:A:910:EDO:H12	2.46	0.45
1:C:202:GLU:OE1	1:C:204:THR:HB	2.17	0.45
5:A:904:2YG:C6	5:A:904:2YG:H26	2.47	0.45
1:C:143:ASP:OD2	1:C:195:LYS:NZ	2.38	0.45
1:A:202:GLU:O	1:A:224:PRO:HD2	2.17	0.44
1:B:61:GLY:O	1:B:62:ASN:HB2	2.17	0.43
1:C:154:PHE:HB3	1:C:155:PRO:HD3	2.01	0.43
1:B:224:PRO:O	2:B:901:NAD:H2N	2.19	0.43
1:B:71:THR:HG22	1:B:255:LEU:HD11	2.01	0.42
2:B:901:NAD:C3N	5:B:904:2YG:H26	2.48	0.42
1:C:166:ARG:HD3	1:C:187:ILE:HD13	2.00	0.42
1:A:202:GLU:CD	1:A:204:THR:HB	2.40	0.42
1:B:167:VAL:HB	1:B:186:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ILE:HB	1:D:230:ILE:HG22	2.02	0.41
1:A:98:GLU:OE1	1:A:114:LYS:CD	2.67	0.41
1:D:144:VAL:HG23	1:D:199:ILE:HG22	2.03	0.41
1:B:145:LEU:HD12	1:B:214:VAL:HG11	2.02	0.41
1:D:109:LEU:HD12	1:D:109:LEU:C	2.41	0.41
5:A:904:2YG:C10	5:A:904:2YG:H15	2.50	0.41
1:B:202:GLU:O	1:B:224:PRO:HD2	2.20	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	257/260 (99%)	247 (96%)	10 (4%)	0	100	100
1	B	257/260 (99%)	245 (95%)	11 (4%)	1 (0%)	34	32
1	C	257/260 (99%)	246 (96%)	10 (4%)	1 (0%)	34	32
1	D	256/260 (98%)	246 (96%)	10 (4%)	0	100	100
All	All	1027/1040 (99%)	984 (96%)	41 (4%)	2 (0%)	47	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	141	SER
1	B	247	LEU

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	214/215 (100%)	203 (95%)	11 (5%)	24	22
1	B	214/215 (100%)	206 (96%)	8 (4%)	34	35
1	C	214/215 (100%)	200 (94%)	14 (6%)	17	14
1	D	213/215 (99%)	199 (93%)	14 (7%)	16	14
All	All	855/860 (99%)	808 (94%)	47 (6%)	21	19

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LEU
1	A	7	ASP
1	A	137	LEU
1	A	145	LEU
1	A	160	LEU
1	A	174	GLU
1	A	176	LEU
1	A	204	THR
1	A	217	GLU
1	A	235	ARG
1	B	106	ARG
1	B	137	LEU
1	B	145	LEU
1	B	166	ARG
1	B	178	GLU
1	B	233	GLU
1	B	235	ARG
1	B	242	LEU
1	C	1	MET
1	C	21	SER
1	C	42	PHE
1	C	45	SER
1	C	82	ASP
1	C	137	LEU
1	C	138	LYS
1	C	145	LEU
1	C	164	ASP
1	C	166	ARG
1	C	204	THR

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Mol	Chain	Res	Type
1	C	214	VAL
1	C	217	GLU
1	C	242	LEU
1	D	7	ASP
1	D	11	ASN
1	D	14	MET
1	D	17	GLN
1	D	43	SER
1	D	95	ASN
1	D	145	LEU
1	D	162	GLN
1	D	164	ASP
1	D	176	LEU
1	D	182	SER
1	D	184	LEU
1	D	235	ARG
1	D	242	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	162	GLN
1	A	208	ASN
1	A	218	ASN
1	B	13	ASN
1	B	72	GLN
1	B	162	GLN
1	B	218	ASN
1	C	17	GLN
1	D	11	ASN
1	D	72	GLN
1	D	95	ASN
1	D	162	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	GOL	A	906	-	5,5,5	0.26	0	5,5,5	0.55	0
6	GOL	A	907	-	5,5,5	0.46	0	5,5,5	0.19	0
2	NAD	D	901	-	42,48,48	0.86	2 (4%)	50,73,73	1.30	7 (14%)
6	GOL	B	905	-	5,5,5	0.47	0	5,5,5	0.57	0
6	GOL	A	905	-	5,5,5	0.20	0	5,5,5	0.27	0
5	2YG	B	904	-	14,18,18	0.30	0	15,21,21	0.78	0
2	NAD	C	901	4	42,48,48	0.88	3 (7%)	50,73,73	1.44	8 (16%)
5	2YG	D	904	-	9,14,18	0.52	0	11,17,21	0.87	0
7	EDO	A	908	-	3,3,3	0.36	0	2,2,2	0.56	0
7	EDO	A	910	-	3,3,3	0.39	0	2,2,2	0.55	0
5	2YG	A	904	-	14,18,18	0.48	0	15,21,21	0.83	0
8	PEG	B	906	-	6,6,6	0.36	0	5,5,5	0.93	0
5	2YG	C	904	-	9,14,18	0.57	0	11,17,21	0.70	0
7	EDO	A	909	-	3,3,3	0.44	0	2,2,2	0.52	0
2	NAD	A	901	4	42,48,48	1.46	4 (9%)	50,73,73	1.83	11 (22%)
2	NAD	B	901	4	42,48,48	1.02	3 (7%)	50,73,73	1.57	11 (22%)

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	GOL	A	906	-	-	0/4/4/4	-
6	GOL	A	907	-	-	4/4/4/4	-
2	NAD	D	901	-	-	5/26/62/62	0/5/5/5
6	GOL	B	905	-	-	2/4/4/4	-
6	GOL	A	905	-	-	2/4/4/4	-
5	2YG	B	904	-	-	6/17/21/21	-
2	NAD	C	901	4	-	6/26/62/62	0/5/5/5
5	2YG	D	904	-	-	2/12/16/21	-
7	EDO	A	908	-	-	1/1/1/1	-
7	EDO	A	910	-	-	1/1/1/1	-
5	2YG	A	904	-	-	5/17/21/21	-
8	PEG	B	906	-	-	1/4/4/4	-
5	2YG	C	904	-	-	4/12/16/21	-
7	EDO	A	909	-	-	1/1/1/1	-
2	NAD	A	901	4	-	4/26/62/62	0/5/5/5
2	NAD	B	901	4	-	5/26/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	NAD	C4N-C3N	6.73	1.50	1.39
2	A	901	NAD	C5N-C4N	2.96	1.45	1.38
2	A	901	NAD	O4D-C1D	2.62	1.44	1.41
2	B	901	NAD	O4D-C1D	2.46	1.44	1.41
2	B	901	NAD	C3N-C7N	2.28	1.54	1.50
2	C	901	NAD	C5A-C4A	2.12	1.46	1.40
2	C	901	NAD	O4D-C1D	2.12	1.44	1.41
2	A	901	NAD	C5A-C4A	2.11	1.46	1.40
2	D	901	NAD	C5A-C4A	2.10	1.46	1.40
2	B	901	NAD	C7N-N7N	2.07	1.36	1.33
2	C	901	NAD	C2A-N3A	2.06	1.35	1.32
2	D	901	NAD	C2A-N3A	2.03	1.35	1.32

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	NAD	C5N-C4N-C3N	-6.54	112.61	120.34
2	B	901	NAD	N3A-C2A-N1A	-4.46	121.71	128.68
2	A	901	NAD	N3A-C2A-N1A	-4.40	121.81	128.68
2	C	901	NAD	N3A-C2A-N1A	-4.04	122.36	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	NAD	PN-O3-PA	-3.99	119.14	132.83
2	D	901	NAD	N3A-C2A-N1A	-3.82	122.70	128.68
2	B	901	NAD	C3N-C7N-N7N	3.70	122.19	117.75
2	C	901	NAD	PN-O3-PA	-3.65	120.30	132.83
2	A	901	NAD	C1B-N9A-C4A	-3.48	120.53	126.64
2	B	901	NAD	PN-O3-PA	-3.46	120.95	132.83
2	B	901	NAD	C1B-N9A-C4A	-3.45	120.58	126.64
2	A	901	NAD	C4A-C5A-N7A	-3.41	105.84	109.40
2	C	901	NAD	C1B-N9A-C4A	-3.25	120.93	126.64
2	C	901	NAD	C3N-C7N-N7N	2.98	121.33	117.75
2	B	901	NAD	C4A-C5A-N7A	-2.94	106.34	109.40
2	D	901	NAD	C3N-C7N-N7N	2.84	121.16	117.75
2	A	901	NAD	C6N-C5N-C4N	2.80	123.51	119.44
2	A	901	NAD	C2A-N1A-C6A	2.78	123.50	118.75
2	D	901	NAD	PN-O3-PA	-2.77	123.33	132.83
2	C	901	NAD	C4A-C5A-N7A	-2.75	106.54	109.40
2	B	901	NAD	O7N-C7N-N7N	-2.74	118.69	122.58
2	D	901	NAD	C3N-C2N-N1N	2.59	122.96	120.43
2	C	901	NAD	C3N-C2N-N1N	2.56	122.93	120.43
2	B	901	NAD	O2A-PA-O1A	2.48	124.50	112.24
2	C	901	NAD	O4D-C1D-C2D	-2.45	103.35	106.93
2	C	901	NAD	O7N-C7N-N7N	-2.43	119.12	122.58
2	A	901	NAD	O7N-C7N-N7N	-2.40	119.17	122.58
2	D	901	NAD	O7N-C7N-N7N	-2.33	119.26	122.58
2	D	901	NAD	C1B-N9A-C4A	-2.30	122.61	126.64
2	D	901	NAD	C4A-C5A-N7A	-2.30	107.00	109.40
2	A	901	NAD	C3N-C7N-N7N	2.28	120.48	117.75
2	B	901	NAD	C3N-C2N-N1N	2.26	122.64	120.43
2	B	901	NAD	C2N-C3N-C4N	-2.25	115.70	118.26
2	B	901	NAD	C2A-N1A-C6A	2.17	122.47	118.75
2	A	901	NAD	C3N-C2N-N1N	2.15	122.53	120.43
2	B	901	NAD	O4D-C1D-C2D	-2.15	103.79	106.93
2	A	901	NAD	O2N-PN-O1N	2.06	122.44	112.24

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	907	GOL	O1-C1-C2-C3
6	A	907	GOL	C1-C2-C3-O3
6	A	907	GOL	O2-C2-C3-O3
2	C	901	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	C	901	NAD	O4D-C1D-N1N-C6N
2	C	901	NAD	C2D-C1D-N1N-C2N
2	C	901	NAD	C2D-C1D-N1N-C6N
5	D	904	2YG	N1-C5-C6-N2
6	B	905	GOL	C1-C2-C3-O3
5	C	904	2YG	N1-C5-C6-C7
5	C	904	2YG	O-C5-C6-C7
5	B	904	2YG	N1-C5-C6-N2
5	B	904	2YG	N1-C5-C6-C7
5	A	904	2YG	N1-C5-C6-N2
5	A	904	2YG	N1-C5-C6-C7
5	A	904	2YG	O-C5-C6-N2
5	A	904	2YG	O-C5-C6-C7
2	D	901	NAD	O4D-C1D-N1N-C2N
2	D	901	NAD	O4D-C1D-N1N-C6N
2	D	901	NAD	C2D-C1D-N1N-C2N
2	D	901	NAD	C2D-C1D-N1N-C6N
2	A	901	NAD	O4D-C1D-N1N-C2N
2	A	901	NAD	O4D-C1D-N1N-C6N
2	A	901	NAD	C2D-C1D-N1N-C2N
2	B	901	NAD	O4D-C1D-N1N-C2N
2	B	901	NAD	O4D-C1D-N1N-C6N
2	B	901	NAD	C2D-C1D-N1N-C2N
6	B	905	GOL	O2-C2-C3-O3
5	A	904	2YG	C5-C6-C7-C8
6	A	905	GOL	O1-C1-C2-C3
6	A	907	GOL	O1-C1-C2-O2
6	A	905	GOL	O1-C1-C2-O2
7	A	909	EDO	O1-C1-C2-O2
5	C	904	2YG	N1-C5-C6-N2
5	B	904	2YG	C7-C8-C9-C10
5	B	904	2YG	O-C5-C6-C7
5	D	904	2YG	O-C5-C6-N2
5	C	904	2YG	O-C5-C6-N2
5	B	904	2YG	N3-C10-C9-C8
2	C	901	NAD	O4B-C4B-C5B-O5B
5	B	904	2YG	O-C5-C6-N2
8	B	906	PEG	O2-C3-C4-O4
7	A	910	EDO	O1-C1-C2-O2
7	A	908	EDO	O1-C1-C2-O2
2	A	901	NAD	O4B-C4B-C5B-O5B
2	B	901	NAD	C2D-C1D-N1N-C6N

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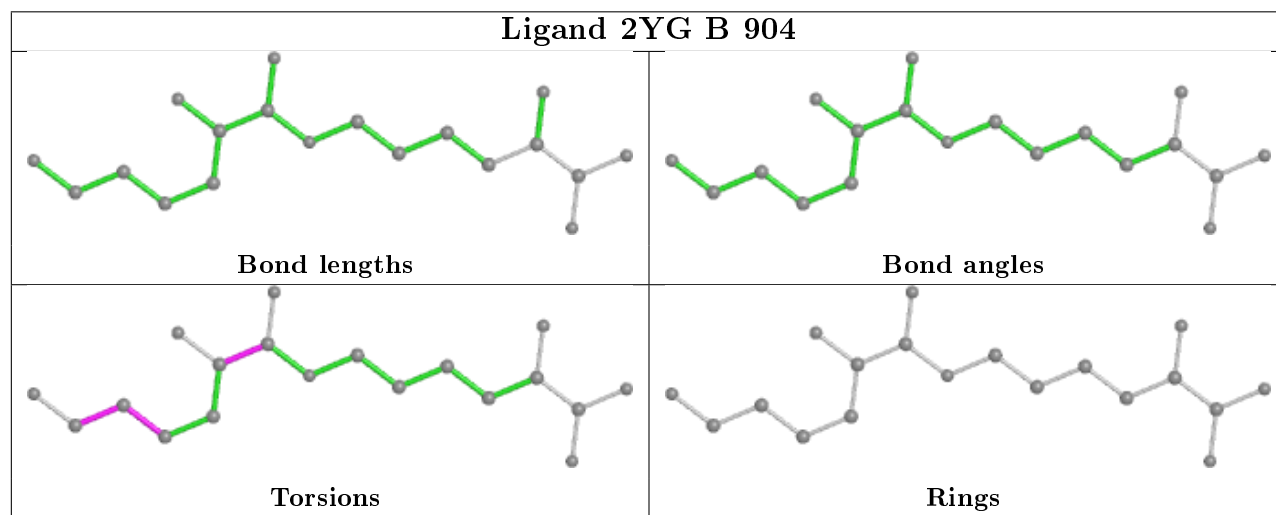
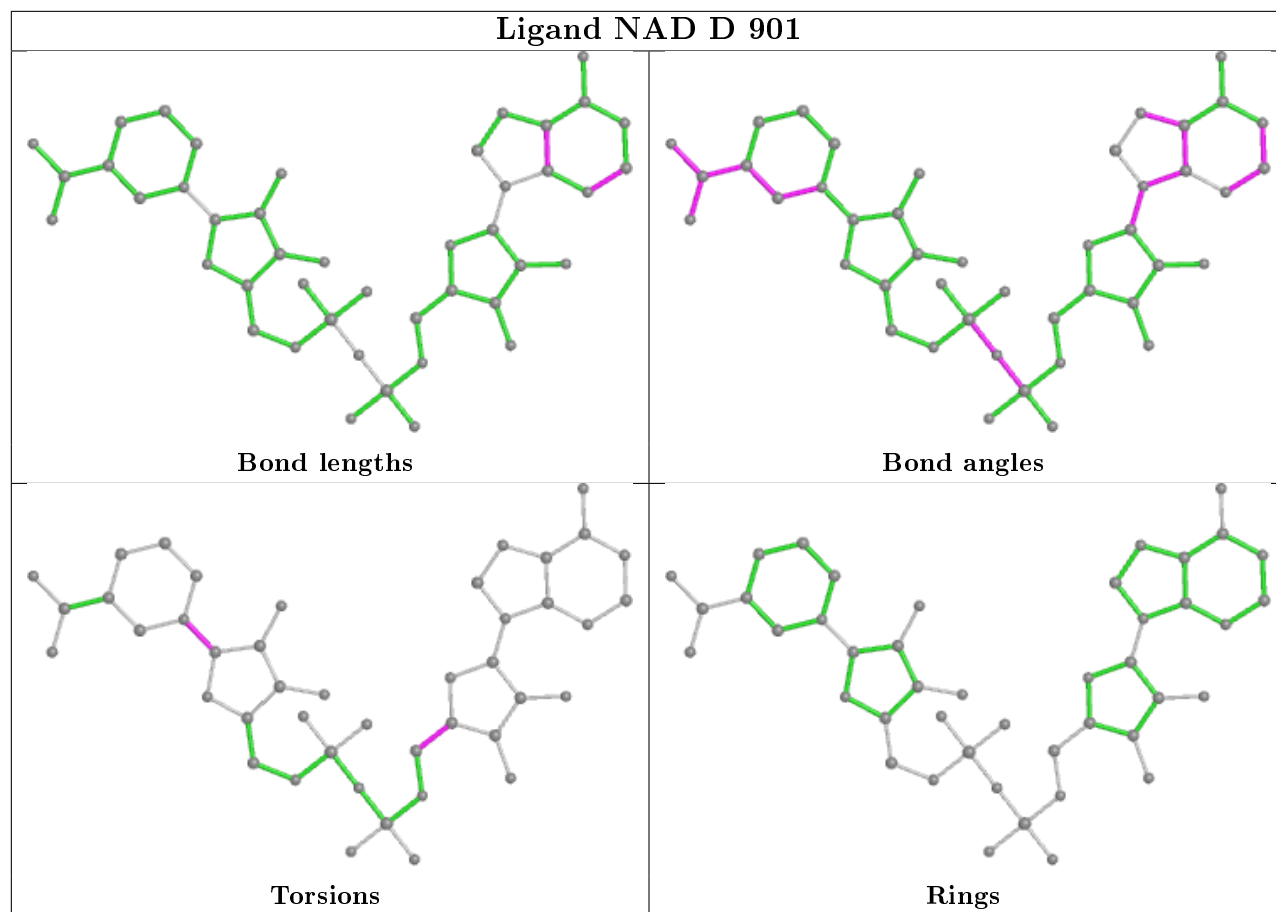
Mol	Chain	Res	Type	Atoms
2	C	901	NAD	C3B-C4B-C5B-O5B
2	D	901	NAD	O4B-C4B-C5B-O5B
2	B	901	NAD	O4B-C4B-C5B-O5B

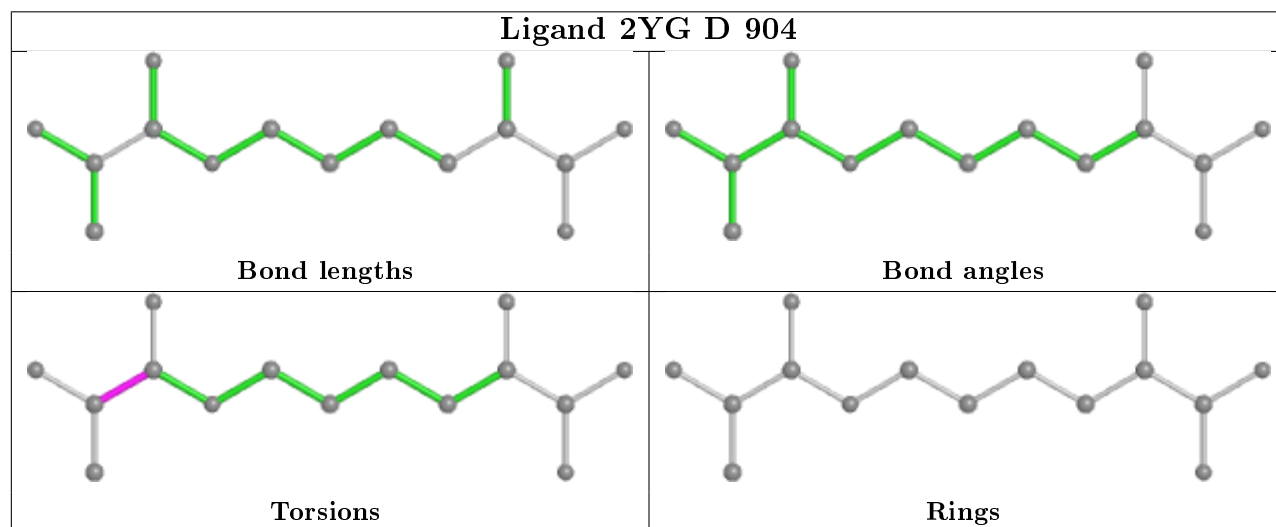
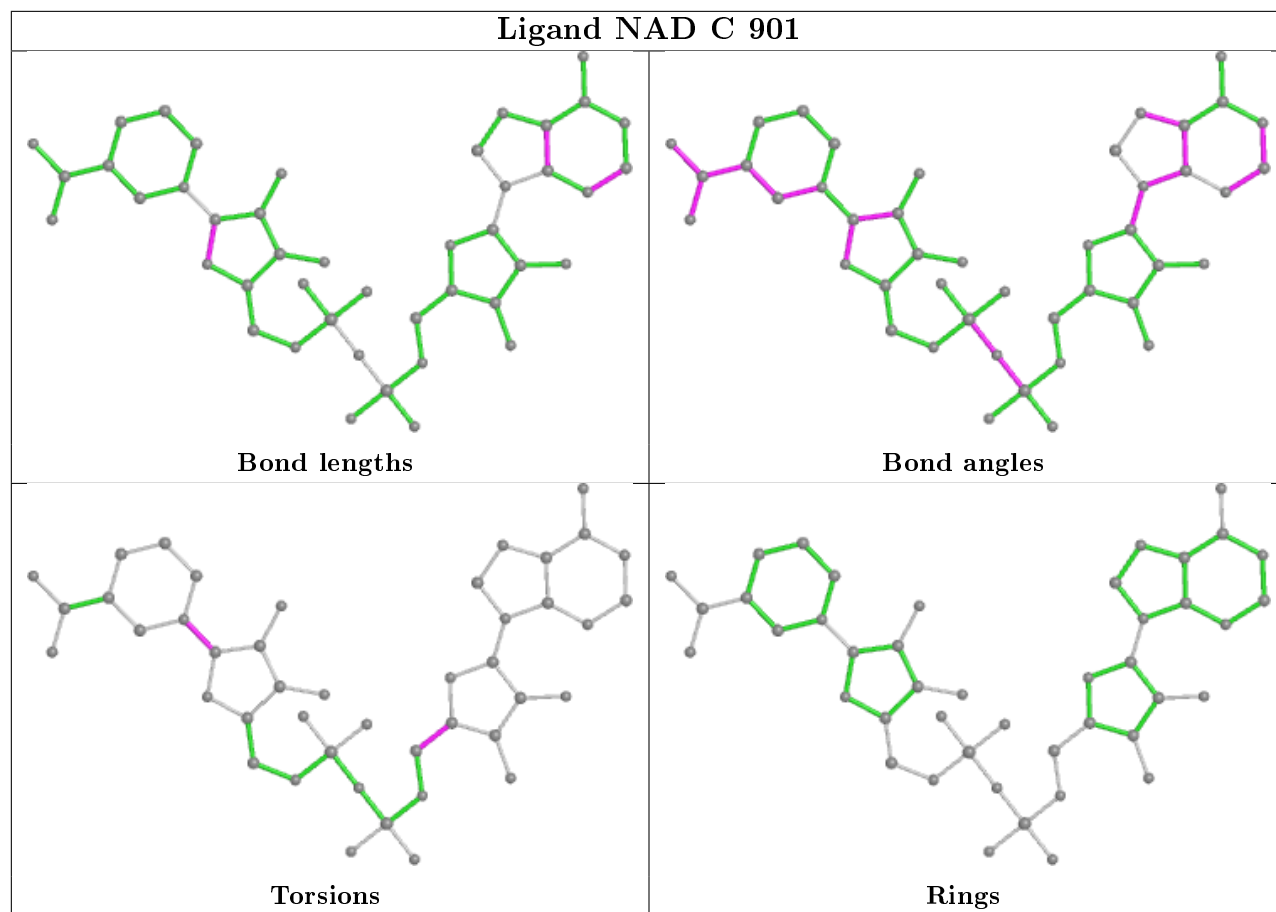
There are no ring outliers.

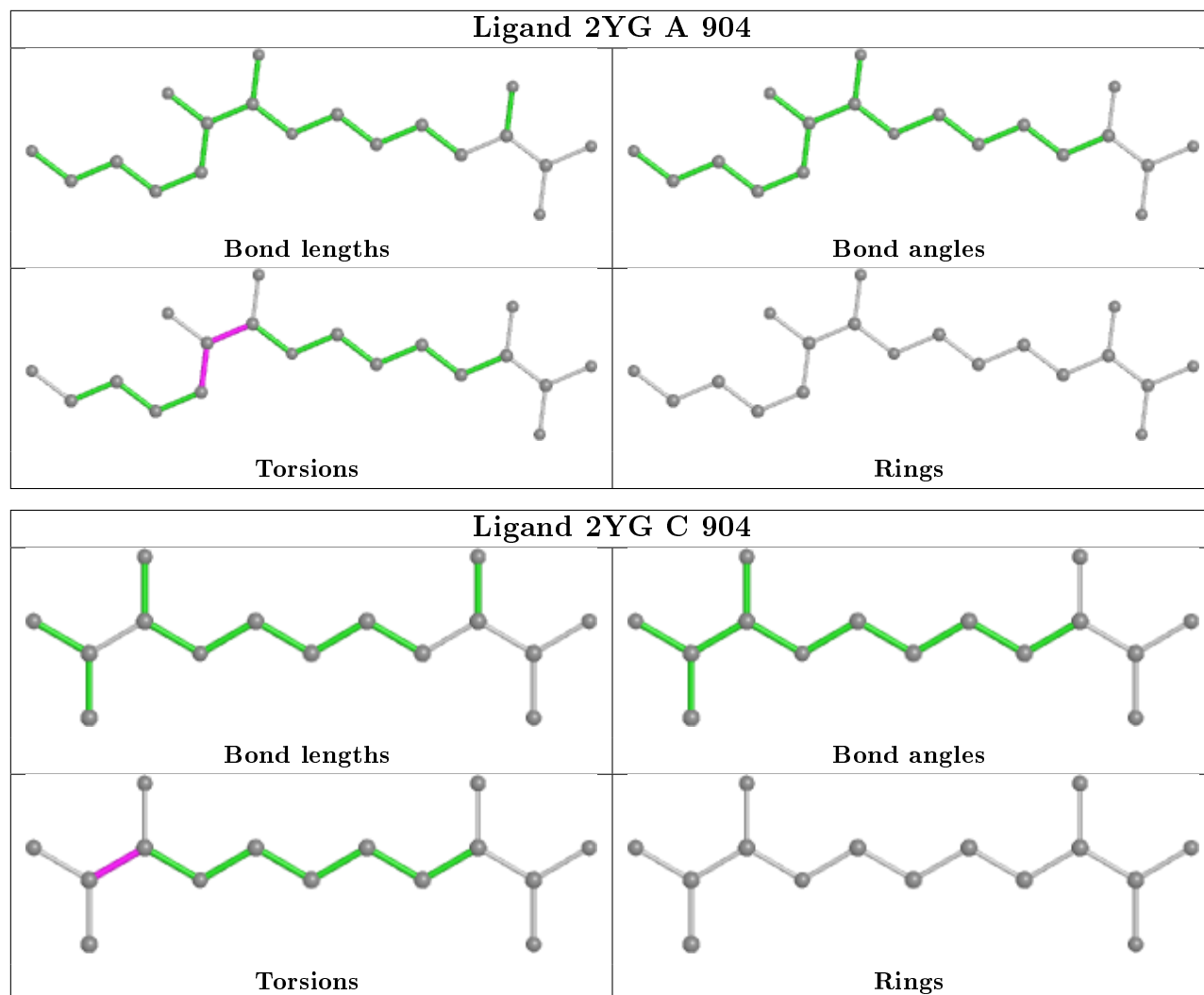
6 monomers are involved in 22 short contacts:

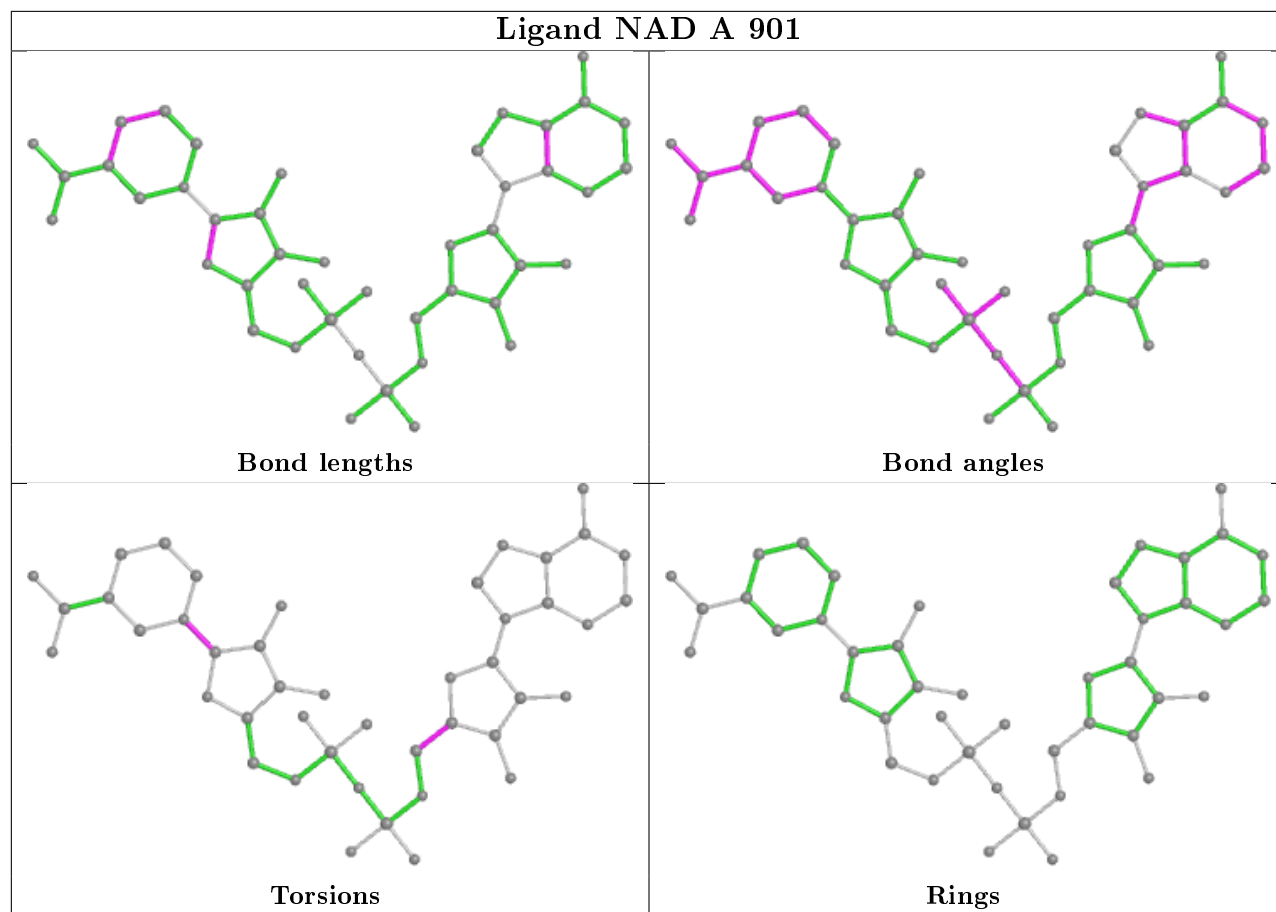
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	904	2YG	8	0
7	A	910	EDO	4	0
5	A	904	2YG	7	0
7	A	909	EDO	2	0
2	A	901	NAD	4	0
2	B	901	NAD	7	0

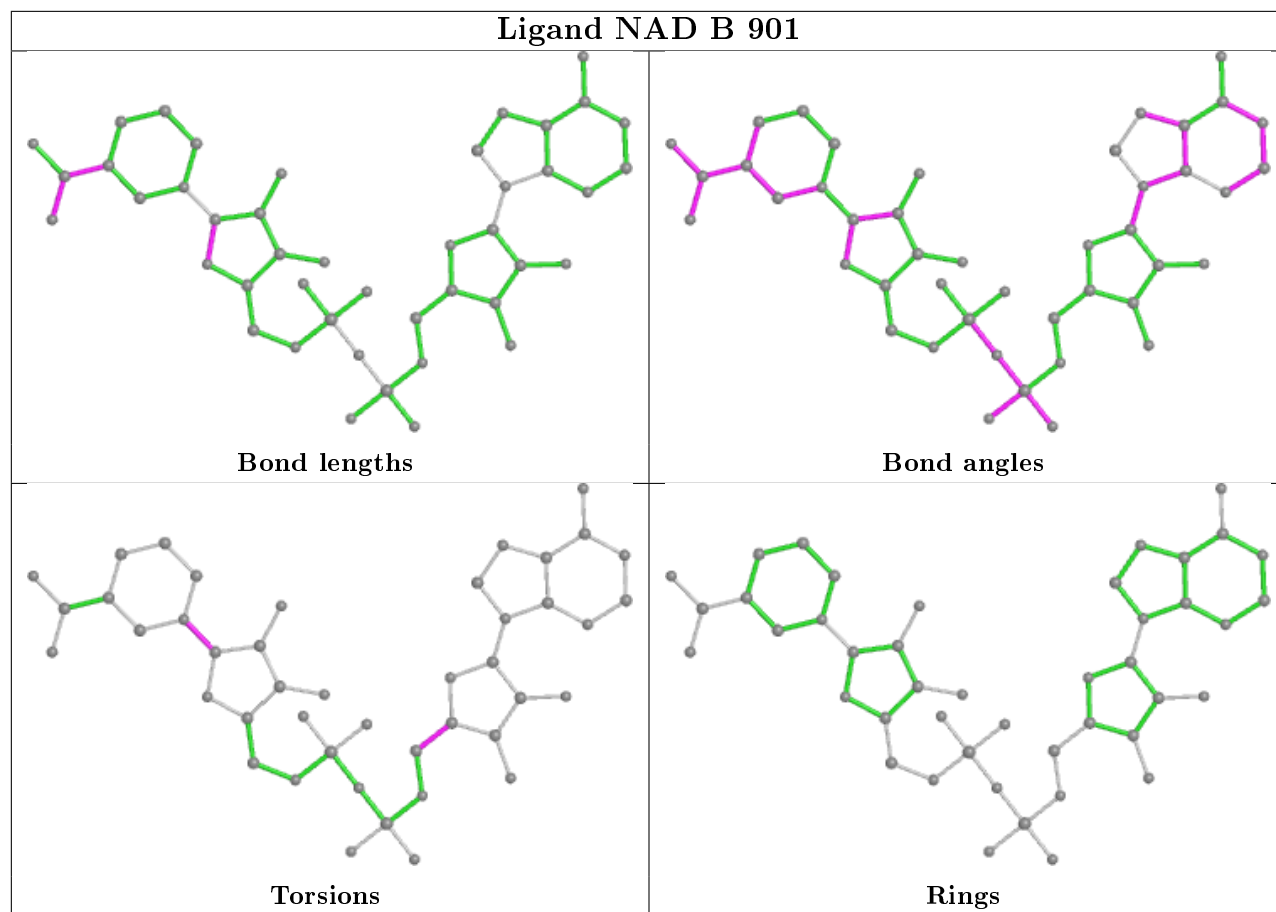
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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	259/260 (99%)	0.11	6 (2%) 60 65	19, 24, 49, 94	0
1	B	259/260 (99%)	0.17	12 (4%) 32 38	19, 25, 52, 96	0
1	C	259/260 (99%)	0.84	50 (19%) 1 1	42, 58, 81, 95	0
1	D	258/260 (99%)	1.02	60 (23%) 0 0	40, 65, 95, 119	0
All	All	1035/1040 (99%)	0.53	128 (12%) 4 5	19, 48, 86, 119	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	ILE	7.2
1	A	1	MET	6.9
1	D	192	ALA	6.8
1	D	2	ALA	5.7
1	D	7	ASP	5.6
1	D	14	MET	5.5
1	C	192	ALA	5.4
1	C	1	MET	5.2
1	D	140	ASP	5.1
1	C	2	ALA	5.0
1	C	140	ASP	4.8
1	C	42	PHE	4.7
1	B	192	ALA	4.7
1	C	193	ASN	4.6
1	B	1	MET	4.4
1	D	141	SER	4.3
1	C	14	MET	4.2
1	D	186	ILE	4.0
1	C	9	LEU	4.0
1	D	106	ARG	4.0
1	D	164	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	7	ASP	3.9
1	B	193	ASN	3.8
1	D	193	ASN	3.7
1	D	142	LYS	3.7
1	D	162	GLN	3.6
1	D	3	LEU	3.6
1	C	179	ARG	3.6
1	C	175	THR	3.6
1	C	82	ASP	3.6
1	D	9	LEU	3.5
1	D	190	ASP	3.5
1	C	75	GLY	3.5
1	D	4	LEU	3.4
1	C	227	PRO	3.4
1	D	185	GLY	3.4
1	C	182	SER	3.4
1	D	166	ARG	3.3
1	C	162	GLN	3.3
1	D	5	THR	3.2
1	D	75	GLY	3.1
1	A	192	ALA	3.0
1	A	140	ASP	3.0
1	D	12	ILE	3.0
1	A	2	ALA	3.0
1	C	185	GLY	2.9
1	C	183	ASN	2.9
1	D	232	GLU	2.9
1	A	227	PRO	2.9
1	B	191	PRO	2.9
1	D	48	VAL	2.8
1	C	142	LYS	2.8
1	C	96	GLY	2.8
1	D	11	ASN	2.8
1	D	175	THR	2.8
1	D	215	LEU	2.8
1	D	236	ASP	2.7
1	C	11	ASN	2.7
1	D	174	GLU	2.7
1	A	193	ASN	2.7
1	D	13	ASN	2.7
1	C	218	ASN	2.6
1	D	17	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	8	ASP	2.6
1	D	82	ASP	2.6
1	D	138	LYS	2.6
1	C	186	ILE	2.6
1	C	226	ILE	2.6
1	B	190	ASP	2.6
1	C	18	LYS	2.6
1	D	242	LEU	2.6
1	D	6	PRO	2.6
1	D	178	GLU	2.6
1	C	54	THR	2.5
1	C	235	ARG	2.5
1	D	179	ARG	2.5
1	D	160	LEU	2.5
1	C	141	SER	2.5
1	C	215	LEU	2.5
1	C	191	PRO	2.5
1	B	179	ARG	2.5
1	C	164	ASP	2.4
1	C	233	GLU	2.4
1	B	2	ALA	2.4
1	C	25	GLU	2.4
1	D	218	ASN	2.4
1	C	177	LEU	2.4
1	D	56	GLY	2.4
1	D	182	SER	2.4
1	C	232	GLU	2.4
1	C	106	ARG	2.4
1	D	233	GLU	2.4
1	D	132	ILE	2.4
1	B	232	GLU	2.3
1	C	10	ILE	2.3
1	B	194	PRO	2.3
1	C	5	THR	2.3
1	C	213	ALA	2.3
1	D	44	SER	2.3
1	D	139	ALA	2.2
1	D	143	ASP	2.2
1	D	42	PHE	2.2
1	C	94	GLN	2.2
1	C	45	SER	2.2
1	D	239	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	235	ARG	2.2
1	D	64	SER	2.2
1	D	16	LEU	2.2
1	D	29	LEU	2.2
1	D	191	PRO	2.2
1	C	174	GLU	2.1
1	C	178	GLU	2.1
1	C	13	ASN	2.1
1	D	168	TYR	2.1
1	D	24	GLN	2.1
1	C	138	LYS	2.1
1	C	181	THR	2.1
1	B	99	ILE	2.1
1	B	227	PRO	2.1
1	C	57	ASN	2.1
1	B	7	ASP	2.0
1	D	96	GLY	2.0
1	D	31	ILE	2.0
1	C	166	ARG	2.0
1	C	72	GLN	2.0
1	C	36	LYS	2.0
1	D	18	LYS	2.0
1	D	183	ASN	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 carbohydrates 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.

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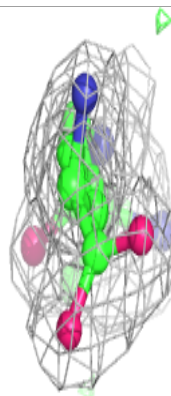
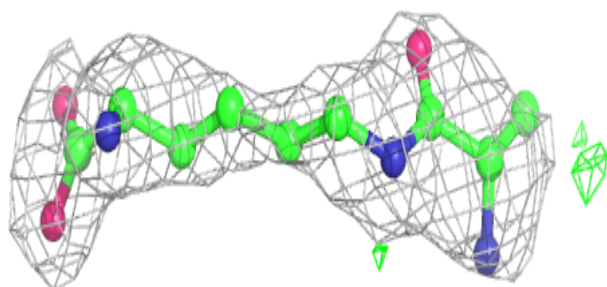
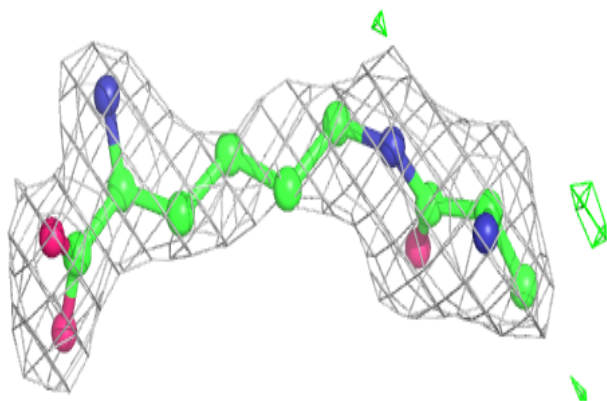
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	D	903	1/1	0.76	0.23	85,85,85,85	0
6	GOL	A	907	6/6	0.78	0.21	46,59,60,69	0
6	GOL	A	905	6/6	0.80	0.21	50,64,70,78	0
4	MG	C	903	1/1	0.88	0.42	82,82,82,82	0
5	2YG	C	904	15/19	0.91	0.20	46,61,66,70	0
3	NA	C	902	1/1	0.91	0.16	60,60,60,60	0
5	2YG	D	904	15/19	0.91	0.15	49,54,68,70	0
6	GOL	B	905	6/6	0.92	0.15	33,37,46,46	0
6	GOL	A	906	6/6	0.92	0.20	49,55,61,66	0
7	EDO	A	910	4/4	0.93	0.17	32,41,51,59	0
8	PEG	B	906	7/7	0.93	0.22	30,39,45,48	0
7	EDO	A	908	4/4	0.93	0.16	44,44,48,53	0
3	NA	D	902	1/1	0.93	0.16	51,51,51,51	0
5	2YG	A	904	19/19	0.94	0.17	26,33,46,52	0
7	EDO	A	909	4/4	0.95	0.12	29,35,41,50	0
2	NAD	D	901	44/44	0.95	0.13	40,48,70,95	0
5	2YG	B	904	19/19	0.95	0.15	22,27,45,49	0
2	NAD	C	901	44/44	0.95	0.11	45,53,64,68	0
3	NA	B	902	1/1	0.96	0.16	43,43,43,43	0
2	NAD	B	901	44/44	0.96	0.10	23,31,37,45	0
4	MG	A	903	1/1	0.97	0.11	39,39,39,39	0
3	NA	A	902	1/1	0.97	0.11	39,39,39,39	0
2	NAD	A	901	44/44	0.97	0.09	21,25,33,35	0
4	MG	B	903	1/1	0.97	0.13	38,38,38,38	0

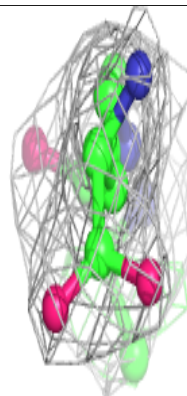
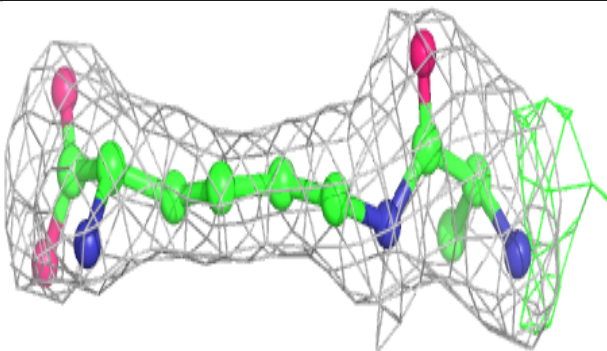
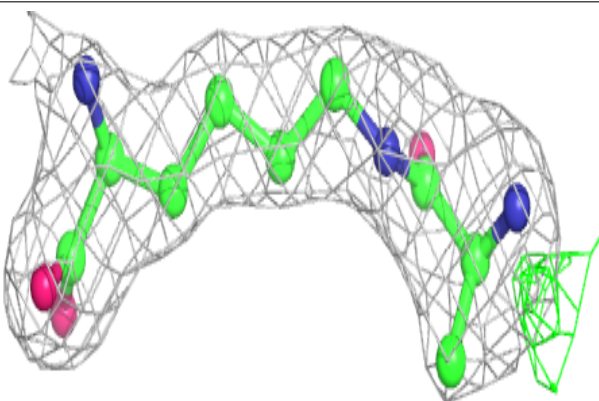
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 2YG C 904:

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

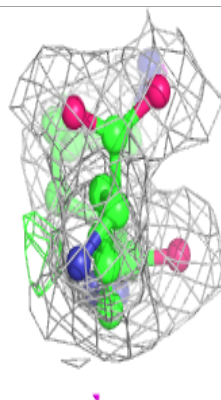
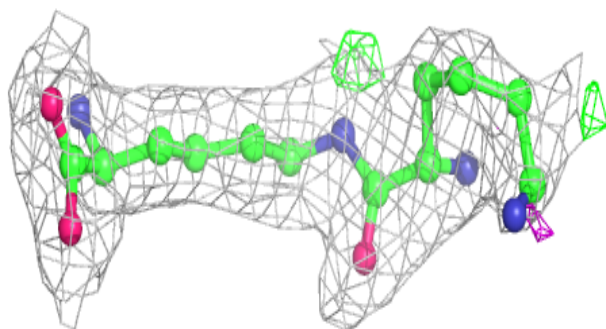
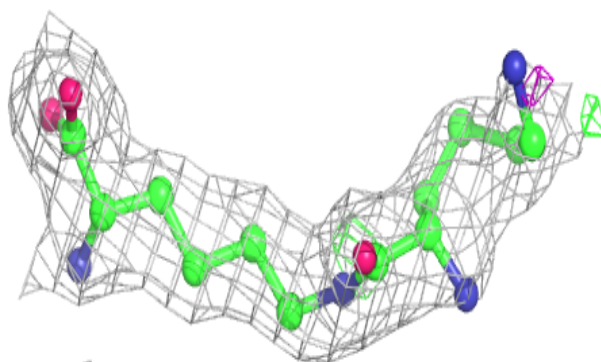
**Electron density around 2YG D 904:**

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

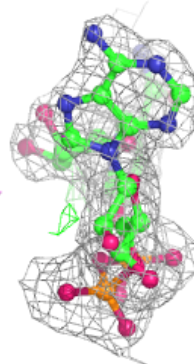
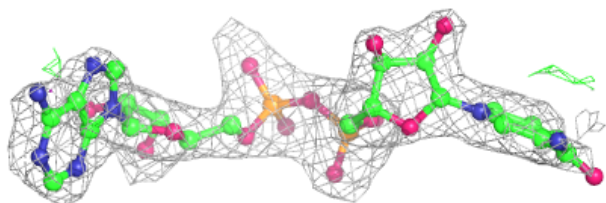
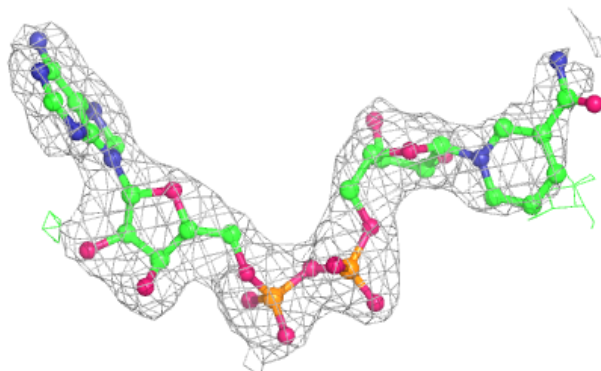


Electron density around 2YG A 904:

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

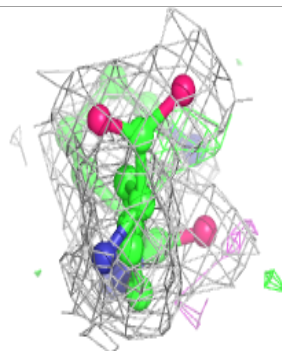
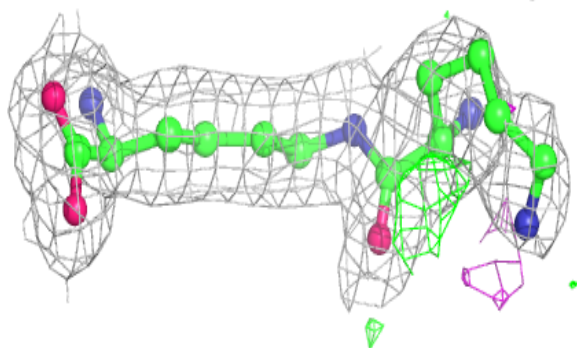
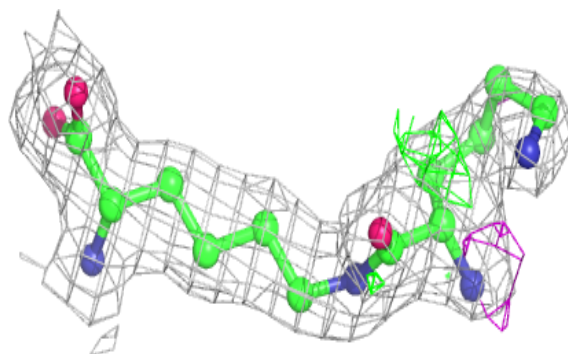
**Electron density around NAD D 901:**

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

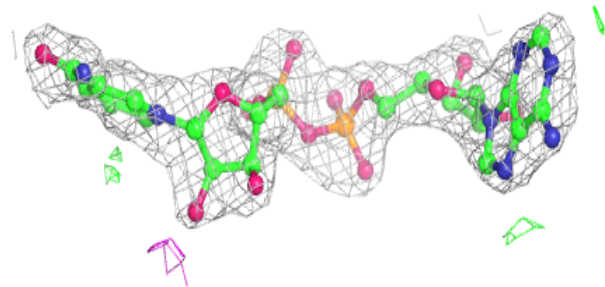
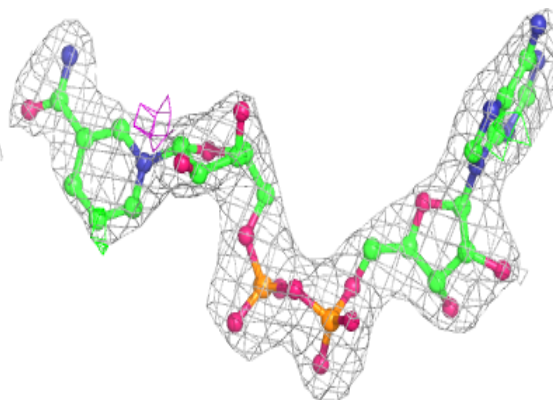


Electron density around 2YG B 904:

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

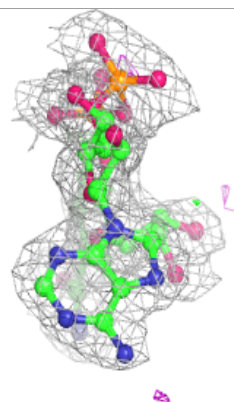
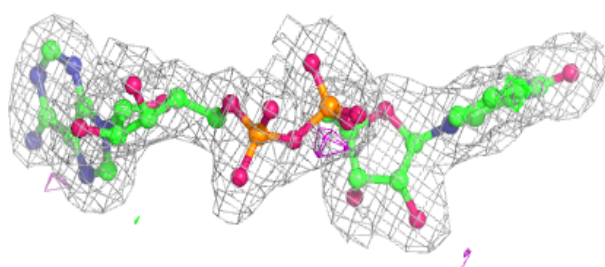
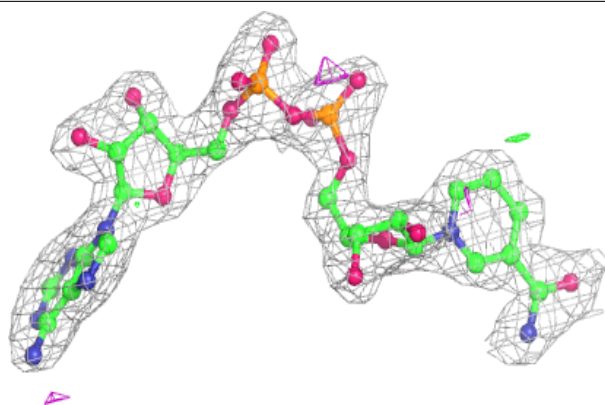
**Electron density around NAD C 901:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

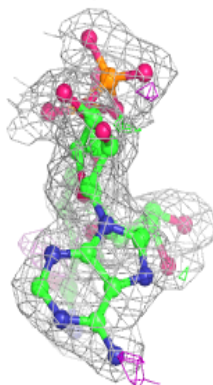
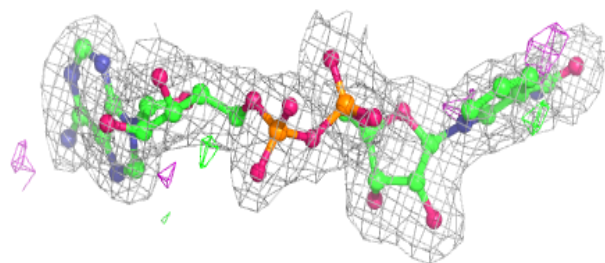
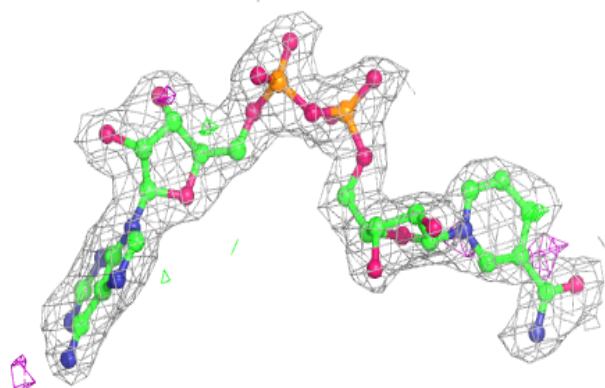


Electron density around NAD B 901:

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

**Electron density around NAD A 901:**

$2mF_o-DF_c$ (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.