



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 05:10 AM JST

PDB ID : 7EPM
Title : human LDHC complexed with NAD⁺ and ethylamino acetic acid
Authors : Yu, Y.; Chen, Q.
Deposited on : 2021-04-27
Resolution : 3.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

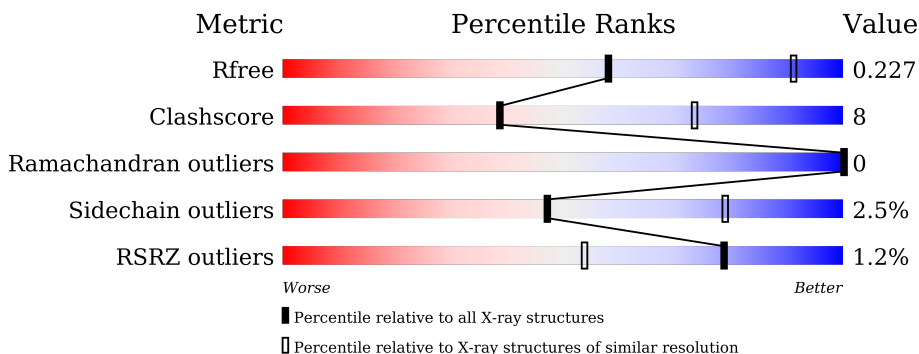
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	341	 82% 15% ...
1	B	341	 77% 18% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	407	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10310 atoms, of which 5058 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.

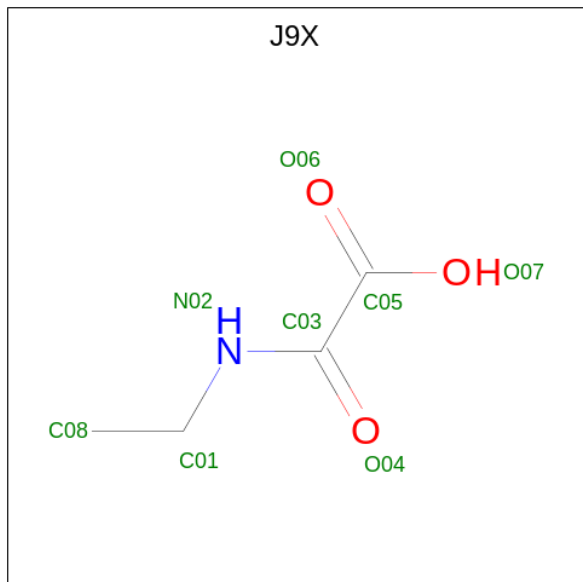
- Molecule 1 is a protein called L-lactate dehydrogenase C chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	335	5065	1640	2491	437	485	12	0	0	0
1	B	326	5005	1595	2503	425	470	12	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

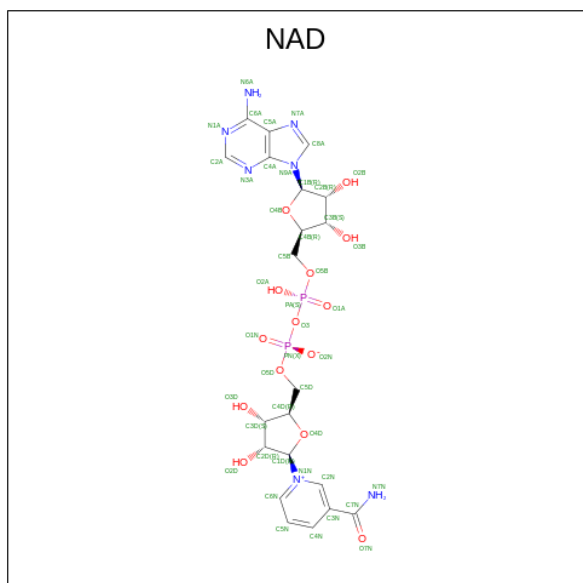
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P07864
A	2	ALA	-	expression tag	UNP P07864
A	56	GLU	LEU	engineered mutation	UNP P07864
A	332	GLN	ILE	engineered mutation	UNP P07864
A	334	LEU	-	expression tag	UNP P07864
A	335	GLU	-	expression tag	UNP P07864
A	336	HIS	-	expression tag	UNP P07864
A	337	HIS	-	expression tag	UNP P07864
A	338	HIS	-	expression tag	UNP P07864
A	339	HIS	-	expression tag	UNP P07864
A	340	HIS	-	expression tag	UNP P07864
A	341	HIS	-	expression tag	UNP P07864
B	1	MET	-	initiating methionine	UNP P07864
B	2	ALA	-	expression tag	UNP P07864
B	56	GLU	LEU	engineered mutation	UNP P07864
B	332	GLN	ILE	engineered mutation	UNP P07864
B	334	LEU	-	expression tag	UNP P07864
B	335	GLU	-	expression tag	UNP P07864
B	336	HIS	-	expression tag	UNP P07864
B	337	HIS	-	expression tag	UNP P07864
B	338	HIS	-	expression tag	UNP P07864
B	339	HIS	-	expression tag	UNP P07864
B	340	HIS	-	expression tag	UNP P07864
B	341	HIS	-	expression tag	UNP P07864

- Molecule 2 is 2-(ethylamino)-2-oxidanylidene-ethanoic acid (three-letter code: J9X) (formula: $C_4H_7NO_3$) (labeled as "Ligand of Interest" by depositor).



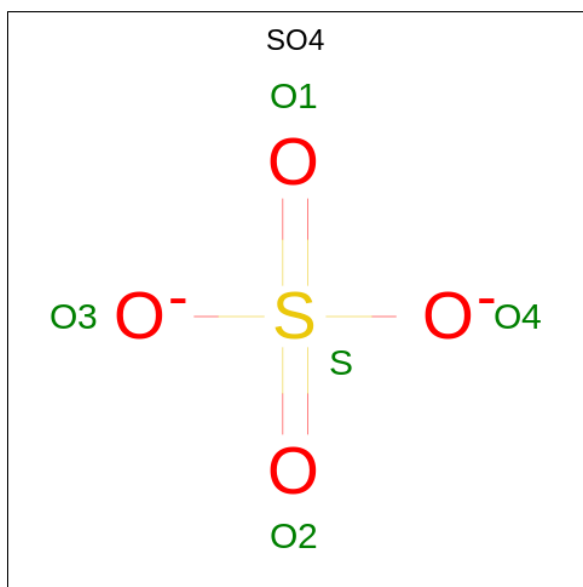
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			
2	A	1	Total	14	4	6	1	3	0	0
2	B	1	Total	14	4	6	1	3	0	0

- 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	
			Total	C	H	N	O			P
3	A	1	70	21	26	7	14	2	0	0
3	B	1	70	21	26	7	14	2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O S		
4	A	1	5	4 1	0	0
4	A	1	5	4 1	0	0
4	A	1	5	4 1	0	0
4	B	1	5	4 1	0	0
4	B	1	5	4 1	0	0
4	B	1	5	4 1	0	0
4	B	1	5	4 1	0	0
4	B	1	5	4 1	0	0
4	B	1	5	4 1	0	0

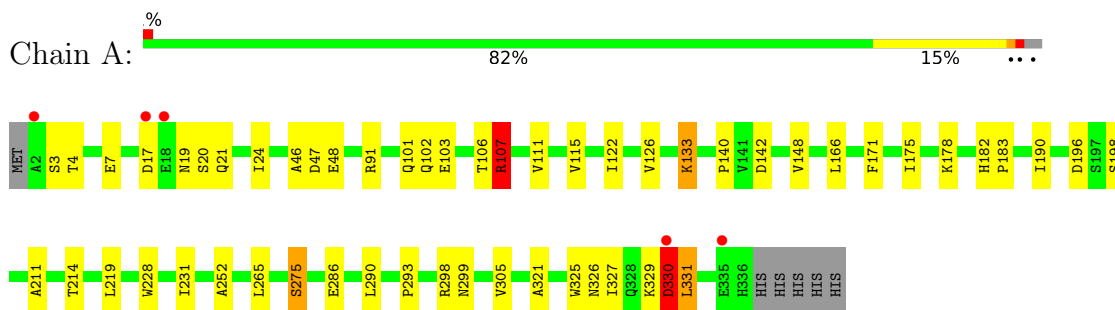
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total	O	0	0
			15	15		
5	B	12	Total	O	0	0
			12	12		

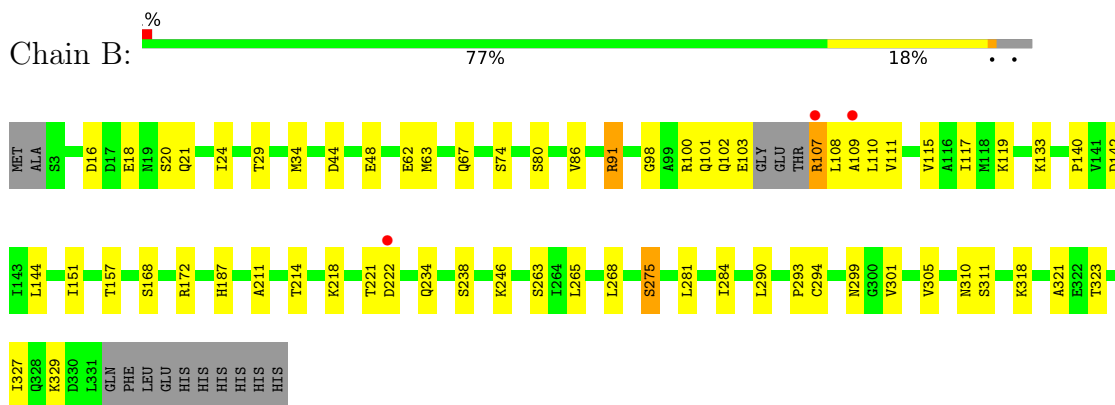
3 Residue-property plots [i](#)

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: L-lactate dehydrogenase C chain



- Molecule 1: L-lactate dehydrogenase C chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	177.89Å 177.89Å 179.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.47 – 3.00 44.47 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.47-3.00) 98.7 (44.47-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472, PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.203 , 0.227 0.203 , 0.227	Depositor DCC
R_{free} test set	1358 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtrriage
Anisotropy	0.037	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10310	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: NAD, J9X, SO4

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	0.50	4/2616 (0.2%)	0.96	7/3541 (0.2%)
1	B	0.36	0/2541	0.55	2/3438 (0.1%)
All	All	0.44	4/5157 (0.1%)	0.79	9/6979 (0.1%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	330	ASP	CB-CG	8.22	1.69	1.51
1	A	107	ARG	CG-CD	-6.83	1.34	1.51
1	A	107	ARG	CB-CG	-6.42	1.35	1.52
1	A	329	LYS	CB-CG	5.00	1.66	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	107	ARG	NE-CZ-NH1	-27.39	106.61	120.30
1	A	107	ARG	NE-CZ-NH2	23.29	131.94	120.30
1	A	107	ARG	CD-NE-CZ	-14.73	102.98	123.60
1	A	107	ARG	CG-CD-NE	-13.31	83.84	111.80
1	A	330	ASP	CB-CG-OD2	13.06	130.05	118.30
1	A	331	LEU	CA-CB-CG	-9.17	94.21	115.30
1	A	330	ASP	OD1-CG-OD2	-8.69	106.78	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	B	91	ARG	CG-CD-NE	-6.34	98.49	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	ASP	Sidechain

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	2574	2491	2656	36	1
1	B	2502	2503	2593	44	2
2	A	8	6	0	0	0
2	B	8	6	0	0	0
3	A	44	26	25	0	0
3	B	44	26	25	1	0
4	A	15	0	0	1	0
4	B	30	0	0	4	0
5	A	15	0	0	1	0
5	B	12	0	0	1	0
All	All	5252	5058	5299	79	2

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 8.

All (79) 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:B:311:SER:OG	4:B:407:SO4:O1	1.93	0.86
1:A:327:ILE:HA	1:A:330:ASP:HB2	1.63	0.80
1:A:326:ASN:O	1:A:330:ASP:N	2.17	0.76
1:B:108:LEU:HD23	1:B:108:LEU:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLU:HG3	1:A:140:PRO:HB3	1.75	0.68
1:B:20:SER:OG	1:B:48:GLU:OE1	2.08	0.67
1:B:101:GLN:HG2	1:B:102:GLN:H	1.59	0.67
1:A:4:THR:HG22	1:A:7:GLU:HB2	1.79	0.65
1:A:102:GLN:O	1:A:106:THR:HG21	1.96	0.65
1:B:234:GLN:O	1:B:238:SER:OG	2.14	0.64
1:B:24:ILE:HD11	1:B:265:LEU:HD11	1.82	0.61
1:B:16:ASP:OD1	5:B:501:HOH:O	2.16	0.60
1:A:142:ASP:OD1	1:A:275:SER:OG	2.20	0.60
1:B:142:ASP:OD1	1:B:275:SER:OG	2.20	0.59
1:B:63:MET:O	1:B:67:GLN:HG3	2.04	0.57
1:A:286:GLU:HG2	1:A:325:TRP:CD2	2.39	0.57
1:B:91:ARG:NH2	1:B:91:ARG:HG2	2.18	0.57
1:A:178:LYS:HD3	1:A:228:TRP:CZ2	2.41	0.56
1:B:107:ARG:HE	1:B:110:LEU:CD1	2.18	0.56
1:B:311:SER:OG	4:B:407:SO4:S	2.64	0.55
1:B:18:GLU:OE2	1:B:18:GLU:HA	2.07	0.55
1:B:119:LYS:HA	1:B:151:ILE:HD13	1.88	0.54
1:A:47:ASP:OD2	5:A:501:HOH:O	2.18	0.54
1:B:294:CYS:HB3	1:B:301:VAL:HG13	1.90	0.53
1:B:34:MET:HG3	1:B:62:GLU:OE1	2.08	0.53
1:A:122:ILE:HG13	1:A:148:VAL:HG22	1.92	0.52
1:A:133:LYS:HE2	1:A:299:ASN:HA	1.92	0.52
1:B:172:ARG:NH1	4:B:405:SO4:O3	2.43	0.52
1:A:20:SER:OG	1:A:48:GLU:OE1	2.24	0.52
1:B:18:GLU:OE1	1:B:48:GLU:OE1	2.28	0.52
1:A:327:ILE:C	1:A:330:ASP:H	2.12	0.51
1:B:29:THR:HB	1:B:34:MET:SD	2.51	0.51
1:A:4:THR:HG23	1:A:7:GLU:H	1.75	0.51
1:A:190:ILE:CG2	1:A:198:SER:HB2	2.40	0.51
1:A:293:PRO:HB2	1:A:305:VAL:HB	1.92	0.50
1:B:218:LYS:O	1:B:221:THR:OG1	2.31	0.49
1:B:103:GLU:HG3	1:B:140:PRO:HB3	1.95	0.48
1:B:168:SER:O	1:B:172:ARG:HG3	2.13	0.48
1:B:310:ASN:ND2	4:B:406:SO4:O1	2.39	0.48
1:A:286:GLU:HG2	1:A:325:TRP:CE2	2.49	0.48
1:B:293:PRO:HB2	1:B:305:VAL:HB	1.95	0.48
1:B:21:GLN:O	1:B:91:ARG:HD2	2.14	0.48
1:A:115:VAL:HG21	1:A:331:LEU:HD13	1.96	0.48
1:B:100:ARG:NH1	3:B:402:NAD:O1N	2.46	0.47
1:B:323:THR:O	1:B:327:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ALA:O	1:A:214:THR:HB	2.15	0.47
4:A:405:SO4:O1	1:B:187:HIS:NE2	2.48	0.47
1:A:19:ASN:OD1	1:A:19:ASN:N	2.49	0.46
1:B:111:VAL:O	1:B:115:VAL:HG23	2.16	0.46
1:B:101:GLN:OE1	1:B:111:VAL:HG22	2.15	0.46
1:A:24:ILE:HD11	1:A:265:LEU:HD11	1.97	0.45
1:A:166:LEU:HD11	1:A:252:ALA:HB1	1.97	0.45
1:B:290:LEU:HD11	1:B:321:ALA:HA	1.98	0.45
1:A:103:GLU:OE1	1:A:142:ASP:HB2	2.17	0.45
1:B:140:PRO:O	1:B:144:LEU:HG	2.17	0.45
1:A:24:ILE:HG13	1:A:46:ALA:HB2	1.99	0.45
1:B:44:ASP:OD2	1:B:74:SER:HB2	2.17	0.44
1:B:101:GLN:CG	1:B:102:GLN:H	2.28	0.44
1:A:102:GLN:C	1:A:106:THR:HG21	2.38	0.43
1:A:103:GLU:HG3	1:A:140:PRO:CB	2.47	0.43
1:A:107:ARG:HA	1:A:107:ARG:HD2	1.62	0.43
1:B:263:SER:HA	1:B:268:LEU:HD12	2.01	0.43
1:B:211:ALA:O	1:B:214:THR:HB	2.19	0.43
1:A:219:LEU:HD11	1:A:228:TRP:CG	2.54	0.42
1:A:122:ILE:O	1:A:126:VAL:HG23	2.20	0.42
1:A:228:TRP:CE3	1:A:231:ILE:HD12	2.55	0.42
1:A:290:LEU:HD11	1:A:321:ALA:HA	2.02	0.42
1:B:86:VAL:HG22	1:B:86:VAL:O	2.19	0.42
1:B:107:ARG:NH1	1:B:109:ALA:HB3	2.35	0.42
1:B:281:LEU:O	1:B:284:ILE:HG12	2.19	0.42
1:A:21:GLN:HE21	1:A:91:ARG:HH12	1.68	0.41
1:A:171:PHE:O	1:A:175:ILE:HG13	2.19	0.41
1:B:98:GLY:HA2	1:B:117:ILE:HD12	2.02	0.41
1:A:101:GLN:HE22	1:A:111:VAL:HG22	1.85	0.41
1:B:34:MET:HG3	1:B:62:GLU:CD	2.40	0.41
1:A:182:HIS:HB2	1:B:268:LEU:O	2.19	0.41
1:A:182:HIS:ND1	1:A:183:PRO:HD2	2.36	0.41
1:B:101:GLN:NE2	1:B:110:LEU:HB3	2.36	0.40
1:B:157:THR:HB	1:B:301:VAL:O	2.20	0.40

All (2) 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:B:62:GLU:OE1	1:B:246:LYS:NZ[10_554]	2.06	0.14
1:A:17:ASP:OD1	1:B:299:ASN:HD21[10_554]	1.48	0.12

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	333/341 (98%)	325 (98%)	8 (2%)	0	100	100
1	B	322/341 (94%)	314 (98%)	8 (2%)	0	100	100
All	All	655/682 (96%)	639 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	289/295 (98%)	282 (98%)	7 (2%)	49	79
1	B	282/295 (96%)	275 (98%)	7 (2%)	47	79
All	All	571/590 (97%)	557 (98%)	14 (2%)	47	79

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	107	ARG
1	A	133	LYS
1	A	196	ASP
1	A	275	SER
1	A	298	ARG
1	A	330	ASP
1	B	80	SER

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Mol	Chain	Res	Type
1	B	107	ARG
1	B	133	LYS
1	B	222	ASP
1	B	275	SER
1	B	318	LYS
1	B	329	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	HIS
1	B	232	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAD	A	402	-	42,48,48	2.89	15 (35%)	50,73,73	1.94	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	404	-	4,4,4	0.16	0	6,6,6	0.16	0
4	SO4	B	408	-	4,4,4	0.16	0	6,6,6	0.16	0
4	SO4	B	403	-	4,4,4	0.14	0	6,6,6	0.18	0
4	SO4	B	404	-	4,4,4	0.12	0	6,6,6	0.13	0
2	J9X	A	401	-	7,7,7	1.55	2 (28%)	7,8,8	1.83	3 (42%)
4	SO4	A	405	-	4,4,4	0.16	0	6,6,6	0.19	0
2	J9X	B	401	-	7,7,7	1.71	2 (28%)	7,8,8	2.05	3 (42%)
4	SO4	B	406	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	405	-	4,4,4	0.20	0	6,6,6	0.26	0
4	SO4	A	403	-	4,4,4	0.19	0	6,6,6	0.26	0
3	NAD	B	402	-	42,48,48	2.69	14 (33%)	50,73,73	1.82	13 (26%)
4	SO4	B	407	-	4,4,4	0.14	0	6,6,6	0.10	0

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	A	402	-	-	11/26/62/62	0/5/5/5
2	J9X	A	401	-	-	3/6/7/7	-
3	NAD	B	402	-	-	11/26/62/62	0/5/5/5
2	J9X	B	401	-	-	3/6/7/7	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NAD	O4D-C1D	11.77	1.57	1.41
3	B	402	NAD	O4D-C1D	10.29	1.55	1.41
3	A	402	NAD	C2N-N1N	5.50	1.41	1.35
3	A	402	NAD	O5D-C5D	-5.38	1.24	1.44
3	B	402	NAD	PA-O5B	5.37	1.81	1.59
3	A	402	NAD	PA-O5B	5.05	1.79	1.59
3	B	402	NAD	C2N-N1N	5.04	1.41	1.35
3	B	402	NAD	PN-O5D	4.89	1.79	1.59
3	B	402	NAD	O5D-C5D	-4.66	1.26	1.44
3	A	402	NAD	PN-O5D	4.57	1.77	1.59
3	B	402	NAD	O4B-C1B	-3.88	1.35	1.41
3	B	402	NAD	C2A-N1A	3.61	1.40	1.33
3	A	402	NAD	O4D-C4D	3.59	1.53	1.45
3	A	402	NAD	C2A-N1A	3.38	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	J9X	C03-C05	2.90	1.57	1.54
3	A	402	NAD	C7N-N7N	2.83	1.38	1.33
3	B	402	NAD	C3N-C7N	2.82	1.54	1.50
3	A	402	NAD	C4A-N3A	2.81	1.39	1.35
3	B	402	NAD	C6N-N1N	-2.80	1.28	1.35
3	A	402	NAD	C2B-C3B	2.77	1.60	1.53
3	A	402	NAD	C6N-N1N	-2.74	1.28	1.35
3	A	402	NAD	C2B-C1B	2.69	1.57	1.53
3	B	402	NAD	O4D-C4D	2.64	1.50	1.45
3	A	402	NAD	O2B-C2B	-2.58	1.36	1.43
2	A	401	J9X	C03-N02	2.55	1.38	1.33
2	A	401	J9X	O07-C05	-2.49	1.23	1.30
3	B	402	NAD	O5B-C5B	-2.42	1.35	1.44
3	A	402	NAD	C3N-C7N	2.34	1.54	1.50
2	B	401	J9X	O07-C05	-2.32	1.23	1.30
3	B	402	NAD	O4B-C4B	-2.25	1.40	1.45
3	B	402	NAD	O2B-C2B	-2.20	1.37	1.43
3	A	402	NAD	O5B-C5B	-2.11	1.36	1.44
3	B	402	NAD	C7N-N7N	2.04	1.36	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAD	O4D-C4D-C3D	-4.93	95.35	105.11
3	B	402	NAD	O4D-C4D-C3D	-4.38	96.44	105.11
3	A	402	NAD	O4B-C1B-C2B	-4.35	100.56	106.93
3	B	402	NAD	O4D-C4D-C5D	3.82	121.96	109.37
3	B	402	NAD	C2N-C3N-C4N	-3.81	113.94	118.26
3	A	402	NAD	C2N-C3N-C4N	-3.78	113.98	118.26
3	B	402	NAD	O5D-PN-O1N	-3.56	95.14	109.07
3	A	402	NAD	O5D-PN-O1N	-3.51	95.35	109.07
3	B	402	NAD	O7N-C7N-N7N	-3.51	117.59	122.58
3	A	402	NAD	O4D-C4D-C5D	3.32	120.28	109.37
2	B	401	J9X	O04-C03-N02	-3.25	117.34	123.30
2	A	401	J9X	O06-C05-C03	-3.07	115.33	122.18
2	B	401	J9X	O06-C05-C03	-3.01	115.48	122.18
3	A	402	NAD	O4B-C4B-C5B	2.99	119.22	109.37
3	A	402	NAD	O7N-C7N-N7N	-2.99	118.33	122.58
3	A	402	NAD	PN-O3-PA	-2.94	122.74	132.83
3	B	402	NAD	O4D-C1D-C2D	-2.88	102.71	106.93
3	B	402	NAD	PN-O3-PA	-2.68	123.63	132.83
3	B	402	NAD	O7N-C7N-C3N	2.68	122.83	119.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAD	O4D-C1D-C2D	-2.61	103.11	106.93
2	A	401	J9X	O04-C03-N02	-2.52	118.68	123.30
3	A	402	NAD	O2B-C2B-C1B	2.52	120.14	110.85
3	A	402	NAD	C1B-N9A-C4A	-2.50	122.24	126.64
3	B	402	NAD	O3B-C3B-C4B	-2.45	103.96	111.05
2	A	401	J9X	O07-C05-O06	2.42	129.13	123.61
3	B	402	NAD	C3N-C2N-N1N	2.34	122.72	120.43
3	A	402	NAD	C3N-C2N-N1N	2.28	122.66	120.43
3	B	402	NAD	O4B-C4B-C5B	2.26	116.82	109.37
3	B	402	NAD	C2B-C3B-C4B	2.24	106.99	102.64
3	A	402	NAD	O4B-C4B-C3B	-2.21	100.74	105.11
3	B	402	NAD	C3D-C2D-C1D	2.18	104.25	100.98
2	B	401	J9X	O07-C05-O06	2.16	128.55	123.61
3	A	402	NAD	C2N-C3N-C7N	2.11	125.58	119.46
3	A	402	NAD	C3N-C7N-N7N	2.10	120.27	117.75

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	J9X	N02-C03-C05-O06
2	A	401	J9X	N02-C03-C05-O07
2	A	401	J9X	O04-C03-C05-O06
2	B	401	J9X	N02-C03-C05-O06
2	B	401	J9X	N02-C03-C05-O07
2	B	401	J9X	O04-C03-C05-O06
3	A	402	NAD	C5B-O5B-PA-O2A
3	A	402	NAD	C5B-O5B-PA-O3
3	A	402	NAD	O4B-C4B-C5B-O5B
3	A	402	NAD	O4D-C1D-N1N-C2N
3	A	402	NAD	C2D-C1D-N1N-C2N
3	A	402	NAD	C2D-C1D-N1N-C6N
3	B	402	NAD	C5B-O5B-PA-O3
3	B	402	NAD	C5D-O5D-PN-O1N
3	B	402	NAD	C5D-O5D-PN-O2N
3	B	402	NAD	O4D-C1D-N1N-C2N
3	B	402	NAD	C2D-C1D-N1N-C2N
3	B	402	NAD	C2D-C1D-N1N-C6N
3	A	402	NAD	C3D-C4D-C5D-O5D
3	B	402	NAD	O4B-C4B-C5B-O5B
3	A	402	NAD	C3B-C4B-C5B-O5B
3	B	402	NAD	O4D-C4D-C5D-O5D

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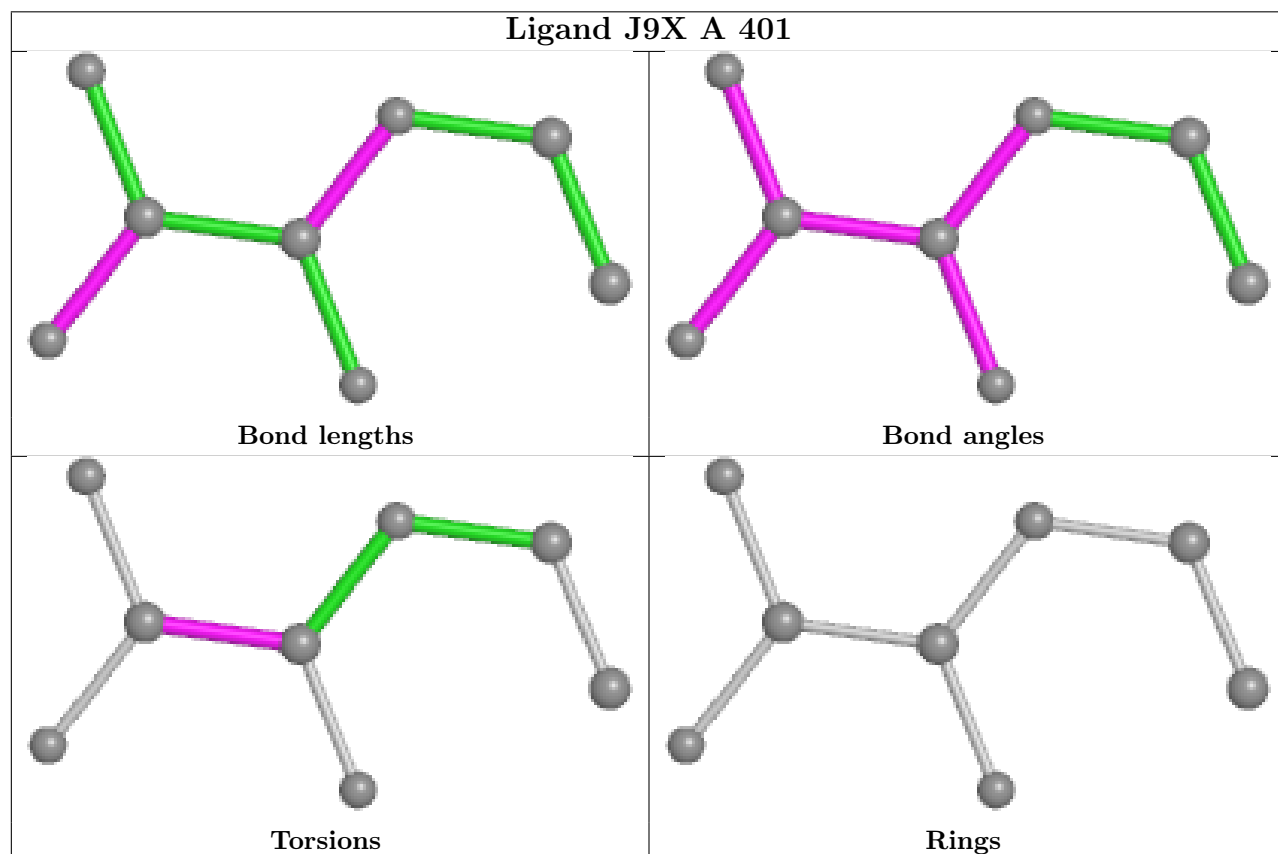
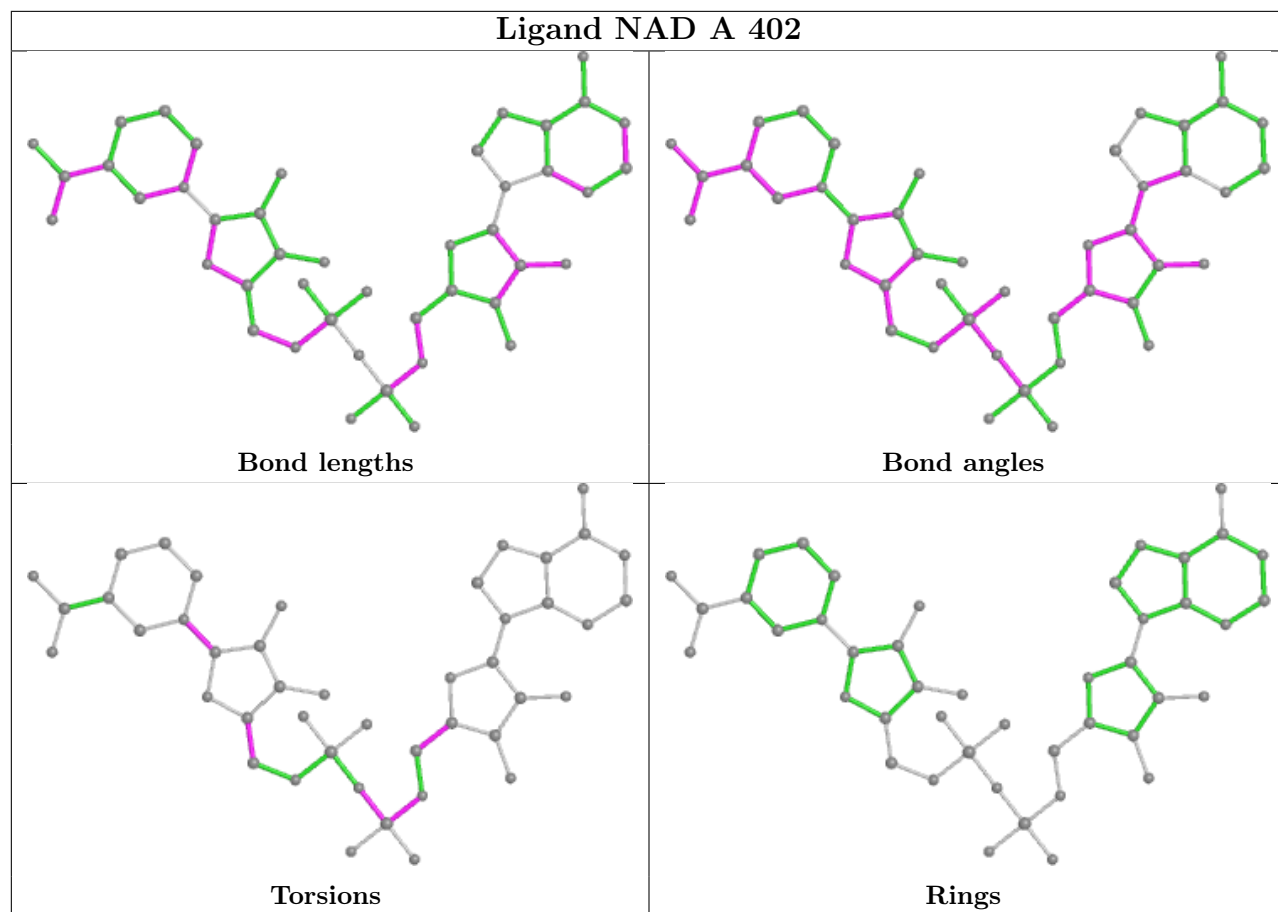
Mol	Chain	Res	Type	Atoms
3	B	402	NAD	C3D-C4D-C5D-O5D
3	A	402	NAD	O4D-C4D-C5D-O5D
3	A	402	NAD	C5B-O5B-PA-O1A
3	A	402	NAD	PN-O3-PA-O1A
3	B	402	NAD	C5D-O5D-PN-O3
3	B	402	NAD	C5B-O5B-PA-O1A

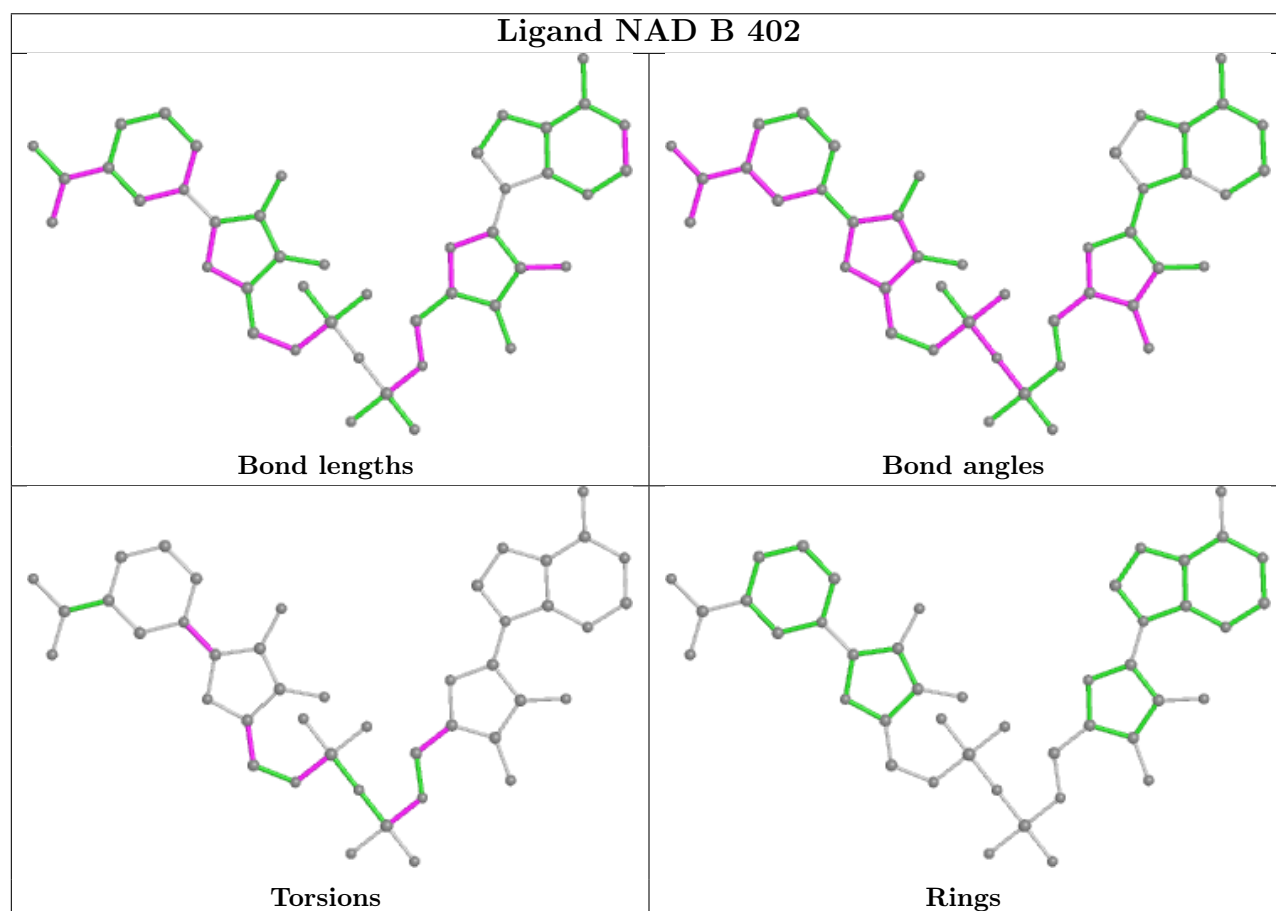
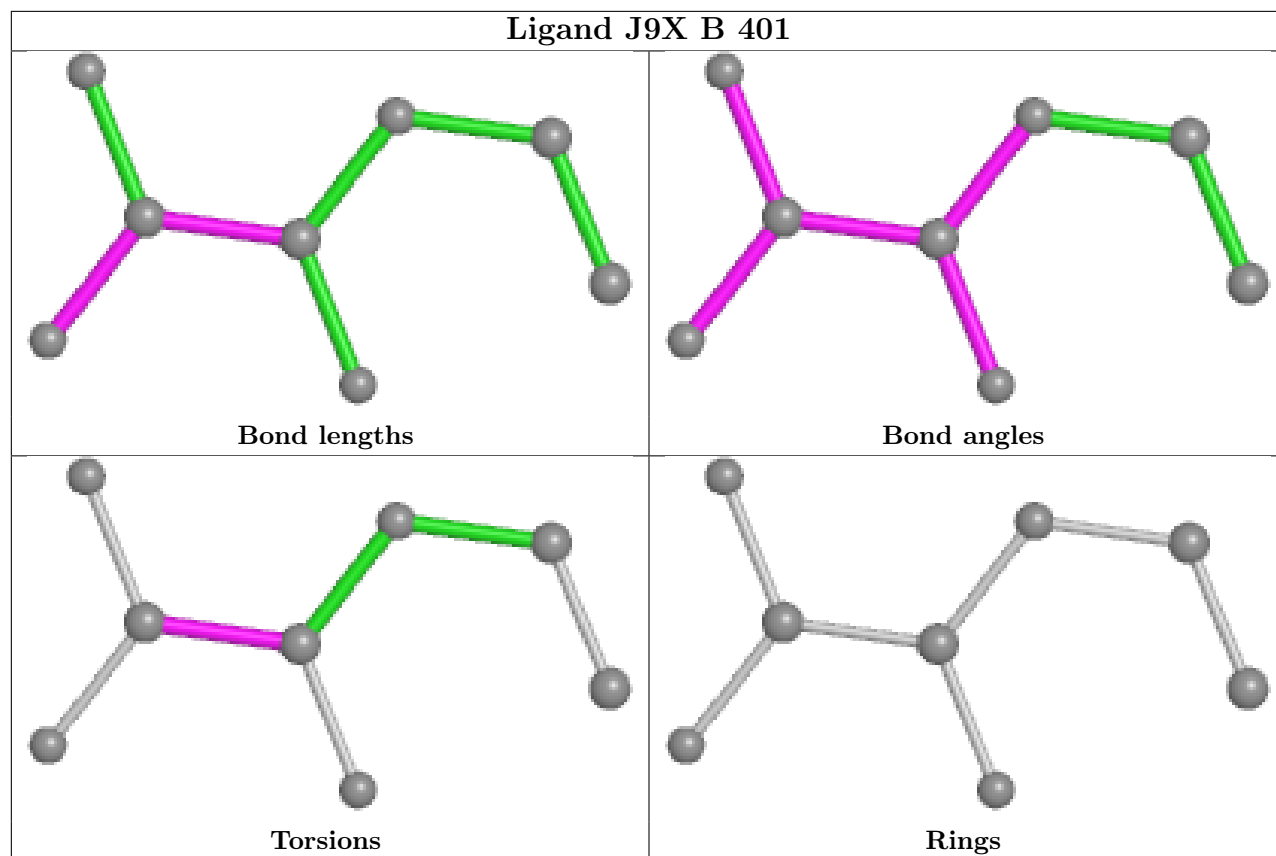
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	SO4	1	0
4	B	406	SO4	1	0
4	B	405	SO4	1	0
3	B	402	NAD	1	0
4	B	407	SO4	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	335/341 (98%)	-0.28	5 (1%)	73 46	31, 47, 79, 159	0
1	B	326/341 (95%)	-0.23	3 (0%)	84 63	33, 47, 91, 130	0
All	All	661/682 (96%)	-0.25	8 (1%)	79 54	31, 47, 85, 159	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	3.8
1	A	18	GLU	3.5
1	A	335	GLU	2.8
1	B	107	ARG	2.5
1	B	109	ALA	2.2
1	B	222	ASP	2.2
1	A	330	ASP	2.1
1	A	17	ASP	2.1

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,

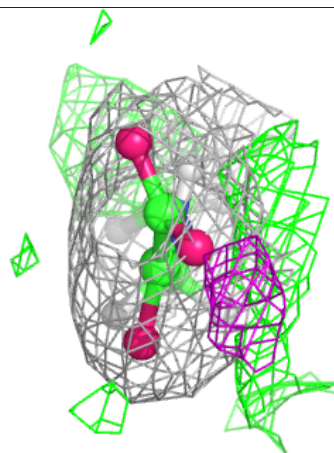
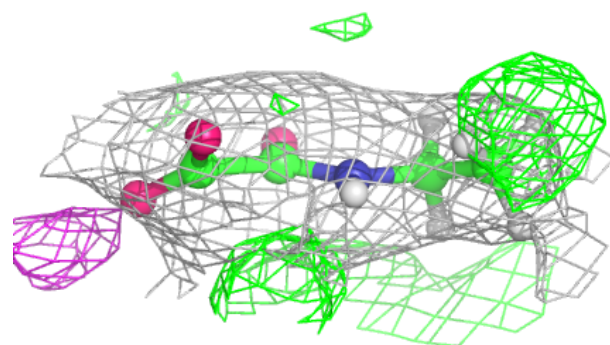
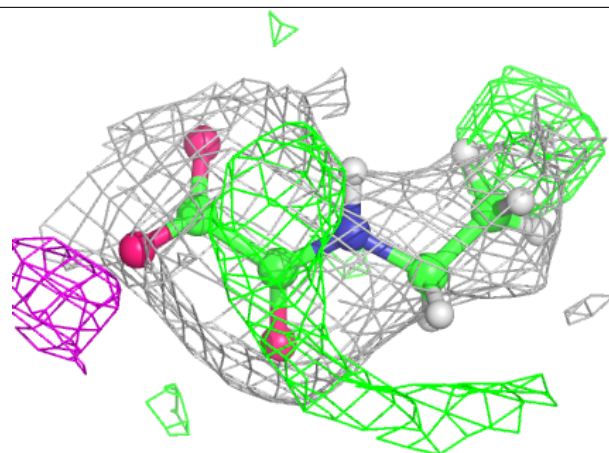
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	404	5/5	0.73	0.23	102,109,151,216	0
4	SO4	B	406	5/5	0.75	0.31	127,135,141,215	0
4	SO4	B	408	5/5	0.78	0.34	84,93,108,170	0
4	SO4	A	403	5/5	0.86	0.34	74,79,81,111	0
4	SO4	B	403	5/5	0.86	0.27	81,88,101,112	0
4	SO4	B	407	5/5	0.89	0.20	122,124,131,155	0
2	J9X	B	401	8/8	0.90	0.20	48,58,75,75	0
2	J9X	A	401	8/8	0.92	0.25	39,53,70,70	0
3	NAD	B	402	44/44	0.95	0.18	39,47,59,73	0
3	NAD	A	402	44/44	0.95	0.20	33,45,57,75	0
4	SO4	B	404	5/5	0.95	0.16	69,70,103,109	0
4	SO4	B	405	5/5	0.97	0.21	38,40,43,45	0
4	SO4	A	405	5/5	0.98	0.16	42,42,45,46	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.

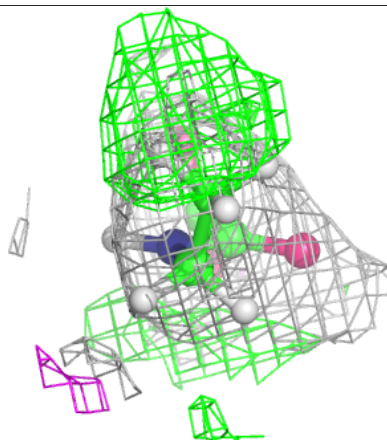
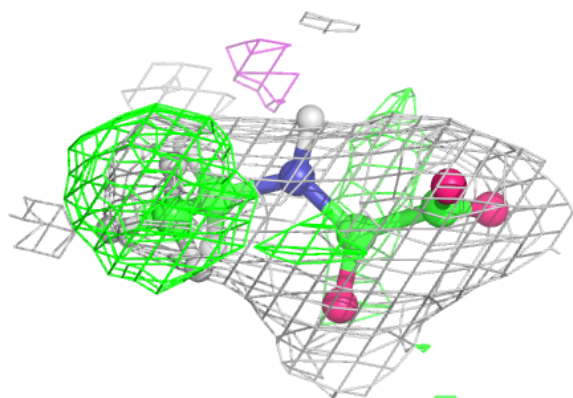
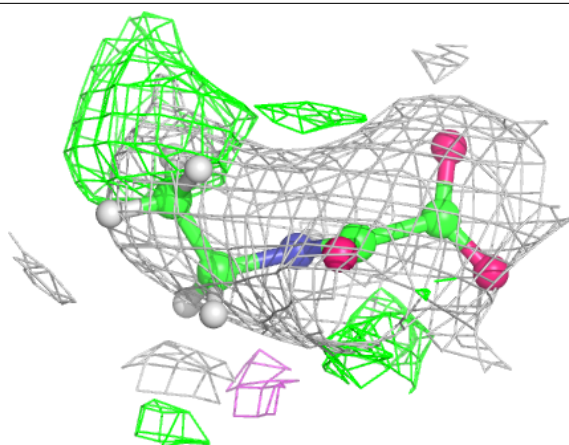
Electron density around J9X B 401:

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

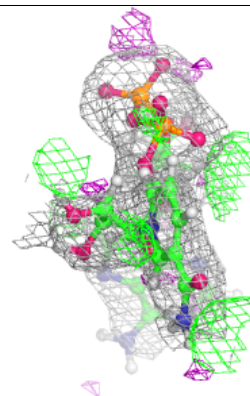
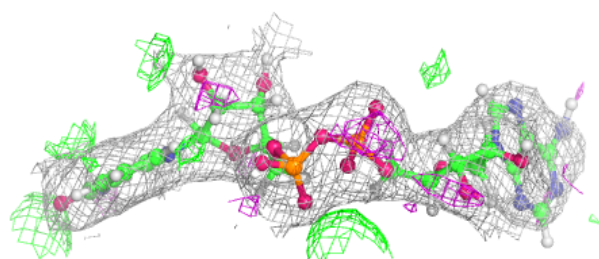
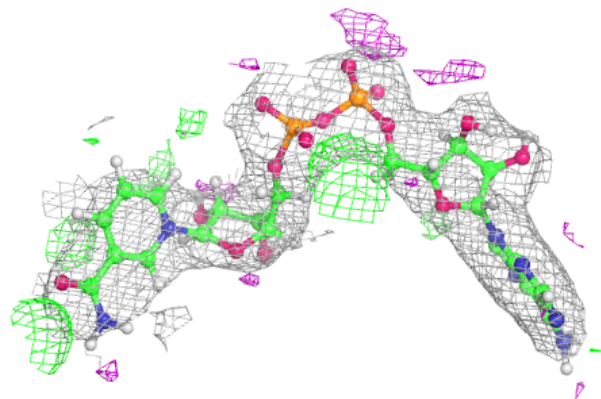


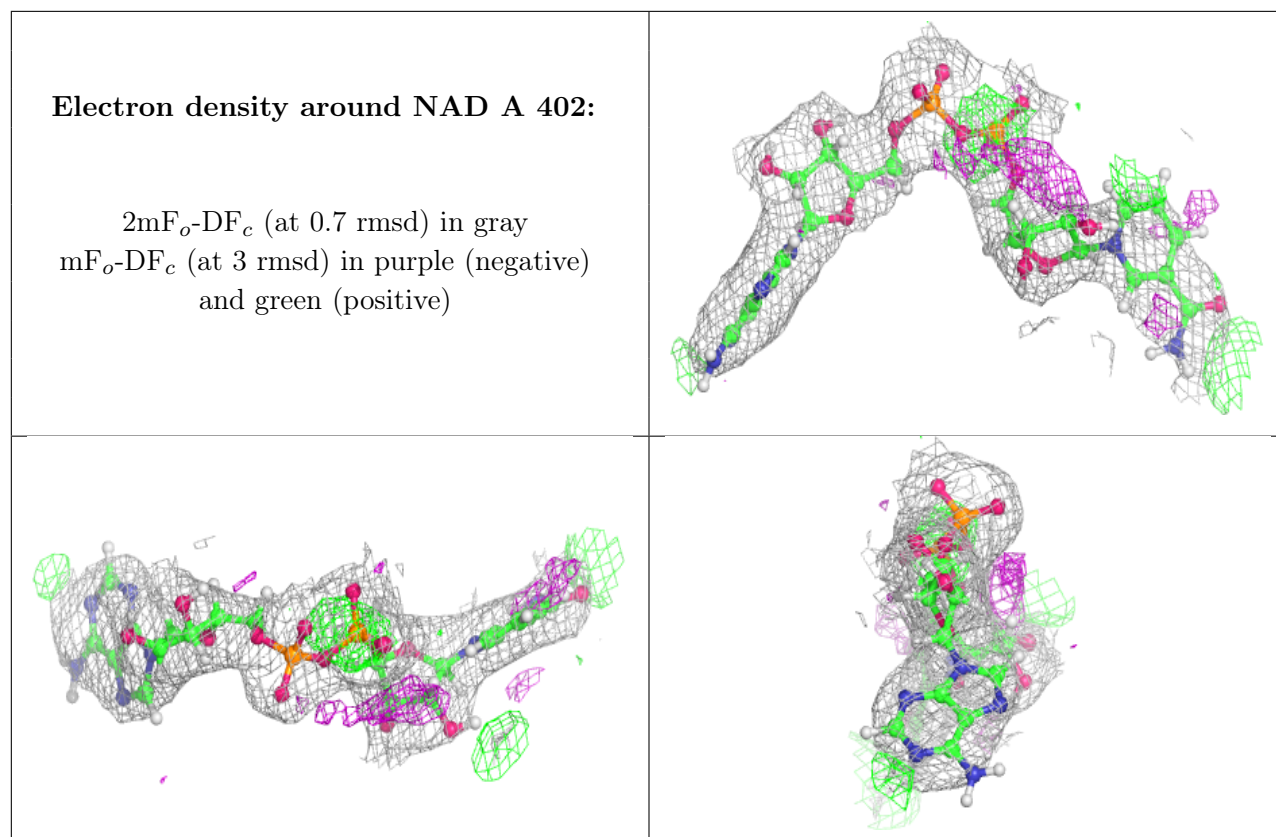
Electron density around J9X A 401:

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

**Electron density around NAD B 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.