



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:53 AM UTC

PDB ID : 7BSL / pdb_00007bsl
Title : Crystal Structure of human ME2 R67A mutant
Authors : Chen, W.L.; Tai, S.C.; Hung, H.C.; Ho, M.C.
Deposited on : 2020-03-30
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

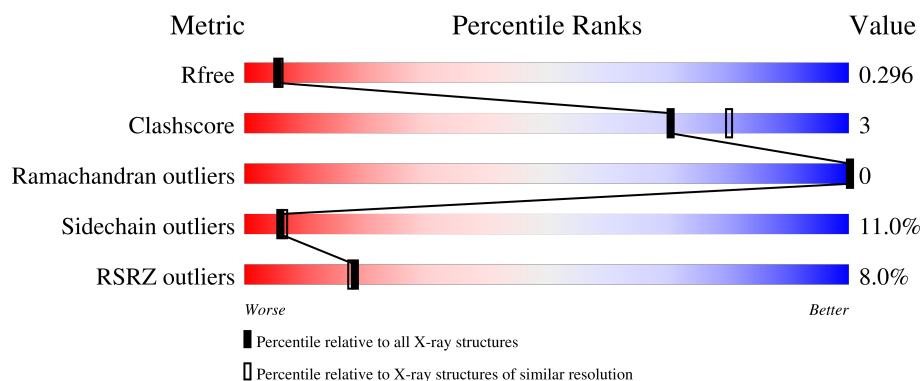
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	566	8% 79% 16% • •
1	B	566	8% 81% 14% • •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8875 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.

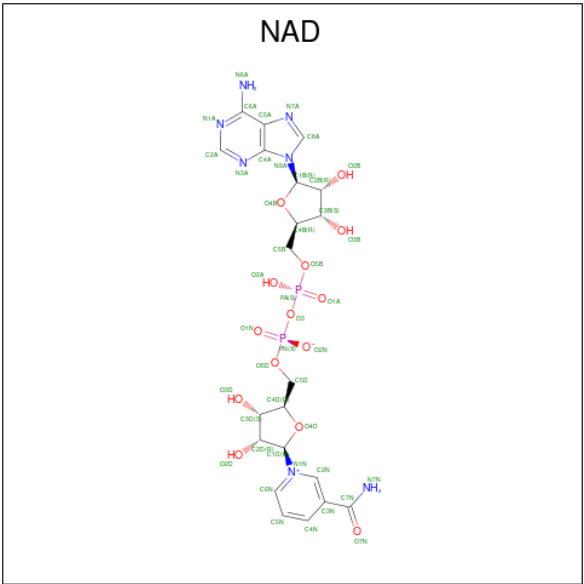
- Molecule 1 is a protein called NAD-dependent malic enzyme, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			4272	2731	729	789	23			
1	B	551	Total	C	N	O	S	0	0	0
			4344	2781	738	802	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP P23368
A	67	ALA	ARG	engineered mutation	UNP P23368
B	19	MET	-	initiating methionine	UNP P23368
B	67	ALA	ARG	engineered mutation	UNP P23368

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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

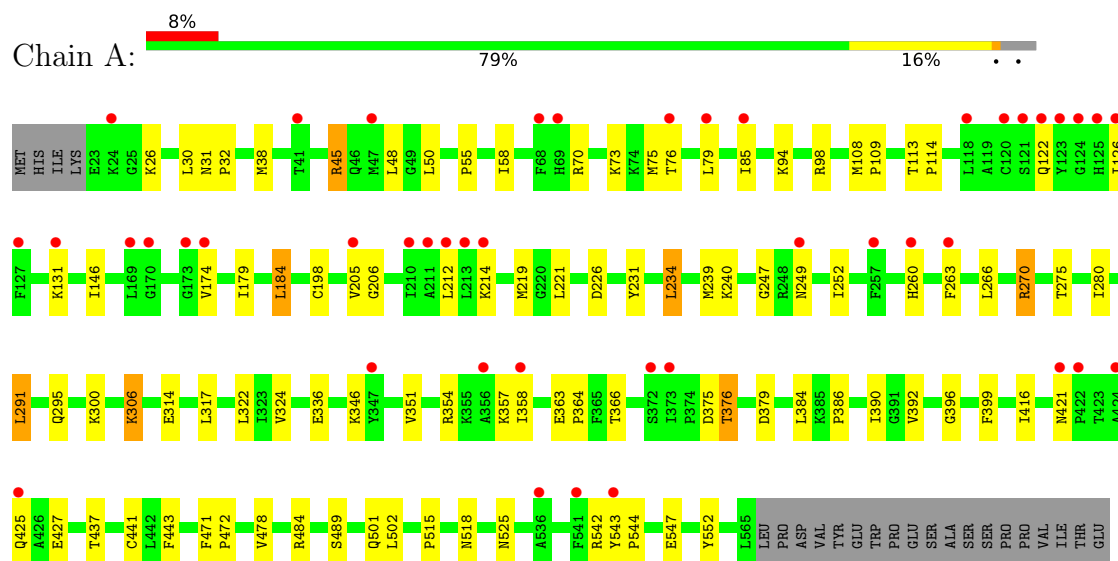
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		
3	B	43	Total	O	0	0
			43	43		

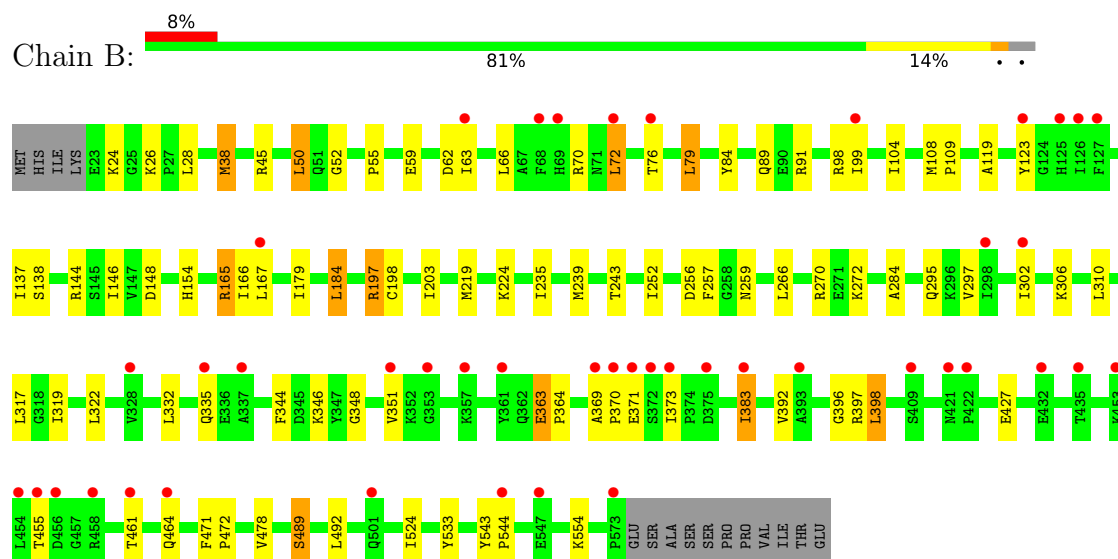
3 Residue-property plots [i](#)

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: NAD-dependent malic enzyme, mitochondrial



- Molecule 1: NAD-dependent malic enzyme, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.20Å 191.15Å 59.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.22 – 2.55 29.22 – 2.55	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.22-2.55) 90.5 (29.22-2.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.249 , 0.297 0.250 , 0.296	Depositor DCC
R_{free} test set	2039 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 23.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8875	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.03	0/4361	1.48	2/5902 (0.0%)
1	B	1.02	0/4438	1.45	0/6011
All	All	1.02	0/8799	1.46	2/11913 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	GLY	CA-C-O	-5.76	118.48	122.22
1	A	206	GLY	CA-C-O	-5.53	118.15	122.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4272	0	4312	31	0
1	B	4344	0	4375	32	0
2	A	88	0	52	0	0
2	B	88	0	52	1	0
3	A	40	0	0	0	0
3	B	43	0	0	0	0
All	All	8875	0	8791	60	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 (60) 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:239:MET:HE1	1:A:252:ILE:HG21	1.66	0.76
1:A:501:GLN:HE22	1:A:525:ASN:HD22	1.35	0.74
1:B:239:MET:HE1	1:B:252:ILE:HG21	1.71	0.72
1:B:184:LEU:HG	1:B:198:CYS:HB3	1.79	0.65
1:A:184:LEU:HG	1:A:198:CYS:HB3	1.83	0.60
1:B:165:ARG:O	1:B:165:ARG:HG3	2.02	0.59
1:A:55:PRO:HG2	1:B:219:MET:HE2	1.85	0.59
1:A:31:ASN:HD22	1:A:32:PRO:HD2	1.69	0.57
1:A:263:PHE:CD1	1:A:280:ILE:HD11	2.38	0.57
1:A:266:LEU:O	1:A:270:ARG:HB3	2.05	0.56
1:A:146:ILE:HG23	1:B:52:GLY:HA3	1.89	0.54
1:B:370:PRO:HG2	1:B:383:ILE:HD11	1.89	0.53
1:A:363:GLU:N	1:A:364:PRO:HD2	2.24	0.52
1:A:249:ASN:HD22	1:A:484:ARG:HG3	1.74	0.52
1:B:79:LEU:HD21	1:B:119:ALA:HA	1.92	0.52
1:B:45:ARG:HA	1:B:50:LEU:HB2	1.94	0.50
1:B:266:LEU:O	1:B:270:ARG:HB2	2.12	0.50
1:A:543:TYR:HA	1:A:544:PRO:C	2.36	0.50
1:A:205:VAL:HG22	1:A:226:ASP:HB3	1.93	0.50
1:A:45:ARG:HA	1:A:50:LEU:HB2	1.94	0.50
1:B:62:ASP:OD1	1:B:98:ARG:NH2	2.45	0.49
1:A:108:MET:N	1:A:109:PRO:HD2	2.28	0.48
1:B:108:MET:N	1:B:109:PRO:HD2	2.28	0.48
1:B:154:HIS:O	1:B:197:ARG:HD3	2.13	0.48
1:B:284:ALA:HA	1:B:319:ILE:HG12	1.96	0.47
1:B:165:ARG:HG2	1:B:257:PHE:O	2.13	0.47
1:B:543:TYR:HA	1:B:544:PRO:C	2.39	0.47
1:B:369:ALA:HB1	1:B:373:ILE:HD11	1.96	0.47
1:A:542:ARG:HG2	1:A:552:TYR:OH	2.15	0.47
1:A:109:PRO:HA	1:A:113:THR:O	2.15	0.47
1:A:205:VAL:HG21	1:A:231:TYR:HD1	1.80	0.46
1:A:396:GLY:HA2	1:A:425:GLN:HA	1.98	0.46
1:B:471:PHE:CG	1:B:472:PRO:HD3	2.52	0.45
1:A:219:MET:HE2	1:B:55:PRO:HG2	1.98	0.45
1:B:310:LEU:HD21	1:B:398:LEU:HD23	1.99	0.45
1:A:515:PRO:HG2	1:A:518:ASN:HD22	1.83	0.44
1:B:396:GLY:O	1:B:427:GLU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:THR:HG21	1:A:441:CYS:SG	2.58	0.43
1:A:358:ILE:HD13	1:A:366:THR:HG21	2.01	0.43
1:B:398:LEU:HD12	1:B:398:LEU:HA	1.83	0.43
1:B:165:ARG:O	1:B:165:ARG:CG	2.65	0.43
1:A:291:LEU:HD21	1:A:390:ILE:HD11	2.00	0.43
1:A:399:PHE:CG	1:A:427:GLU:HB3	2.54	0.43
1:A:306:LYS:HB3	1:A:386:PRO:HA	2.01	0.42
1:A:471:PHE:CG	1:A:472:PRO:HD3	2.54	0.42
1:B:166:ILE:HD13	1:B:256:ASP:HB3	2.02	0.42
1:B:272:LYS:HB3	1:B:272:LYS:HE3	1.90	0.42
1:B:72:LEU:HG	1:B:84:TYR:HD2	1.84	0.42
1:B:259:ASN:ND2	2:B:601:NAD:C5N	2.83	0.42
1:A:376:THR:HG22	1:A:379:ASP:H	1.84	0.41
1:B:363:GLU:N	1:B:364:PRO:CD	2.84	0.41
1:B:184:LEU:HD12	1:B:184:LEU:HA	1.86	0.41
1:B:344:PHE:CZ	1:B:348:GLY:HA2	2.55	0.41
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.85	0.41
1:B:38:MET:HG2	1:B:59:GLU:HG3	2.02	0.41
1:A:542:ARG:NH1	1:A:544:PRO:O	2.54	0.40
1:B:489:SER:HB2	1:B:533:TYR:CZ	2.56	0.40
1:A:416:ILE:O	1:A:443:PHE:HA	2.21	0.40
1:A:113:THR:HA	1:A:114:PRO:HA	1.89	0.40
1:B:144:ARG:NH1	1:B:148:ASP:OD1	2.53	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	541/566 (96%)	522 (96%)	19 (4%)	0	100	100
1	B	549/566 (97%)	536 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1090/1132 (96%)	1058 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	458/480 (95%)	408 (89%)	50 (11%)	6	7
1	B	466/480 (97%)	414 (89%)	52 (11%)	6	6
All	All	924/960 (96%)	822 (89%)	102 (11%)	6	6

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	30	LEU
1	A	38	MET
1	A	45	ARG
1	A	48	LEU
1	A	58	ILE
1	A	70	ARG
1	A	73	LYS
1	A	75	MET
1	A	76	THR
1	A	79	LEU
1	A	85	ILE
1	A	94	LYS
1	A	98	ARG
1	A	122	GLN
1	A	126	ILE
1	A	131	LYS
1	A	174	VAL
1	A	179	ILE
1	A	184	LEU

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Mol	Chain	Res	Type
1	A	212	LEU
1	A	214	LYS
1	A	221	LEU
1	A	234	LEU
1	A	240	LYS
1	A	260	HIS
1	A	270	ARG
1	A	275	THR
1	A	291	LEU
1	A	295	GLN
1	A	300	LYS
1	A	306	LYS
1	A	314	GLU
1	A	317	LEU
1	A	322	LEU
1	A	324	VAL
1	A	336	GLU
1	A	346	LYS
1	A	351	VAL
1	A	354	ARG
1	A	357	LYS
1	A	375	ASP
1	A	376	THR
1	A	384	LEU
1	A	392	VAL
1	A	421	ASN
1	A	478	VAL
1	A	489	SER
1	A	502	LEU
1	A	547	GLU
1	B	24	LYS
1	B	26	LYS
1	B	28	LEU
1	B	38	MET
1	B	50	LEU
1	B	63	ILE
1	B	66	LEU
1	B	70	ARG
1	B	72	LEU
1	B	76	THR
1	B	79	LEU
1	B	89	GLN

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Mol	Chain	Res	Type
1	B	91	ARG
1	B	99	ILE
1	B	104	ILE
1	B	123	TYR
1	B	137	ILE
1	B	138	SER
1	B	146	ILE
1	B	165	ARG
1	B	167	LEU
1	B	179	ILE
1	B	184	LEU
1	B	197	ARG
1	B	203	ILE
1	B	224	LYS
1	B	235	ILE
1	B	243	THR
1	B	295	GLN
1	B	297	VAL
1	B	302	ILE
1	B	306	LYS
1	B	317	LEU
1	B	322	LEU
1	B	332	LEU
1	B	335	GLN
1	B	346	LYS
1	B	351	VAL
1	B	363	GLU
1	B	371	GLU
1	B	383	ILE
1	B	392	VAL
1	B	397	ARG
1	B	398	LEU
1	B	455	THR
1	B	461	THR
1	B	464	GLN
1	B	478	VAL
1	B	489	SER
1	B	492	LEU
1	B	524	ILE
1	B	554	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	35	ASN
1	A	46	GLN
1	A	61	GLN
1	A	122	GLN
1	A	209	ASN
1	A	249	ASN
1	A	253	GLN
1	A	330	ASN
1	A	338	GLN
1	A	482	ASN
1	A	501	GLN
1	A	518	ASN
1	B	61	GLN
1	B	249	ASN
1	B	259	ASN
1	B	295	GLN
1	B	338	GLN
1	B	367	HIS
1	B	382	ASN
1	B	464	GLN
1	B	485	HIS
1	B	501	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	601	-	46,48,48	1.23	7 (15%)	64,73,73	1.64	12 (18%)
2	NAD	A	602	-	46,48,48	1.20	6 (13%)	64,73,73	1.56	11 (17%)
2	NAD	B	602	-	46,48,48	1.24	6 (13%)	64,73,73	1.59	12 (18%)
2	NAD	A	601	-	46,48,48	1.25	7 (15%)	64,73,73	1.62	13 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	601	-	-	8/30/62/62	0/5/5/5
2	NAD	A	602	-	-	17/30/62/62	0/5/5/5
2	NAD	B	602	-	-	11/30/62/62	0/5/5/5
2	NAD	A	601	-	-	13/30/62/62	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	NAD	C5A-C4A	4.71	1.47	1.39
2	A	601	NAD	C5A-C4A	4.64	1.47	1.39
2	B	601	NAD	C5A-C4A	4.63	1.47	1.39
2	A	602	NAD	C5A-C4A	4.54	1.47	1.39
2	B	601	NAD	C5A-C6A	2.81	1.48	1.41
2	A	601	NAD	C5A-C6A	2.79	1.48	1.41
2	B	602	NAD	C5A-C6A	2.78	1.48	1.41
2	A	602	NAD	C5A-C6A	2.71	1.48	1.41
2	A	601	NAD	PA-O3	2.54	1.62	1.59
2	B	602	NAD	C8A-N7A	2.45	1.36	1.31
2	B	601	NAD	C8A-N7A	2.40	1.36	1.31
2	B	602	NAD	O4D-C1D	2.39	1.44	1.40
2	A	602	NAD	C8A-N7A	2.38	1.36	1.31
2	A	601	NAD	C8A-N7A	2.36	1.36	1.31
2	A	602	NAD	C5A-N7A	-2.36	1.34	1.39
2	A	601	NAD	PN-O3	2.35	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	NAD	C5A-N7A	-2.30	1.34	1.39
2	B	601	NAD	C5A-N7A	-2.27	1.34	1.39
2	B	601	NAD	O4D-C1D	2.26	1.43	1.40
2	A	601	NAD	C5A-N7A	-2.25	1.35	1.39
2	B	601	NAD	PN-O3	2.21	1.61	1.59
2	A	601	NAD	O4D-C1D	2.20	1.43	1.40
2	A	602	NAD	C4A-N9A	-2.09	1.33	1.37
2	B	602	NAD	C4A-N9A	-2.06	1.33	1.37
2	A	602	NAD	O4D-C1D	2.06	1.43	1.40
2	B	601	NAD	PA-O3	2.03	1.61	1.59

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAD	C5A-C4A-N3A	-5.71	118.85	126.72
2	A	601	NAD	C5A-C4A-N3A	-5.68	118.90	126.72
2	B	602	NAD	C5A-C4A-N3A	-5.39	119.29	126.72
2	A	602	NAD	C5A-C4A-N3A	-5.34	119.37	126.72
2	B	601	NAD	N3A-C4A-N9A	4.50	134.82	127.17
2	A	601	NAD	N3A-C4A-N9A	4.46	134.76	127.17
2	A	602	NAD	N3A-C4A-N9A	4.23	134.36	127.17
2	B	602	NAD	N3A-C4A-N9A	4.22	134.34	127.17
2	B	602	NAD	N3A-C2A-N1A	-3.95	122.61	128.58
2	B	601	NAD	C2A-N3A-C4A	3.94	121.44	111.83
2	A	601	NAD	C2A-N3A-C4A	3.92	121.40	111.83
2	A	601	NAD	N3A-C2A-N1A	-3.92	122.65	128.58
2	A	602	NAD	N3A-C2A-N1A	-3.88	122.71	128.58
2	B	601	NAD	N3A-C2A-N1A	-3.87	122.72	128.58
2	B	602	NAD	C2A-N3A-C4A	3.85	121.24	111.83
2	A	602	NAD	C2A-N3A-C4A	3.80	121.11	111.83
2	B	601	NAD	C4A-C5A-N7A	-3.62	106.44	110.58
2	B	602	NAD	C4A-C5A-N7A	-3.54	106.53	110.58
2	A	601	NAD	C4A-C5A-N7A	-3.51	106.57	110.58
2	A	602	NAD	C4A-C5A-N7A	-3.42	106.67	110.58
2	A	602	NAD	C4D-O4D-C1D	-3.04	107.14	109.92
2	A	602	NAD	C4A-N9A-C8A	2.96	108.85	105.74
2	B	601	NAD	C4A-N9A-C8A	2.92	108.80	105.74
2	B	602	NAD	C4A-N9A-C8A	2.92	108.80	105.74
2	B	601	NAD	O4B-C1B-N9A	2.88	113.62	108.09
2	B	601	NAD	C5A-N7A-C8A	2.81	107.86	103.45
2	A	601	NAD	C5A-N7A-C8A	2.76	107.78	103.45
2	A	601	NAD	C4A-N9A-C8A	2.73	108.60	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	NAD	C5A-N7A-C8A	2.68	107.66	103.45
2	B	602	NAD	C4D-O4D-C1D	2.66	112.36	109.92
2	A	602	NAD	C5A-N7A-C8A	2.62	107.57	103.45
2	B	602	NAD	C6A-C5A-N7A	2.44	136.79	132.09
2	A	602	NAD	C6A-C5A-N7A	2.37	136.66	132.09
2	B	601	NAD	N9A-C8A-N7A	-2.37	110.58	113.94
2	B	601	NAD	C6A-C5A-N7A	2.36	136.63	132.09
2	B	602	NAD	N9A-C8A-N7A	-2.33	110.64	113.94
2	A	602	NAD	N9A-C8A-N7A	-2.33	110.64	113.94
2	A	601	NAD	N9A-C8A-N7A	-2.28	110.69	113.94
2	A	601	NAD	C6A-C5A-N7A	2.28	136.48	132.09
2	B	602	NAD	C2A-N1A-C6A	2.25	122.42	118.73
2	B	601	NAD	C4D-O4D-C1D	2.24	111.98	109.92
2	A	601	NAD	C3N-C7N-N7N	2.23	120.48	117.74
2	A	602	NAD	C2A-N1A-C6A	2.19	122.32	118.73
2	A	601	NAD	C6N-N1N-C2N	-2.17	120.03	121.88
2	A	601	NAD	C2A-N1A-C6A	2.16	122.28	118.73
2	B	601	NAD	C2A-N1A-C6A	2.10	122.19	118.73
2	A	601	NAD	O4B-C1B-N9A	2.10	112.13	108.09
2	B	602	NAD	C6N-N1N-C2N	-2.06	120.13	121.88

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAD	C5B-O5B-PA-O1A
2	A	601	NAD	C5D-O5D-PN-O3
2	A	601	NAD	C5D-O5D-PN-O2N
2	A	601	NAD	O4D-C1D-N1N-C2N
2	A	601	NAD	O4D-C1D-N1N-C6N
2	A	602	NAD	C5B-O5B-PA-O1A
2	A	602	NAD	C5B-O5B-PA-O3
2	A	602	NAD	C5D-O5D-PN-O3
2	A	602	NAD	C5D-O5D-PN-O1N
2	A	602	NAD	O4D-C1D-N1N-C2N
2	B	601	NAD	C5D-O5D-PN-O1N
2	B	601	NAD	C2N-C3N-C7N-O7N
2	B	601	NAD	C2N-C3N-C7N-N7N
2	B	602	NAD	C5B-O5B-PA-O1A
2	B	602	NAD	O4D-C1D-N1N-C2N
2	B	601	NAD	C4N-C3N-C7N-O7N
2	B	601	NAD	C4N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
2	A	602	NAD	O4D-C4D-C5D-O5D
2	A	602	NAD	C3D-C4D-C5D-O5D
2	B	602	NAD	C3D-C4D-C5D-O5D
2	B	602	NAD	C2N-C3N-C7N-O7N
2	B	602	NAD	C2N-C3N-C7N-N7N
2	A	602	NAD	C3B-C4B-C5B-O5B
2	B	602	NAD	O4D-C4D-C5D-O5D
2	B	602	NAD	C4N-C3N-C7N-N7N
2	B	602	NAD	C4N-C3N-C7N-O7N
2	A	602	NAD	O4B-C4B-C5B-O5B
2	A	602	NAD	C4D-C5D-O5D-PN
2	B	601	NAD	O4B-C4B-C5B-O5B
2	A	601	NAD	PN-O3-PA-O1A
2	A	602	NAD	PA-O3-PN-O1N
2	A	601	NAD	C4D-C5D-O5D-PN
2	A	601	NAD	C5B-O5B-PA-O2A
2	A	601	NAD	C5B-O5B-PA-O3
2	A	602	NAD	C5B-O5B-PA-O2A
2	A	602	NAD	C5D-O5D-PN-O2N
2	B	602	NAD	C5B-O5B-PA-O2A
2	B	602	NAD	C5B-O5B-PA-O3
2	B	602	NAD	C5D-O5D-PN-O1N
2	A	601	NAD	PN-O3-PA-O2A
2	A	601	NAD	C2D-C1D-N1N-C2N
2	A	601	NAD	C2D-C1D-N1N-C6N
2	B	601	NAD	O4D-C4D-C5D-O5D
2	A	602	NAD	C4N-C3N-C7N-N7N
2	A	602	NAD	O4D-C1D-N1N-C6N
2	A	602	NAD	C4N-C3N-C7N-O7N
2	A	602	NAD	PA-O3-PN-O2N
2	B	601	NAD	PA-O3-PN-O1N
2	A	601	NAD	O4B-C4B-C5B-O5B

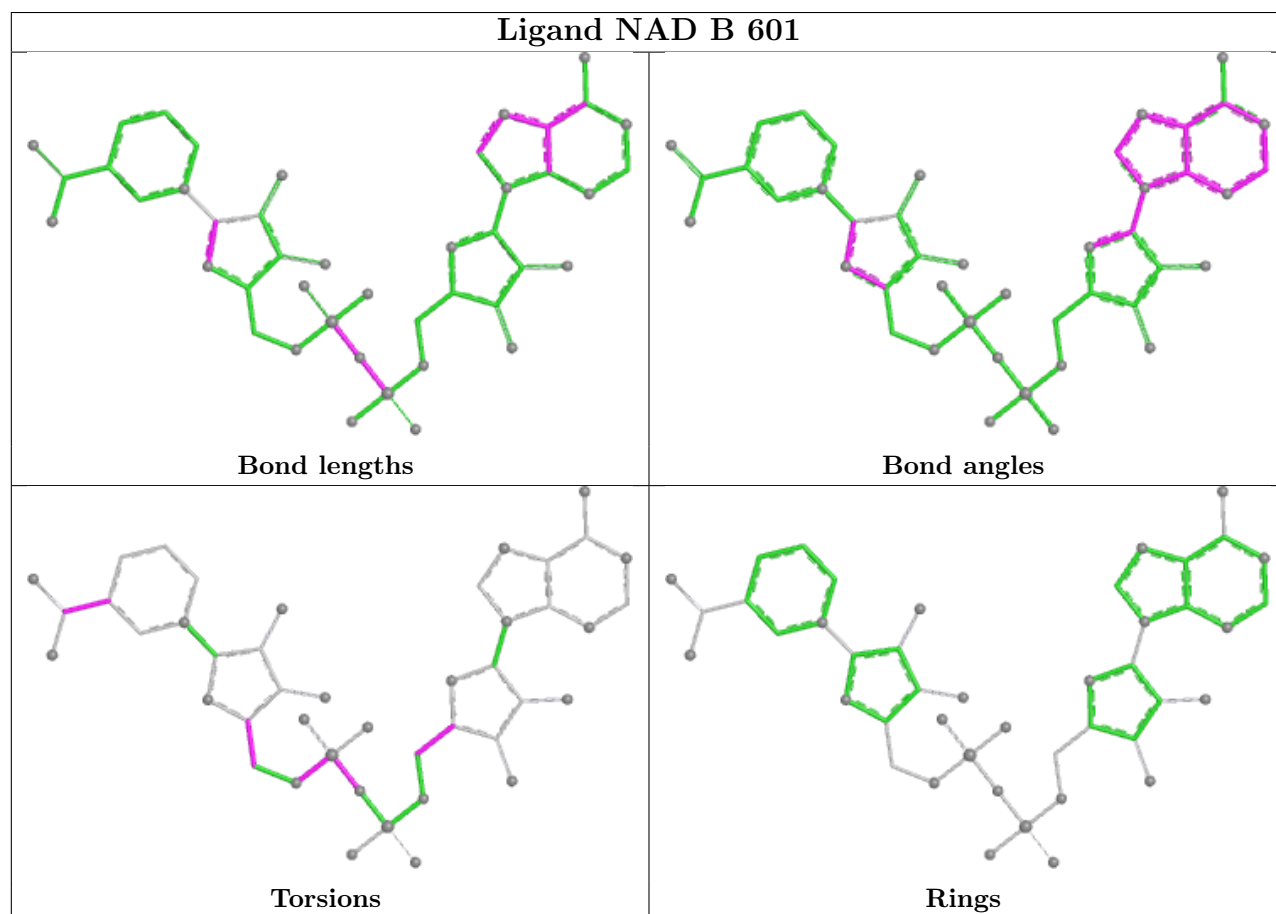
There are no ring outliers.

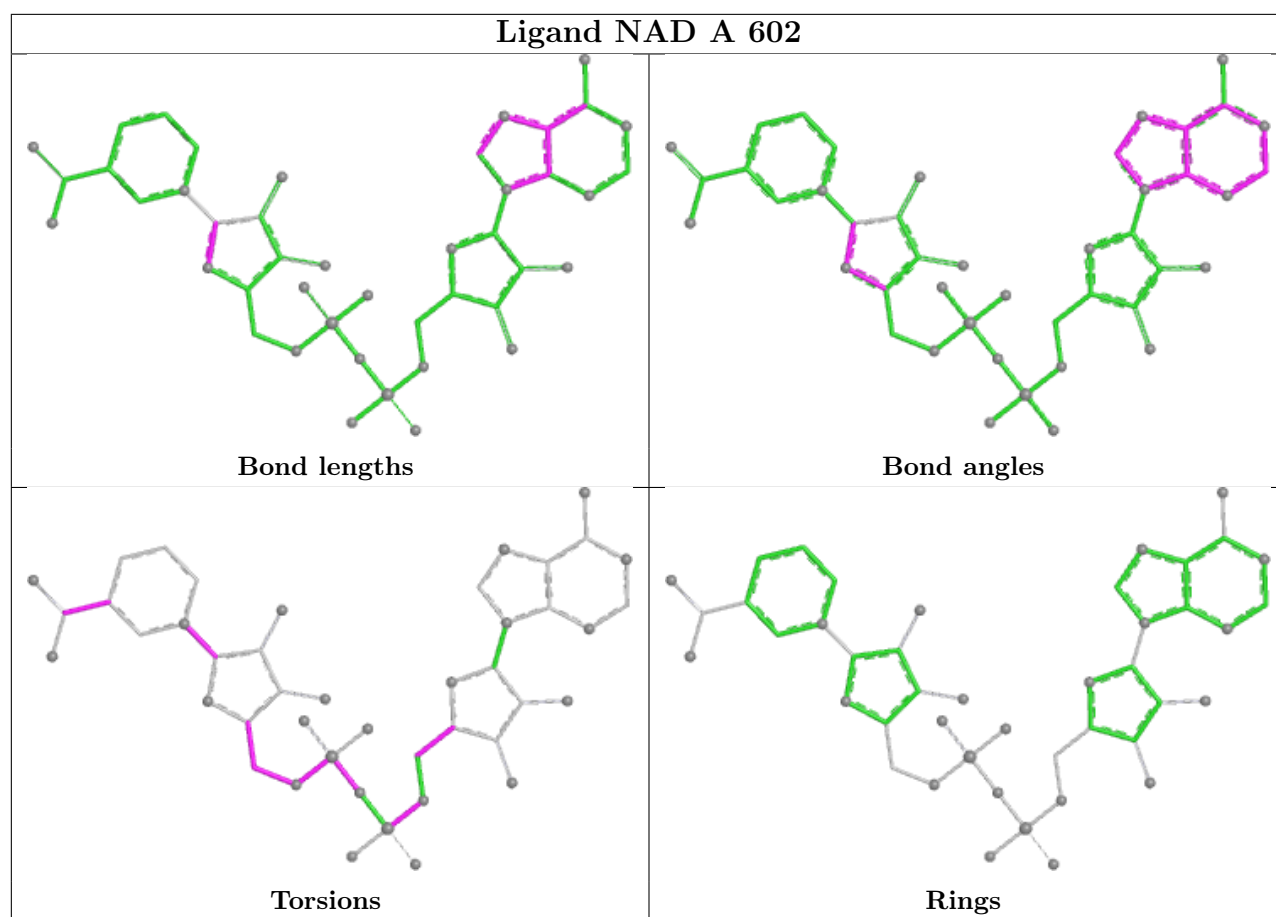
1 monomer is involved in 1 short contact:

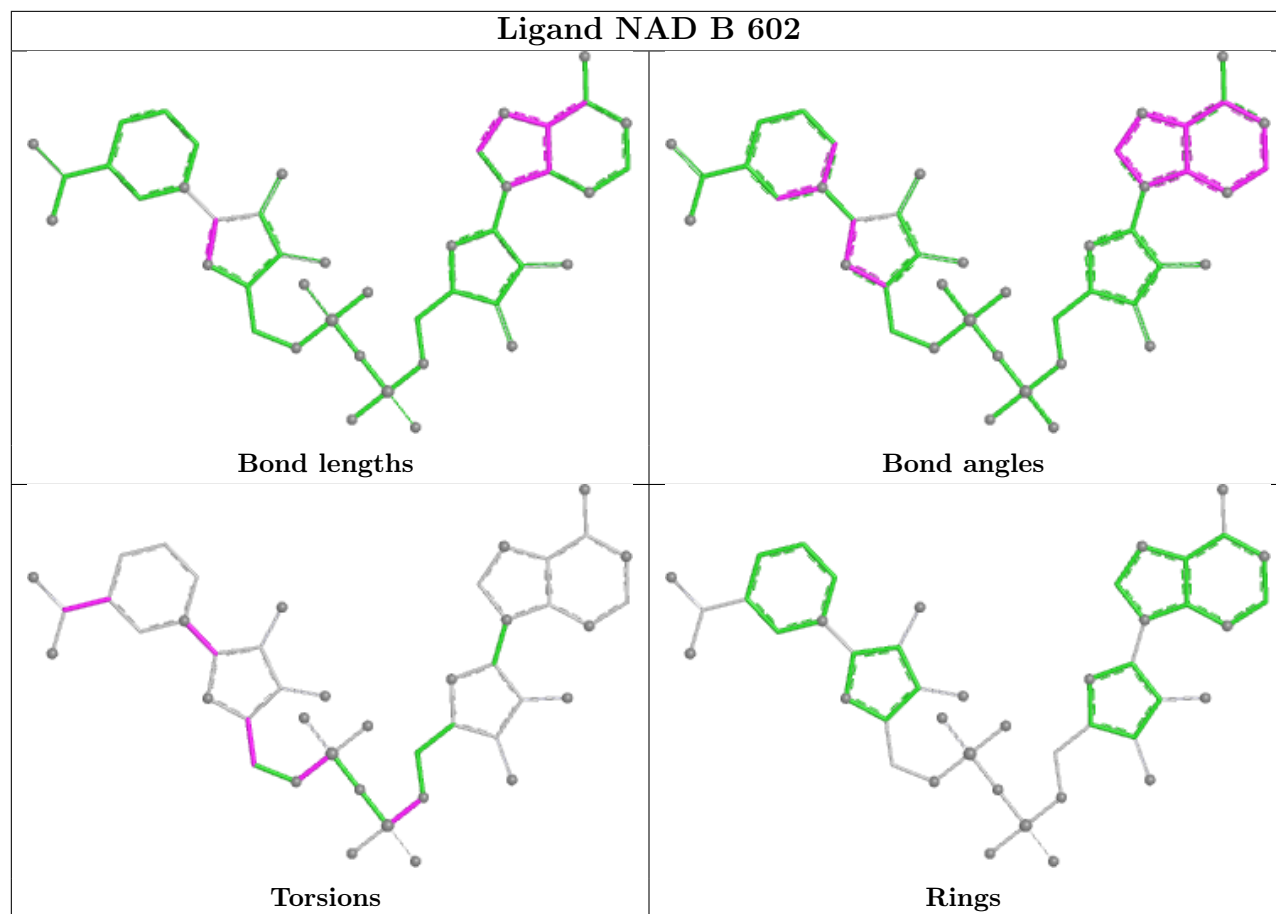
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	NAD	1	0

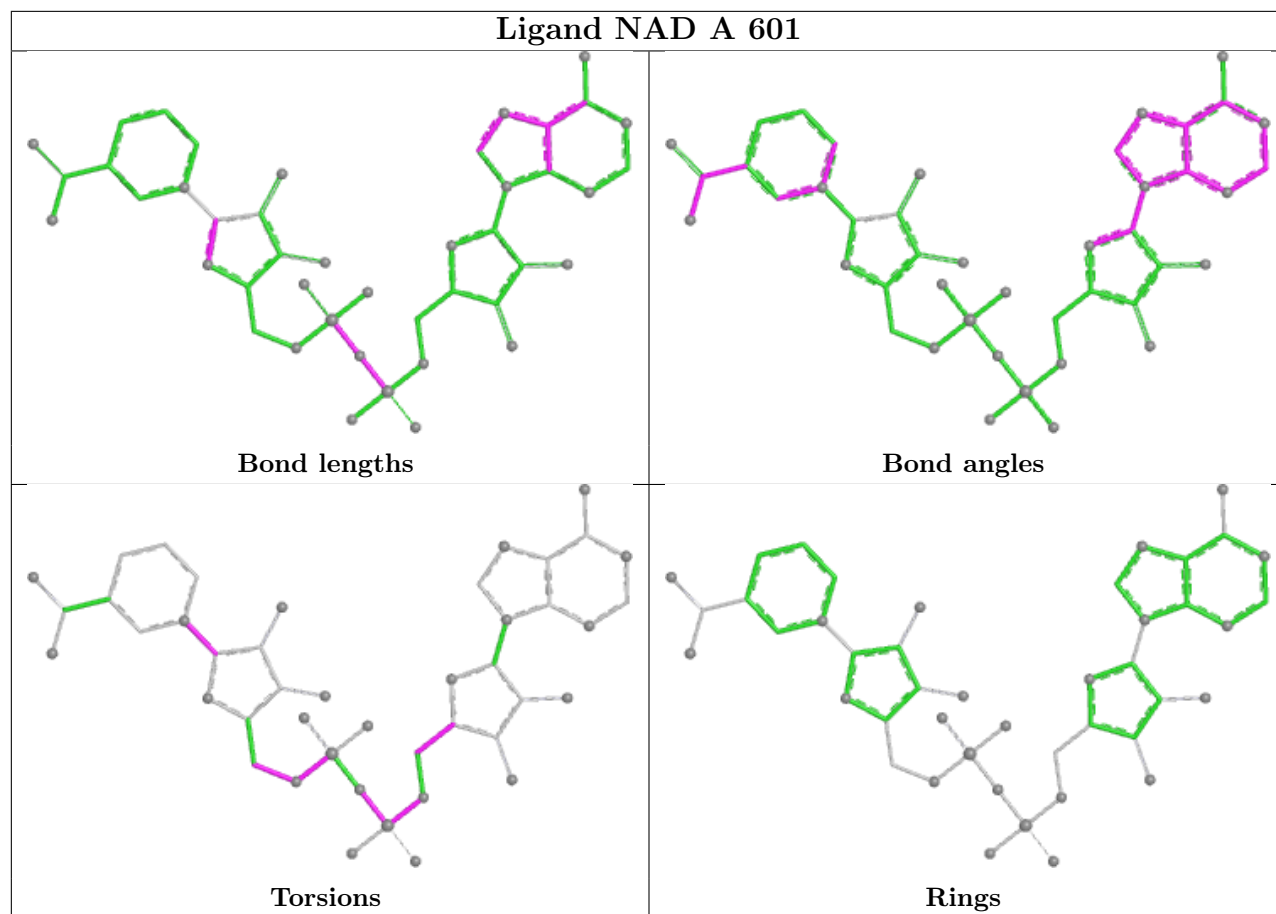
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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	543/566 (95%)	0.72	44 (8%)	18 17	22, 35, 58, 78	0
1	B	551/566 (97%)	0.72	44 (7%)	18 18	24, 37, 62, 76	0
All	All	1094/1132 (96%)	0.72	88 (8%)	18 18	22, 36, 61, 78	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	123	TYR	5.7
1	A	421	ASN	4.9
1	A	123	TYR	4.8
1	A	124	GLY	4.4
1	B	298	ILE	4.0
1	B	421	ASN	3.8
1	A	263	PHE	3.7
1	A	122	GLN	3.5
1	A	126	ILE	3.5
1	B	455	THR	3.3
1	B	383	ILE	3.3
1	A	543	TYR	3.0
1	B	126	ILE	2.9
1	B	302	ILE	2.9
1	B	353	GLY	2.9
1	A	85	ILE	2.8
1	A	76	THR	2.8
1	A	249	ASN	2.7
1	B	99	ILE	2.7
1	A	174	VAL	2.7
1	A	68	PHE	2.6
1	B	68	PHE	2.6
1	A	118	LEU	2.6
1	B	167	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	432	GLU	2.6
1	A	127	PHE	2.6
1	B	127	PHE	2.6
1	A	212	LEU	2.5
1	A	120	CYS	2.5
1	A	211	ALA	2.5
1	A	372	SER	2.5
1	B	435	THR	2.5
1	B	361	TYR	2.5
1	A	69	HIS	2.5
1	A	210	ILE	2.5
1	A	169	LEU	2.5
1	A	121	SER	2.5
1	B	422	PRO	2.4
1	A	425	GLN	2.4
1	B	464	GLN	2.4
1	A	173	GLY	2.4
1	B	375	ASP	2.4
1	A	347	TYR	2.4
1	B	547	GLU	2.4
1	A	213	LEU	2.4
1	A	24	LYS	2.4
1	A	424	ALA	2.4
1	B	371	GLU	2.4
1	B	357	LYS	2.3
1	A	356	ALA	2.3
1	A	422	PRO	2.3
1	B	76	THR	2.3
1	A	257	PHE	2.3
1	B	125	HIS	2.3
1	A	358	ILE	2.3
1	B	456	ASP	2.3
1	A	536	ALA	2.2
1	A	214	LYS	2.2
1	B	409	SER	2.2
1	B	328	VAL	2.2
1	A	41	THR	2.2
1	B	373	ILE	2.2
1	B	393	ALA	2.2
1	A	260	HIS	2.2
1	B	453	LYS	2.2
1	B	573	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	337	ALA	2.2
1	B	458	ARG	2.2
1	A	125	HIS	2.1
1	B	369	ALA	2.1
1	B	501	GLN	2.1
1	B	544	PRO	2.1
1	B	69	HIS	2.1
1	A	170	GLY	2.1
1	B	372	SER	2.1
1	A	47	MET	2.1
1	A	541	PHE	2.1
1	A	205	VAL	2.1
1	B	454	LEU	2.1
1	B	351	VAL	2.1
1	B	72	LEU	2.1
1	A	131	LYS	2.1
1	B	335	GLN	2.0
1	A	373	ILE	2.0
1	B	461	THR	2.0
1	A	79	LEU	2.0
1	B	63	ILE	2.0
1	B	370	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	A	601	44/44	0.60	0.24	68,90,110,110	0

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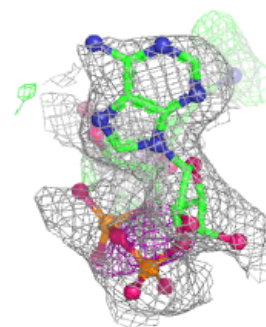
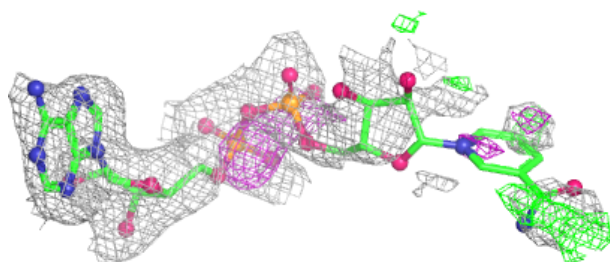
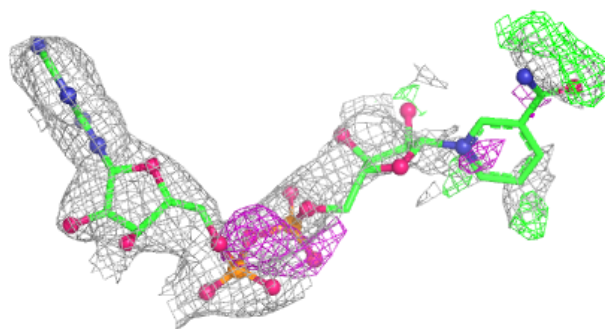
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	B	601	44/44	0.73	0.21	65,90,115,115	0
2	NAD	B	602	44/44	0.80	0.20	40,58,102,103	0
2	NAD	A	602	44/44	0.83	0.16	40,59,93,94	0

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.

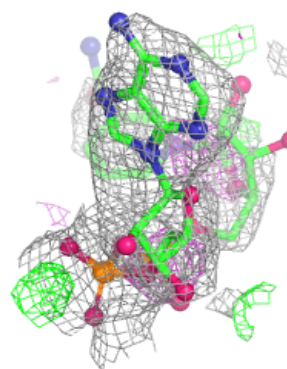
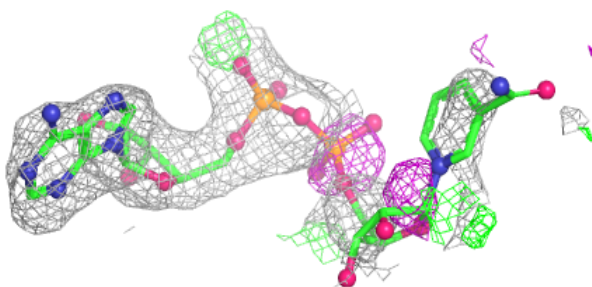
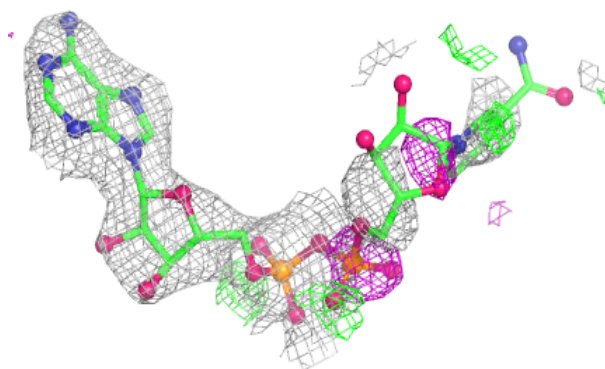
Electron density around NAD A 601:

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



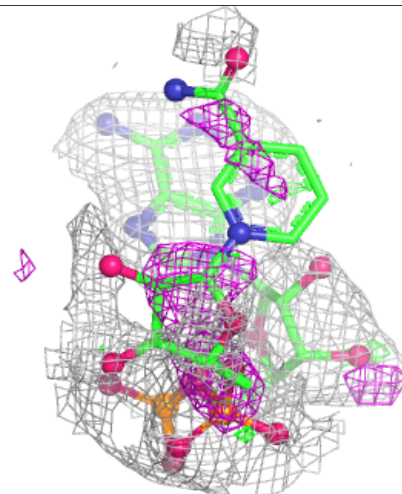
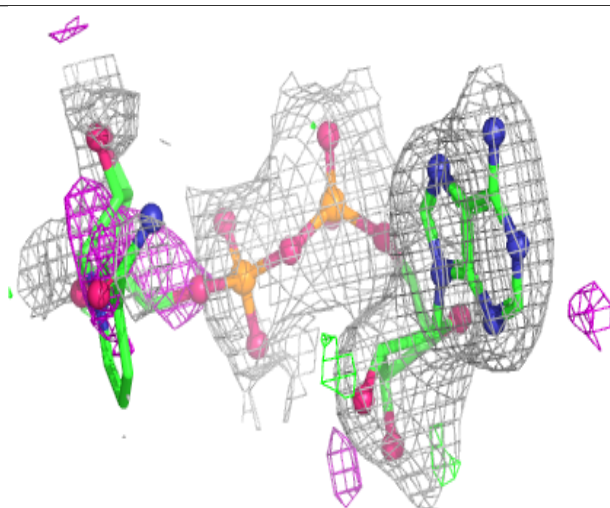
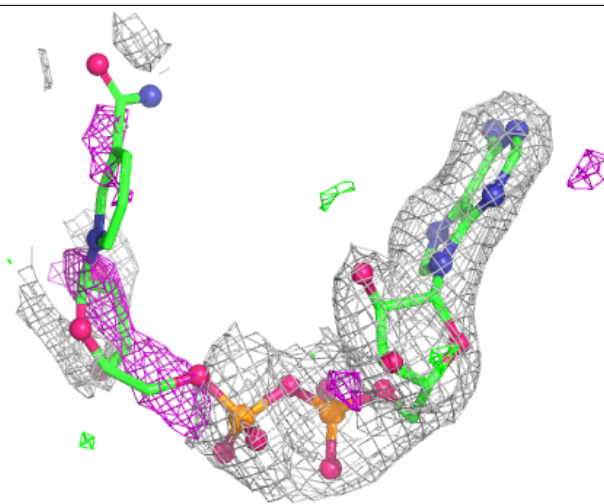
Electron density around NAD B 601:

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



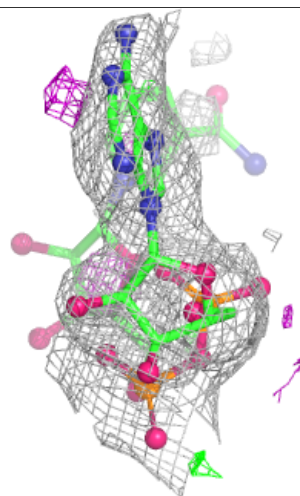
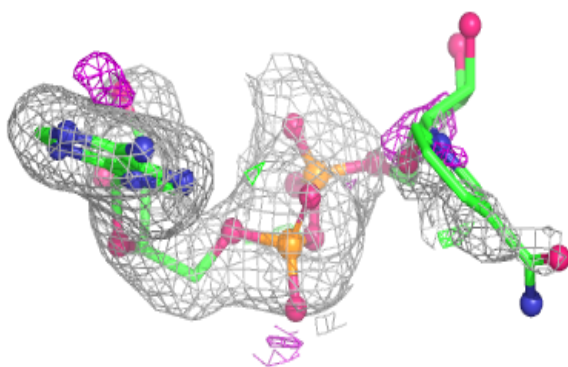
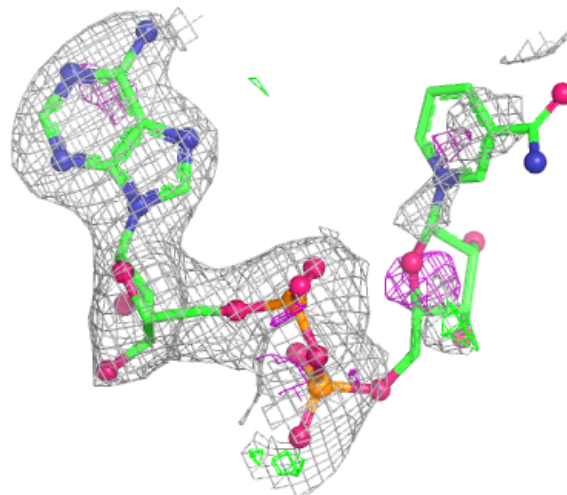
Electron density around NAD B 602:

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



Electron density around NAD A 602:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.