



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:55 AM UTC

PDB ID : 7BSK / pdb_00007bsk
Title : Crystal structure of human ME2 R67Q 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

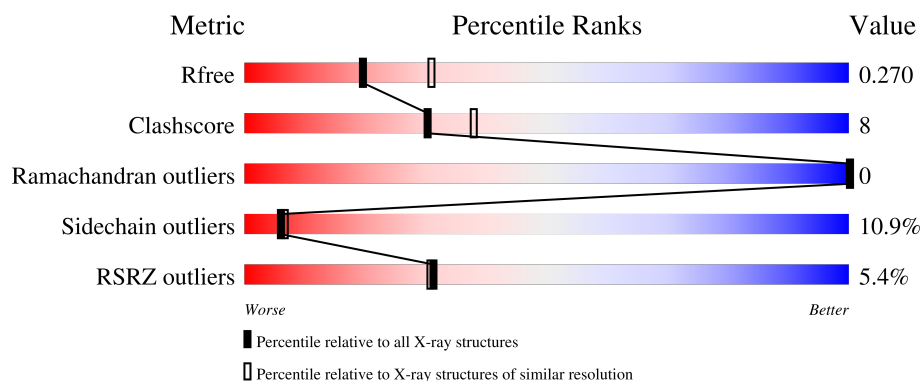
1 Overall quality at a glance

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	6% 72% 20% • •
1	B	566	5% 77% 17% • •

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		

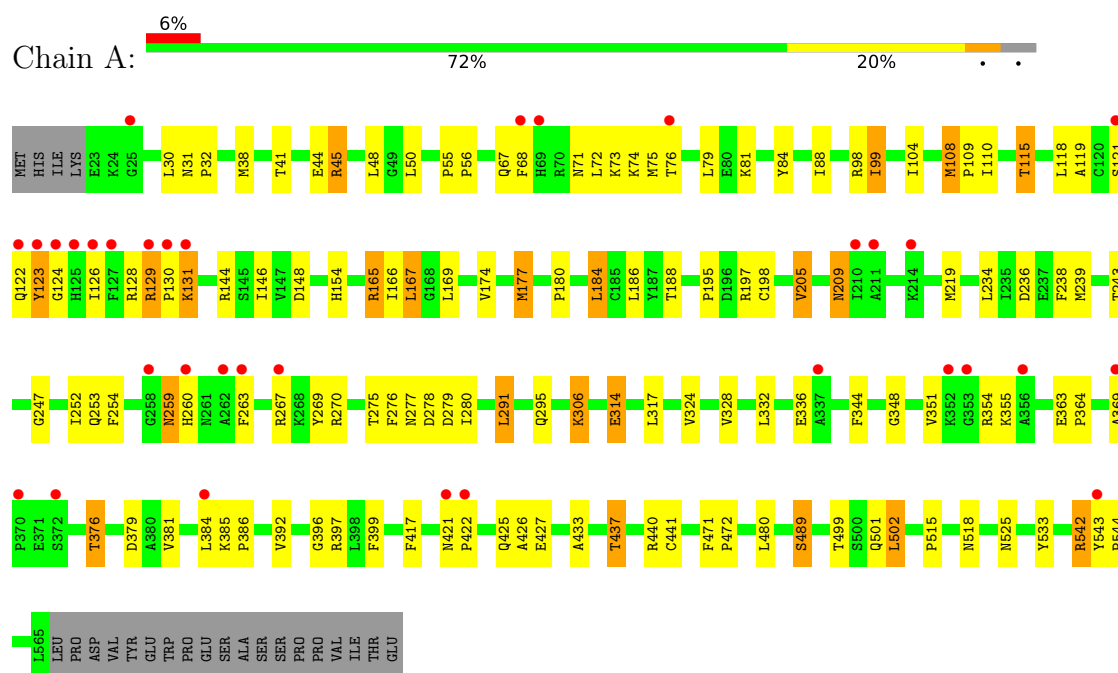
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		
3	B	52	Total	O	0	0
			52	52		

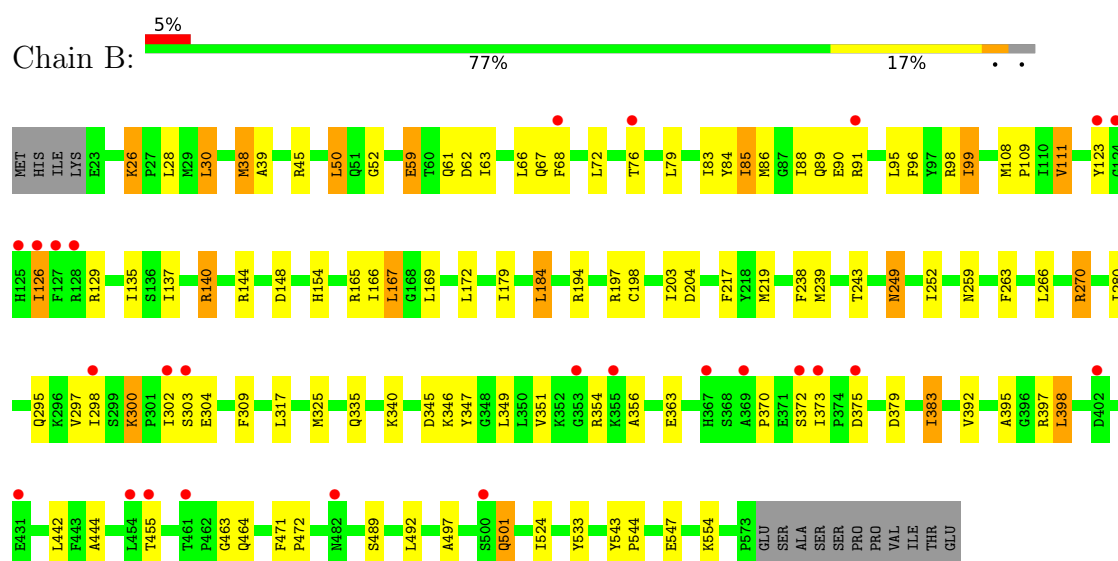
3 Residue-property plots [i](#)

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	117.85Å 191.41Å 58.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 2.55 29.48 – 2.55	Depositor EDS
% Data completeness (in resolution range)	90.2 (29.48-2.55) 90.2 (29.48-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.226 , 0.278 0.226 , 0.270	Depositor DCC
R_{free} test set	1999 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 18.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8893	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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	1.01	0/4365	1.46	1/5907 (0.0%)
1	B	1.02	0/4442	1.44	2/6016 (0.0%)
All	All	1.01	0/8807	1.45	3/11923 (0.0%)

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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	GLY	CA-C-O	-6.57	117.95	122.22
1	B	300	LYS	CA-C-N	6.34	127.77	119.84
1	B	300	LYS	C-N-CA	6.34	127.77	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	309	PHE	Peptide

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	4276	0	4315	81	0
1	B	4348	0	4378	71	0
2	A	88	0	52	0	0
2	B	88	0	52	6	0
3	A	41	0	0	1	0
3	B	52	0	0	0	0
All	All	8893	0	8797	147	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 8.

All (147) 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:263:PHE:CD1	1:A:280:ILE:HD11	2.04	0.93
1:B:259:ASN:HD21	2:B:601:NAD:C5N	1.83	0.91
1:B:239:MET:HE1	1:B:252:ILE:HG21	1.55	0.89
1:B:259:ASN:ND2	2:B:601:NAD:C5N	2.36	0.88
1:A:154:HIS:O	1:A:197:ARG:HG2	1.77	0.84
1:A:501:GLN:HE22	1:A:525:ASN:HD22	1.27	0.83
1:B:68:PHE:CD2	1:B:99:ILE:HD12	2.14	0.83
1:B:137:ILE:O	1:B:140:ARG:HG2	1.80	0.80
1:A:109:PRO:O	1:A:115:THR:HG23	1.81	0.80
1:B:61:GLN:NE2	1:B:98:ARG:HG3	1.96	0.80
1:B:303:SER:HA	1:B:340:LYS:HE2	1.66	0.78
1:B:154:HIS:O	1:B:197:ARG:HD3	1.83	0.77
1:B:85:ILE:HG13	1:B:99:ILE:HD11	1.64	0.77
1:B:68:PHE:CD1	1:B:88:ILE:HD11	2.19	0.77
1:B:68:PHE:CE1	1:B:88:ILE:HD11	2.22	0.74
1:A:279:ASP:OD1	3:A:701:HOH:O	2.05	0.73
1:A:239:MET:HE1	1:A:252:ILE:HG21	1.70	0.73
1:B:68:PHE:CE1	1:B:84:TYR:CE2	2.76	0.73
1:A:396:GLY:HA2	1:A:425:GLN:HA	1.74	0.69
1:A:68:PHE:CZ	1:A:72:LEU:HD22	2.27	0.69
1:A:238:PHE:CD2	1:A:239:MET:HE2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLN:HG2	1:B:217:PHE:CG	2.30	0.67
1:B:144:ARG:NH1	1:B:148:ASP:OD1	2.28	0.67
1:A:124:GLY:O	1:A:128:ARG:NH2	2.27	0.66
1:A:165:ARG:O	1:A:165:ARG:NH1	2.29	0.65
1:B:83:ILE:HD11	1:B:123:TYR:CE2	2.31	0.65
1:B:62:ASP:OD1	1:B:98:ARG:NH2	2.29	0.64
1:A:129:ARG:HE	1:A:130:PRO:HD2	1.62	0.64
1:B:249:ASN:H	1:B:249:ASN:HD22	1.45	0.64
1:A:437:THR:HG21	1:A:441:CYS:HB3	1.80	0.64
1:B:259:ASN:ND2	2:B:601:NAD:H5N	2.10	0.64
1:B:83:ILE:HD11	1:B:123:TYR:CD2	2.33	0.63
1:B:68:PHE:CE1	1:B:88:ILE:CD1	2.83	0.61
1:A:277:ASN:HD22	1:A:280:ILE:H	1.47	0.61
1:A:433:ALA:O	1:A:437:THR:HB	2.00	0.61
1:B:38:MET:HB3	1:B:59:GLU:HG3	1.81	0.61
1:B:68:PHE:CE2	1:B:99:ILE:HD12	2.36	0.61
1:B:370:PRO:HG2	1:B:383:ILE:HD11	1.83	0.60
1:A:109:PRO:O	1:A:115:THR:CG2	2.49	0.60
1:B:68:PHE:CZ	1:B:84:TYR:CD2	2.89	0.59
1:B:95:LEU:O	1:B:99:ILE:HG23	2.02	0.59
1:A:31:ASN:HD22	1:A:32:PRO:HD2	1.68	0.59
1:B:184:LEU:HG	1:B:198:CYS:HB3	1.85	0.58
1:A:291:LEU:HD13	1:A:417:PHE:CE2	2.39	0.58
1:A:184:LEU:HG	1:A:198:CYS:HB3	1.86	0.58
1:A:68:PHE:CD1	1:A:88:ILE:HD11	2.39	0.57
1:A:177:MET:HA	1:A:177:MET:HE3	1.88	0.56
1:B:38:MET:HB3	1:B:59:GLU:CG	2.34	0.56
1:B:395:ALA:HB3	1:B:398:LEU:HD22	1.87	0.56
1:A:437:THR:HG21	1:A:441:CYS:CB	2.36	0.56
1:B:347:TYR:CD2	1:B:356:ALA:HB1	2.41	0.55
1:A:263:PHE:HB3	1:A:314:GLU:CD	2.31	0.55
1:B:300:LYS:HE3	1:B:304:GLU:HG2	1.90	0.54
1:B:259:ASN:HD21	2:B:601:NAD:C4N	2.21	0.54
1:B:61:GLN:HE21	1:B:98:ARG:HG3	1.73	0.53
1:A:259:ASN:HD22	1:A:259:ASN:N	2.07	0.53
1:B:68:PHE:CE1	1:B:84:TYR:CZ	2.97	0.52
1:B:68:PHE:CD1	1:B:88:ILE:CD1	2.91	0.52
1:A:41:THR:HG23	1:A:44:GLU:H	1.73	0.52
1:A:499:THR:O	1:A:502:LEU:HB2	2.10	0.52
1:A:238:PHE:CE2	1:A:239:MET:HE2	2.45	0.51
1:B:194:ARG:HG3	2:B:602:NAD:C6A	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASN:C	1:A:209:ASN:HD22	2.18	0.51
1:A:263:PHE:CD1	1:A:263:PHE:N	2.78	0.51
1:B:39:ALA:HA	1:B:59:GLU:O	2.10	0.51
1:A:79:LEU:HD21	1:A:122:GLN:OE1	2.11	0.51
1:A:165:ARG:HE	1:A:259:ASN:HD21	1.58	0.50
1:A:177:MET:O	1:A:180:PRO:HD2	2.11	0.50
1:B:45:ARG:HA	1:B:50:LEU:HB2	1.94	0.50
1:A:167:LEU:CD1	1:A:422:PRO:HG3	2.41	0.50
1:B:444:ALA:HA	1:B:463:GLY:O	2.12	0.50
1:A:144:ARG:NH1	1:A:148:ASP:OD1	2.44	0.49
1:A:146:ILE:HG23	1:B:52:GLY:HA3	1.95	0.49
1:A:68:PHE:CE2	1:A:99:ILE:HD12	2.48	0.49
1:A:489:SER:HB2	1:A:533:TYR:OH	2.12	0.49
1:B:165:ARG:O	1:B:165:ARG:HG3	2.12	0.49
1:B:379:ASP:O	1:B:383:ILE:HG23	2.13	0.49
1:A:263:PHE:HD1	1:A:280:ILE:HD11	1.71	0.49
1:B:86:MET:CE	1:B:111:VAL:HG22	2.43	0.49
1:B:543:TYR:HA	1:B:544:PRO:C	2.37	0.49
1:B:86:MET:HE3	1:B:111:VAL:HG22	1.94	0.48
1:A:68:PHE:CD1	1:A:88:ILE:CD1	2.97	0.48
1:B:166:ILE:HG13	1:B:172:LEU:HD12	1.95	0.48
1:A:471:PHE:CG	1:A:472:PRO:HD3	2.48	0.48
1:A:344:PHE:CZ	1:A:348:GLY:HA2	2.48	0.47
1:B:370:PRO:CG	1:B:383:ILE:HD11	2.45	0.47
1:A:68:PHE:CE1	1:A:84:TYR:CE2	3.02	0.47
1:B:108:MET:N	1:B:109:PRO:CD	2.78	0.47
1:B:68:PHE:CZ	1:B:84:TYR:CE2	3.02	0.47
1:B:489:SER:HB2	1:B:533:TYR:CZ	2.50	0.47
1:A:167:LEU:HD12	1:A:422:PRO:HG3	1.97	0.47
1:B:68:PHE:CE2	1:B:99:ILE:CD1	2.97	0.47
1:A:253:GLN:OE1	1:A:276:PHE:CE2	2.68	0.47
1:B:26:LYS:HG2	1:B:30:LEU:HD13	1.97	0.46
1:A:376:THR:HG22	1:A:379:ASP:H	1.80	0.46
1:B:266:LEU:O	1:B:270:ARG:HB2	2.15	0.46
1:A:56:PRO:HG2	1:B:204:ASP:OD2	2.16	0.46
1:A:55:PRO:HG2	1:B:219:MET:HE2	1.97	0.45
1:B:379:ASP:O	1:B:383:ILE:CG2	2.64	0.45
1:B:471:PHE:CG	1:B:472:PRO:HD3	2.52	0.45
1:A:205:VAL:O	1:A:205:VAL:CG1	2.65	0.45
1:A:169:LEU:HD22	1:A:169:LEU:N	2.31	0.44
1:A:399:PHE:CG	1:A:427:GLU:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:MET:N	1:A:109:PRO:HD2	2.33	0.44
1:A:131:LYS:HA	1:A:131:LYS:CE	2.48	0.44
1:B:325:MET:HE2	1:B:492:LEU:HD12	1.98	0.44
1:A:437:THR:CG2	1:A:441:CYS:H	2.31	0.44
1:A:104:ILE:O	1:A:108:MET:HB2	2.18	0.43
1:A:306:LYS:HB3	1:A:386:PRO:HA	2.00	0.43
1:A:71:ASN:ND2	1:B:126:ILE:HA	2.33	0.43
1:B:68:PHE:CD2	1:B:99:ILE:CD1	2.95	0.43
1:A:45:ARG:HA	1:A:50:LEU:HB2	2.00	0.43
1:A:128:ARG:HB2	1:A:219:MET:CE	2.49	0.43
1:A:328:VAL:HA	1:A:332:LEU:O	2.18	0.43
1:A:397:ARG:NH1	1:A:426:ALA:O	2.51	0.43
1:A:489:SER:HB2	1:A:533:TYR:CZ	2.54	0.43
1:A:236:ASP:OD1	1:A:269:TYR:OH	2.32	0.43
1:A:437:THR:O	1:A:437:THR:HG23	2.19	0.43
1:A:471:PHE:N	1:A:472:PRO:CD	2.82	0.43
1:A:437:THR:HG23	1:A:440:ARG:H	1.84	0.43
1:A:351:VAL:HG21	1:A:369:ALA:HA	2.00	0.42
1:B:345:ASP:HB2	2:B:601:NAD:O2B	2.19	0.42
1:A:515:PRO:HG2	1:A:518:ASN:HD22	1.84	0.42
1:A:381:VAL:O	1:A:385:LYS:HA	2.20	0.42
1:A:72:LEU:HD11	1:A:81:LYS:HG2	2.01	0.42
1:A:188:THR:HG21	1:A:195:PRO:HG3	2.00	0.42
1:A:131:LYS:HA	1:A:131:LYS:HE3	2.02	0.42
1:B:68:PHE:CE1	1:B:84:TYR:CD2	3.08	0.42
1:B:135:ILE:O	1:B:203:ILE:HA	2.20	0.42
1:A:344:PHE:CE2	1:A:348:GLY:HA2	2.54	0.42
1:B:90:GLU:OE1	1:B:129:ARG:NH1	2.52	0.42
1:B:266:LEU:O	1:B:270:ARG:CB	2.68	0.41
1:B:86:MET:HE1	1:B:96:PHE:CZ	2.55	0.41
1:A:68:PHE:CE1	1:A:88:ILE:HD12	2.55	0.41
1:A:363:GLU:N	1:A:364:PRO:HD2	2.36	0.41
1:A:239:MET:HE3	1:A:254:PHE:CZ	2.56	0.41
1:A:542:ARG:CD	1:A:542:ARG:C	2.93	0.41
1:A:543:TYR:HA	1:A:544:PRO:C	2.45	0.41
1:B:238:PHE:CE2	1:B:239:MET:HE2	2.56	0.41
1:B:298:ILE:HD11	1:B:442:LEU:HD12	2.03	0.41
1:A:110:ILE:HA	1:A:115:THR:CG2	2.52	0.40
1:A:263:PHE:O	1:A:267:ARG:HG3	2.21	0.40
1:B:263:PHE:CD1	1:B:280:ILE:HD11	2.56	0.40
1:B:167:LEU:HD12	1:B:167:LEU:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:ALA:O	1:B:501:GLN:HG3	2.21	0.40
1:A:119:ALA:O	1:A:123:TYR:HB2	2.21	0.40
1:B:165:ARG:O	1:B:165:ARG:CG	2.70	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%)	527 (96%)	22 (4%)	0	100	100
All	All	1090/1132 (96%)	1049 (96%)	41 (4%)	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	459/481 (95%)	407 (89%)	52 (11%)	5	6
1	B	467/481 (97%)	418 (90%)	49 (10%)	6	8
All	All	926/962 (96%)	825 (89%)	101 (11%)	6	7

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	38	MET
1	A	45	ARG
1	A	48	LEU
1	A	73	LYS
1	A	74	LYS
1	A	75	MET
1	A	76	THR
1	A	98	ARG
1	A	99	ILE
1	A	108	MET
1	A	115	THR
1	A	118	LEU
1	A	121	SER
1	A	123	TYR
1	A	126	ILE
1	A	129	ARG
1	A	131	LYS
1	A	165	ARG
1	A	166	ILE
1	A	167	LEU
1	A	174	VAL
1	A	177	MET
1	A	184	LEU
1	A	186	LEU
1	A	205	VAL
1	A	209	ASN
1	A	234	LEU
1	A	243	THR
1	A	259	ASN
1	A	260	HIS
1	A	270	ARG
1	A	275	THR
1	A	278	ASP
1	A	291	LEU
1	A	295	GLN
1	A	306	LYS
1	A	314	GLU
1	A	317	LEU
1	A	324	VAL
1	A	336	GLU
1	A	354	ARG
1	A	355	LYS

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Mol	Chain	Res	Type
1	A	376	THR
1	A	384	LEU
1	A	392	VAL
1	A	421	ASN
1	A	437	THR
1	A	480	LEU
1	A	489	SER
1	A	502	LEU
1	A	542	ARG
1	B	26	LYS
1	B	28	LEU
1	B	30	LEU
1	B	38	MET
1	B	50	LEU
1	B	59	GLU
1	B	63	ILE
1	B	66	LEU
1	B	67	GLN
1	B	72	LEU
1	B	76	THR
1	B	79	LEU
1	B	85	ILE
1	B	89	GLN
1	B	91	ARG
1	B	99	ILE
1	B	111	VAL
1	B	126	ILE
1	B	140	ARG
1	B	167	LEU
1	B	169	LEU
1	B	179	ILE
1	B	184	LEU
1	B	243	THR
1	B	249	ASN
1	B	270	ARG
1	B	295	GLN
1	B	297	VAL
1	B	302	ILE
1	B	317	LEU
1	B	335	GLN
1	B	346	LYS
1	B	349	LEU

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Mol	Chain	Res	Type
1	B	351	VAL
1	B	354	ARG
1	B	363	GLU
1	B	372	SER
1	B	373	ILE
1	B	375	ASP
1	B	383	ILE
1	B	392	VAL
1	B	397	ARG
1	B	398	LEU
1	B	455	THR
1	B	464	GLN
1	B	501	GLN
1	B	524	ILE
1	B	547	GLU
1	B	554	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	46	GLN
1	A	67	GLN
1	A	71	ASN
1	A	153	ASN
1	A	209	ASN
1	A	249	ASN
1	A	253	GLN
1	A	259	ASN
1	A	277	ASN
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	67	GLN
1	B	89	GLN
1	B	122	GLN
1	B	230	GLN
1	B	249	ASN
1	B	259	ASN

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Mol	Chain	Res	Type
1	B	338	GLN
1	B	482	ASN
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	602	-	46,48,48	1.28	6 (13%)	64,73,73	1.66	12 (18%)
2	NAD	B	601	-	46,48,48	1.21	7 (15%)	64,73,73	1.71	12 (18%)
2	NAD	A	601	-	46,48,48	1.34	7 (15%)	64,73,73	1.69	14 (21%)
2	NAD	A	602	-	46,48,48	1.24	7 (15%)	64,73,73	1.65	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	602	-	-	8/30/62/62	0/5/5/5
2	NAD	B	601	-	-	8/30/62/62	0/5/5/5
2	NAD	A	601	-	-	13/30/62/62	0/5/5/5
2	NAD	A	602	-	-	15/30/62/62	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	NAD	C5A-C4A	4.69	1.47	1.39
2	A	601	NAD	C5A-C4A	4.54	1.47	1.39
2	B	601	NAD	C5A-C4A	4.31	1.46	1.39
2	A	602	NAD	C5A-C4A	4.10	1.46	1.39
2	A	601	NAD	PA-O3	3.26	1.63	1.59
2	A	601	NAD	PN-O3	3.22	1.63	1.59
2	A	602	NAD	C5A-N7A	-2.98	1.33	1.39
2	B	602	NAD	C5A-C6A	2.90	1.49	1.41
2	B	602	NAD	O4D-C1D	2.86	1.44	1.40
2	B	602	NAD	C8A-N7A	2.72	1.36	1.31
2	A	601	NAD	C5A-C6A	2.56	1.48	1.41
2	B	601	NAD	C5A-C6A	2.51	1.48	1.41
2	A	602	NAD	C4A-N9A	-2.51	1.32	1.37
2	A	602	NAD	C8A-N7A	2.49	1.36	1.31
2	A	602	NAD	PN-O3	2.47	1.62	1.59
2	A	601	NAD	C8A-N7A	2.43	1.36	1.31
2	B	601	NAD	O4D-C1D	2.41	1.44	1.40
2	A	602	NAD	O4D-C1D	2.41	1.44	1.40
2	B	601	NAD	C5A-N7A	-2.39	1.34	1.39
2	B	602	NAD	C5A-N7A	-2.35	1.34	1.39
2	A	601	NAD	O4D-C1D	2.31	1.43	1.40
2	B	601	NAD	C8A-N7A	2.21	1.35	1.31
2	B	602	NAD	C4A-N9A	-2.16	1.33	1.37
2	A	601	NAD	C5A-N7A	-2.13	1.35	1.39
2	B	601	NAD	PN-O3	2.07	1.61	1.59
2	A	602	NAD	C5A-C6A	2.06	1.46	1.41
2	B	601	NAD	C4A-N9A	-2.04	1.33	1.37

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	NAD	C5A-C4A-N3A	-5.34	119.36	126.72
2	B	601	NAD	C5A-C4A-N3A	-5.13	119.66	126.72
2	A	602	NAD	C5A-C4A-N3A	-5.04	119.78	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NAD	C5A-C4A-N3A	-4.93	119.93	126.72
2	B	601	NAD	N3A-C4A-N9A	4.44	134.72	127.17
2	B	601	NAD	N3A-C2A-N1A	-4.31	122.06	128.58
2	A	601	NAD	N3A-C2A-N1A	-4.31	122.06	128.58
2	A	601	NAD	N3A-C4A-N9A	4.18	134.28	127.17
2	A	602	NAD	N3A-C4A-N9A	4.16	134.24	127.17
2	B	602	NAD	N3A-C2A-N1A	-4.06	122.43	128.58
2	A	602	NAD	N3A-C2A-N1A	-4.02	122.50	128.58
2	B	602	NAD	C2A-N3A-C4A	3.91	121.38	111.83
2	B	602	NAD	C4A-C5A-N7A	-3.87	106.15	110.58
2	B	601	NAD	C2A-N3A-C4A	3.87	121.27	111.83
2	A	601	NAD	C2A-N3A-C4A	3.77	121.05	111.83
2	B	602	NAD	N3A-C4A-N9A	3.73	133.51	127.17
2	A	602	NAD	C2A-N3A-C4A	3.62	120.68	111.83
2	A	602	NAD	C4D-O4D-C1D	-3.52	106.70	109.92
2	B	601	NAD	C4A-N9A-C8A	3.51	109.43	105.74
2	A	601	NAD	C4A-N9A-C8A	3.51	109.42	105.74
2	A	602	NAD	C4A-N9A-C8A	3.21	109.11	105.74
2	B	601	NAD	O4B-C1B-N9A	3.20	114.24	108.09
2	A	601	NAD	C4A-C5A-N7A	-3.19	106.94	110.58
2	A	602	NAD	O4B-C1B-N9A	-3.14	102.06	108.09
2	B	602	NAD	C6N-N1N-C2N	-3.05	119.28	121.88
2	B	601	NAD	C4A-C5A-N7A	-3.05	107.10	110.58
2	B	601	NAD	C4D-O4D-C1D	2.89	112.58	109.92
2	A	601	NAD	C6N-N1N-C2N	-2.89	119.42	121.88
2	A	602	NAD	C4A-C5A-N7A	-2.88	107.28	110.58
2	A	602	NAD	C2B-C1B-N9A	2.75	120.14	113.30
2	B	602	NAD	C5A-N7A-C8A	2.74	107.76	103.45
2	B	602	NAD	C6A-C5A-N7A	2.70	137.30	132.09
2	A	601	NAD	C5A-N7A-C8A	2.66	107.63	103.45
2	A	601	NAD	C4D-O4D-C1D	-2.65	107.50	109.92
2	A	601	NAD	N9A-C8A-N7A	-2.63	110.21	113.94
2	B	601	NAD	C5A-N7A-C8A	2.60	107.53	103.45
2	A	601	NAD	C2A-N1A-C6A	2.58	122.97	118.73
2	B	601	NAD	N9A-C8A-N7A	-2.55	110.32	113.94
2	A	601	NAD	C6A-C5A-N7A	2.52	136.95	132.09
2	B	601	NAD	C2A-N1A-C6A	2.45	122.75	118.73
2	B	602	NAD	C4A-N9A-C8A	2.40	108.26	105.74
2	A	602	NAD	N9A-C8A-N7A	-2.38	110.56	113.94
2	B	602	NAD	C2A-N1A-C6A	2.35	122.59	118.73
2	B	601	NAD	C6A-C5A-N7A	2.30	136.51	132.09
2	A	602	NAD	C5A-N7A-C8A	2.29	107.05	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	NAD	N9A-C8A-N7A	-2.29	110.69	113.94
2	A	601	NAD	C4A-N9A-C1B	-2.27	121.32	126.63
2	B	602	NAD	C2B-C1B-N9A	2.19	118.74	113.30
2	A	602	NAD	C2A-N1A-C6A	2.17	122.29	118.73
2	A	601	NAD	O7N-C7N-N7N	-2.13	119.54	122.62
2	A	602	NAD	C6A-C5A-N7A	2.03	136.01	132.09

There are no chirality outliers.

All (44) 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-O1N
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	601	NAD	C2D-C1D-N1N-C2N
2	A	601	NAD	C2D-C1D-N1N-C6N
2	A	602	NAD	C5B-O5B-PA-O1A
2	A	602	NAD	C5B-O5B-PA-O2A
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	C3D-C4D-C5D-O5D
2	A	602	NAD	O4D-C1D-N1N-C2N
2	A	602	NAD	O4D-C1D-N1N-C6N
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	C5D-O5D-PN-O1N
2	B	602	NAD	C2D-C1D-N1N-C2N
2	B	602	NAD	C2D-C1D-N1N-C6N
2	B	601	NAD	C4N-C3N-C7N-N7N
2	B	601	NAD	C4N-C3N-C7N-O7N
2	A	602	NAD	O4B-C4B-C5B-O5B
2	A	602	NAD	C3B-C4B-C5B-O5B
2	A	602	NAD	O4D-C4D-C5D-O5D
2	B	601	NAD	O4B-C4B-C5B-O5B
2	B	601	NAD	O4D-C4D-C5D-O5D
2	B	601	NAD	C3D-C4D-C5D-O5D
2	B	602	NAD	O4D-C4D-C5D-O5D

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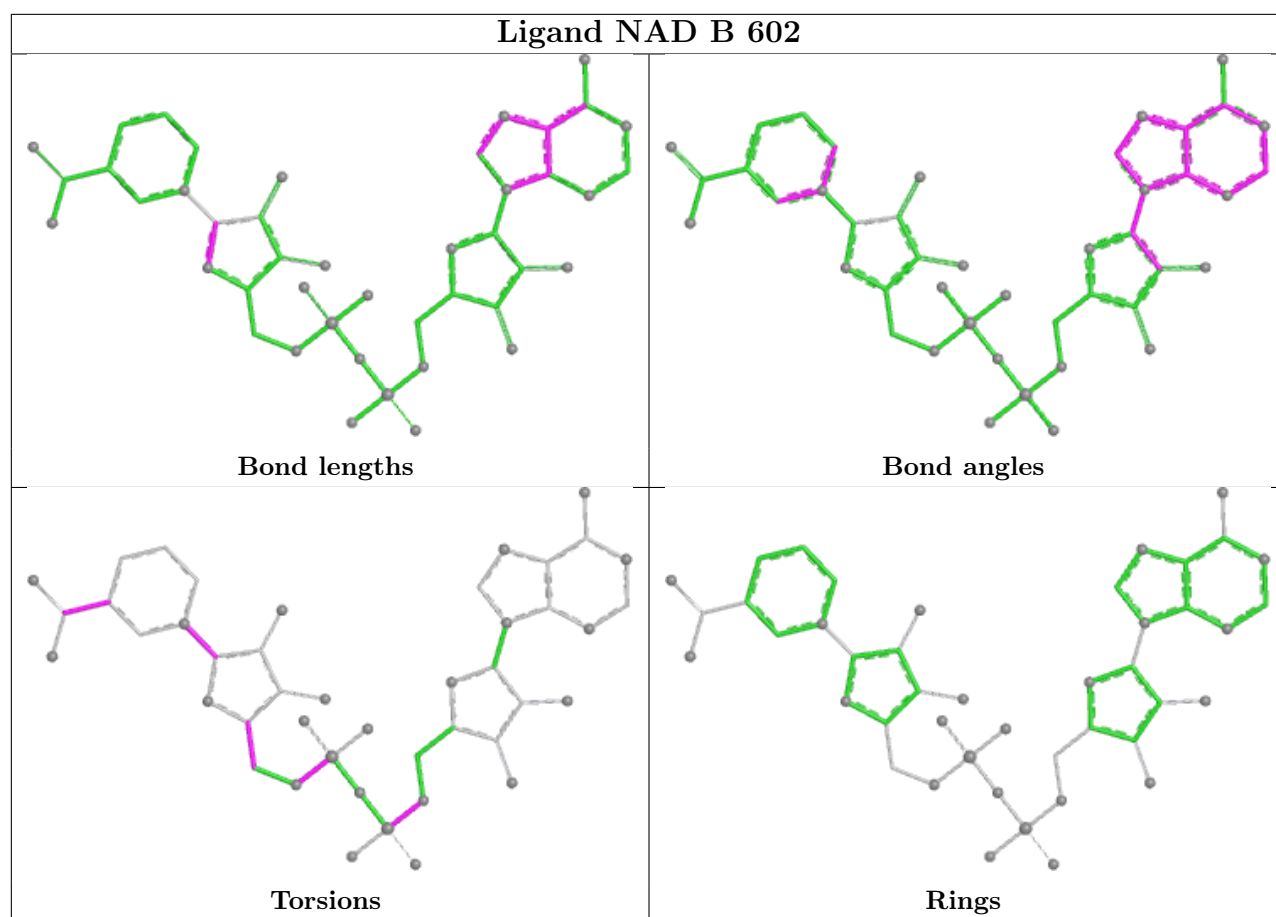
Mol	Chain	Res	Type	Atoms
2	B	602	NAD	C3D-C4D-C5D-O5D
2	A	602	NAD	C4D-C5D-O5D-PN
2	B	601	NAD	C3B-C4B-C5B-O5B
2	A	601	NAD	PA-O3-PN-O5D
2	A	601	NAD	C5B-O5B-PA-O2A
2	A	601	NAD	C5B-O5B-PA-O3
2	A	601	NAD	C4D-C5D-O5D-PN
2	A	601	NAD	PN-O3-PA-O2A
2	B	602	NAD	C4N-C3N-C7N-N7N
2	B	602	NAD	C4N-C3N-C7N-O7N
2	A	602	NAD	C4N-C3N-C7N-N7N
2	A	602	NAD	C4N-C3N-C7N-O7N
2	A	602	NAD	PA-O3-PN-O2N

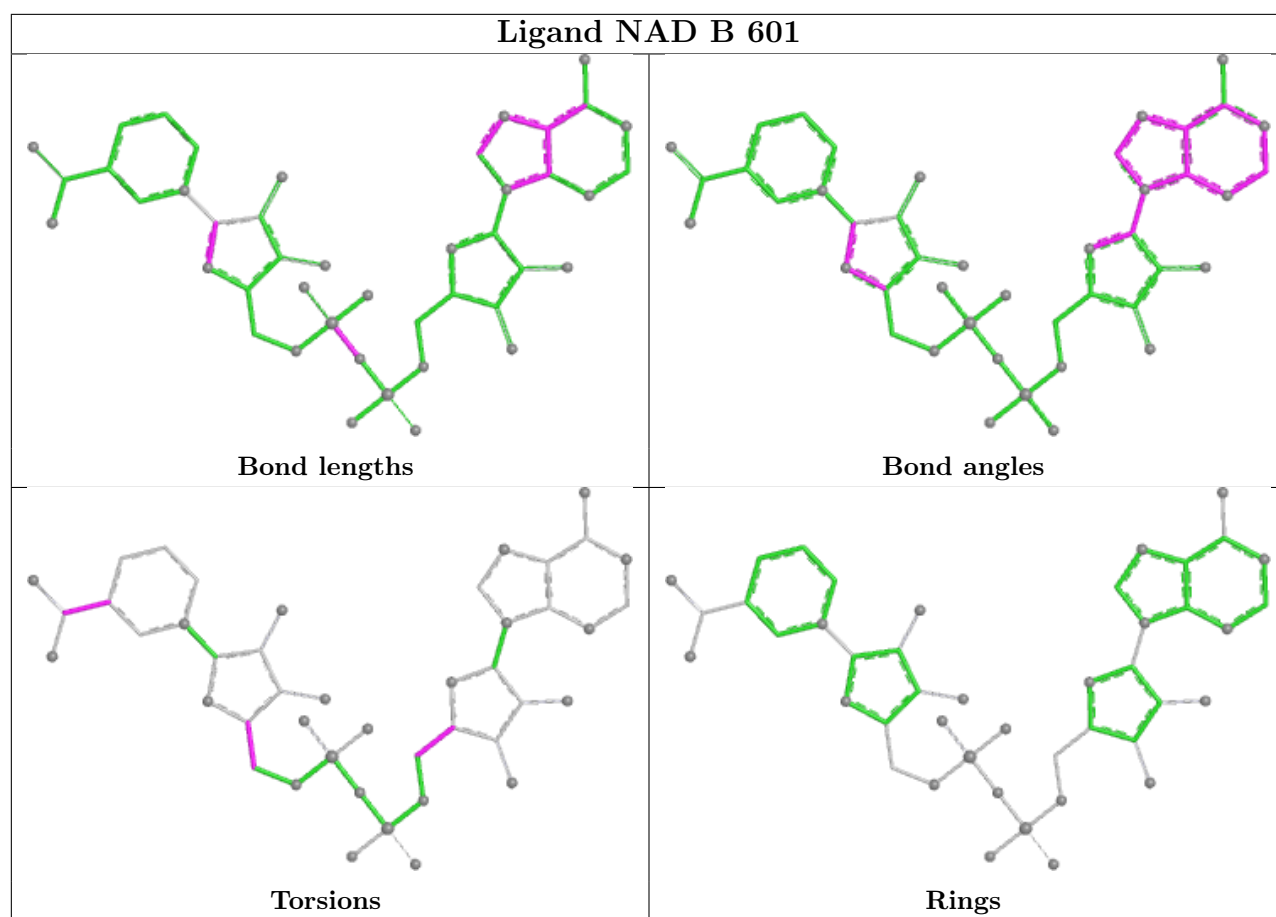
There are no ring outliers.

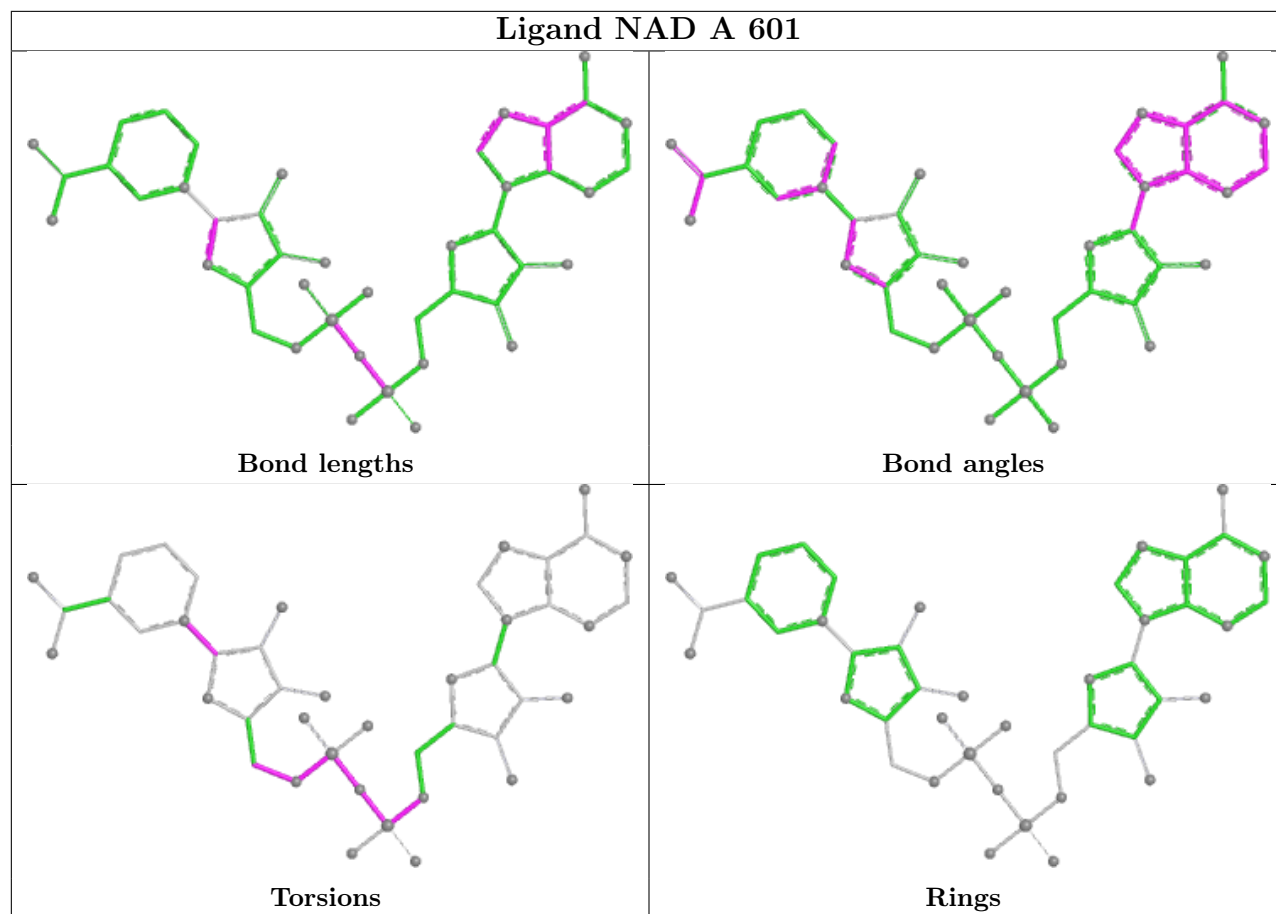
2 monomers are involved in 6 short contacts:

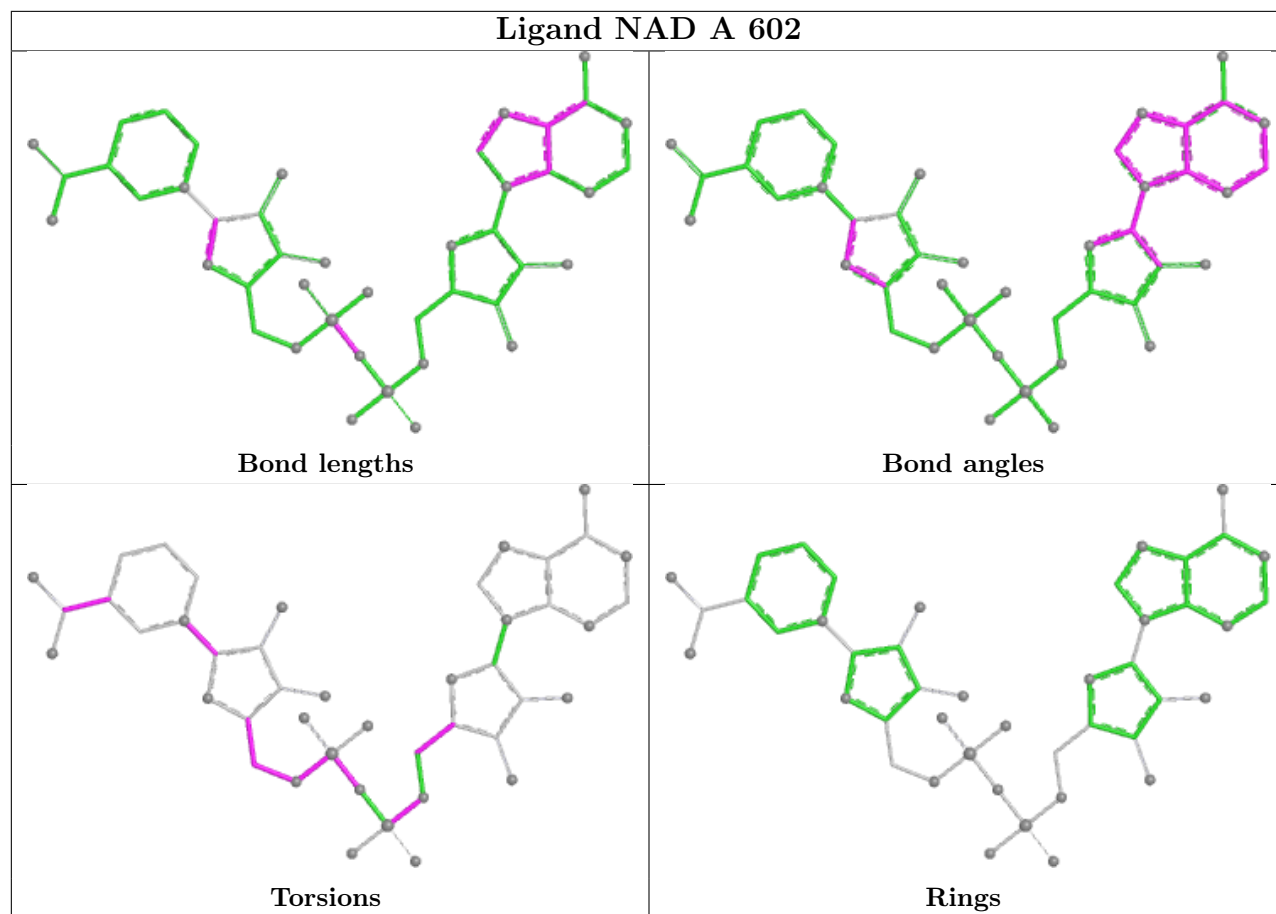
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	NAD	1	0
2	B	601	NAD	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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%)	0.36	33 (6%) 27 26	21, 38, 68, 144	0
1	B	551/566 (97%)	0.33	26 (4%) 36 36	22, 40, 70, 111	0
All	All	1094/1132 (96%)	0.35	59 (5%) 31 31	21, 39, 69, 144	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	TYR	7.4
1	A	126	ILE	7.2
1	A	124	GLY	6.2
1	A	131	LYS	6.0
1	A	125	HIS	5.4
1	A	130	PRO	5.2
1	A	263	PHE	4.8
1	A	127	PHE	4.6
1	B	455	THR	4.1
1	B	126	ILE	3.6
1	B	127	PHE	3.6
1	A	211	ALA	3.6
1	A	76	THR	3.5
1	A	210	ILE	3.4
1	A	353	GLY	3.4
1	B	353	GLY	3.3
1	A	122	GLN	3.2
1	B	125	HIS	3.1
1	A	260	HIS	3.0
1	A	121	SER	2.9
1	B	298	ILE	2.9
1	A	421	ASN	2.8
1	B	123	TYR	2.8
1	B	302	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	422	PRO	2.7
1	A	129	ARG	2.7
1	B	482	ASN	2.7
1	A	369	ALA	2.6
1	A	214	LYS	2.6
1	A	543	TYR	2.6
1	B	124	GLY	2.6
1	B	68	PHE	2.5
1	A	68	PHE	2.5
1	A	372	SER	2.5
1	A	267	ARG	2.4
1	B	369	ALA	2.4
1	A	262	ALA	2.4
1	A	352	LYS	2.3
1	A	384	LEU	2.3
1	B	454	LEU	2.3
1	B	91	ARG	2.3
1	B	431	GLU	2.2
1	A	25	GLY	2.2
1	B	372	SER	2.2
1	B	373	ILE	2.2
1	B	500	SER	2.2
1	B	355	LYS	2.2
1	B	367	HIS	2.1
1	A	258	GLY	2.1
1	B	461	THR	2.1
1	B	375	ASP	2.1
1	B	402	ASP	2.1
1	A	69	HIS	2.1
1	B	303	SER	2.1
1	A	337	ALA	2.0
1	B	128	ARG	2.0
1	B	76	THR	2.0
1	A	370	PRO	2.0
1	A	356	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

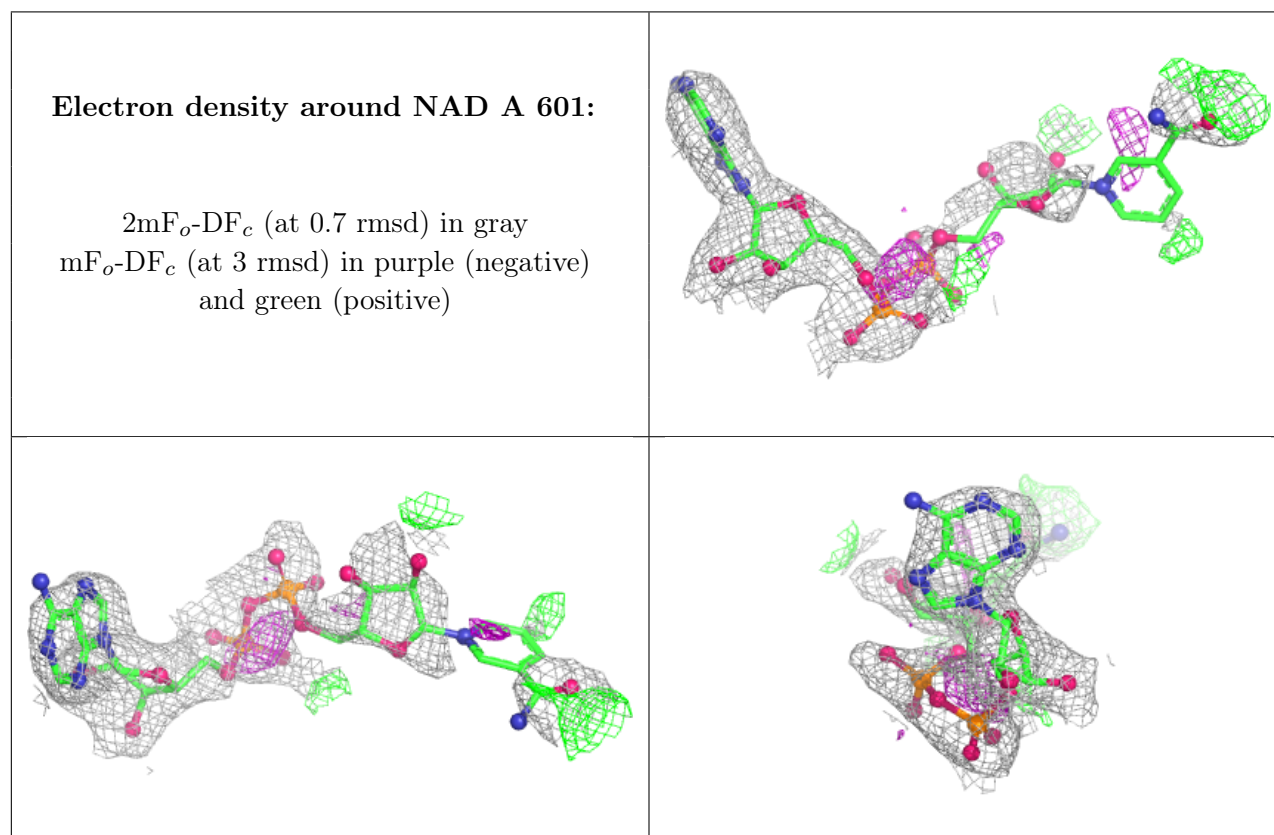
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

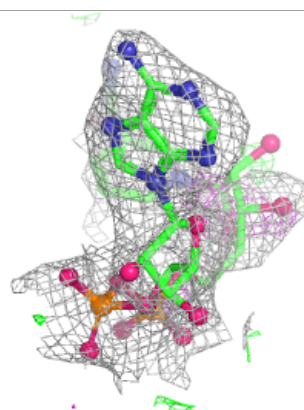
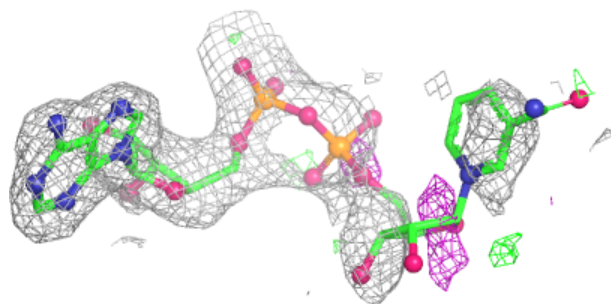
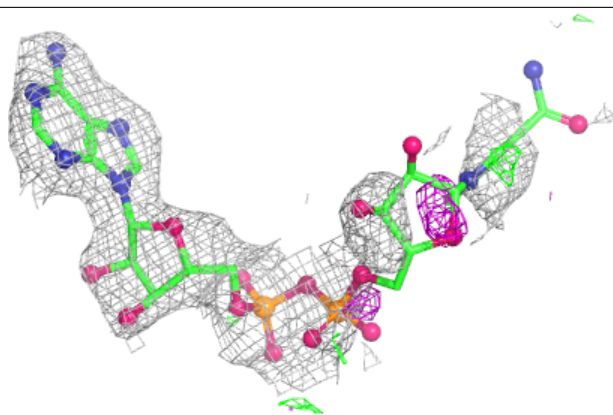
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	A	601	44/44	0.71	0.21	64,107,123,124	0
2	NAD	B	601	44/44	0.83	0.16	49,91,135,138	0
2	NAD	B	602	44/44	0.85	0.15	33,59,129,130	0
2	NAD	A	602	44/44	0.89	0.14	30,52,119,121	0

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



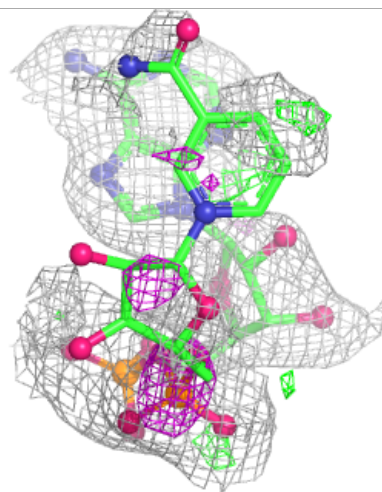
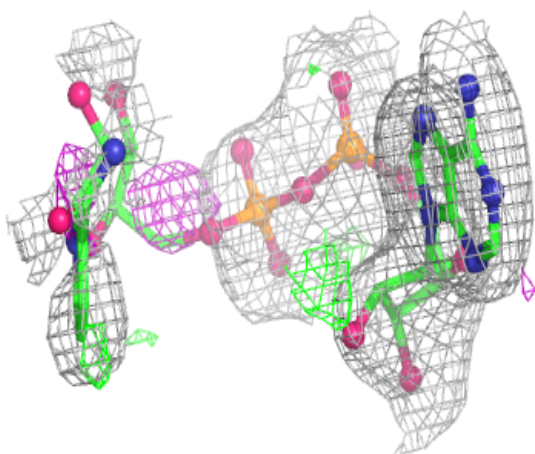
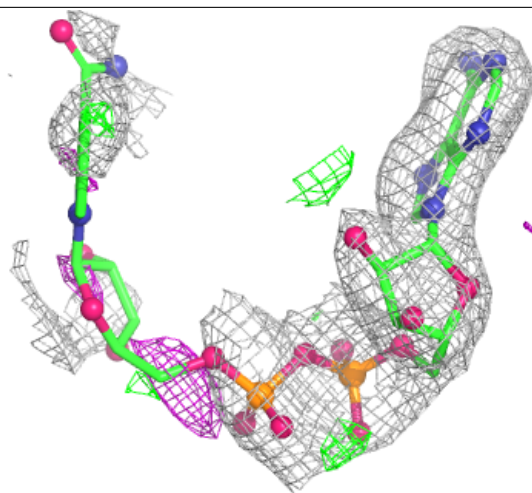
Electron density around NAD B 601:

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



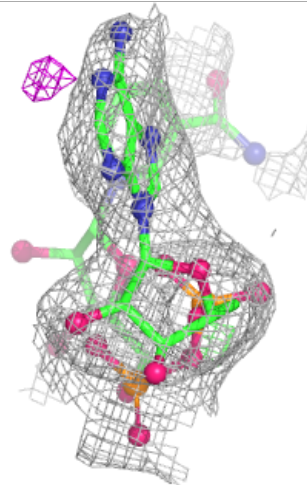
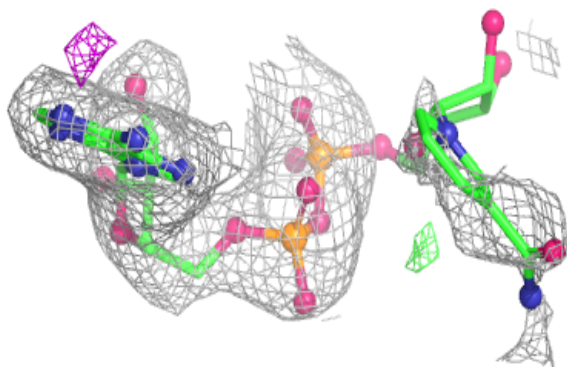
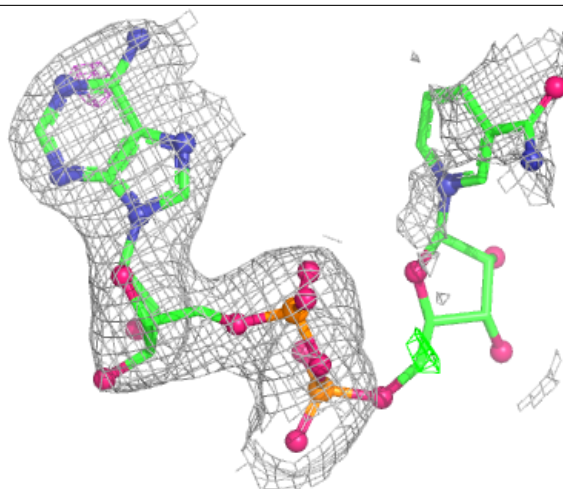
Electron density around NAD B 602:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.