



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:30 PM UTC

PDB ID : 6G1M / pdb_00006g1m
Title : Amine Dehydrogenase from *Petrotoga mobilis*; open and closed form
Authors : Beloti, L.; Frese, A.; Mayol, O.; Vaxelaire-Vergne, C.; Grogan, G.
Deposited on : 2018-03-21
Resolution : 2.32 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

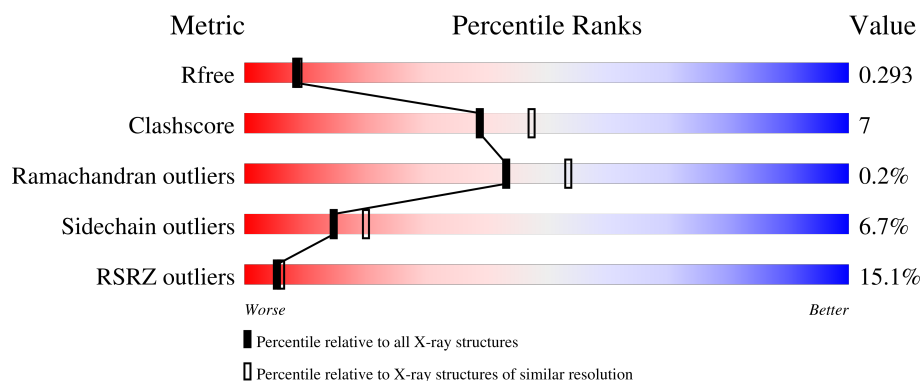
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	338	29% 82% 15% ..
1	B	338	11% 79% 17% ..
1	C	338	8% 82% 15% ..
1	D	338	11% 82% 15% ..

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
3	PO4	A	402	-	X	-	-
3	PO4	D	402	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10224 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 Dihydrodipicolinate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2402	1544	396	450	12			
1	B	332	Total	C	N	O	S	0	0	0
			2458	1580	404	462	12			
1	C	335	Total	C	N	O	S	0	0	0
			2485	1598	409	466	12			
1	D	334	Total	C	N	O	S	0	0	0
			2423	1559	402	450	12			

There are 4 discrepancies between the modelled and reference sequences:

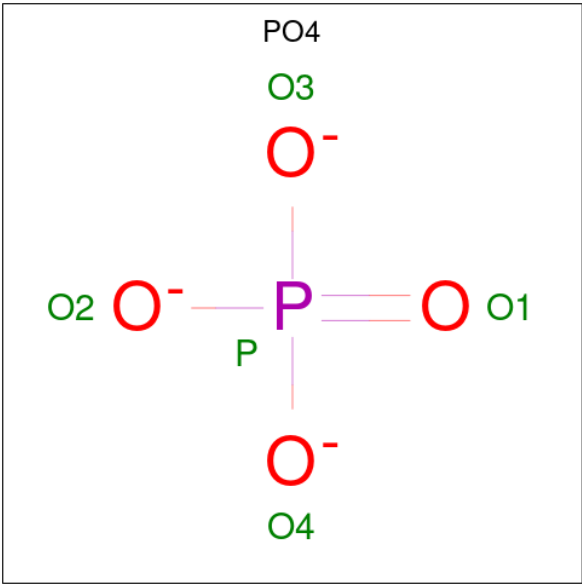
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP A9BHL2
B	1	SER	-	expression tag	UNP A9BHL2
C	1	SER	-	expression tag	UNP A9BHL2
D	1	SER	-	expression tag	UNP A9BHL2

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

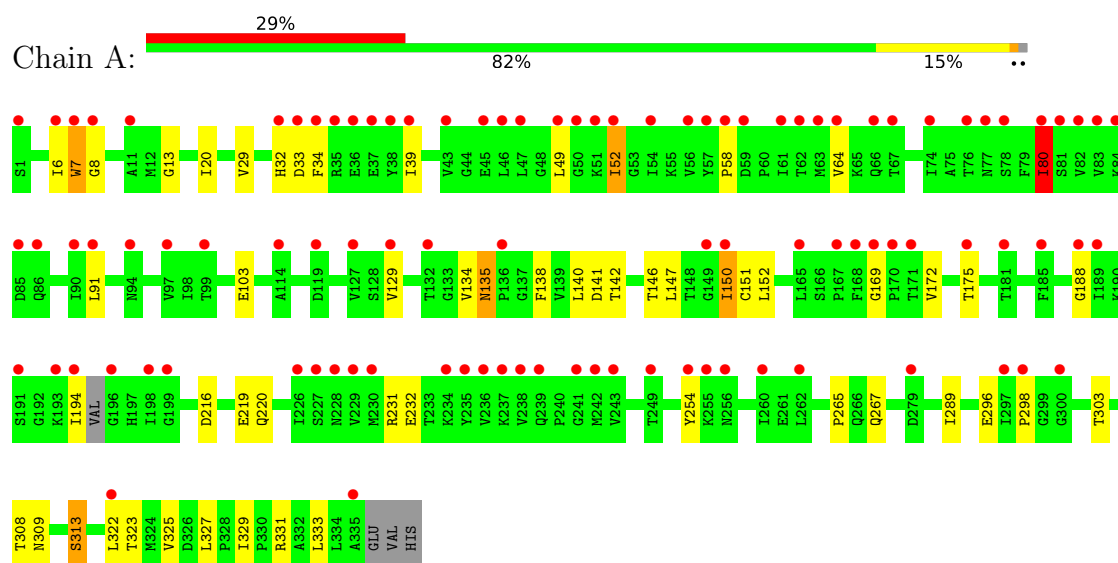
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	72	Total	O	0	0
			72	72		
4	C	84	Total	O	0	0
			84	84		
4	D	63	Total	O	0	0
			63	63		

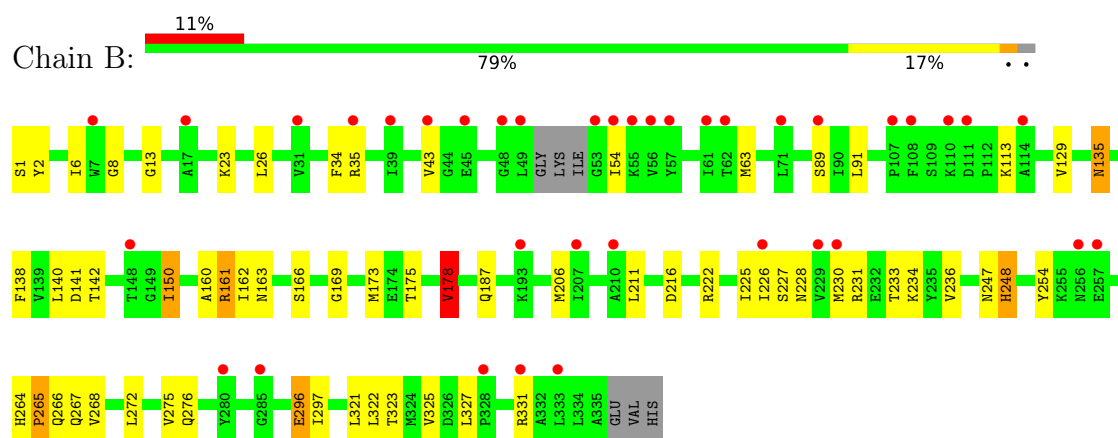
3 Residue-property plots [i](#)

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.

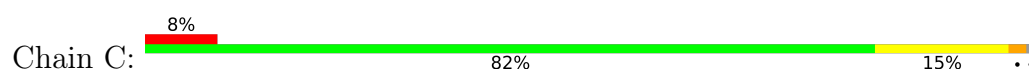
• Molecule 1: Dihydrodipicolinate reductase

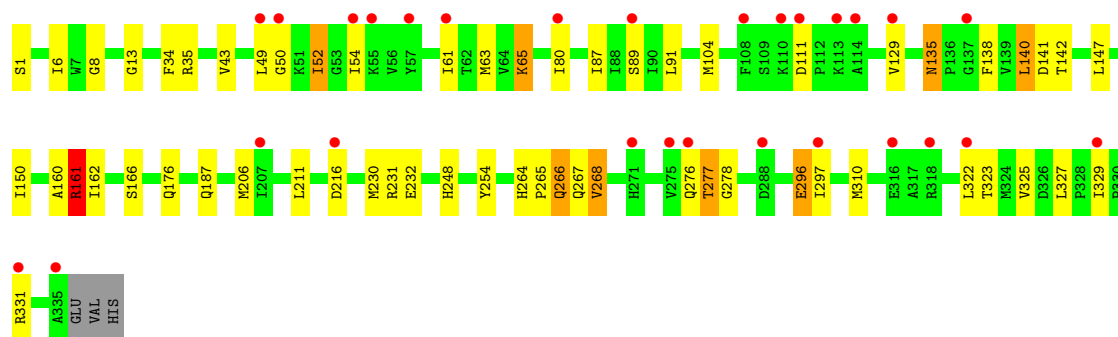


• Molecule 1: Dihydrodipicolinate reductase

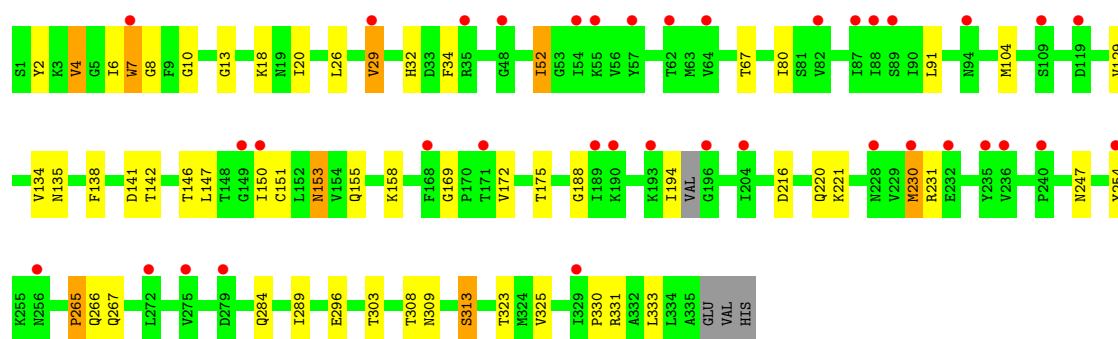
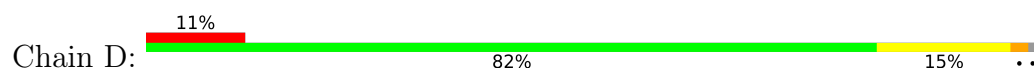


• Molecule 1: Dihydrodipicolinate reductase





● Molecule 1: Dihydrodipicolinate reductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.11Å 83.64Å 125.71Å 90.00° 94.28° 90.00°	Depositor
Resolution (Å)	125.36 – 2.32 125.36 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.4 (125.36-2.32) 99.4 (125.36-2.32)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.248 , 0.295 (Not available) , 0.293	Depositor DCC
R_{free} test set	3155 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10224	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.96% 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, PO4

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	0.99	2/2446 (0.1%)	1.09	6/3347 (0.2%)
1	B	1.12	7/2503 (0.3%)	1.11	5/3410 (0.1%)
1	C	1.12	7/2531 (0.3%)	1.12	11/3448 (0.3%)
1	D	1.03	3/2468 (0.1%)	1.09	5/3372 (0.1%)
All	All	1.07	19/9948 (0.2%)	1.10	27/13577 (0.2%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	VAL	C-O	-8.12	1.14	1.23
1	C	135	ASN	C-N	7.79	1.49	1.34
1	B	135	ASN	C-N	7.68	1.48	1.34
1	A	135	ASN	C-N	7.57	1.48	1.34
1	D	135	ASN	C-N	7.33	1.48	1.34
1	B	265	PRO	C-O	-6.97	1.14	1.23
1	C	265	PRO	C-O	-6.65	1.16	1.23
1	C	1	SER	C-N	-6.46	1.24	1.33
1	B	178	VAL	C-O	-6.34	1.17	1.24
1	C	135	ASN	C-O	-6.22	1.16	1.24
1	D	265	PRO	C-O	-5.90	1.17	1.23
1	C	162	ILE	C-O	-5.80	1.17	1.24
1	B	248	HIS	C-O	-5.74	1.17	1.24
1	B	160	ALA	C-O	-5.46	1.17	1.23
1	C	160	ALA	C-O	-5.43	1.17	1.23
1	C	248	HIS	C-O	-5.39	1.17	1.24
1	A	265	PRO	C-O	-5.34	1.17	1.23
1	D	266	GLN	C-O	-5.08	1.18	1.24
1	B	296	GLU	C-O	-5.08	1.17	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	SER	O-C-N	7.81	135.50	123.00
1	A	80	ILE	CB-CA-C	-7.60	102.24	111.97
1	D	52	ILE	N-CA-CB	-7.36	103.57	112.33
1	A	52	ILE	N-CA-CB	-6.38	104.06	112.36
1	A	169	GLY	N-CA-C	6.28	119.83	112.23
1	C	278	GLY	N-CA-C	6.18	119.34	111.37
1	A	80	ILE	CA-CB-CG1	6.07	120.72	110.40
1	B	162	ILE	CB-CA-C	5.98	119.18	110.98
1	C	206	MET	CG-SD-CE	-5.89	87.94	100.90
1	B	206	MET	CG-SD-CE	-5.80	88.14	100.90
1	C	162	ILE	N-CA-C	-5.78	99.55	107.99
1	C	161	ARG	CG-CD-NE	-5.75	99.35	112.00
1	B	169	GLY	N-CA-C	5.74	119.18	112.23
1	C	162	ILE	CB-CA-C	5.67	118.75	110.98
1	A	7	TRP	CB-CA-C	5.65	118.88	109.56
1	D	7	TRP	CB-CA-C	5.56	118.73	109.56
1	D	4	VAL	CB-CA-C	5.50	118.97	110.50
1	A	329	ILE	CB-CA-C	5.49	116.26	110.88
1	D	169	GLY	N-CA-C	5.48	118.86	112.23
1	D	52	ILE	CB-CA-C	5.48	116.53	110.62
1	C	1	SER	CA-C-N	-5.45	114.03	122.09
1	C	1	SER	C-N-CA	-5.45	114.03	122.09
1	B	162	ILE	N-CA-C	-5.37	100.15	107.99
1	C	268	VAL	CG1-CB-CG2	5.08	121.98	110.80
1	C	268	VAL	N-CA-CB	-5.03	104.12	110.31
1	B	268	VAL	N-CA-CB	5.03	116.49	110.31
1	C	52	ILE	N-CA-CB	5.00	119.48	111.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2402	0	2344	31	0
1	B	2458	0	2453	38	0
1	C	2485	0	2494	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2423	0	2385	40	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	1	0
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	A	51	0	0	3	0
4	B	72	0	0	2	0
4	C	84	0	0	1	0
4	D	63	0	0	3	0
All	All	10224	0	9780	134	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 7.

All (134) 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:D:153:ASN:HD21	1:D:155:GLN:NE2	1.37	1.20
1:C:176:GLN:NE2	1:C:266:GLN:HG3	1.77	0.99
1:C:231:ARG:HH12	1:C:267:GLN:HE21	1.13	0.97
1:D:153:ASN:ND2	1:D:155:GLN:NE2	2.16	0.93
1:A:231:ARG:HH12	1:A:267:GLN:HE21	1.18	0.91
1:D:231:ARG:HH12	1:D:267:GLN:HE21	1.17	0.89
1:B:2:TYR:HB2	1:B:26:LEU:HD23	1.57	0.86
1:D:153:ASN:ND2	1:D:155:GLN:HE22	1.70	0.86
1:C:80:ILE:HD13	1:C:111:ASP:OD2	1.79	0.83
1:D:153:ASN:HD21	1:D:155:GLN:HE22	0.84	0.82
1:D:142:THR:O	1:D:146:THR:HG23	1.82	0.80
1:A:142:THR:O	1:A:146:THR:HG23	1.82	0.79
1:A:33:ASP:O	1:A:39:ILE:HD11	1.82	0.79
1:C:277:THR:HG23	1:C:296:GLU:HB3	1.65	0.78
1:B:276:GLN:H	1:B:276:GLN:CD	1.88	0.78
1:C:329:ILE:HG23	1:D:146:THR:HG22	1.64	0.78
1:B:161:ARG:NH2	1:B:297:ILE:O	2.16	0.77
1:B:231:ARG:HH22	1:B:267:GLN:NE2	1.83	0.76
1:C:176:GLN:HE22	1:C:266:GLN:HG3	1.51	0.75
1:D:7:TRP:O	1:D:32:HIS:O	2.05	0.75
1:A:7:TRP:O	1:A:32:HIS:O	2.05	0.74
1:B:231:ARG:NH2	1:B:267:GLN:HE21	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:GLN:H	1:B:276:GLN:NE2	1.85	0.73
1:D:80:ILE:HD11	1:D:104:MET:SD	2.30	0.71
1:C:80:ILE:HG21	1:C:111:ASP:OD2	1.90	0.70
1:D:313:SER:OG	4:D:501:HOH:O	1.99	0.69
1:D:230:MET:HE2	4:D:561:HOH:O	1.91	0.69
1:A:219:GLU:OE1	4:A:502:HOH:O	2.10	0.69
1:B:231:ARG:HH22	1:B:267:GLN:HE21	1.36	0.66
1:D:80:ILE:CD1	1:D:104:MET:SD	2.83	0.66
1:B:163:ASN:HD22	1:B:266:GLN:HG2	1.61	0.64
1:A:231:ARG:HH12	1:A:267:GLN:NE2	1.94	0.63
1:A:313:SER:OG	4:A:501:HOH:O	2.09	0.63
1:B:227:SER:OG	1:B:231:ARG:HD2	1.98	0.62
1:B:231:ARG:NH2	1:B:267:GLN:NE2	2.47	0.61
1:D:231:ARG:HH12	1:D:267:GLN:NE2	1.93	0.60
1:D:134:VAL:HG13	1:D:303:THR:N	2.17	0.60
1:A:134:VAL:HG13	1:A:303:THR:N	2.17	0.59
2:A:401:NAD:H6N	2:A:401:NAD:H52N	1.85	0.58
1:B:2:TYR:HB2	1:B:26:LEU:CD2	2.32	0.58
1:C:176:GLN:HE22	1:C:266:GLN:CG	2.17	0.57
1:A:91:LEU:HD21	1:A:129:VAL:HG22	1.86	0.57
1:C:91:LEU:HD21	1:C:129:VAL:HG22	1.87	0.56
1:D:91:LEU:HD21	1:D:129:VAL:HG22	1.88	0.56
1:A:8:GLY:O	1:A:13:GLY:HA3	2.06	0.56
1:A:80:ILE:HG12	1:A:103:GLU:OE1	2.05	0.56
1:C:329:ILE:HD12	1:D:146:THR:HG22	1.89	0.55
1:B:178:VAL:HG23	1:B:236:VAL:HG21	1.89	0.55
1:B:216:ASP:OD2	1:B:254:TYR:O	2.25	0.55
1:C:8:GLY:O	1:C:13:GLY:HA3	2.07	0.55
1:D:8:GLY:O	1:D:13:GLY:HA3	2.07	0.55
1:A:188:GLY:HA3	1:A:194:ILE:HD12	1.89	0.54
1:B:8:GLY:O	1:B:13:GLY:HA3	2.07	0.54
1:B:226:ILE:HD12	1:B:226:ILE:O	2.08	0.54
1:B:91:LEU:HD21	1:B:129:VAL:HG22	1.89	0.54
1:A:231:ARG:NH1	1:A:267:GLN:HE21	1.99	0.54
1:A:39:ILE:HD12	1:A:58:PRO:HA	1.90	0.53
1:A:216:ASP:OD2	1:A:254:TYR:O	2.27	0.53
1:B:178:VAL:CG2	1:B:236:VAL:HG21	2.38	0.53
1:C:216:ASP:OD2	1:C:254:TYR:O	2.25	0.53
1:D:216:ASP:OD2	1:D:254:TYR:O	2.26	0.53
1:B:135:ASN:HD21	1:B:140:LEU:HD12	1.73	0.53
1:D:323:THR:OG1	1:D:325:VAL:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ARG:NH1	1:D:267:GLN:HE21	1.98	0.53
1:A:323:THR:OG1	1:A:325:VAL:HG22	2.09	0.53
1:C:323:THR:OG1	1:C:325:VAL:HG22	2.09	0.52
1:D:221:LYS:CB	4:D:537:HOH:O	2.56	0.52
1:D:188:GLY:HA3	1:D:194:ILE:HD12	1.90	0.52
1:B:43:VAL:HG22	1:B:54:ILE:HB	1.92	0.52
1:B:323:THR:OG1	1:B:325:VAL:HG22	2.10	0.52
1:B:276:GLN:O	1:B:276:GLN:HG2	2.09	0.51
1:C:43:VAL:HG22	1:C:54:ILE:HB	1.91	0.51
1:C:322:LEU:HD13	1:C:327:LEU:HD21	1.93	0.51
1:B:138:PHE:HA	1:B:142:THR:HB	1.94	0.50
1:B:233:THR:HG22	1:B:234:LYS:N	2.25	0.50
1:C:230:MET:HE3	1:C:232:GLU:HB2	1.93	0.50
1:C:161:ARG:NH2	1:C:297:ILE:O	2.37	0.49
1:A:138:PHE:HA	1:A:142:THR:HB	1.95	0.49
1:C:138:PHE:HA	1:C:142:THR:HB	1.93	0.48
1:A:172:VAL:HA	1:A:175:THR:HG22	1.96	0.48
1:B:264:HIS:N	1:B:265:PRO:HD3	2.28	0.48
1:B:91:LEU:HD21	1:B:129:VAL:CG2	2.44	0.48
1:B:231:ARG:HG2	1:B:272:LEU:HD12	1.96	0.48
1:D:91:LEU:HD21	1:D:129:VAL:CG2	2.45	0.47
1:D:172:VAL:O	1:D:175:THR:HG22	2.14	0.47
1:B:322:LEU:HD13	1:B:327:LEU:HD21	1.96	0.47
1:C:329:ILE:HD12	1:D:146:THR:CG2	2.44	0.47
1:A:322:LEU:HD13	1:A:327:LEU:HD21	1.95	0.47
1:C:61:ILE:HG22	1:C:65:LYS:HD2	1.97	0.47
1:D:2:TYR:HB2	1:D:26:LEU:HD23	1.97	0.47
1:D:138:PHE:HA	1:D:142:THR:HB	1.96	0.47
1:A:172:VAL:O	1:A:175:THR:HG22	2.15	0.46
1:D:80:ILE:HD13	1:D:104:MET:SD	2.55	0.46
1:B:175:THR:HA	4:B:504:HOH:O	2.15	0.46
1:C:91:LEU:HD21	1:C:129:VAL:CG2	2.44	0.46
1:A:91:LEU:HD21	1:A:129:VAL:CG2	2.45	0.46
1:A:138:PHE:CE2	1:B:150:ILE:CD1	2.99	0.46
1:D:158:LYS:CD	1:D:284:GLN:NE2	2.79	0.46
1:D:172:VAL:HA	1:D:175:THR:HG22	1.97	0.46
1:A:152:LEU:O	1:B:23:LYS:NZ	2.48	0.45
1:C:310:MET:HA	4:C:512:HOH:O	2.16	0.45
1:C:277:THR:HG23	1:C:296:GLU:H	1.81	0.45
1:B:247:ASN:HA	1:B:265:PRO:HA	1.99	0.45
1:A:135:ASN:ND2	1:A:140:LEU:HD12	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:CYS:SG	1:A:289:ILE:HD11	2.58	0.44
1:A:309:ASN:ND2	1:A:333:LEU:H	2.15	0.44
1:C:329:ILE:CG2	1:D:146:THR:HG22	2.41	0.44
1:D:151:CYS:SG	1:D:289:ILE:HD11	2.58	0.44
1:A:20:ILE:CD1	1:A:308:THR:HG23	2.48	0.44
1:D:309:ASN:ND2	1:D:333:LEU:H	2.16	0.43
1:D:216:ASP:CG	1:D:254:TYR:O	2.61	0.43
1:C:216:ASP:CG	1:C:254:TYR:O	2.61	0.43
1:B:216:ASP:CG	1:B:254:TYR:O	2.61	0.43
1:D:20:ILE:CD1	1:D:308:THR:HG23	2.48	0.43
1:A:150:ILE:CD1	1:A:289:ILE:HD11	2.49	0.43
1:C:176:GLN:NE2	1:C:266:GLN:CG	2.65	0.43
1:A:298:PRO:HB3	4:A:540:HOH:O	2.19	0.43
1:B:163:ASN:ND2	1:B:266:GLN:HG2	2.30	0.42
1:C:147:LEU:HD23	1:C:147:LEU:HA	1.87	0.42
1:C:161:ARG:HB3	1:C:264:HIS:ND1	2.33	0.42
1:D:247:ASN:HA	1:D:265:PRO:HA	2.01	0.42
1:A:216:ASP:CG	1:A:254:TYR:O	2.62	0.42
1:C:135:ASN:ND2	1:C:140:LEU:HD22	2.34	0.42
1:D:10:GLY:HA3	2:D:401:NAD:O5B	2.19	0.42
1:B:173:MET:HB3	1:B:178:VAL:HG22	2.02	0.42
1:C:87:ILE:HD13	1:C:104:MET:HE2	2.02	0.41
1:A:138:PHE:CE2	1:B:150:ILE:HD12	2.55	0.41
1:B:228:ASN:ND2	4:B:501:HOH:O	2.22	0.41
1:B:225:ILE:HD13	1:B:267:GLN:HG3	2.02	0.41
1:C:111:ASP:N	1:C:111:ASP:OD1	2.53	0.41
1:D:151:CYS:SG	1:D:289:ILE:CD1	3.09	0.41
1:C:329:ILE:HD11	1:D:330:PRO:HD3	2.03	0.40
1:D:29:VAL:HG13	1:D:67:THR:HB	2.03	0.40
1:B:222:ARG:HD3	1:B:248:HIS:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	330/338 (98%)	319 (97%)	11 (3%)	0	100	100
1	B	328/338 (97%)	319 (97%)	9 (3%)	0	100	100
1	C	333/338 (98%)	319 (96%)	12 (4%)	2 (1%)	21	25
1	D	330/338 (98%)	320 (97%)	10 (3%)	0	100	100
All	All	1321/1352 (98%)	1277 (97%)	42 (3%)	2 (0%)	43	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	52	ILE
1	C	50	GLY

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	243/287 (85%)	228 (94%)	15 (6%)	16	23
1	B	258/287 (90%)	240 (93%)	18 (7%)	14	18
1	C	262/287 (91%)	242 (92%)	20 (8%)	12	16
1	D	247/287 (86%)	232 (94%)	15 (6%)	17	23
All	All	1010/1148 (88%)	942 (93%)	68 (7%)	15	20

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	29	VAL
1	A	34	PHE
1	A	49	LEU
1	A	52	ILE
1	A	64	VAL

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Mol	Chain	Res	Type
1	A	80	ILE
1	A	141	ASP
1	A	147	LEU
1	A	150	ILE
1	A	220	GLN
1	A	232	GLU
1	A	296	GLU
1	A	313	SER
1	A	331	ARG
1	B	1	SER
1	B	6	ILE
1	B	34	PHE
1	B	35	ARG
1	B	63	MET
1	B	89	SER
1	B	113	LYS
1	B	141	ASP
1	B	150	ILE
1	B	161	ARG
1	B	166	SER
1	B	178	VAL
1	B	187	GLN
1	B	211	LEU
1	B	230	MET
1	B	296	GLU
1	B	321	LEU
1	B	331	ARG
1	C	6	ILE
1	C	34	PHE
1	C	35	ARG
1	C	49	LEU
1	C	63	MET
1	C	65	LYS
1	C	89	SER
1	C	140	LEU
1	C	141	ASP
1	C	150	ILE
1	C	161	ARG
1	C	166	SER
1	C	187	GLN
1	C	211	LEU
1	C	266	GLN

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Mol	Chain	Res	Type
1	C	268	VAL
1	C	276	GLN
1	C	277	THR
1	C	296	GLU
1	C	331	ARG
1	D	4	VAL
1	D	6	ILE
1	D	18	LYS
1	D	29	VAL
1	D	34	PHE
1	D	52	ILE
1	D	141	ASP
1	D	147	LEU
1	D	150	ILE
1	D	153	ASN
1	D	220	GLN
1	D	230	MET
1	D	296	GLU
1	D	313	SER
1	D	331	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	126	ASN
1	A	135	ASN
1	A	155	GLN
1	A	266	GLN
1	A	267	GLN
1	A	309	ASN
1	B	86	GLN
1	B	94	ASN
1	B	126	ASN
1	B	135	ASN
1	B	155	GLN
1	B	163	ASN
1	B	267	GLN
1	B	276	GLN
1	C	86	GLN
1	C	94	ASN
1	C	135	ASN

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Mol	Chain	Res	Type
1	C	155	GLN
1	C	176	GLN
1	C	267	GLN
1	C	294	ASN
1	D	86	GLN
1	D	94	ASN
1	D	126	ASN
1	D	135	ASN
1	D	155	GLN
1	D	176	GLN
1	D	220	GLN
1	D	266	GLN
1	D	267	GLN
1	D	284	GLN
1	D	309	ASN

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](#)

6 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	C	401	-	46,48,48	0.80	1 (2%)	64,73,73	0.88	3 (4%)
2	NAD	D	401	-	46,48,48	0.83	1 (2%)	64,73,73	0.77	1 (1%)
3	PO4	A	402	-	4,4,4	3.94	4 (100%)	6,6,6	0.58	0
2	NAD	B	401	-	46,48,48	0.82	2 (4%)	64,73,73	0.88	3 (4%)
3	PO4	D	402	-	4,4,4	3.50	4 (100%)	6,6,6	0.52	0
2	NAD	A	401	-	46,48,48	0.96	3 (6%)	64,73,73	1.05	5 (7%)

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	C	401	-	-	5/30/62/62	0/5/5/5
2	NAD	D	401	-	-	6/30/62/62	0/5/5/5
2	NAD	A	401	-	-	8/30/62/62	0/5/5/5
2	NAD	B	401	-	-	4/30/62/62	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	PO4	P-O2	-4.85	1.40	1.54
3	A	402	PO4	P-O4	-4.23	1.42	1.54
3	D	402	PO4	P-O1	-4.16	1.41	1.50
3	D	402	PO4	P-O3	-3.75	1.43	1.54
3	A	402	PO4	P-O3	-3.41	1.44	1.54
3	D	402	PO4	P-O2	-3.05	1.45	1.54
3	A	402	PO4	P-O1	-3.00	1.43	1.50
3	D	402	PO4	P-O4	-2.88	1.46	1.54
2	A	401	NAD	PA-O3	-2.64	1.56	1.59
2	A	401	NAD	O5D-C5D	-2.16	1.36	1.44
2	C	401	NAD	PN-O2N	-2.14	1.45	1.55
2	B	401	NAD	PN-O2N	-2.13	1.45	1.55
2	A	401	NAD	PN-O3	-2.05	1.57	1.59
2	B	401	NAD	PA-O2A	-2.00	1.46	1.55
2	D	401	NAD	PA-O2A	-2.00	1.46	1.55

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAD	C6N-N1N-C2N	-3.09	119.25	121.88
2	B	401	NAD	C6N-N1N-C2N	-2.89	119.42	121.88
2	A	401	NAD	PN-O5D-C5D	-2.84	105.08	121.35
2	C	401	NAD	O3B-C3B-C4B	-2.69	103.37	111.08
2	A	401	NAD	C2D-C3D-C4D	-2.57	97.64	102.61
2	C	401	NAD	C6N-N1N-C2N	-2.57	119.69	121.88
2	A	401	NAD	O3-PN-O1N	-2.46	103.30	110.70
2	D	401	NAD	O3B-C3B-C2B	2.41	119.55	111.82
2	B	401	NAD	O3B-C3B-C2B	2.29	119.15	111.82
2	B	401	NAD	C4D-O4D-C1D	2.17	111.92	109.92
2	C	401	NAD	C4D-O4D-C1D	2.07	111.82	109.92
2	A	401	NAD	C5D-C4D-C3D	-2.07	107.76	115.21

There are no chirality outliers.

All (23) torsion outliers are listed below:

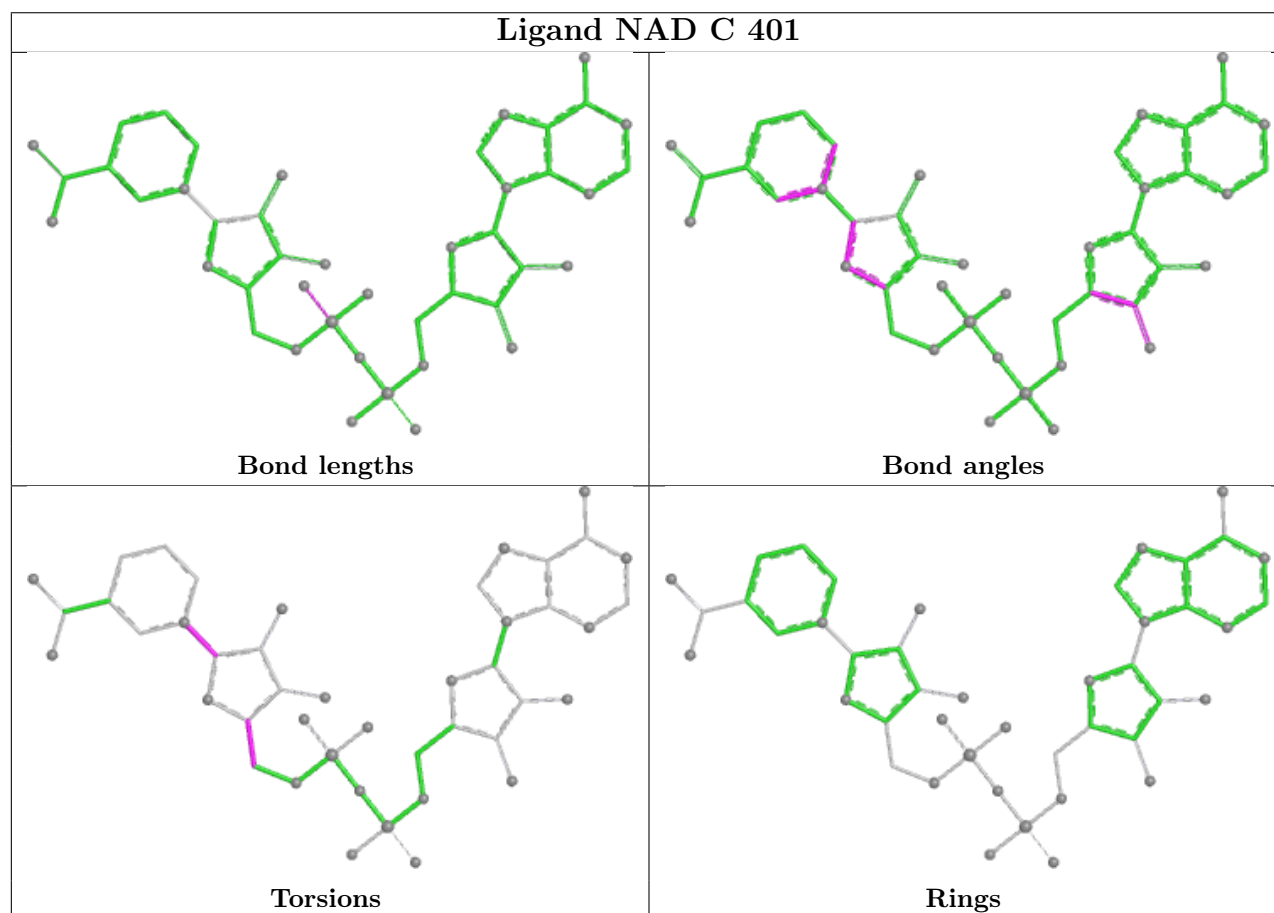
Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5B-O5B-PA-O1A
2	A	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	O4D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	C2D-C1D-N1N-C2N
2	B	401	NAD	C2D-C1D-N1N-C6N
2	C	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	C2D-C1D-N1N-C2N
2	C	401	NAD	C2D-C1D-N1N-C6N
2	D	401	NAD	O4D-C1D-N1N-C2N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	C2D-C1D-N1N-C6N
2	A	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	C3B-C4B-C5B-O5B
2	A	401	NAD	O4D-C4D-C5D-O5D
2	A	401	NAD	C3D-C4D-C5D-O5D
2	D	401	NAD	O4D-C4D-C5D-O5D
2	D	401	NAD	C3D-C4D-C5D-O5D
2	A	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C4D-C5D-O5D
2	A	401	NAD	PA-O3-PN-O1N

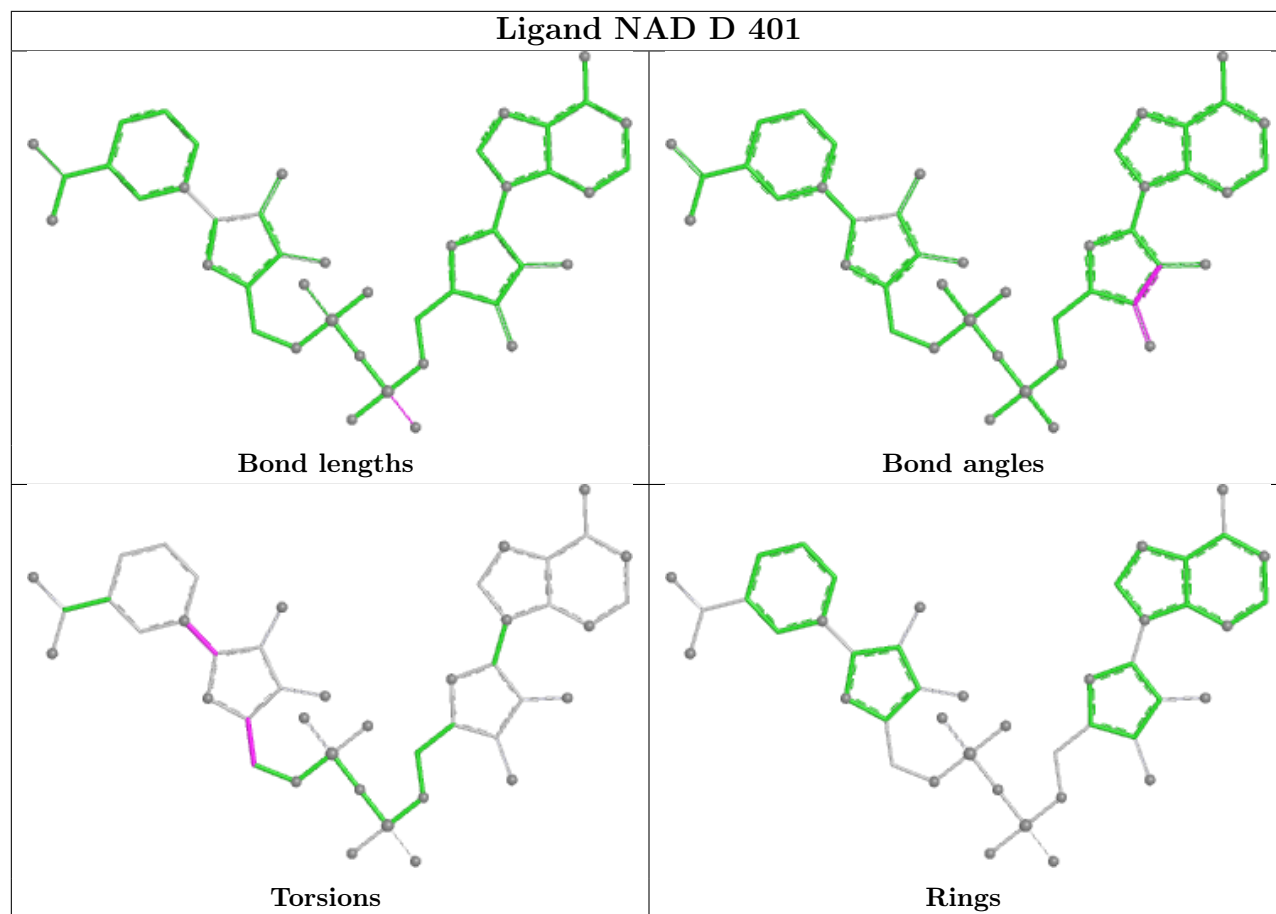
There are no ring outliers.

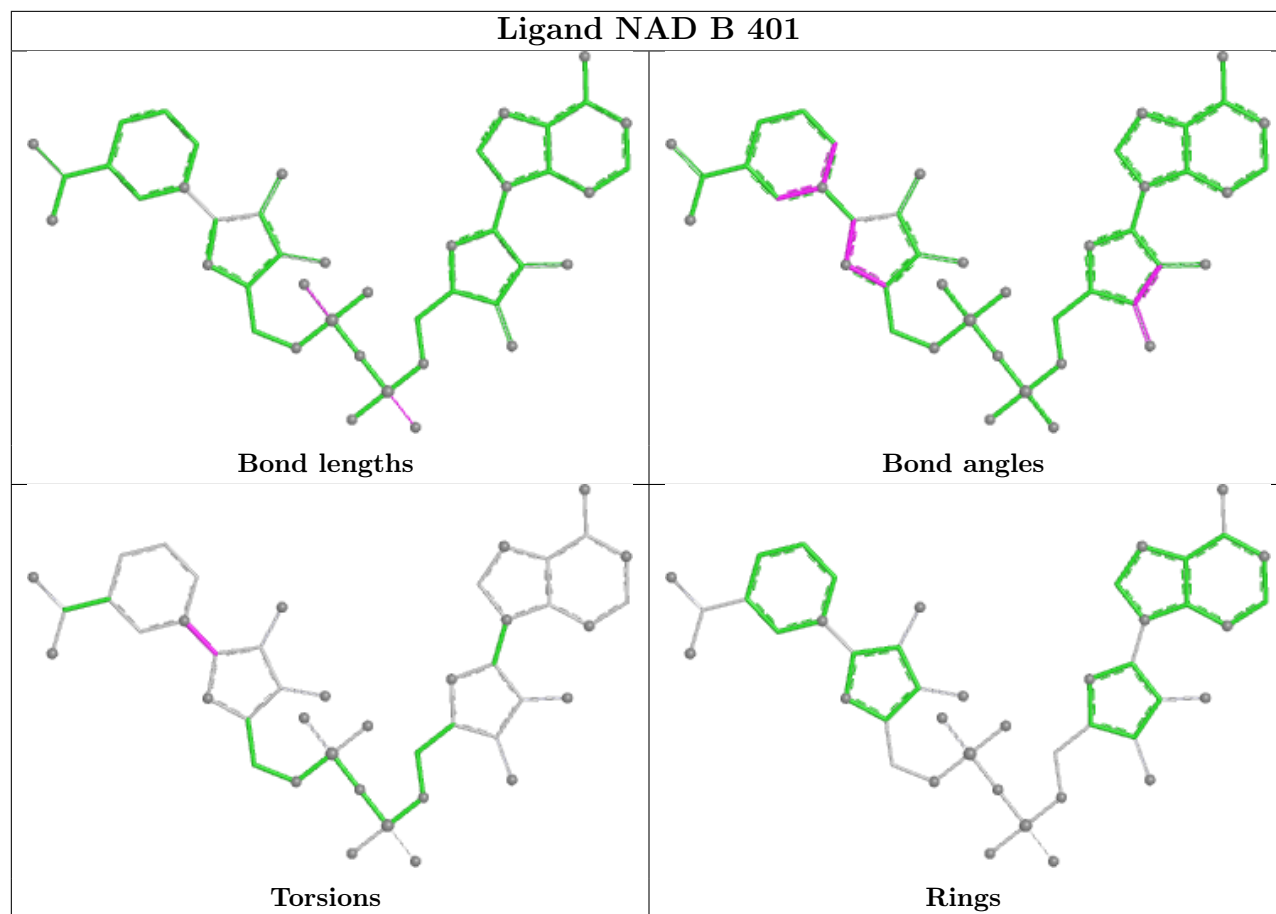
2 monomers are involved in 2 short contacts:

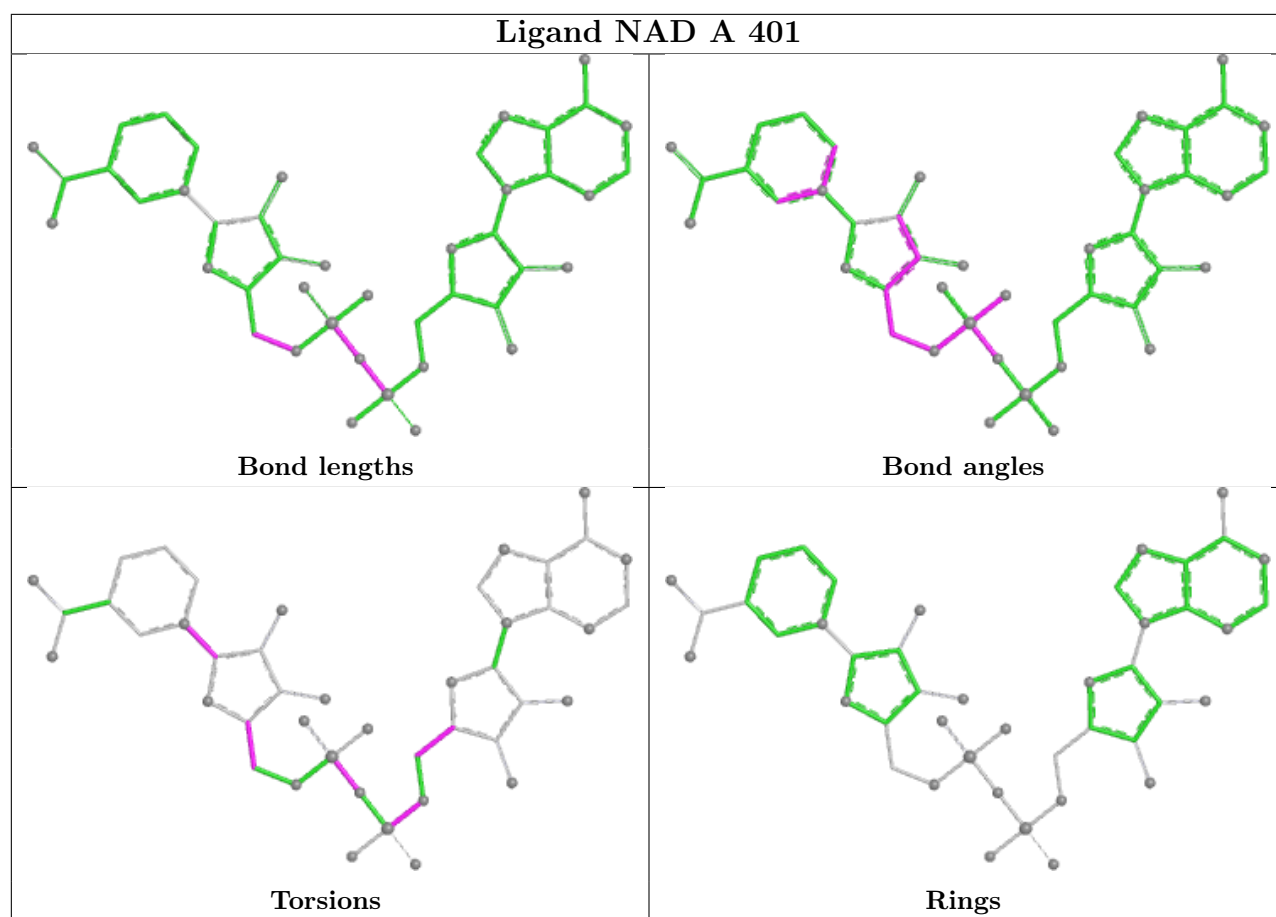
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	NAD	1	0
2	A	401	NAD	1	0

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	334/338 (98%)	1.60	99 (29%) 1 1	23, 40, 63, 86	0
1	B	332/338 (98%)	1.14	37 (11%) 10 11	18, 32, 53, 66	0
1	C	335/338 (99%)	0.96	28 (8%) 17 19	18, 29, 45, 70	0
1	D	334/338 (98%)	1.01	37 (11%) 10 11	20, 34, 53, 69	0
All	All	1335/1352 (98%)	1.18	201 (15%) 5 6	18, 34, 56, 86	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	LEU	5.1
1	A	7	TRP	4.7
1	A	52	ILE	4.7
1	A	235	TYR	4.6
1	A	35	ARG	4.6
1	A	171	THR	4.4
1	D	189	ILE	4.3
1	A	47	LEU	4.2
1	A	238	VAL	4.0
1	A	33	ASP	4.0
1	D	279	ASP	3.9
1	B	54	ILE	3.9
1	A	335	ALA	3.9
1	A	82	VAL	3.8
1	D	171	THR	3.7
1	A	167	PRO	3.7
1	B	53	GLY	3.7
1	A	227	SER	3.6
1	A	168	PHE	3.6
1	D	94	ASN	3.6
1	B	48	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	49	LEU	3.4
1	C	89	SER	3.4
1	A	189	ILE	3.4
1	A	67	THR	3.3
1	C	111	ASP	3.3
1	D	235	TYR	3.3
1	A	80	ILE	3.3
1	A	38	TYR	3.3
1	C	50	GLY	3.3
1	A	56	VAL	3.2
1	A	149	GLY	3.2
1	A	254	TYR	3.2
1	A	74	ILE	3.2
1	A	198	ILE	3.2
1	B	39	ILE	3.2
1	A	1	SER	3.1
1	A	234	LYS	3.1
1	B	110	LYS	3.1
1	A	37	GLU	3.1
1	A	54	ILE	3.1
1	C	61	ILE	3.1
1	A	199	GLY	3.1
1	A	34	PHE	3.0
1	D	48	GLY	3.0
1	D	168	PHE	3.0
1	A	58	PRO	3.0
1	A	76	THR	2.9
1	B	62	THR	2.9
1	B	111	ASP	2.9
1	A	169	GLY	2.9
1	A	188	GLY	2.9
1	A	279	ASP	2.9
1	D	240	PRO	2.9
1	D	88	ILE	2.9
1	A	94	ASN	2.9
1	A	237	LYS	2.8
1	B	56	VAL	2.8
1	D	54	ILE	2.8
1	D	228	ASN	2.8
1	C	335	ALA	2.8
1	D	256	ASN	2.8
1	A	78	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	108	PHE	2.8
1	B	285	GLY	2.8
1	A	83	VAL	2.7
1	A	229	VAL	2.7
1	C	54	ILE	2.7
1	A	193	LYS	2.7
1	C	113	LYS	2.7
1	A	43	VAL	2.7
1	C	275	VAL	2.7
1	A	300	GLY	2.7
1	C	137	GLY	2.7
1	D	193	LYS	2.7
1	A	256	ASN	2.6
1	A	6	ILE	2.6
1	A	255	LYS	2.6
1	A	196	GLY	2.6
1	A	239	GLN	2.6
1	A	8	GLY	2.6
1	A	243	VAL	2.6
1	A	194	ILE	2.6
1	C	49	LEU	2.5
1	A	114	ALA	2.5
1	A	77	ASN	2.5
1	A	260	ILE	2.5
1	C	329	ILE	2.5
1	B	333	LEU	2.5
1	A	241	GLY	2.5
1	D	149	GLY	2.5
1	D	190	LYS	2.5
1	B	45	GLU	2.5
1	B	331	ARG	2.5
1	A	51	LYS	2.5
1	C	110	LYS	2.5
1	A	50	GLY	2.5
1	A	64	VAL	2.5
1	C	129	VAL	2.5
1	B	57	TYR	2.5
1	A	228	ASN	2.5
1	B	148	THR	2.4
1	A	61	ILE	2.4
1	B	31	VAL	2.4
1	B	226	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	229	VAL	2.4
1	A	81	SER	2.4
1	A	226	ILE	2.4
1	C	57	TYR	2.4
1	A	129	VAL	2.4
1	A	242	MET	2.4
1	A	32	HIS	2.4
1	C	271	HIS	2.4
1	A	36	GLU	2.4
1	A	45	GLU	2.4
1	D	57	TYR	2.3
1	A	132	THR	2.3
1	A	230	MET	2.3
1	A	49	LEU	2.3
1	C	316	GLU	2.3
1	D	232	GLU	2.3
1	D	7	TRP	2.3
1	A	11	ALA	2.3
1	A	63	MET	2.3
1	D	329	ILE	2.3
1	A	150	ILE	2.3
1	D	29	VAL	2.3
1	D	272	LEU	2.3
1	A	170	PRO	2.3
1	D	196	GLY	2.3
1	D	35	ARG	2.3
1	D	254	TYR	2.3
1	A	249	THR	2.3
1	A	90	ILE	2.3
1	C	80	ILE	2.3
1	D	87	ILE	2.3
1	D	236	VAL	2.3
1	B	230	MET	2.2
1	B	17	ALA	2.2
1	B	55	LYS	2.2
1	B	61	ILE	2.2
1	C	108	PHE	2.2
1	D	82	VAL	2.2
1	C	216	ASP	2.2
1	B	107	PRO	2.2
1	D	230	MET	2.2
1	A	66	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	99	THR	2.2
1	A	39	ILE	2.2
1	C	297	ILE	2.2
1	B	71	LEU	2.2
1	C	322	LEU	2.2
1	D	150	ILE	2.2
1	A	97	VAL	2.2
1	A	119	ASP	2.2
1	A	127	VAL	2.2
1	B	43	VAL	2.2
1	D	119	ASP	2.2
1	C	276	GLN	2.2
1	B	210	ALA	2.2
1	D	89	SER	2.2
1	D	109	SER	2.2
1	A	297	ILE	2.1
1	B	207	ILE	2.1
1	A	236	VAL	2.1
1	D	275	VAL	2.1
1	A	84	LYS	2.1
1	B	193	LYS	2.1
1	B	257	GLU	2.1
1	A	181	THR	2.1
1	A	165	LEU	2.1
1	A	59	ASP	2.1
1	B	256	ASN	2.1
1	A	175	THR	2.1
1	B	35	ARG	2.1
1	B	89	SER	2.1
1	B	114	ALA	2.1
1	C	114	ALA	2.1
1	C	55	LYS	2.1
1	B	280	TYR	2.1
1	D	204	ILE	2.1
1	A	86	GLN	2.1
1	D	62	THR	2.1
1	C	207	ILE	2.1
1	A	57	TYR	2.1
1	A	298	PRO	2.1
1	B	328	PRO	2.1
1	C	331	ARG	2.1
1	D	55	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	85	ASP	2.0
1	A	262	LEU	2.0
1	A	322	LEU	2.0
1	C	288	ASP	2.0
1	A	136	PRO	2.0
1	D	64	VAL	2.0
1	A	185	PHE	2.0
1	B	7	TRP	2.0
1	A	62	THR	2.0
1	A	191	SER	2.0
1	A	91	LEU	2.0
1	C	318	ARG	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](#)

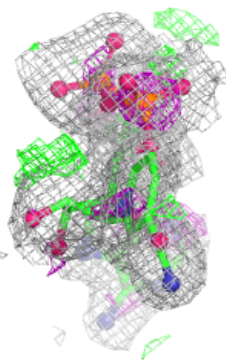
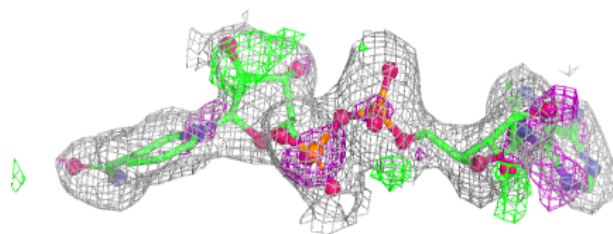
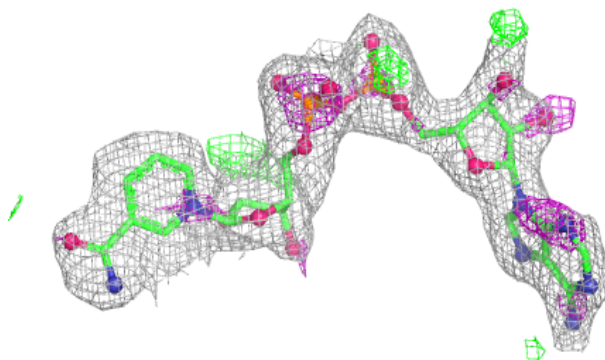
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	A	401	44/44	0.87	0.11	20,20,20,20	0
3	PO4	A	402	5/5	0.90	0.12	44,44,53,56	0
2	NAD	C	401	44/44	0.93	0.09	20,20,20,20	0
2	NAD	D	401	44/44	0.93	0.09	20,20,20,20	0
2	NAD	B	401	44/44	0.93	0.08	20,20,20,20	0
3	PO4	D	402	5/5	0.93	0.12	37,38,40,50	0

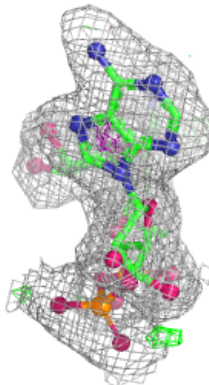
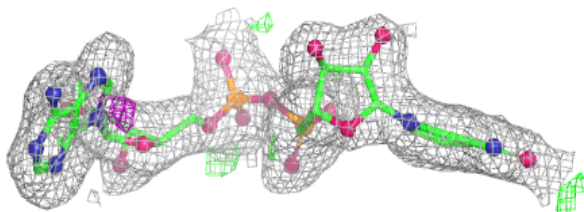
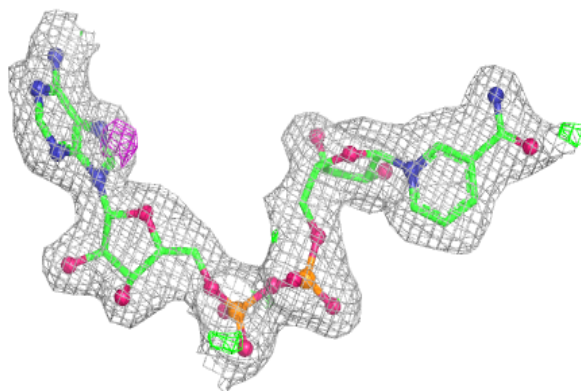
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD 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)

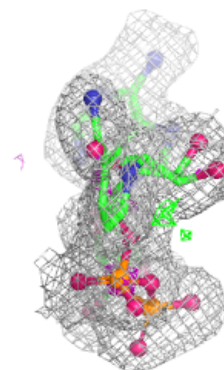
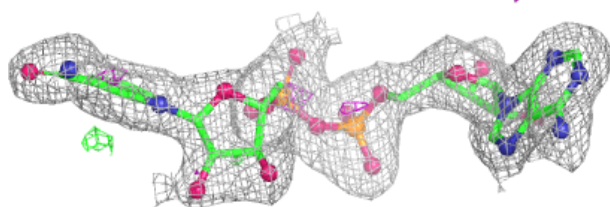
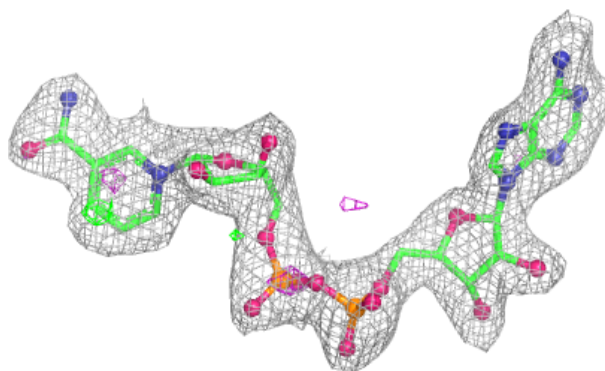
**Electron density around NAD C 401:**

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

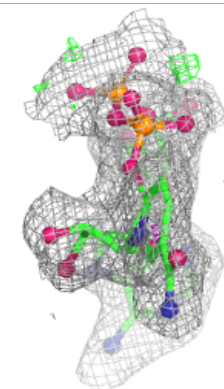
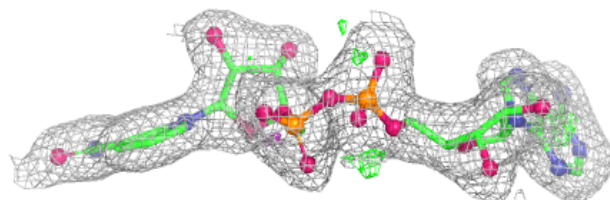
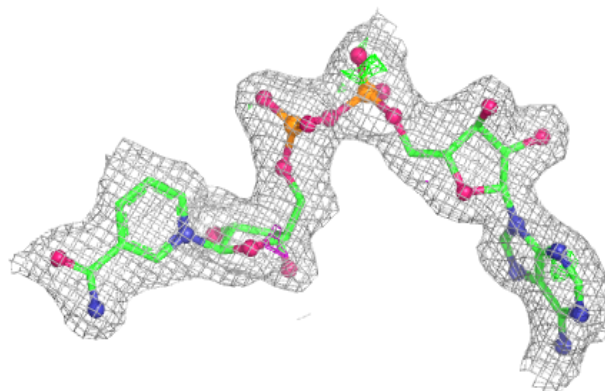


Electron density around NAD D 401:

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

**Electron density around NAD B 401:**

$2mF_o-DF_c$ (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.