



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:57 PM UTC

PDB ID : 9PG6 / pdb_00009pg6
Title : Crystal structure of Glyceraldehyde-3-phosphate dehydrogenase from *Bordetella pertussis* (NAD bound)
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2025-07-07
Resolution : 2.15 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

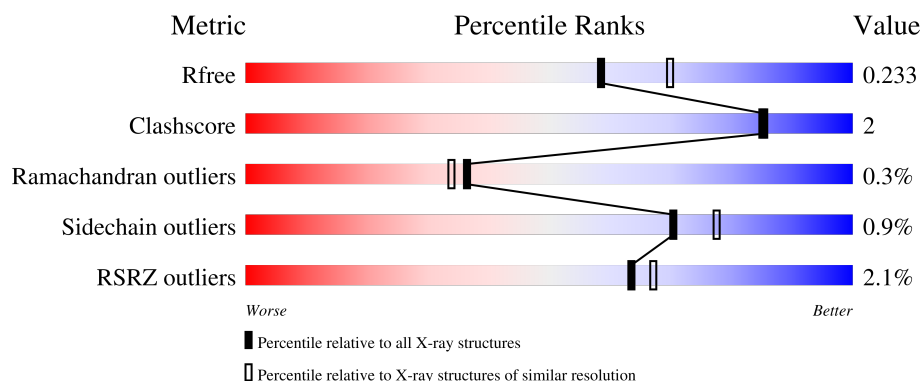
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	344	3% 93% 7% ..
1	B	344	2% 90% 7% ..
1	C	344	% 92% 5% .
1	D	344	2% 90% 8% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	344	3% 90% 8% •
1	F	344	2% 93% 5% •
1	G	344	% 93% 5% •
1	H	344	% 93% 5% ••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21477 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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	3	0
			2558	1608	447	494	9			
1	B	336	Total	C	N	O	S	0	4	0
			2573	1618	454	492	9			
1	C	336	Total	C	N	O	S	0	1	0
			2556	1608	446	492	10			
1	D	336	Total	C	N	O	S	0	4	0
			2573	1618	452	493	10			
1	E	336	Total	C	N	O	S	0	4	0
			2558	1608	449	492	9			
1	F	336	Total	C	N	O	S	0	2	0
			2553	1605	447	492	9			
1	G	336	Total	C	N	O	S	0	7	0
			2591	1629	458	495	9			
1	H	337	Total	C	N	O	S	0	3	0
			2574	1618	452	494	10			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q7VZB9
A	-6	ALA	-	expression tag	UNP Q7VZB9
A	-5	HIS	-	expression tag	UNP Q7VZB9
A	-4	HIS	-	expression tag	UNP Q7VZB9
A	-3	HIS	-	expression tag	UNP Q7VZB9
A	-2	HIS	-	expression tag	UNP Q7VZB9
A	-1	HIS	-	expression tag	UNP Q7VZB9
A	0	HIS	-	expression tag	UNP Q7VZB9
B	-7	MET	-	expression tag	UNP Q7VZB9
B	-6	ALA	-	expression tag	UNP Q7VZB9
B	-5	HIS	-	expression tag	UNP Q7VZB9
B	-4	HIS	-	expression tag	UNP Q7VZB9
B	-3	HIS	-	expression tag	UNP Q7VZB9

Continued on next page...

Continued from previous page...

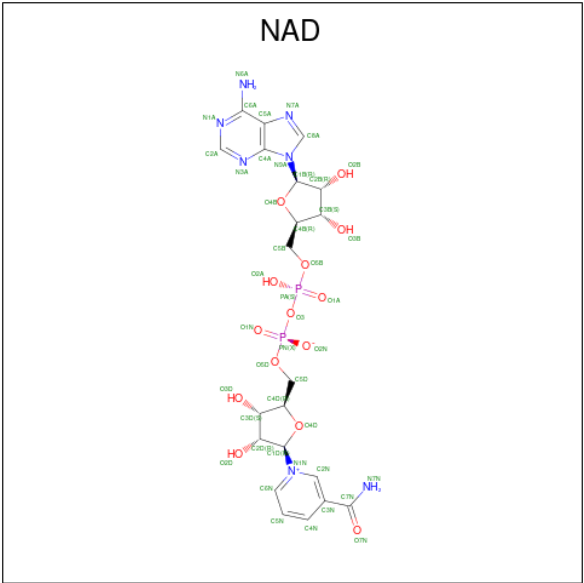
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q7VZB9
B	-1	HIS	-	expression tag	UNP Q7VZB9
B	0	HIS	-	expression tag	UNP Q7VZB9
C	-7	MET	-	expression tag	UNP Q7VZB9
C	-6	ALA	-	expression tag	UNP Q7VZB9
C	-5	HIS	-	expression tag	UNP Q7VZB9
C	-4	HIS	-	expression tag	UNP Q7VZB9
C	-3	HIS	-	expression tag	UNP Q7VZB9
C	-2	HIS	-	expression tag	UNP Q7VZB9
C	-1	HIS	-	expression tag	UNP Q7VZB9
C	0	HIS	-	expression tag	UNP Q7VZB9
D	-7	MET	-	expression tag	UNP Q7VZB9
D	-6	ALA	-	expression tag	UNP Q7VZB9
D	-5	HIS	-	expression tag	UNP Q7VZB9
D	-4	HIS	-	expression tag	UNP Q7VZB9
D	-3	HIS	-	expression tag	UNP Q7VZB9
D	-2	HIS	-	expression tag	UNP Q7VZB9
D	-1	HIS	-	expression tag	UNP Q7VZB9
D	0	HIS	-	expression tag	UNP Q7VZB9
E	-7	MET	-	expression tag	UNP Q7VZB9
E	-6	ALA	-	expression tag	UNP Q7VZB9
E	-5	HIS	-	expression tag	UNP Q7VZB9
E	-4	HIS	-	expression tag	UNP Q7VZB9
E	-3	HIS	-	expression tag	UNP Q7VZB9
E	-2	HIS	-	expression tag	UNP Q7VZB9
E	-1	HIS	-	expression tag	UNP Q7VZB9
E	0	HIS	-	expression tag	UNP Q7VZB9
F	-7	MET	-	expression tag	UNP Q7VZB9
F	-6	ALA	-	expression tag	UNP Q7VZB9
F	-5	HIS	-	expression tag	UNP Q7VZB9
F	-4	HIS	-	expression tag	UNP Q7VZB9
F	-3	HIS	-	expression tag	UNP Q7VZB9
F	-2	HIS	-	expression tag	UNP Q7VZB9
F	-1	HIS	-	expression tag	UNP Q7VZB9
F	0	HIS	-	expression tag	UNP Q7VZB9
G	-7	MET	-	expression tag	UNP Q7VZB9
G	-6	ALA	-	expression tag	UNP Q7VZB9
G	-5	HIS	-	expression tag	UNP Q7VZB9
G	-4	HIS	-	expression tag	UNP Q7VZB9
G	-3	HIS	-	expression tag	UNP Q7VZB9
G	-2	HIS	-	expression tag	UNP Q7VZB9
G	-1	HIS	-	expression tag	UNP Q7VZB9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q7VZB9
H	-7	MET	-	expression tag	UNP Q7VZB9
H	-6	ALA	-	expression tag	UNP Q7VZB9
H	-5	HIS	-	expression tag	UNP Q7VZB9
H	-4	HIS	-	expression tag	UNP Q7VZB9
H	-3	HIS	-	expression tag	UNP Q7VZB9
H	-2	HIS	-	expression tag	UNP Q7VZB9
H	-1	HIS	-	expression tag	UNP Q7VZB9
H	0	HIS	-	expression tag	UNP Q7VZB9

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

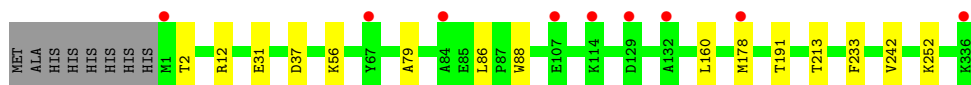
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total	O	0	0
			65	65		
4	B	62	Total	O	0	0
			62	62		
4	C	77	Total	O	0	0
			77	77		
4	D	80	Total	O	0	0
			80	80		
4	E	64	Total	O	0	0
			64	64		
4	F	70	Total	O	0	0
			70	70		
4	G	83	Total	O	0	0
			83	83		
4	H	83	Total	O	0	0
			83	83		

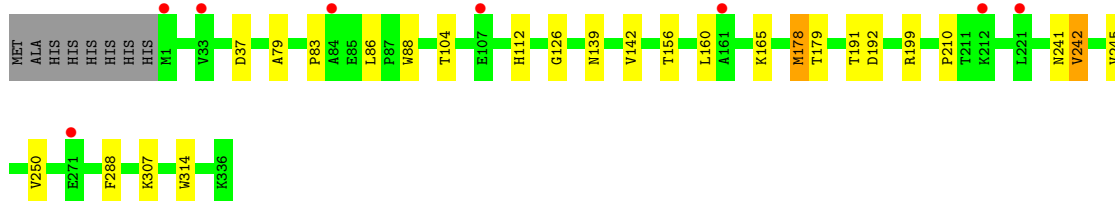
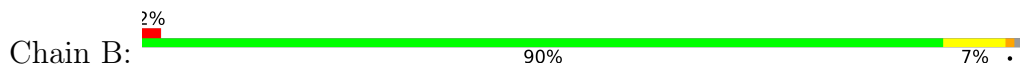
3 Residue-property plots [i](#)

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: Glyceraldehyde-3-phosphate dehydrogenase



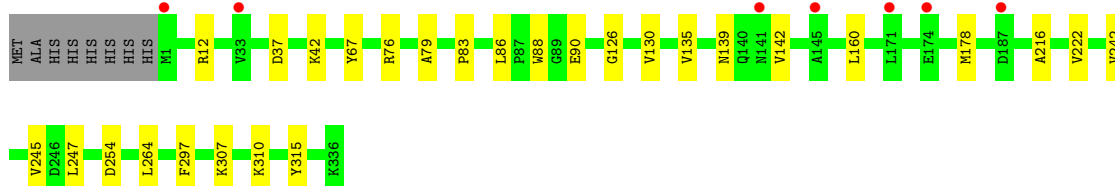
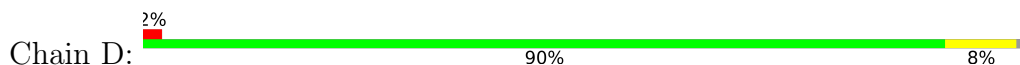
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



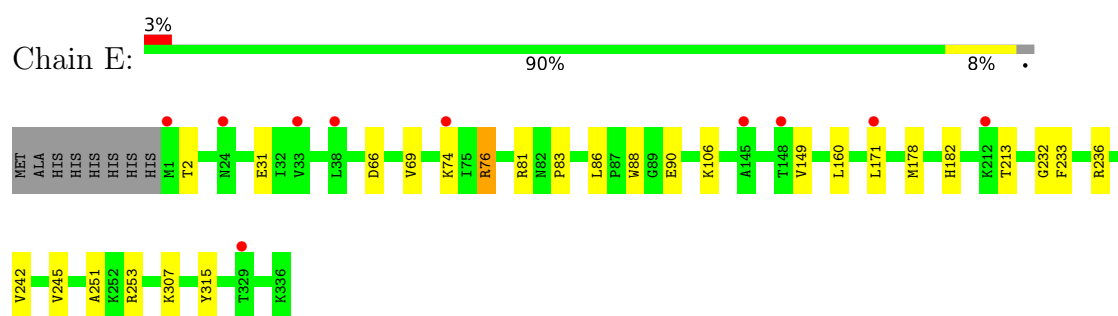
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



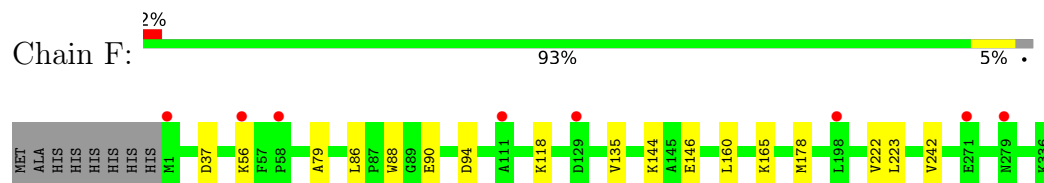
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



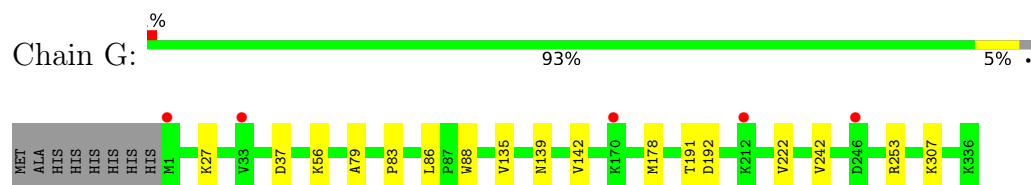
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



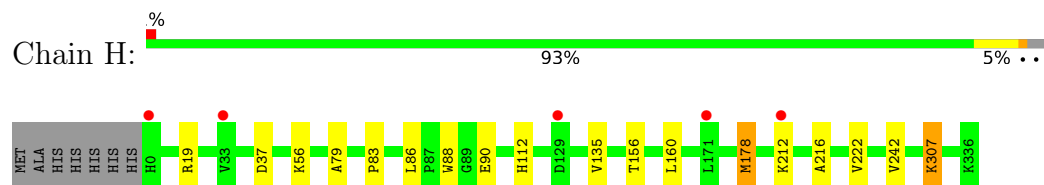
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.83Å 130.06Å 140.97Å 90.00° 90.86° 90.00°	Depositor
Resolution (Å)	49.03 – 2.15 49.03 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.03-2.15) 99.8 (49.03-2.15)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.16Å)	Xtriage
Refinement program	PHENIX (dev_5438: ???)	Depositor
R, R_{free}	0.193 , 0.230 0.199 , 0.233	Depositor DCC
R_{free} test set	7791 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21477	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1735e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.21	0/2611	0.43	0/3551
1	B	0.20	0/2629	0.41	0/3571
1	C	0.23	0/2603	0.46	0/3536
1	D	0.20	0/2629	0.44	0/3572
1	E	0.19	0/2614	0.41	0/3555
1	F	0.20	0/2603	0.43	0/3539
1	G	0.24	0/2656	0.45	0/3608
1	H	0.24	0/2628	0.44	0/3571
All	All	0.21	0/20973	0.43	0/28503

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	E	0	2
1	H	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	76[A]	ARG	Sidechain
1	E	76[B]	ARG	Sidechain
1	H	19	ARG	Sidechain

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	2558	0	2568	7	0
1	B	2573	0	2601	15	0
1	C	2556	0	2580	8	0
1	D	2573	0	2601	15	0
1	E	2558	0	2566	18	0
1	F	2553	0	2564	7	0
1	G	2591	0	2624	9	0
1	H	2574	0	2589	13	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	0	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
2	G	44	0	26	0	0
2	H	44	0	26	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	A	65	0	0	0	0
4	B	62	0	0	0	0
4	C	77	0	0	0	0
4	D	80	0	0	0	0
4	E	64	0	0	0	0
4	F	70	0	0	0	0
4	G	83	0	0	0	0
4	H	83	0	0	1	0
All	All	21477	0	20901	90	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 2.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LEU:HD22	1:B:178:MET:HE3	1.55	0.87
1:D:160:LEU:HD22	1:D:178:MET:HE3	1.65	0.77
1:H:160:LEU:HD22	1:H:178:MET:HE2	1.73	0.69
1:E:66:ASP:HB3	1:E:76[B]:ARG:HH21	1.57	0.69
1:E:160:LEU:HD22	1:E:178:MET:HE3	1.79	0.64
1:B:156:THR:HG22	1:B:178:MET:HE1	1.81	0.63
1:D:86:LEU:HD13	1:D:88:TRP:CZ2	2.38	0.59
1:E:251:ALA:O	1:E:307:LYS:CE	2.52	0.58
1:A:86:LEU:HD13	1:A:88:TRP:CZ2	2.39	0.58
1:E:86:LEU:HD13	1:E:88:TRP:CZ2	2.40	0.57
1:H:86:LEU:HD13	1:H:88:TRP:CZ2	2.39	0.57
1:B:156:THR:CG2	1:B:178:MET:HE1	2.35	0.56
1:E:251:ALA:O	1:E:307:LYS:HE3	2.05	0.56
1:E:83:PRO:HA	1:E:86:LEU:HD12	1.88	0.56
1:B:86:LEU:HD13	1:B:88:TRP:CZ2	2.40	0.56
1:F:160:LEU:HD22	1:F:178:MET:HE3	1.88	0.56
1:F:165:LYS:HD2	1:F:223:LEU:HD21	1.89	0.55
1:H:37:ASP:O	1:H:79:ALA:HA	2.08	0.53
1:C:135:VAL:HG23	1:C:222:VAL:HG11	1.90	0.53
1:D:135:VAL:HG23	1:D:222:VAL:HG11	1.90	0.53
1:D:37:ASP:O	1:D:79:ALA:HA	2.08	0.53
1:E:171:LEU:HD23	1:E:253:ARG:NH2	2.26	0.51
1:E:178:MET:HE2	1:E:245:VAL:HG13	1.94	0.50
1:C:86:LEU:HD13	1:C:88:TRP:CZ2	2.47	0.50
1:C:37:ASP:O	1:C:79:ALA:HA	2.12	0.48
1:E:69:VAL:HG22	1:E:74:LYS:HG2	1.95	0.48
1:D:264:LEU:HD13	1:D:297:PHE:CE1	2.49	0.48
1:F:86:LEU:HD13	1:F:88:TRP:CZ2	2.48	0.48
1:B:37:ASP:O	1:B:79:ALA:HA	2.14	0.48
1:G:86:LEU:HD13	1:G:88:TRP:CZ2	2.49	0.47
1:F:94:ASP:OD1	1:F:118:LYS:HE3	2.15	0.47
1:F:144:LYS:NZ	1:F:146:GLU:OE2	2.40	0.47
1:E:251:ALA:O	1:E:307:LYS:HE2	2.14	0.47
1:G:37:ASP:O	1:G:79:ALA:HA	2.14	0.47
1:H:135:VAL:HG23	1:H:222:VAL:HG11	1.96	0.47
1:H:83:PRO:HB3	1:H:112:HIS:CE1	2.49	0.47
1:H:156:THR:CG2	1:H:178:MET:HE1	2.46	0.46
1:H:212:LYS:HD2	4:H:533:HOH:O	2.14	0.46
1:D:83:PRO:HA	1:D:86:LEU:HD12	1.97	0.46
1:D:254:ASP:OD1	1:D:307:LYS:HG3	2.15	0.46
1:H:83:PRO:HA	1:H:86:LEU:HD12	1.98	0.46
1:C:111:ALA:HA	1:C:114:LYS:HG3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:LYS:HA	1:E:149:VAL:HG11	1.98	0.45
1:C:10:TYR:CE2	1:C:15:ARG:HG2	2.52	0.45
1:G:139:ASN:O	1:G:142:VAL:HG22	2.17	0.45
1:G:253:ARG:HA	1:G:307:LYS:HE3	1.98	0.45
1:E:106:LYS:HG3	1:E:149:VAL:HB	1.98	0.45
1:C:83:PRO:HA	1:C:86:LEU:HD12	1.98	0.45
1:B:139:ASN:O	1:B:142:VAL:HG22	2.17	0.45
1:A:37:ASP:O	1:A:79:ALA:HA	2.17	0.45
1:B:83:PRO:HB3	1:B:112:HIS:CE1	2.53	0.44
1:E:66:ASP:HB3	1:E:76[B]:ARG:NH2	2.30	0.44
1:F:37:ASP:O	1:F:79:ALA:HA	2.18	0.44
1:F:135:VAL:HG23	1:F:222:VAL:HG11	2.00	0.44
1:A:12:ARG:HG2	2:A:401:NAD:O2A	2.18	0.43
1:D:67:TYR:CE2	1:D:76[B]:ARG:HG2	2.53	0.43
1:E:2:THR:HG21	1:E:31:GLU:HG2	1.99	0.43
1:H:307:LYS:HB3	1:H:307:LYS:HE3	1.86	0.43
1:B:250:VAL:CG1	1:B:307:LYS:HE2	2.48	0.43
1:D:126:GLY:HA3	1:D:130:VAL:HG11	2.00	0.43
1:A:160:LEU:HD22	1:A:178:MET:SD	2.59	0.43
1:H:178:MET:HG2	1:H:216:ALA:HB2	2.01	0.43
1:D:160:LEU:HD11	1:D:247:LEU:HD22	2.00	0.42
1:D:245:VAL:HG23	1:D:315:TYR:CE1	2.54	0.42
1:G:178:MET:HE2	1:G:178:MET:HB2	1.88	0.42
1:B:179:THR:OG1	1:D:310:LYS:HE2	2.19	0.42
1:E:213:THR:HG22	1:E:233:PHE:HA	2.00	0.42
1:A:191:THR:HG23	1:D:12:ARG:HD3	2.02	0.41
1:G:88:TRP:HA	1:G:88:TRP:CE3	2.55	0.41
1:G:191:THR:O	1:G:192:ASP:C	2.63	0.41
1:H:86:LEU:HD13	1:H:88:TRP:HZ2	1.84	0.41
1:A:213:THR:HG22	1:A:233:PHE:HA	2.02	0.41
1:B:178:MET:HE2	1:B:245:VAL:HG22	2.03	0.41
1:B:191:THR:O	1:B:192:ASP:C	2.63	0.41
1:E:178:MET:HG3	1:E:232:GLY:HA3	2.02	0.41
1:A:2:THR:HG21	1:A:31:GLU:HG2	2.02	0.41
1:B:199[A]:ARG:HD2	1:B:210:PRO:O	2.20	0.41
1:E:182:HIS:HB3	1:E:236:ARG:HD3	2.03	0.41
1:G:83:PRO:HA	1:G:86:LEU:HD12	2.02	0.41
1:B:288:PHE:CE2	1:B:314:TRP:CD1	3.08	0.41
1:C:178:MET:HG2	1:C:179:THR:N	2.36	0.41
1:D:178:MET:HG2	1:D:216:ALA:HB2	2.03	0.41
1:H:88:TRP:CE3	1:H:88:TRP:HA	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:HIS:HB3	1:C:236:ARG:HD3	2.03	0.40
1:D:139:ASN:O	1:D:142:VAL:HG22	2.21	0.40
1:B:104:THR:O	1:B:126:GLY:HA2	2.20	0.40
1:E:245:VAL:HG23	1:E:315:TYR:CE1	2.56	0.40
1:B:241:ASN:O	1:B:242:VAL:HB	2.22	0.40
1:G:135:VAL:HG23	1:G:222:VAL:HG11	2.02	0.40
1:H:88:TRP:HA	1:H:88:TRP:HE3	1.87	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	337/344 (98%)	328 (97%)	8 (2%)	1 (0%)	36	34
1	B	338/344 (98%)	328 (97%)	9 (3%)	1 (0%)	36	34
1	C	335/344 (97%)	325 (97%)	9 (3%)	1 (0%)	36	34
1	D	338/344 (98%)	328 (97%)	9 (3%)	1 (0%)	36	34
1	E	338/344 (98%)	330 (98%)	7 (2%)	1 (0%)	36	34
1	F	336/344 (98%)	326 (97%)	9 (3%)	1 (0%)	36	34
1	G	341/344 (99%)	332 (97%)	8 (2%)	1 (0%)	36	34
1	H	338/344 (98%)	328 (97%)	9 (3%)	1 (0%)	36	34
All	All	2701/2752 (98%)	2625 (97%)	68 (2%)	8 (0%)	36	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	VAL
1	B	242	VAL
1	C	242	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	242	VAL
1	E	242	VAL
1	F	242	VAL
1	G	242	VAL
1	H	242	VAL

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	279/286 (98%)	277 (99%)	2 (1%)	76	82
1	B	281/286 (98%)	279 (99%)	2 (1%)	76	82
1	C	280/286 (98%)	276 (99%)	4 (1%)	59	66
1	D	282/286 (99%)	280 (99%)	2 (1%)	76	82
1	E	278/286 (97%)	276 (99%)	2 (1%)	76	82
1	F	278/286 (97%)	276 (99%)	2 (1%)	76	82
1	G	284/286 (99%)	282 (99%)	2 (1%)	76	82
1	H	281/286 (98%)	277 (99%)	4 (1%)	59	66
All	All	2243/2288 (98%)	2223 (99%)	20 (1%)	70	77

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	252	LYS
1	B	165	LYS
1	B	178	MET
1	C	27	LYS
1	C	56	LYS
1	C	107	GLU
1	C	114	LYS
1	D	42	LYS
1	D	90	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	81	ARG
1	E	90	GLU
1	F	56	LYS
1	F	90	GLU
1	G	27	LYS
1	G	56	LYS
1	H	56	LYS
1	H	90	GLU
1	H	178	MET
1	H	307	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	296	ASN
1	F	241	ASN
1	F	289	ASN
1	G	227	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	C	401	-	46,48,48	1.16	2 (4%)	64,73,73	0.91	2 (3%)
2	NAD	B	401	-	46,48,48	1.14	2 (4%)	64,73,73	0.94	2 (3%)
2	NAD	A	401	-	46,48,48	1.20	2 (4%)	64,73,73	0.95	3 (4%)
2	NAD	G	401	-	46,48,48	1.17	3 (6%)	64,73,73	0.97	5 (7%)
2	NAD	H	401	-	46,48,48	1.09	1 (2%)	64,73,73	0.94	3 (4%)
2	NAD	F	401	-	46,48,48	1.18	2 (4%)	64,73,73	1.01	5 (7%)
2	NAD	E	401	-	46,48,48	1.13	2 (4%)	64,73,73	0.91	3 (4%)
2	NAD	D	401	-	46,48,48	1.05	3 (6%)	64,73,73	1.03	4 (6%)

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	-	-	4/30/62/62	0/5/5/5
2	NAD	B	401	-	-	9/30/62/62	0/5/5/5
2	NAD	A	401	-	-	4/30/62/62	0/5/5/5
2	NAD	G	401	-	-	5/30/62/62	0/5/5/5
2	NAD	H	401	-	-	6/30/62/62	0/5/5/5
2	NAD	F	401	-	-	4/30/62/62	0/5/5/5
2	NAD	E	401	-	-	6/30/62/62	0/5/5/5
2	NAD	D	401	-	-	4/30/62/62	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	PA-O3	5.95	1.65	1.59
2	F	401	NAD	PA-O3	5.79	1.65	1.59
2	G	401	NAD	PA-O3	5.69	1.65	1.59
2	C	401	NAD	PA-O3	5.67	1.65	1.59
2	H	401	NAD	PA-O3	5.53	1.65	1.59
2	B	401	NAD	PA-O3	5.47	1.65	1.59
2	E	401	NAD	PA-O3	5.13	1.65	1.59
2	D	401	NAD	PA-O3	5.12	1.65	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	NAD	PN-O3	3.48	1.63	1.59
2	F	401	NAD	PN-O3	3.26	1.63	1.59
2	A	401	NAD	PN-O3	3.20	1.62	1.59
2	G	401	NAD	PN-O3	3.16	1.62	1.59
2	B	401	NAD	PN-O3	3.13	1.62	1.59
2	C	401	NAD	PN-O3	3.12	1.62	1.59
2	D	401	NAD	O4D-C1D	-2.18	1.38	1.40
2	D	401	NAD	PN-O3	2.17	1.61	1.59
2	G	401	NAD	O4D-C1D	-2.15	1.38	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAD	O3-PA-O1A	-3.31	100.75	110.70
2	H	401	NAD	O3-PA-O1A	-2.85	102.13	110.70
2	D	401	NAD	O2A-PA-O1A	2.64	124.72	112.44
2	F	401	NAD	O3-PA-O1A	-2.59	102.92	110.70
2	B	401	NAD	O2A-PA-O1A	2.59	124.47	112.44
2	H	401	NAD	O2A-PA-O1A	2.55	124.30	112.44
2	A	401	NAD	O2A-PA-O1A	2.54	124.28	112.44
2	F	401	NAD	O7N-C7N-N7N	2.53	126.27	122.62
2	G	401	NAD	O2A-PA-O1A	2.50	124.06	112.44
2	C	401	NAD	O2A-PA-O1A	2.43	123.75	112.44
2	G	401	NAD	O7N-C7N-N7N	2.41	126.10	122.62
2	E	401	NAD	O2A-PA-O1A	2.41	123.65	112.44
2	C	401	NAD	O3-PA-O1A	-2.37	103.56	110.70
2	F	401	NAD	C2B-C1B-N9A	2.31	119.04	113.30
2	E	401	NAD	O7N-C7N-N7N	2.25	125.87	122.62
2	A	401	NAD	O3-PA-O1A	-2.16	104.20	110.70
2	F	401	NAD	O7N-C7N-C3N	-2.15	116.97	119.60
2	D	401	NAD	C2B-C1B-N9A	2.14	118.62	113.30
2	G	401	NAD	O7N-C7N-C3N	-2.12	117.01	119.60
2	F	401	NAD	O2A-PA-O1A	2.11	122.26	112.44
2	A	401	NAD	O7N-C7N-N7N	2.11	125.66	122.62
2	D	401	NAD	C6N-N1N-C1D	-2.10	115.60	119.73
2	G	401	NAD	O3-PA-O1A	-2.09	104.42	110.70
2	E	401	NAD	O3-PA-O1A	-2.07	104.48	110.70
2	H	401	NAD	C6N-N1N-C1D	-2.05	115.70	119.73
2	B	401	NAD	C2B-C1B-N9A	2.04	118.38	113.30
2	G	401	NAD	C6N-N1N-C1D	-2.02	115.77	119.73

There are no chirality outliers.

All (42) torsion outliers are listed below:

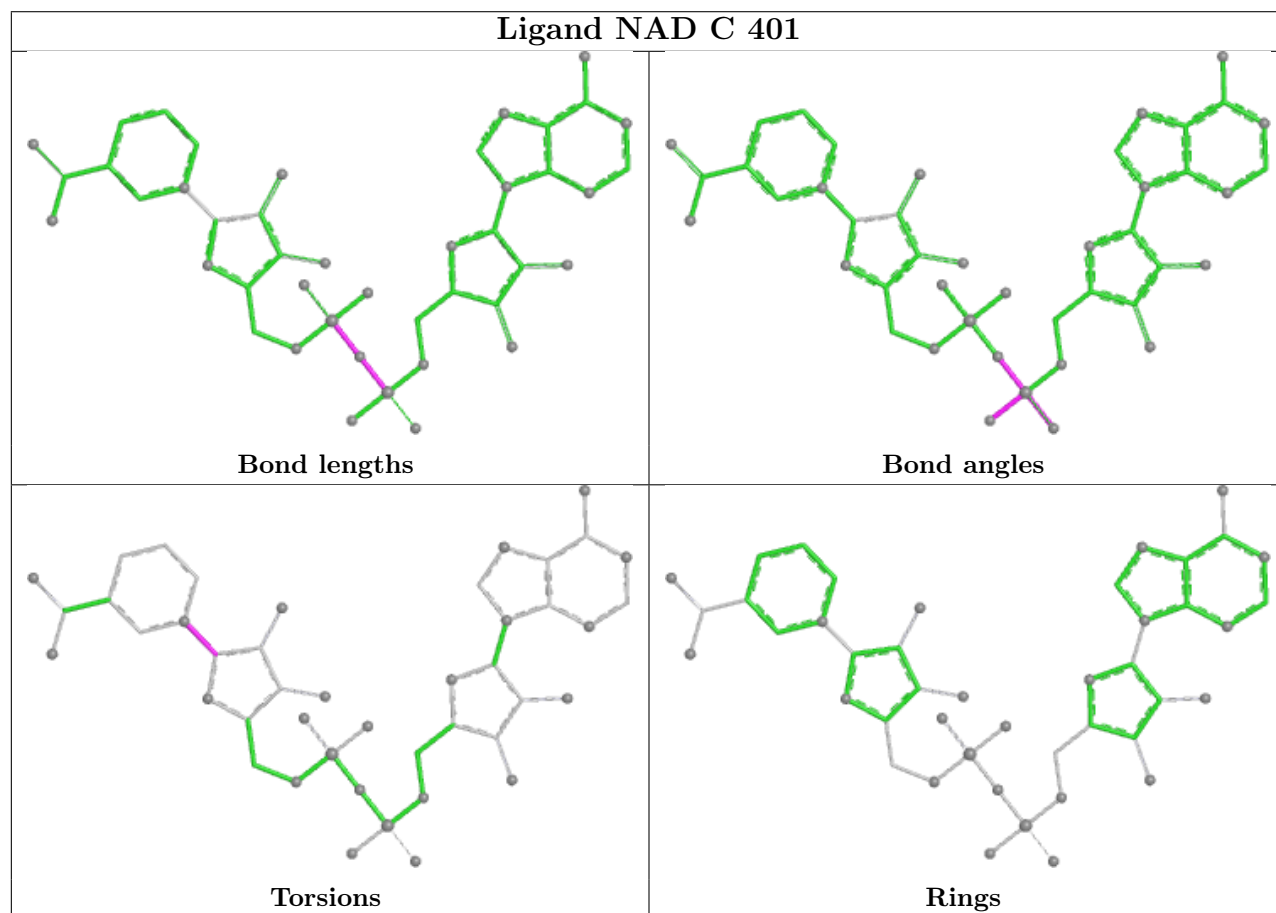
Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	C5B-O5B-PA-O1A
2	B	401	NAD	C5D-O5D-PN-O2N
2	B	401	NAD	O4D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	C2D-C1D-N1N-C2N
2	B	401	NAD	C2D-C1D-N1N-C6N
2	C	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	C2D-C1D-N1N-C6N
2	D	401	NAD	O4D-C1D-N1N-C2N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	C2D-C1D-N1N-C6N
2	E	401	NAD	O4D-C1D-N1N-C2N
2	E	401	NAD	O4D-C1D-N1N-C6N
2	E	401	NAD	C2D-C1D-N1N-C6N
2	F	401	NAD	O4D-C1D-N1N-C2N
2	F	401	NAD	O4D-C1D-N1N-C6N
2	G	401	NAD	O4D-C1D-N1N-C2N
2	G	401	NAD	O4D-C1D-N1N-C6N
2	G	401	NAD	C2D-C1D-N1N-C2N
2	G	401	NAD	C2D-C1D-N1N-C6N
2	H	401	NAD	O4D-C1D-N1N-C2N
2	H	401	NAD	O4D-C1D-N1N-C6N
2	H	401	NAD	C2D-C1D-N1N-C2N
2	H	401	NAD	C2D-C1D-N1N-C6N
2	B	401	NAD	C5D-O5D-PN-O3
2	H	401	NAD	C5D-O5D-PN-O2N
2	A	401	NAD	C2D-C1D-N1N-C6N
2	C	401	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	C2D-C1D-N1N-C2N
2	E	401	NAD	C2D-C1D-N1N-C2N
2	F	401	NAD	C2D-C1D-N1N-C6N
2	H	401	NAD	O4B-C4B-C5B-O5B
2	E	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	O4B-C4B-C5B-O5B
2	G	401	NAD	C2B-C1B-N9A-C8A
2	A	401	NAD	C2B-C1B-N9A-C8A
2	E	401	NAD	C2B-C1B-N9A-C8A
2	B	401	NAD	C2B-C1B-N9A-C8A
2	F	401	NAD	C2B-C1B-N9A-C8A

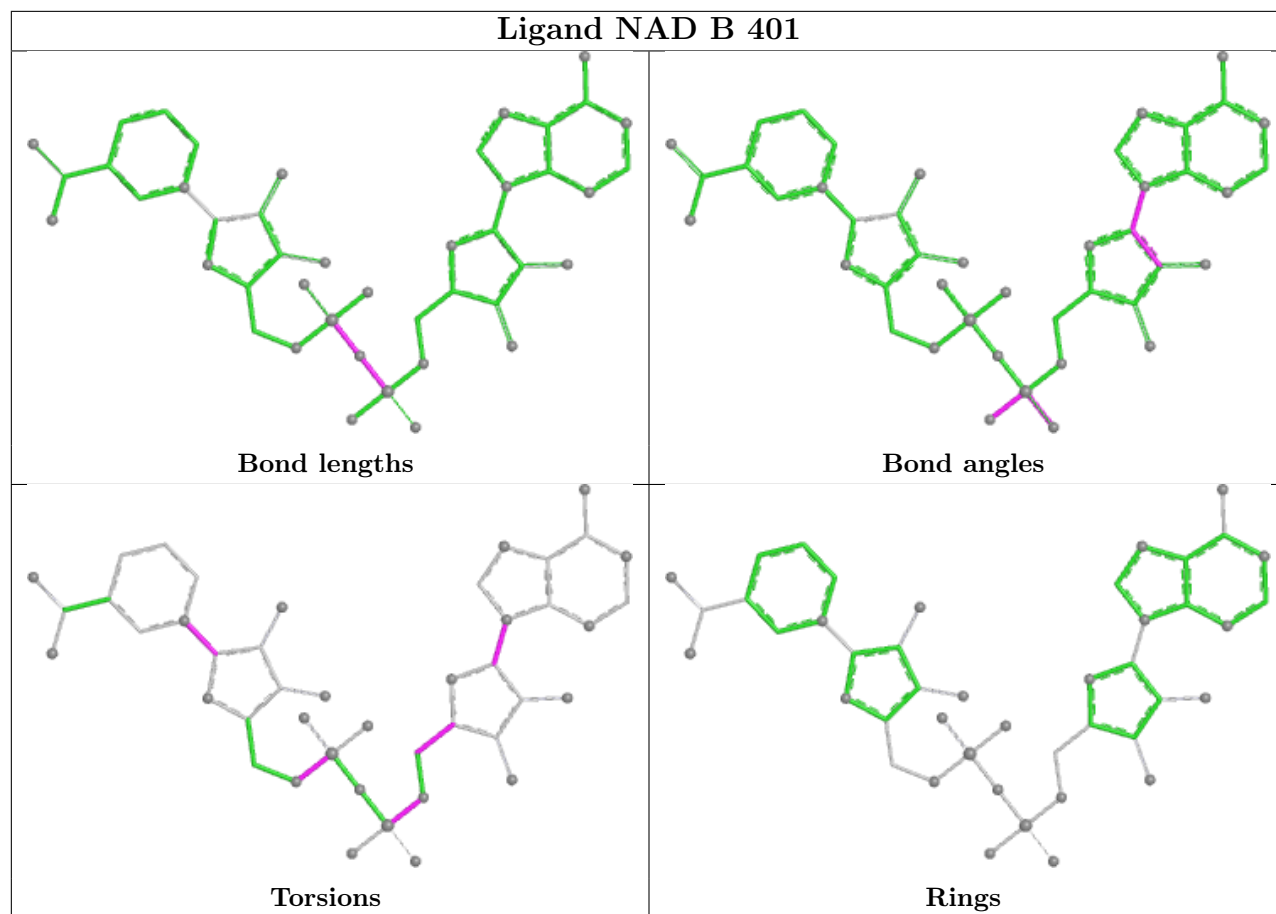
There are no ring outliers.

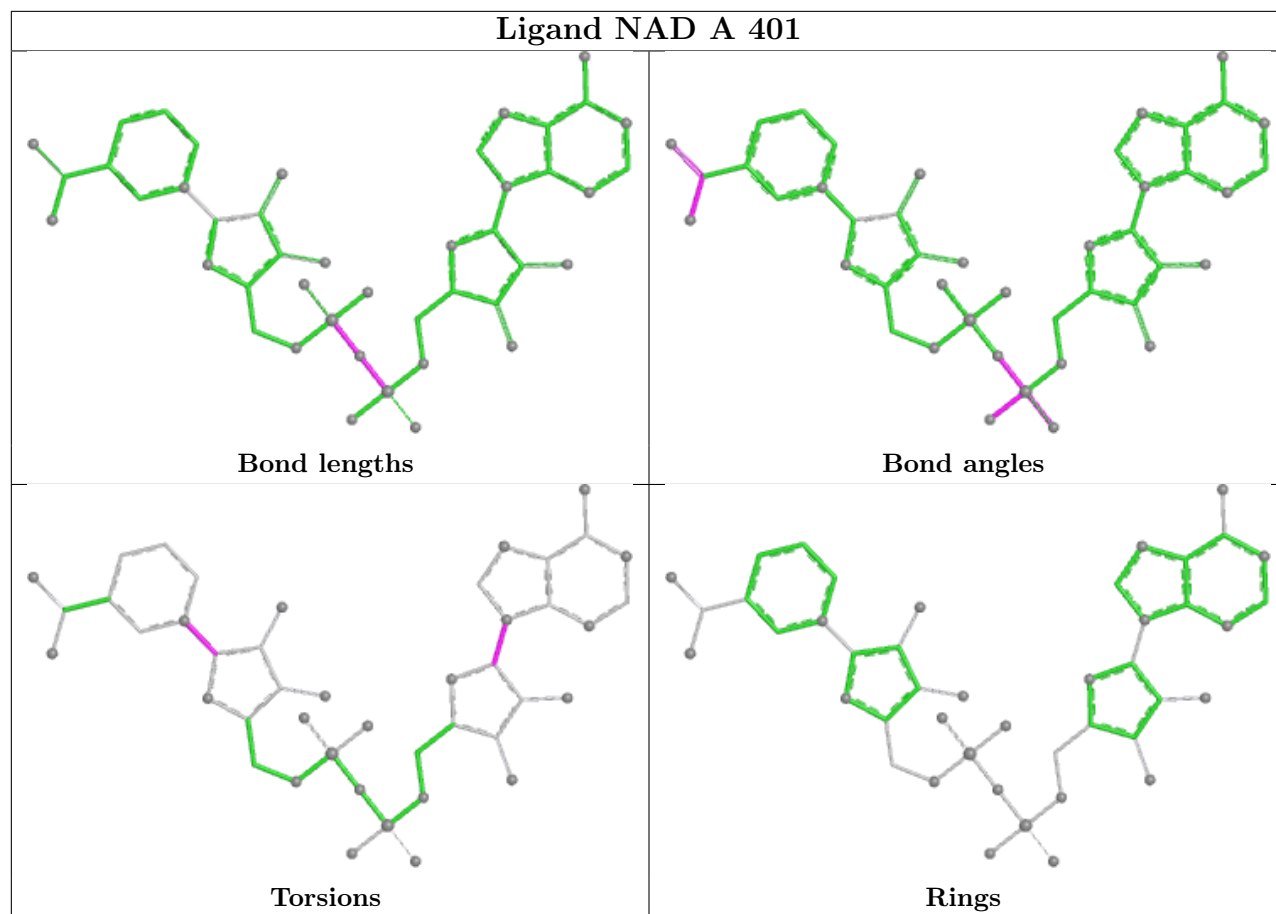
1 monomer is involved in 1 short contact:

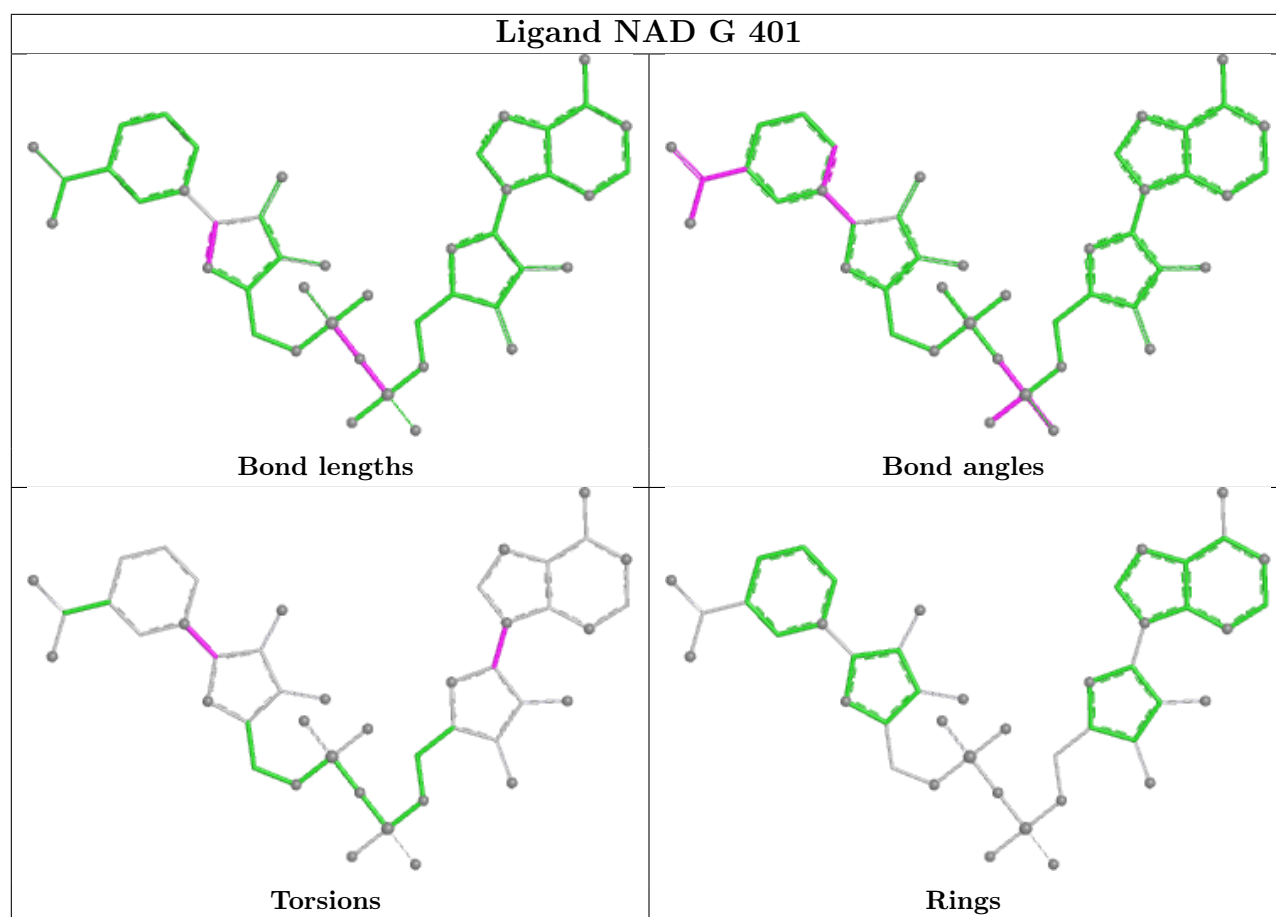
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAD	1	0

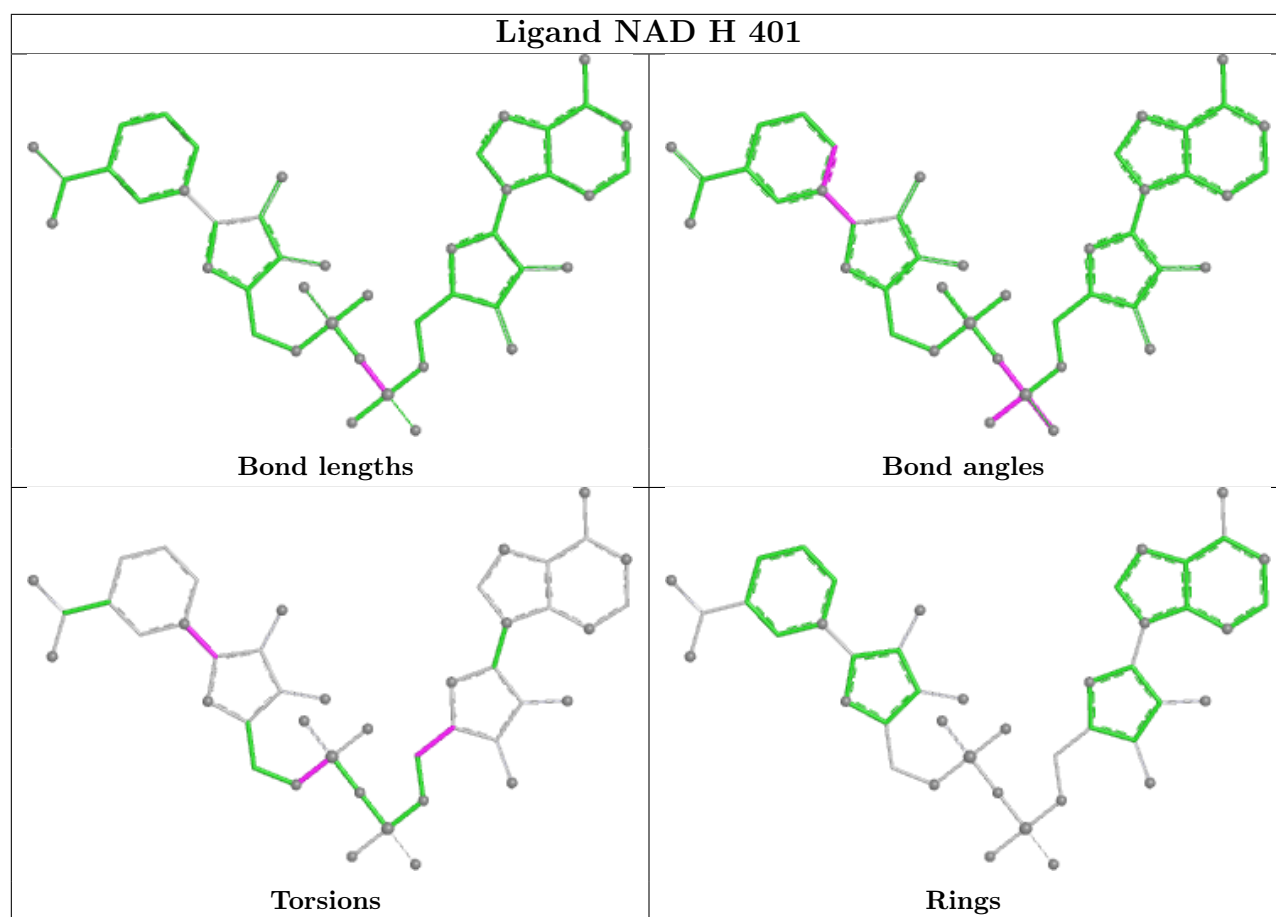
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

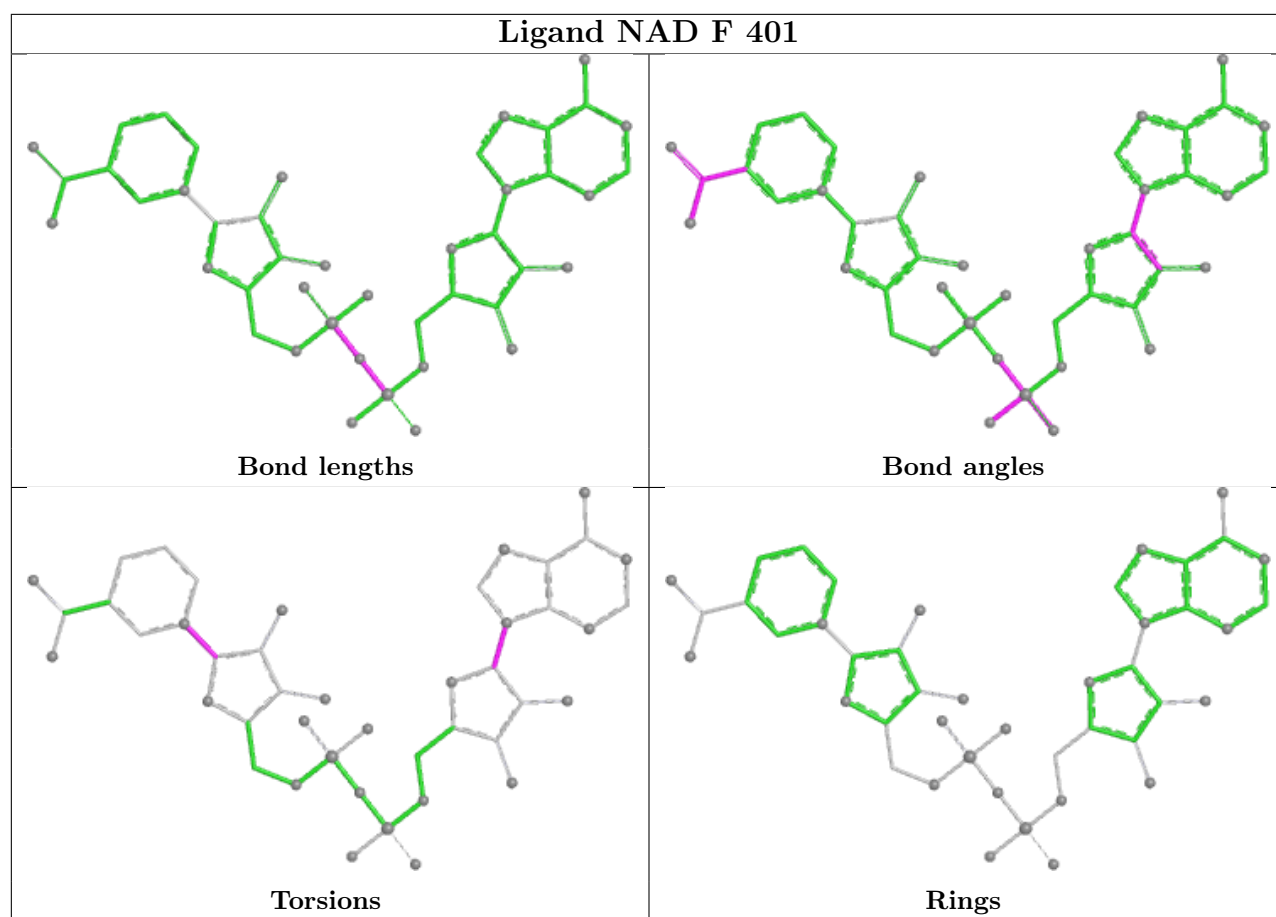


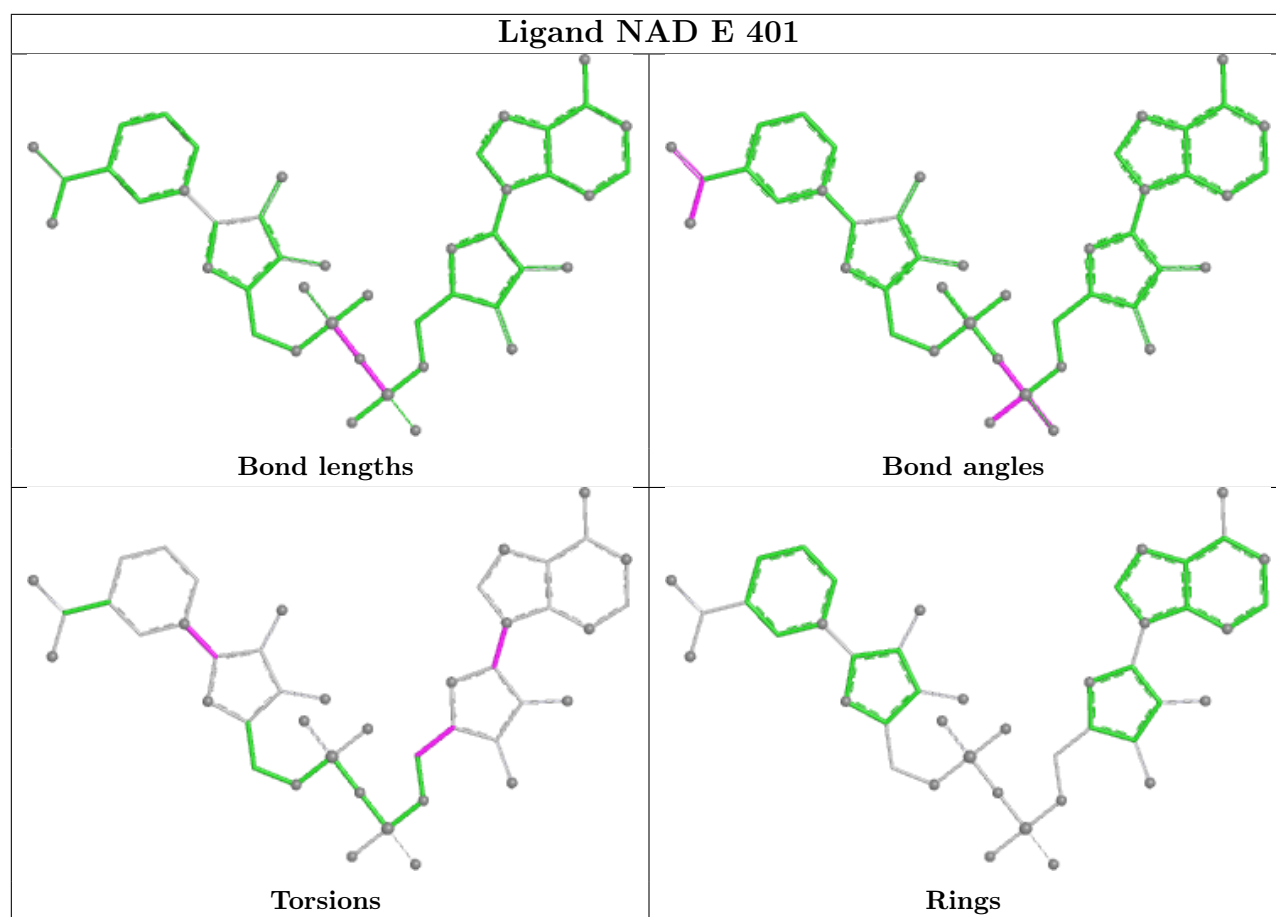


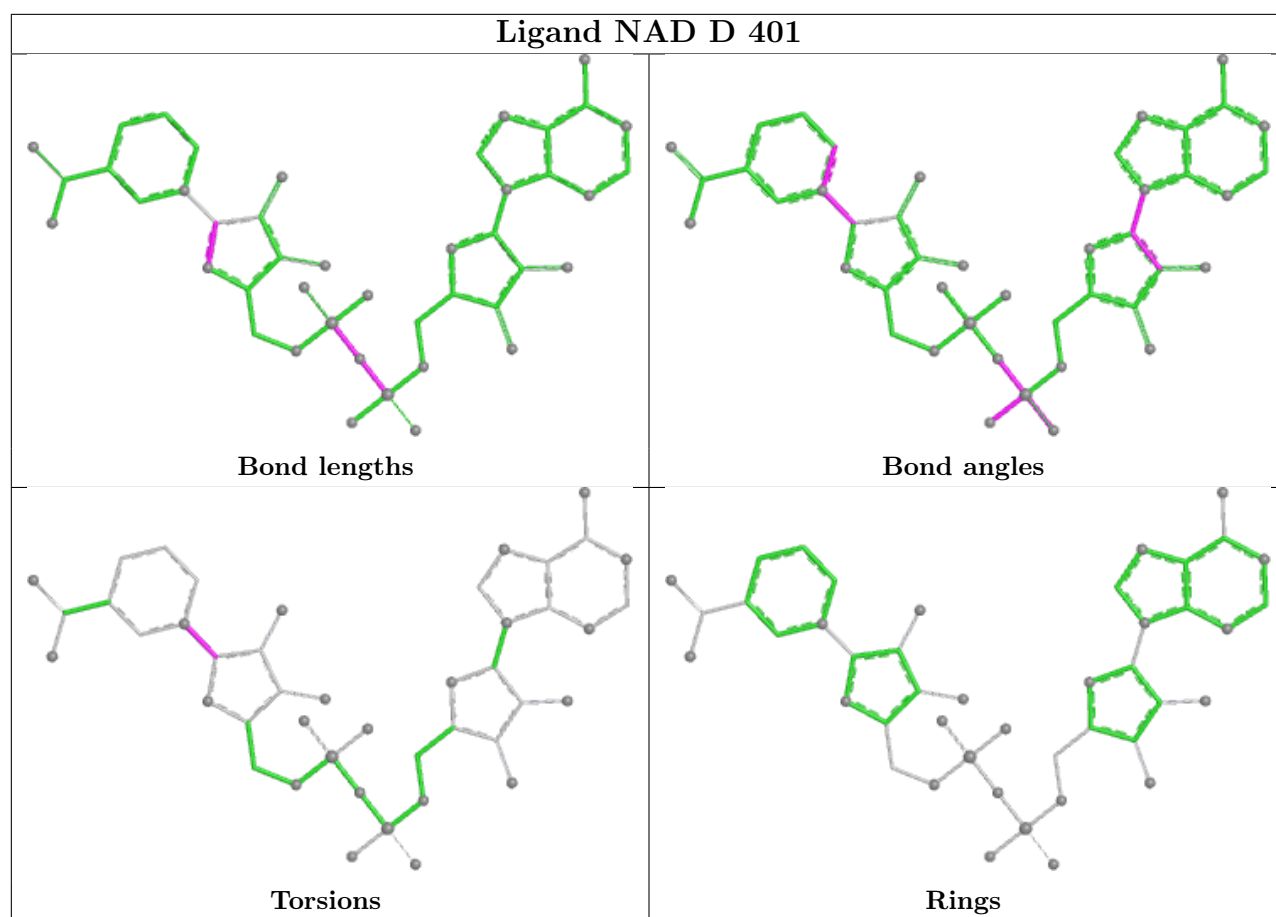












5.7 Other polymers [i](#)

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	336/344 (97%)	0.48	9 (2%)	56	60	23, 38, 57, 82	3 (0%)
1	B	336/344 (97%)	0.53	8 (2%)	59	63	17, 39, 58, 78	4 (1%)
1	C	336/344 (97%)	0.40	4 (1%)	76	79	20, 34, 53, 81	1 (0%)
1	D	336/344 (97%)	0.41	7 (2%)	63	67	20, 35, 54, 82	4 (1%)
1	E	336/344 (97%)	0.66	10 (2%)	52	56	16, 39, 59, 89	4 (1%)
1	F	336/344 (97%)	0.60	8 (2%)	59	63	16, 39, 57, 85	2 (0%)
1	G	336/344 (97%)	0.45	5 (1%)	72	76	18, 34, 53, 69	7 (2%)
1	H	337/344 (97%)	0.35	5 (1%)	72	76	20, 34, 53, 96	3 (0%)
All	All	2689/2752 (97%)	0.49	56 (2%)	63	67	16, 37, 56, 96	28 (1%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	129	ASP	4.0
1	D	171	LEU	3.6
1	A	67	TYR	3.5
1	C	1	MET	3.4
1	B	212	LYS	3.1
1	G	170	LYS	3.0
1	E	145	ALA	3.0
1	A	1	MET	2.8
1	G	1	MET	2.8
1	H	129	ASP	2.8
1	B	33	VAL	2.8
1	H	212	LYS	2.8
1	D	187	ASP	2.8
1	D	1	MET	2.7
1	B	221	LEU	2.7
1	E	33	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	0	HIS	2.7
1	F	129	ASP	2.7
1	F	58	PRO	2.7
1	E	1	MET	2.7
1	F	1	MET	2.6
1	B	84	ALA	2.6
1	B	107	GLU	2.6
1	E	24	ASN	2.5
1	C	107	GLU	2.5
1	F	271	GLU	2.5
1	E	171	LEU	2.5
1	A	178	MET	2.4
1	F	198	LEU	2.4
1	G	212	LYS	2.4
1	H	171	LEU	2.4
1	B	271	GLU	2.4
1	G	246	ASP	2.4
1	G	33	VAL	2.4
1	A	132	ALA	2.3
1	A	107	GLU	2.3
1	H	33	VAL	2.3
1	A	84	ALA	2.3
1	A	114	LYS	2.3
1	F	111	ALA	2.3
1	C	102	PHE	2.2
1	E	212	LYS	2.2
1	B	1	MET	2.2
1	D	174	GLU	2.2
1	A	336	LYS	2.2
1	A	129	ASP	2.2
1	E	74	LYS	2.2
1	D	145	ALA	2.1
1	E	38	LEU	2.1
1	F	279[A]	ASN	2.1
1	E	148	THR	2.1
1	E	329	THR	2.1
1	D	33	VAL	2.1
1	D	141	ASN	2.1
1	B	161	ALA	2.1
1	F	56	LYS	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](#)

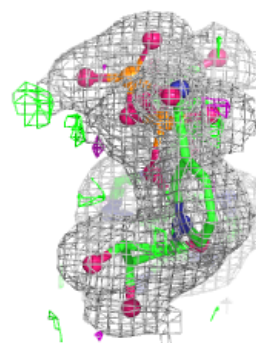
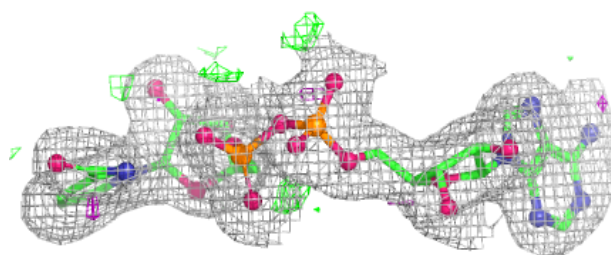
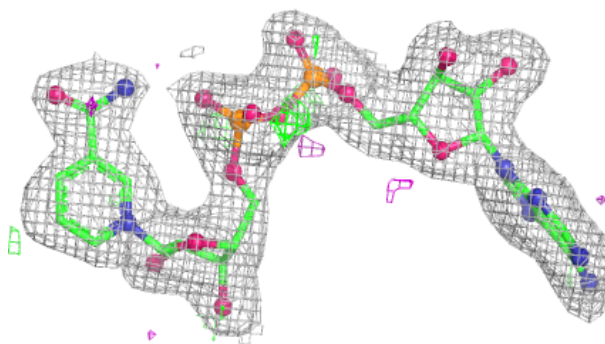
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	MG	B	402	1/1	0.74	0.19	53,53,53,53	0
3	MG	A	402	1/1	0.89	0.18	57,57,57,57	0
3	MG	D	402	1/1	0.91	0.04	30,30,30,30	0
3	MG	F	402	1/1	0.94	0.05	53,53,53,53	0
2	NAD	A	401	44/44	0.95	0.08	25,32,39,41	0
2	NAD	F	401	44/44	0.95	0.07	23,32,37,43	0
2	NAD	G	401	44/44	0.96	0.06	18,26,31,35	0
2	NAD	H	401	44/44	0.96	0.06	20,28,31,35	0
2	NAD	C	401	44/44	0.96	0.07	23,29,35,38	0
2	NAD	D	401	44/44	0.96	0.07	20,28,32,34	0
2	NAD	E	401	44/44	0.96	0.07	28,35,40,42	0
2	NAD	B	401	44/44	0.96	0.07	24,31,36,42	0
3	MG	H	402	1/1	0.99	0.03	31,31,31,31	0

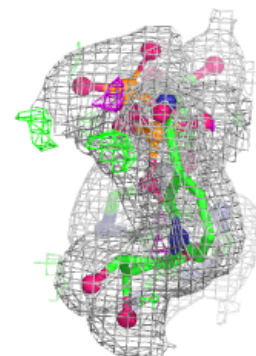
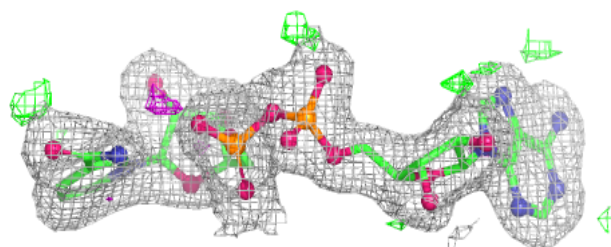
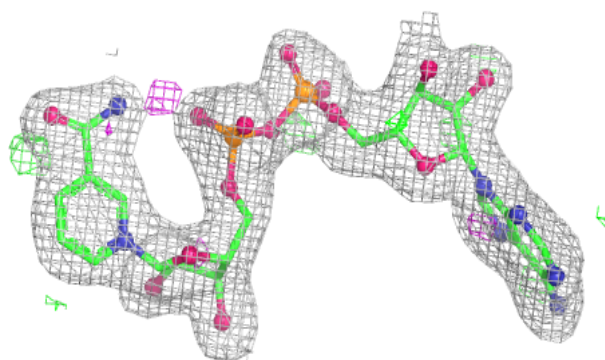
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

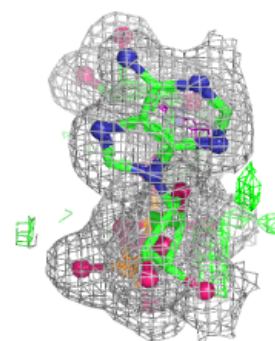
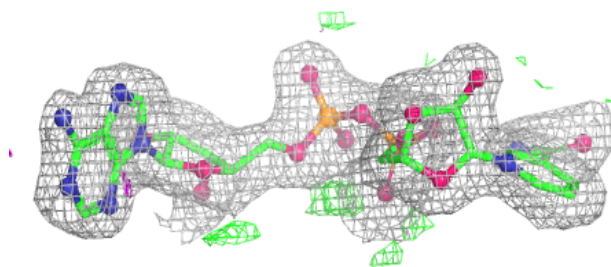
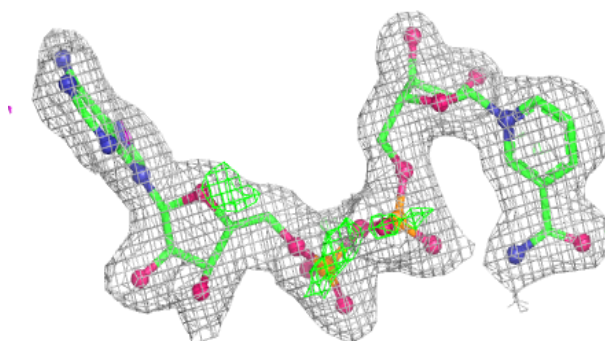
**Electron density around NAD F 401:**

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

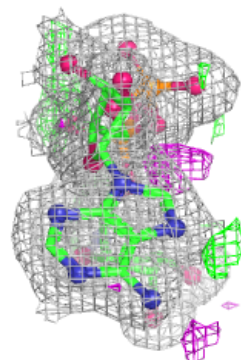
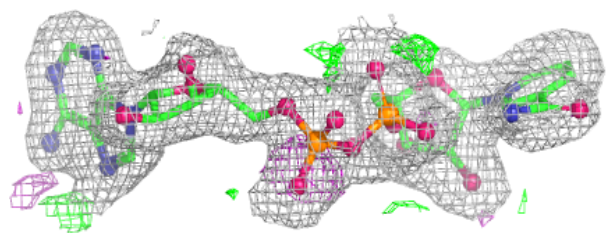
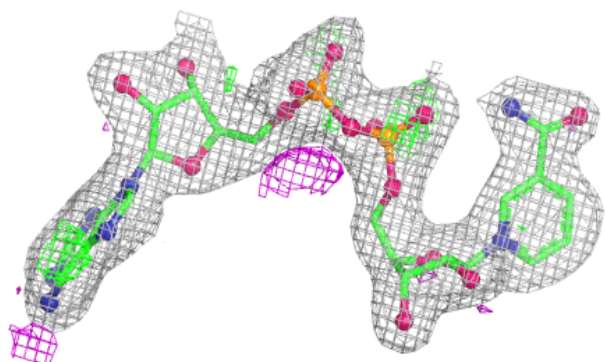


Electron density around NAD G 401:

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

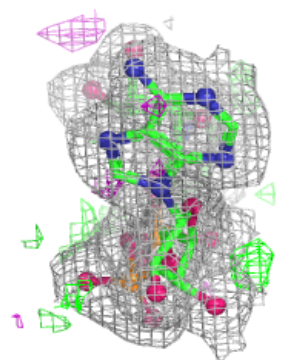
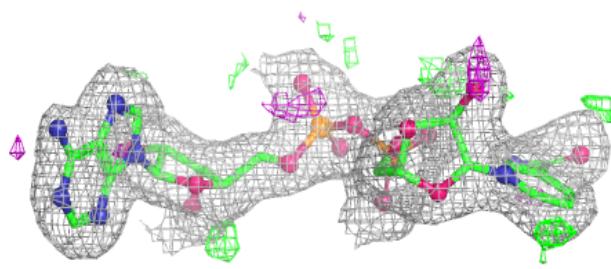
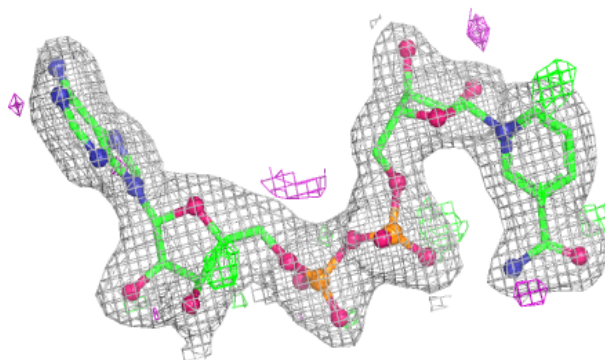
**Electron density around NAD H 401:**

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

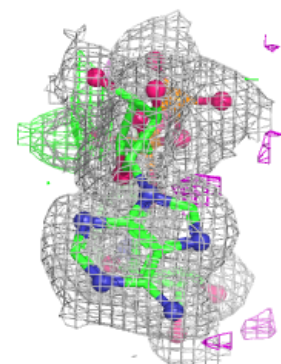
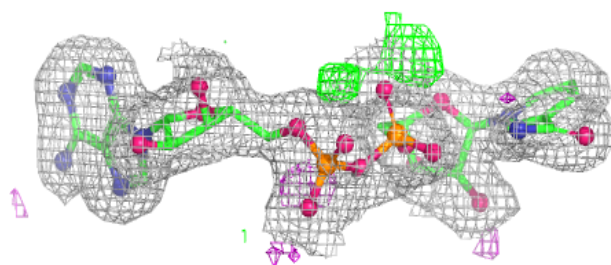
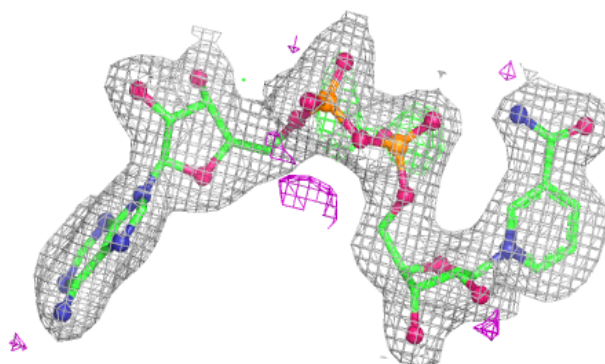


Electron density around NAD C 401:

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

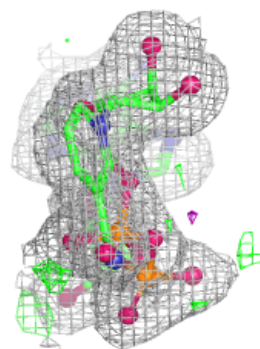
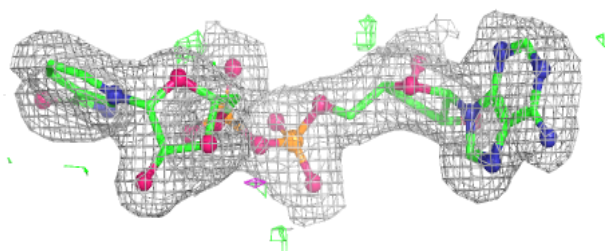
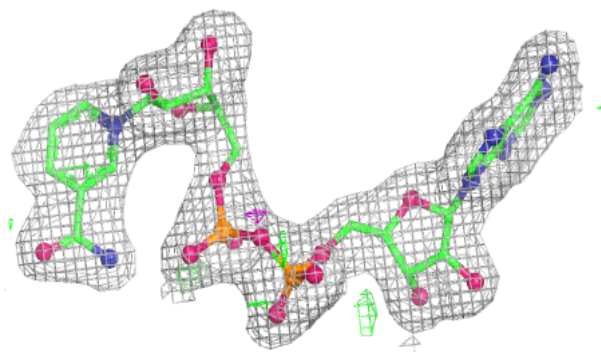
**Electron density around NAD D 401:**

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

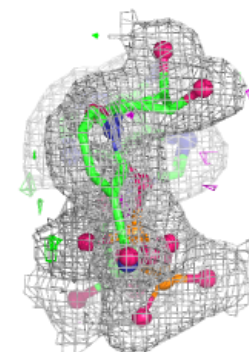
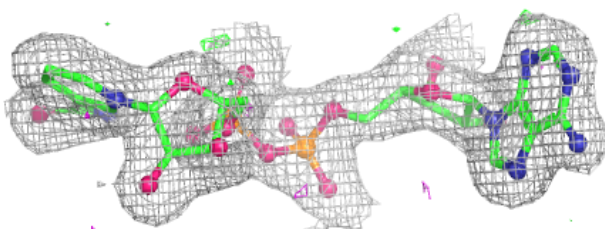
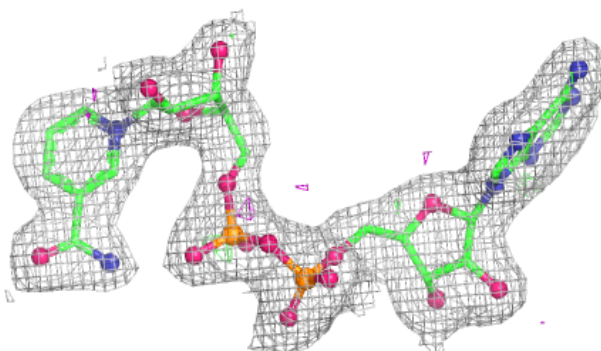


Electron density around NAD E 401:

$2mF_o-DF_c$ (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.