



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:51 AM UTC

PDB ID : 8P5F / pdb_00008p5f
Title : Human wild-type GAPDH,orthorhombic form
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Deposited on : 2023-05-24
Resolution : 1.82 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

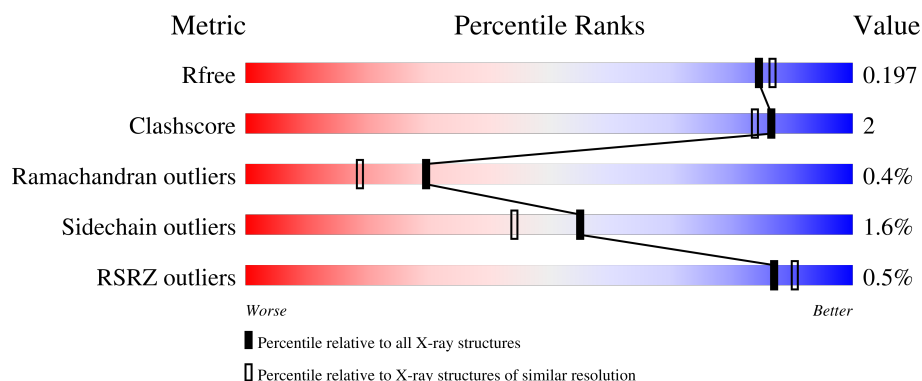
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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.

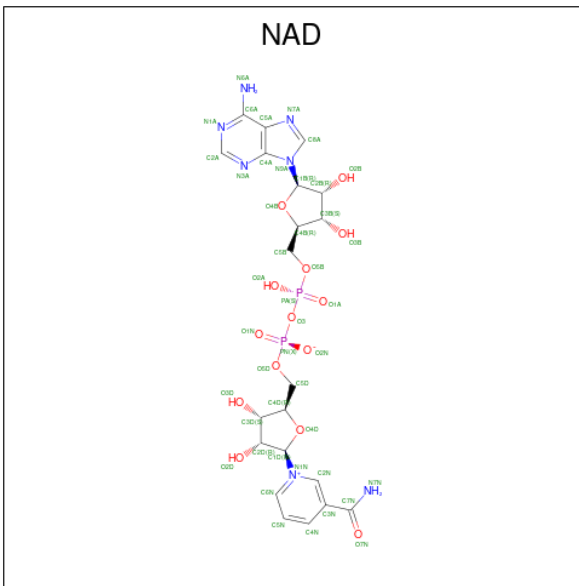
Mol	Chain	Length	Quality of chain
1	AAA	335	95% 5%
1	DDD	335	95% 5% .
1	EEE	335	90% 8% ..
1	GGG	335	% 90% 10% .

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	AAA	334	Total 2532	C 1600	N 439	O 480	S 13	0	1	0
1	DDD	333	Total 2538	C 1604	N 439	O 482	S 13	0	2	0
1	EEE	333	Total 2535	C 1604	N 438	O 481	S 12	0	2	0
1	GGG	333	Total 2533	C 1601	N 441	O 479	S 12	0	1	0

- 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	AAA	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	DDD	1	Total 44	C 21	N 7	O 14	P 2	0	0

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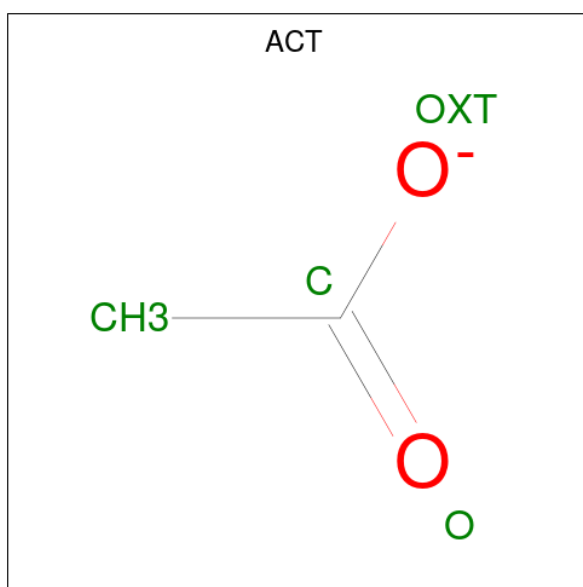
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	EEE	1	Total	C	N	O	P	0
			44	21	7	14	2	
2	GGG	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	EEE	2	Total	Zn	0	0
			2	2		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	EEE	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	241	Total	O	0	0
			241	241		
5	DDD	239	Total	O	0	0
			239	239		
5	EEE	173	Total	O	0	0
			173	173		

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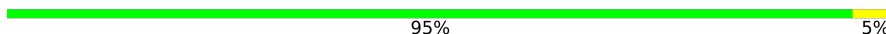
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	GGG	102	Total 102	O 102	0	0

3 Residue-property plots [i](#)

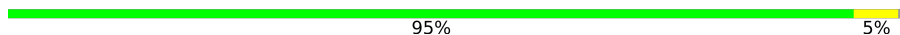
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

Chain AAA: 



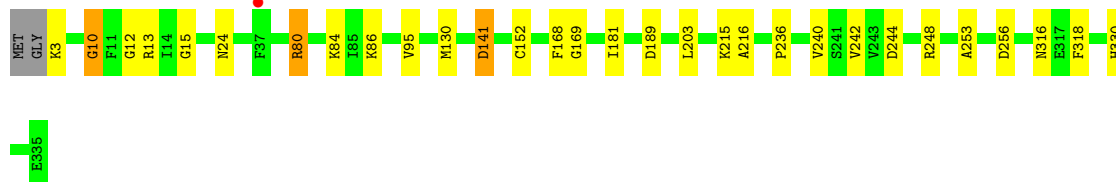
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain DDD: 

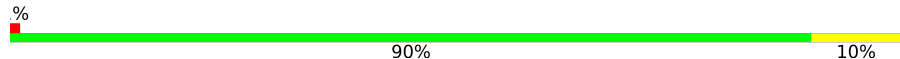


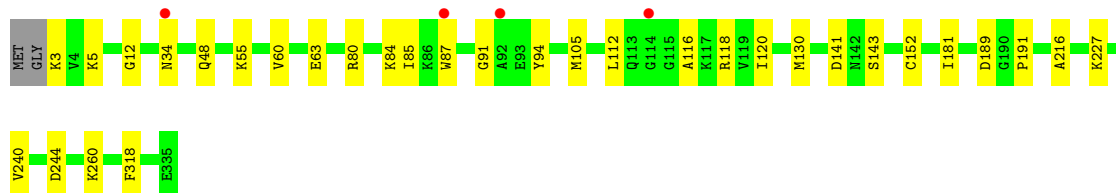
- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain EEE: 



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain GGG: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.82Å 132.81Å 146.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 1.82 14.99 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.8 (14.99-1.82) 99.8 (14.99-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.160 , 0.189 0.170 , 0.197	Depositor DCC
R_{free} test set	6994 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.0	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	0.97	EDS
Total number of atoms	11075	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 3.14% 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: ZN, ACT, NAD, CSD

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	AAA	1.14	3/2579 (0.1%)	1.27	2/3488 (0.1%)
1	DDD	1.11	2/2576 (0.1%)	1.24	4/3487 (0.1%)
1	EEE	1.13	3/2583 (0.1%)	1.29	7/3495 (0.2%)
1	GGG	1.11	1/2578 (0.0%)	1.36	2/3487 (0.1%)
All	All	1.12	9/10316 (0.1%)	1.29	15/13957 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	121	ILE	C-O	7.80	1.32	1.24
1	AAA	329	ALA	C-O	7.66	1.33	1.24
1	DDD	165	HIS	CE1-NE2	7.23	1.39	1.32
1	EEE	242	VAL	C-O	6.37	1.30	1.24
1	EEE	10	GLY	C-O	5.77	1.31	1.23
1	DDD	317	GLU	C-O	5.68	1.30	1.24
1	AAA	269	PRO	C-O	-5.61	1.17	1.24
1	GGG	191	PRO	C-O	-5.57	1.17	1.23
1	EEE	95	VAL	C-O	5.41	1.29	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GGG	244	ASP	CA-CB-CG	7.83	120.43	112.60
1	EEE	244	ASP	CA-CB-CG	6.87	119.47	112.60
1	DDD	39	ASP	CA-CB-CG	6.86	119.46	112.60
1	AAA	244	ASP	CA-CB-CG	6.10	118.70	112.60
1	DDD	20	ARG	CB-CA-C	-6.07	101.35	110.88
1	EEE	24	ASN	CA-CB-CG	5.96	118.56	112.60
1	AAA	244	ASP	N-CA-CB	-5.53	101.92	110.65
1	GGG	189	ASP	CA-CB-CG	5.38	117.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EEE	141	ASP	CA-CB-CG	5.34	117.94	112.60
1	EEE	80	ARG	N-CA-C	-5.30	105.67	111.82
1	EEE	189	ASP	CA-CB-CG	5.24	117.84	112.60
1	DDD	131	PHE	CA-CB-CG	-5.12	108.69	113.80
1	EEE	236	PRO	N-CA-CB	5.07	105.95	102.35
1	DDD	28	VAL	CA-C-O	-5.03	116.71	121.64
1	EEE	244	ASP	CB-CA-C	5.01	118.81	110.74

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	AAA	2532	0	2532	12	0
1	DDD	2538	0	2539	10	0
1	EEE	2535	0	2539	20	0
1	GGG	2533	0	2537	14	0
2	AAA	44	0	26	0	0
2	DDD	44	0	26	1	0
2	EEE	44	0	26	3	0
2	GGG	44	0	26	1	0
3	EEE	2	0	0	0	0
4	EEE	4	0	3	0	0
5	AAA	241	0	0	3	0
5	DDD	239	0	0	0	0
5	EEE	173	0	0	3	0
5	GGG	102	0	0	2	0
All	All	11075	0	10254	44	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 (44) 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:AAA:24:ASN:HB2	5:AAA:710:HOH:O	1.59	1.00
1:DDD:203[B]:LEU:HB2	1:EEE:203[B]:LEU:HD21	1.43	0.98
1:DDD:203[B]:LEU:HD13	1:EEE:203[B]:LEU:HD22	1.54	0.89
1:AAA:248:ARG:HD2	1:EEE:248:ARG:HD2	1.57	0.85
1:DDD:203[A]:LEU:HD22	1:EEE:181:ILE:HD13	1.68	0.75
1:EEE:330:HIS:ND1	5:EEE:501:HOH:O	2.20	0.75
1:GGG:227:LYS:HE3	5:GGG:520:HOH:O	1.89	0.72
1:DDD:203[B]:LEU:HD13	1:EEE:203[B]:LEU:CD2	2.21	0.69
1:GGG:130:MET:HE1	1:GGG:216:ALA:HB1	1.79	0.65
1:GGG:12:GLY:HA3	2:GGG:401:NAD:O5B	1.98	0.63
1:AAA:203:LEU:HD22	1:GGG:181:ILE:HD13	1.81	0.62
1:AAA:248:ARG:CD	1:EEE:248:ARG:HD2	2.29	0.62
1:EEE:203[A]:LEU:HD12	5:EEE:521:HOH:O	2.02	0.59
1:AAA:248:ARG:HD2	1:EEE:248:ARG:CD	2.30	0.59
1:AAA:172:GLU:OE2	1:AAA:248:ARG:HD3	2.03	0.57
1:AAA:130[B]:MET:HE1	1:AAA:216:ALA:HB1	1.86	0.56
1:AAA:187:THR:HB	1:GGG:181:ILE:HD12	1.89	0.55
1:DDD:181:ILE:HD13	1:EEE:203[B]:LEU:HD12	1.88	0.55
1:DDD:203[A]:LEU:HD22	1:EEE:181:ILE:CD1	2.37	0.54
1:GGG:227:LYS:CE	5:GGG:520:HOH:O	2.49	0.53
1:EEE:130:MET:HE1	1:EEE:216:ALA:HB1	1.90	0.53
1:GGG:141:ASP:OD1	1:GGG:143:SER:OG	2.26	0.53
1:GGG:94:TYR:CE1	1:GGG:118:ARG:HD2	2.45	0.52
1:EEE:86:LYS:HE2	5:EEE:662:HOH:O	2.10	0.51
1:GGG:5:LYS:HD2	1:GGG:91:GLY:O	2.10	0.51
1:DDD:203[B]:LEU:CB	1:EEE:203[B]:LEU:HD21	2.29	0.50
1:AAA:145:LYS:HD2	5:AAA:508:HOH:O	2.13	0.47
1:EEE:152:CSD:HB2	2:EEE:401:NAD:H5N	1.97	0.47
1:AAA:315:ASP:OD1	1:AAA:315:ASP:C	2.59	0.46
1:EEE:10:GLY:O	1:EEE:15:GLY:HA3	2.16	0.46
1:DDD:12:GLY:HA3	2:DDD:401:NAD:O5B	2.15	0.46
1:GGG:34:ASN:ND2	1:GGG:85:ILE:HD11	2.31	0.46
1:DDD:248:ARG:HA	1:DDD:306:HIS:O	2.16	0.45
1:GGG:112:LEU:HD23	1:GGG:116:ALA:O	2.17	0.45
1:AAA:130[B]:MET:HE3	1:AAA:130[B]:MET:HB3	1.73	0.45
1:GGG:120:ILE:N	1:GGG:120:ILE:HD12	2.32	0.45
1:GGG:48:GLN:O	1:GGG:55:LYS:HA	2.17	0.44
1:EEE:168:PHE:CD1	1:EEE:253:ALA:HB2	2.53	0.44
1:GGG:85:ILE:HG21	1:GGG:87:TRP:CE2	2.53	0.43
1:EEE:12:GLY:HA3	2:EEE:401:NAD:O5B	2.18	0.43
1:DDD:93:GLU:HG3	1:DDD:117:LYS:HG3	1.99	0.43
1:AAA:145:LYS:CE	5:AAA:508:HOH:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:316:ASN:O	2:EEE:401:NAD:H4N	2.19	0.42
1:EEE:12:GLY:O	1:EEE:13:ARG:C	2.61	0.41

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	AAA	332/335 (99%)	322 (97%)	9 (3%)	1 (0%)	36	26
1	DDD	331/335 (99%)	318 (96%)	12 (4%)	1 (0%)	36	26
1	EEE	332/335 (99%)	320 (96%)	10 (3%)	2 (1%)	21	11
1	GGG	331/335 (99%)	317 (96%)	13 (4%)	1 (0%)	36	26
All	All	1326/1340 (99%)	1277 (96%)	44 (3%)	5 (0%)	30	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	240	VAL
1	DDD	240	VAL
1	EEE	240	VAL
1	GGG	240	VAL
1	EEE	169	GLY

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	AAA	270/270 (100%)	269 (100%)	1 (0%)	84	81
1	DDD	270/270 (100%)	269 (100%)	1 (0%)	84	81
1	EEE	271/270 (100%)	264 (97%)	7 (3%)	40	23
1	GGG	270/270 (100%)	262 (97%)	8 (3%)	36	17
All	All	1081/1080 (100%)	1064 (98%)	17 (2%)	55	44

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	215	LYS
1	DDD	318	PHE
1	EEE	3	LYS
1	EEE	80	ARG
1	EEE	84	LYS
1	EEE	141	ASP
1	EEE	215	LYS
1	EEE	256	ASP
1	EEE	318	PHE
1	GGG	3	LYS
1	GGG	60	VAL
1	GGG	63	GLU
1	GGG	80	ARG
1	GGG	84	LYS
1	GGG	105	MET
1	GGG	260	LYS
1	GGG	318	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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$
1	CSD	DDD	152[B]	1	4,7,8	1.30	1 (25%)	1,8,10	0.19	0
1	CSD	AAA	152	1	4,7,8	1.50	1 (25%)	1,8,10	1.01	0
1	CSD	GGG	152	1	4,7,8	1.95	1 (25%)	1,8,10	2.73	1 (100%)
1	CSD	EEE	152	1	4,7,8	1.35	0	1,8,10	0.13	0
1	CSD	DDD	152[A]	1	4,7,8	0.88	0	1,8,10	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	DDD	152[B]	1	-	0/2/6/8	-
1	CSD	AAA	152	1	-	1/2/6/8	-
1	CSD	GGG	152	1	-	1/2/6/8	-
1	CSD	EEE	152	1	-	1/2/6/8	-
1	CSD	DDD	152[A]	1	-	1/2/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	GGG	152	CSD	OD1-SG	3.32	1.50	1.47
1	AAA	152	CSD	OD1-SG	2.53	1.50	1.47
1	DDD	152[B]	CSD	OD1-SG	2.02	1.49	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GGG	152	CSD	OD1-SG-CB	2.73	110.64	105.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	DDD	152[A]	CSD	CA-CB-SG-OD1
1	EEE	152	CSD	CA-CB-SG-OD1
1	GGG	152	CSD	CA-CB-SG-OD1
1	AAA	152	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	EEE	152	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
4	ACT	EEE	403	3	3,3,3	0.86	0	3,3,3	1.96	1 (33%)
2	NAD	AAA	401	-	46,48,48	1.23	4 (8%)	64,73,73	0.89	2 (3%)
2	NAD	GGG	401	-	46,48,48	1.12	2 (4%)	64,73,73	0.70	1 (1%)
2	NAD	DDD	401	-	46,48,48	1.05	3 (6%)	64,73,73	0.71	0
2	NAD	EEE	401	-	46,48,48	1.29	3 (6%)	64,73,73	0.88	3 (4%)

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	AAA	401	-	-	5/30/62/62	0/5/5/5
2	NAD	GGG	401	-	-	6/30/62/62	0/5/5/5
2	NAD	EEE	401	-	-	5/30/62/62	0/5/5/5
2	NAD	DDD	401	-	-	5/30/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	GGG	401	NAD	C2N-N1N	6.19	1.41	1.35
2	EEE	401	NAD	C2N-N1N	5.33	1.40	1.35
2	DDD	401	NAD	C2N-N1N	5.29	1.40	1.35
2	AAA	401	NAD	C2N-N1N	4.18	1.39	1.35
2	AAA	401	NAD	O4D-C1D	4.12	1.46	1.40
2	EEE	401	NAD	PA-O3	4.07	1.63	1.59
2	EEE	401	NAD	PN-O3	3.63	1.63	1.59
2	AAA	401	NAD	PN-O3	3.22	1.63	1.59
2	GGG	401	NAD	O4D-C1D	3.07	1.44	1.40
2	AAA	401	NAD	C4N-C3N	2.94	1.43	1.39
2	DDD	401	NAD	PA-O3	2.10	1.61	1.59
2	DDD	401	NAD	PN-O3	2.03	1.61	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EEE	401	NAD	C6N-N1N-C2N	-3.37	119.01	121.88
2	GGG	401	NAD	C6N-N1N-C2N	-3.15	119.20	121.88
2	EEE	401	NAD	O3-PA-O1A	-2.81	102.24	110.70
2	AAA	401	NAD	O3-PA-O1A	-2.80	102.28	110.70
4	EEE	403	ACT	O-C-CH3	-2.67	111.57	122.53
2	AAA	401	NAD	C6N-N1N-C2N	-2.35	119.88	121.88
2	EEE	401	NAD	O2A-PA-O1A	2.32	123.22	112.44

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	401	NAD	O4D-C1D-N1N-C2N
2	AAA	401	NAD	O4D-C1D-N1N-C6N
2	AAA	401	NAD	C2D-C1D-N1N-C2N
2	AAA	401	NAD	C2D-C1D-N1N-C6N
2	DDD	401	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	DDD	401	NAD	O4D-C1D-N1N-C6N
2	DDD	401	NAD	C2D-C1D-N1N-C2N
2	DDD	401	NAD	C2D-C1D-N1N-C6N
2	EEE	401	NAD	O4D-C1D-N1N-C2N
2	EEE	401	NAD	O4D-C1D-N1N-C6N
2	EEE	401	NAD	C2D-C1D-N1N-C2N
2	EEE	401	NAD	C2D-C1D-N1N-C6N
2	GGG	401	NAD	O4D-C1D-N1N-C2N
2	GGG	401	NAD	O4D-C1D-N1N-C6N
2	GGG	401	NAD	C2D-C1D-N1N-C2N
2	GGG	401	NAD	C2D-C1D-N1N-C6N
2	GGG	401	NAD	O4B-C4B-C5B-O5B
2	EEE	401	NAD	C4N-C3N-C7N-N7N
2	DDD	401	NAD	C2B-C1B-N9A-C8A
2	GGG	401	NAD	C2B-C1B-N9A-C8A
2	AAA	401	NAD	C2B-C1B-N9A-C8A

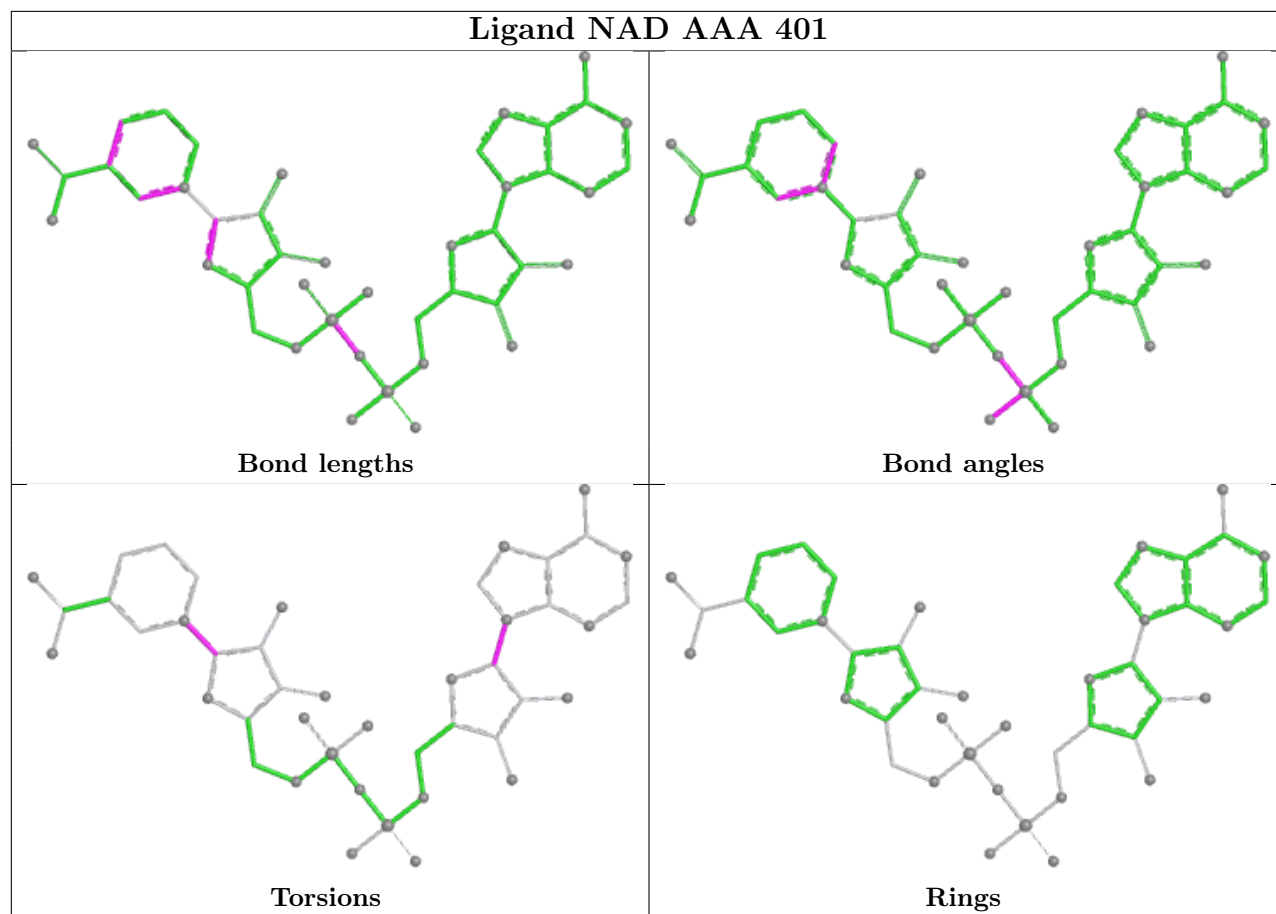
There are no ring outliers.

3 monomers are involved in 5 short contacts:

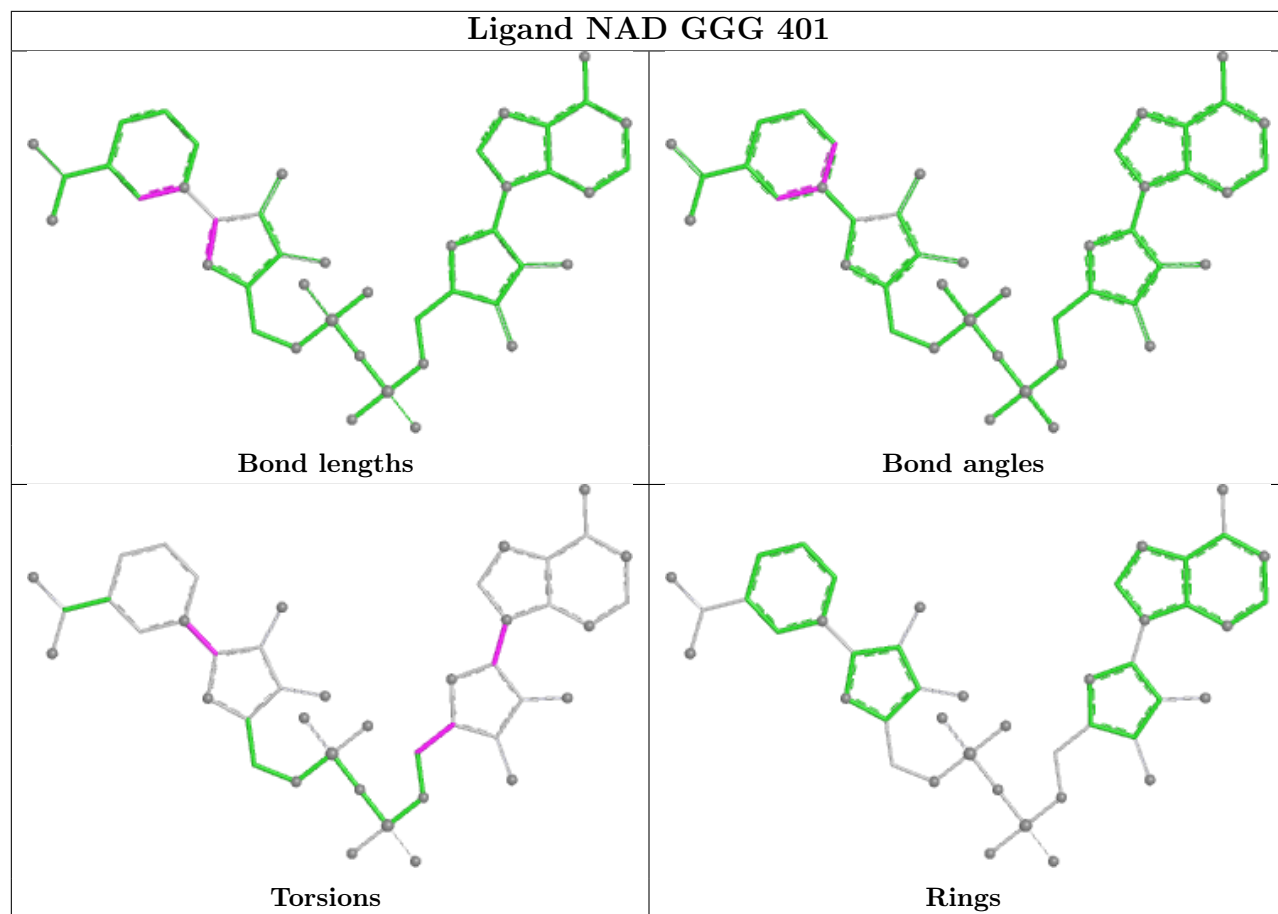
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	GGG	401	NAD	1	0
2	DDD	401	NAD	1	0
2	EEE	401	NAD	3	0

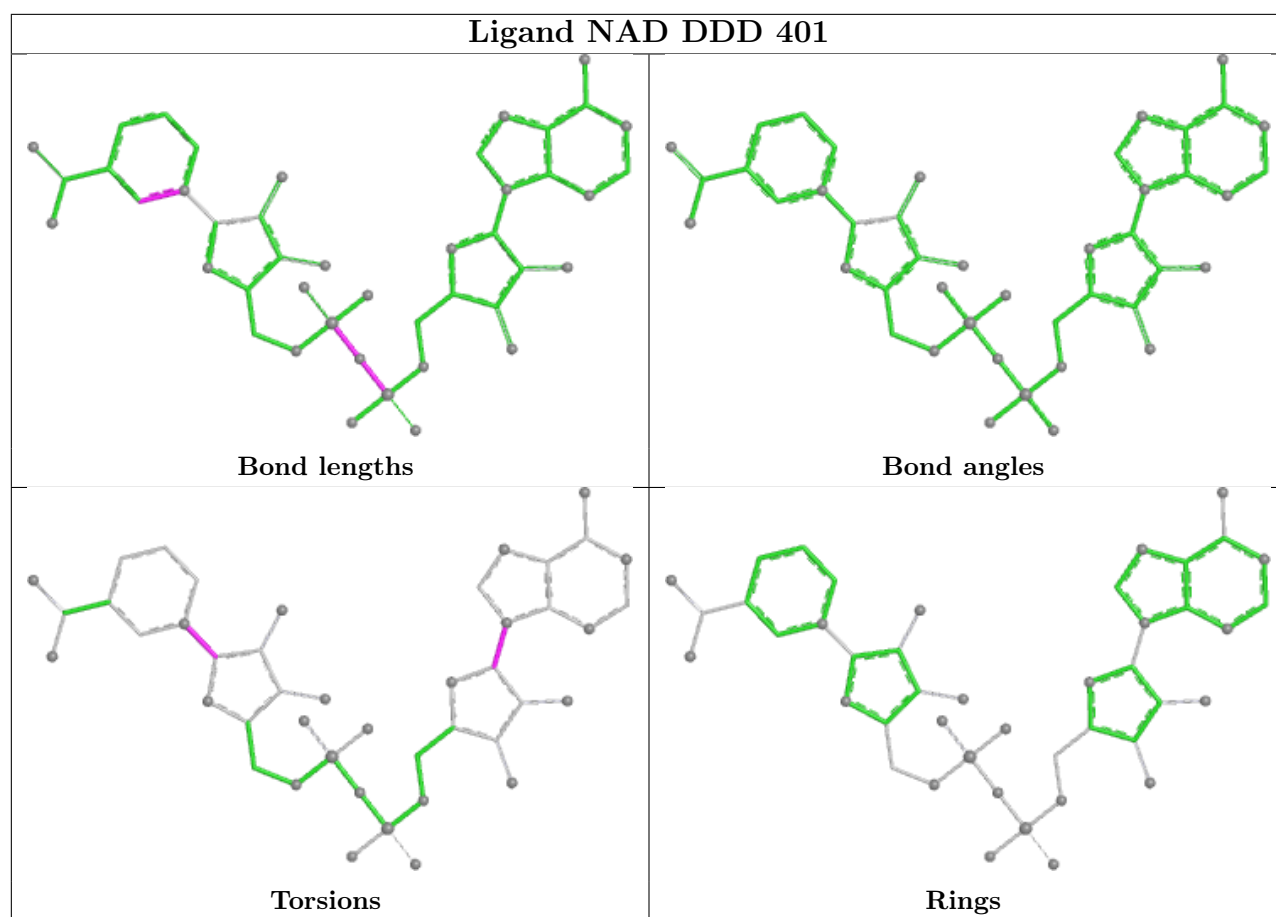
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

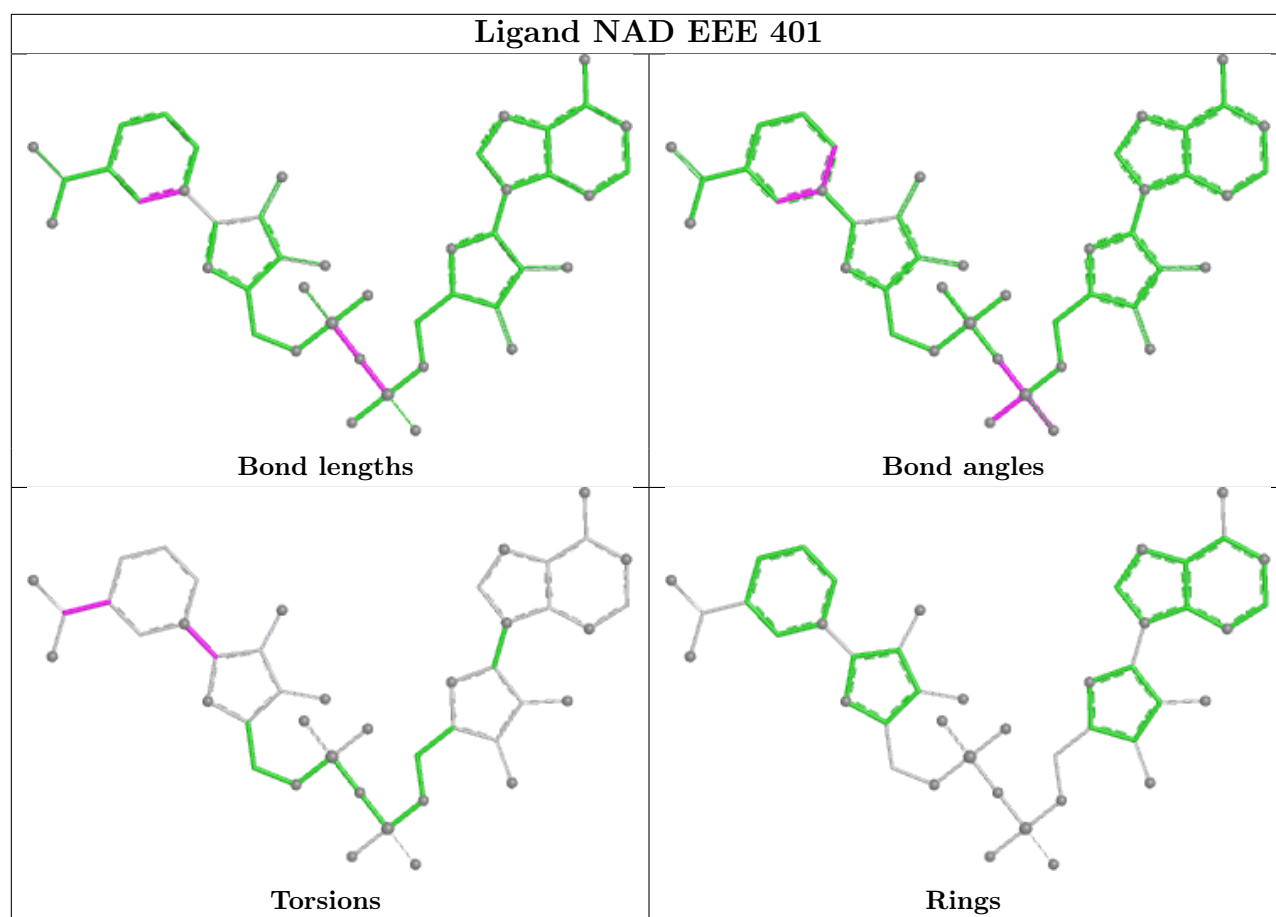
Ligand NAD AAA 401



Ligand NAD GGG 401







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	333/335 (99%)	-0.43	1 (0%) 90 93	27, 36, 54, 74	1 (0%)
1	DDD	332/335 (99%)	-0.48	0 100 100	22, 36, 54, 72	1 (0%)
1	EEE	332/335 (99%)	-0.29	1 (0%) 90 93	21, 40, 61, 84	2 (0%)
1	GGG	332/335 (99%)	0.11	4 (1%) 76 82	21, 50, 87, 111	1 (0%)
All	All	1329/1340 (99%)	-0.27	6 (0%) 87 90	21, 39, 72, 111	5 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	2	GLY	5.8
1	GGG	114	GLY	2.4
1	GGG	92	ALA	2.4
1	GGG	87	TRP	2.4
1	EEE	37	PHE	2.2
1	GGG	34	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSD	GGG	152	8/9	0.95	0.07	36,40,52,55	0
1	CSD	EEE	152	8/9	0.96	0.07	33,34,43,48	0
1	CSD	DDD	152[A]	8/9	0.97	0.07	27,31,37,43	8
1	CSD	DDD	152[B]	8/9	0.97	0.07	27,30,36,38	8
1	CSD	AAA	152	8/9	0.98	0.05	30,32,39,49	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

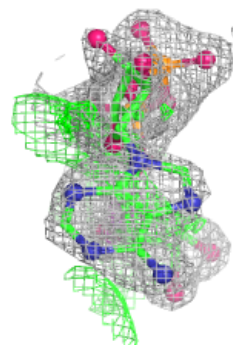
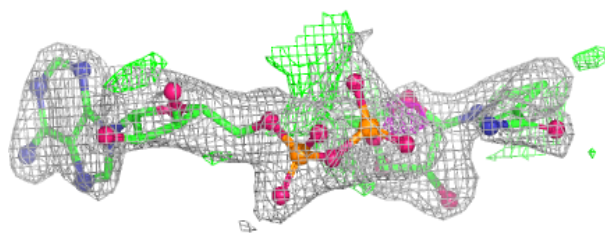
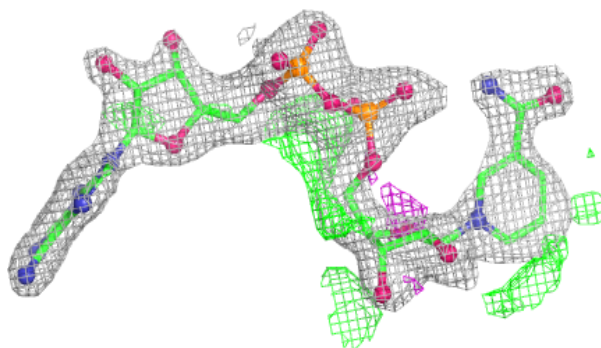
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GGG	401	44/44	0.84	0.12	42,53,61,63	44
2	NAD	EEE	401	44/44	0.93	0.09	39,44,50,52	0
4	ACT	EEE	403	4/4	0.94	0.12	38,43,48,51	0
3	ZN	EEE	402	1/1	0.96	0.10	38,38,38,38	0
2	NAD	AAA	401	44/44	0.98	0.05	29,33,37,38	0
3	ZN	EEE	404	1/1	0.98	0.05	38,38,38,38	0
2	NAD	DDD	401	44/44	0.98	0.05	30,34,37,40	0

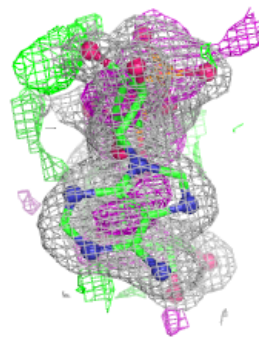
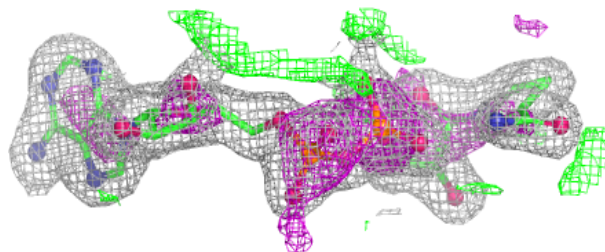
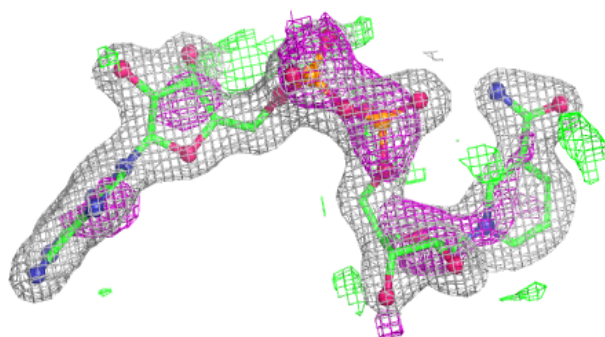
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD GGG 401:

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

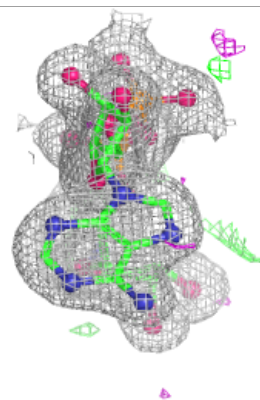
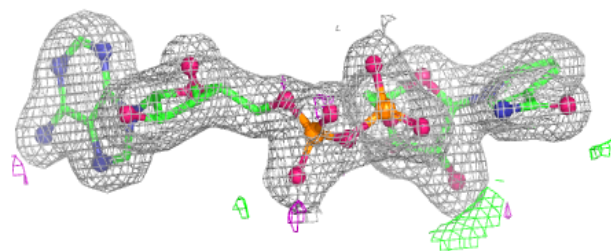
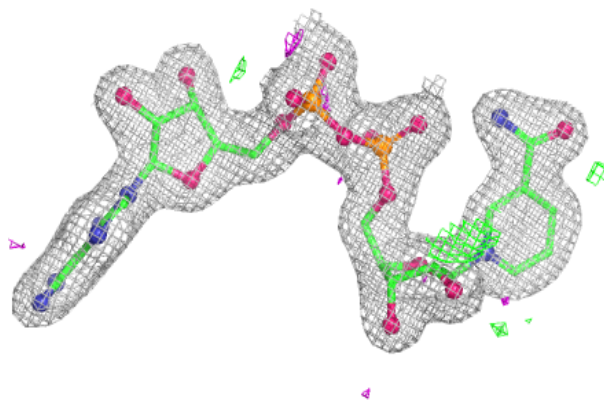
**Electron density around NAD EEE 401:**

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

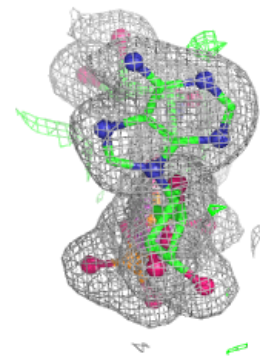
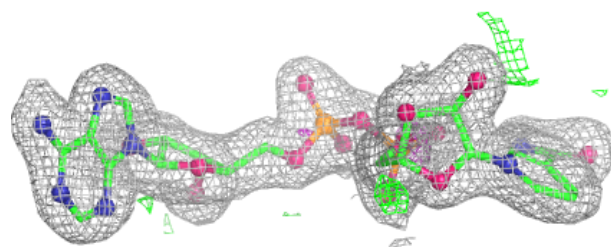
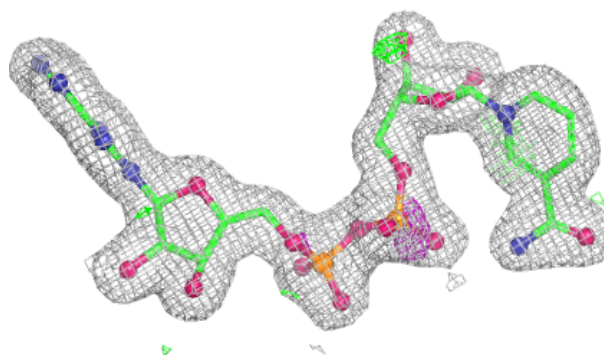


Electron density around NAD AAA 401:

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

**Electron density around NAD DDD 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.