



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 09:33 am BST

PDB ID : 4ZVV
Title : Lactate dehydrogenase A in complex with a trisubstituted piperidine-2,4-dione inhibitor GNE-140
Authors : Li, Y.; Chen, Z.; Eigenbrot, C.
Deposited on : 2015-05-18
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

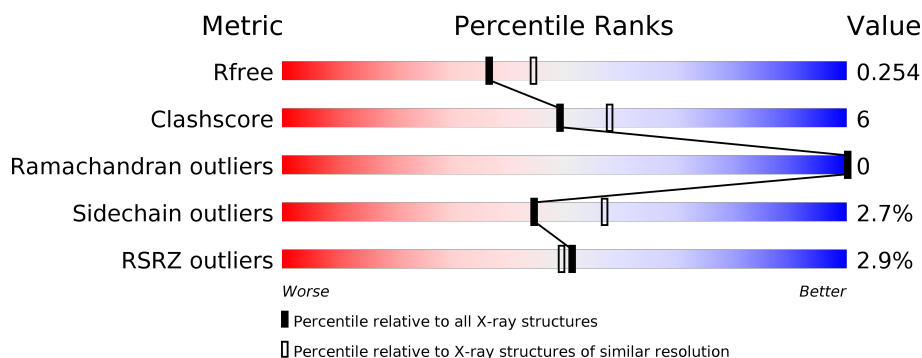
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	332	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>.</div> </div> </div>
1	B	332	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div>
1	C	332	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>
1	D	332	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>.</div> </div> </div>

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 L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total 2568	C 1639	N 439	O 477	S 13	0	0	0
1	B	331	Total 2568	C 1639	N 439	O 477	S 13	0	0	0
1	C	331	Total 2568	C 1639	N 439	O 477	S 13	0	0	0
1	D	331	Total 2572	C 1642	N 439	O 478	S 13	0	1	0

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



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

Continued on next page...

Continued from previous page...

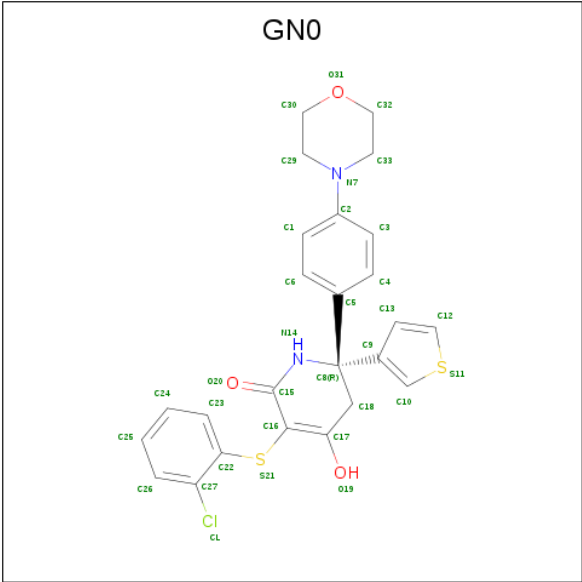
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is (2 {R})-5-(2-chlorophenyl)sulfanyl-2-(4-morpholin-4-ylphenyl)-4-oxidanyl-2-thiophen-3-yl-1,3-dihydropyridin-6-one (three-letter code: GN0) (formula: C₂₅H₂₃ClN₂O₃S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			33	25	1	2	3	2		
4	B	1	Total	C	Cl	N	O	S	0	0
			33	25	1	2	3	2		
4	C	1	Total	C	Cl	N	O	S	0	0
			33	25	1	2	3	2		
4	D	1	Total	C	Cl	N	O	S	0	0
			33	25	1	2	3	2		

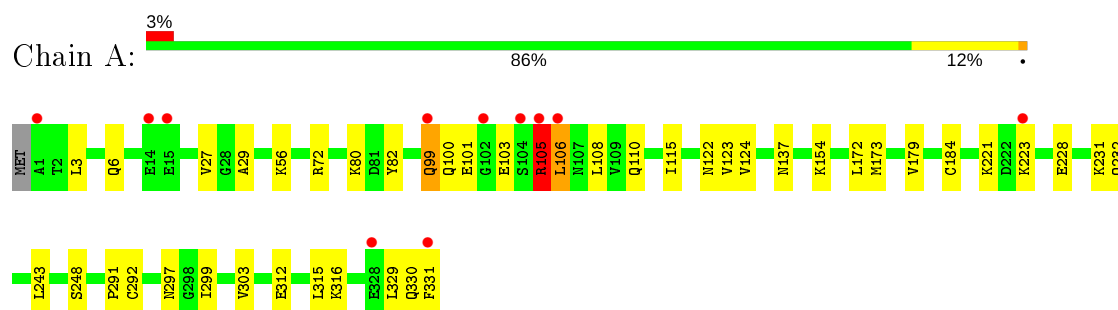
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	71	Total	O	0	0
			71	71		
5	C	82	Total	O	0	0
			82	82		
5	D	84	Total	O	0	0
			84	84		

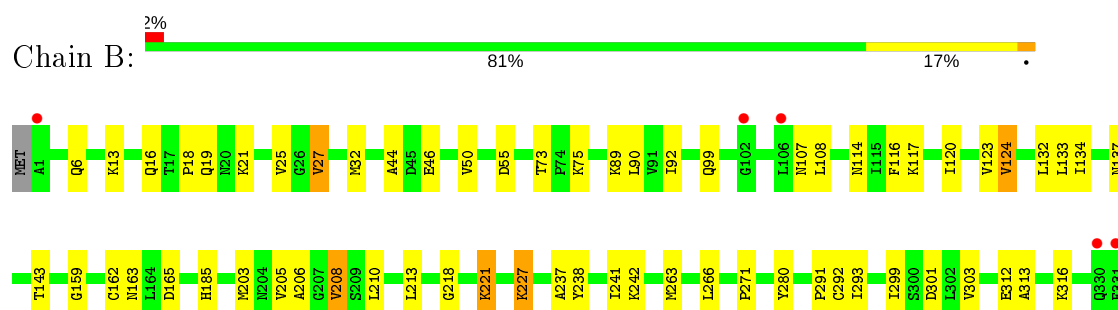
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

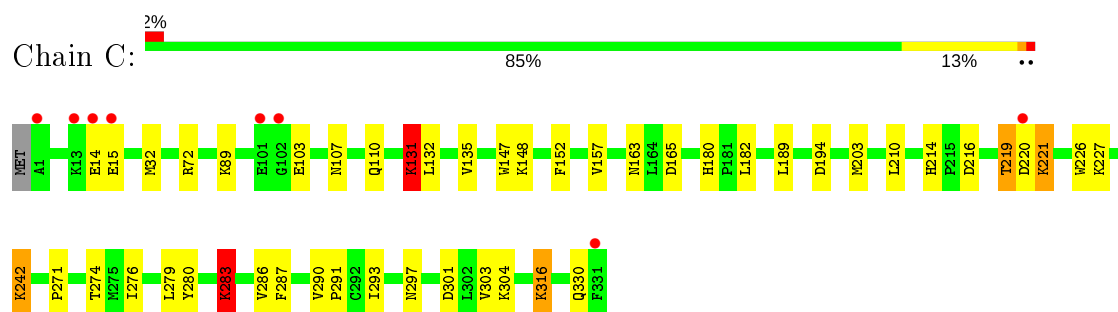
• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain

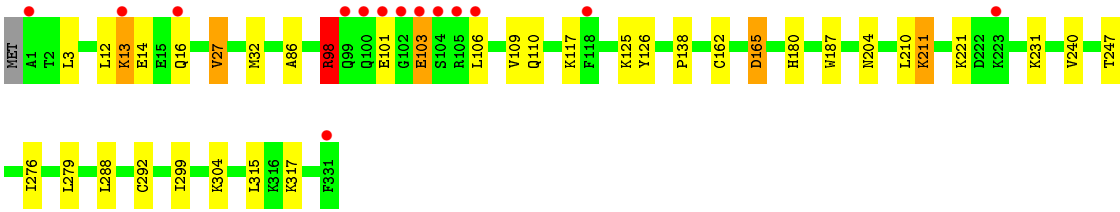


• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.16 Å 81.29 Å 102.47 Å 90.00° 98.31° 90.00°	Depositor
Resolution (Å)	38.45 – 2.20 38.45 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.45-2.20) 85.8 (38.45-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.64 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.232 , 0.259 0.229 , 0.254	Depositor DCC
R_{free} test set	1152 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 24.2	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	0.93	EDS
Total number of atoms	10928	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 3.97% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GN0, SO4, 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	0.67	10/2612 (0.4%)	0.55	2/3532 (0.1%)
1	B	0.50	1/2612 (0.0%)	0.50	1/3532 (0.0%)
1	C	0.59	9/2612 (0.3%)	0.51	1/3532 (0.0%)
1	D	0.73	13/2619 (0.5%)	0.61	4/3541 (0.1%)
All	All	0.63	33/10455 (0.3%)	0.54	8/14137 (0.1%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	13	LYS	CA-C	16.53	1.96	1.52
1	B	13	LYS	CB-CG	-11.04	1.22	1.52
1	D	13	LYS	CB-CG	-10.90	1.23	1.52
1	A	101	GLU	CG-CD	-10.49	1.36	1.51
1	A	101	GLU	CD-OE1	10.43	1.37	1.25
1	C	242	LYS	CE-NZ	10.06	1.74	1.49
1	C	283	LYS	CE-NZ	9.08	1.71	1.49
1	D	98	ARG	CZ-NH2	8.29	1.43	1.33
1	D	103	GLU	CD-OE1	8.11	1.34	1.25
1	A	105	ARG	CG-CD	7.10	1.69	1.51
1	A	99	GLN	CD-NE2	6.79	1.49	1.32
1	D	117	LYS	CE-NZ	6.51	1.65	1.49
1	A	80	LYS	CE-NZ	6.50	1.65	1.49
1	D	101	GLU	CB-CG	6.41	1.64	1.52
1	C	15	GLU	CB-CG	-6.26	1.40	1.52
1	A	99	GLN	CG-CD	6.06	1.65	1.51
1	A	231	LYS	CD-CE	5.99	1.66	1.51
1	A	106	LEU	CG-CD1	5.97	1.74	1.51
1	D	13	LYS	C-N	-5.84	1.20	1.34
1	D	231	LYS	CD-CE	5.82	1.65	1.51
1	C	242	LYS	CD-CE	5.77	1.65	1.51
1	C	221	LYS	CE-NZ	5.67	1.63	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	211	LYS	CE-NZ	5.59	1.63	1.49
1	C	14	GLU	CB-CG	-5.55	1.41	1.52
1	D	14	GLU	CB-CG	5.38	1.62	1.52
1	C	227	LYS	CE-NZ	5.34	1.62	1.49
1	A	154	LYS	CE-NZ	5.33	1.62	1.49
1	D	103	GLU	CG-CD	-5.27	1.44	1.51
1	D	103	GLU	CD-OE2	5.24	1.31	1.25
1	A	223	LYS	CE-NZ	5.10	1.61	1.49
1	C	131	LYS	CD-CE	5.09	1.64	1.51
1	C	148	LYS	CD-CE	5.06	1.63	1.51
1	D	103	GLU	CB-CG	5.04	1.61	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	13	LYS	CB-CA-C	12.89	136.18	110.40
1	D	13	LYS	CB-CG-CD	9.71	136.84	111.60
1	D	98	ARG	NE-CZ-NH1	-8.77	115.92	120.30
1	A	105	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	D	13	LYS	CA-CB-CG	-5.79	100.66	113.40
1	A	101	GLU	OE1-CD-OE2	-5.62	116.56	123.30
1	C	242	LYS	CD-CE-NZ	-5.55	98.92	111.70
1	B	13	LYS	CA-CB-CG	5.54	125.59	113.40

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	2568	0	2656	35	0
1	B	2568	0	2656	46	0
1	C	2568	0	2656	31	0
1	D	2572	0	2660	30	0
2	A	44	0	26	2	0
2	B	44	0	26	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	44	0	26	1	0
2	D	44	0	26	0	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	33	0	0	0	0
4	B	33	0	0	0	0
4	C	33	0	0	0	0
4	D	33	0	0	0	0
5	A	72	0	0	0	0
5	B	71	0	0	1	0
5	C	82	0	0	0	0
5	D	84	0	0	0	0
All	All	10928	0	10732	126	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 6.

All (126) 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:C:283:LYS:NZ	1:C:283:LYS:CE	1.71	1.50
1:C:242:LYS:CE	1:C:242:LYS:NZ	1.74	1.49
1:D:13:LYS:C	1:D:13:LYS:CA	1.95	1.34
1:A:99:GLN:NE2	1:A:103:GLU:OE2	1.91	1.03
1:B:227:LYS:HE3	1:B:227:LYS:N	1.81	0.95
1:A:106:LEU:O	1:A:106:LEU:HD13	1.72	0.89
1:A:99:GLN:HE21	1:A:100:GLN:H	1.24	0.85
1:B:227:LYS:HE3	1:B:227:LYS:H	1.47	0.78
1:A:99:GLN:HE21	1:A:100:GLN:N	1.81	0.77
1:B:134:ILE:CG2	1:B:159:GLY:HA2	2.15	0.76
1:A:99:GLN:NE2	1:A:100:GLN:H	1.84	0.75
1:A:105:ARG:HD2	1:A:106:LEU:H	1.52	0.74
1:A:27:VAL:O	1:A:27:VAL:HG12	1.88	0.73
1:B:134:ILE:HG22	1:B:159:GLY:HA2	1.70	0.73
1:B:90:LEU:HB2	1:B:263:MET:CE	2.24	0.67
1:C:242:LYS:CD	1:C:242:LYS:NZ	2.58	0.66
1:B:313:ALA:HA	1:B:316:LYS:HE3	1.77	0.66
1:B:44:ALA:O	1:B:73:THR:HG22	1.96	0.65
1:C:103:GLU:HG3	1:C:107:ASN:HD22	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ILE:HD12	1:B:301:ASP:HB2	1.78	0.64
1:B:116:PHE:HZ	1:B:134:ILE:HD11	1.62	0.64
1:C:291:PRO:HG2	1:C:303:VAL:HB	1.82	0.62
1:A:110:GLN:HE21	1:A:330:GLN:H	1.45	0.61
1:B:134:ILE:HG21	1:B:143:THR:OG1	2.01	0.61
1:C:283:LYS:CD	1:C:283:LYS:NZ	2.63	0.61
1:B:218:GLY:H	1:B:227:LYS:HZ1	1.49	0.59
1:B:292:CYS:HB3	1:B:299:ILE:HG23	1.85	0.59
1:C:110:GLN:HE22	1:C:330:GLN:H	1.49	0.59
1:A:27:VAL:O	1:A:27:VAL:CG1	2.51	0.58
1:A:110:GLN:NE2	1:A:330:GLN:H	2.02	0.57
1:D:98:ARG:CD	1:D:103:GLU:OE1	2.52	0.57
1:C:214:HIS:HB2	1:D:3:LEU:HD13	1.87	0.57
1:C:203:MET:HG2	1:C:210:LEU:HD22	1.87	0.57
1:A:105:ARG:HD2	1:A:106:LEU:N	2.19	0.56
1:C:219:THR:HG23	1:C:221:LYS:H	1.70	0.56
1:B:90:LEU:HB2	1:B:263:MET:HE3	1.87	0.56
1:A:173:MET:SD	1:A:184:CYS:HB3	2.46	0.56
1:D:276:ILE:HG22	1:D:279:LEU:HB2	1.87	0.56
1:D:27:VAL:HG13	1:D:27:VAL:O	2.07	0.55
1:D:27:VAL:HG22	1:D:32:MET:SD	2.48	0.54
1:A:3:LEU:CD1	1:B:213:LEU:HD11	2.36	0.54
1:C:180:HIS:CE1	1:C:182:LEU:HD12	2.42	0.54
1:D:240:VAL:HG11	1:D:247:THR:HG22	1.89	0.54
1:B:206:ALA:HA	1:D:187:TRP:CZ2	2.43	0.54
1:D:276:ILE:HG13	1:D:288:LEU:HB2	1.89	0.54
1:A:291:PRO:HB2	1:A:303:VAL:HB	1.89	0.54
1:D:292:CYS:HB3	1:D:299:ILE:HG23	1.89	0.53
1:B:116:PHE:CZ	1:B:134:ILE:HD11	2.45	0.52
1:B:203:MET:HB3	1:B:210:LEU:HD12	1.91	0.52
1:D:98:ARG:HD3	1:D:103:GLU:OE1	2.10	0.52
1:B:120:ILE:O	1:B:124:VAL:HG13	2.09	0.52
1:B:291:PRO:HB2	1:B:303:VAL:HB	1.92	0.52
1:C:274:THR:O	1:C:287:PHE:HA	2.10	0.52
1:D:98:ARG:NE	1:D:103:GLU:OE1	2.42	0.52
1:A:99:GLN:NE2	1:A:100:GLN:N	2.51	0.52
1:A:292:CYS:HB3	1:A:299:ILE:HG23	1.91	0.51
1:B:114:ASN:HA	1:B:117:LYS:HE2	1.91	0.51
1:A:115:ILE:HG23	2:A:401:NAD:N6A	2.26	0.51
1:A:297:ASN:ND2	1:D:16:GLN:NE2	2.58	0.51
1:A:297:ASN:OD1	1:D:16:GLN:NE2	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:VAL:O	2:C:401:NAD:H2N	2.09	0.51
1:C:293:ILE:HD12	1:C:301:ASP:HB2	1.93	0.51
1:B:92:ILE:HG12	1:B:133:LEU:HD23	1.93	0.50
1:B:134:ILE:HG23	1:B:159:GLY:HA2	1.92	0.48
1:B:25:VAL:HG13	1:B:50:VAL:HG22	1.93	0.48
1:A:297:ASN:CG	1:D:16:GLN:HE22	2.16	0.48
1:C:163:ASN:HA	1:C:271:PRO:HG2	1.95	0.48
1:B:99:GLN:HB2	1:B:108:LEU:HD22	1.95	0.48
1:B:16:GLN:OE1	1:C:297:ASN:ND2	2.47	0.47
1:C:132:LEU:HD13	1:C:152:PHE:HE2	1.79	0.47
1:D:125:LYS:HE3	1:D:126:TYR:CZ	2.48	0.47
1:D:98:ARG:HD2	1:D:98:ARG:N	2.30	0.47
1:C:32:MET:HA	1:C:32:MET:CE	2.44	0.47
1:A:137:ASN:HB2	2:A:401:NAD:O2D	2.15	0.47
1:C:32:MET:HA	1:C:32:MET:HE2	1.97	0.46
1:B:19:GLN:O	1:B:89:LYS:HE2	2.15	0.46
1:A:312:GLU:HG2	1:A:316:LYS:NZ	2.31	0.46
1:A:179:VAL:HG13	1:A:184:CYS:SG	2.56	0.45
1:A:297:ASN:CG	1:D:16:GLN:NE2	2.70	0.45
1:A:106:LEU:HD13	1:A:106:LEU:C	2.37	0.45
1:C:219:THR:HG23	1:C:221:LYS:N	2.32	0.45
1:C:216:ASP:O	1:C:219:THR:HG22	2.17	0.45
1:D:86:ALA:HA	1:D:126:TYR:HB3	1.99	0.45
1:B:221:LYS:HD2	1:B:221:LYS:H	1.82	0.45
1:C:316:LYS:HE3	1:C:316:LYS:HB2	1.68	0.45
1:B:218:GLY:H	1:B:227:LYS:NZ	2.14	0.44
1:D:276:ILE:HG22	1:D:276:ILE:O	2.17	0.44
1:B:46:GLU:OE1	1:B:75:LYS:HD3	2.18	0.44
1:A:297:ASN:ND2	1:D:16:GLN:HE21	2.16	0.44
1:B:266:LEU:O	1:D:180:HIS:HB2	2.18	0.44
1:C:89:LYS:O	1:C:131:LYS:HE2	2.18	0.44
1:D:106:LEU:HD22	1:D:110:GLN:HB3	2.00	0.44
1:B:27:VAL:O	1:B:27:VAL:HG13	2.18	0.43
1:A:172:LEU:HD13	1:A:232:GLN:HB3	2.00	0.43
1:A:6:GLN:O	1:D:304:LYS:HE2	2.18	0.43
1:A:82:TYR:CG	1:A:122:ASN:HB3	2.54	0.43
1:D:162:CYS:HA	1:D:165:ASP:OD1	2.19	0.43
1:D:204:ASN:HA	1:D:210:LEU:HD13	2.00	0.43
1:B:137:ASN:HB2	2:B:401:NAD:O2D	2.19	0.43
1:B:162:CYS:HA	1:B:165:ASP:OD1	2.19	0.42
1:A:243:LEU:HB3	1:B:55:ASP:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLN:O	1:C:304:LYS:HE3	2.19	0.42
1:D:109:VAL:HG22	1:D:138:PRO:HG2	2.01	0.42
1:B:27:VAL:HG22	1:B:32:MET:SD	2.60	0.42
1:A:228:GLU:O	1:A:232:GLN:HB2	2.20	0.42
1:B:238:TYR:O	1:B:242:LYS:HG3	2.20	0.42
1:B:280:TYR:HB3	1:B:312:GLU:HG2	2.01	0.41
1:B:237:ALA:O	1:B:241:ILE:HG12	2.19	0.41
1:C:276:ILE:HG22	1:C:286:VAL:HG13	2.02	0.41
1:B:185:HIS:O	1:B:203:MET:HA	2.20	0.41
1:A:99:GLN:OE1	1:A:108:LEU:HD22	2.21	0.41
1:C:132:LEU:HD13	1:C:152:PHE:CE2	2.54	0.41
1:C:147:TRP:HA	1:C:157:VAL:HG21	2.03	0.41
1:C:279:LEU:HD13	1:C:280:TYR:CD2	2.55	0.41
1:A:29:ALA:HB1	1:A:248:SER:HB3	2.03	0.41
1:A:297:ASN:HD21	1:D:16:GLN:HE21	1.68	0.41
1:C:189:LEU:HD22	1:C:290:VAL:HA	2.03	0.40
1:B:123:VAL:HG11	1:B:132:LEU:HD21	2.03	0.40
1:A:297:ASN:HD21	1:D:16:GLN:NE2	2.18	0.40
1:C:226:TRP:CE2	1:D:3:LEU:HD23	2.57	0.40
1:B:205:VAL:O	1:B:208:VAL:HG13	2.21	0.40
1:C:132:LEU:CD1	1:C:152:PHE:HE2	2.34	0.40
1:B:18:PRO:HB2	1:B:21:LYS:HB2	2.03	0.40
1:B:218:GLY:H	1:B:227:LYS:HE2	1.86	0.40
1:B:163:ASN:HA	1:B:271:PRO:HG2	2.03	0.40
1:B:73:THR:HG23	5:B:514:HOH:O	2.21	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	329/332 (99%)	321 (98%)	8 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	329/332 (99%)	323 (98%)	6 (2%)	0	100	100
1	C	329/332 (99%)	322 (98%)	7 (2%)	0	100	100
1	D	330/332 (99%)	323 (98%)	7 (2%)	0	100	100
All	All	1317/1328 (99%)	1289 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	287/288 (100%)	278 (97%)	9 (3%)	40	51
1	B	287/288 (100%)	281 (98%)	6 (2%)	53	67
1	C	287/288 (100%)	279 (97%)	8 (3%)	43	56
1	D	288/288 (100%)	280 (97%)	8 (3%)	43	56
All	All	1149/1152 (100%)	1118 (97%)	31 (3%)	44	57

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LYS
1	A	72	ARG
1	A	105	ARG
1	A	123	VAL
1	A	124	VAL
1	A	221	LYS
1	A	315	LEU
1	A	329	LEU
1	A	331	PHE
1	B	27	VAL
1	B	107	ASN
1	B	124	VAL
1	B	208	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	221	LYS
1	B	227	LYS
1	C	72	ARG
1	C	131	LYS
1	C	165	ASP
1	C	194	ASP
1	C	219	THR
1	C	220	ASP
1	C	283	LYS
1	C	316	LYS
1	D	12	LEU
1	D	27	VAL
1	D	98	ARG
1	D	165	ASP
1	D	211	LYS
1	D	221	LYS
1	D	315	LEU
1	D	317	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	110	GLN
1	A	297	ASN
1	C	107	ASN
1	C	110	GLN
1	C	297	ASN
1	D	16	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 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
3	SO4	B	403	-	4,4,4	0.11	0	6,6,6	0.05	0
3	SO4	A	404	-	4,4,4	0.13	0	6,6,6	0.07	0
2	NAD	C	401	-	42,48,48	1.08	2 (4%)	50,73,73	1.52	8 (16%)
2	NAD	A	401	-	42,48,48	1.02	3 (7%)	50,73,73	1.08	3 (6%)
4	GN0	D	403	-	34,37,37	1.31	5 (14%)	37,53,53	1.97	7 (18%)
3	SO4	B	402	-	4,4,4	0.16	0	6,6,6	0.04	0
3	SO4	D	402	-	4,4,4	0.16	0	6,6,6	0.08	0
4	GN0	C	403	-	34,37,37	1.20	4 (11%)	37,53,53	1.98	5 (13%)
4	GN0	B	404	-	34,37,37	1.28	5 (14%)	37,53,53	1.89	7 (18%)
2	NAD	D	401	-	42,48,48	1.04	2 (4%)	50,73,73	1.18	6 (12%)
3	SO4	C	402	-	4,4,4	0.13	0	6,6,6	0.13	0
2	NAD	B	401	-	42,48,48	1.02	2 (4%)	50,73,73	1.08	3 (6%)
3	SO4	A	402	-	4,4,4	0.12	0	6,6,6	0.08	0
4	GN0	A	405	-	34,37,37	1.41	5 (14%)	37,53,53	1.90	9 (24%)
3	SO4	A	403	-	4,4,4	0.13	0	6,6,6	0.09	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
2	NAD	C	401	-	-	15/26/62/62	0/5/5/5
2	NAD	A	401	-	-	8/26/62/62	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GN0	D	403	-	-	3/14/46/46	0/5/5/5
4	GN0	C	403	-	-	1/14/46/46	0/5/5/5
4	GN0	B	404	-	-	3/14/46/46	0/5/5/5
2	NAD	D	401	-	-	7/26/62/62	0/5/5/5
2	NAD	B	401	-	-	7/26/62/62	0/5/5/5
4	GN0	A	405	-	-	2/14/46/46	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	GN0	C8-C9	-4.47	1.48	1.53
4	D	403	GN0	C8-C9	-4.32	1.48	1.53
4	B	404	GN0	C8-C9	-4.25	1.48	1.53
4	C	403	GN0	C8-C9	-4.20	1.48	1.53
4	A	405	GN0	C8-C5	-2.99	1.50	1.53
4	D	403	GN0	C8-C5	-2.91	1.50	1.53
4	A	405	GN0	C16-S21	-2.90	1.71	1.76
4	B	404	GN0	O19-C17	-2.86	1.25	1.32
4	A	405	GN0	O19-C17	-2.84	1.25	1.32
4	C	403	GN0	O19-C17	-2.84	1.25	1.32
4	D	403	GN0	O19-C17	-2.80	1.25	1.32
4	B	404	GN0	C8-C5	-2.77	1.50	1.53
2	C	401	NAD	C3N-C7N	-2.63	1.46	1.50
2	B	401	NAD	C7N-N7N	2.48	1.37	1.33
2	C	401	NAD	C7N-N7N	2.47	1.37	1.33
4	D	403	GN0	C10-C9	2.46	1.38	1.37
2	D	401	NAD	C7N-N7N	2.43	1.37	1.33
2	A	401	NAD	C7N-N7N	2.42	1.37	1.33
4	B	404	GN0	C10-C9	2.38	1.38	1.37
4	B	404	GN0	C16-S21	-2.35	1.72	1.76
4	C	403	GN0	C10-C9	2.33	1.38	1.37
2	D	401	NAD	C3N-C7N	-2.30	1.47	1.50
4	D	403	GN0	C16-S21	-2.21	1.72	1.76
4	A	405	GN0	C10-C9	2.20	1.38	1.37
2	A	401	NAD	C2B-C1B	-2.08	1.50	1.53
2	A	401	NAD	C3N-C7N	-2.07	1.47	1.50
4	C	403	GN0	C8-C5	-2.07	1.51	1.53
2	B	401	NAD	C3N-C7N	-2.07	1.47	1.50

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	403	GN0	C8-N14-C15	8.64	123.76	117.33
4	D	403	GN0	C8-N14-C15	8.22	123.45	117.33
4	B	404	GN0	C8-N14-C15	7.61	123.00	117.33
4	A	405	GN0	C8-N14-C15	6.33	122.05	117.33
2	C	401	NAD	O5D-PN-O1N	-5.18	88.81	109.07
4	A	405	GN0	C33-N7-C29	4.27	120.93	111.52
4	C	403	GN0	C33-N7-C29	4.23	120.86	111.52
4	D	403	GN0	C33-N7-C29	4.08	120.52	111.52
4	B	404	GN0	C33-N7-C29	4.07	120.50	111.52
4	C	403	GN0	O19-C17-C16	4.04	130.97	121.91
2	C	401	NAD	C3N-C7N-N7N	-3.94	113.03	117.75
4	A	405	GN0	O19-C17-C16	3.85	130.54	121.91
4	B	404	GN0	O19-C17-C16	3.83	130.51	121.91
2	C	401	NAD	O2N-PN-O1N	3.75	130.78	112.24
4	D	403	GN0	O19-C17-C16	3.71	130.23	121.91
2	D	401	NAD	C3N-C7N-N7N	-3.71	113.30	117.75
4	A	405	GN0	O31-C32-C33	-3.48	104.12	111.80
4	A	405	GN0	O31-C30-C29	-3.15	104.86	111.80
2	B	401	NAD	C3N-C7N-N7N	-3.07	114.07	117.75
2	A	401	NAD	C3N-C7N-N7N	-3.06	114.08	117.75
2	C	401	NAD	O7N-C7N-N7N	2.75	126.48	122.58
4	C	403	GN0	O19-C17-C18	-2.70	108.06	114.38
2	C	401	NAD	O2N-PN-O5D	-2.60	95.69	107.75
4	D	403	GN0	C18-C8-N14	2.53	111.15	108.09
4	D	403	GN0	O31-C30-C29	-2.50	106.28	111.80
4	A	405	GN0	C22-S21-C16	2.46	105.93	102.81
4	B	404	GN0	O19-C17-C18	-2.43	108.67	114.38
2	B	401	NAD	O4B-C1B-C2B	-2.34	103.50	106.93
4	A	405	GN0	C18-C8-N14	2.33	110.91	108.09
4	A	405	GN0	O20-C15-N14	2.33	124.49	121.74
4	B	404	GN0	C18-C8-N14	2.29	110.86	108.09
4	D	403	GN0	O19-C17-C18	-2.27	109.05	114.38
4	D	403	GN0	O31-C32-C33	-2.27	106.80	111.80
4	B	404	GN0	O20-C15-N14	2.25	124.40	121.74
2	C	401	NAD	C2N-C3N-C4N	2.23	120.78	118.26
2	C	401	NAD	O4B-C1B-C2B	-2.19	103.73	106.93
2	D	401	NAD	O7N-C7N-N7N	2.19	125.69	122.58
4	A	405	GN0	O19-C17-C18	-2.11	109.42	114.38
4	C	403	GN0	O31-C30-C29	-2.11	107.16	111.80
2	A	401	NAD	O7N-C7N-N7N	2.10	125.56	122.58
2	A	401	NAD	O2A-PA-O1A	2.07	122.47	112.24
2	C	401	NAD	PN-O3-PA	-2.06	125.74	132.83
2	D	401	NAD	O4B-C1B-C2B	-2.06	103.92	106.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	GN0	O31-C30-C29	-2.06	107.26	111.80
2	B	401	NAD	O7N-C7N-N7N	2.06	125.50	122.58
2	D	401	NAD	C2N-C3N-C4N	2.04	120.57	118.26
2	D	401	NAD	O2N-PN-O1N	2.02	122.23	112.24
2	D	401	NAD	O2A-PA-O1A	2.01	122.19	112.24

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	NAD	C5B-O5B-PA-O2A
2	C	401	NAD	C5D-O5D-PN-O1N
2	C	401	NAD	C5D-O5D-PN-O2N
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	A	401	NAD	C5B-O5B-PA-O2A
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	C2D-C1D-N1N-C2N
4	D	403	GN0	C17-C16-S21-C22
4	B	404	GN0	C17-C16-S21-C22
2	D	401	NAD	C5B-O5B-PA-O2A
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	B	401	NAD	O4D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	O4D-C4D-C5D-O5D
2	C	401	NAD	C3D-C4D-C5D-O5D
2	B	401	NAD	O4B-C4B-C5B-O5B
4	C	403	GN0	C17-C16-S21-C22
2	C	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	C3B-C4B-C5B-O5B
2	C	401	NAD	C5B-O5B-PA-O3
2	A	401	NAD	C5B-O5B-PA-O3
4	B	404	GN0	C15-C16-S21-C22
4	A	405	GN0	C17-C16-S21-C22
2	D	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	PN-O3-PA-O1A

Continued on next page...

Continued from previous page...

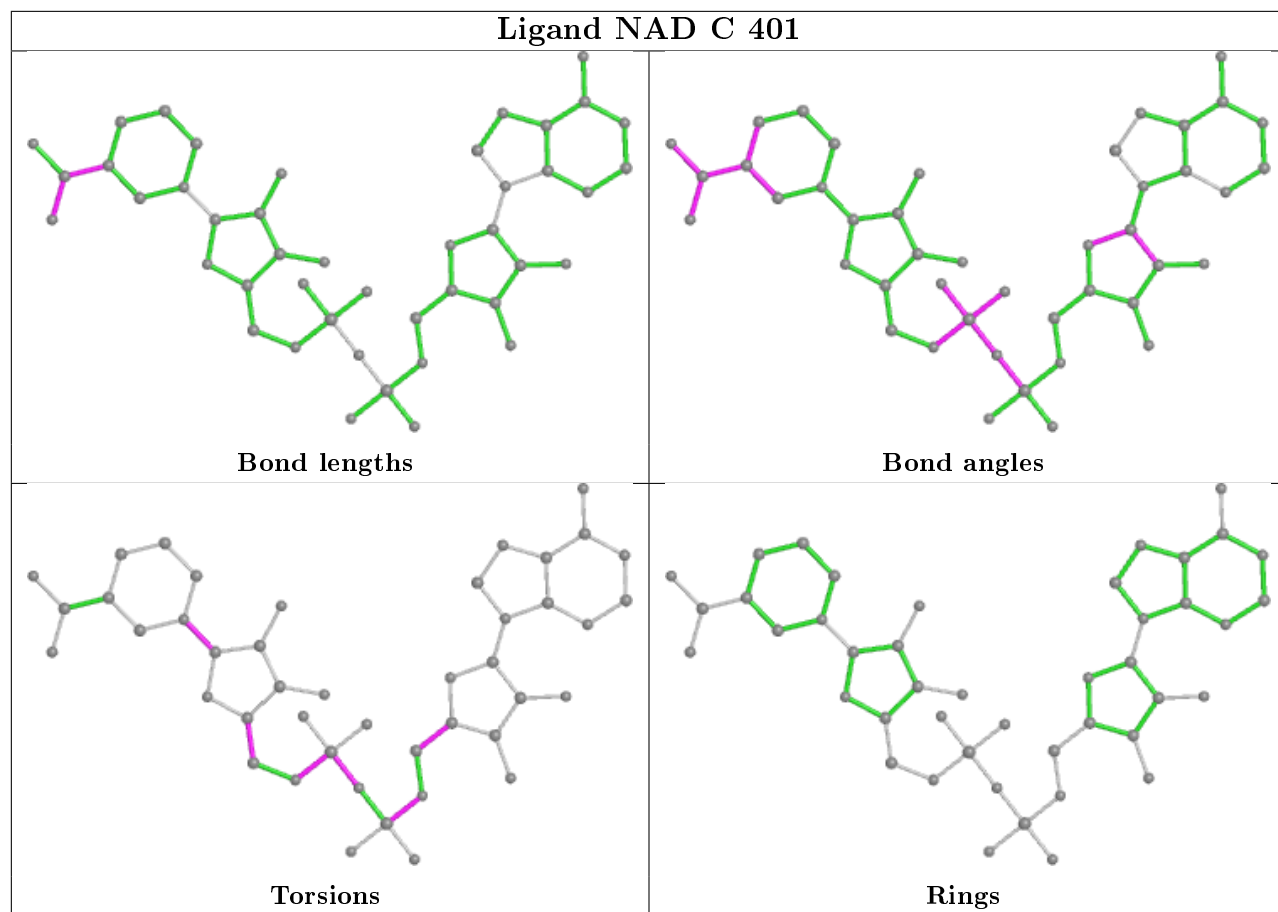
Mol	Chain	Res	Type	Atoms
2	C	401	NAD	C3B-C4B-C5B-O5B
2	A	401	NAD	O4B-C4B-C5B-O5B
2	C	401	NAD	C5D-O5D-PN-O3
2	A	401	NAD	C2D-C1D-N1N-C6N
2	D	401	NAD	C5B-O5B-PA-O3
2	B	401	NAD	C2D-C1D-N1N-C2N
2	B	401	NAD	C2D-C1D-N1N-C6N
2	C	401	NAD	PA-O3-PN-O1N
4	D	403	GN0	C15-C16-S21-C22
4	A	405	GN0	C15-C16-S21-C22
2	C	401	NAD	C5B-O5B-PA-O1A
2	A	401	NAD	C5B-O5B-PA-O1A
4	D	403	GN0	C4-C5-C8-C9
4	B	404	GN0	C6-C5-C8-C9

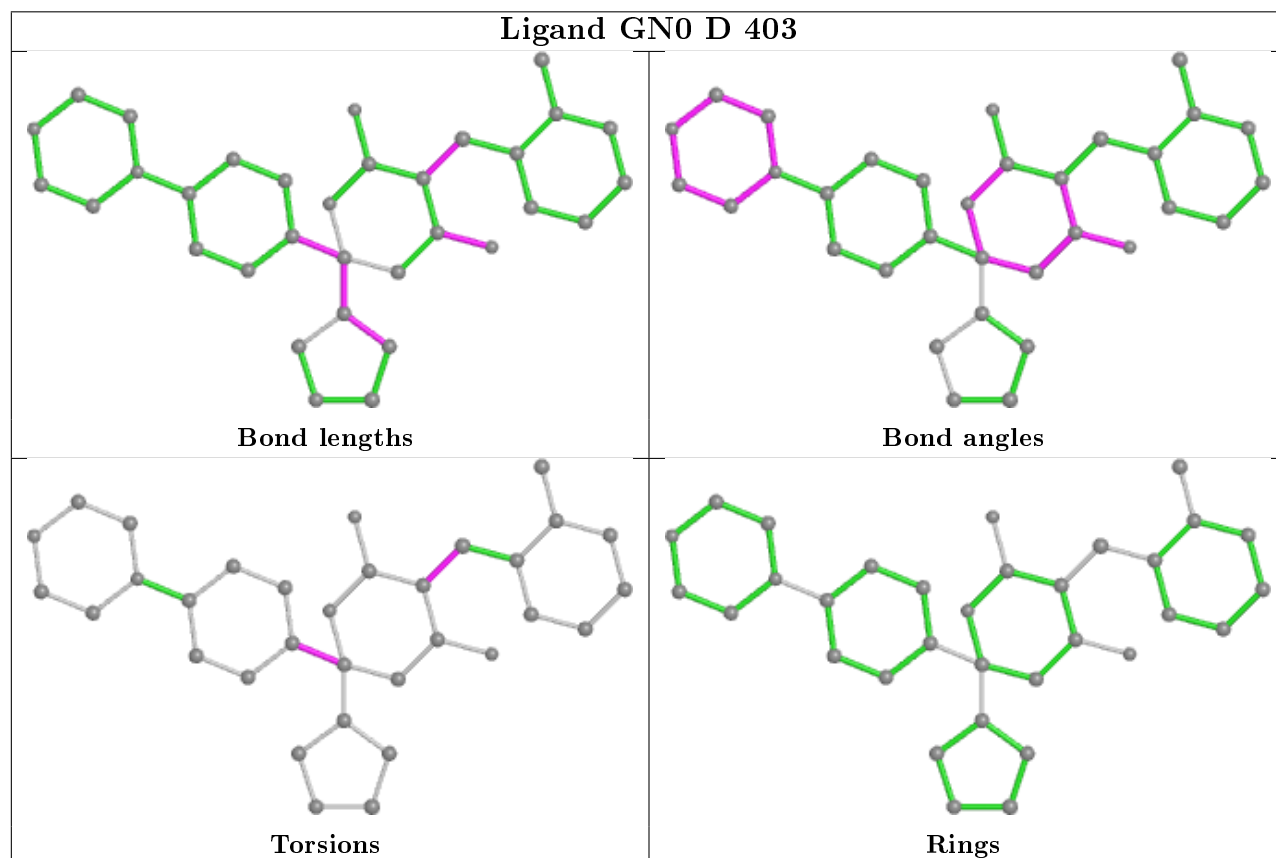
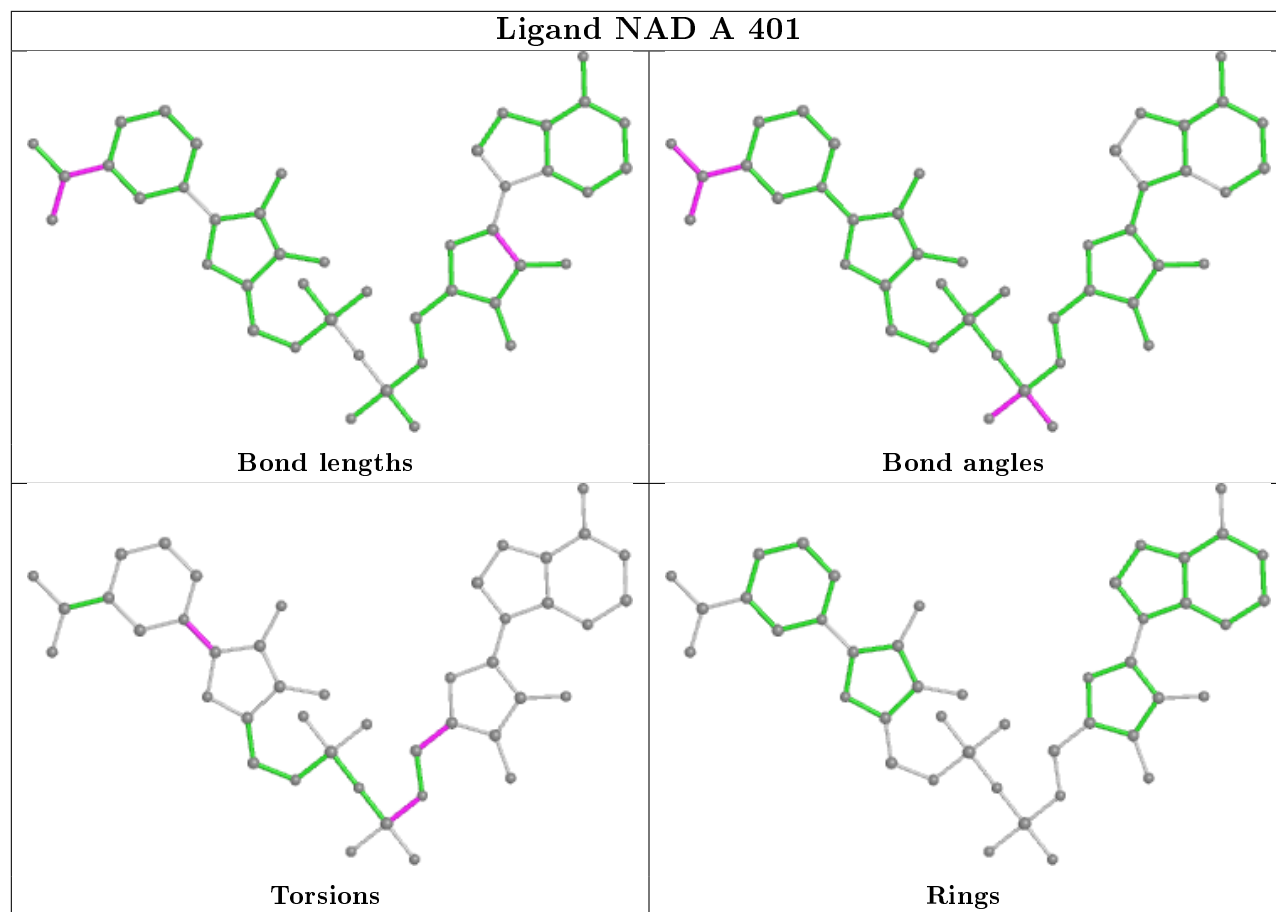
There are no ring outliers.

3 monomers are involved in 4 short contacts:

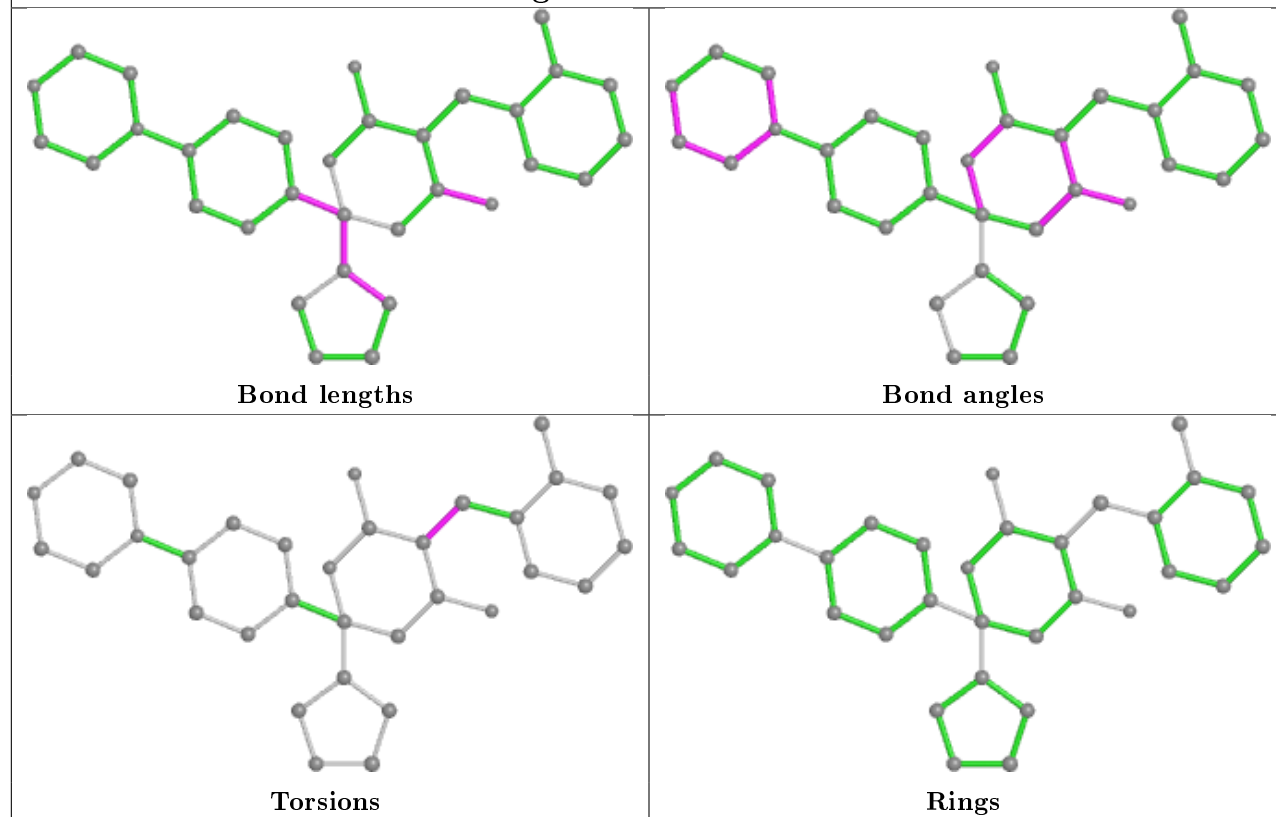
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	NAD	1	0
2	A	401	NAD	2	0
2	B	401	NAD	1	0

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.

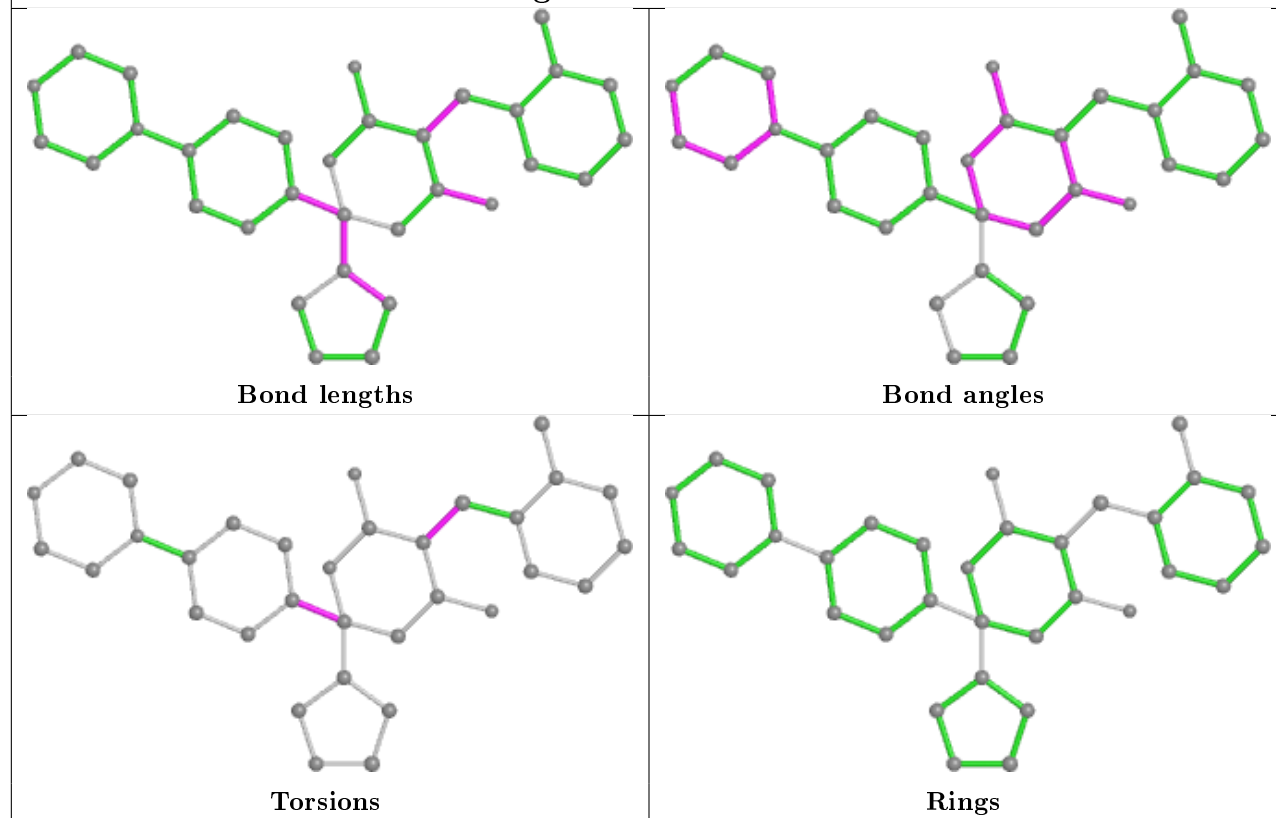


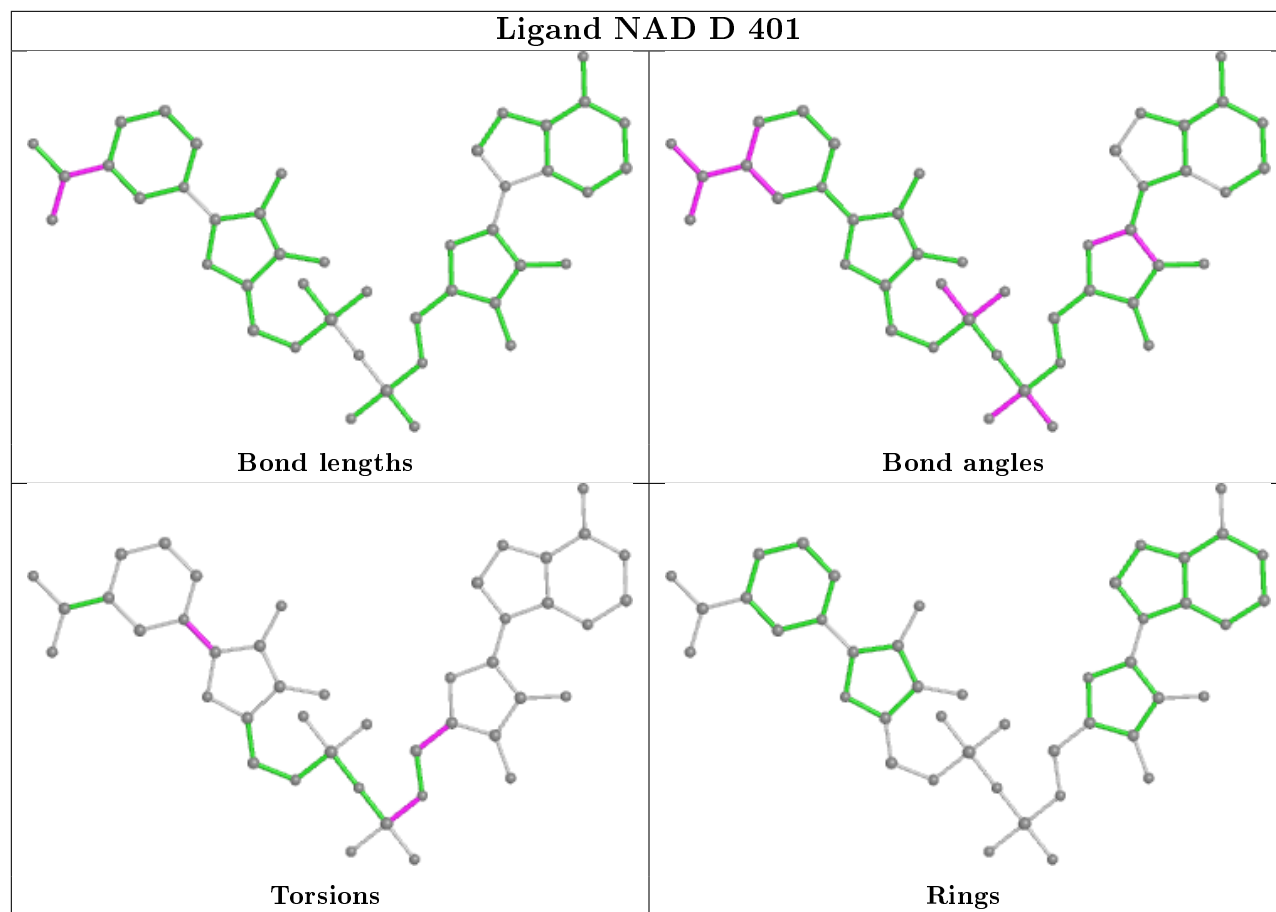


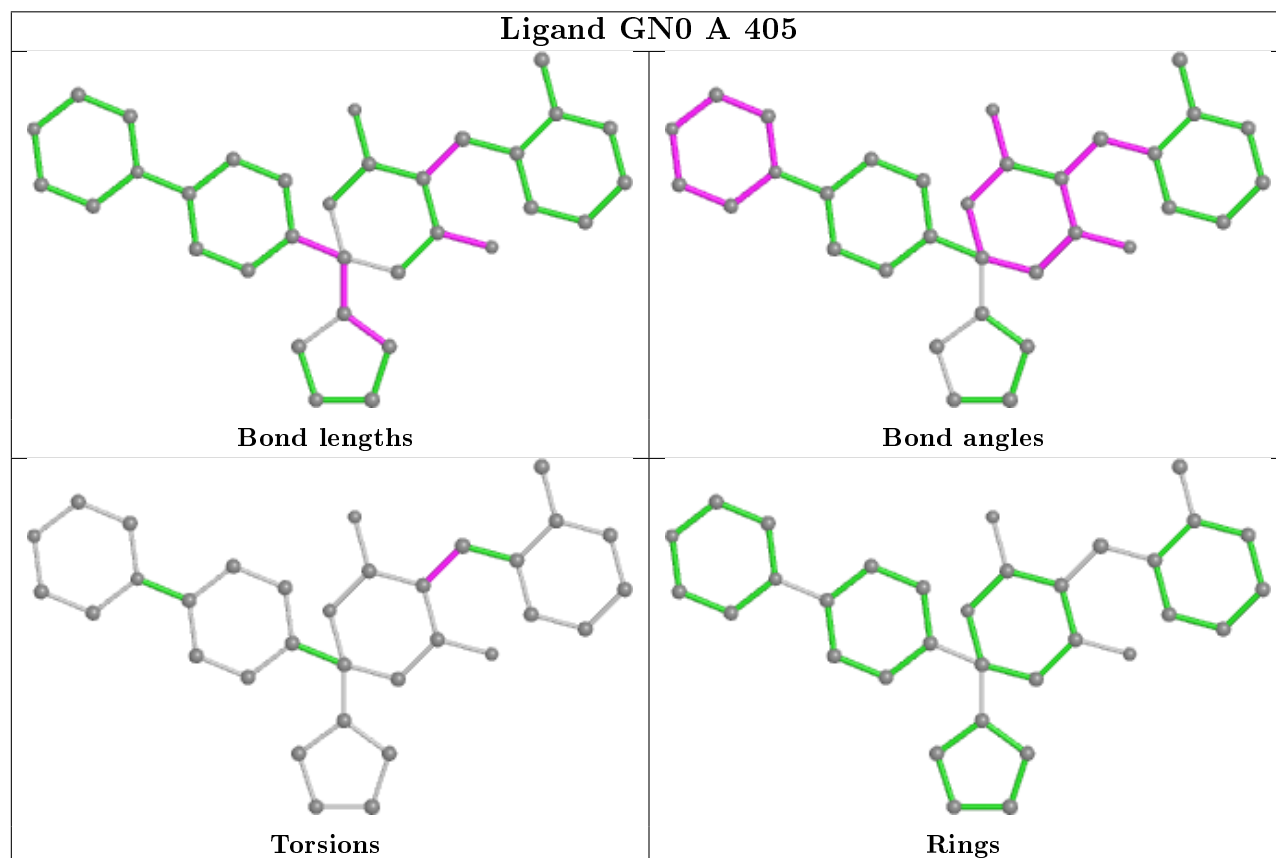
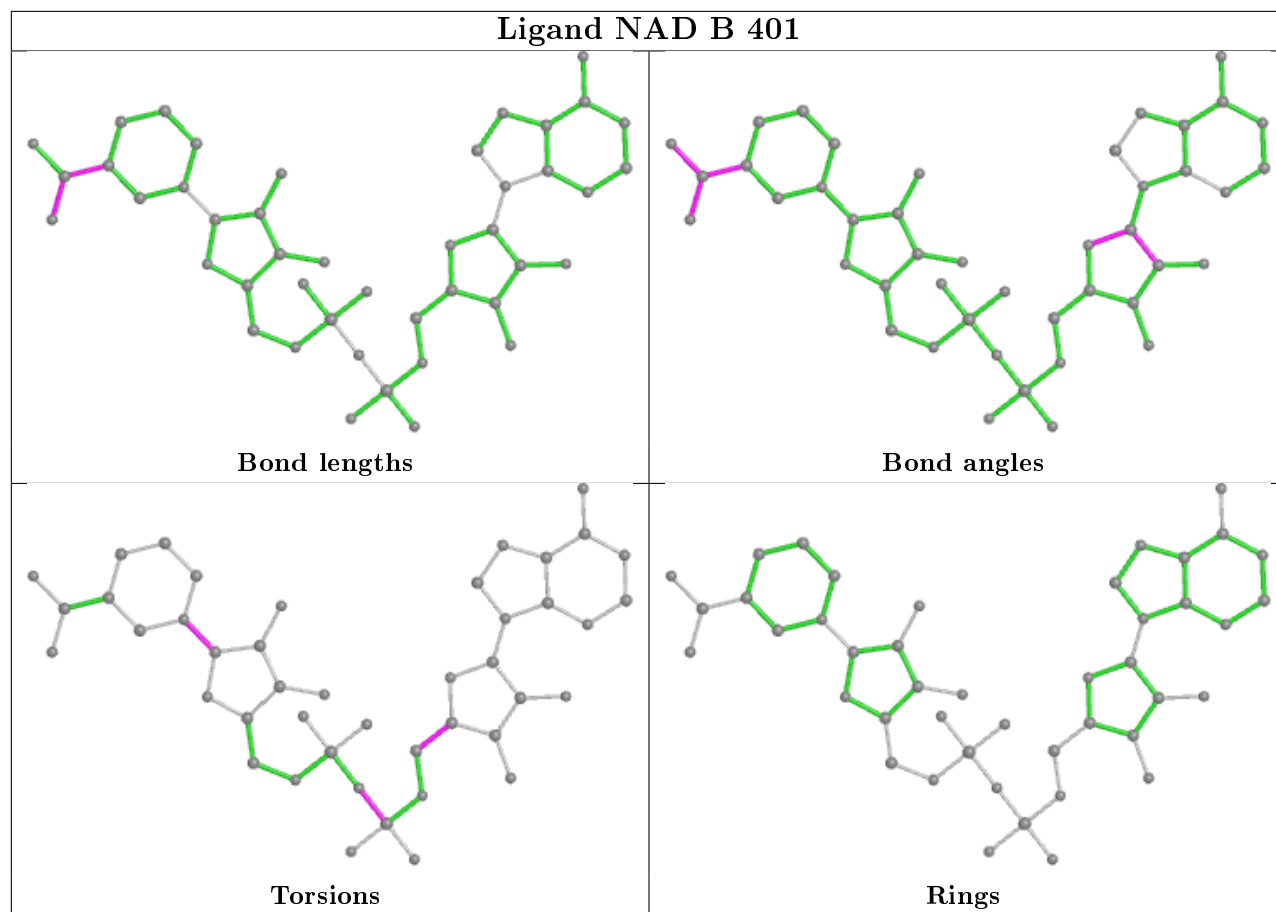
Ligand GN0 C 403



Ligand GN0 B 404







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	331/332 (99%)	0.08	11 (3%) 46 44	28, 35, 50, 66	0
1	B	331/332 (99%)	0.07	5 (1%) 73 72	26, 34, 48, 57	1 (0%)
1	C	331/332 (99%)	0.08	8 (2%) 59 56	26, 33, 46, 55	2 (0%)
1	D	331/332 (99%)	0.10	14 (4%) 36 34	27, 32, 49, 62	1 (0%)
All	All	1324/1328 (99%)	0.08	38 (2%) 51 49	26, 34, 49, 66	4 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	ALA	6.6
1	D	331	PHE	5.5
1	A	105	ARG	5.1
1	D	102	GLY	4.9
1	D	104	SER	4.9
1	D	105	ARG	4.0
1	C	331	PHE	3.9
1	D	1	ALA	3.8
1	A	331	PHE	3.5
1	D	118	PHE	3.5
1	B	106	LEU	3.5
1	D	100	GLN	3.4
1	D	99	GLN	3.3
1	A	106	LEU	3.3
1	C	101	GLU	3.2
1	A	1	ALA	3.1
1	A	223	LYS	3.1
1	C	15	GLU	2.9
1	D	101	GLU	2.9
1	B	331	PHE	2.8
1	A	104	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	106	LEU	2.8
1	D	13	LYS	2.6
1	D	223	LYS	2.6
1	B	1	ALA	2.6
1	A	15	GLU	2.5
1	A	102	GLY	2.5
1	B	102	GLY	2.4
1	A	328	GLU	2.4
1	D	103	GLU	2.3
1	C	13	LYS	2.3
1	B	330	GLN	2.3
1	A	99	GLN	2.2
1	C	14	GLU	2.2
1	A	14	GLU	2.1
1	C	102	GLY	2.1
1	D	16	GLN	2.1
1	C	220	ASP	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

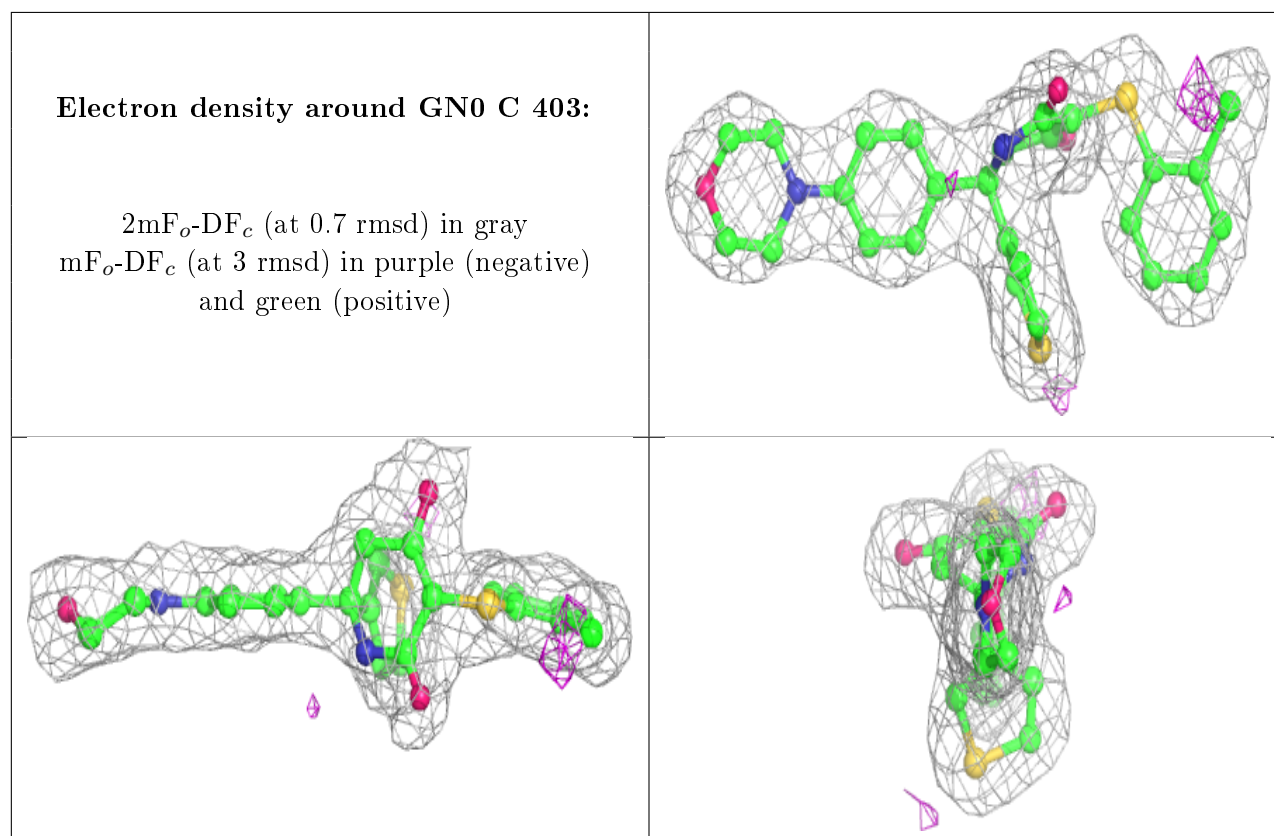
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	402	5/5	0.77	0.38	31,32,32,32	5
3	SO4	B	403	5/5	0.89	0.15	45,46,47,47	0
3	SO4	A	403	5/5	0.89	0.22	51,52,52,53	0
3	SO4	A	402	5/5	0.91	0.24	56,56,57,57	0
4	GN0	C	403	33/33	0.91	0.12	34,36,36,38	0
3	SO4	D	402	5/5	0.93	0.16	50,51,51,51	0

Continued on next page...

Continued from previous page...

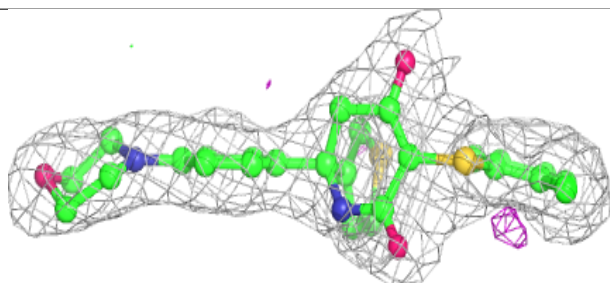
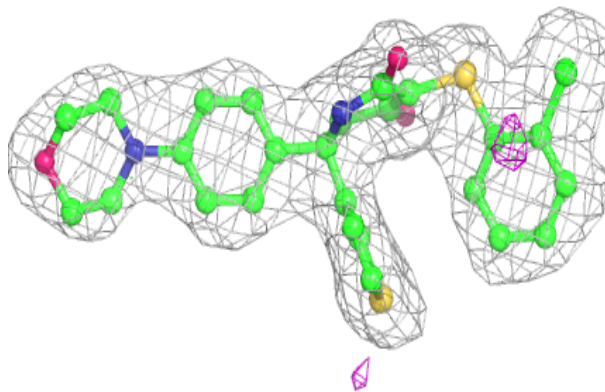
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GN0	A	405	33/33	0.93	0.11	34,35,36,38	0
4	GN0	D	403	33/33	0.93	0.12	32,34,35,35	0
2	NAD	C	401	44/44	0.94	0.12	30,32,35,35	0
2	NAD	A	401	44/44	0.94	0.12	34,35,40,40	0
3	SO4	C	402	5/5	0.94	0.12	49,50,50,51	0
4	GN0	B	404	33/33	0.95	0.11	34,36,40,40	0
3	SO4	A	404	5/5	0.95	0.11	50,50,51,51	5
2	NAD	B	401	44/44	0.95	0.10	31,33,35,35	0
2	NAD	D	401	44/44	0.96	0.09	28,31,34,34	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.

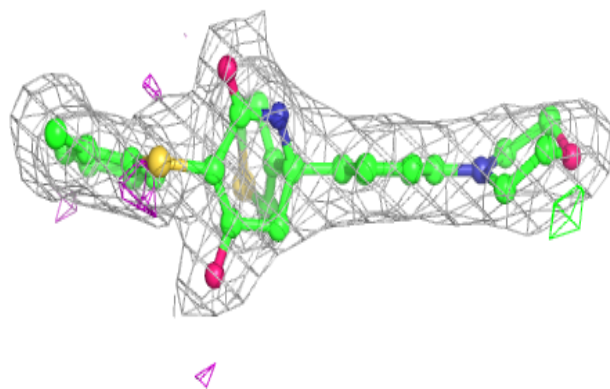
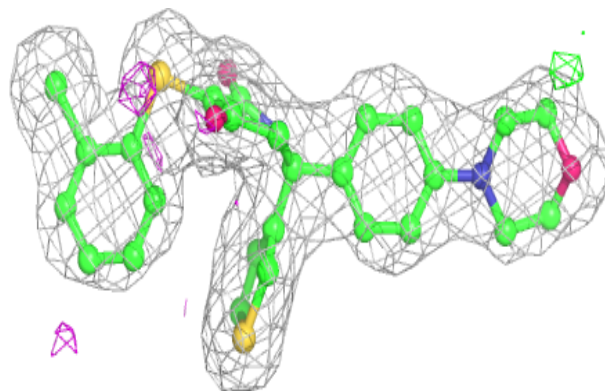


Electron density around GN0 A 405:

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

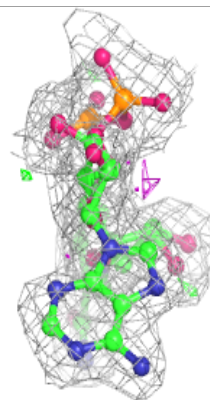
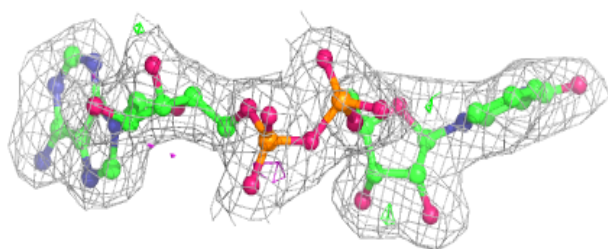
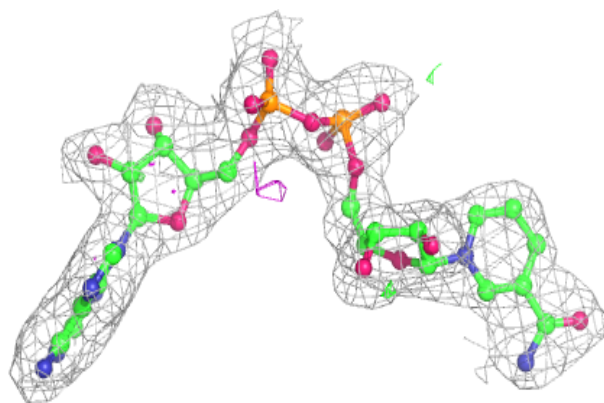
**Electron density around GN0 D 403:**

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

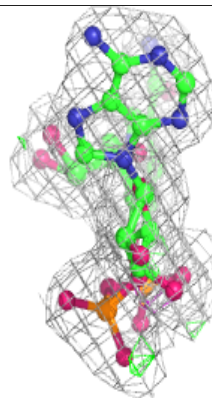
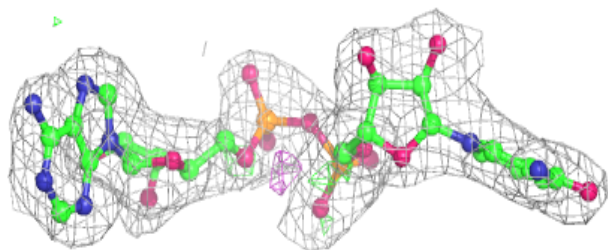
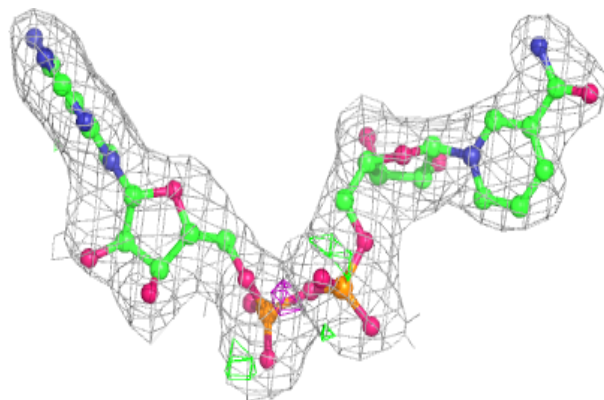


Electron density around NAD C 401:

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

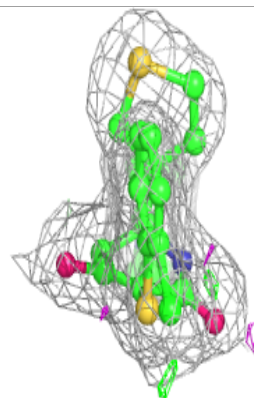
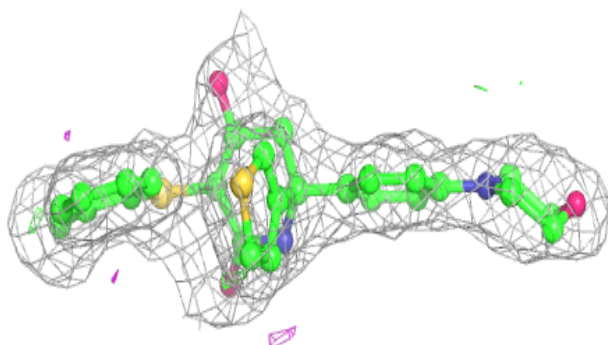
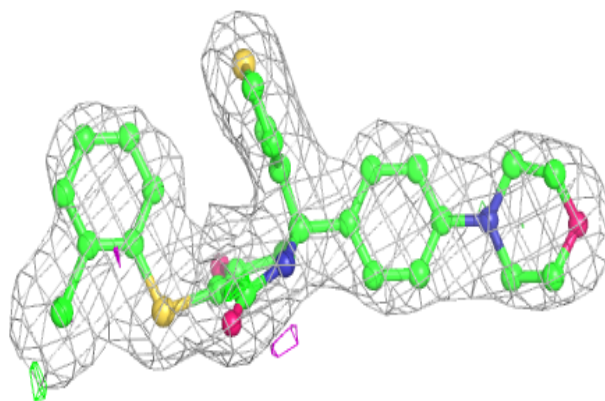
**Electron density around NAD A 401:**

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

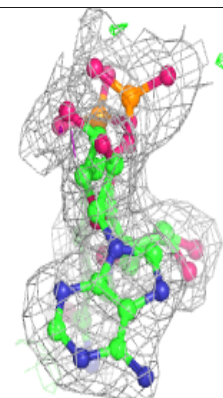
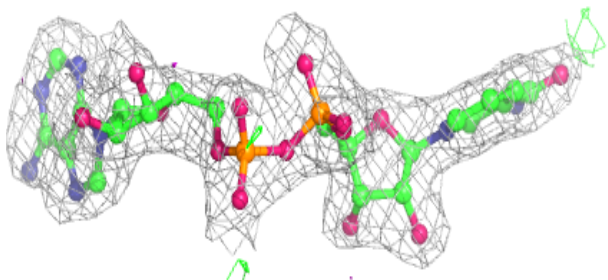
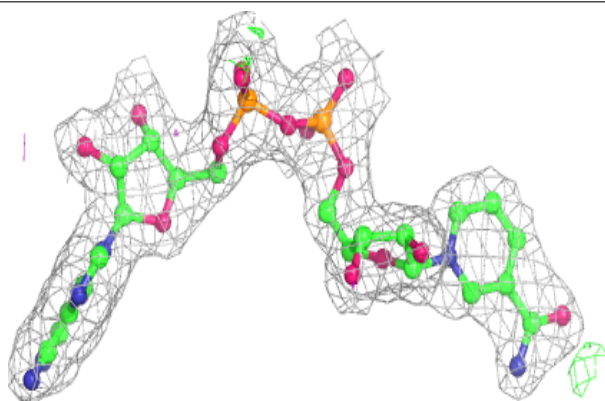


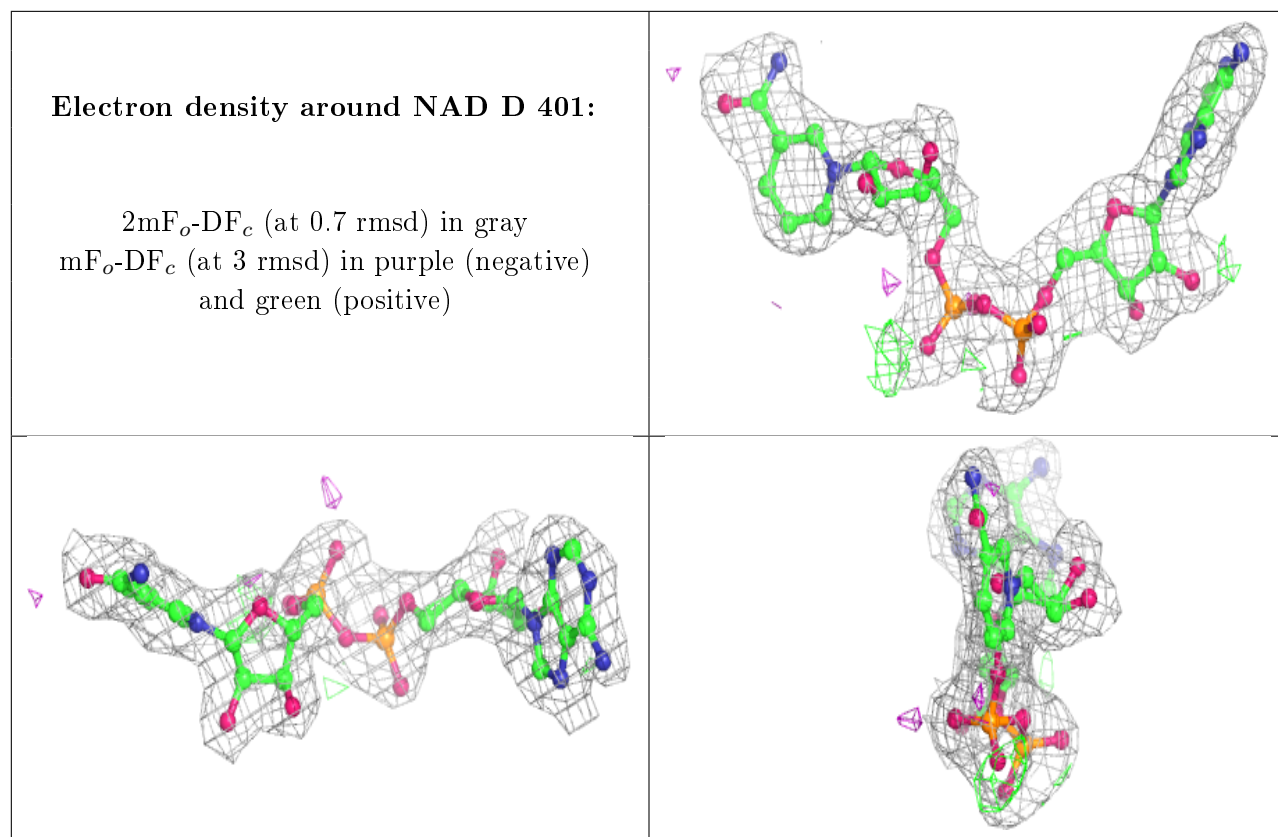
Electron density around GN0 B 404:

$2mF_o-DF_c$ (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.