



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:00 PM UTC

PDB ID : 8JFM / pdb_00008jfm
Title : Crystal structure of enoyl-ACP reductase FabI in complex with NADH from *Helicobacter pylori*
Authors : Song, W.Y.; Zhang, L.
Deposited on : 2023-05-18
Resolution : 2.21 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

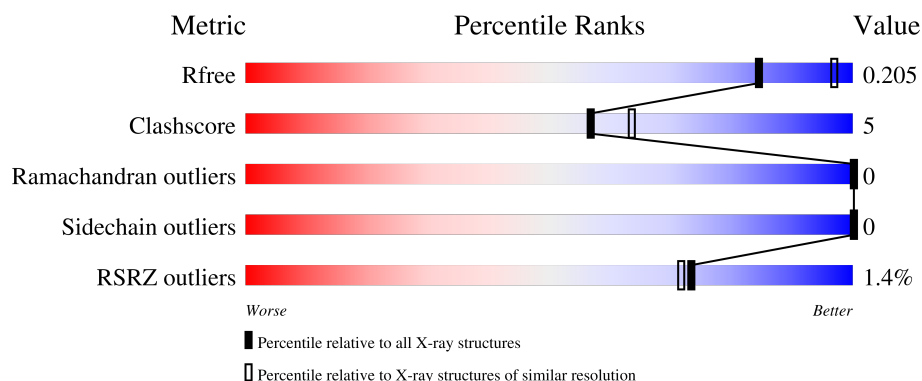
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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 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	273	2% 90% 10%
1	B	273	2% 87% 11% .
1	C	273	2% 86% 11% .
1	D	273	2% 85% 13% .
1	E	273	2% 89% 10% .

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Mol	Chain	Length	Quality of chain
1	F	273	% 91% 7%
1	G	273	2% 89% 10%
1	H	273	% 92% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17995 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	1	0
			2084	1332	348	395	9			
1	B	267	Total	C	N	O	S	0	0	0
			2038	1305	340	384	9			
1	C	267	Total	C	N	O	S	0	0	0
			2042	1308	341	384	9			
1	D	268	Total	C	N	O	S	0	0	0
			2047	1310	341	387	9			
1	E	269	Total	C	N	O	S	0	0	0
			2056	1316	343	388	9			
1	F	267	Total	C	N	O	S	0	0	0
			2038	1305	340	384	9			
1	G	269	Total	C	N	O	S	0	0	0
			2056	1316	343	388	9			
1	H	269	Total	C	N	O	S	0	0	0
			2056	1316	343	388	9			

- 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	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		
3	B	148	Total	O	0	0
			148	148		
3	C	156	Total	O	0	0
			156	156		
3	D	120	Total	O	0	0
			120	120		

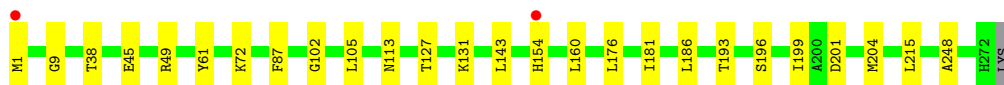
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	172	Total 172	O 172	0	0
3	F	192	Total 192	O 192	0	0
3	G	159	Total 159	O 159	0	0
3	H	133	Total 133	O 133	0	0

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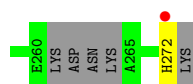
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



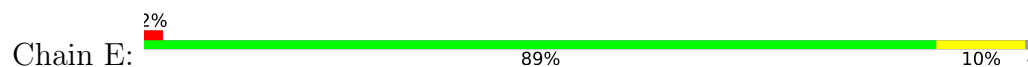
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|------------|------|------|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ASV
LYS | A265 | H772 | LYS | M1 | G9 | Q31 | T38 | L44 | R47 | Y59 | V60 | Y61 | D86 | F87 | F94 | A115 | M116 | E117 | A138 | Y151 | H154 | Y155 | N156 | V157 | A168 | L176 | T181 | R182 | P190 | I191 | T199 | A200 | D201 | N218 | M229 | V239 | M255 | E259 | G1J | LYS |
|------------|------|------|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

-
- GLU
LYS
ASP
ASN
LYS
ALA
T266
H272
K273
- M1
G2
K5
G9
Q31
T38
Y39
L40
L44
E45
K46
R47
P60
I51
E54
Y61
S66
S77
F87
L105
I118
H154
H179
M180
I181
R182
P190
R192
T193
S196
A200
M209
S237
G238
V239
M255
T255

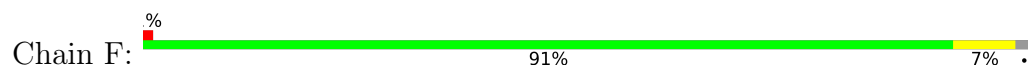
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- | Country | Publications |
|---------|--------------|
| M1 | 10 |
| G2 | 8 |
| K5 | 6 |
| G9 | 5 |
| G32 | 4 |
| T38 | 3 |
| Y39 | 2 |
| L40 | 1 |
| L44 | 1 |
| E45 | 1 |
| E46 | 1 |
| R47 | 1 |
| Y61 | 1 |
| E62 | 1 |
| L63 | 1 |
| L74 | 1 |
| F87 | 1 |
| L100 | 1 |
| S103 | 1 |
| E106 | 1 |
| E125 | 1 |
| L143 | 1 |
| L146 | 1 |
| M152 | 1 |
| L176 | 1 |
| H179 | 1 |
| L180 | 1 |
| I181 | 1 |
| L186 | 1 |
| I199 | 1 |
| A200 | 1 |
| D201 | 1 |
| F202 | 1 |
| R203 | 1 |
| M204 | 1 |
| L215 | 1 |
| R216 | 1 |
| K217 | 1 |
| L218 | 1 |



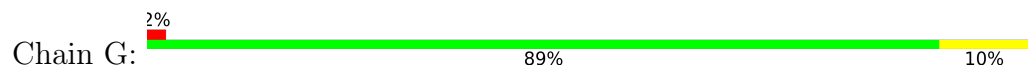
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.81Å 110.55Å 142.94Å 90.00° 99.12° 90.00°	Depositor
Resolution (Å)	46.47 – 2.21 46.47 – 2.21	Depositor EDS
% Data completeness (in resolution range)	93.7 (46.47-2.21) 93.8 (46.47-2.21)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.153 , 0.205 0.154 , 0.205	Depositor DCC
R_{free} test set	5207 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17995	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/2125	0.56	0/2873
1	B	0.50	4/2075 (0.2%)	0.61	2/2806 (0.1%)
1	C	0.35	0/2079	0.59	1/2810 (0.0%)
1	D	0.30	0/2084	0.55	1/2818 (0.0%)
1	E	0.33	0/2093	0.52	0/2829
1	F	0.34	0/2075	0.53	0/2806
1	G	0.34	0/2093	0.55	0/2829
1	H	0.31	0/2093	0.53	0/2829
All	All	0.36	4/16717 (0.0%)	0.55	4/22600 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	157	VAL	C-O	-8.60	1.13	1.24
1	B	155	TYR	C-O	-7.44	1.15	1.24
1	B	156	ASN	C-O	-6.07	1.18	1.24
1	B	151	TYR	C-O	-6.04	1.16	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	203	ARG	CB-CG-CD	8.40	130.61	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ARG	CG-CD-NE	5.63	124.39	112.00
1	B	155	TYR	CB-CA-C	5.34	119.93	110.85
1	C	1	MET	CG-SD-CE	-5.28	89.28	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	154	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2084	0	2114	22	0
1	B	2038	0	2066	26	0
1	C	2042	0	2074	27	0
1	D	2047	0	2072	27	0
1	E	2056	0	2085	22	0
1	F	2038	0	2066	16	0
1	G	2056	0	2085	23	0
1	H	2056	0	2085	16	0
2	A	44	0	26	0	0
2	B	44	0	26	3	0
2	C	44	0	26	3	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	2	0
3	A	146	0	0	2	1
3	B	148	0	0	5	0
3	C	156	0	0	1	0
3	D	120	0	0	6	0
3	E	172	0	0	1	0
3	F	192	0	0	6	1
3	G	159	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	133	0	0	2	1
All	All	17995	0	16855	155	2

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 5.

All (155) 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:154:HIS:HD2	3:B:442:HOH:O	1.50	0.93
1:F:72:LYS:NZ	3:F:401:HOH:O	2.04	0.88
1:C:5:LYS:NZ	3:C:401:HOH:O	2.08	0.85
1:H:8:LYS:NZ	3:H:401:HOH:O	2.16	0.77
1:D:40:LEU:HB3	1:D:44:LEU:HD22	1.68	0.76
1:F:1:MET:HG2	1:G:1:MET:HG2	1.69	0.74
1:C:193:THR:H	1:C:196:SER:HB2	1.54	0.73
1:B:265:ALA:N	3:B:401:HOH:O	2.23	0.71
1:A:1:MET:HE1	1:D:2:GLY:HA2	1.73	0.71
1:A:193:THR:H	1:A:196:SER:HB2	1.58	0.69
1:F:8:LYS:NZ	3:F:403:HOH:O	2.22	0.68
1:B:31:GLN:HE22	1:C:1:MET:HE1	1.59	0.67
1:E:259:GLU:HG3	1:E:268:LEU:HD21	1.76	0.66
1:E:199:ILE:HG22	1:E:201:ASP:H	1.60	0.66
1:F:270:ASP:OD1	3:F:402:HOH:O	2.14	0.65
1:B:31:GLN:NE2	1:C:1:MET:HE1	2.12	0.65
1:A:199:ILE:HG22	1:A:201:ASP:H	1.63	0.63
1:D:1:MET:HG3	1:D:2:GLY:H	1.63	0.63
1:A:72:LYS:NZ	3:A:402:HOH:O	2.31	0.62
1:B:191:ILE:H	2:B:301:NAD:H72N	1.50	0.59
1:E:87:PHE:HB2	1:E:232:LEU:HD22	1.84	0.59
1:B:154:HIS:CD2	3:B:442:HOH:O	2.37	0.59
1:B:31:GLN:HE22	1:C:1:MET:CE	2.16	0.59
1:D:146:LEU:HD23	1:D:152:MET:HE2	1.86	0.58
1:D:125:GLU:OE2	3:D:401:HOH:O	2.17	0.58
1:A:127:THR:O	1:A:131:LYS:HB2	2.04	0.57
1:A:49:ARG:NH1	3:A:404:HOH:O	2.38	0.56
1:E:258:VAL:HG21	1:G:204:MET:HE1	1.87	0.56
1:E:222:GLU:H	1:E:222:GLU:CD	2.11	0.56
1:E:1:MET:HE1	1:H:31:GLN:HE22	1.71	0.56
1:D:179:HIS:ND1	3:D:405:HOH:O	2.33	0.55
1:C:105:LEU:HD11	1:D:176:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:269:TRP:O	1:G:272:HIS:HB3	2.06	0.55
1:H:8:LYS:HG3	1:H:34:THR:HB	1.88	0.55
1:D:103:SER:OG	1:D:106:GLU:HG2	2.07	0.54
1:A:102:GLY:O	1:A:154:HIS:ND1	2.39	0.54
1:F:38:THR:HA	1:F:61:TYR:O	2.08	0.53
1:G:38:THR:HA	1:G:61:TYR:O	2.09	0.52
1:C:2:GLY:H	1:C:5:LYS:HZ2	1.57	0.52
1:C:38:THR:HA	1:C:61:TYR:O	2.10	0.52
1:C:61:TYR:CE1	1:C:77:SER:HB3	2.45	0.51
1:A:1:MET:HE1	1:D:2:GLY:CA	2.39	0.51
1:E:38:THR:HA	1:E:61:TYR:O	2.11	0.51
1:D:199:ILE:HG22	1:D:201:ASP:H	1.76	0.51
1:D:38:THR:HA	1:D:61:TYR:O	2.11	0.51
1:C:190:PRO:HA	2:C:301:NAD:H71N	1.76	0.51
1:C:191:ILE:H	2:C:301:NAD:H72N	1.58	0.51
1:B:255:MET:HE1	1:D:204:MET:HE1	1.91	0.50
1:C:47:ARG:O	1:C:50:PRO:HD2	2.10	0.50
1:B:38:THR:HA	1:B:61:TYR:O	2.11	0.50
1:C:51:ILE:O	1:C:54:GLU:HG2	2.12	0.50
1:G:199:ILE:HG22	1:G:200:ALA:O	2.12	0.49
1:B:151:TYR:CD2	1:B:151:TYR:C	2.90	0.49
1:A:204:MET:HE1	1:C:255:MET:HE1	1.95	0.49
1:E:49:ARG:HB2	1:E:50:PRO:HD3	1.94	0.49
1:A:9:GLY:HA3	1:A:87:PHE:CE2	2.47	0.49
1:D:272:HIS:NE2	3:D:404:HOH:O	2.32	0.49
1:G:40:LEU:HB3	1:G:44:LEU:HD13	1.94	0.49
1:H:9:GLY:HA3	1:H:87:PHE:CZ	2.48	0.49
1:G:176:LEU:HD21	1:H:105:LEU:HD11	1.95	0.48
1:F:209:ASN:ND2	3:F:405:HOH:O	2.36	0.48
1:G:97:LYS:NZ	1:G:198:GLY:HA3	2.29	0.48
1:B:1:MET:HE1	1:C:31:GLN:HE22	1.79	0.47
1:H:176:LEU:HB3	1:H:181:ILE:HB	1.95	0.47
1:H:65:VAL:HG22	2:H:301:NAD:N1A	2.29	0.47
1:C:39:TYR:CD1	1:C:45:GLU:HB2	2.50	0.47
1:C:1:MET:O	1:C:1:MET:HG2	2.13	0.47
1:D:63:LEU:HD22	1:D:74:LEU:HD22	1.97	0.47
1:D:215:LEU:HB2	1:D:248:ALA:HB1	1.97	0.47
1:B:229:MET:HE3	1:B:229:MET:HB3	1.78	0.47
1:D:47:ARG:N	1:D:47:ARG:HD2	2.30	0.46
1:A:38:THR:HA	1:A:61:TYR:O	2.15	0.46
1:F:68:GLU:HG2	1:F:125:GLU:OE2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:MET:HE2	3:E:405:HOH:O	2.15	0.46
1:H:39:TYR:CD2	1:H:60:VAL:HG12	2.51	0.46
1:E:127:THR:HG21	1:E:176:LEU:HD11	1.98	0.46
1:F:31:GLN:HE22	1:G:1:MET:CE	2.29	0.45
1:H:169:VAL:HG21	1:H:185:ALA:HB2	1.98	0.45
1:B:9:GLY:HA3	1:B:87:PHE:CE2	2.52	0.45
1:D:39:TYR:CD1	1:D:45:GLU:HB2	2.52	0.45
1:G:176:LEU:HB3	1:G:181:ILE:HB	1.99	0.45
1:C:190:PRO:HG3	1:C:209:ASN:ND2	2.31	0.45
1:B:176:LEU:HB3	1:B:181:ILE:HB	1.98	0.45
1:F:1:MET:HG2	1:G:1:MET:CG	2.43	0.45
1:D:9:GLY:HA3	1:D:87:PHE:CZ	2.52	0.45
1:D:100:LEU:HD12	1:D:199:ILE:HD11	1.99	0.45
1:E:9:GLY:HA3	1:E:87:PHE:CE2	2.51	0.45
1:D:9:GLY:HA3	1:D:87:PHE:CE2	2.51	0.45
1:A:45:GLU:HG2	1:A:49:ARG:HG3	1.99	0.44
1:C:179:HIS:HB2	1:C:181:ILE:HD12	1.99	0.44
1:F:46:LYS:HG3	1:F:47:ARG:HD2	1.99	0.44
1:A:215:LEU:HD12	1:A:248:ALA:HA	1.99	0.44
1:E:72:LYS:HB3	1:E:73:PRO:HD3	1.98	0.44
1:H:97:LYS:HE2	1:H:198:GLY:O	2.17	0.44
1:D:1:MET:CG	1:D:2:GLY:H	2.30	0.44
1:D:143:LEU:HD13	1:D:186:LEU:HB3	1.99	0.44
1:F:1:MET:CE	1:G:31:GLN:HE22	2.30	0.44
1:B:190:PRO:HA	2:B:301:NAD:H71N	1.82	0.44
1:H:8:LYS:HB2	1:H:8:LYS:HE2	1.81	0.44
1:A:204:MET:HE3	1:A:204:MET:HB3	1.87	0.44
1:E:1:MET:CE	1:H:31:GLN:HE22	2.31	0.43
1:D:217:LYS:NZ	3:D:406:HOH:O	2.35	0.43
1:E:259:GLU:HG3	1:E:268:LEU:CD2	2.45	0.43
1:A:105:LEU:HD11	1:B:176:LEU:HD21	2.00	0.43
1:D:176:LEU:HB3	1:D:181:ILE:HB	2.00	0.43
1:C:40:LEU:HB3	1:C:44:LEU:HD12	2.00	0.43
1:D:5:LYS:HA	1:D:32:GLY:O	2.18	0.43
1:B:86:ASP:O	1:B:138:ALA:HA	2.19	0.43
1:A:113:ASN:ND2	1:B:117:GLU:OE2	2.48	0.43
1:C:66:SER:HB3	1:C:118:ILE:HD11	2.00	0.43
1:E:97:LYS:NZ	1:E:198:GLY:O	2.51	0.43
1:C:9:GLY:HA2	1:C:87:PHE:O	2.19	0.43
1:A:143:LEU:HD13	1:A:186:LEU:HB3	2.01	0.42
1:C:182:ARG:HD2	1:C:239:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:MET:HB2	1:E:204:MET:HE2	1.86	0.42
1:F:218:ASN:HB3	3:F:418:HOH:O	2.18	0.42
1:D:204:MET:HE3	1:D:204:MET:HB3	1.86	0.42
1:F:87:PHE:HB2	1:F:232:LEU:HD22	2.01	0.42
1:E:207:LYS:HA	1:E:207:LYS:HD3	1.79	0.42
1:G:131:LYS:HB3	1:G:131:LYS:HE2	1.91	0.42
1:E:208:TRP:CZ3	1:G:267:LEU:HD11	2.55	0.42
1:F:155:TYR:CZ	1:F:158:MET:HG3	2.54	0.42
1:A:1:MET:HE2	3:D:513:HOH:O	2.19	0.42
1:A:176:LEU:HB3	1:A:181:ILE:HB	2.02	0.42
1:B:44:LEU:HD21	3:B:507:HOH:O	2.18	0.42
1:B:182:ARG:HD2	1:B:239:VAL:O	2.19	0.42
1:H:79:LYS:HD3	1:H:133:LEU:HD22	2.02	0.42
3:F:490:HOH:O	1:G:1:MET:HE2	2.20	0.42
1:B:94:PHE:O	1:B:115:ALA:HA	2.20	0.41
1:A:160:LEU:HD11	1:B:168:ALA:HA	2.02	0.41
1:E:59:TYR:HB3	1:E:61:TYR:OH	2.20	0.41
1:G:127:THR:HG22	1:H:105:LEU:HD21	2.02	0.41
1:E:1:MET:HE2	3:H:479:HOH:O	2.20	0.41
1:E:66:SER:HB3	1:E:118:ILE:HD11	2.02	0.41
1:C:1:MET:N	1:C:5:LYS:NZ	2.68	0.41
1:H:65:VAL:HG22	2:H:301:NAD:C6A	2.51	0.41
1:B:9:GLY:HA3	1:B:87:PHE:CZ	2.55	0.41
1:A:45:GLU:OE1	1:A:49:ARG:NE	2.52	0.41
1:B:190:PRO:HA	2:B:301:NAD:N7N	2.36	0.41
1:C:182:ARG:NE	1:C:237:SER:HA	2.36	0.41
1:G:47:ARG:HD2	1:G:47:ARG:N	2.35	0.41
1:G:47:ARG:C	1:G:50:PRO:HD2	2.45	0.41
1:G:201:ASP:O	1:G:205:ILE:HG13	2.21	0.41
1:C:190:PRO:HA	2:C:301:NAD:N7N	2.34	0.40
1:B:59:TYR:HB3	1:B:61:TYR:OH	2.21	0.40
1:B:218:ASN:HB3	3:B:439:HOH:O	2.20	0.40
1:G:9:GLY:HA3	1:G:87:PHE:CZ	2.55	0.40
1:D:200:ALA:O	3:D:402:HOH:O	2.22	0.40
1:F:9:GLY:HA3	1:F:87:PHE:CZ	2.57	0.40
1:G:59:TYR:HB3	1:G:61:TYR:OH	2.21	0.40
1:G:67:LYS:HZ2	1:G:67:LYS:HG2	1.74	0.40
1:E:204:MET:HE1	1:G:267:LEU:HG	2.03	0.40
1:A:9:GLY:HA3	1:A:87:PHE:CZ	2.57	0.40
1:C:9:GLY:HA3	1:C:87:PHE:CE2	2.56	0.40
1:F:208:TRP:CZ3	1:H:267:LEU:HD11	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:472:HOH:O	3:H:514:HOH:O[1_545]	2.14	0.06
3:F:530:HOH:O	3:G:463:HOH:O[2_446]	2.16	0.04

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	271/273 (99%)	264 (97%)	7 (3%)	0	100	100
1	B	263/273 (96%)	255 (97%)	8 (3%)	0	100	100
1	C	263/273 (96%)	258 (98%)	5 (2%)	0	100	100
1	D	264/273 (97%)	258 (98%)	6 (2%)	0	100	100
1	E	265/273 (97%)	259 (98%)	6 (2%)	0	100	100
1	F	263/273 (96%)	255 (97%)	8 (3%)	0	100	100
1	G	265/273 (97%)	259 (98%)	6 (2%)	0	100	100
1	H	265/273 (97%)	258 (97%)	7 (3%)	0	100	100
All	All	2119/2184 (97%)	2066 (98%)	53 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	225/225 (100%)	225 (100%)	0	100	100
1	B	219/225 (97%)	219 (100%)	0	100	100
1	C	220/225 (98%)	220 (100%)	0	100	100
1	D	220/225 (98%)	220 (100%)	0	100	100
1	E	221/225 (98%)	221 (100%)	0	100	100
1	F	219/225 (97%)	219 (100%)	0	100	100
1	G	221/225 (98%)	221 (100%)	0	100	100
1	H	221/225 (98%)	221 (100%)	0	100	100
All	All	1766/1800 (98%)	1766 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	263	ASN
1	A	272	HIS
1	B	53	GLN
1	B	128	ASN
1	C	26	GLN
1	C	128	ASN
1	D	251	HIS
1	E	179	HIS
1	F	128	ASN
1	F	136	ASN
1	F	218	ASN
1	H	26	GLN
1	H	30	ASN
1	H	113	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	D	301	-	46,48,48	0.75	1 (2%)	64,73,73	0.99	3 (4%)
2	NAD	C	301	-	46,48,48	1.06	3 (6%)	64,73,73	1.08	2 (3%)
2	NAD	A	301	-	46,48,48	0.84	1 (2%)	64,73,73	0.90	3 (4%)
2	NAD	H	301	-	46,48,48	1.02	3 (6%)	64,73,73	1.04	4 (6%)
2	NAD	E	301	-	46,48,48	0.79	0	64,73,73	0.90	3 (4%)
2	NAD	F	301	-	46,48,48	1.06	2 (4%)	64,73,73	1.10	3 (4%)
2	NAD	G	301	-	46,48,48	0.72	0	64,73,73	1.02	3 (4%)
2	NAD	B	301	-	46,48,48	0.79	1 (2%)	64,73,73	0.84	2 (3%)

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	D	301	-	-	6/30/62/62	0/5/5/5
2	NAD	C	301	-	-	5/30/62/62	0/5/5/5
2	NAD	A	301	-	-	7/30/62/62	0/5/5/5
2	NAD	H	301	-	-	6/30/62/62	0/5/5/5
2	NAD	E	301	-	-	7/30/62/62	0/5/5/5
2	NAD	F	301	-	-	6/30/62/62	0/5/5/5
2	NAD	G	301	-	-	6/30/62/62	0/5/5/5
2	NAD	B	301	-	-	7/30/62/62	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAD	C2N-N1N	3.23	1.38	1.35
2	H	301	NAD	PA-O2A	-2.59	1.43	1.55
2	C	301	NAD	PA-O2A	-2.57	1.43	1.55
2	B	301	NAD	C2N-N1N	2.51	1.37	1.35
2	F	301	NAD	PA-O2A	-2.51	1.43	1.55
2	C	301	NAD	C5N-C4N	-2.38	1.34	1.38
2	H	301	NAD	C5N-C4N	-2.33	1.34	1.38
2	F	301	NAD	C5N-C4N	-2.28	1.35	1.38
2	D	301	NAD	C5N-C4N	-2.07	1.35	1.38
2	H	301	NAD	PN-O2N	-2.03	1.45	1.55
2	C	301	NAD	PN-O2N	-2.01	1.46	1.55

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAD	C6N-N1N-C2N	-4.72	117.86	121.88
2	G	301	NAD	O4B-C1B-N9A	4.53	116.79	108.09
2	F	301	NAD	C6N-N1N-C2N	-4.48	118.06	121.88
2	F	301	NAD	O4B-C1B-N9A	4.21	116.17	108.09
2	C	301	NAD	O4B-C1B-N9A	4.15	116.05	108.09
2	H	301	NAD	C6N-N1N-C2N	-4.13	118.36	121.88
2	A	301	NAD	C6N-N1N-C2N	-3.69	118.74	121.88
2	D	301	NAD	O4B-C1B-N9A	3.54	114.88	108.09
2	D	301	NAD	C6N-N1N-C2N	-3.38	119.00	121.88
2	G	301	NAD	C6N-N1N-C2N	-3.35	119.03	121.88
2	A	301	NAD	O4B-C1B-N9A	3.23	114.29	108.09
2	E	301	NAD	O4B-C1B-N9A	2.92	113.70	108.09
2	B	301	NAD	C6N-N1N-C2N	-2.78	119.51	121.88
2	B	301	NAD	O4B-C1B-N9A	2.66	113.20	108.09
2	H	301	NAD	O4B-C1B-C2B	-2.41	101.45	106.62
2	G	301	NAD	C4B-O4B-C1B	-2.39	104.20	109.47
2	H	301	NAD	C4A-N9A-C1B	-2.25	121.36	126.63
2	D	301	NAD	O3-PN-O1N	-2.25	103.92	110.70
2	E	301	NAD	C3N-C7N-N7N	2.23	120.48	117.74
2	E	301	NAD	C6N-N1N-C2N	-2.23	119.98	121.88
2	F	301	NAD	C4B-O4B-C1B	-2.12	104.79	109.47
2	H	301	NAD	C1B-N9A-C8A	2.05	131.65	127.09
2	A	301	NAD	O4B-C1B-C2B	-2.01	102.31	106.62

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAD	C5D-O5D-PN-O3
2	A	301	NAD	C5D-O5D-PN-O1N
2	A	301	NAD	C5D-O5D-PN-O2N
2	A	301	NAD	O4D-C1D-N1N-C2N
2	A	301	NAD	O4D-C1D-N1N-C6N
2	A	301	NAD	C2D-C1D-N1N-C6N
2	B	301	NAD	C5D-O5D-PN-O3
2	B	301	NAD	C5D-O5D-PN-O1N
2	B	301	NAD	C5D-O5D-PN-O2N
2	B	301	NAD	O4D-C1D-N1N-C2N
2	B	301	NAD	O4D-C1D-N1N-C6N
2	B	301	NAD	C2D-C1D-N1N-C6N
2	C	301	NAD	PN-O3-PA-O5B
2	C	301	NAD	C5D-O5D-PN-O3
2	C	301	NAD	C5D-O5D-PN-O1N
2	C	301	NAD	C5D-O5D-PN-O2N
2	C	301	NAD	O4D-C1D-N1N-C2N
2	D	301	NAD	PN-O3-PA-O5B
2	D	301	NAD	C5D-O5D-PN-O3
2	D	301	NAD	C5D-O5D-PN-O1N
2	D	301	NAD	C5D-O5D-PN-O2N
2	D	301	NAD	O4D-C1D-N1N-C6N
2	D	301	NAD	C2D-C1D-N1N-C6N
2	E	301	NAD	PN-O3-PA-O5B
2	E	301	NAD	C5D-O5D-PN-O3
2	E	301	NAD	C5D-O5D-PN-O1N
2	E	301	NAD	C5D-O5D-PN-O2N
2	F	301	NAD	C5D-O5D-PN-O3
2	F	301	NAD	C5D-O5D-PN-O1N
2	F	301	NAD	C5D-O5D-PN-O2N
2	F	301	NAD	O4D-C1D-N1N-C2N
2	G	301	NAD	PN-O3-PA-O5B
2	G	301	NAD	C5D-O5D-PN-O3
2	G	301	NAD	C5D-O5D-PN-O1N
2	G	301	NAD	C5D-O5D-PN-O2N
2	G	301	NAD	O4D-C1D-N1N-C6N
2	G	301	NAD	C2D-C1D-N1N-C6N
2	H	301	NAD	C5D-O5D-PN-O3
2	H	301	NAD	C5D-O5D-PN-O1N
2	H	301	NAD	C5D-O5D-PN-O2N
2	H	301	NAD	O4D-C1D-N1N-C2N
2	A	301	NAD	PN-O3-PA-O5B
2	B	301	NAD	PN-O3-PA-O5B

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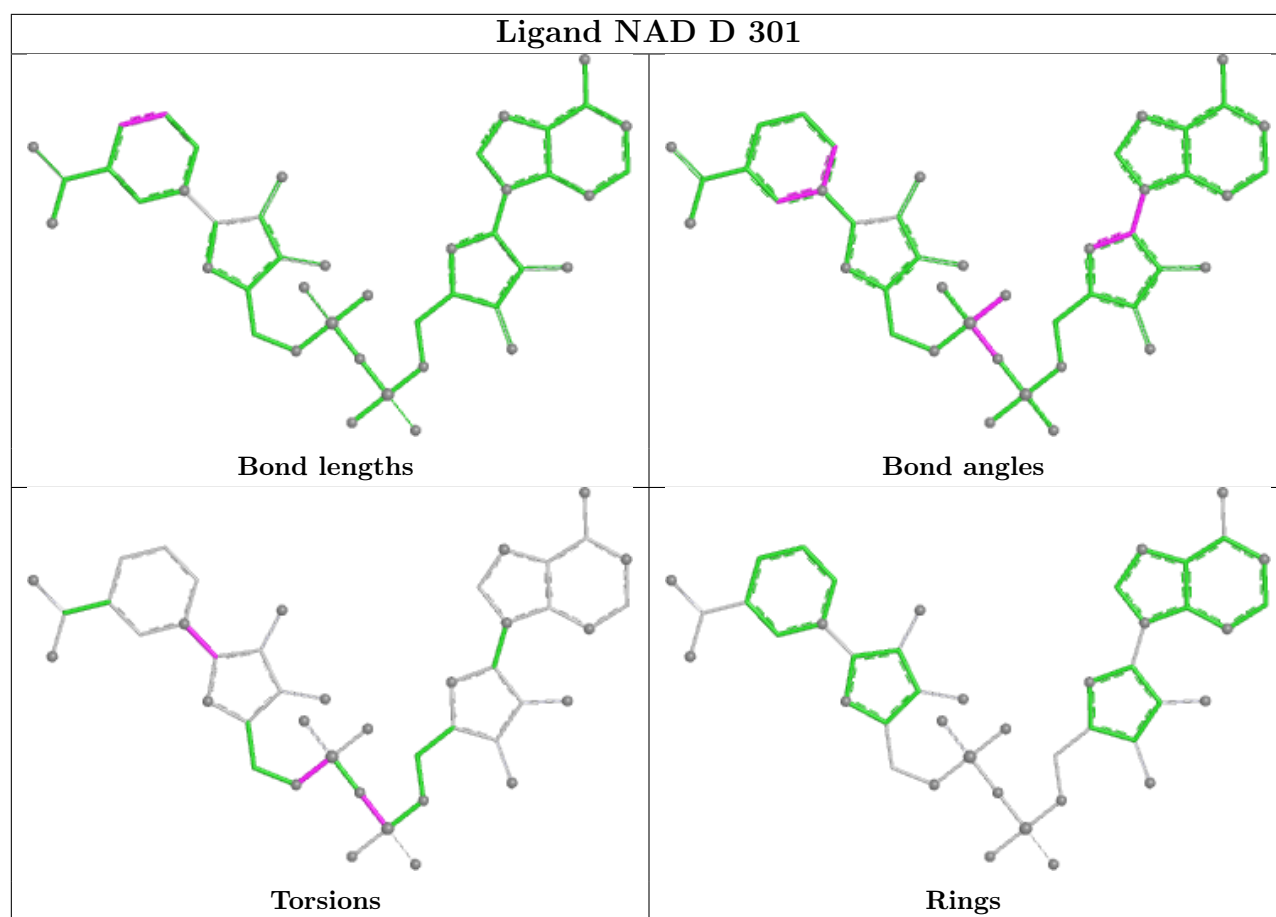
Mol	Chain	Res	Type	Atoms
2	F	301	NAD	PN-O3-PA-O5B
2	H	301	NAD	PN-O3-PA-O5B
2	E	301	NAD	C2D-C1D-N1N-C6N
2	E	301	NAD	O4D-C1D-N1N-C6N
2	F	301	NAD	O4D-C1D-N1N-C6N
2	H	301	NAD	O4D-C1D-N1N-C6N
2	E	301	NAD	O4B-C4B-C5B-O5B

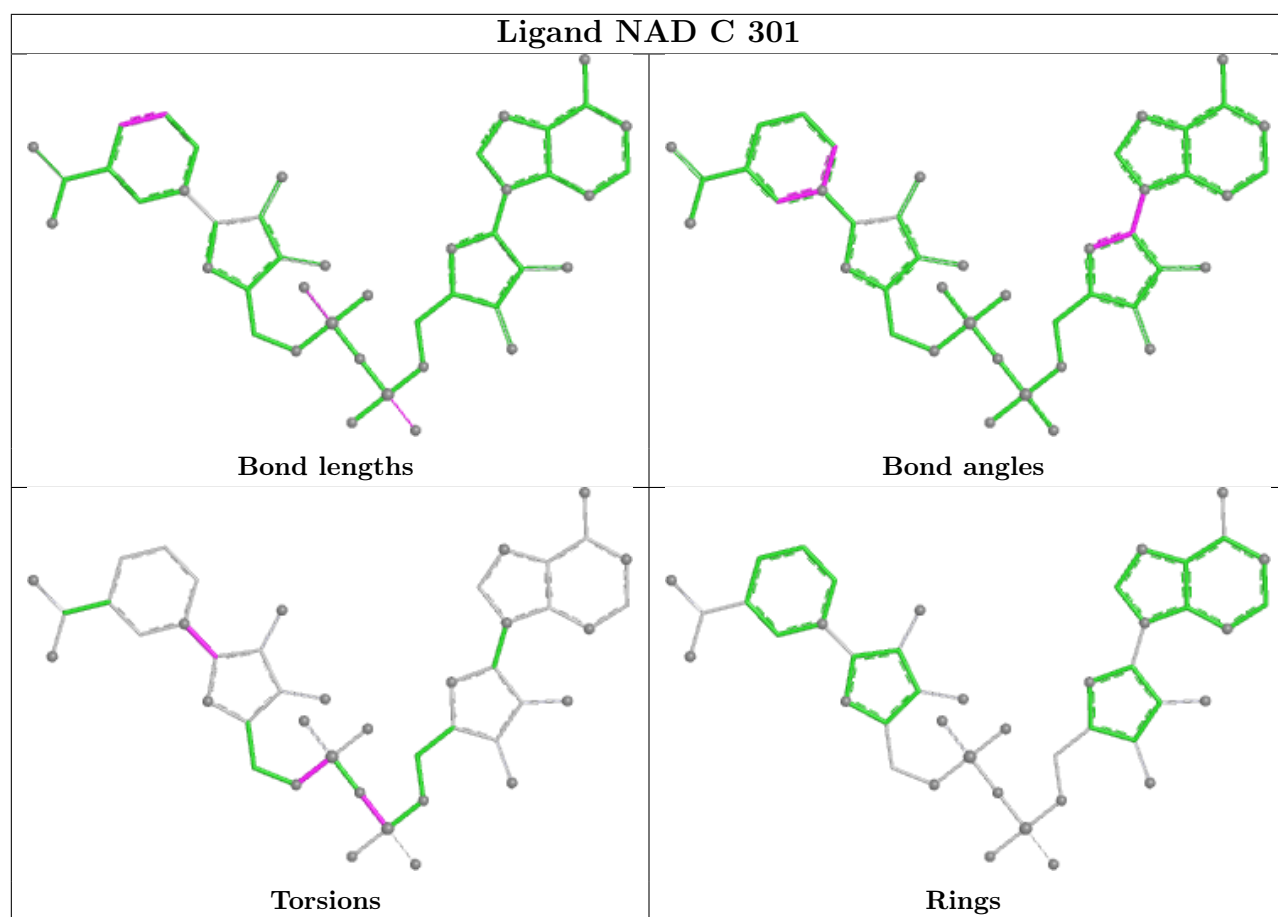
There are no ring outliers.

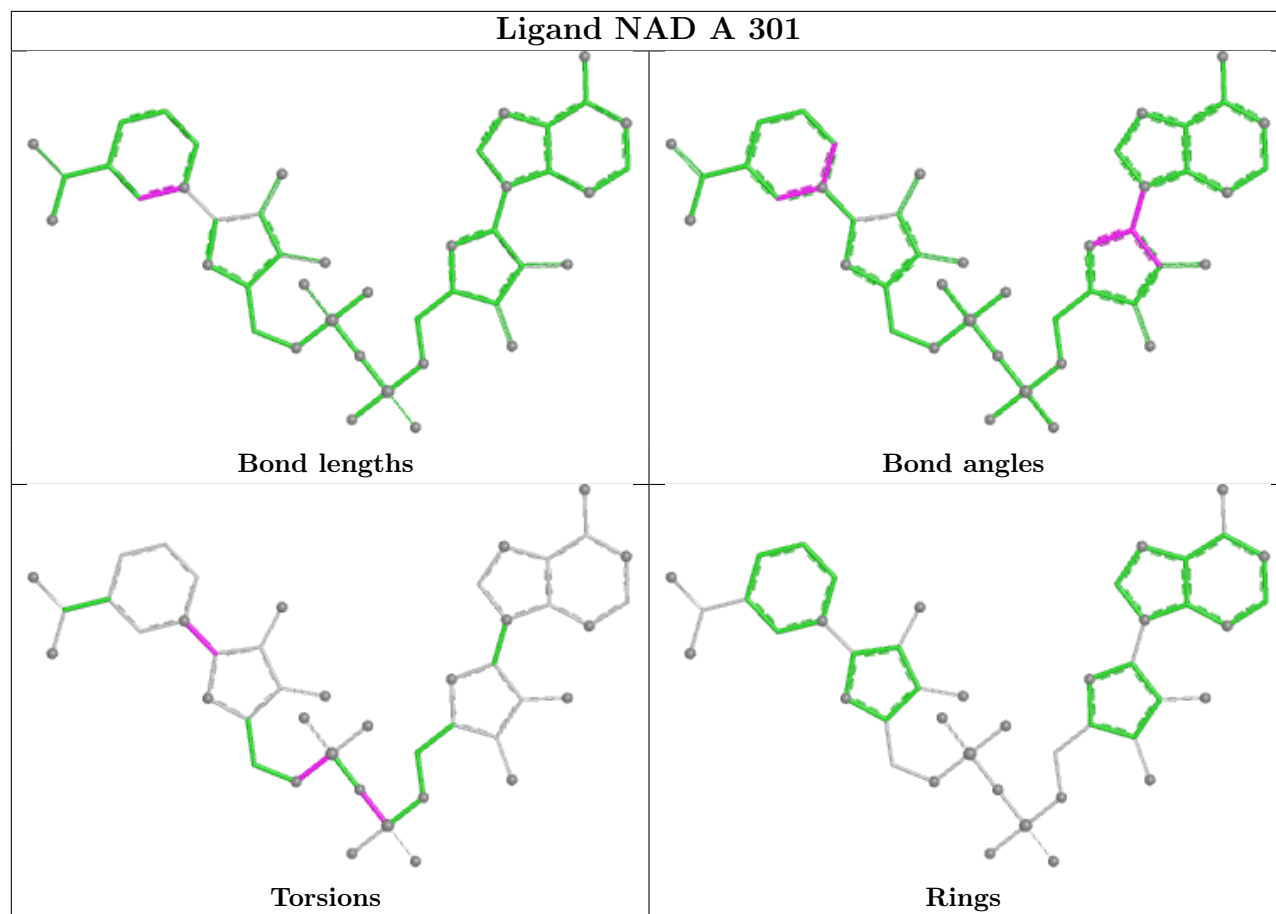
3 monomers are involved in 8 short contacts:

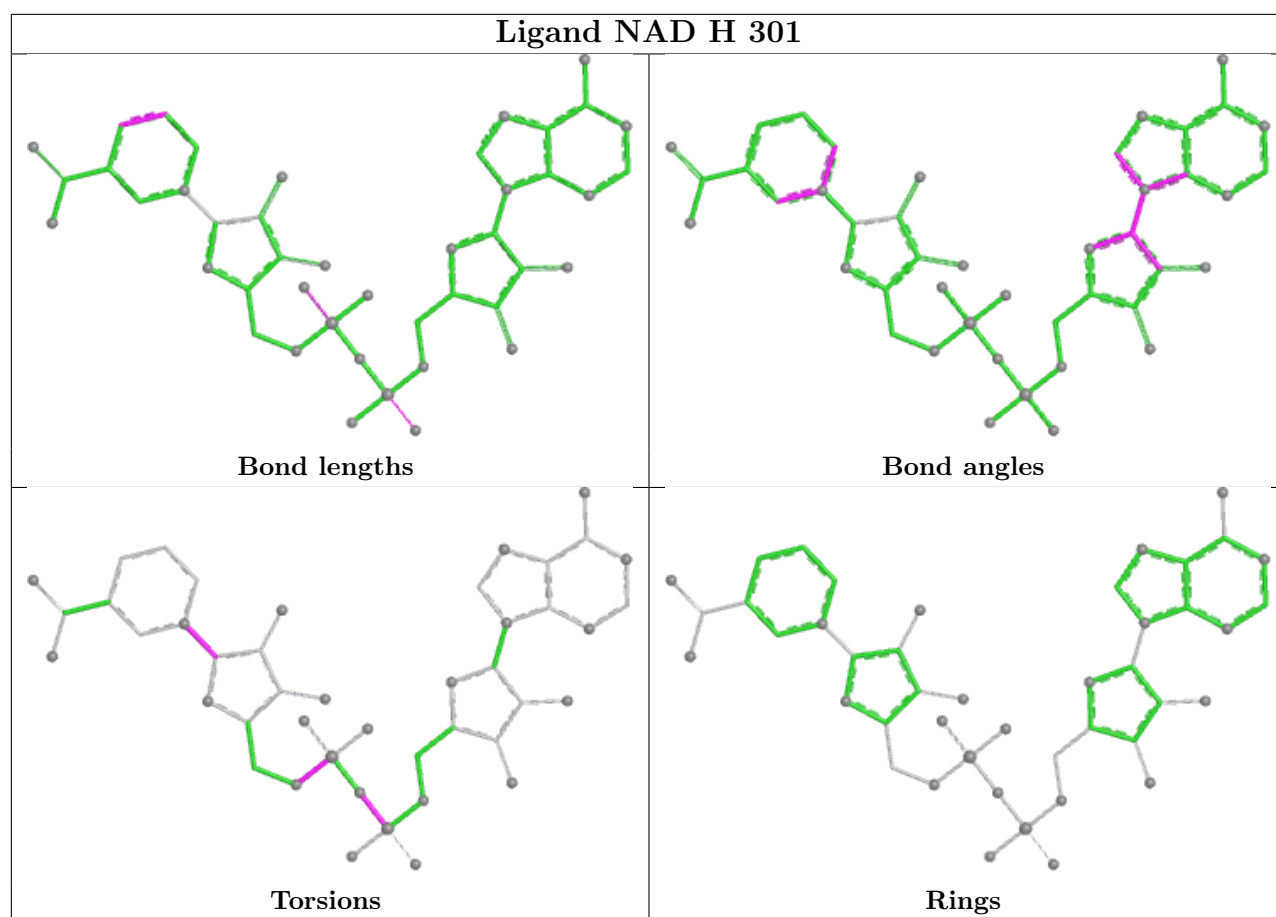
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	NAD	3	0
2	H	301	NAD	2	0
2	B	301	NAD	3	0

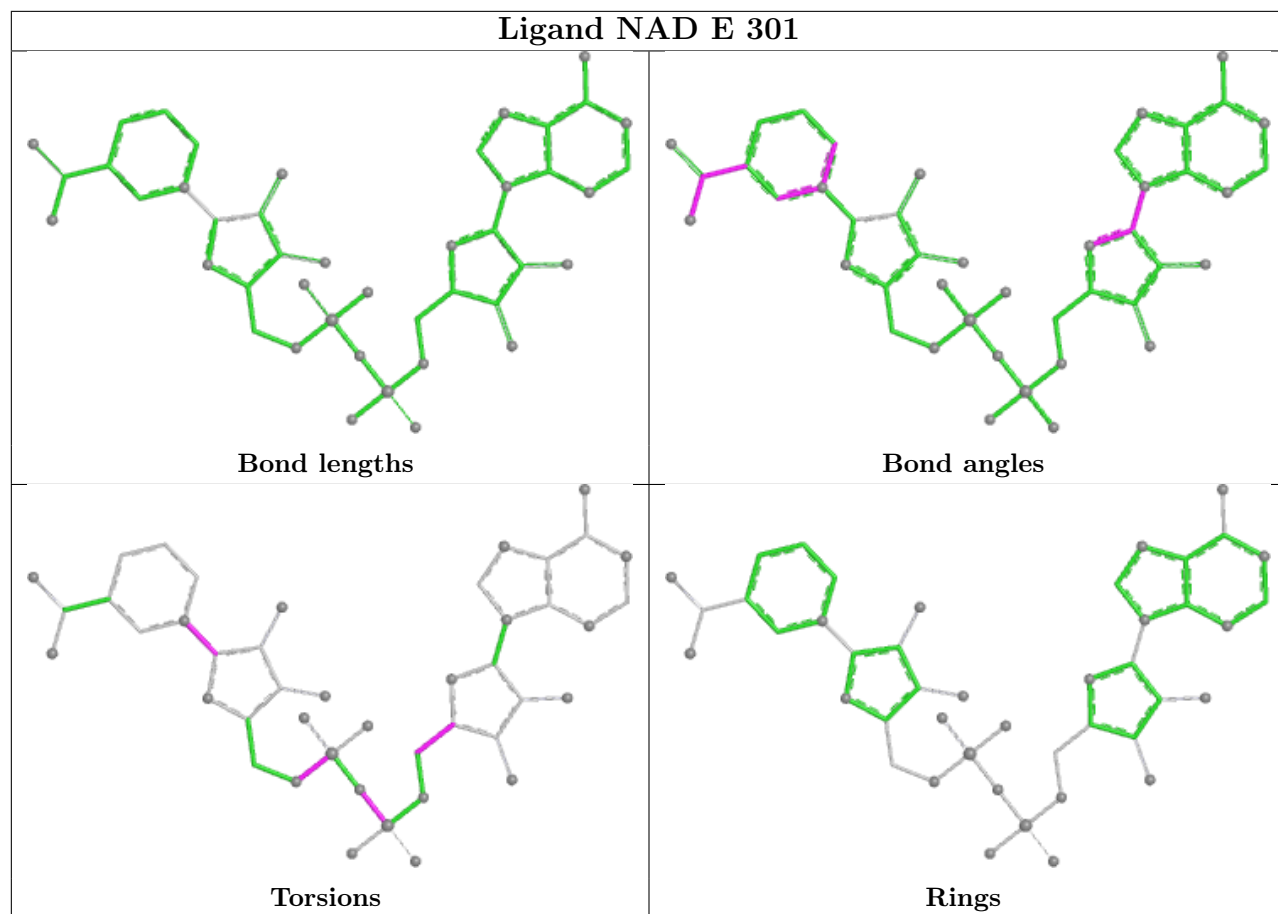
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

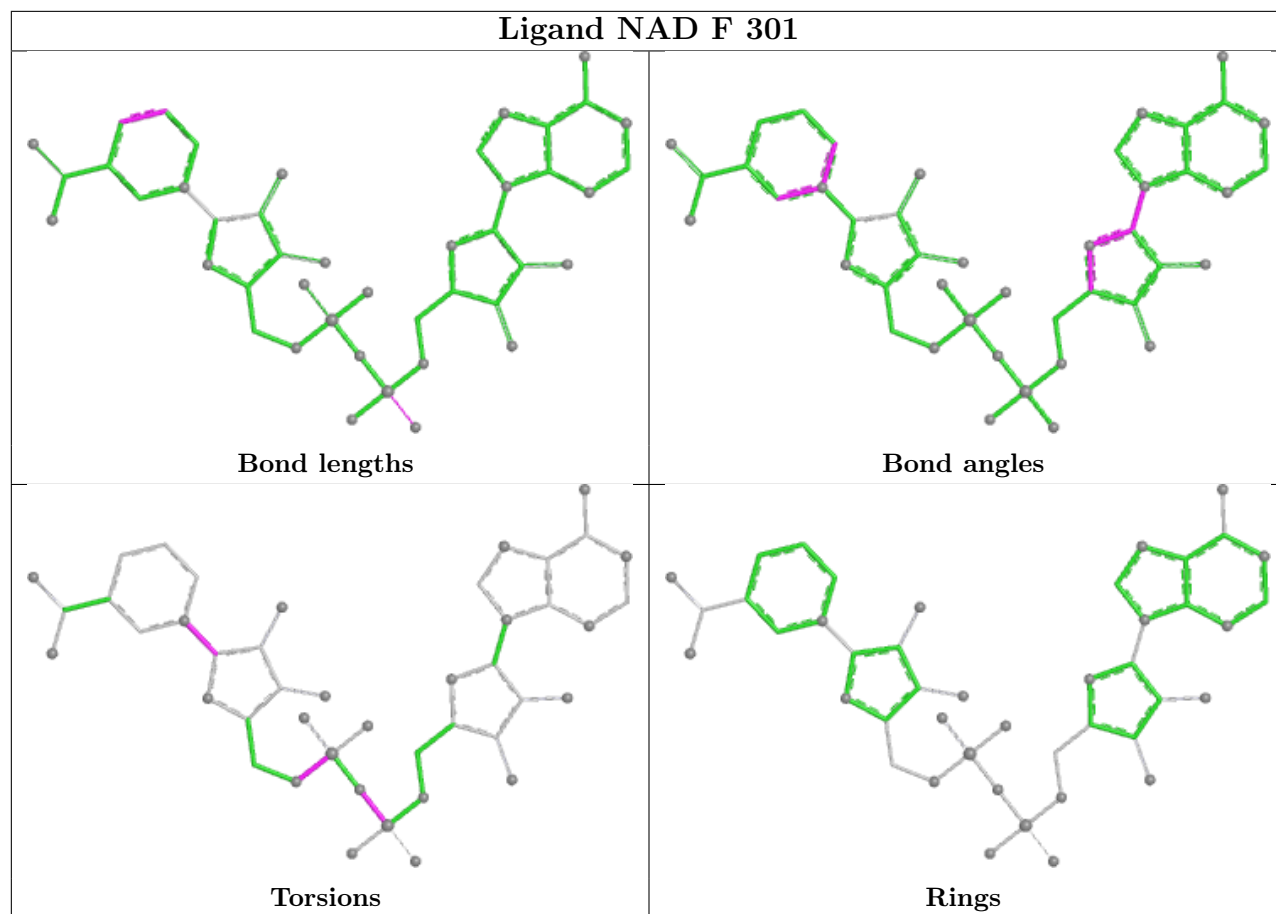


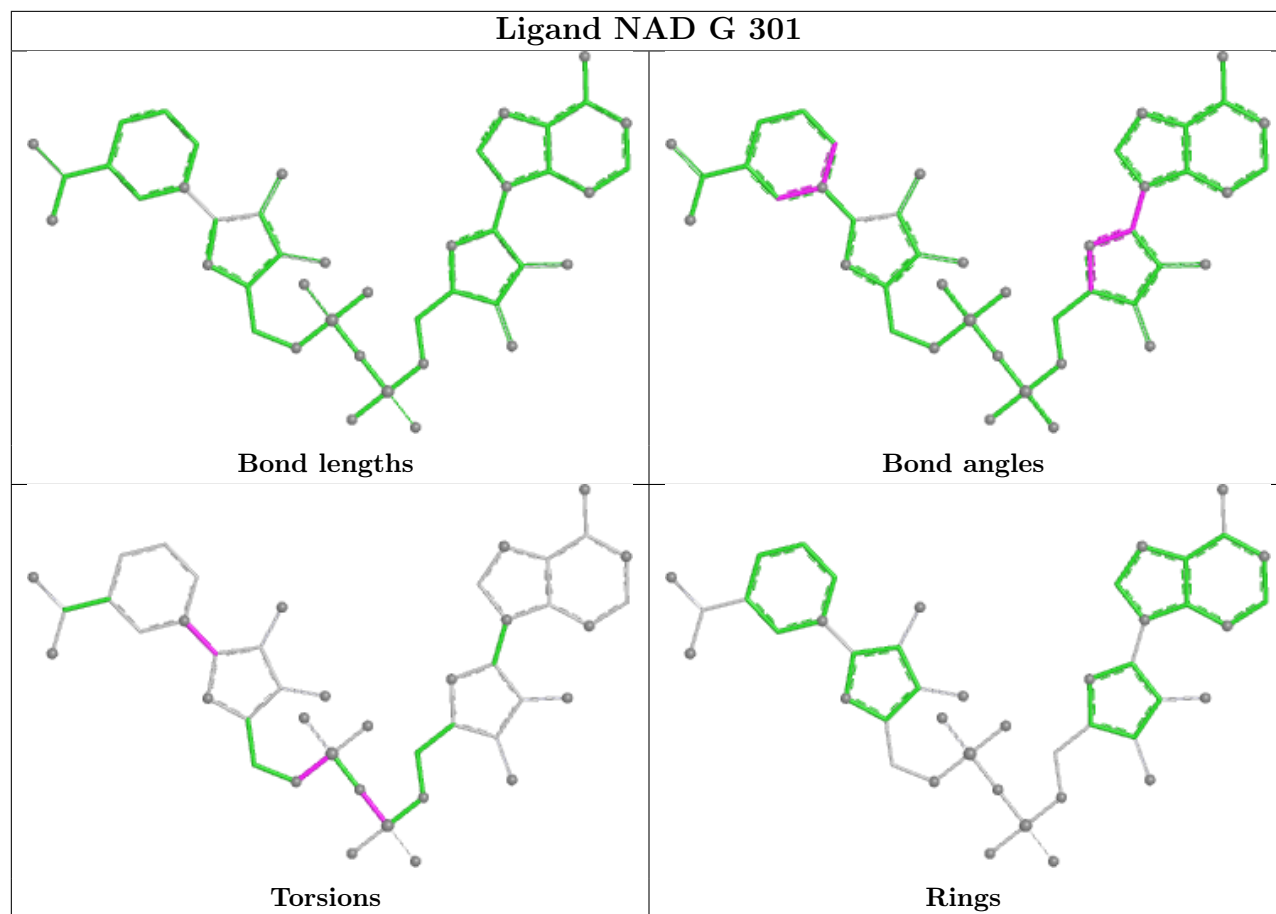


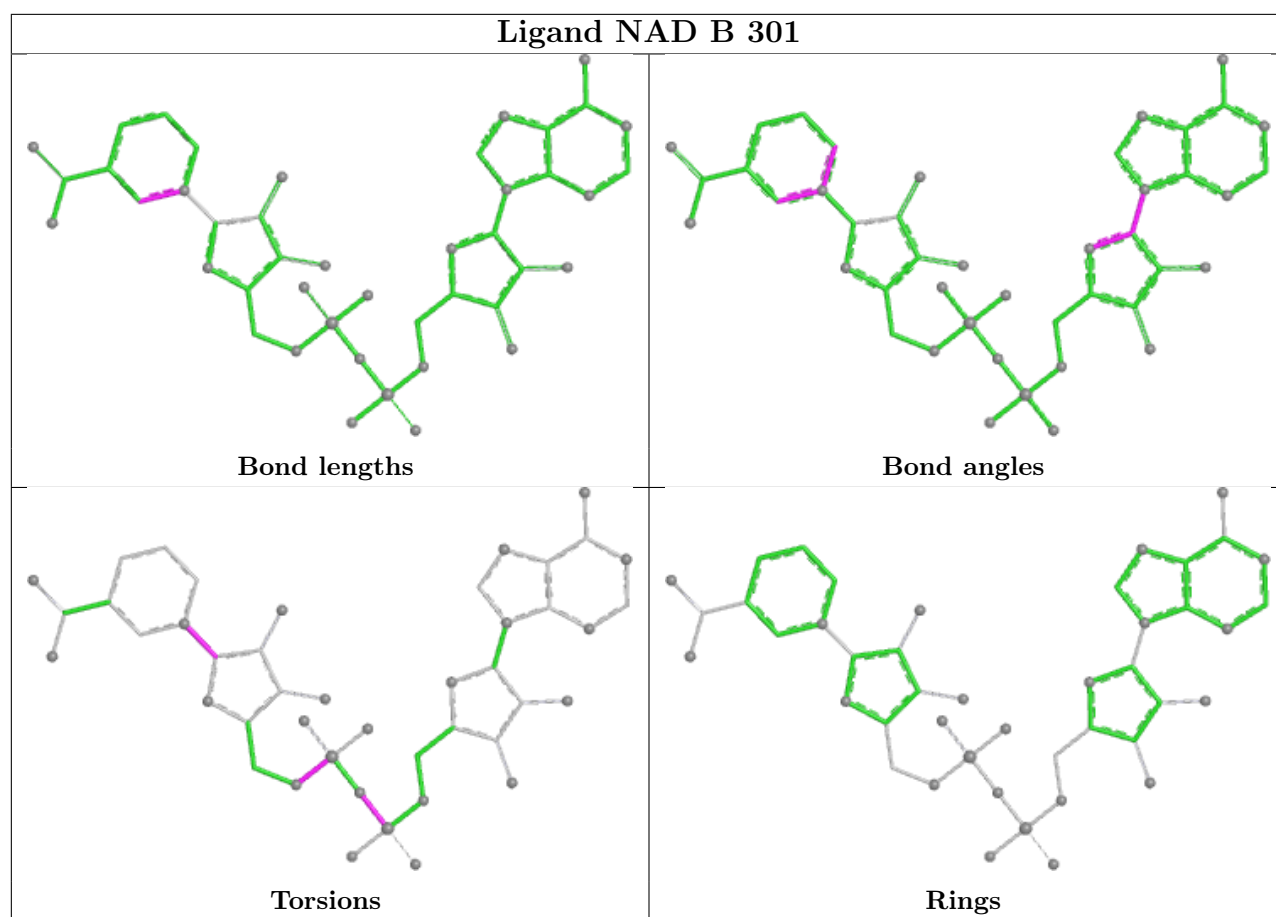












5.7 Other polymers [i](#)

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	272/273 (99%)	-0.35	2 (0%) 84 83	16, 26, 49, 59	1 (0%)
1	B	267/273 (97%)	-0.42	3 (1%) 78 77	16, 24, 46, 58	0
1	C	267/273 (97%)	-0.38	4 (1%) 72 70	18, 26, 45, 60	0
1	D	268/273 (98%)	-0.18	5 (1%) 66 64	21, 31, 52, 77	0
1	E	269/273 (98%)	-0.49	6 (2%) 62 60	16, 23, 48, 67	0
1	F	267/273 (97%)	-0.47	3 (1%) 78 77	16, 23, 42, 55	0
1	G	269/273 (98%)	-0.40	5 (1%) 66 64	17, 25, 46, 73	0
1	H	269/273 (98%)	-0.37	2 (0%) 84 83	17, 25, 50, 68	0
All	All	2148/2184 (98%)	-0.38	30 (1%) 73 72	16, 25, 48, 77	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	201	ASP	4.3
1	F	1	MET	4.3
1	D	1	MET	3.9
1	G	199	ILE	3.8
1	E	272	HIS	3.4
1	B	201	ASP	3.4
1	E	201	ASP	3.1
1	F	265	ALA	3.0
1	H	1	MET	2.9
1	B	199	ILE	2.9
1	E	200	ALA	2.8
1	D	200	ALA	2.8
1	E	199	ILE	2.7
1	C	154	HIS	2.6
1	F	272	HIS	2.6
1	G	272	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	101	GLU	2.6
1	B	200	ALA	2.5
1	C	200	ALA	2.4
1	C	273	LYS	2.4
1	E	197	SER	2.3
1	E	260	GLU	2.2
1	G	200	ALA	2.2
1	D	199	ILE	2.2
1	A	1	MET	2.2
1	D	272	HIS	2.2
1	G	198	GLY	2.2
1	A	154	HIS	2.1
1	C	272	HIS	2.1
1	H	272	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

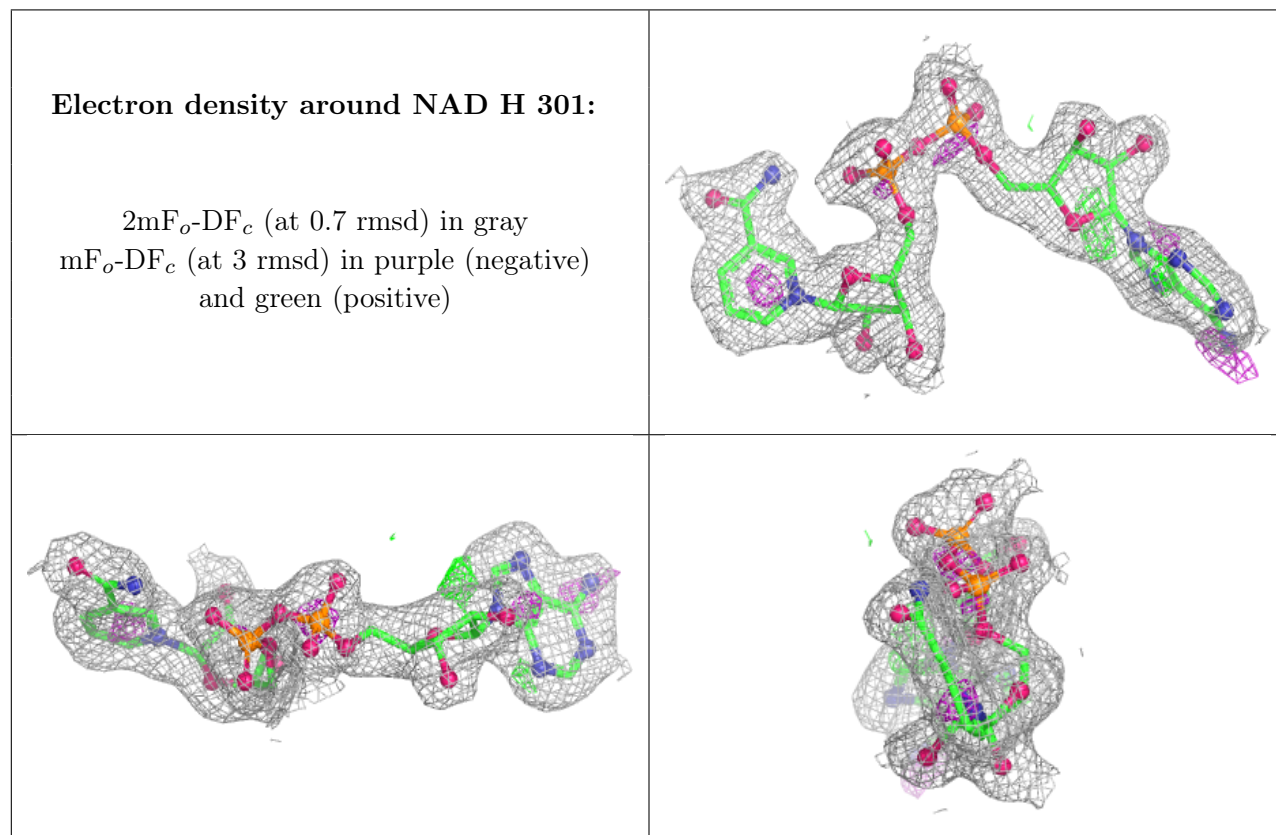
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

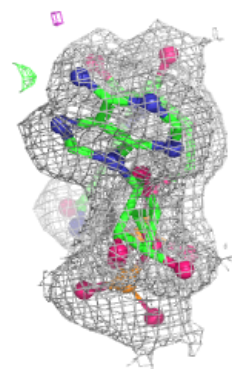
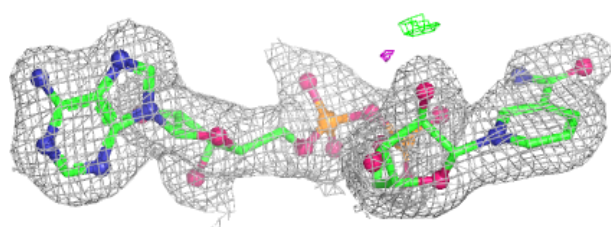
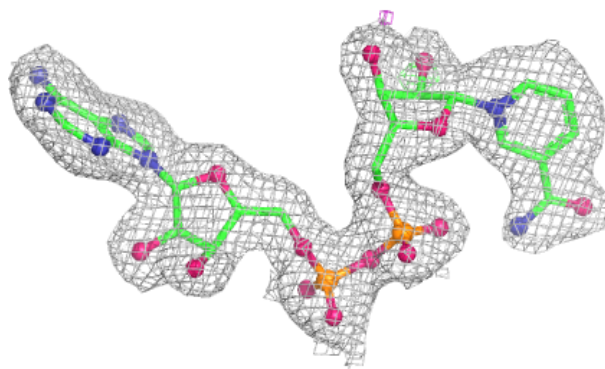
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	H	301	44/44	0.94	0.07	17,24,31,33	0
2	NAD	F	301	44/44	0.97	0.05	16,21,26,27	0
2	NAD	D	301	44/44	0.97	0.05	21,30,37,39	0
2	NAD	A	301	44/44	0.98	0.05	17,24,29,31	0
2	NAD	E	301	44/44	0.98	0.04	16,22,25,26	0
2	NAD	B	301	44/44	0.98	0.05	17,21,24,28	0
2	NAD	G	301	44/44	0.98	0.04	19,23,27,29	0
2	NAD	C	301	44/44	0.98	0.05	17,24,30,33	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.

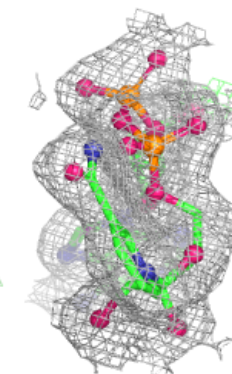
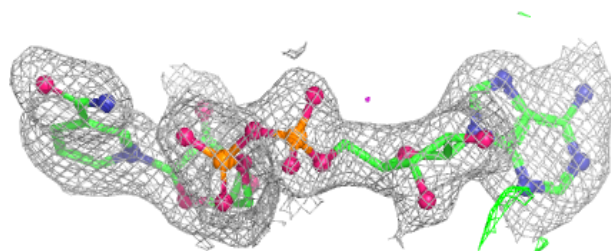
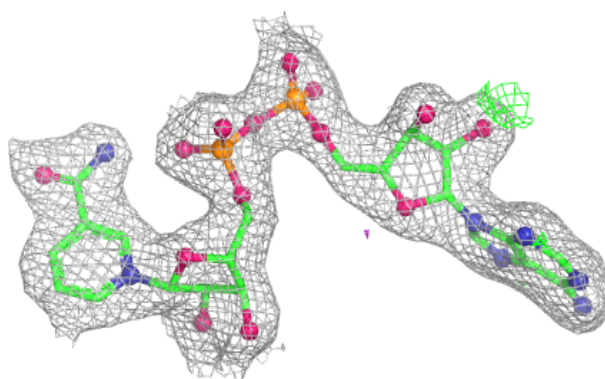


Electron density around NAD F 301:

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

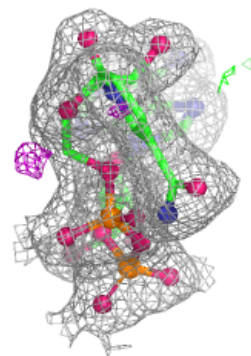
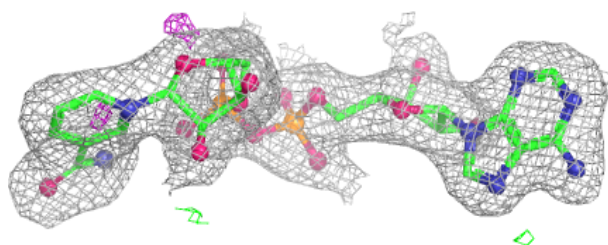
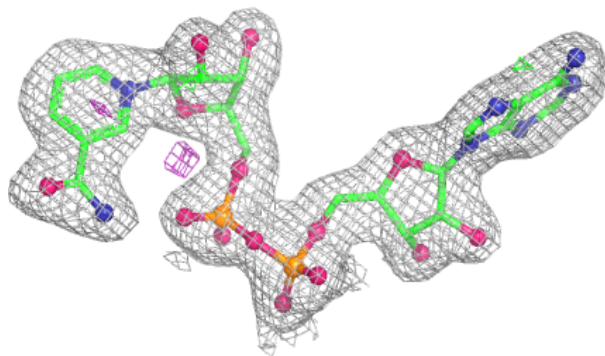
**Electron density around NAD D 301:**

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

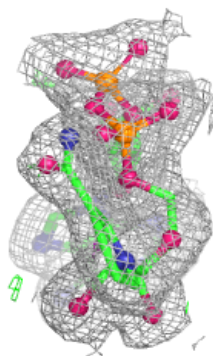
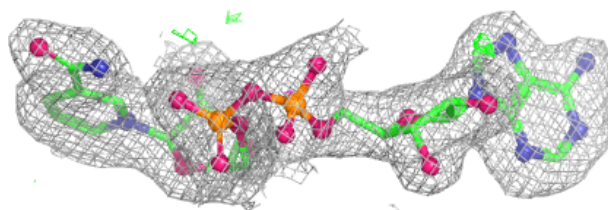
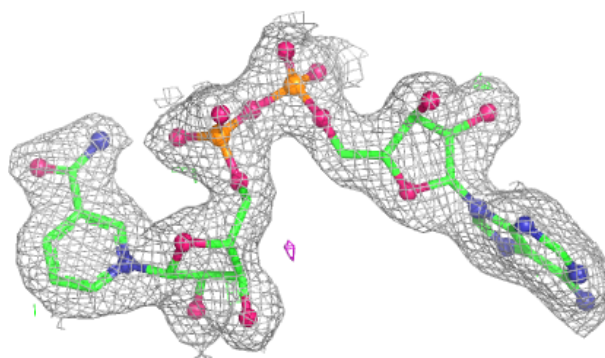


Electron density around NAD A 301:

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

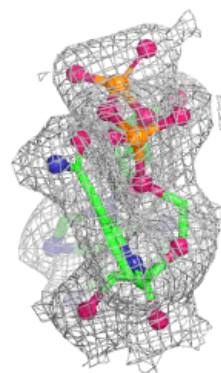
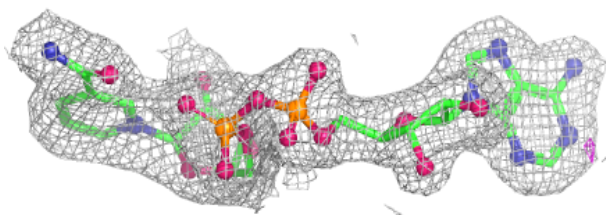
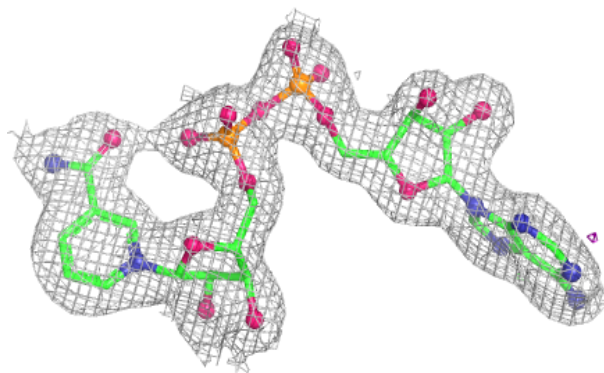
**Electron density around NAD E 301:**

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

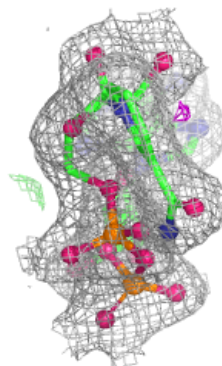
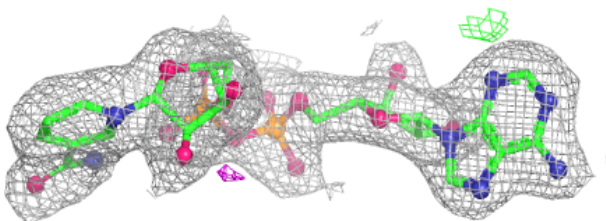
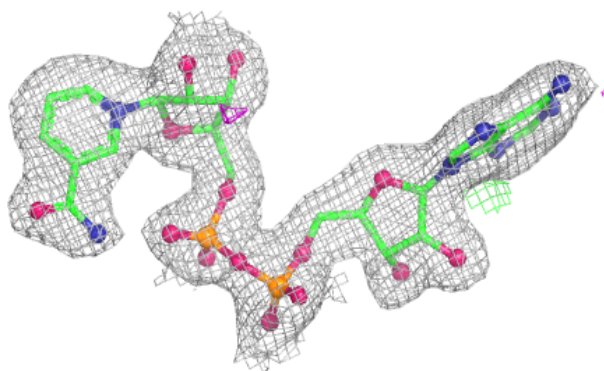


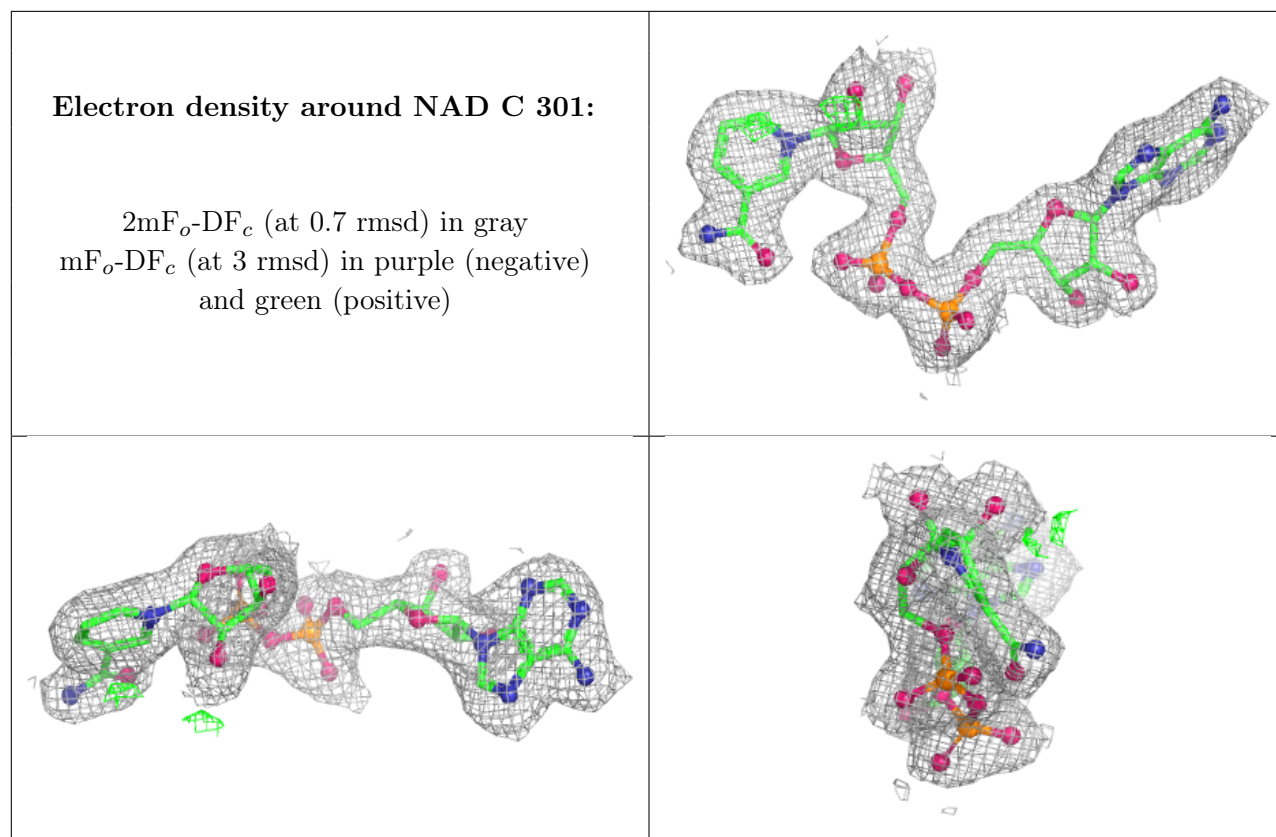
Electron density around NAD B 301:

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

**Electron density around NAD G 301:**

$2mF_o-DF_c$ (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.