



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:25 PM UTC

PDB ID : 3IJR / pdb_00003ijr
Title : 2.05 Angstrom resolution crystal structure of a short chain dehydrogenase from Bacillus anthracis str. 'Ames Ancestor' in complex with NAD+
Authors : Halavaty, A.S.; Minasov, G.; Skarina, T.; Onopriyenko, O.; Gordon, E.; Kwon, K.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2009-08-04
Resolution : 2.05 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](#) ①) were used in the production of this report:

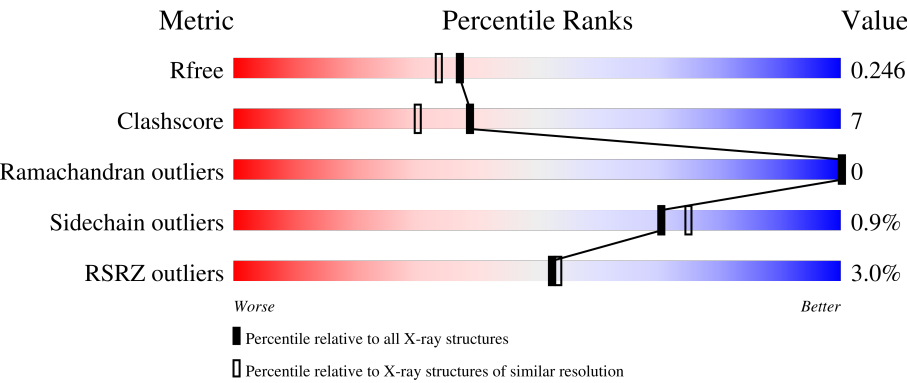
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	291	% 88% 8% .
1	B	291	2% 86% 10% ..
1	C	291	89% 8% .
1	D	291	% 88% 8% .
1	E	291	10% 79% 16% ..

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Mol	Chain	Length	Quality of chain
1	F	291	3% 80% 19%
1	G	291	% 82% 14% • •
1	H	291	4% 87% 12% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19037 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 Oxidoreductase, short chain dehydrogenase/reductase family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	Se	0	7	0
			2211	1392	374	439	2	4			
1	B	283	Total	C	N	O	S	Se	0	3	0
			2195	1386	371	432	2	4			
1	C	281	Total	C	N	O	S	Se	0	6	0
			2201	1390	371	434	2	4			
1	D	281	Total	C	N	O	S	Se	0	6	0
			2197	1385	371	435	2	4			
1	E	280	Total	C	N	O	S	Se	0	2	0
			2157	1361	364	426	2	4			
1	F	290	Total	C	N	O	S	Se	0	5	0
			2263	1425	383	448	2	5			
1	G	281	Total	C	N	O	S	Se	0	5	0
			2190	1381	370	433	2	4			
1	H	289	Total	C	N	O	S	Se	0	5	0
			2257	1423	383	444	2	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q81UV8
A	-1	ASN	-	expression tag	UNP Q81UV8
A	0	ALA	-	expression tag	UNP Q81UV8
B	-2	SER	-	expression tag	UNP Q81UV8
B	-1	ASN	-	expression tag	UNP Q81UV8
B	0	ALA	-	expression tag	UNP Q81UV8
C	-2	SER	-	expression tag	UNP Q81UV8
C	-1	ASN	-	expression tag	UNP Q81UV8
C	0	ALA	-	expression tag	UNP Q81UV8
D	-2	SER	-	expression tag	UNP Q81UV8
D	-1	ASN	-	expression tag	UNP Q81UV8
D	0	ALA	-	expression tag	UNP Q81UV8
E	-2	SER	-	expression tag	UNP Q81UV8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP Q81UV8
E	0	ALA	-	expression tag	UNP Q81UV8
F	-2	SER	-	expression tag	UNP Q81UV8
F	-1	ASN	-	expression tag	UNP Q81UV8
F	0	ALA	-	expression tag	UNP Q81UV8
G	-2	SER	-	expression tag	UNP Q81UV8
G	-1	ASN	-	expression tag	UNP Q81UV8
G	0	ALA	-	expression tag	UNP Q81UV8
H	-2	SER	-	expression tag	UNP Q81UV8
H	-1	ASN	-	expression tag	UNP Q81UV8
H	0	ALA	-	expression tag	UNP Q81UV8

- # NAD

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



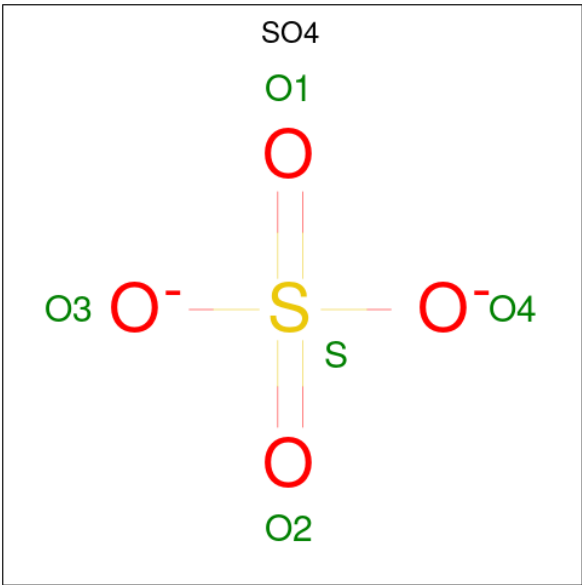
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

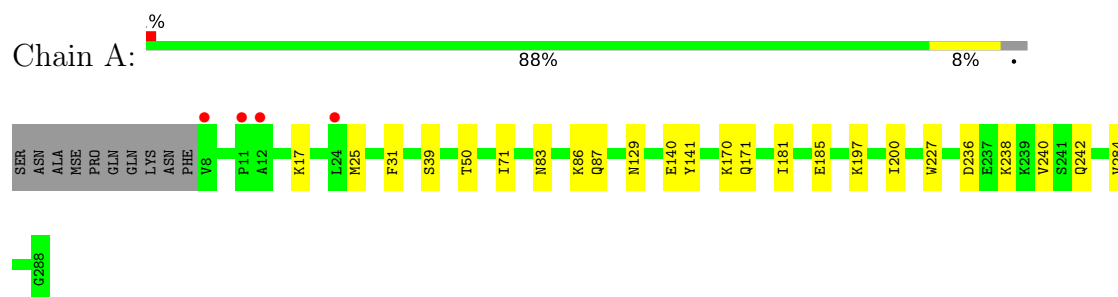
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	170	Total 172	O 172	0	5
5	B	127	Total 127	O 127	0	0
5	C	149	Total 151	O 151	0	3
5	D	132	Total 132	O 132	0	1
5	E	68	Total 68	O 68	0	0
5	F	79	Total 79	O 79	0	1
5	G	105	Total 105	O 105	0	0
5	H	102	Total 102	O 102	0	1

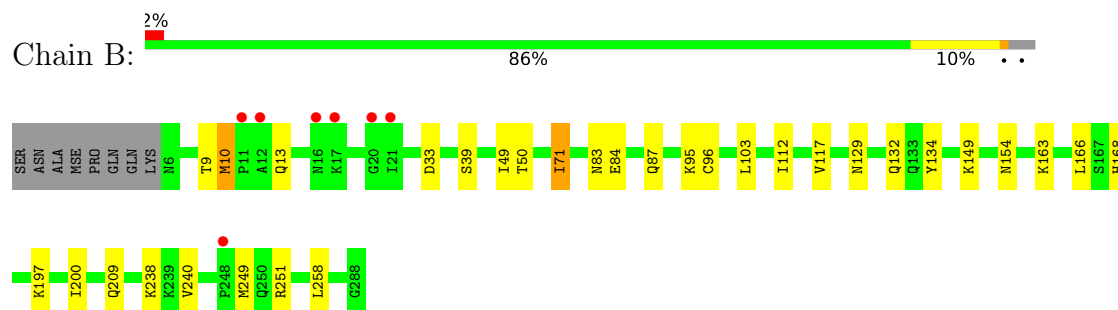
3 Residue-property plots [i](#)

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.

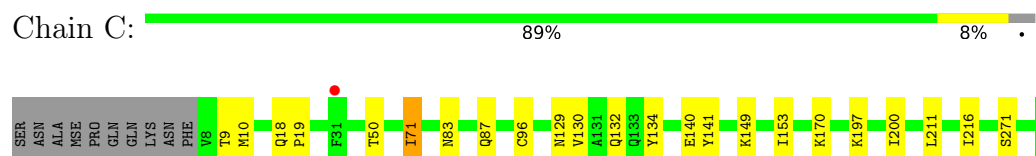
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family



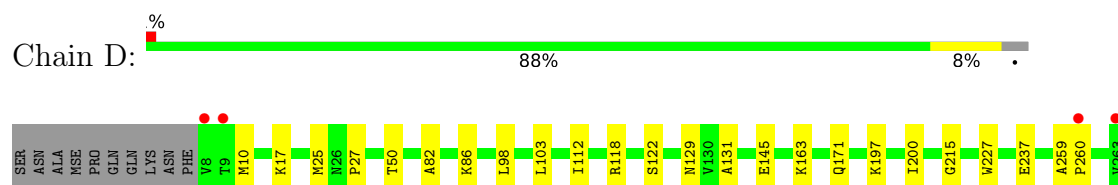
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family



- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family



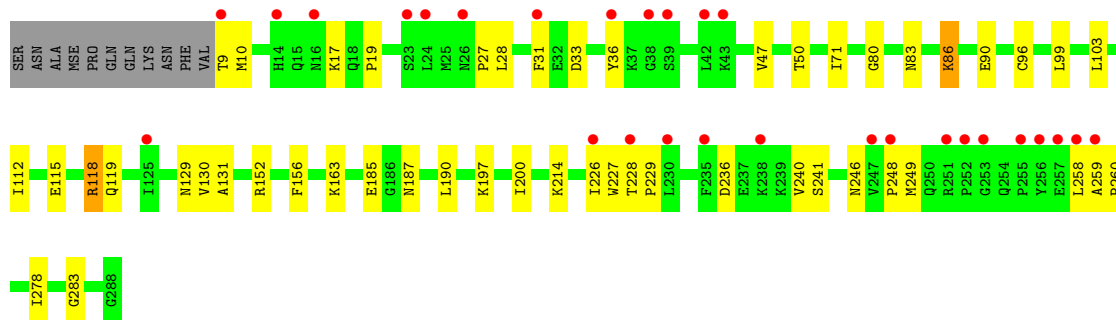
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family





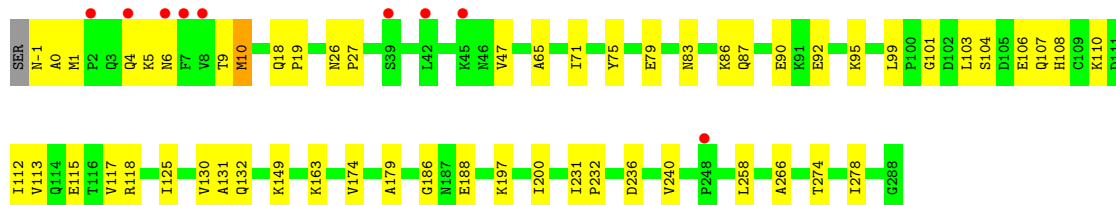
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family

Chain E:



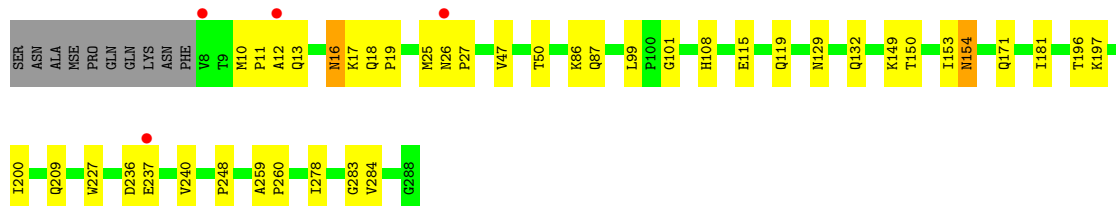
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family

Chain F:



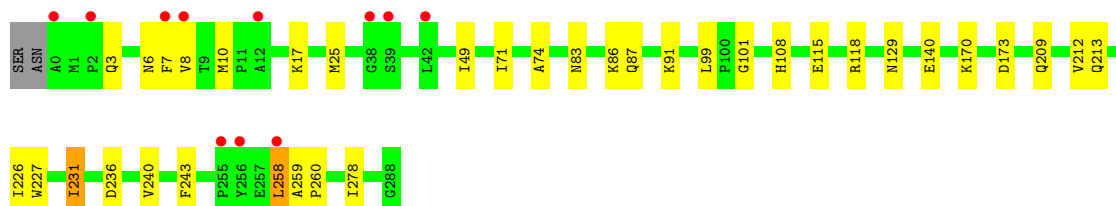
- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family

Chain G:



- Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	112.75Å 123.20Å 169.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.05 30.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.05) 99.6 (30.00-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.157 , 0.193 0.220 , 0.246	Depositor DCC
R_{free} test set	7373 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.7	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	19037	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.93% 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: NAD, SO4, MG

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	0.71	0/2248	0.91	1/3042 (0.0%)
1	B	0.71	0/2233	0.90	4/3022 (0.1%)
1	C	0.69	0/2238	0.86	1/3027 (0.0%)
1	D	0.65	0/2234	0.89	1/3022 (0.0%)
1	E	0.56	0/2194	0.88	2/2969 (0.1%)
1	F	0.60	0/2301	0.89	5/3112 (0.2%)
1	G	0.61	0/2227	0.87	2/3013 (0.1%)
1	H	0.59	0/2295	0.89	1/3103 (0.0%)
All	All	0.64	0/17970	0.89	17/24310 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	186	GLY	N-CA-C	-6.86	103.74	112.65
1	A	71	ILE	N-CA-C	6.23	116.84	107.75
1	H	71	ILE	N-CA-C	6.02	116.54	107.75
1	C	71	ILE	N-CA-C	6.00	116.51	107.75
1	F	104	SER	N-CA-C	-5.89	106.05	113.18
1	F	179	ALA	CA-C-O	5.67	121.23	117.94
1	B	166	LEU	N-CA-C	5.64	117.43	111.28
1	B	33	ASP	N-CA-C	-5.57	101.50	109.24
1	G	154	ASN	N-CA-C	5.42	118.11	111.82
1	B	71	ILE	N-CA-C	5.36	115.62	108.11
1	B	154	ASN	N-CA-C	5.36	118.04	111.82
1	F	71	ILE	N-CA-C	5.32	115.55	108.11
1	E	71	ILE	N-CA-C	5.28	115.50	108.11
1	E	47	VAL	N-CA-C	5.25	116.14	108.53
1	D	237	GLU	N-CA-C	5.14	116.57	111.07
1	G	47	VAL	N-CA-C	5.11	115.26	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	174	VAL	N-CA-C	5.10	115.08	108.35

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	2211	0	2178	19	0
1	B	2195	0	2169	23	0
1	C	2201	0	2183	23	0
1	D	2197	0	2173	21	0
1	E	2157	0	2135	57	0
1	F	2263	0	2231	49	0
1	G	2190	0	2168	30	1
1	H	2257	0	2234	29	0
2	A	44	0	25	1	0
2	B	44	0	25	1	0
2	C	44	0	25	6	0
2	D	44	0	25	1	0
2	E	44	0	25	5	0
2	F	44	0	26	4	0
2	G	44	0	26	0	0
2	H	44	0	25	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	10	0	0	0	0
4	B	5	0	0	1	0
4	C	20	0	0	1	0
4	D	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	5	0	0	1	0
4	F	10	0	0	1	0
4	G	10	0	0	0	0
4	H	5	0	0	0	0
5	A	172	0	0	5	0
5	B	127	0	0	3	0
5	C	151	0	0	0	0
5	D	132	0	0	2	0
5	E	68	0	0	14	0
5	F	79	0	0	6	0
5	G	105	0	0	1	0
5	H	102	0	0	1	0
All	All	19037	0	17673	244	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:MSE:HE2	1:D:227:TRP:CE2	1.89	1.06
1:G:10:MSE:HE2	1:G:227:TRP:CZ2	1.95	1.00
1:A:185[B]:GLU:OE2	1:A:284:VAL:HG11	1.60	1.00
1:G:10:MSE:HE1	1:G:27:PRO:HD2	1.41	0.99
1:H:3:GLN:NE2	1:H:6:ASN:HD22	1.64	0.96
1:A:181:ILE:HD11	1:A:185[B]:GLU:OE2	1.69	0.93
1:D:10:MSE:CE	1:D:227:TRP:CE2	2.53	0.90
1:D:10:MSE:HE2	1:D:227:TRP:CD2	2.06	0.90
1:G:16:ASN:C	1:G:16:ASN:HD22	1.82	0.86
1:A:83[B]:ASN:HB3	5:A:720[B]:HOH:O	1.77	0.84
1:E:10:MSE:HE2	1:E:227:TRP:CE2	2.12	0.84
1:E:99:LEU:HD11	5:E:695:HOH:O	1.79	0.81
1:H:87[B]:GLN:HE21	1:H:87[B]:GLN:HA	1.44	0.80
1:H:3:GLN:HE22	1:H:6:ASN:HD22	1.28	0.80
1:A:171:GLN:HG3	5:A:388:HOH:O	1.84	0.78
1:G:132:GLN:HE22	1:G:149:LYS:HE2	1.48	0.78
1:H:3:GLN:HE22	1:H:6:ASN:ND2	1.81	0.78
1:G:10:MSE:HE2	1:G:227:TRP:CE2	2.19	0.77
1:A:83[B]:ASN:O	1:A:87[B]:GLN:HG2	1.86	0.76
1:E:118:ARG:HG3	1:E:118:ARG:HH11	1.51	0.76
1:F:1:MSE:CE	5:F:649:HOH:O	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:MSE:HE2	1:F:10:MSE:HA	1.69	0.74
1:C:10:MSE:HE2	1:C:10:MSE:HA	1.71	0.73
1:A:185[B]:GLU:OE2	1:A:284:VAL:CG1	2.37	0.73
1:C:130[B]:VAL:HG11	1:C:153:ILE:HD11	1.70	0.73
1:E:130:VAL:HG23	2:E:301:NAD:C1B	2.19	0.72
1:H:3:GLN:NE2	1:H:6:ASN:ND2	2.33	0.72
1:F:9:THR:O	1:F:10:MSE:HE3	1.89	0.72
1:E:96:CYS:CB	5:E:694:HOH:O	2.39	0.71
2:A:301:NAD:N7N	5:A:816:HOH:O	2.21	0.70
1:F:1:MSE:HE3	5:F:649:HOH:O	1.92	0.69
1:F:65:ALA:O	1:F:92[B]:GLU:HG2	1.93	0.69
1:E:28:LEU:HD22	5:E:707:HOH:O	1.92	0.69
1:B:9:THR:O	1:B:10:MSE:HE3	1.93	0.68
1:C:132:GLN:HE22	1:C:149:LYS:HE2	1.56	0.68
1:B:10:MSE:HA	1:B:10:MSE:HE2	1.76	0.68
1:E:99:LEU:CD2	1:E:115:GLU:HG2	2.23	0.68
1:C:130[A]:VAL:HG23	2:C:301:NAD:N9A	2.11	0.66
1:G:171:GLN:NE2	5:G:627:HOH:O	2.27	0.65
1:C:130[A]:VAL:HG23	2:C:301:NAD:C1B	2.26	0.65
1:F:4:GLN:NE2	1:F:5:LYS:O	2.30	0.65
1:C:9:THR:O	1:C:10:MSE:HE3	1.97	0.65
1:E:10:MSE:HE3	1:E:27:PRO:HD2	1.77	0.65
1:C:9:THR:O	1:C:10:MSE:CE	2.45	0.64
1:F:4:GLN:NE2	1:F:6:ASN:OD1	2.30	0.64
1:B:83:ASN:O	1:B:87[A]:GLN:HG2	1.99	0.63
1:G:10:MSE:CE	1:G:27:PRO:HD2	2.25	0.62
1:E:90:GLU:HG3	5:E:694:HOH:O	1.99	0.62
1:F:95:LYS:NZ	5:F:566:HOH:O	2.28	0.62
1:E:118:ARG:HH11	1:E:118:ARG:CG	2.11	0.61
1:F:1:MSE:HE2	5:F:649:HOH:O	1.99	0.61
1:F:103:LEU:HD21	1:F:112:ILE:HD13	1.82	0.61
1:F:99:LEU:CD2	1:F:115:GLU:HG2	2.30	0.61
1:E:10:MSE:HE2	1:E:227:TRP:CD2	2.35	0.61
1:E:10:MSE:CE	1:E:27:PRO:HD2	2.31	0.60
1:G:10:MSE:HE3	1:G:11:PRO:HD2	1.82	0.60
1:B:84:GLU:O	1:B:87[B]:GLN:HG2	2.02	0.59
1:D:10:MSE:CE	1:D:27:PRO:HD2	2.33	0.59
1:E:9:THR:HG21	5:E:862:HOH:O	2.01	0.59
1:E:228:THR:HB	1:E:229:PRO:HD2	1.82	0.59
1:H:83:ASN:O	1:H:87[B]:GLN:HG2	2.02	0.59
1:C:197:LYS:HD3	1:C:200:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:MSE:HE2	1:G:227:TRP:CH2	2.36	0.59
1:D:10:MSE:CE	1:D:227:TRP:CZ2	2.86	0.58
1:F:132:GLN:HE22	1:F:149:LYS:HE2	1.67	0.58
1:E:99:LEU:HD21	1:E:115:GLU:CG	2.34	0.58
1:B:49:ILE:HG23	1:B:49:ILE:O	2.04	0.57
1:F:115:GLU:OE1	1:F:118:ARG:NH1	2.38	0.57
1:F:99:LEU:HD22	1:F:115:GLU:HG2	1.87	0.57
1:G:16:ASN:C	1:G:16:ASN:ND2	2.56	0.57
1:G:10:MSE:CE	1:G:227:TRP:CZ2	2.80	0.56
1:E:31:PHE:HB3	5:E:445:HOH:O	2.06	0.56
1:E:10:MSE:HE2	1:E:227:TRP:CZ2	2.40	0.56
1:H:87[B]:GLN:HE21	1:H:87[B]:GLN:CA	2.15	0.56
1:A:181:ILE:CD1	1:A:185[B]:GLU:OE2	2.51	0.55
1:C:140[A]:GLU:HG2	1:C:141:TYR:CD1	2.42	0.54
1:E:248:PRO:HG2	1:E:283:GLY:O	2.07	0.54
1:F:131:ALA:HB3	2:F:301:NAD:H3D	1.90	0.54
1:B:197:LYS:HD3	1:B:200:ILE:HD12	1.90	0.54
1:G:25:MSE:HE2	1:G:227:TRP:CE2	2.42	0.54
1:A:17:LYS:HD2	1:A:17:LYS:C	2.33	0.54
1:D:197:LYS:HD3	1:D:200:ILE:HD12	1.89	0.54
1:F:-1:ASN:HA	1:F:188:GLU:OE2	2.08	0.54
1:G:50:THR:O	1:G:129:ASN:HB3	2.08	0.54
1:E:197:LYS:HD3	1:E:200:ILE:HD12	1.90	0.53
1:E:96:CYS:HB3	5:E:694:HOH:O	2.04	0.53
1:G:13:GLN:NE2	1:G:26:ASN:O	2.41	0.53
1:C:271:SER:HA	4:C:328:SO4:O4	2.09	0.53
1:H:118:ARG:NE	5:H:782:HOH:O	2.39	0.53
1:A:31:PHE:HB3	5:A:309:HOH:O	2.09	0.53
1:D:145[A]:GLU:OE1	1:D:145[A]:GLU:N	2.40	0.53
5:D:625:HOH:O	1:H:8:VAL:HG21	2.08	0.53
1:H:87[B]:GLN:HA	1:H:87[B]:GLN:NE2	2.20	0.53
1:E:249:MSE:HE3	1:F:274:THR:HG22	1.91	0.53
1:F:92[B]:GLU:HG3	1:F:92[B]:GLU:O	2.09	0.53
1:E:86:LYS:HG2	5:E:694:HOH:O	2.09	0.52
1:E:163:LYS:NZ	4:E:319:SO4:O3	2.42	0.51
1:H:101:GLY:HA3	1:H:108:HIS:CE1	2.46	0.51
1:B:129:ASN:ND2	2:B:301:NAD:H4D	2.25	0.51
1:G:101:GLY:HA3	1:G:108:HIS:CE1	2.45	0.51
1:B:117:VAL:HG21	1:B:168:HIS:CE1	2.45	0.51
1:E:80:GLY:HA2	5:E:331:HOH:O	2.11	0.51
1:G:153:ILE:HG23	1:G:154:ASN:OD1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:LYS:N	1:H:173:ASP:OD2	2.34	0.51
1:B:132:GLN:NE2	1:B:134:TYR:OH	2.43	0.51
1:F:92[B]:GLU:O	1:F:92[B]:GLU:CG	2.59	0.51
1:D:10:MSE:HE3	1:D:27:PRO:HD2	1.92	0.50
1:C:130[B]:VAL:HG11	1:C:153:ILE:CD1	2.41	0.50
1:E:278:ILE:HD12	1:F:278:ILE:HD12	1.93	0.50
1:F:107:GLN:HB2	5:F:379:HOH:O	2.10	0.50
1:E:96:CYS:SG	5:E:694:HOH:O	2.59	0.50
1:F:4:GLN:CD	1:F:6:ASN:OD1	2.55	0.50
1:F:101:GLY:HA3	1:F:108:HIS:CE1	2.46	0.50
1:F:4:GLN:OE1	1:F:6:ASN:OD1	2.30	0.50
1:H:99:LEU:CD2	1:H:115:GLU:HG2	2.42	0.49
1:D:131:ALA:HB3	2:D:301:NAD:H3D	1.95	0.49
1:E:187:ASN:ND2	1:E:190:LEU:HD12	2.27	0.49
1:F:65:ALA:C	1:F:92[B]:GLU:HG2	2.37	0.49
1:B:84:GLU:OE1	5:B:724:HOH:O	2.20	0.49
1:F:130:VAL:HG12	2:F:301:NAD:H1B	1.95	0.49
1:D:25:MSE:HE2	1:D:227:TRP:CE2	2.48	0.49
1:E:99:LEU:HD21	1:E:115:GLU:HG3	1.95	0.49
1:F:10:MSE:HA	1:F:10:MSE:CE	2.41	0.48
1:C:9:THR:O	1:C:10:MSE:HE2	2.13	0.48
1:E:236:ASP:O	1:E:240:VAL:HG23	2.13	0.48
1:G:99:LEU:CD2	1:G:115:GLU:HG2	2.44	0.48
1:G:150:THR:HG22	1:G:196:THR:HG21	1.95	0.48
1:B:71:ILE:O	1:B:96:CYS:HA	2.14	0.48
1:C:18:GLN:HA	1:C:19:PRO:C	2.38	0.48
1:C:130[B]:VAL:HG22	2:C:301:NAD:H1B	1.95	0.48
1:C:132:GLN:NE2	1:C:134:TYR:OH	2.46	0.48
1:E:9:THR:HB	1:E:241:SER:O	2.14	0.48
1:C:50:THR:O	1:C:129:ASN:HB3	2.14	0.48
1:F:197:LYS:HD3	1:F:200:ILE:HD12	1.96	0.48
1:D:10:MSE:HE2	1:D:227:TRP:CZ2	2.45	0.48
1:H:7:PHE:HB2	1:H:10:MSE:HE1	1.94	0.48
1:B:103:LEU:HD21	1:B:112:ILE:HD13	1.96	0.47
1:A:238:LYS:NZ	1:A:242:GLN:HE22	2.12	0.47
1:C:130[A]:VAL:CG2	2:C:301:NAD:C4A	2.92	0.47
1:E:33:ASP:HB3	1:E:36:TYR:HB2	1.97	0.47
1:E:86:LYS:NZ	1:E:86:LYS:HB3	2.29	0.47
1:A:39:SER:HB3	1:B:39:SER:HB3	1.96	0.47
1:B:117:VAL:HG21	1:B:168:HIS:ND1	2.30	0.47
1:H:49:ILE:HG23	1:H:49:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:ARG:CG	1:E:118:ARG:NH1	2.76	0.47
1:B:249:MSE:HE1	1:B:251:ARG:HH21	1.80	0.47
1:E:185[B]:GLU:O	1:H:209[B]:GLN:NE2	2.48	0.47
1:G:278:ILE:HD12	1:H:278:ILE:HD12	1.95	0.47
1:E:259:ALA:HB3	1:E:260:PRO:HD3	1.96	0.46
1:F:125:ILE:HD13	1:F:266:ALA:HB1	1.97	0.46
1:B:209[B]:GLN:NE2	5:B:686:HOH:O	2.48	0.46
1:C:129:ASN:ND2	2:C:301:NAD:H4D	2.30	0.46
1:E:99:LEU:HD21	1:E:115:GLU:HG2	1.93	0.46
1:D:259:ALA:HB3	1:D:260:PRO:HD3	1.97	0.46
1:H:236:ASP:O	1:H:240:VAL:HG23	2.15	0.46
1:H:226:ILE:CD1	1:H:258:LEU:HD11	2.46	0.46
1:D:10:MSE:HE3	1:D:227:TRP:CZ2	2.51	0.46
1:D:171[A]:GLN:HG3	1:D:215:GLY:HA3	1.97	0.46
1:E:246:ASN:OD1	1:E:246:ASN:N	2.39	0.46
1:G:10:MSE:CE	1:G:227:TRP:CE2	2.94	0.46
1:E:248:PRO:HG2	1:E:283:GLY:C	2.41	0.45
1:H:129:ASN:ND2	2:H:301:NAD:H4D	2.31	0.45
1:C:83:ASN:O	1:C:87:GLN:HG2	2.15	0.45
1:G:197:LYS:HD3	1:G:200:ILE:HD12	1.98	0.45
1:B:132:GLN:NE2	1:B:149:LYS:HE2	2.31	0.45
1:G:12:ALA:HB1	1:G:237:GLU:HB2	1.99	0.45
1:E:99:LEU:CD2	1:E:115:GLU:CG	2.92	0.45
1:F:19:PRO:HG3	2:F:301:NAD:C8A	2.47	0.45
1:G:181:ILE:HD11	1:G:284:VAL:HG11	1.98	0.45
1:A:197:LYS:HD3	1:A:200:ILE:HD12	1.98	0.45
1:E:115:GLU:CD	1:E:118:ARG:HH12	2.25	0.45
1:A:236:ASP:O	1:A:240:VAL:HG23	2.16	0.45
1:D:103:LEU:HD21	1:D:112:ILE:HD13	1.99	0.45
1:F:75:TYR:OH	1:F:79:GLU:OE2	2.26	0.45
1:G:248:PRO:HG2	1:G:283:GLY:O	2.17	0.45
1:H:231:ILE:HG12	1:H:243:PHE:CZ	2.52	0.45
1:E:99:LEU:HD22	1:E:115:GLU:HG2	1.96	0.45
1:E:103:LEU:HD21	1:E:112:ILE:HD13	1.99	0.45
1:E:249:MSE:HE3	1:F:274:THR:CG2	2.47	0.45
1:A:83[A]:ASN:O	1:A:86:LYS:HB3	2.16	0.44
1:F:163:LYS:NZ	4:F:326:SO4:O2	2.46	0.44
1:B:132:GLN:HE22	1:B:149:LYS:HE2	1.82	0.44
1:E:130:VAL:HG23	2:E:301:NAD:O4B	2.17	0.44
1:F:83[B]:ASN:O	1:F:87:GLN:HG2	2.17	0.44
1:E:131:ALA:HB3	2:E:301:NAD:H3D	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:LYS:NZ	5:F:618:HOH:O	2.51	0.44
1:D:50:THR:O	1:D:129:ASN:HB3	2.18	0.44
1:E:214:LYS:HE2	5:E:436:HOH:O	2.18	0.44
1:E:226:ILE:HD12	1:E:258:LEU:HD21	1.99	0.44
1:F:101:GLY:HA3	1:F:108:HIS:NE2	2.33	0.44
1:G:25:MSE:CE	1:G:227:TRP:CE2	3.00	0.44
1:B:13:GLN:HG2	1:B:240:VAL:HG11	1.99	0.43
1:E:86:LYS:CG	5:E:694:HOH:O	2.66	0.43
1:E:17:LYS:HE3	1:E:19:PRO:O	2.18	0.43
1:D:10:MSE:HE1	1:D:27:PRO:HD2	1.99	0.43
1:E:83:ASN:HB3	5:E:331:HOH:O	2.18	0.43
1:H:25:MSE:CE	1:H:227:TRP:CE2	3.00	0.43
1:B:95:LYS:NZ	5:B:843:HOH:O	2.33	0.43
1:A:140:GLU:HG2	1:A:141:TYR:CD1	2.54	0.43
1:B:163:LYS:NZ	4:B:318:SO4:O3	2.40	0.43
1:G:18:GLN:HA	1:G:19:PRO:C	2.43	0.43
1:B:95:LYS:HG3	1:B:96:CYS:N	2.34	0.42
1:A:50:THR:O	1:A:129:ASN:HB3	2.19	0.42
1:F:106:GLU:HG2	1:F:110:LYS:HE3	2.01	0.42
1:E:130:VAL:HG23	2:E:301:NAD:N9A	2.33	0.42
1:F:26:ASN:HA	1:F:27:PRO:HA	1.90	0.42
1:G:17:LYS:HB2	1:G:17:LYS:HE3	1.81	0.42
1:C:130[A]:VAL:HG21	1:C:153:ILE:HD11	2.00	0.42
1:F:9:THR:O	1:F:10:MSE:CE	2.64	0.42
1:G:259:ALA:HB3	1:G:260:PRO:HD3	2.02	0.42
1:F:86:LYS:NZ	1:F:90:GLU:OE2	2.47	0.42
1:F:132:GLN:NE2	1:F:149:LYS:HE2	2.34	0.42
1:A:185[B]:GLU:CD	1:A:284:VAL:HG11	2.39	0.42
1:D:10:MSE:CE	1:D:227:TRP:NE1	2.82	0.42
1:E:9:THR:CG2	5:E:862:HOH:O	2.64	0.42
1:H:259:ALA:HB3	1:H:260:PRO:HD3	2.02	0.42
1:F:83[A]:ASN:O	1:F:86:LYS:HB3	2.20	0.41
1:H:7:PHE:CB	1:H:10:MSE:HE1	2.50	0.41
1:H:74:ALA:HA	1:H:99:LEU:O	2.20	0.41
1:C:130[A]:VAL:HG23	2:C:301:NAD:C4A	2.50	0.41
1:F:18:GLN:HA	1:F:19:PRO:C	2.46	0.41
1:H:212:VAL:HG13	1:H:213:GLN:N	2.35	0.41
1:F:47:VAL:HG22	1:F:125:ILE:HB	2.02	0.41
1:F:231:ILE:HB	1:F:232:PRO:CD	2.50	0.41
1:E:130:VAL:HG23	2:E:301:NAD:H1B	1.98	0.41
1:D:163:LYS:NZ	4:D:324:SO4:O1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:THR:O	1:E:129:ASN:HB3	2.21	0.41
1:A:25:MSE:HE2	1:A:227:TRP:CE2	2.55	0.41
1:F:0:ALA:HB2	1:G:209:GLN:OE1	2.21	0.41
1:E:152:ARG:HA	1:E:156:PHE:CD2	2.56	0.41
1:H:25:MSE:HE2	1:H:227:TRP:CE2	2.55	0.41
1:B:50:THR:O	1:B:129:ASN:HB3	2.21	0.41
1:C:71:ILE:O	1:C:96:CYS:HA	2.21	0.41
1:A:86:LYS:NZ	5:A:313:HOH:O	2.54	0.40
1:D:82:ALA:HB1	1:D:98:LEU:HD22	2.04	0.40
1:E:115:GLU:OE2	1:E:119:GLN:NE2	2.54	0.40
1:F:236[B]:ASP:O	1:F:240:VAL:HG23	2.21	0.40
1:C:211:LEU:HB3	1:C:216:ILE:HB	2.03	0.40
1:D:122[B]:SER:OG	5:D:590:HOH:O	2.21	0.40
1:F:113:VAL:O	1:F:117:VAL:HG23	2.22	0.40
1:E:163:LYS:HG3	1:H:140:GLU:HA	2.03	0.40
1:G:236:ASP:O	1:G:240:VAL:HG23	2.22	0.40
1:H:91:LYS:HB2	1:H:91:LYS:HE3	1.93	0.40
1:F:103:LEU:HD12	2:F:301:NAD:C2A	2.52	0.40

All (1) 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)
1:G:86:LYS:NZ	1:G:119:GLN:O[2_455]	2.19	0.01

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	286/291 (98%)	275 (96%)	11 (4%)	0	100	100
1	B	284/291 (98%)	272 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	285/291 (98%)	274 (96%)	11 (4%)	0	100	100
1	D	285/291 (98%)	275 (96%)	10 (4%)	0	100	100
1	E	280/291 (96%)	269 (96%)	11 (4%)	0	100	100
1	F	293/291 (101%)	280 (96%)	13 (4%)	0	100	100
1	G	284/291 (98%)	275 (97%)	9 (3%)	0	100	100
1	H	292/291 (100%)	284 (97%)	8 (3%)	0	100	100
All	All	2289/2328 (98%)	2204 (96%)	85 (4%)	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	242/239 (101%)	241 (100%)	1 (0%)	84	88
1	B	240/239 (100%)	237 (99%)	3 (1%)	61	63
1	C	241/239 (101%)	240 (100%)	1 (0%)	84	88
1	D	241/239 (101%)	238 (99%)	3 (1%)	63	65
1	E	236/239 (99%)	234 (99%)	2 (1%)	73	77
1	F	248/239 (104%)	246 (99%)	2 (1%)	73	77
1	G	240/239 (100%)	238 (99%)	2 (1%)	73	77
1	H	247/239 (103%)	243 (98%)	4 (2%)	55	56
All	All	1935/1912 (101%)	1917 (99%)	18 (1%)	70	75

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LYS
1	B	10	MSE
1	B	238	LYS
1	B	258	LEU

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Mol	Chain	Res	Type
1	C	170	LYS
1	D	17	LYS
1	D	86	LYS
1	D	118	ARG
1	E	86	LYS
1	E	118	ARG
1	F	10	MSE
1	F	258	LEU
1	G	16	ASN
1	G	87	GLN
1	H	17	LYS
1	H	86	LYS
1	H	231	ILE
1	H	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	242	GLN
1	A	250	GLN
1	B	128	ASN
1	B	129	ASN
1	B	132	GLN
1	B	250	GLN
1	B	276	GLN
1	C	128	ASN
1	C	129	ASN
1	C	132	GLN
1	C	171	GLN
1	C	276	GLN
1	D	30	GLN
1	D	83	ASN
1	D	128	ASN
1	D	276	GLN
1	E	87	GLN
1	E	128	ASN
1	E	133	GLN
1	E	250	GLN
1	F	4	GLN
1	F	87	GLN
1	F	107	GLN

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Mol	Chain	Res	Type
1	F	128	ASN
1	F	129	ASN
1	F	132	GLN
1	G	16	ASN
1	G	30	GLN
1	G	128	ASN
1	G	129	ASN
1	G	132	GLN
1	G	171	GLN
1	G	250	GLN
1	G	276	GLN
1	H	3	GLN
1	H	128	ASN
1	H	129	ASN
1	H	137	GLN
1	H	213	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	H	301	3	46,48,48	1.86	8 (17%)	64,73,73	1.62	10 (15%)
2	NAD	G	301	3	46,48,48	1.74	6 (13%)	64,73,73	1.58	10 (15%)
4	SO4	C	328	-	4,4,4	0.26	0	6,6,6	0.26	0
2	NAD	C	301	3	46,48,48	1.81	4 (8%)	64,73,73	1.78	16 (25%)
4	SO4	B	318	-	4,4,4	0.23	0	6,6,6	0.19	0
4	SO4	F	322	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SO4	C	321	-	4,4,4	0.30	0	6,6,6	0.30	0
4	SO4	C	320	-	4,4,4	0.19	0	6,6,6	0.18	0
2	NAD	B	301	3	46,48,48	1.81	7 (15%)	64,73,73	1.69	15 (23%)
4	SO4	E	319	-	4,4,4	0.19	0	6,6,6	0.14	0
4	SO4	H	325	-	4,4,4	0.19	0	6,6,6	0.12	0
4	SO4	A	317	-	4,4,4	0.29	0	6,6,6	0.54	0
2	NAD	E	301	3	46,48,48	1.76	6 (13%)	64,73,73	1.68	13 (20%)
4	SO4	A	323	-	4,4,4	0.23	0	6,6,6	0.22	0
2	NAD	D	301	3	46,48,48	1.70	4 (8%)	64,73,73	1.74	17 (26%)
4	SO4	F	326	-	4,4,4	0.25	0	6,6,6	0.13	0
2	NAD	F	301	3	46,48,48	1.74	6 (13%)	64,73,73	1.72	12 (18%)
4	SO4	D	324	-	4,4,4	0.24	0	6,6,6	0.16	0
2	NAD	A	301	3	46,48,48	1.76	5 (10%)	64,73,73	1.70	13 (20%)
4	SO4	G	329	-	4,4,4	0.22	0	6,6,6	0.09	0
4	SO4	G	330	-	4,4,4	0.23	0	6,6,6	0.27	0
4	SO4	C	327	-	4,4,4	0.22	0	6,6,6	0.17	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	H	301	3	-	7/30/62/62	0/5/5/5
2	NAD	A	301	3	-	6/30/62/62	0/5/5/5
2	NAD	G	301	3	-	4/30/62/62	0/5/5/5
2	NAD	C	301	3	-	4/30/62/62	0/5/5/5
2	NAD	E	301	3	-	7/30/62/62	0/5/5/5
2	NAD	B	301	3	-	5/30/62/62	0/5/5/5
2	NAD	D	301	3	-	3/30/62/62	0/5/5/5
2	NAD	F	301	3	-	5/30/62/62	0/5/5/5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NAD	O7N-C7N	9.59	1.42	1.24
2	H	301	NAD	O7N-C7N	9.58	1.42	1.24
2	E	301	NAD	O7N-C7N	9.45	1.41	1.24
2	A	301	NAD	O7N-C7N	9.45	1.41	1.24
2	G	301	NAD	O7N-C7N	9.31	1.41	1.24
2	B	301	NAD	O7N-C7N	9.27	1.41	1.24
2	C	301	NAD	O7N-C7N	9.16	1.41	1.24
2	D	301	NAD	O7N-C7N	8.97	1.40	1.24
2	C	301	NAD	PA-O3	4.92	1.64	1.59
2	A	301	NAD	PA-O3	3.67	1.63	1.59
2	H	301	NAD	PN-O3	3.47	1.63	1.59
2	B	301	NAD	PN-O3	3.15	1.62	1.59
2	H	301	NAD	PA-O3	2.99	1.62	1.59
2	B	301	NAD	PA-O3	2.89	1.62	1.59
2	H	301	NAD	C2A-N1A	2.83	1.39	1.33
2	B	301	NAD	C2A-N3A	2.70	1.38	1.33
2	D	301	NAD	C2A-N1A	2.69	1.38	1.33
2	E	301	NAD	PN-O3	2.62	1.62	1.59
2	C	301	NAD	C2A-N3A	2.59	1.38	1.33
2	D	301	NAD	C2A-N3A	2.56	1.38	1.33
2	B	301	NAD	C2A-N1A	2.55	1.38	1.33
2	G	301	NAD	PA-O3	2.55	1.62	1.59
2	E	301	NAD	C2A-N3A	2.53	1.38	1.33
2	D	301	NAD	C8A-N7A	2.44	1.36	1.31
2	F	301	NAD	C2A-N1A	2.42	1.38	1.33
2	E	301	NAD	C2A-N1A	2.42	1.38	1.33
2	F	301	NAD	C8A-N7A	2.39	1.36	1.31
2	E	301	NAD	PA-O3	2.39	1.62	1.59
2	H	301	NAD	C2A-N3A	2.36	1.38	1.33
2	F	301	NAD	C2N-N1N	2.33	1.37	1.35
2	G	301	NAD	C2A-N1A	2.33	1.38	1.33
2	B	301	NAD	C8A-N7A	2.31	1.36	1.31
2	G	301	NAD	PN-O3	2.30	1.62	1.59
2	H	301	NAD	C5A-N7A	-2.28	1.34	1.39
2	F	301	NAD	C2A-N3A	2.26	1.37	1.33
2	C	301	NAD	C2A-N1A	2.25	1.37	1.33
2	A	301	NAD	C5A-N7A	-2.16	1.35	1.39
2	G	301	NAD	C8A-N7A	2.16	1.35	1.31
2	G	301	NAD	C2A-N3A	2.15	1.37	1.33
2	A	301	NAD	C2A-N3A	2.15	1.37	1.33
2	B	301	NAD	C2N-N1N	2.11	1.37	1.35
2	H	301	NAD	C8A-N7A	2.08	1.35	1.31
2	E	301	NAD	C8A-N7A	2.06	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	NAD	C2N-N1N	2.04	1.37	1.35
2	A	301	NAD	PN-O3	2.03	1.61	1.59
2	F	301	NAD	C5A-N7A	-2.00	1.35	1.39

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	NAD	N3A-C2A-N1A	-6.09	119.36	128.58
2	C	301	NAD	N3A-C2A-N1A	-6.04	119.44	128.58
2	D	301	NAD	N3A-C2A-N1A	-5.83	119.75	128.58
2	E	301	NAD	N3A-C2A-N1A	-5.77	119.84	128.58
2	A	301	NAD	N3A-C2A-N1A	-5.63	120.06	128.58
2	H	301	NAD	N3A-C2A-N1A	-5.61	120.09	128.58
2	G	301	NAD	N3A-C2A-N1A	-5.59	120.12	128.58
2	B	301	NAD	N3A-C2A-N1A	-5.36	120.47	128.58
2	H	301	NAD	N9A-C8A-N7A	-4.48	107.57	113.94
2	E	301	NAD	N9A-C8A-N7A	-4.40	107.69	113.94
2	A	301	NAD	C5A-C4A-N3A	-4.39	120.68	126.72
2	B	301	NAD	C5A-C4A-N3A	-4.28	120.83	126.72
2	C	301	NAD	N9A-C8A-N7A	-4.27	107.88	113.94
2	F	301	NAD	C5A-C4A-N3A	-4.15	121.00	126.72
2	G	301	NAD	C5A-C4A-N3A	-4.11	121.05	126.72
2	B	301	NAD	N9A-C8A-N7A	-4.09	108.13	113.94
2	A	301	NAD	N9A-C8A-N7A	-4.06	108.17	113.94
2	H	301	NAD	C5A-C4A-N3A	-4.06	121.12	126.72
2	G	301	NAD	N9A-C8A-N7A	-4.02	108.24	113.94
2	F	301	NAD	N9A-C8A-N7A	-3.98	108.29	113.94
2	E	301	NAD	C5A-C4A-N3A	-3.95	121.28	126.72
2	D	301	NAD	C5A-C4A-N3A	-3.95	121.28	126.72
2	F	301	NAD	O4B-C1B-N9A	3.95	115.67	108.09
2	D	301	NAD	N9A-C8A-N7A	-3.89	108.42	113.94
2	C	301	NAD	C5A-C4A-N3A	-3.77	121.53	126.72
2	E	301	NAD	C5A-N7A-C8A	3.74	109.33	103.45
2	C	301	NAD	C5A-N7A-C8A	3.70	109.26	103.45
2	A	301	NAD	C4D-O4D-C1D	-3.69	106.54	109.92
2	G	301	NAD	C5A-N7A-C8A	3.61	109.13	103.45
2	A	301	NAD	C5A-N7A-C8A	3.59	109.09	103.45
2	H	301	NAD	C5A-N7A-C8A	3.56	109.05	103.45
2	F	301	NAD	C5A-N7A-C8A	3.47	108.90	103.45
2	B	301	NAD	C5A-N7A-C8A	3.46	108.88	103.45
2	F	301	NAD	C2A-N3A-C4A	3.40	120.12	111.83
2	C	301	NAD	C2A-N3A-C4A	3.33	119.95	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAD	O4B-C1B-N9A	3.32	114.46	108.09
2	B	301	NAD	O4B-C1B-N9A	3.31	114.45	108.09
2	A	301	NAD	C2A-N3A-C4A	3.28	119.84	111.83
2	G	301	NAD	C2A-N3A-C4A	3.26	119.80	111.83
2	H	301	NAD	C2A-N3A-C4A	3.25	119.76	111.83
2	D	301	NAD	C5A-N7A-C8A	3.24	108.54	103.45
2	D	301	NAD	C2A-N3A-C4A	3.20	119.66	111.83
2	B	301	NAD	C3N-C7N-N7N	3.16	121.63	117.74
2	B	301	NAD	C2A-N3A-C4A	3.16	119.54	111.83
2	E	301	NAD	C2A-N3A-C4A	3.15	119.52	111.83
2	C	301	NAD	O4B-C1B-N9A	3.09	114.02	108.09
2	A	301	NAD	N3A-C4A-N9A	3.08	132.40	127.17
2	C	301	NAD	O2N-PN-O3	2.99	115.34	107.27
2	B	301	NAD	N3A-C4A-N9A	2.97	132.22	127.17
2	G	301	NAD	O4B-C1B-N9A	2.95	113.76	108.09
2	A	301	NAD	O4B-C1B-N9A	2.93	113.72	108.09
2	D	301	NAD	O3-PN-O1N	-2.92	101.92	110.70
2	C	301	NAD	C3N-C7N-N7N	2.91	121.33	117.74
2	G	301	NAD	C4A-C5A-N7A	-2.86	107.31	110.58
2	H	301	NAD	N3A-C4A-N9A	2.85	132.02	127.17
2	E	301	NAD	O4B-C1B-N9A	2.80	113.47	108.09
2	D	301	NAD	C4D-O4D-C1D	-2.79	107.37	109.92
2	C	301	NAD	C4A-C5A-N7A	-2.74	107.44	110.58
2	E	301	NAD	N3A-C4A-N9A	2.73	131.82	127.17
2	H	301	NAD	C4A-N9A-C8A	2.70	108.57	105.74
2	F	301	NAD	C4A-C5A-N7A	-2.69	107.51	110.58
2	E	301	NAD	C2B-C1B-N9A	-2.66	106.69	113.30
2	D	301	NAD	C3N-C7N-N7N	2.66	121.01	117.74
2	E	301	NAD	C3N-C7N-N7N	2.61	120.95	117.74
2	E	301	NAD	C4A-C5A-N7A	-2.60	107.61	110.58
2	E	301	NAD	O3-PN-O1N	-2.59	102.91	110.70
2	C	301	NAD	O3-PN-O1N	-2.59	102.92	110.70
2	E	301	NAD	C4A-N9A-C8A	2.58	108.45	105.74
2	C	301	NAD	O7N-C7N-N7N	-2.55	118.93	122.62
2	F	301	NAD	O7N-C7N-N7N	-2.55	118.93	122.62
2	C	301	NAD	C4D-O4D-C1D	-2.55	107.59	109.92
2	A	301	NAD	O7N-C7N-N7N	-2.52	118.98	122.62
2	D	301	NAD	C4A-C5A-N7A	-2.51	107.71	110.58
2	H	301	NAD	C4D-O4D-C1D	-2.49	107.65	109.92
2	C	301	NAD	N3A-C4A-N9A	2.45	131.33	127.17
2	B	301	NAD	O7N-C7N-N7N	-2.42	119.12	122.62
2	D	301	NAD	N3A-C4A-N9A	2.42	131.28	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAD	C4A-N9A-C8A	2.41	108.27	105.74
2	F	301	NAD	N3A-C4A-N9A	2.38	131.22	127.17
2	C	301	NAD	O3-PA-O1A	-2.36	103.60	110.70
2	G	301	NAD	N3A-C4A-N9A	2.36	131.18	127.17
2	B	301	NAD	C4A-C5A-N7A	-2.35	107.89	110.58
2	E	301	NAD	C4D-O4D-C1D	-2.33	107.79	109.92
2	A	301	NAD	C4A-C5A-N7A	-2.33	107.92	110.58
2	D	301	NAD	C2B-C1B-N9A	-2.32	107.53	113.30
2	H	301	NAD	C4A-C5A-N7A	-2.31	107.94	110.58
2	B	301	NAD	O2A-PA-O3	2.30	113.48	107.27
2	B	301	NAD	C4A-N9A-C8A	2.29	108.14	105.74
2	B	301	NAD	C2B-C1B-N9A	-2.25	107.72	113.30
2	D	301	NAD	O3-PA-O1A	-2.23	104.01	110.70
2	F	301	NAD	C2B-C1B-N9A	-2.22	107.79	113.30
2	D	301	NAD	C5N-C4N-C3N	-2.19	118.21	120.36
2	D	301	NAD	O2N-PN-O1N	2.18	122.60	112.44
2	F	301	NAD	O3-PN-O1N	-2.12	104.32	110.70
2	G	301	NAD	C2B-C1B-N9A	-2.12	108.03	113.30
2	B	301	NAD	O3-PN-O1N	-2.10	104.40	110.70
2	D	301	NAD	C2N-C3N-C4N	2.07	120.66	118.26
2	H	301	NAD	O3-PN-O1N	-2.06	104.50	110.70
2	B	301	NAD	O3-PA-O1A	-2.06	104.52	110.70
2	D	301	NAD	C4A-N9A-C8A	2.05	107.89	105.74
2	G	301	NAD	C3B-C2B-C1B	2.05	105.33	101.46
2	A	301	NAD	C4A-N9A-C8A	2.04	107.88	105.74
2	A	301	NAD	O3-PN-O1N	-2.03	104.59	110.70
2	C	301	NAD	C2B-C1B-N9A	-2.03	108.27	113.30
2	A	301	NAD	O3-PA-O1A	-2.02	104.64	110.70
2	F	301	NAD	O7N-C7N-C3N	2.00	122.05	119.60

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAD	PN-O3-PA-O5B
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	B	301	NAD	C5D-O5D-PN-O3
2	B	301	NAD	C5D-O5D-PN-O1N
2	B	301	NAD	C5D-O5D-PN-O2N
2	C	301	NAD	PN-O3-PA-O5B

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Mol	Chain	Res	Type	Atoms
2	C	301	NAD	C5D-O5D-PN-O3
2	D	301	NAD	C5D-O5D-PN-O3
2	D	301	NAD	C5D-O5D-PN-O1N
2	E	301	NAD	C5B-O5B-PA-O1A
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	PN-O3-PA-O5B
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	G	301	NAD	PN-O3-PA-O5B
2	G	301	NAD	C5D-O5D-PN-O3
2	H	301	NAD	PN-O3-PA-O5B
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	E	301	NAD	O4B-C4B-C5B-O5B
2	E	301	NAD	C3B-C4B-C5B-O5B
2	B	301	NAD	PN-O3-PA-O5B
2	D	301	NAD	PN-O3-PA-O5B
2	C	301	NAD	C5D-O5D-PN-O1N
2	G	301	NAD	C5D-O5D-PN-O1N
2	H	301	NAD	C5B-O5B-PA-O2A
2	H	301	NAD	O4B-C4B-C5B-O5B
2	C	301	NAD	C4B-C5B-O5B-PA
2	F	301	NAD	C4B-C5B-O5B-PA
2	G	301	NAD	O4B-C4B-C5B-O5B
2	H	301	NAD	C4B-C5B-O5B-PA
2	A	301	NAD	C4B-C5B-O5B-PA
2	B	301	NAD	C4B-C5B-O5B-PA
2	A	301	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

12 monomers are involved in 24 short contacts:

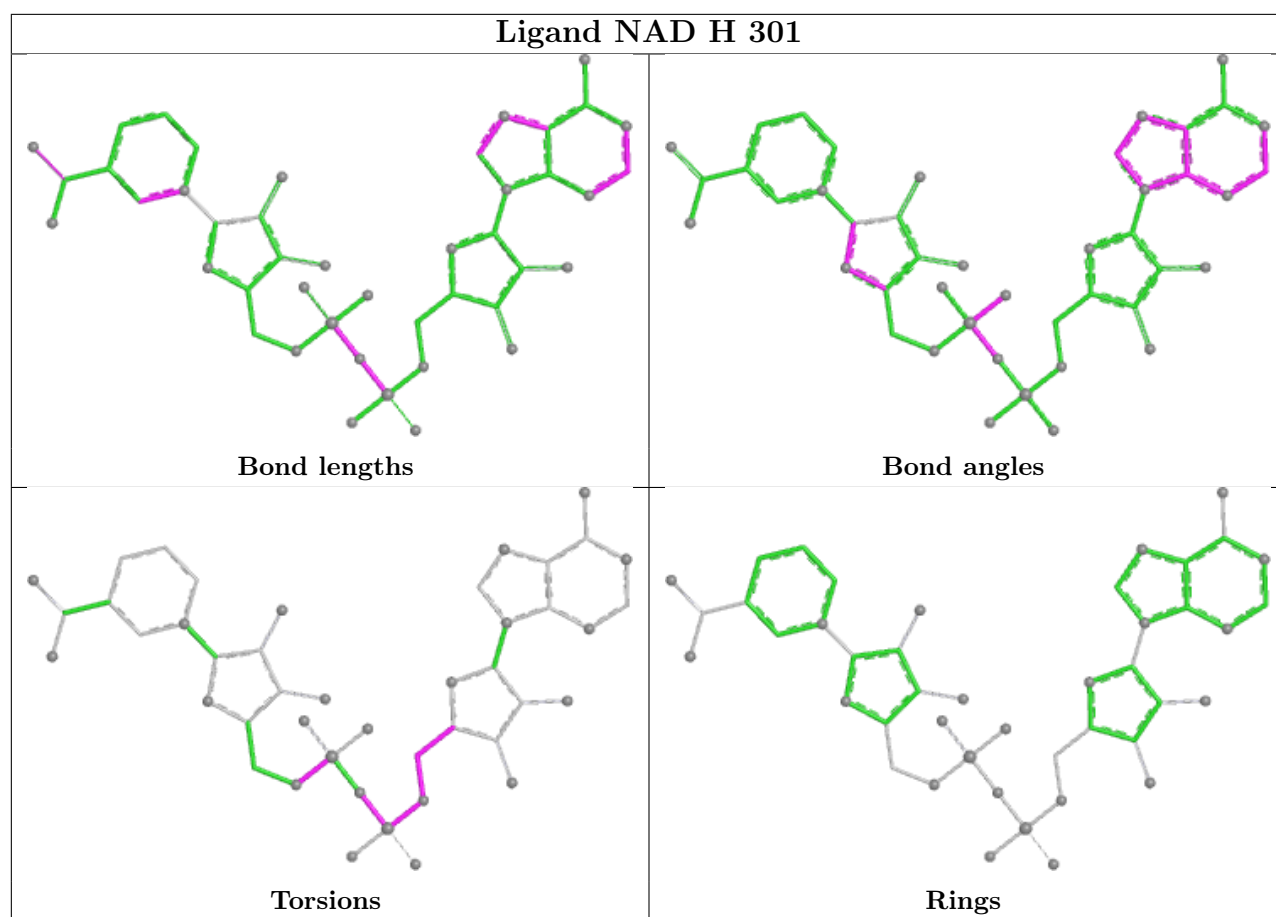
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	NAD	1	0
4	C	328	SO4	1	0
2	C	301	NAD	6	0
4	B	318	SO4	1	0

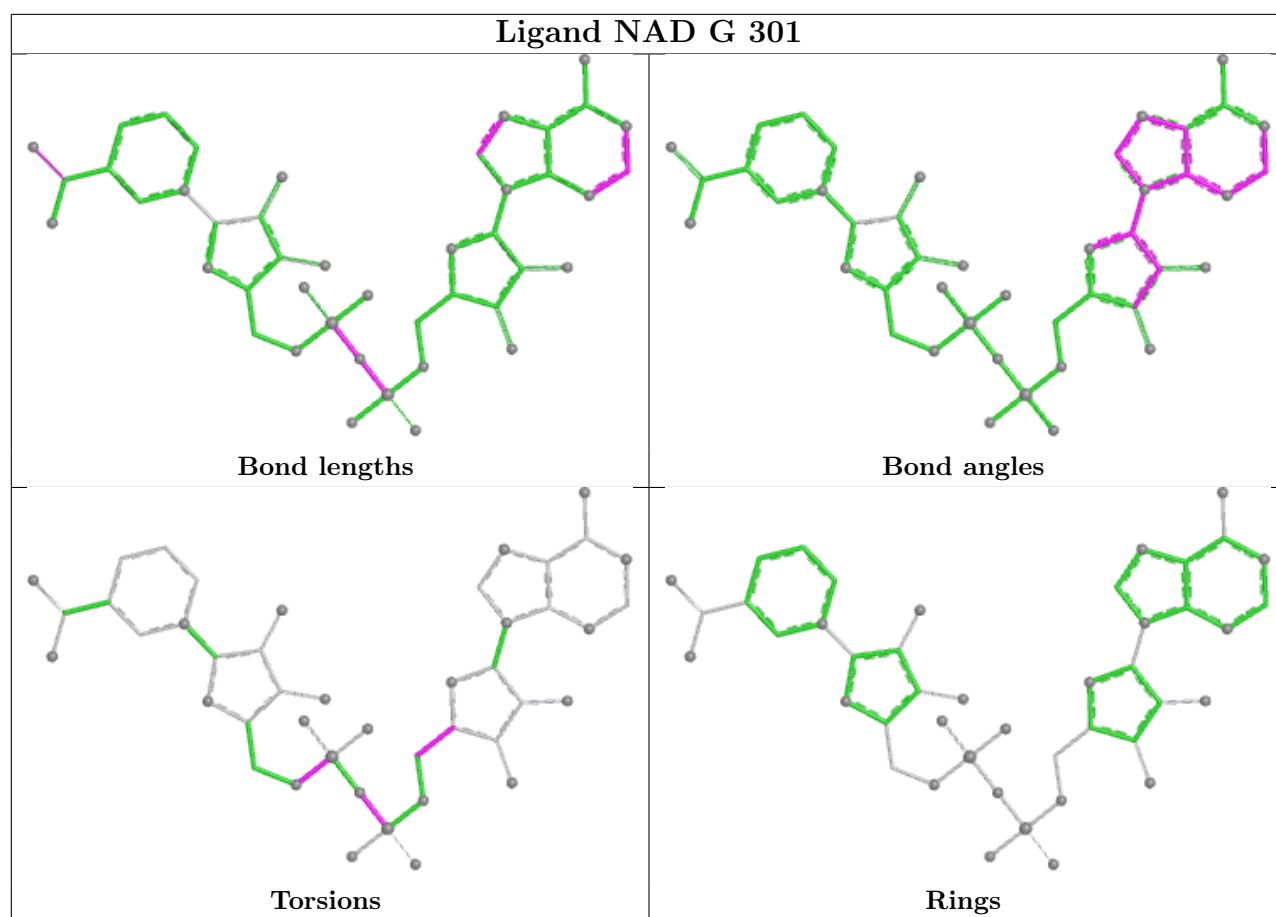
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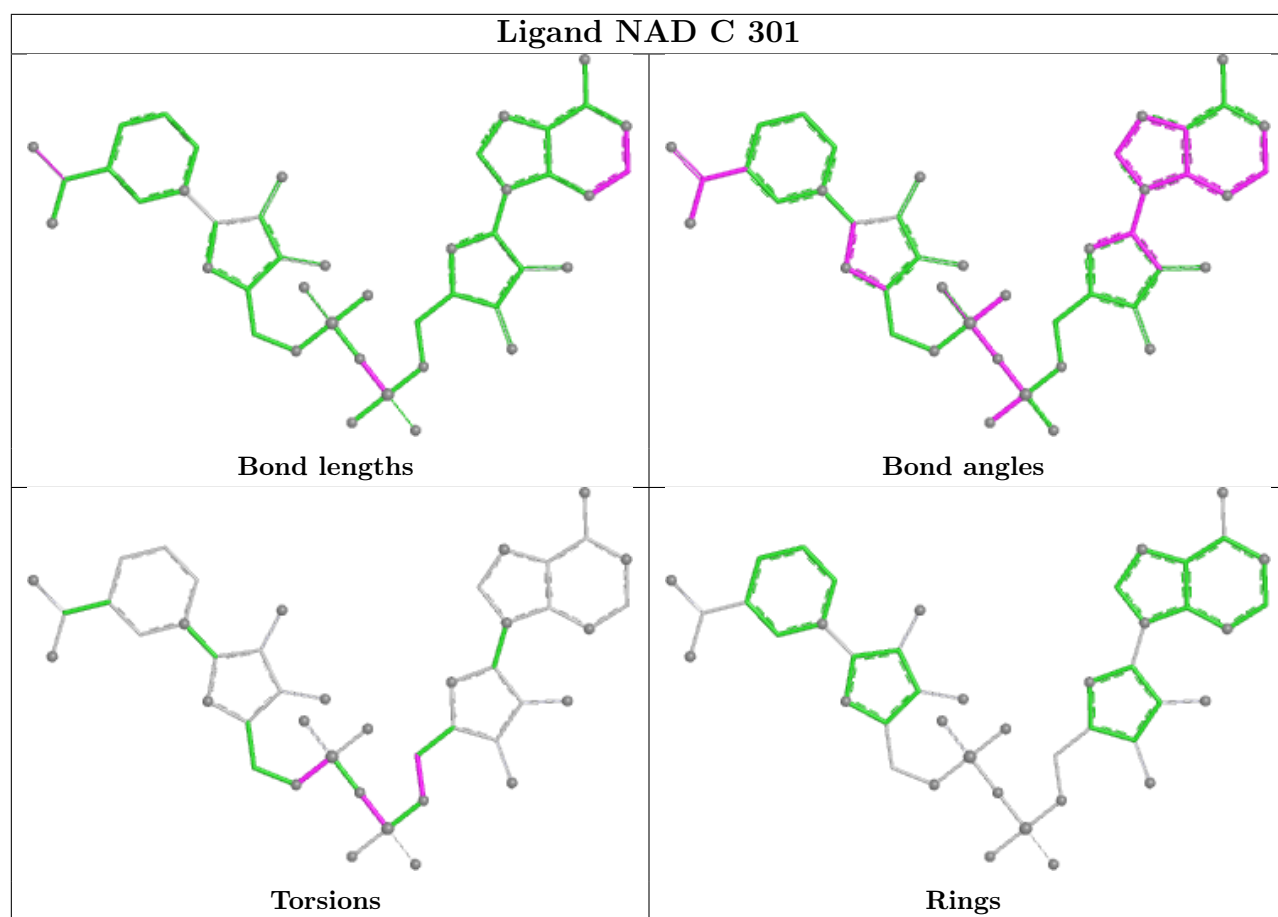
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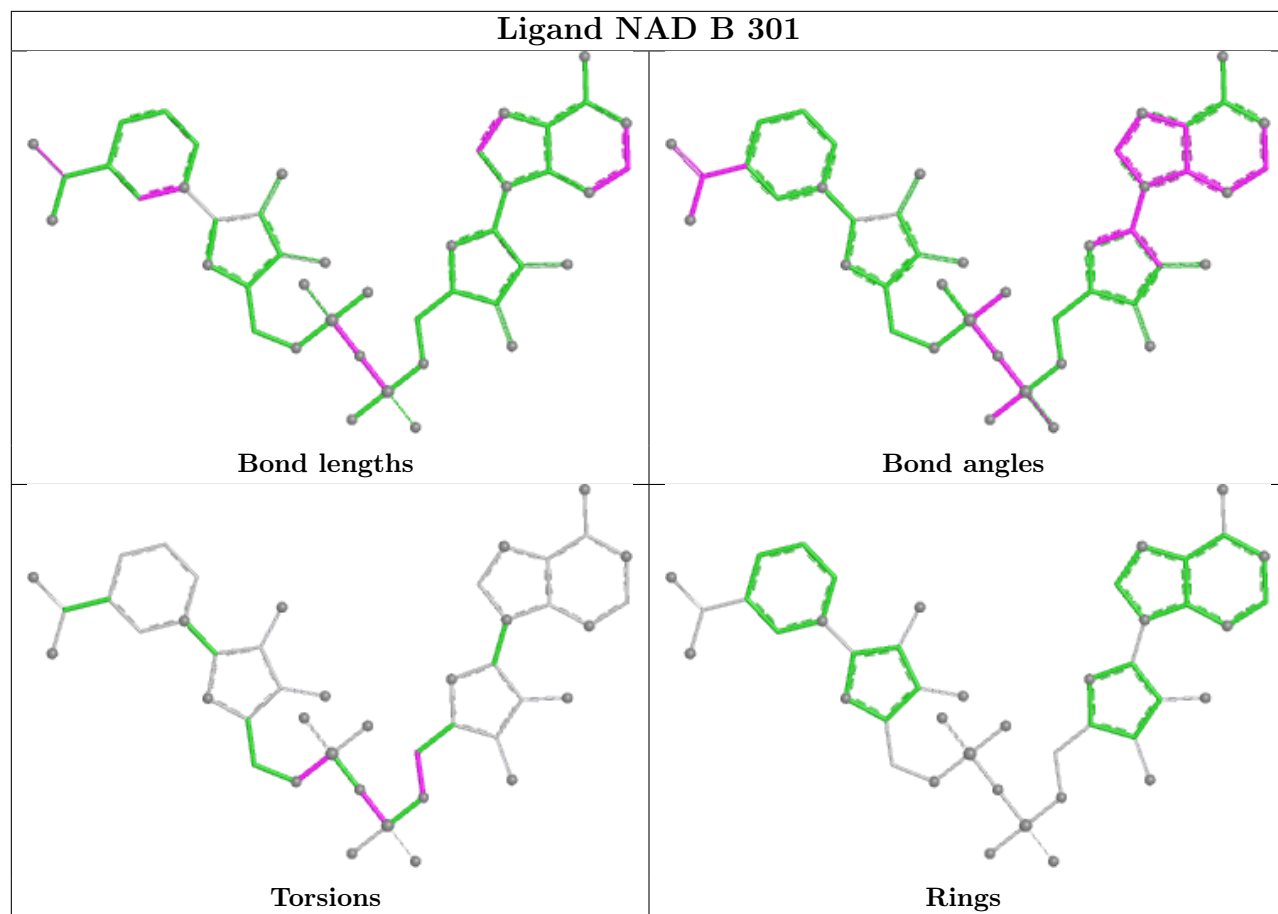
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	NAD	1	0
4	E	319	SO4	1	0
2	E	301	NAD	5	0
2	D	301	NAD	1	0
4	F	326	SO4	1	0
2	F	301	NAD	4	0
4	D	324	SO4	1	0
2	A	301	NAD	1	0

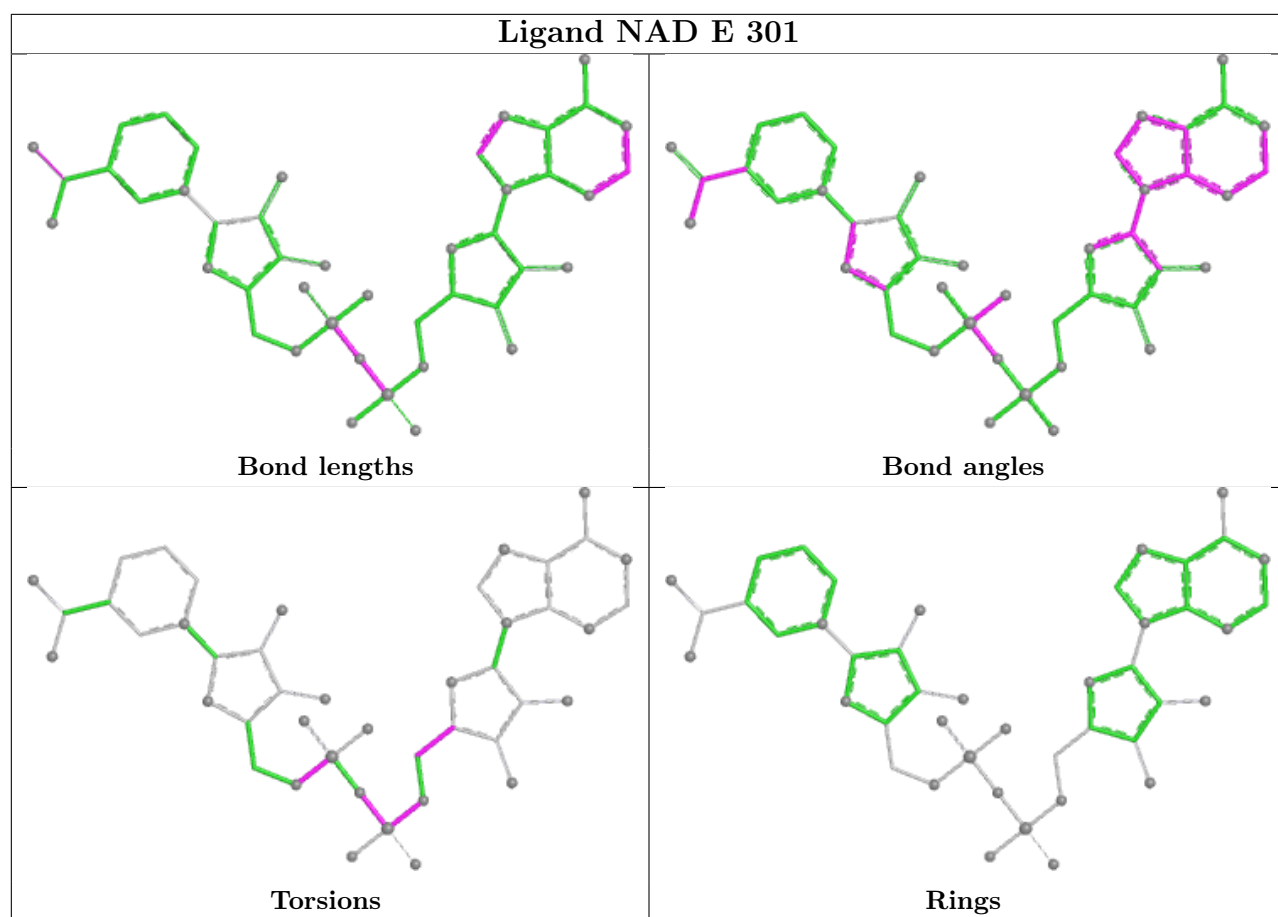
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

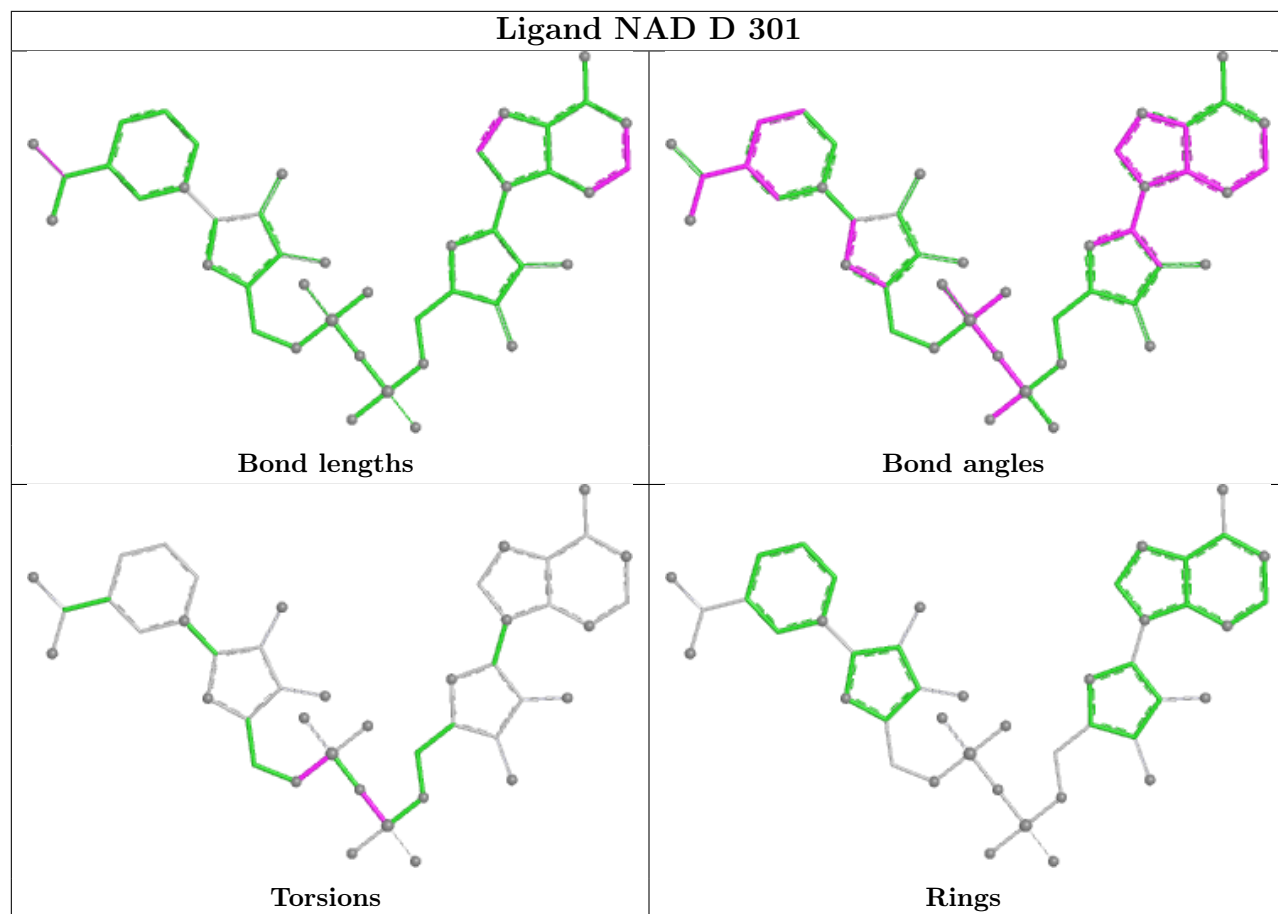


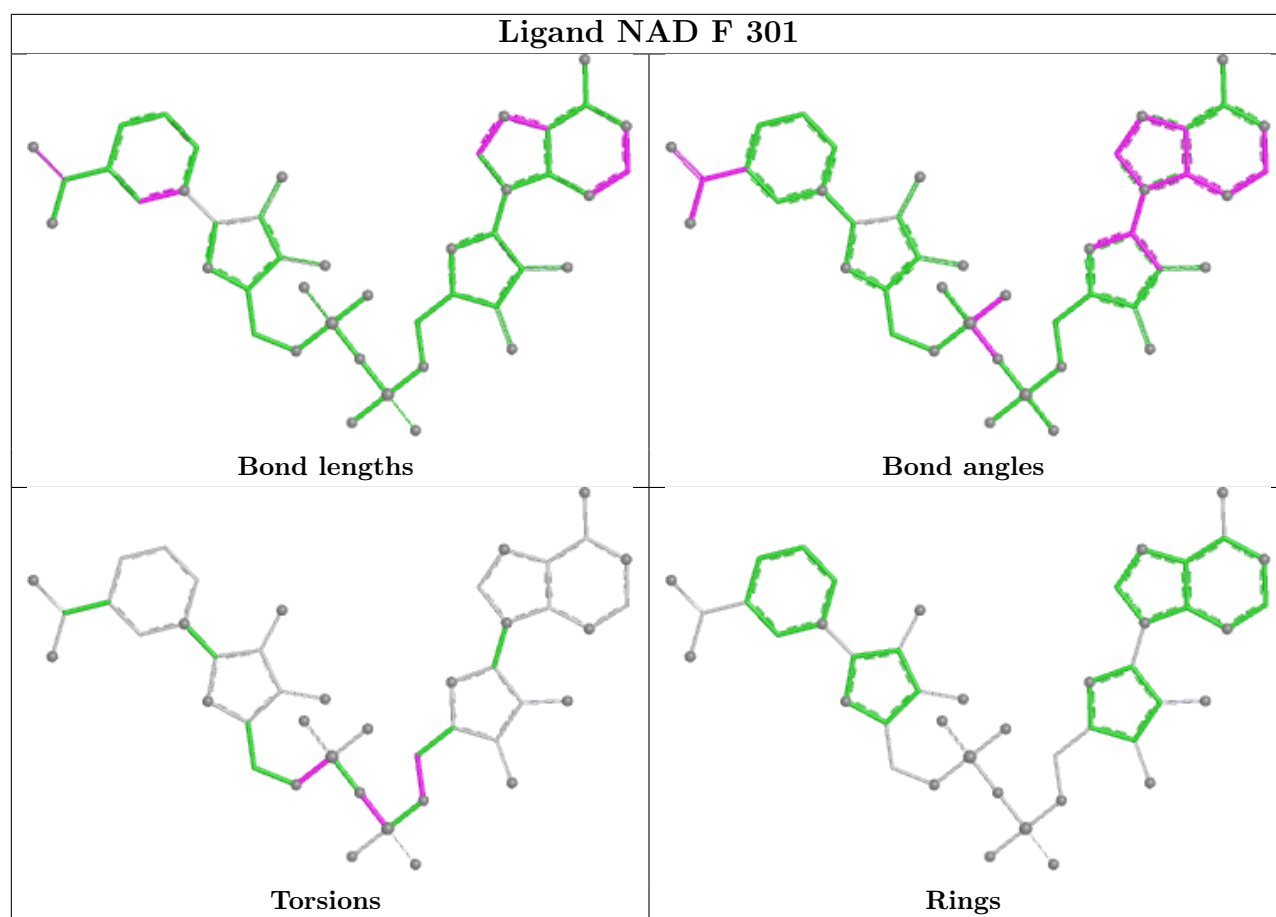


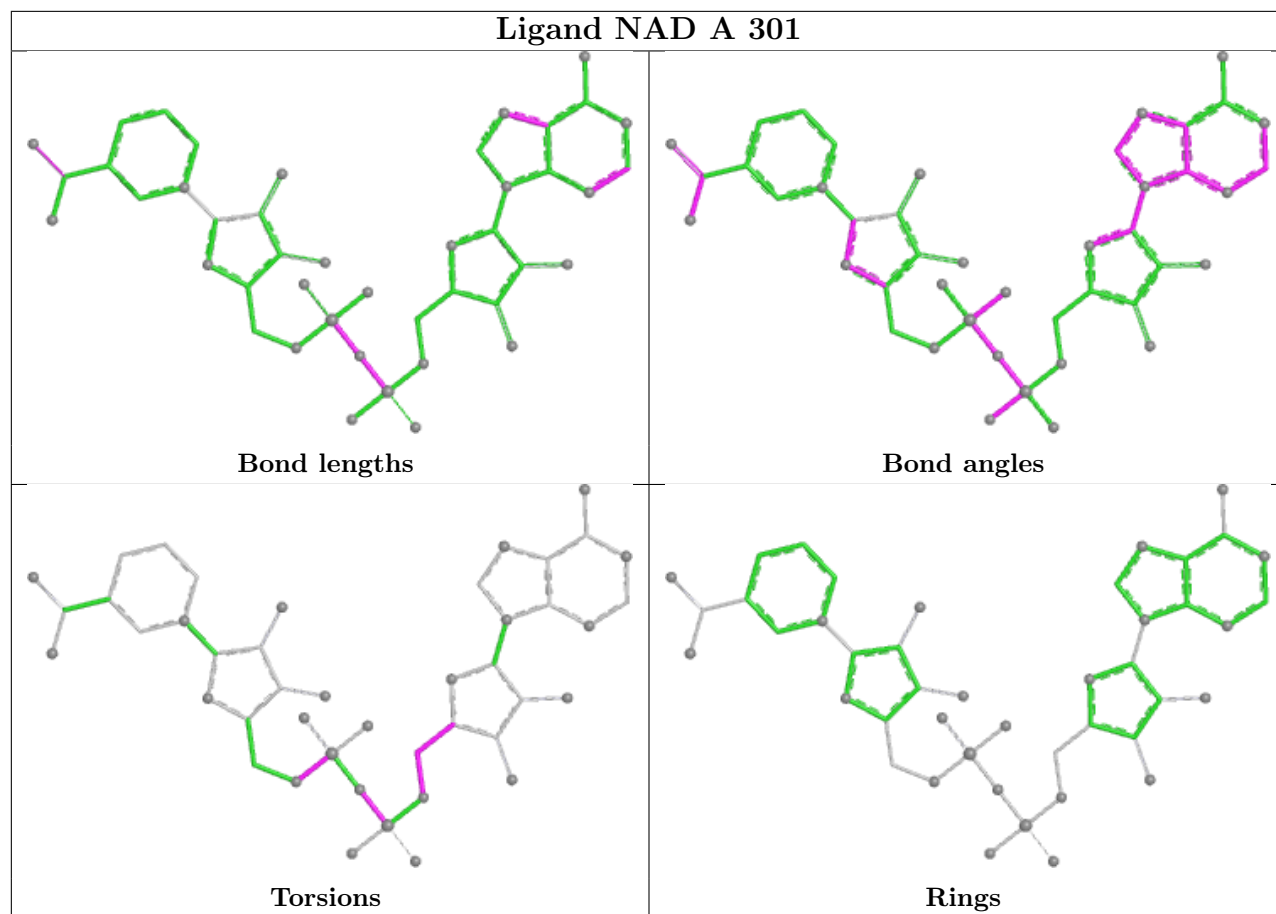












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	277/291 (95%)	-0.10	4 (1%) 73 75	2, 6, 18, 25	7 (2%)
1	B	279/291 (95%)	0.17	7 (2%) 58 60	3, 10, 23, 37	3 (1%)
1	C	277/291 (95%)	-0.16	1 (0%) 88 90	2, 5, 13, 20	6 (2%)
1	D	277/291 (95%)	0.09	4 (1%) 73 75	3, 10, 20, 35	6 (2%)
1	E	276/291 (94%)	0.59	28 (10%) 12 12	3, 12, 20, 24	2 (0%)
1	F	285/291 (97%)	0.25	9 (3%) 50 50	7, 15, 27, 43	5 (1%)
1	G	277/291 (95%)	0.08	4 (1%) 73 75	5, 13, 21, 28	5 (1%)
1	H	284/291 (97%)	0.20	11 (3%) 43 44	3, 14, 24, 28	5 (1%)
All	All	2232/2328 (95%)	0.14	68 (3%) 52 53	2, 12, 21, 43	39 (1%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	259	ALA	9.0
1	E	258	LEU	8.5
1	H	258	LEU	4.9
1	E	256	TYR	4.8
1	E	255	PRO	4.5
1	F	7	PHE	3.8
1	E	257	GLU	3.7
1	B	12	ALA	3.7
1	E	226	ILE	3.7
1	E	42	LEU	3.6
1	A	12	ALA	3.6
1	D	263	VAL	3.4
1	A	8	VAL	3.3
1	F	39	SER	3.3
1	E	9	THR	3.3
1	E	252	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	251	ARG	3.0
1	B	20	GLY	3.0
1	H	2	PRO	2.9
1	E	38	GLY	2.9
1	F	45	LYS	2.9
1	E	253	GLY	2.8
1	E	43	LYS	2.8
1	H	42	LEU	2.7
1	E	248	PRO	2.7
1	H	8	VAL	2.7
1	E	23	SER	2.6
1	E	39	SER	2.6
1	E	238	LYS	2.6
1	A	24	LEU	2.6
1	B	17	LYS	2.6
1	G	237	GLU	2.5
1	H	7	PHE	2.5
1	C	31	PHE	2.5
1	H	38	GLY	2.5
1	H	0	ALA	2.5
1	H	12	ALA	2.4
1	E	24	LEU	2.4
1	B	16	ASN	2.4
1	H	39	SER	2.4
1	H	255	PRO	2.4
1	G	8	VAL	2.4
1	F	248	PRO	2.4
1	D	260	PRO	2.3
1	E	230	LEU	2.3
1	F	42	LEU	2.3
1	F	4	GLN	2.3
1	G	26	ASN	2.3
1	B	21	ILE	2.3
1	F	8	VAL	2.3
1	E	31	PHE	2.2
1	B	248	PRO	2.2
1	E	247	VAL	2.2
1	E	235	PHE	2.2
1	D	9	THR	2.2
1	A	11	PRO	2.2
1	E	125	ILE	2.2
1	E	228	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	12	ALA	2.1
1	E	26	ASN	2.1
1	F	6	ASN	2.1
1	E	36	TYR	2.1
1	F	2	PRO	2.1
1	D	8	VAL	2.1
1	E	16	ASN	2.0
1	B	11	PRO	2.0
1	H	256	TYR	2.0
1	E	14	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.

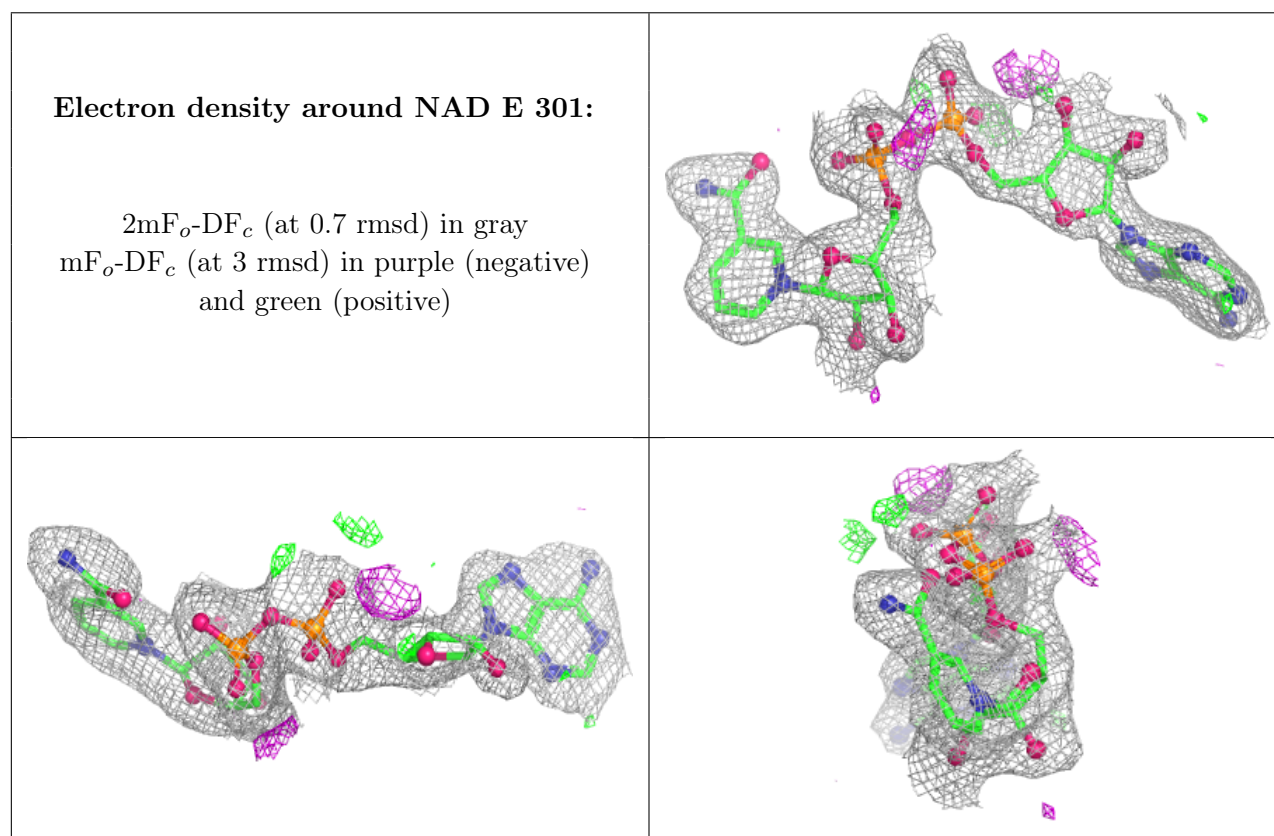
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	F	322	5/5	0.53	0.23	65,66,68,69	5
4	SO4	C	327	5/5	0.62	0.14	78,78,79,80	5
4	SO4	G	330	5/5	0.64	0.27	40,47,48,51	5
4	SO4	H	325	5/5	0.65	0.15	80,81,82,83	5
3	MG	E	300	1/1	0.67	0.12	57,57,57,57	0
3	MG	G	300	1/1	0.70	0.13	54,54,54,54	0
4	SO4	D	324	5/5	0.72	0.12	81,81,82,83	5
4	SO4	C	328	5/5	0.73	0.29	46,46,48,51	5
4	SO4	A	323	5/5	0.74	0.12	68,70,74,74	5
4	SO4	G	329	5/5	0.74	0.17	61,62,63,64	5
4	SO4	F	326	5/5	0.76	0.17	60,61,62,64	5
4	SO4	C	321	5/5	0.76	0.11	62,66,67,67	0
3	MG	C	300	1/1	0.78	0.12	43,43,43,43	0

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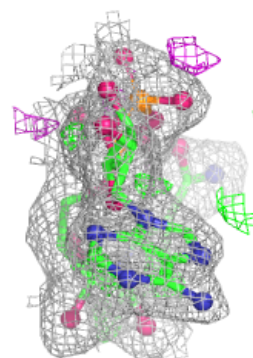
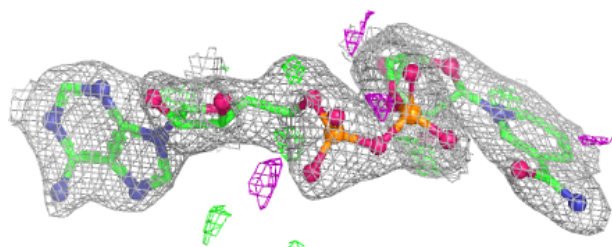
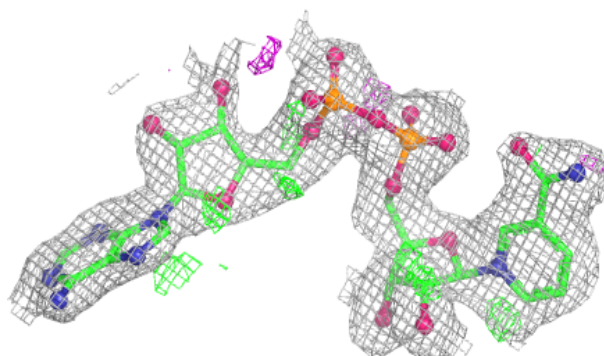
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	E	319	5/5	0.79	0.14	69,69,71,71	5
3	MG	F	300	1/1	0.81	0.12	53,53,53,53	0
4	SO4	B	318	5/5	0.83	0.11	60,61,64,65	5
2	NAD	E	301	44/44	0.84	0.14	41,49,54,54	44
3	MG	A	300	1/1	0.85	0.10	37,37,37,37	1
2	NAD	B	301	44/44	0.86	0.12	27,39,47,49	44
4	SO4	A	317	5/5	0.86	0.12	49,51,52,55	5
3	MG	H	300	1/1	0.87	0.08	53,53,53,53	0
4	SO4	C	320	5/5	0.87	0.14	45,45,49,49	5
2	NAD	F	301	44/44	0.87	0.12	33,44,53,54	44
3	MG	B	300	1/1	0.87	0.07	41,41,41,41	1
2	NAD	G	301	44/44	0.88	0.12	33,41,46,47	44
2	NAD	C	301	44/44	0.90	0.10	27,33,37,38	44
3	MG	D	300	1/1	0.90	0.13	44,44,44,44	0
2	NAD	A	301	44/44	0.91	0.10	26,33,38,39	44
2	NAD	D	301	44/44	0.92	0.10	26,37,42,47	0
2	NAD	H	301	44/44	0.92	0.10	30,38,45,48	44

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.

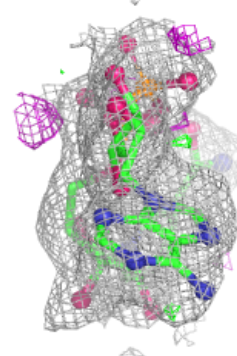
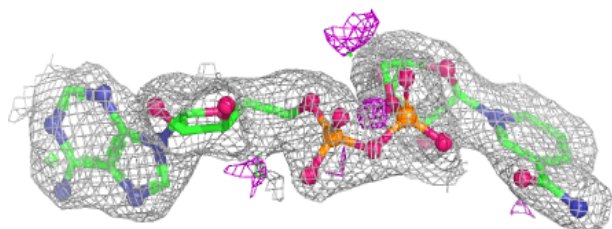
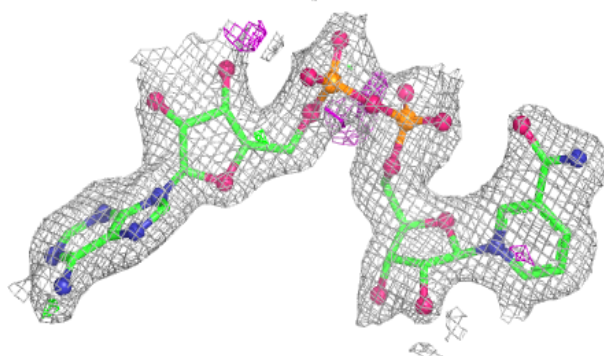


Electron density around NAD B 301:

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

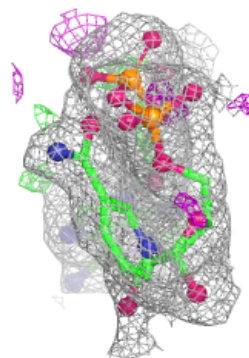
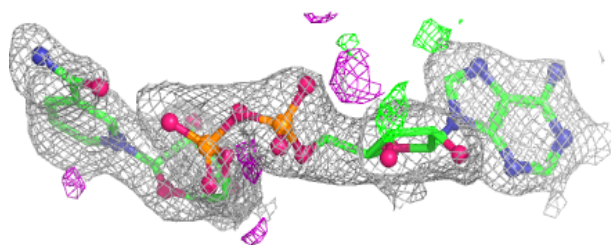
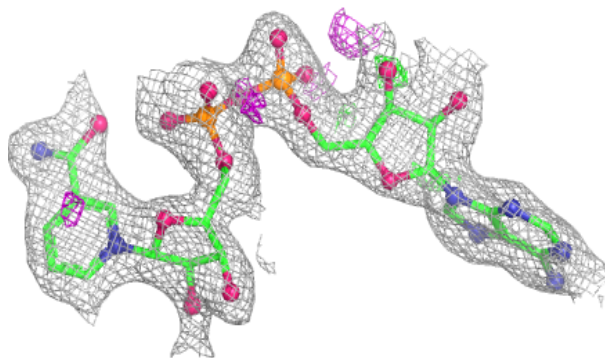
**Electron density around NAD F 301:**

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

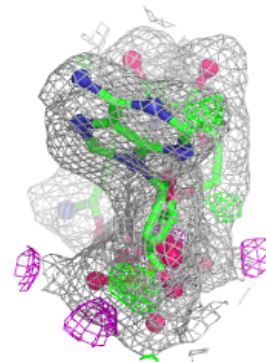
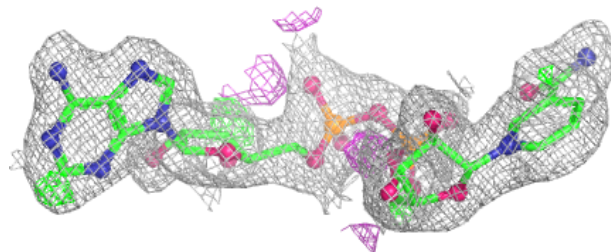
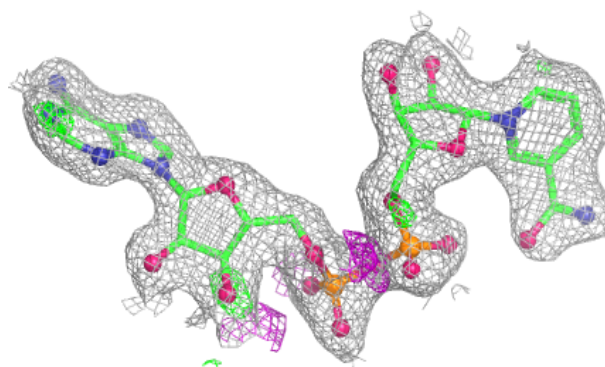


Electron density around NAD G 301:

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

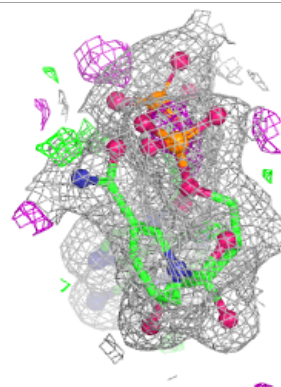
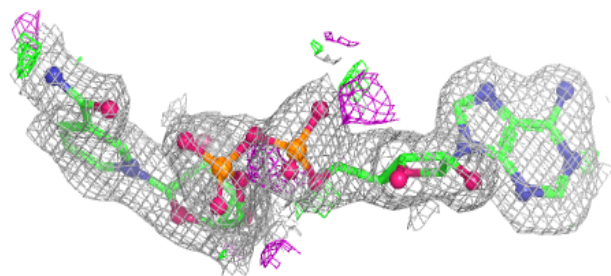
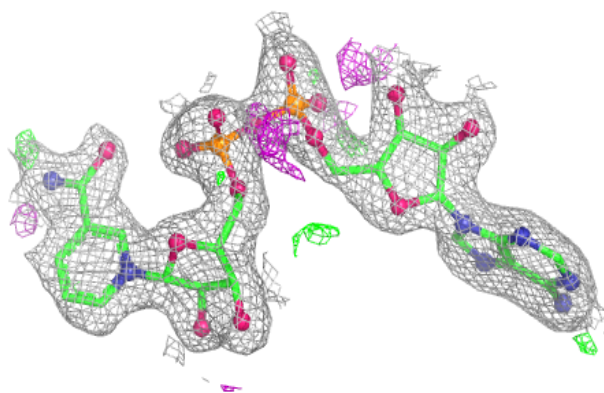
**Electron density around NAD C 301:**

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

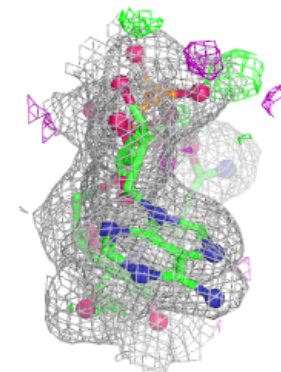
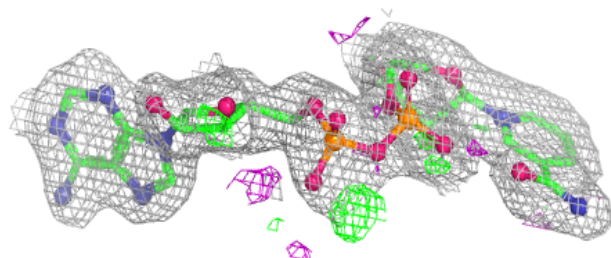
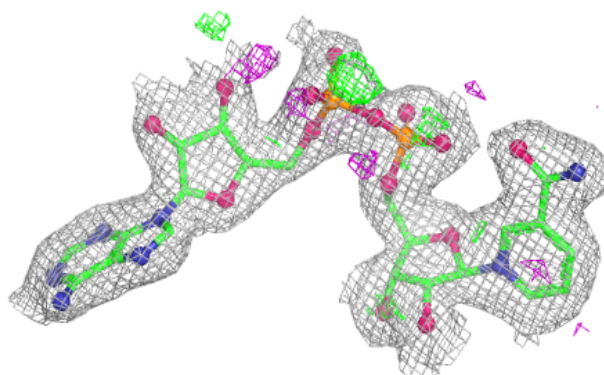


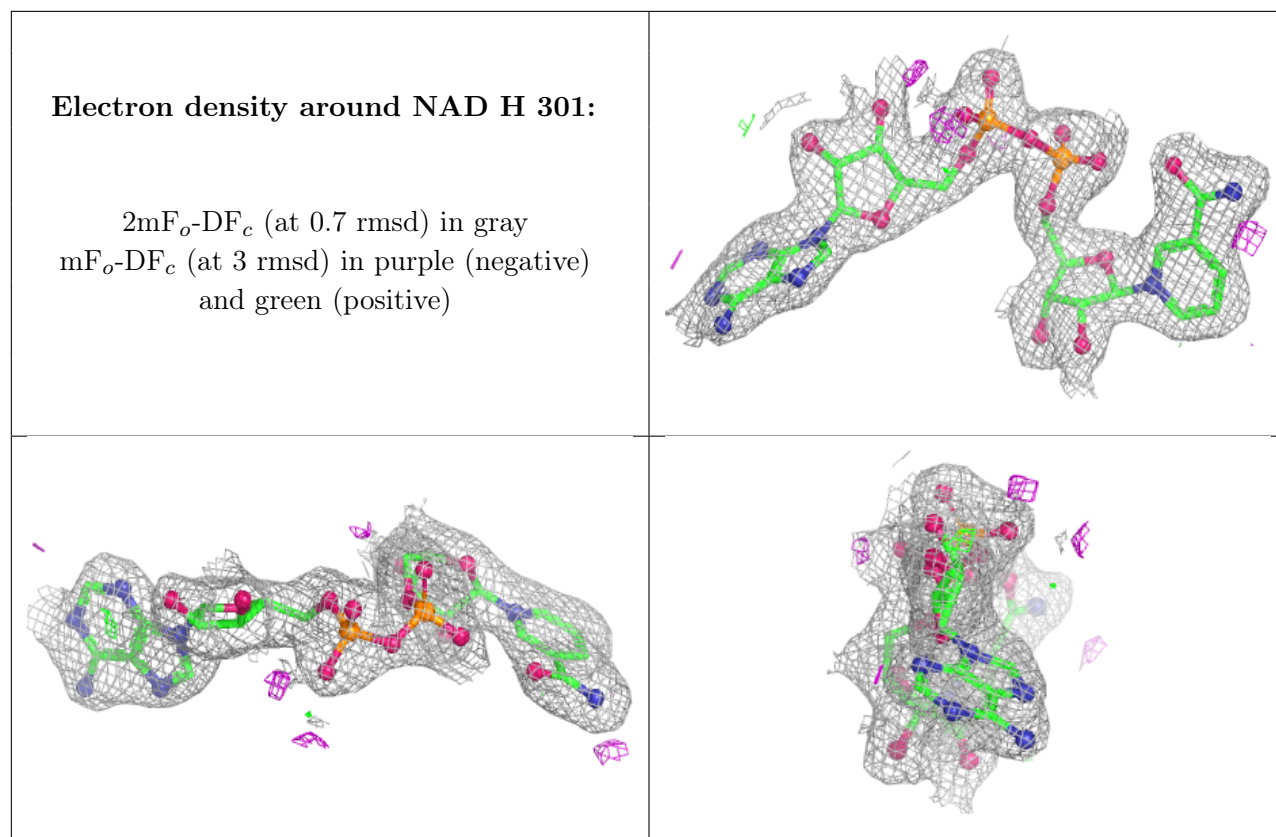
Electron density around NAD A 301:

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

**Electron density around NAD 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.