



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:21 AM UTC

PDB ID : 4FR8 / pdb_00004fr8
Title : Crystal structure of human aldehyde dehydrogenase-2 in complex with nitro-glycerin
Authors : Lang, B.S.; Gruber, K.
Deposited on : 2012-06-26
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 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

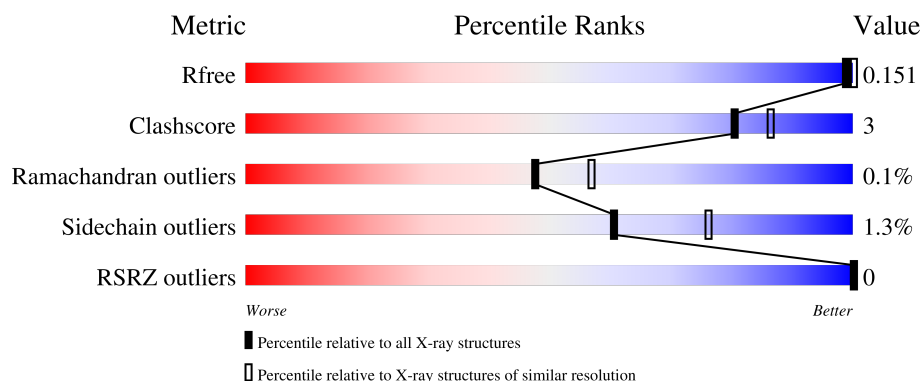
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

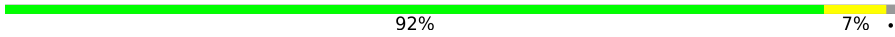
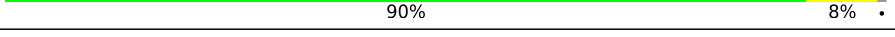
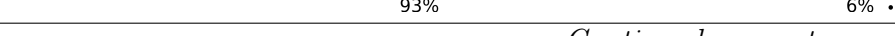
The reported resolution of this entry is 2.20 Å.

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	500	
1	B	500	
1	C	500	
1	D	500	
1	E	500	

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Mol	Chain	Length	Quality of chain
1	F	500	 90% 8% •
1	G	500	 94% 5% •
1	H	500	 91% 8% •

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 33739 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 Aldehyde dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	4	0
			3821	2428	652	724	17			
1	B	493	Total	C	N	O	S	0	2	0
			3810	2422	651	720	17			
1	C	496	Total	C	N	O	S	0	3	0
			3836	2437	656	726	17			
1	D	493	Total	C	N	O	S	0	6	0
			3841	2438	657	729	17			
1	E	493	Total	C	N	O	S	0	3	0
			3816	2425	652	721	18			
1	F	493	Total	C	N	O	S	0	2	0
			3808	2420	651	720	17			
1	G	494	Total	C	N	O	S	0	2	0
			3816	2425	653	722	16			
1	H	493	Total	C	N	O	S	0	3	0
			3818	2426	652	723	17			

There are 24 discrepancies between the modelled and reference sequences:

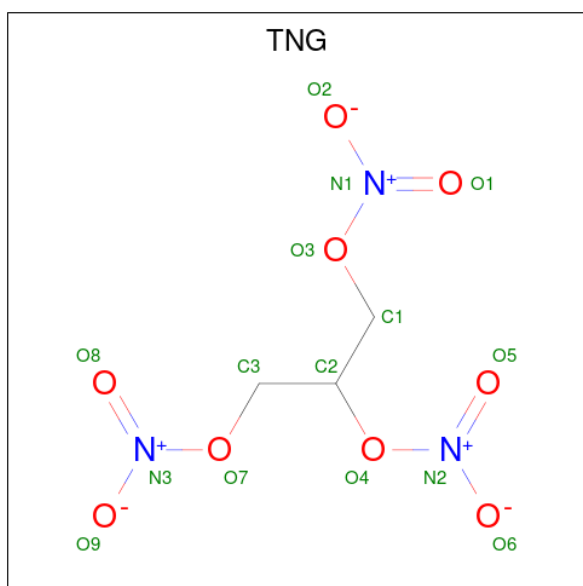
Chain	Residue	Modelled	Actual	Comment	Reference
A	268	GLN	GLU	engineered mutation	UNP P05091
A	301	SER	CYS	engineered mutation	UNP P05091
A	303	SER	CYS	engineered mutation	UNP P05091
B	268	GLN	GLU	engineered mutation	UNP P05091
B	301	SER	CYS	engineered mutation	UNP P05091
B	303	SER	CYS	engineered mutation	UNP P05091
C	268	GLN	GLU	engineered mutation	UNP P05091
C	301	SER	CYS	engineered mutation	UNP P05091
C	303	SER	CYS	engineered mutation	UNP P05091
D	268	GLN	GLU	engineered mutation	UNP P05091
D	301	SER	CYS	engineered mutation	UNP P05091
D	303	SER	CYS	engineered mutation	UNP P05091
E	268	GLN	GLU	engineered mutation	UNP P05091

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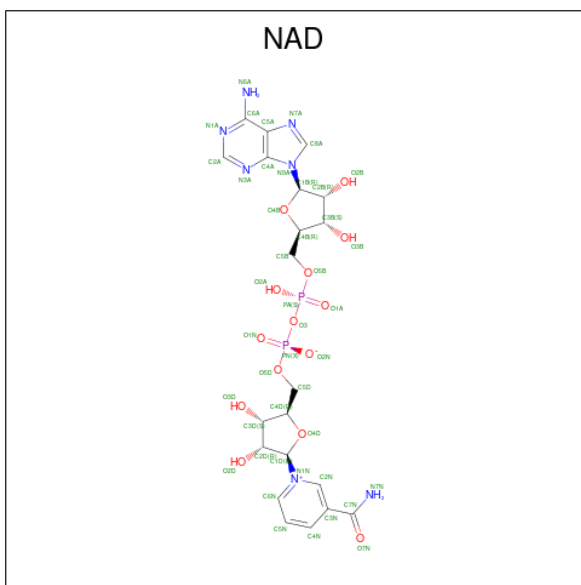
Chain	Residue	Modelled	Actual	Comment	Reference
E	301	SER	CYS	engineered mutation	UNP P05091
E	303	SER	CYS	engineered mutation	UNP P05091
F	268	GLN	GLU	engineered mutation	UNP P05091
F	301	SER	CYS	engineered mutation	UNP P05091
F	303	SER	CYS	engineered mutation	UNP P05091
G	268	GLN	GLU	engineered mutation	UNP P05091
G	301	SER	CYS	engineered mutation	UNP P05091
G	303	SER	CYS	engineered mutation	UNP P05091
H	268	GLN	GLU	engineered mutation	UNP P05091
H	301	SER	CYS	engineered mutation	UNP P05091
H	303	SER	CYS	engineered mutation	UNP P05091

- Molecule 2 is propane-1,2,3-triyl trinitrate (CCD ID: TNG) (formula: $C_3H_5N_3O_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	3	3	9		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).

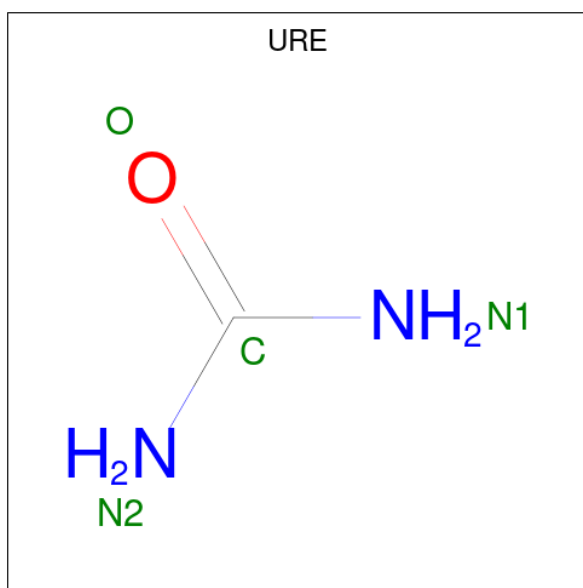


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 35	C 15	N 5	O 13	P 2	0	0
3	C	1	Total 35	C 15	N 5	O 13	P 2	0	0
3	D	1	Total 35	C 15	N 5	O 13	P 2	0	0
3	F	1	Total 35	C 15	N 5	O 13	P 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is UREA (CCD ID: URE) (formula: $\text{CH}_4\text{N}_2\text{O}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			4	1	2	1		
5	B	1	Total	C	N	O	0	0
			4	1	2	1		
5	C	1	Total	C	N	O	0	0
			4	1	2	1		
5	C	1	Total	C	N	O	0	0
			4	1	2	1		
5	D	1	Total	C	N	O	0	0
			4	1	2	1		
5	E	1	Total	C	N	O	0	0
			4	1	2	1		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

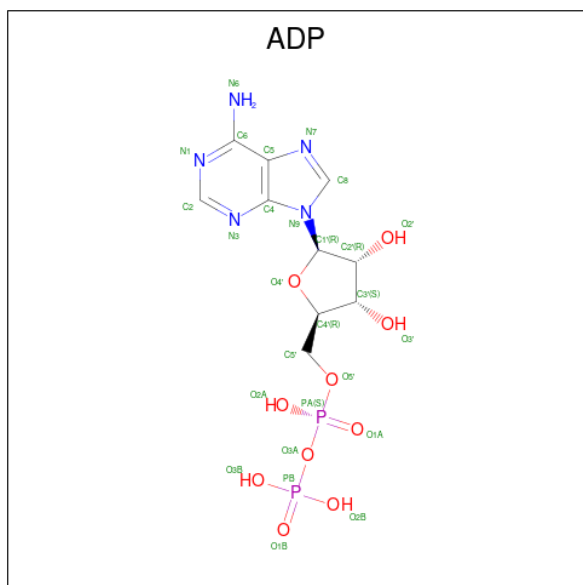
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	B	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		
6	E	1	Total	Na	0	0
			1	1		

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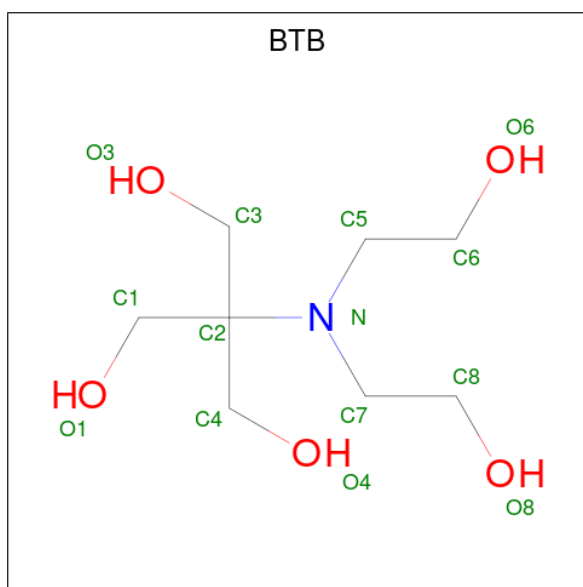
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Na	0	0
			1	1		
6	G	1	Total	Na	0	0
			1	1		
6	H	1	Total	Na	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

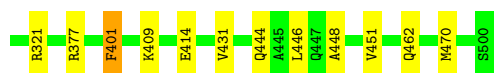
- Molecule 8 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	1	Total	C	N	O	0	0
			14	8	1	5		

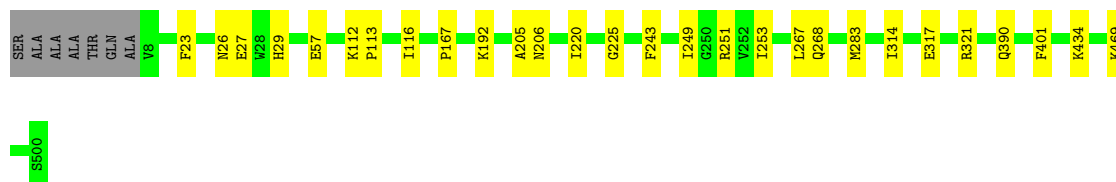
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	344	Total	O	0	0
			344	344		
9	B	380	Total	O	0	0
			380	380		
9	C	361	Total	O	0	0
			361	361		
9	D	398	Total	O	0	0
			398	398		
9	E	323	Total	O	0	0
			323	323		
9	F	325	Total	O	0	0
			325	325		
9	G	338	Total	O	0	0
			338	338		
9	H	387	Total	O	0	0
			387	387		



- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain E: 93% 6% .



- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain F: 90% 8% .



- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain G: 94% 5% .



- Molecule 1: Aldehyde dehydrogenase, mitochondrial

Chain H: 91% 8% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.66Å 175.92Å 102.30Å 90.00° 95.01° 90.00°	Depositor
Resolution (Å)	37.07 – 2.20 37.07 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.07-2.20) 95.3 (37.07-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.132 , 0.167 0.130 , 0.151	Depositor DCC
R_{free} test set	9049 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 19.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.218 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33739	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: ADP, NA, URE, NAD, MG, TNG, BTB

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	0.34	0/3905	0.73	2/5298 (0.0%)
1	B	0.34	0/3894	0.73	1/5282 (0.0%)
1	C	0.34	0/3920	0.75	2/5319 (0.0%)
1	D	0.35	0/3925	0.71	1/5324 (0.0%)
1	E	0.33	0/3900	0.73	1/5290 (0.0%)
1	F	0.34	0/3892	0.72	1/5280 (0.0%)
1	G	0.34	0/3900	0.73	2/5291 (0.0%)
1	H	0.34	0/3902	0.72	2/5293 (0.0%)
All	All	0.34	0/31238	0.73	12/42377 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	199	LEU	N-CA-C	6.86	118.41	111.07
1	G	312	GLU	N-CA-C	6.30	118.18	111.31
1	G	199	LEU	N-CA-C	6.26	117.77	111.07
1	H	199	LEU	N-CA-C	6.12	117.62	111.07
1	C	199	LEU	N-CA-C	6.05	117.54	111.07
1	B	199	LEU	N-CA-C	5.81	117.28	111.07
1	C	166	ILE	N-CA-C	5.76	114.23	107.84
1	A	166	ILE	N-CA-C	5.63	114.08	107.84
1	E	469	LYS	CB-CA-C	-5.58	110.12	116.54
1	H	166	ILE	N-CA-C	5.15	113.56	107.84
1	A	469	LYS	CB-CA-C	-5.06	110.72	116.54
1	D	199	LEU	N-CA-C	5.05	116.47	111.07

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	3821	0	3763	29	0
1	B	3810	0	3757	17	0
1	C	3836	0	3781	27	0
1	D	3841	0	3776	24	0
1	E	3816	0	3760	12	0
1	F	3808	0	3753	25	0
1	G	3816	0	3761	13	0
1	H	3818	0	3760	19	0
2	A	15	0	5	3	0
3	A	35	0	19	2	0
3	C	35	0	19	2	0
3	D	35	0	19	3	0
3	F	35	0	19	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	4	0	4	0	0
5	B	4	0	4	0	0
5	C	8	0	8	0	0
5	D	4	0	4	0	0
5	E	4	0	4	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	B	27	0	12	0	0
7	E	27	0	12	2	0
7	G	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	27	0	12	2	0
8	G	14	0	19	1	0
9	A	344	0	0	5	0
9	B	380	0	0	6	0
9	C	361	0	0	4	0
9	D	398	0	0	2	0
9	E	323	0	0	0	0
9	F	325	0	0	4	0
9	G	338	0	0	1	0
9	H	387	0	0	2	0
All	All	33739	0	30283	159	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 3.

All (159) 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:A:459:PHE:CZ	2:A:601:TNG:H2	2.10	0.86
1:B:46:GLU:OE2	1:B:377:ARG:NH1	2.23	0.70
1:A:166:ILE:HD11	1:A:193:VAL:HG12	1.72	0.69
1:A:459:PHE:CE1	2:A:601:TNG:H2	2.29	0.67
7:E:1001:ADP:O1B	7:E:1001:ADP:O1A	2.12	0.65
1:B:498:LYS:NZ	1:C:80:ASP:OD1	2.31	0.64
1:D:203:TYR:O	1:D:206[B]:ASN:ND2	2.31	0.64
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.36	0.61
1:B:251:ARG:HH21	1:B:470:MET:HE1	1.66	0.60
1:H:205:ALA:HB2	1:H:220:ILE:HD12	1.85	0.58
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.39	0.57
1:C:90:ARG:NE	9:C:1262:HOH:O	2.24	0.57
1:F:86:ARG:HD2	9:F:1226:HOH:O	2.04	0.57
1:A:149:ASP:HA	1:A:498:LYS:HB2	1.86	0.57
1:F:205:ALA:HB2	1:F:220:ILE:HD12	1.87	0.56
1:A:347:GLU:HG2	1:A:351:LYS:HE3	1.87	0.56
1:H:202:LEU:HD21	1:H:222:PRO:HG3	1.89	0.55
1:A:459:PHE:CZ	2:A:601:TNG:C3	2.88	0.55
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.88	0.55
1:B:317:GLU:HG2	1:B:321:ARG:HD2	1.89	0.54
1:C:489:LYS:HD2	1:D:451:VAL:HG23	1.89	0.54
1:D:321:ARG:NH1	9:D:1462:HOH:O	2.40	0.54
7:H:1001:ADP:O1A	7:H:1001:ADP:O1B	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:PRO:HD2	1:G:108:LEU:HD22	1.91	0.53
3:D:1001:NAD:O1A	3:D:1001:NAD:O1N	2.27	0.53
1:A:302[B]:CYS:SG	1:A:427:LEU:HD21	2.48	0.53
1:C:90:ARG:NH1	9:C:1265:HOH:O	2.42	0.53
1:A:427:LEU:HB2	1:A:471:SER:HB3	1.92	0.52
1:C:317:GLU:OE2	1:C:321:ARG:NH1	2.37	0.52
3:A:1001:NAD:O1A	3:A:1001:NAD:O1N	2.27	0.51
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.46	0.51
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.92	0.51
1:B:155:ARG:HD2	9:B:1376:HOH:O	2.10	0.51
1:E:249:ILE:O	1:E:253:ILE:HG12	2.11	0.51
1:F:329:ARG:HE	1:F:341:GLN:HB2	1.74	0.51
1:C:15:PRO:HD2	1:C:108:LEU:HD22	1.93	0.51
1:F:22:ILE:HG12	1:F:222:PRO:HD2	1.91	0.51
1:E:317:GLU:OE2	1:E:321:ARG:NH1	2.44	0.51
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.46	0.50
1:H:15:PRO:HD2	1:H:108:LEU:HD22	1.93	0.50
1:C:149:ASP:HA	1:C:498:LYS:HB2	1.92	0.50
1:F:284:ASP:OD1	1:F:321:ARG:NH1	2.45	0.49
1:A:262:LEU:HD21	1:B:251:ARG:HA	1.94	0.49
1:E:434:LYS:HD3	9:H:1330:HOH:O	2.10	0.49
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.48	0.49
1:H:225:GLY:HA3	7:H:1001:ADP:C8	2.47	0.49
1:F:258:GLY:HA2	1:F:262:LEU:HD23	1.94	0.49
1:H:317:GLU:O	1:H:321:ARG:HG3	2.13	0.49
3:F:1001:NAD:O1A	3:F:1001:NAD:O1N	2.30	0.48
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.95	0.48
1:B:131:TYR:CE1	1:B:462:GLN:HG3	2.48	0.48
1:A:422:ASN:HB3	9:A:851:HOH:O	2.14	0.48
1:E:283:MET:HE1	1:E:314:ILE:HB	1.95	0.47
9:A:891:HOH:O	1:D:78:ARG:HG2	2.14	0.47
1:C:70:PHE:CZ	1:C:160:GLY:HA2	2.50	0.47
1:B:377:ARG:NH2	9:B:1460:HOH:O	2.47	0.47
1:F:247:THR:HA	1:F:269:LEU:HD13	1.97	0.47
1:G:56:LYS:HE3	9:G:1401:HOH:O	2.14	0.47
1:A:26:ASN:O	1:A:209:LYS:HE2	2.15	0.47
1:F:377:ARG:O	9:F:1419:HOH:O	2.20	0.47
1:E:251:ARG:HA	1:F:262:LEU:HD21	1.98	0.46
1:F:368:LEU:HD12	1:F:385:VAL:HG12	1.97	0.46
1:H:70:PHE:CZ	1:H:160:GLY:HA2	2.50	0.46
1:G:188:VAL:HG12	1:G:217:VAL:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.50	0.45
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.97	0.45
1:C:489:LYS:NZ	1:D:446:LEU:O	2.49	0.45
1:E:243:PHE:HB3	1:E:267:LEU:HD23	1.97	0.45
1:H:112:LYS:NZ	1:H:121:ASP:OD2	2.46	0.45
1:B:112:LYS:NZ	1:B:121:ASP:OD2	2.49	0.45
1:F:283:MET:HE1	1:F:314:ILE:HB	1.98	0.45
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.50	0.45
1:C:427:LEU:HB2	1:C:471:SER:HB3	1.97	0.45
1:H:283:MET:HE1	1:H:314:ILE:HB	1.99	0.45
1:G:131:TYR:CE1	1:G:462:GLN:HG3	2.52	0.45
1:C:155:ARG:CZ	1:D:444:GLN:HG3	2.46	0.45
1:F:112:LYS:HB2	9:F:1178:HOH:O	2.16	0.45
1:B:409:LYS:HG2	9:B:1329:HOH:O	2.16	0.45
1:G:192:LYS:NZ	7:G:1001:ADP:O2'	2.39	0.45
1:A:469:LYS:HA	9:B:1314:HOH:O	2.17	0.44
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.51	0.44
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.52	0.44
1:A:63:VAL:HG11	1:A:235:HIS:CE1	2.52	0.44
1:A:225:GLY:HA3	3:A:1001:NAD:C8A	2.46	0.44
1:C:413:ILE:O	1:C:417:VAL:HG23	2.18	0.44
1:E:225:GLY:HA3	7:E:1001:ADP:C8	2.52	0.44
1:H:21:GLN:HB3	1:H:29:HIS:O	2.17	0.44
1:B:366:LYS:HE3	1:B:366:LYS:HB2	1.67	0.44
1:B:64:LYS:NZ	9:B:1428:HOH:O	2.49	0.44
1:D:166:ILE:HD11	1:D:193:VAL:HG12	1.98	0.44
1:F:321:ARG:HD3	9:F:1408:HOH:O	2.17	0.44
1:F:135:TRP:CE2	1:H:138:LYS:HD3	2.53	0.43
1:A:93:ASP:OD2	9:A:1031:HOH:O	2.21	0.43
1:E:205:ALA:HB2	1:E:220:ILE:HD12	1.99	0.43
1:H:22:ILE:HG12	1:H:222:PRO:HD2	2.00	0.43
1:H:120:VAL:HA	9:H:1320:HOH:O	2.18	0.43
1:F:413:ILE:O	1:F:417:VAL:HG23	2.17	0.43
1:A:498:LYS:HB3	1:A:498:LYS:HE2	1.82	0.43
1:B:230:ALA:HA	9:B:1272:HOH:O	2.19	0.43
1:C:251:ARG:NH2	1:C:470:MET:HE1	2.34	0.43
1:F:161:VAL:HA	1:F:188:VAL:HG23	2.01	0.43
1:D:131:TYR:CE1	1:D:462:GLN:HG3	2.54	0.43
1:B:306:SER:O	1:B:406:GLN:HB2	2.19	0.43
1:G:352:LYS:HE3	1:G:352:LYS:HB2	1.80	0.43
8:G:1004:BTB:H41	8:G:1004:BTB:H72	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:GLN:NE2	9:C:1427:HOH:O	2.52	0.42
1:A:449:GLY:HA3	1:A:466:GLY:O	2.19	0.42
1:C:498:LYS:HE2	1:C:498:LYS:HB3	1.85	0.42
1:A:106:GLU:O	1:A:110:ASN:HB3	2.20	0.42
3:D:1001:NAD:H3B	9:D:1425:HOH:O	2.18	0.42
1:F:131:TYR:CE1	1:F:462:GLN:HG3	2.55	0.42
1:F:366:LYS:HD3	1:F:368:LEU:HD21	2.02	0.42
1:G:192:LYS:HB2	1:G:232:ILE:HD12	1.99	0.42
1:H:366:LYS:HD2	1:H:388:ASP:HB2	2.01	0.42
1:C:131:TYR:CE1	1:C:462:GLN:HG3	2.53	0.42
1:D:249:ILE:O	1:D:253:ILE:HG12	2.20	0.42
1:F:111:GLY:O	1:F:343:PRO:HD2	2.20	0.42
1:H:161:VAL:HA	1:H:188:VAL:HG23	2.01	0.42
1:A:90:ARG:NE	9:A:930:HOH:O	2.33	0.42
1:D:247:THR:HA	1:D:269:LEU:HD13	2.00	0.42
1:D:315:TYR:CG	1:D:409:LYS:HD3	2.54	0.42
1:F:21:GLN:HB3	1:F:29:HIS:O	2.20	0.42
1:A:320:GLU:HG2	9:A:959:HOH:O	2.20	0.42
1:C:444:GLN:HG3	1:D:155:ARG:NH2	2.34	0.42
1:D:377:ARG:NH2	1:H:376:ASP:OD1	2.52	0.42
1:A:443:SER:HA	1:A:451:VAL:HG11	2.02	0.42
1:A:175:GLN:HG3	1:A:191:MET:SD	2.60	0.41
1:A:249:ILE:O	1:A:253:ILE:HG12	2.20	0.41
1:D:401:PHE:CD2	3:D:1001:NAD:H2D	2.55	0.41
1:C:464:PRO:HA	1:C:476:GLU:O	2.21	0.41
3:C:1001:NAD:H3B	9:C:1367:HOH:O	2.19	0.41
1:E:27:GLU:HB2	1:E:29:HIS:HE1	1.84	0.41
1:E:112:LYS:HB3	1:E:112:LYS:HE2	1.87	0.41
1:B:138:LYS:HD3	1:D:135:TRP:CE2	2.55	0.41
1:C:246:SER:HB3	3:C:1001:NAD:O4D	2.20	0.41
1:A:125:VAL:HG21	1:A:172:LEU:HB3	2.01	0.41
1:B:245:GLY:O	1:B:269:LEU:HA	2.21	0.41
1:B:283:MET:HE1	1:B:314:ILE:HB	2.01	0.41
1:C:21:GLN:HB3	1:C:29:HIS:O	2.21	0.41
1:C:489:LYS:HD3	1:D:448:ALA:O	2.20	0.41
1:D:251:ARG:HH21	1:D:470:MET:HE1	1.85	0.41
1:C:390:GLN:HG2	1:C:393:MET:HE3	2.01	0.41
1:G:251:ARG:NH2	1:G:470:MET:HE1	2.36	0.41
1:F:214:PRO:HA	1:F:215:PRO:HD3	1.98	0.41
1:G:70:PHE:CZ	1:G:160:GLY:HA2	2.56	0.41
1:F:11:PRO:HB3	1:F:114:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:131:TYR:CE1	1:H:462:GLN:HG3	2.56	0.41
1:A:135:TRP:CE2	1:C:138:LYS:HD3	2.55	0.41
1:H:121:ASP:O	1:H:125:VAL:HG23	2.21	0.41
1:D:70:PHE:CZ	1:D:160:GLY:HA2	2.56	0.41
1:C:254:GLN:NE2	1:D:254[A]:GLN:OE1	2.54	0.40
1:D:122:LEU:HD13	1:D:122:LEU:HA	1.96	0.40
1:E:113:PRO:HB2	1:E:116:ILE:HG12	2.02	0.40
1:F:138:LYS:HD3	1:H:135:TRP:CE2	2.57	0.40
1:G:336:ASP:OD1	1:G:338:LYS:HB2	2.21	0.40
1:C:251:ARG:HA	1:D:262:LEU:HD21	2.03	0.40
1:F:135:TRP:CG	1:F:482:LEU:HD11	2.56	0.40
1:A:161:VAL:HA	1:A:188:VAL:HG23	2.04	0.40
1:D:21:GLN:HB3	1:D:29:HIS: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	495/500 (99%)	477 (96%)	18 (4%)	0	100	100
1	B	493/500 (99%)	478 (97%)	14 (3%)	1 (0%)	43	51
1	C	497/500 (99%)	480 (97%)	17 (3%)	0	100	100
1	D	497/500 (99%)	481 (97%)	16 (3%)	0	100	100
1	E	494/500 (99%)	475 (96%)	18 (4%)	1 (0%)	43	51
1	F	493/500 (99%)	477 (97%)	16 (3%)	0	100	100
1	G	494/500 (99%)	480 (97%)	14 (3%)	0	100	100
1	H	494/500 (99%)	479 (97%)	15 (3%)	0	100	100
All	All	3957/4000 (99%)	3827 (97%)	128 (3%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	167	PRO
1	E	167	PRO

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	403/402 (100%)	398 (99%)	5 (1%)	63	78
1	B	401/402 (100%)	393 (98%)	8 (2%)	48	64
1	C	404/402 (100%)	400 (99%)	4 (1%)	68	81
1	D	405/402 (101%)	399 (98%)	6 (2%)	57	73
1	E	402/402 (100%)	396 (98%)	6 (2%)	57	73
1	F	401/402 (100%)	397 (99%)	4 (1%)	68	81
1	G	401/402 (100%)	399 (100%)	2 (0%)	81	90
1	H	402/402 (100%)	397 (99%)	5 (1%)	63	78
All	All	3219/3216 (100%)	3179 (99%)	40 (1%)	61	78

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LYS
1	A	268	GLN
1	A	359	THR
1	A	401	PHE
1	A	414	GLU
1	B	90	ARG
1	B	192	LYS
1	B	268	GLN
1	B	362	GLN
1	B	401	PHE
1	B	413	ILE
1	B	416	VAL

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Mol	Chain	Res	Type
1	B	431	VAL
1	C	192	LYS
1	C	268	GLN
1	C	362	GLN
1	C	416	VAL
1	D	192	LYS
1	D	248	GLU
1	D	268	GLN
1	D	401	PHE
1	D	414	GLU
1	D	431	VAL
1	E	57	GLU
1	E	192	LYS
1	E	206	ASN
1	E	268	GLN
1	E	390	GLN
1	E	401	PHE
1	F	268	GLN
1	F	366	LYS
1	F	401	PHE
1	F	414	GLU
1	G	268	GLN
1	G	417	VAL
1	H	27	GLU
1	H	192	LYS
1	H	268	GLN
1	H	352	LYS
1	H	414	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	B	21	GLN
1	B	50	GLN
1	B	254	GLN
1	B	289	GLN
1	B	344	GLN
1	C	254	GLN
1	C	444	GLN
1	D	26	ASN
1	D	71	GLN

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Mol	Chain	Res	Type
1	D	289	GLN
1	D	349	GLN
1	E	206	ASN
1	E	254	GLN
1	F	29	HIS
1	F	497	GLN
1	F	499	ASN
1	G	26	ASN
1	G	206	ASN
1	G	289	GLN
1	H	358	ASN
1	H	444	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 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	$\# Z > 2$
7	ADP	H	1001	4	28,29,29	1.47	5 (17%)	43,45,45	1.85	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ADP	E	1001	4	28,29,29	1.47	5 (17%)	43,45,45	1.84	11 (25%)
7	ADP	G	1001	4	28,29,29	1.41	5 (17%)	43,45,45	1.87	9 (20%)
3	NAD	C	1001	4	38,38,48	1.24	3 (7%)	53,58,73	1.79	12 (22%)
8	BTB	G	1004	-	13,13,13	0.37	0	7,16,16	0.64	0
5	URE	C	1005	-	3,3,3	0.40	0	3,3,3	0.24	0
5	URE	A	604	-	3,3,3	0.39	0	3,3,3	0.28	0
5	URE	B	1003	-	3,3,3	0.46	0	3,3,3	0.41	0
3	NAD	F	1001	4	38,38,48	1.31	5 (13%)	53,58,73	1.73	12 (22%)
5	URE	D	1003	-	3,3,3	0.46	0	3,3,3	0.52	0
5	URE	E	1004	-	3,3,3	0.37	0	3,3,3	0.23	0
3	NAD	A	1001	4	38,38,48	1.30	5 (13%)	53,58,73	1.75	11 (20%)
7	ADP	B	1001	4	28,29,29	1.43	5 (17%)	43,45,45	1.80	8 (18%)
2	TNG	A	601	-	7,14,14	0.96	0	4,17,17	0.71	0
5	URE	C	1003	-	3,3,3	0.45	0	3,3,3	0.37	0
3	NAD	D	1001	4	38,38,48	1.26	5 (13%)	53,58,73	1.74	13 (24%)

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
7	ADP	H	1001	4	-	5/16/32/32	0/3/3/3
7	ADP	E	1001	4	-	7/16/32/32	0/3/3/3
7	ADP	G	1001	4	-	2/16/32/32	0/3/3/3
3	NAD	C	1001	4	-	8/22/51/62	0/4/4/5
8	BTB	G	1004	-	-	4/21/21/21	-
3	NAD	F	1001	4	-	10/22/51/62	0/4/4/5
3	NAD	A	1001	4	-	8/22/51/62	0/4/4/5
7	ADP	B	1001	4	-	2/16/32/32	0/3/3/3
2	TNG	A	601	-	-	5/8/14/14	-
3	NAD	D	1001	4	-	8/22/51/62	0/4/4/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1001	ADP	C5-C4	4.84	1.47	1.39
7	E	1001	ADP	C5-C4	4.78	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1001	NAD	C5A-C4A	4.75	1.47	1.39
7	H	1001	ADP	C5-C4	4.63	1.47	1.39
7	G	1001	ADP	C5-C4	4.62	1.47	1.39
3	C	1001	NAD	C5A-C4A	4.59	1.47	1.39
3	D	1001	NAD	C5A-C4A	4.59	1.47	1.39
3	A	1001	NAD	C5A-C4A	4.47	1.47	1.39
7	H	1001	ADP	PA-O3A	3.20	1.63	1.59
7	E	1001	ADP	PA-O3A	3.07	1.62	1.59
7	G	1001	ADP	C5-C6	2.90	1.49	1.41
3	C	1001	NAD	C5A-C6A	2.85	1.48	1.41
3	F	1001	NAD	C5A-C6A	2.80	1.48	1.41
7	E	1001	ADP	C5-C6	2.76	1.48	1.41
7	H	1001	ADP	C5-C6	2.75	1.48	1.41
3	F	1001	NAD	PN-O3	2.74	1.62	1.59
3	D	1001	NAD	C5A-C6A	2.74	1.48	1.41
3	A	1001	NAD	C5A-C6A	2.69	1.48	1.41
7	B	1001	ADP	C5-C6	2.66	1.48	1.41
3	A	1001	NAD	PN-O3	2.55	1.62	1.59
3	A	1001	NAD	PA-O3	2.54	1.62	1.59
7	B	1001	ADP	PA-O3A	2.32	1.62	1.59
3	D	1001	NAD	C8A-N7A	2.26	1.36	1.31
7	B	1001	ADP	C5-N7	-2.24	1.35	1.39
7	G	1001	ADP	PA-O3A	2.24	1.61	1.59
3	F	1001	NAD	C5A-N7A	-2.21	1.35	1.39
7	H	1001	ADP	C8-N7	2.20	1.35	1.31
3	C	1001	NAD	PN-O3	2.17	1.61	1.59
7	H	1001	ADP	C5-N7	-2.16	1.35	1.39
3	A	1001	NAD	C8A-N7A	2.13	1.35	1.31
7	E	1001	ADP	C8-N7	2.12	1.35	1.31
7	G	1001	ADP	C8-N7	2.10	1.35	1.31
3	F	1001	NAD	C8A-N7A	2.07	1.35	1.31
7	G	1001	ADP	C5-N7	-2.06	1.35	1.39
3	D	1001	NAD	PN-O3	2.05	1.61	1.59
3	D	1001	NAD	C5A-N7A	-2.04	1.35	1.39
7	B	1001	ADP	C8-N7	2.03	1.35	1.31
7	E	1001	ADP	C5-N7	-2.02	1.35	1.39

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1001	ADP	C5-C4-N3	-6.11	118.30	126.72
3	C	1001	NAD	C5A-C4A-N3A	-5.80	118.73	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	1001	ADP	C5-C4-N3	-5.75	118.80	126.72
7	E	1001	ADP	C5-C4-N3	-5.65	118.94	126.72
3	F	1001	NAD	C5A-C4A-N3A	-5.64	118.95	126.72
3	A	1001	NAD	C5A-C4A-N3A	-5.52	119.11	126.72
7	B	1001	ADP	C5-C4-N3	-5.47	119.19	126.72
3	D	1001	NAD	C5A-C4A-N3A	-5.46	119.19	126.72
7	G	1001	ADP	N3-C4-N9	4.89	135.49	127.17
3	C	1001	NAD	N3A-C4A-N9A	4.79	135.31	127.17
7	H	1001	ADP	N3-C4-N9	4.62	135.02	127.17
7	E	1001	ADP	N3-C4-N9	4.54	134.88	127.17
3	F	1001	NAD	N3A-C4A-N9A	4.52	134.86	127.17
3	D	1001	NAD	N3A-C4A-N9A	4.49	134.81	127.17
3	A	1001	NAD	N3A-C4A-N9A	4.49	134.80	127.17
7	B	1001	ADP	N3-C4-N9	4.48	134.78	127.17
3	A	1001	NAD	C2A-N3A-C4A	3.84	121.22	111.83
7	G	1001	ADP	C4-C5-N7	-3.83	106.21	110.58
3	C	1001	NAD	C2A-N3A-C4A	3.80	121.12	111.83
7	H	1001	ADP	C2-N3-C4	3.75	120.99	111.83
3	F	1001	NAD	C2A-N3A-C4A	3.72	120.92	111.83
7	E	1001	ADP	C4-C5-N7	-3.70	106.35	110.58
3	A	1001	NAD	N3A-C2A-N1A	-3.70	122.99	128.58
3	D	1001	NAD	C2A-N3A-C4A	3.70	120.86	111.83
7	G	1001	ADP	C2-N3-C4	3.68	120.83	111.83
7	E	1001	ADP	C2-N3-C4	3.67	120.79	111.83
3	C	1001	NAD	C4A-C5A-N7A	-3.64	106.42	110.58
3	F	1001	NAD	C4A-C5A-N7A	-3.63	106.43	110.58
3	D	1001	NAD	N3A-C2A-N1A	-3.57	123.18	128.58
7	H	1001	ADP	C4-C5-N7	-3.55	106.53	110.58
3	A	1001	NAD	C4A-C5A-N7A	-3.52	106.56	110.58
7	B	1001	ADP	C2-N3-C4	3.48	120.33	111.83
3	F	1001	NAD	N3A-C2A-N1A	-3.45	123.36	128.58
7	E	1001	ADP	N3-C2-N1	-3.43	123.39	128.58
7	B	1001	ADP	C4-C5-N7	-3.42	106.67	110.58
7	H	1001	ADP	N3-C2-N1	-3.42	123.41	128.58
3	C	1001	NAD	N3A-C2A-N1A	-3.36	123.50	128.58
3	D	1001	NAD	C4A-C5A-N7A	-3.32	106.78	110.58
7	B	1001	ADP	N3-C2-N1	-3.12	123.85	128.58
3	A	1001	NAD	C4A-N9A-C8A	3.11	109.00	105.74
7	G	1001	ADP	C5-N7-C8	3.10	108.33	103.45
3	D	1001	NAD	C4A-N9A-C8A	3.00	108.89	105.74
3	C	1001	NAD	C5A-N7A-C8A	2.99	108.14	103.45
7	G	1001	ADP	N3-C2-N1	-2.98	124.07	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1001	NAD	C4A-N9A-C8A	2.97	108.86	105.74
7	E	1001	ADP	C5-N7-C8	2.92	108.04	103.45
3	F	1001	NAD	C5A-N7A-C8A	2.88	107.98	103.45
3	A	1001	NAD	C5A-N7A-C8A	2.84	107.91	103.45
7	H	1001	ADP	C5-N7-C8	2.80	107.85	103.45
7	B	1001	ADP	C5-N7-C8	2.79	107.83	103.45
7	H	1001	ADP	C4-N9-C8	2.71	108.58	105.74
7	E	1001	ADP	C4-N9-C8	2.70	108.57	105.74
7	G	1001	ADP	C4-N9-C8	2.69	108.57	105.74
3	D	1001	NAD	C5A-N7A-C8A	2.69	107.67	103.45
3	C	1001	NAD	C1D-C2D-C3D	2.59	105.78	101.63
3	A	1001	NAD	C6A-C5A-N7A	2.59	137.08	132.09
3	F	1001	NAD	C4A-N9A-C8A	2.59	108.46	105.74
3	F	1001	NAD	O2D-C2D-C3D	-2.58	106.35	111.43
7	B	1001	ADP	C4-N9-C8	2.55	108.42	105.74
3	A	1001	NAD	N9A-C8A-N7A	-2.46	110.45	113.94
3	A	1001	NAD	C1D-C2D-C3D	2.41	105.49	101.63
3	C	1001	NAD	C6A-C5A-N7A	2.41	136.73	132.09
3	C	1001	NAD	N9A-C8A-N7A	-2.34	110.62	113.94
3	D	1001	NAD	N9A-C8A-N7A	-2.31	110.66	113.94
7	E	1001	ADP	C6-C5-N7	2.30	136.52	132.09
3	F	1001	NAD	C6A-C5A-N7A	2.29	136.50	132.09
7	G	1001	ADP	N9-C8-N7	-2.28	110.70	113.94
3	A	1001	NAD	O2D-C2D-C3D	-2.24	107.01	111.43
7	H	1001	ADP	C6-C5-N7	2.23	136.39	132.09
3	D	1001	NAD	C1D-C2D-C3D	2.19	105.12	101.63
3	D	1001	NAD	O2A-PA-O1A	2.18	122.57	112.44
3	D	1001	NAD	C6A-C5A-N7A	2.17	136.28	132.09
7	E	1001	ADP	C2-N1-C6	2.17	122.29	118.73
7	E	1001	ADP	N9-C8-N7	-2.16	110.87	113.94
7	H	1001	ADP	N9-C8-N7	-2.16	110.87	113.94
3	D	1001	NAD	O2D-C2D-C3D	-2.14	107.22	111.43
3	D	1001	NAD	C2A-N1A-C6A	2.13	122.22	118.73
3	F	1001	NAD	C1D-C2D-C3D	2.12	105.02	101.63
3	F	1001	NAD	N9A-C8A-N7A	-2.11	110.94	113.94
3	F	1001	NAD	C2A-N1A-C6A	2.10	122.19	118.73
7	H	1001	ADP	O4'-C1'-N9	2.10	112.13	108.09
7	G	1001	ADP	C6-C5-N7	2.06	136.07	132.09
7	H	1001	ADP	C2-N1-C6	2.06	122.12	118.73
3	C	1001	NAD	O2D-C2D-C3D	-2.04	107.42	111.43
7	B	1001	ADP	N9-C8-N7	-2.03	111.05	113.94
3	C	1001	NAD	O4B-C1B-N9A	2.03	111.98	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	1001	ADP	O4'-C1'-N9	2.01	111.95	108.09

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	TNG	C2-C1-O3-N1
3	A	1001	NAD	C5D-O5D-PN-O3
3	A	1001	NAD	C5D-O5D-PN-O1N
3	C	1001	NAD	C5D-O5D-PN-O1N
3	D	1001	NAD	C5D-O5D-PN-O3
3	D	1001	NAD	C5D-O5D-PN-O1N
3	F	1001	NAD	C5D-O5D-PN-O3
3	F	1001	NAD	C5D-O5D-PN-O1N
8	G	1004	BTB	C1-C2-C3-O3
8	G	1004	BTB	C4-C2-C3-O3
8	G	1004	BTB	N-C2-C3-O3
3	F	1001	NAD	O4D-C4D-C5D-O5D
8	G	1004	BTB	N-C5-C6-O6
2	A	601	TNG	O4-C2-C3-O7
3	A	1001	NAD	O4D-C4D-C5D-O5D
3	F	1001	NAD	C3D-C4D-C5D-O5D
3	A	1001	NAD	C2B-C1B-N9A-C8A
3	C	1001	NAD	C2B-C1B-N9A-C8A
3	D	1001	NAD	C2B-C1B-N9A-C8A
3	F	1001	NAD	C2B-C1B-N9A-C8A
7	B	1001	ADP	C2'-C1'-N9-C8
7	G	1001	ADP	C2'-C1'-N9-C8
7	H	1001	ADP	C2'-C1'-N9-C8
3	A	1001	NAD	PN-O3-PA-O1A
3	D	1001	NAD	PN-O3-PA-O1A
3	F	1001	NAD	PN-O3-PA-O1A
2	A	601	TNG	C2-C3-O7-N3
7	E	1001	ADP	C2'-C1'-N9-C8
3	A	1001	NAD	C5D-O5D-PN-O2N
3	C	1001	NAD	C5D-O5D-PN-O3
3	C	1001	NAD	C5D-O5D-PN-O2N
3	D	1001	NAD	C5D-O5D-PN-O2N
3	F	1001	NAD	C5D-O5D-PN-O2N
7	H	1001	ADP	PA-O3A-PB-O1B
3	C	1001	NAD	PN-O3-PA-O1A
7	E	1001	ADP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	D	1001	NAD	O4D-C4D-C5D-O5D
7	E	1001	ADP	PB-O3A-PA-O1A
3	A	1001	NAD	O4B-C1B-N9A-C8A
3	F	1001	NAD	O4B-C1B-N9A-C8A
7	G	1001	ADP	O4'-C1'-N9-C8
7	H	1001	ADP	O4'-C1'-N9-C8
2	A	601	TNG	O3-C1-C2-O4
7	E	1001	ADP	PA-O3A-PB-O2B
7	E	1001	ADP	PA-O3A-PB-O3B
7	H	1001	ADP	PA-O3A-PB-O2B
7	H	1001	ADP	PA-O3A-PB-O3B
3	D	1001	NAD	O4B-C1B-N9A-C8A
7	B	1001	ADP	O4'-C1'-N9-C8
7	E	1001	ADP	O4'-C1'-N9-C8
3	A	1001	NAD	PN-O3-PA-O2A
3	D	1001	NAD	PA-O3-PN-O2N
3	F	1001	NAD	PN-O3-PA-O2A
7	E	1001	ADP	PB-O3A-PA-O2A
3	C	1001	NAD	O4B-C1B-N9A-C8A
2	A	601	TNG	C1-C2-C3-O7
3	C	1001	NAD	PN-O3-PA-O2A
3	C	1001	NAD	PA-O3-PN-O2N
3	F	1001	NAD	PA-O3-PN-O2N

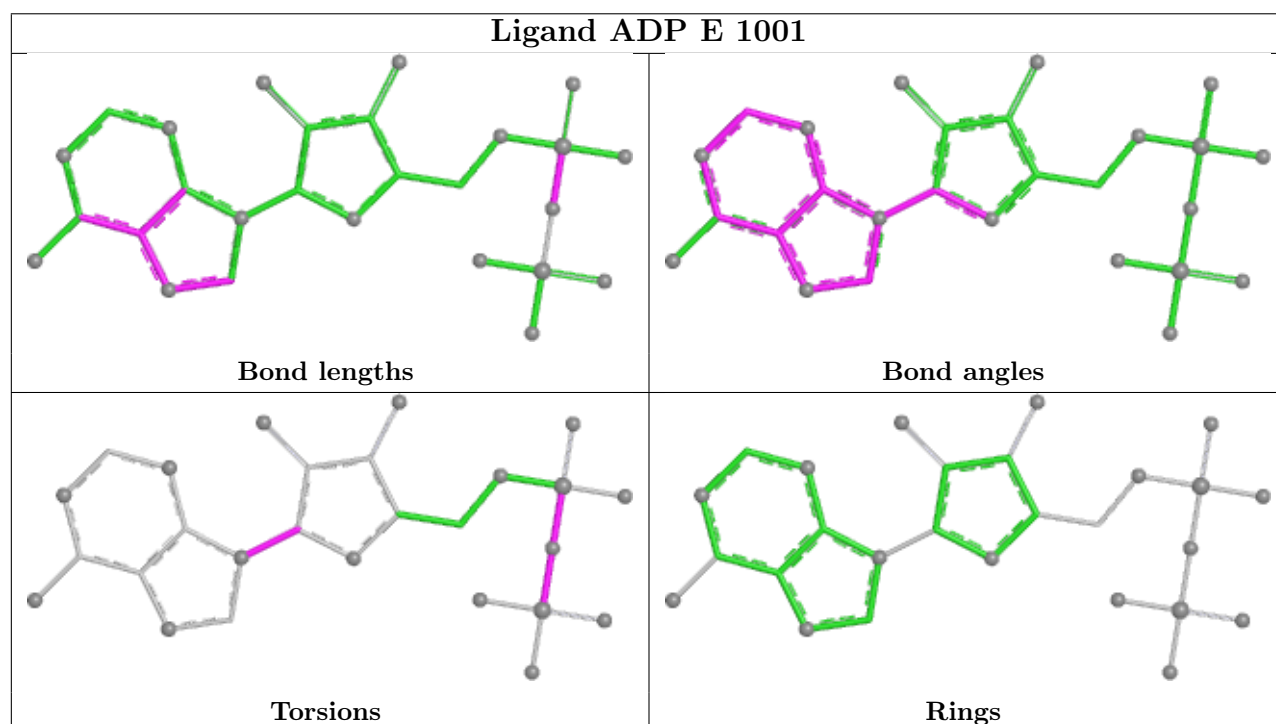
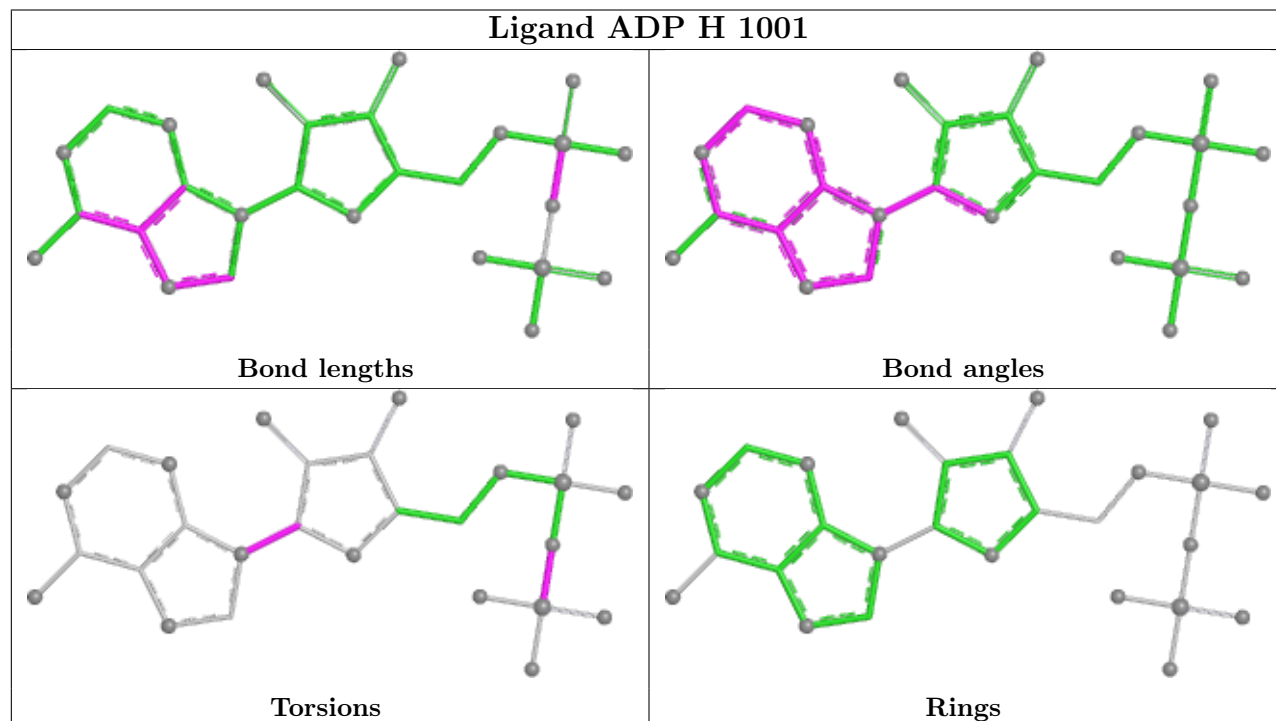
There are no ring outliers.

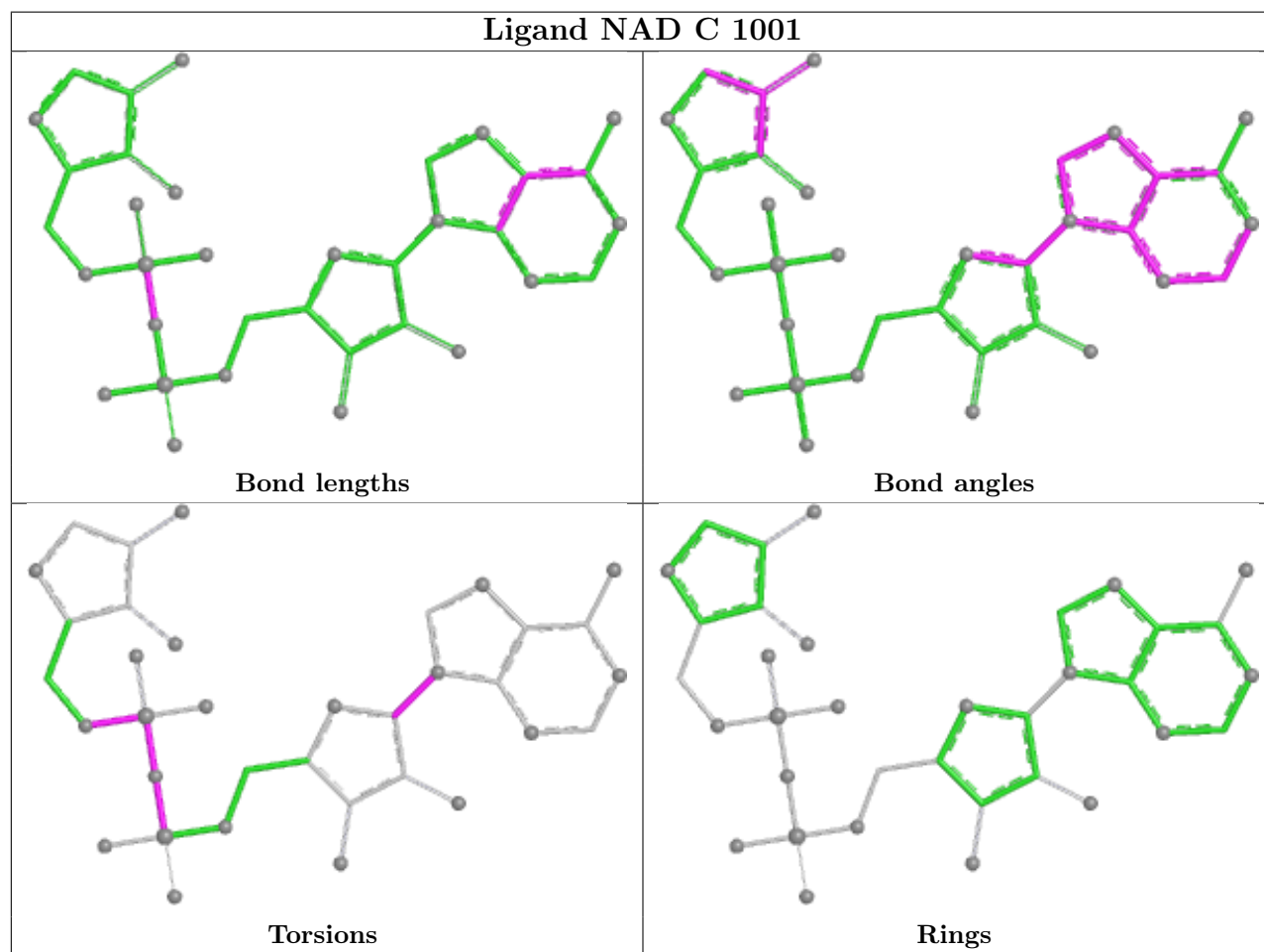
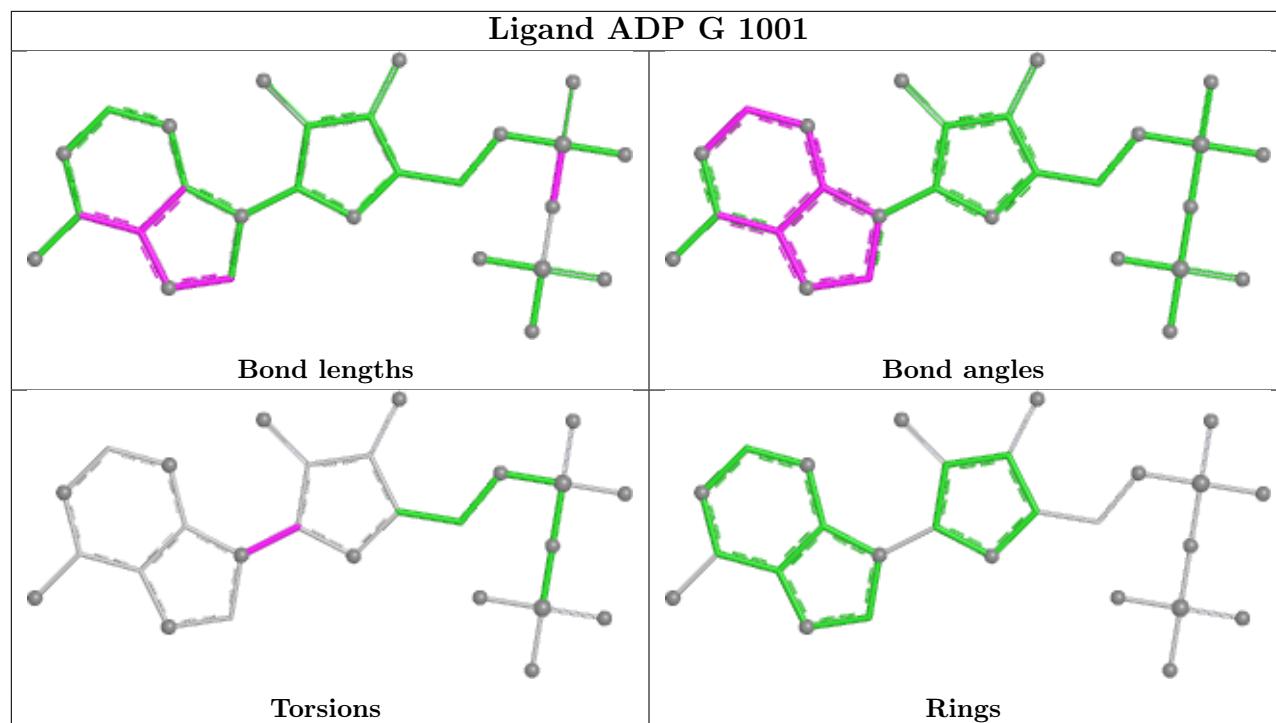
9 monomers are involved in 17 short contacts:

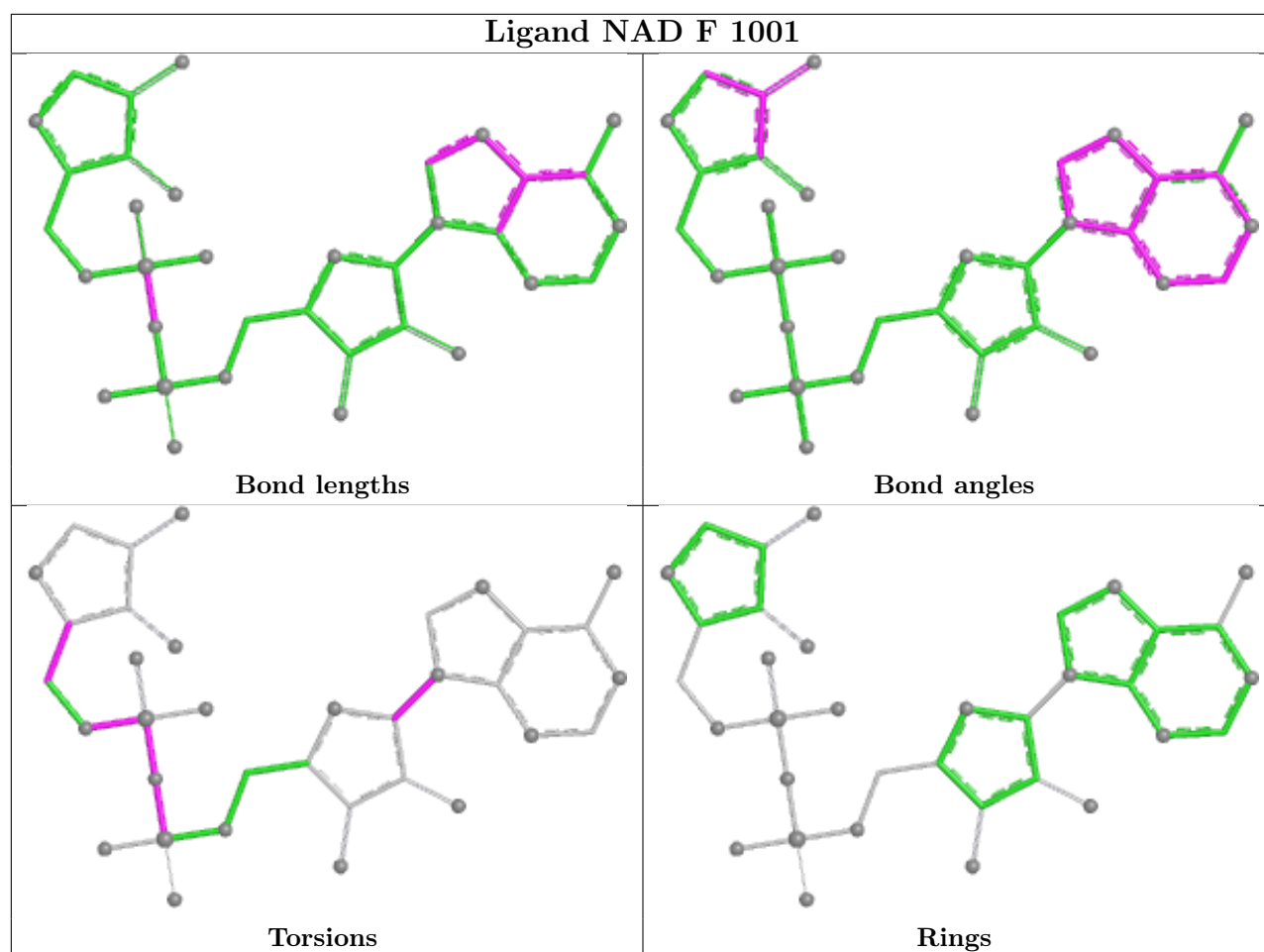
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	1001	ADP	2	0
7	E	1001	ADP	2	0
7	G	1001	ADP	1	0
3	C	1001	NAD	2	0
8	G	1004	BTB	1	0
3	F	1001	NAD	1	0
3	A	1001	NAD	2	0
2	A	601	TNG	3	0
3	D	1001	NAD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

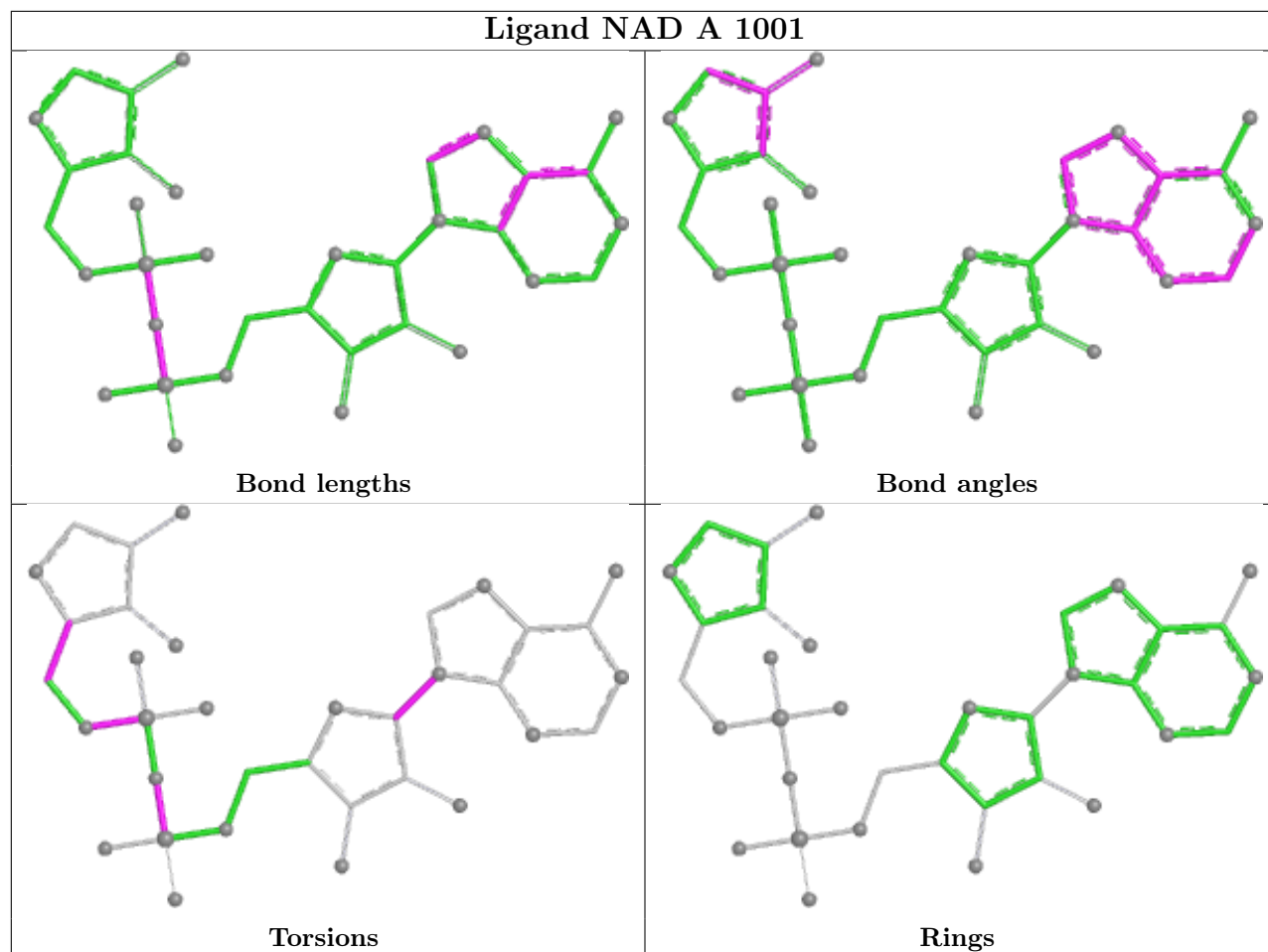
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



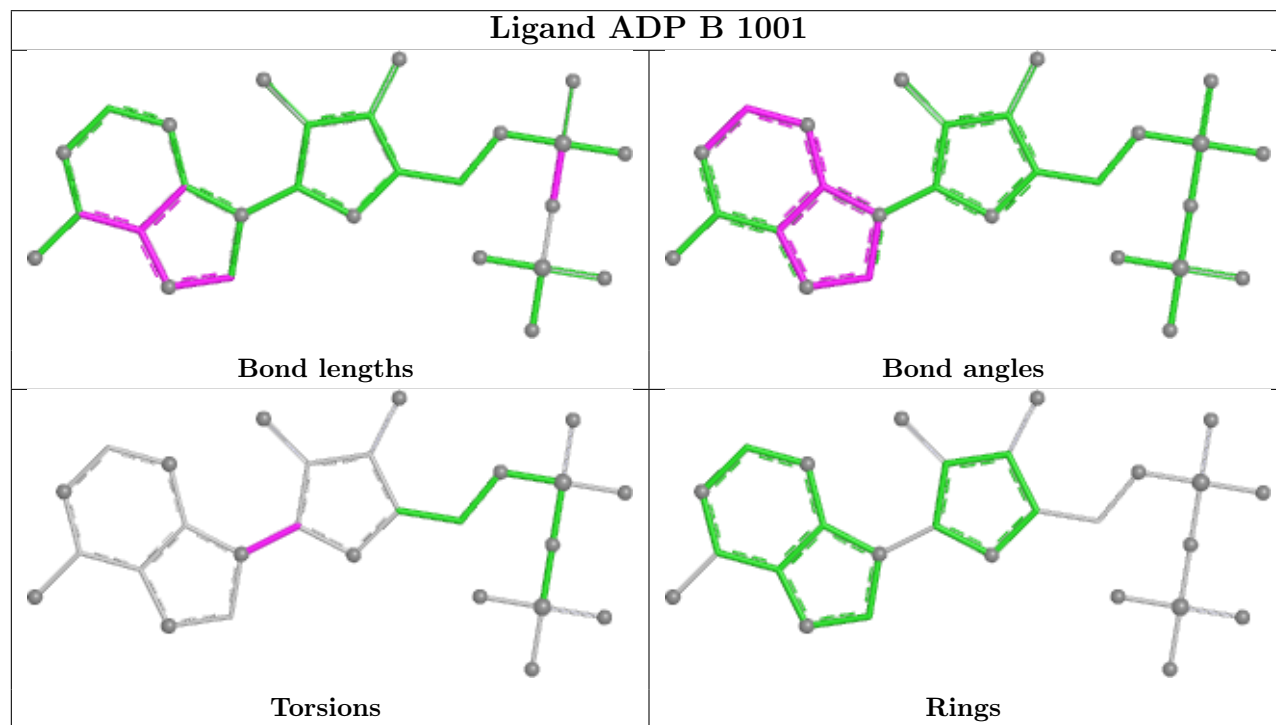


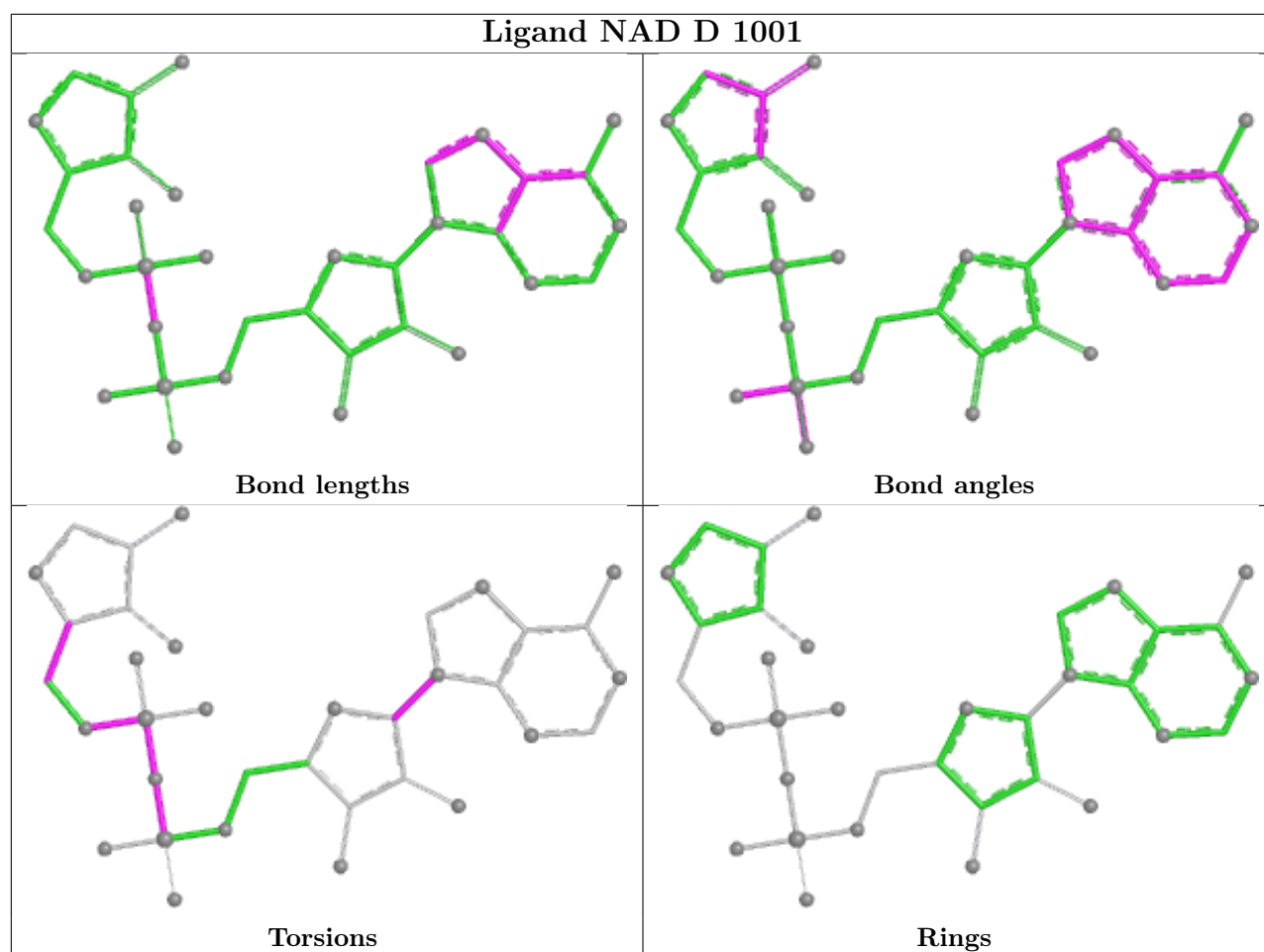


Ligand NAD A 1001



Ligand ADP B 1001





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	493/500 (98%)	-1.74	0 100 100	8, 21, 31, 45	4 (0%)
1	B	493/500 (98%)	-1.75	0 100 100	8, 19, 29, 48	2 (0%)
1	C	496/500 (99%)	-1.74	0 100 100	9, 19, 29, 42	3 (0%)
1	D	493/500 (98%)	-1.77	0 100 100	7, 17, 26, 40	6 (1%)
1	E	493/500 (98%)	-1.72	0 100 100	10, 21, 32, 55	3 (0%)
1	F	493/500 (98%)	-1.70	0 100 100	11, 22, 33, 52	2 (0%)
1	G	494/500 (98%)	-1.73	0 100 100	9, 20, 32, 46	2 (0%)
1	H	493/500 (98%)	-1.77	0 100 100	8, 18, 27, 41	3 (0%)
All	All	3948/4000 (98%)	-1.74	0 100 100	7, 20, 30, 55	25 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

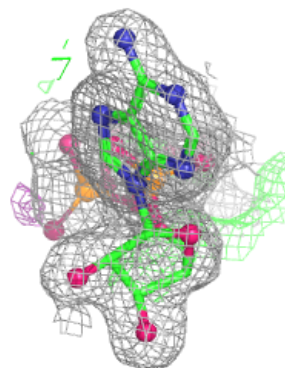
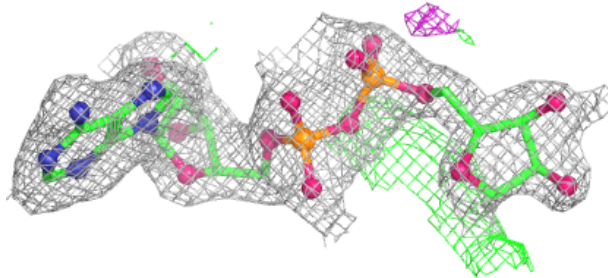
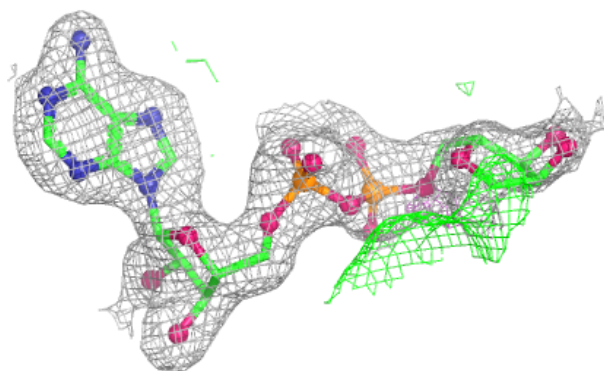
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
4	MG	B	1002	1/1	0.96	0.05	49,49,49,49	0
4	MG	F	1002	1/1	0.96	0.04	52,52,52,52	0
4	MG	H	1002	1/1	0.97	0.05	45,45,45,45	0
4	MG	E	1002	1/1	0.98	0.03	38,38,38,38	0
2	TNG	A	601	15/15	0.98	0.05	22,26,29,29	15
4	MG	G	1002	1/1	0.98	0.08	50,50,50,50	0
4	MG	C	1002	1/1	0.98	0.05	54,54,54,54	0
5	URE	E	1004	4/4	0.98	0.06	32,38,39,40	0
4	MG	D	1002	1/1	0.99	0.04	41,41,41,41	0
3	NAD	D	1001	35/44	0.99	0.02	15,23,37,41	0
3	NAD	F	1001	35/44	0.99	0.02	23,30,47,58	0
4	MG	A	603	1/1	0.99	0.04	44,44,44,44	0
3	NAD	A	1001	35/44	0.99	0.02	20,28,44,51	0
5	URE	A	604	4/4	0.99	0.03	19,24,26,29	0
5	URE	B	1003	4/4	0.99	0.03	17,20,24,27	0
5	URE	C	1003	4/4	0.99	0.02	16,21,23,26	0
5	URE	C	1005	4/4	0.99	0.03	33,40,41,41	0
3	NAD	C	1001	35/44	0.99	0.02	18,24,44,50	0
6	NA	A	605	1/1	0.99	0.02	27,27,27,27	0
6	NA	C	1004	1/1	0.99	0.02	25,25,25,25	0
6	NA	D	1004	1/1	0.99	0.02	25,25,25,25	0
6	NA	E	1003	1/1	0.99	0.02	28,28,28,28	0
6	NA	F	1003	1/1	0.99	0.03	27,27,27,27	0
7	ADP	E	1001	27/27	0.99	0.02	16,26,38,48	0
7	ADP	G	1001	27/27	0.99	0.02	20,25,43,54	0
6	NA	G	1003	1/1	1.00	0.01	27,27,27,27	0
6	NA	H	1003	1/1	1.00	0.01	15,15,15,15	0
7	ADP	B	1001	27/27	1.00	0.02	17,23,45,57	0
5	URE	D	1003	4/4	1.00	0.01	16,24,28,29	0
6	NA	B	1004	1/1	1.00	0.02	23,23,23,23	0
7	ADP	H	1001	27/27	1.00	0.02	18,22,44,49	0
8	BTB	G	1004	14/14	1.00	0.02	15,20,23,24	0

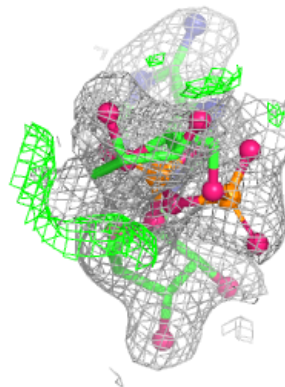
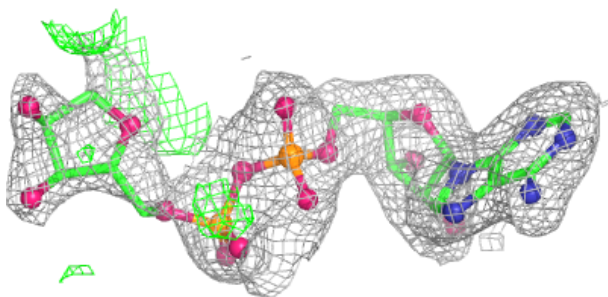
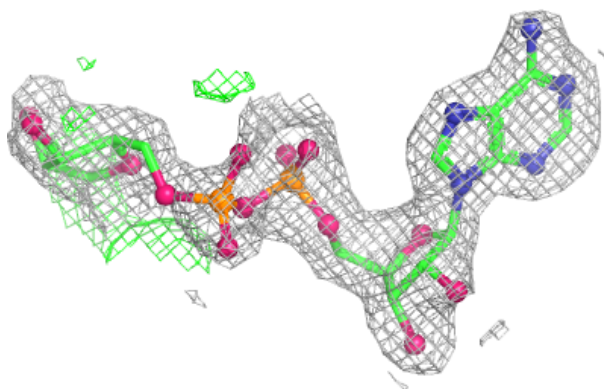
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 1001:

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

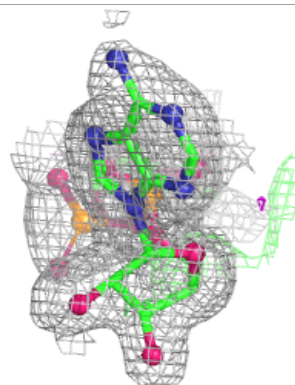
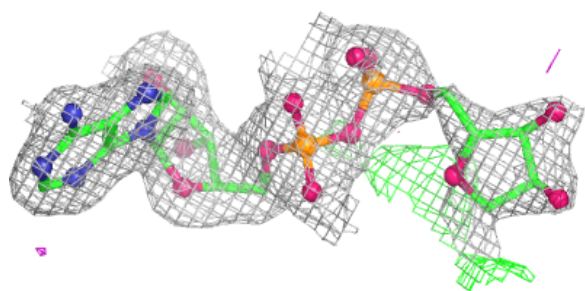
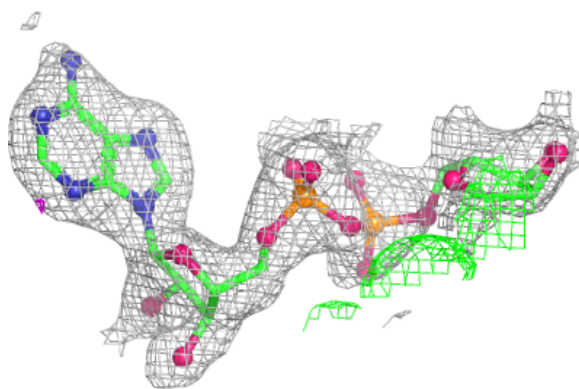
**Electron density around NAD F 1001:**

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

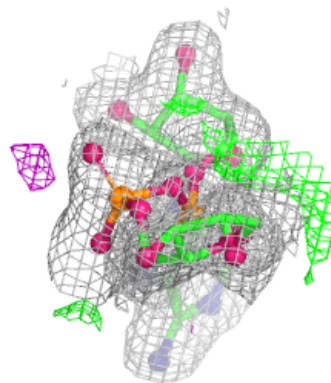
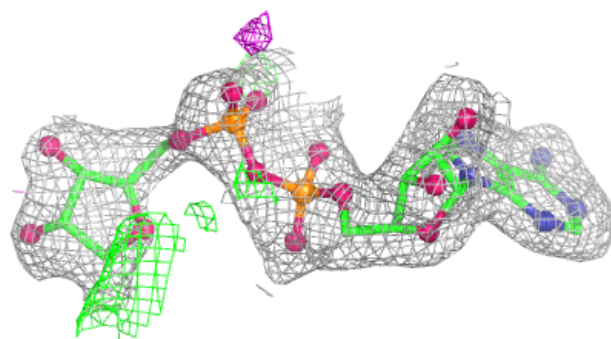
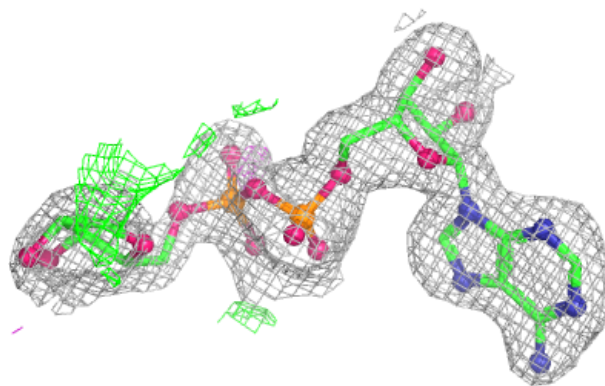


Electron density around NAD A 1001:

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

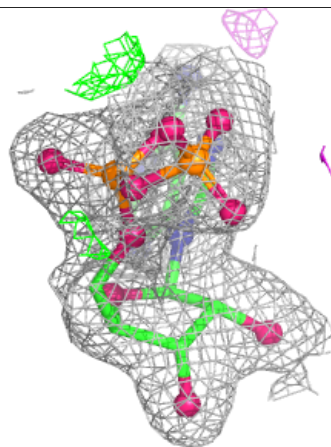
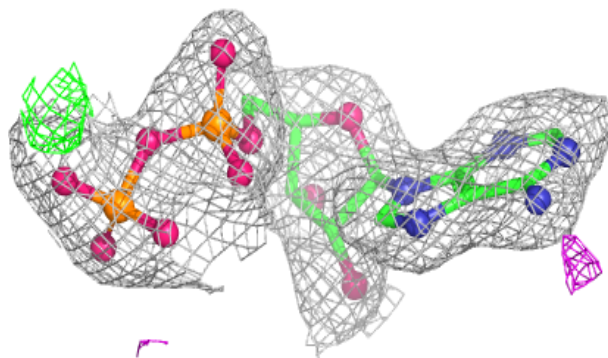
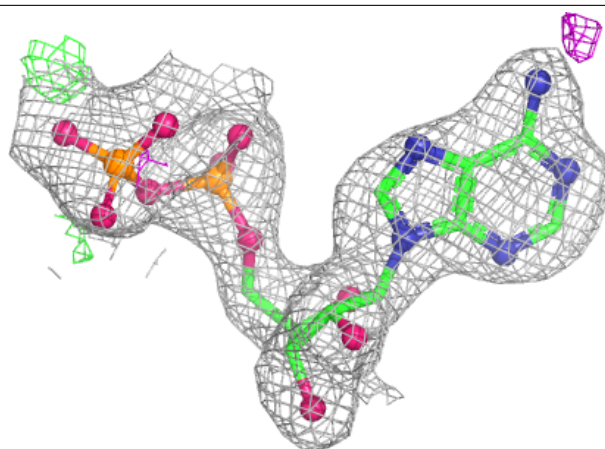
**Electron density around NAD C 1001:**

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

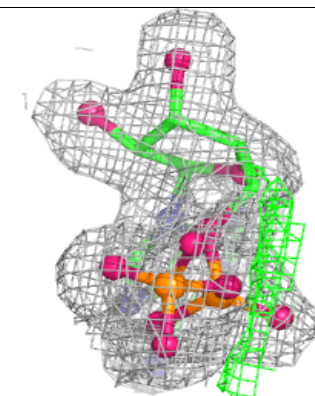
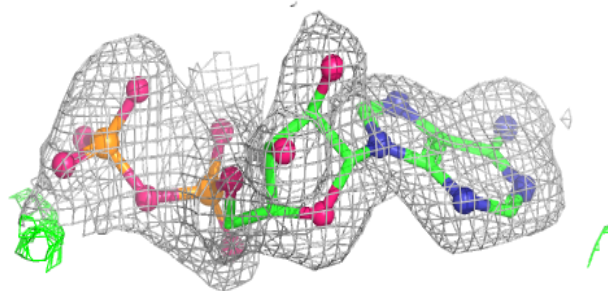
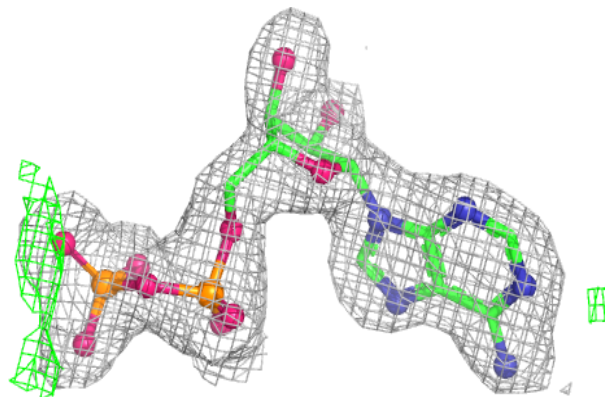


Electron density around ADP E 1001:

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

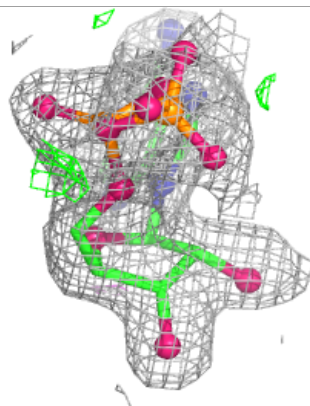
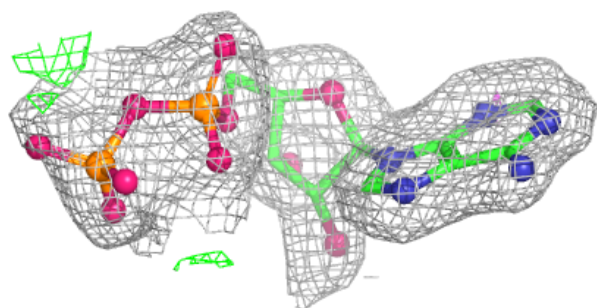
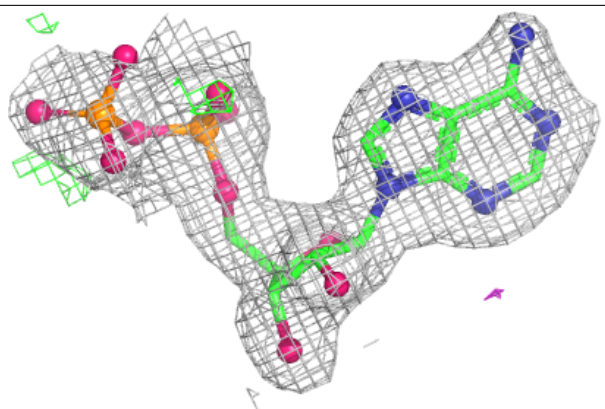
**Electron density around ADP G 1001:**

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

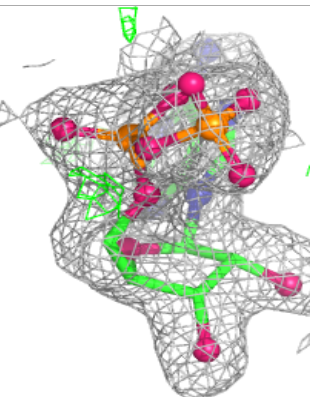
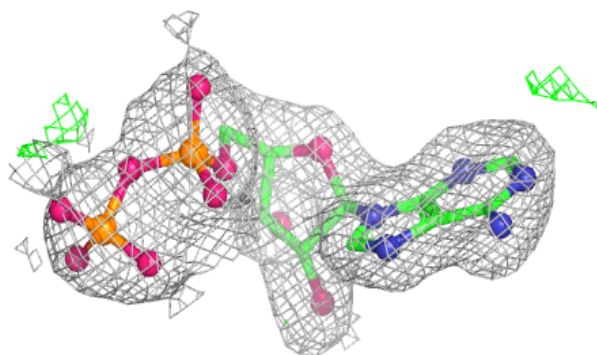
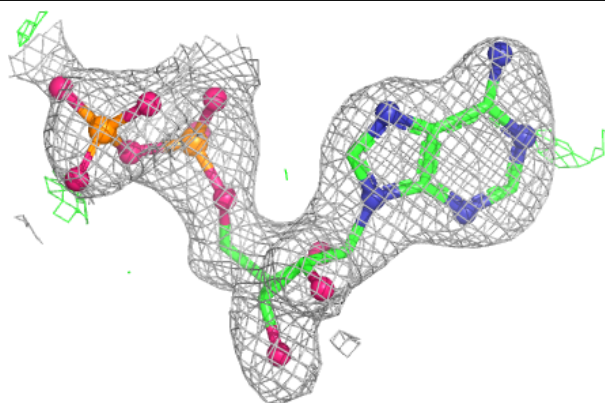


Electron density around ADP B 1001:

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

**Electron density around ADP H 1001:**

$2mF_o-DF_c$ (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.