



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:59 pm BST

PDB ID : 5UX5
Title : Structure of Proline Utilization A (PutA) from *Corynebacterium freiburgense*
Authors : Tanner, J.J.
Deposited on : 2017-02-22
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

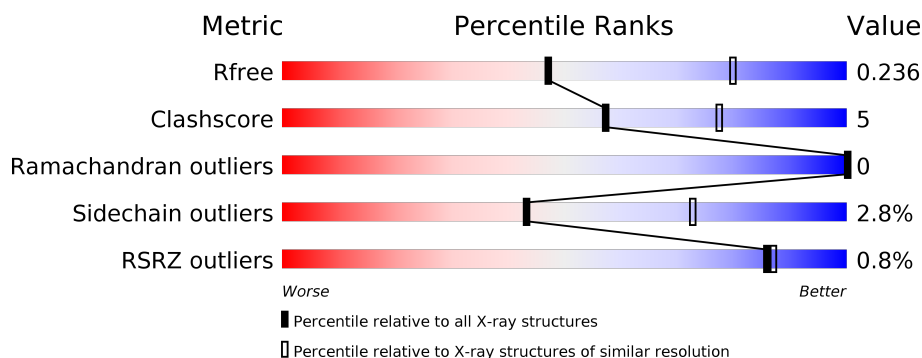
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1076	
1	B	1076	
1	C	1076	
1	D	1076	

2 Entry composition [i](#)

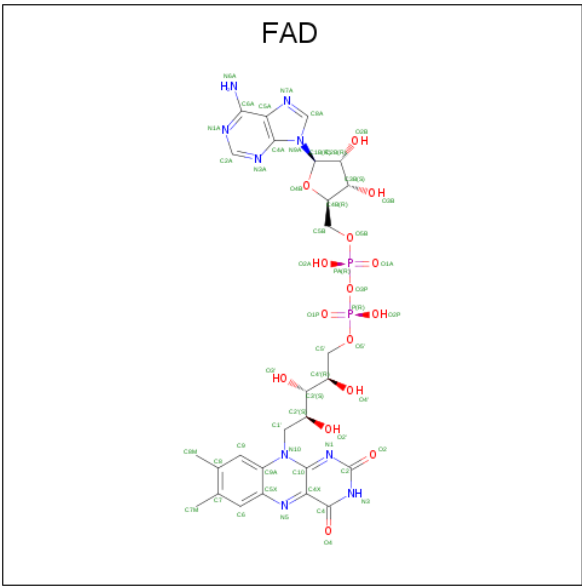
There are 4 unique types of molecules in this entry. The entry contains 29652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BIFUNCTIONAL PROTEIN Proline utilization A (PutA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	963	Total	C	N	O	S	0	0	0
			7388	4665	1302	1402	19			
1	B	962	Total	C	N	O	S	0	0	0
			7314	4621	1289	1384	20			
1	C	962	Total	C	N	O	S	0	0	0
			7277	4602	1285	1371	19			
1	D	962	Total	C	N	O	S	0	0	0
			7301	4614	1284	1384	19			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



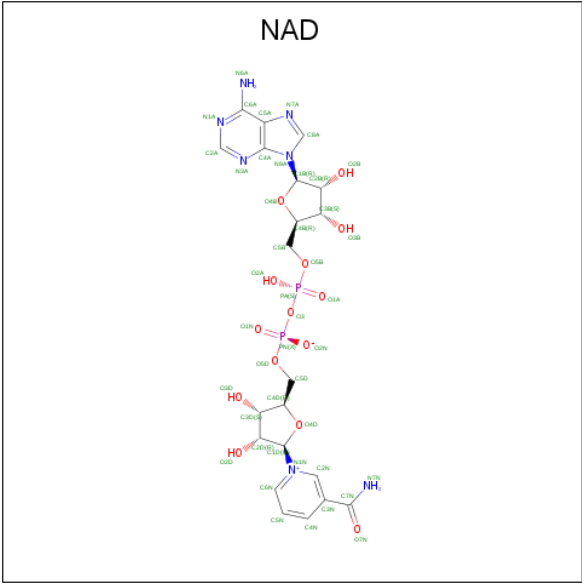
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).

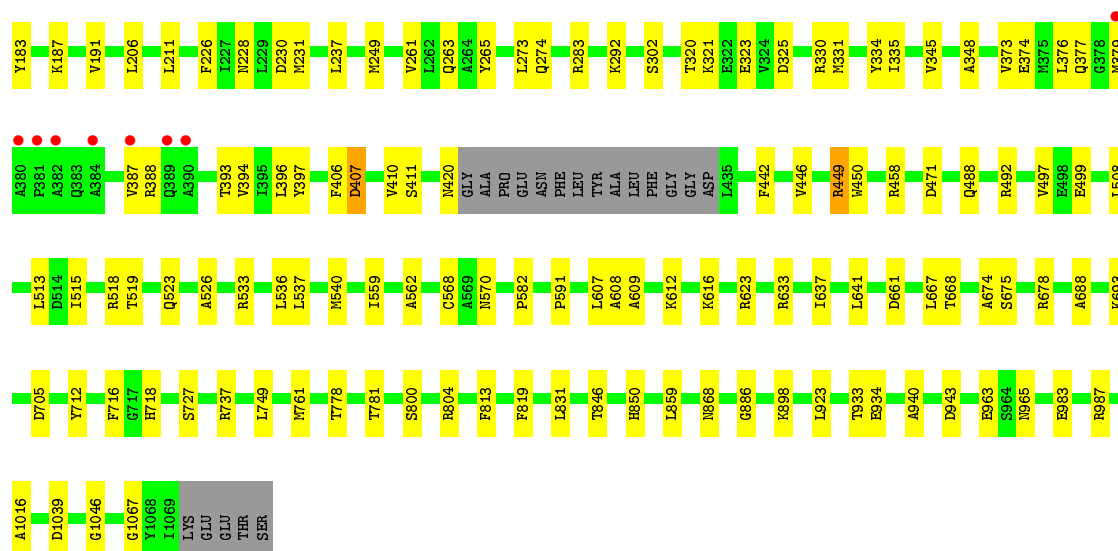


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	B	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	C	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
3	D	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

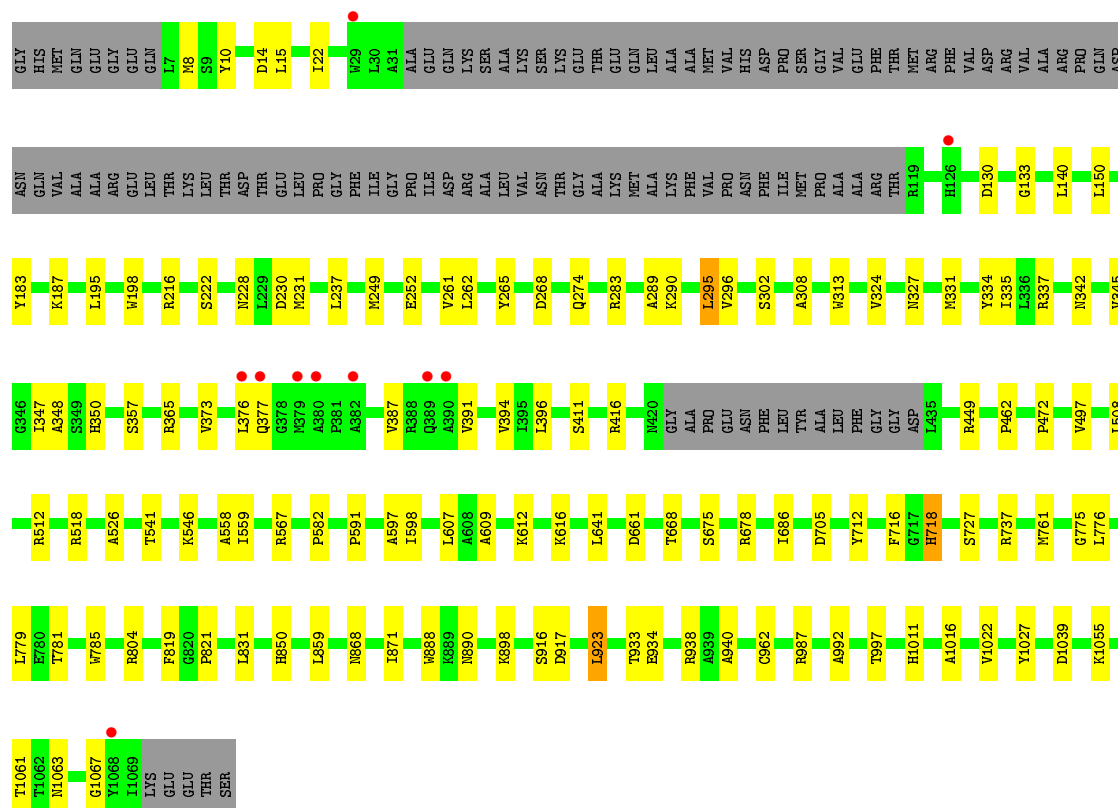
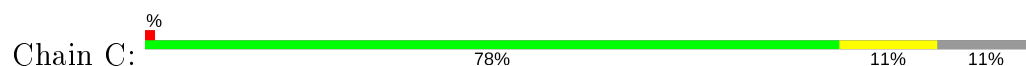
- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



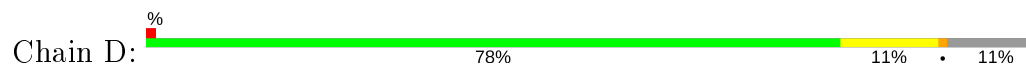
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

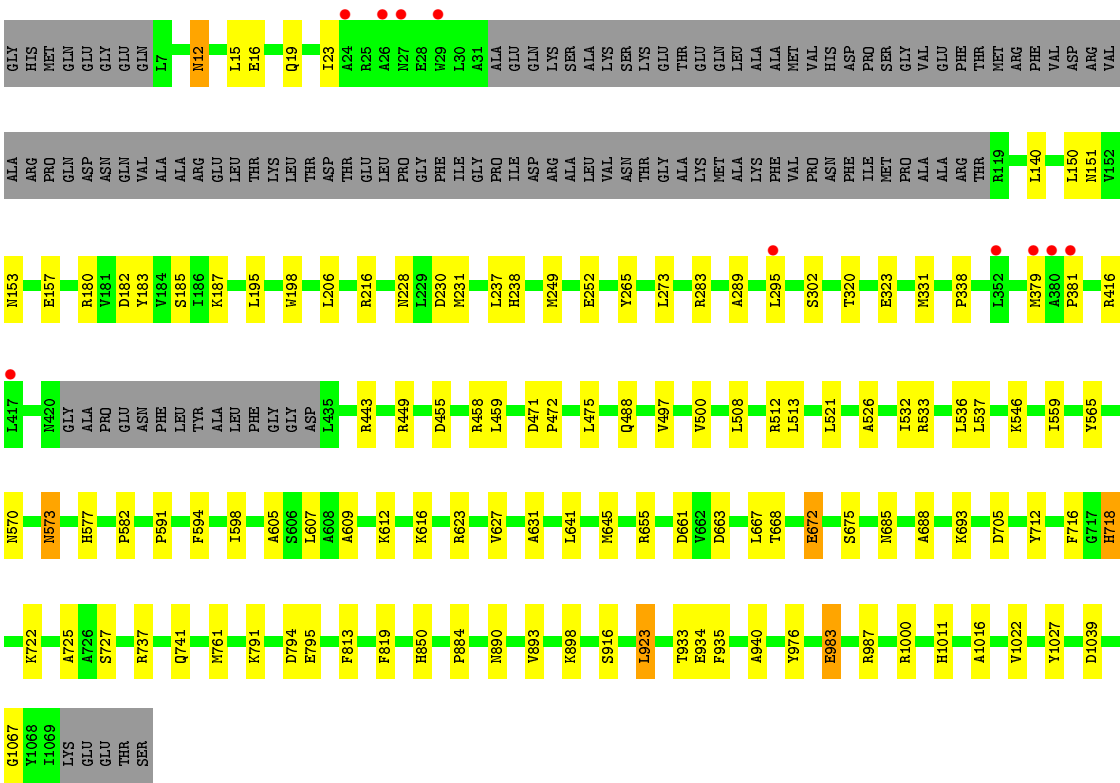


• Molecule 1: BIFUNCTIONAL PROTEIN Proline utilization A (PutA)



• Molecule 1: BIFUNCTIONAL PROTEIN Proline utilization A (PutA)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.96Å 116.36Å 140.73Å 71.48° 89.68° 83.42°	Depositor
Resolution (Å)	63.29 – 2.70 63.29 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (63.29-2.70) 98.4 (63.29-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.183 , 0.236 0.184 , 0.236	Depositor DCC
R_{free} test set	6785 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.8	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	0.94	EDS
Total number of atoms	29652	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAD, FAD

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	0.48	1/7541 (0.0%)	0.65	0/10265
1	B	0.43	1/7466 (0.0%)	0.60	0/10173
1	C	0.42	0/7429	0.59	0/10129
1	D	0.44	0/7453	0.61	0/10160
All	All	0.44	2/29889 (0.0%)	0.61	0/40727

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	568	CYS	CB-SG	-6.26	1.71	1.82
1	A	568	CYS	CB-SG	-5.16	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7388	0	7194	72	0
1	B	7314	0	7078	71	0
1	C	7277	0	7024	64	0
1	D	7301	0	7049	76	0
2	A	53	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	2	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
3	A	35	0	19	1	0
3	B	35	0	19	1	0
3	C	35	0	19	2	0
3	D	35	0	19	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
All	All	29652	0	28545	283	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 5.

All (283) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:ASP:OD2	1:B:737:ARG:NH2	2.11	0.83
1:C:302:SER:HB3	1:C:1067:GLY:HA3	1.67	0.77
1:C:10:TYR:O	1:C:337:ARG:NH2	2.15	0.76
1:A:705:ASP:OD2	1:A:737:ARG:NH2	2.18	0.76
1:D:513:LEU:HD11	1:D:641:LEU:HD11	1.67	0.76
1:B:302:SER:HB3	1:B:1067:GLY:HA3	1.68	0.76
1:C:187:LYS:HG2	1:C:230:ASP:HB2	1.70	0.72
1:B:187:LYS:HG2	1:B:230:ASP:HB2	1.73	0.70
1:A:302:SER:HB3	1:A:1067:GLY:HA3	1.74	0.69
1:B:492:ARG:NH2	1:B:499:GLU:OE1	2.25	0.69
1:D:302:SER:HB3	1:D:1067:GLY:HA3	1.76	0.67
1:A:187:LYS:HG2	1:A:230:ASP:HB2	1.76	0.66
1:A:532:ILE:HD11	1:A:631:ALA:HB2	1.77	0.66
3:C:2002:NAD:O2A	3:C:2002:NAD:H8A	1.95	0.66
1:B:846:THR:HG22	1:B:868:ASN:HB2	1.79	0.65
1:D:688:ALA:HB3	1:D:893:VAL:HB	1.77	0.65
1:D:497:VAL:HG13	1:D:655:ARG:HG2	1.79	0.64
1:A:10:TYR:O	1:A:337:ARG:NH2	2.29	0.64
1:B:191:VAL:HG21	1:B:211:LEU:HD21	1.78	0.64
1:C:705:ASP:OD2	1:C:737:ARG:NH2	2.31	0.63
1:B:616:LYS:NZ	3:B:2002:NAD:O2B	2.33	0.62
1:C:216:ARG:NE	1:C:252:GLU:OE1	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:GLU:CD	1:B:449:ARG:HH22	2.05	0.60
1:B:716:PHE:HB3	1:B:761:MET:HE2	1.83	0.60
1:C:779:LEU:HD11	1:C:785:TRP:CD1	2.36	0.59
1:D:19:GLN:O	1:D:23:ILE:HG13	2.03	0.59
1:C:916:SER:OG	1:C:938:ARG:NH1	2.34	0.59
1:A:688:ALA:HB3	1:A:893:VAL:HB	1.83	0.59
1:C:616:LYS:NZ	3:C:2002:NAD:O2B	2.35	0.58
1:B:488:GLN:HA	1:B:623:ARG:HD2	1.85	0.58
1:D:16:GLU:CD	1:D:449:ARG:HH22	2.07	0.58
1:B:536:LEU:HB3	1:B:540:MET:HE3	1.86	0.58
1:D:672:GLU:N	1:D:672:GLU:OE1	2.32	0.58
1:A:185:SER:HB3	1:A:228:ASN:HB3	1.86	0.57
1:D:228:ASN:ND2	1:D:230:ASP:OD1	2.38	0.57
1:D:705:ASP:OD2	1:D:737:ARG:NH2	2.38	0.57
1:A:716:PHE:HB3	1:A:761:MET:HE2	1.87	0.56
1:D:716:PHE:HB3	1:D:761:MET:HE2	1.86	0.56
1:B:536:LEU:HB3	1:B:540:MET:CE	2.36	0.56
1:B:508:LEU:HD11	1:B:661:ASP:HB3	1.88	0.56
1:A:933:THR:HG21	1:A:983:GLU:OE2	2.06	0.56
1:A:1022:VAL:HB	1:A:1027:TYR:CE2	2.39	0.56
1:D:923:LEU:HD11	1:D:940:ALA:HB1	1.88	0.56
1:C:591:PRO:HD3	1:C:668:THR:HB	1.88	0.55
1:A:249:MET:SD	1:A:283:ARG:HG3	2.45	0.55
1:B:591:PRO:HD3	1:B:668:THR:HB	1.88	0.55
1:D:693:LYS:HE2	1:D:813:PHE:O	2.07	0.55
1:B:749:LEU:HD13	1:B:761:MET:HE2	1.87	0.55
1:B:633:ARG:NH1	1:B:637:ILE:O	2.38	0.55
1:C:231:MET:HE1	1:C:237:LEU:HA	1.89	0.55
1:C:296:VAL:HG12	1:C:348:ALA:HB3	1.88	0.54
1:D:1016:ALA:HB3	1:D:1039:ASP:HA	1.89	0.54
1:D:508:LEU:HD11	1:D:661:ASP:HB3	1.87	0.54
1:A:591:PRO:HD3	1:A:668:THR:HB	1.89	0.54
1:A:228:ASN:HD21	1:A:261:VAL:HG23	1.71	0.54
1:D:216:ARG:NE	1:D:252:GLU:OE1	2.26	0.54
1:D:231:MET:HE1	1:D:237:LEU:HA	1.89	0.54
1:D:616:LYS:NZ	3:D:2002:NAD:O2B	2.42	0.53
1:A:332:MET:HE1	1:A:357:SER:HB3	1.91	0.53
1:D:12:ASN:N	1:D:12:ASN:HD22	2.06	0.53
1:B:582:PRO:HB3	1:B:609:ALA:O	2.08	0.53
1:D:185:SER:HB3	1:D:228:ASN:HB3	1.91	0.53
1:A:274:GLN:HG2	1:A:334:TYR:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ASP:HB3	1:B:133:GLY:HA3	1.89	0.53
1:D:15:LEU:HD12	1:D:449:ARG:HD3	1.91	0.53
1:A:487:PRO:HG2	1:A:539:VAL:HB	1.89	0.53
1:A:508:LEU:HD11	1:A:661:ASP:HB3	1.90	0.53
1:C:831:LEU:HD23	1:C:859:LEU:HD23	1.90	0.53
1:D:238:HIS:CE1	1:D:475:LEU:HD11	2.43	0.52
1:A:933:THR:HG22	1:A:935:PHE:H	1.72	0.52
1:C:716:PHE:HB3	1:C:761:MET:HE2	1.91	0.52
1:C:923:LEU:HD11	1:C:940:ALA:HB1	1.91	0.52
1:D:526:ALA:HB1	1:D:559:ILE:HG23	1.89	0.52
1:C:776:LEU:HD21	1:C:821:PRO:HD2	1.92	0.52
1:B:943:ASP:OD1	1:B:1046:GLY:HA3	2.10	0.52
1:C:678:ARG:HD2	1:C:686:ILE:HG21	1.92	0.52
1:D:140:LEU:HD23	1:D:150:LEU:HD12	1.91	0.52
1:D:320:THR:OG1	1:D:323:GLU:HG3	2.10	0.51
1:B:716:PHE:HB3	1:B:761:MET:CE	2.41	0.51
1:C:327:ASN:O	1:C:331:MET:HG3	2.10	0.51
1:B:148:TYR:CZ	1:B:388:ARG:HD3	2.45	0.51
1:C:198:TRP:CZ2	1:C:472:PRO:HG3	2.45	0.51
1:C:890:ASN:HA	1:C:1011:HIS:NE2	2.25	0.51
1:A:489:PRO:HD2	1:A:623:ARG:HD2	1.93	0.51
1:A:867:GLY:O	1:A:898:LYS:NZ	2.39	0.50
1:B:442:PHE:O	1:B:446:VAL:HG23	2.11	0.50
1:A:329:LEU:HA	1:A:332:MET:HE2	1.93	0.50
1:C:607:LEU:HD22	1:C:641:LEU:HD22	1.94	0.50
1:A:488:GLN:HA	1:A:623:ARG:HD2	1.93	0.50
1:C:324:VAL:HG21	2:C:2001:FAD:N3A	2.28	0.49
1:C:508:LEU:HD11	1:C:661:ASP:HB3	1.93	0.49
1:C:283:ARG:NH2	1:C:289:ALA:O	2.45	0.49
1:D:546:LYS:HG2	1:D:718:HIS:CE1	2.47	0.49
1:B:933:THR:HG22	1:B:934:GLU:N	2.27	0.49
1:B:886:GLY:O	1:B:898:LYS:NZ	2.44	0.49
1:A:917:ASP:OD1	1:B:570:ASN:HB3	2.11	0.49
1:A:976:TYR:OH	1:A:1000:ARG:NH1	2.44	0.49
1:B:923:LEU:HD11	1:B:940:ALA:HB1	1.94	0.49
1:B:320:THR:OG1	1:B:323:GLU:HG3	2.13	0.49
1:D:249:MET:SD	1:D:283:ARG:HG3	2.52	0.49
1:D:157:GLU:HG2	1:D:741:GLN:NE2	2.28	0.48
1:A:308:ALA:HB1	1:A:313:TRP:O	2.12	0.48
1:A:526:ALA:HB1	1:A:559:ILE:HG23	1.94	0.48
1:B:693:LYS:HE2	1:B:813:PHE:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:LYS:HG2	1:C:718:HIS:CE1	2.49	0.48
1:D:238:HIS:NE2	1:D:475:LEU:HD11	2.29	0.48
1:C:249:MET:SD	1:C:283:ARG:HG3	2.54	0.48
1:B:274:GLN:HG2	1:B:334:TYR:CZ	2.48	0.48
1:D:667:LEU:O	1:D:688:ALA:HA	2.14	0.48
1:B:933:THR:HG21	1:B:983:GLU:OE2	2.13	0.48
1:D:890:ASN:HA	1:D:1011:HIS:NE2	2.29	0.48
1:A:376:LEU:HD23	1:A:397:TYR:HB3	1.95	0.47
1:A:20:GLU:OE2	1:A:443:ARG:NH1	2.47	0.47
1:C:295:LEU:HD11	1:C:331:MET:HB2	1.95	0.47
1:C:868:ASN:OD1	1:C:898:LYS:NZ	2.47	0.47
1:A:582:PRO:HB3	1:A:609:ALA:O	2.13	0.47
1:B:667:LEU:O	1:B:688:ALA:HA	2.13	0.47
1:A:295:LEU:HD22	1:A:331:MET:HE3	1.95	0.47
1:D:500:VAL:HA	1:D:645:MET:HE1	1.97	0.47
1:A:594:PHE:HB2	1:A:598:ILE:HD12	1.97	0.47
1:C:387:VAL:O	1:C:391:VAL:HG22	2.14	0.47
1:D:488:GLN:HA	1:D:623:ARG:HD2	1.96	0.47
1:C:345:VAL:HG12	1:C:347:ILE:HD12	1.97	0.47
1:D:458:ARG:HD2	1:D:471:ASP:OD2	2.14	0.47
1:B:607:LEU:HD22	1:B:641:LEU:HD22	1.97	0.46
1:C:582:PRO:HB3	1:C:609:ALA:O	2.16	0.46
1:D:976:TYR:OH	1:D:1000:ARG:NH1	2.46	0.46
1:C:140:LEU:HD23	1:C:150:LEU:HD12	1.98	0.46
1:C:228:ASN:HD21	1:C:261:VAL:HG23	1.79	0.46
1:B:519:THR:O	1:B:523:GLN:HG2	2.15	0.46
1:A:268:ASP:OD1	1:A:268:ASP:N	2.49	0.46
1:A:376:LEU:HG	2:A:2001:FAD:HM82	1.98	0.46
1:B:778:THR:O	1:B:804:ARG:NH2	2.48	0.46
1:C:716:PHE:HB3	1:C:761:MET:CE	2.46	0.46
1:C:308:ALA:HB1	1:C:313:TRP:O	2.16	0.46
1:D:532:ILE:HD11	1:D:631:ALA:HB2	1.98	0.46
1:A:222:SER:HA	1:A:223:PRO:C	2.32	0.45
1:C:1022:VAL:HB	1:C:1027:TYR:CE2	2.52	0.45
1:B:231:MET:HE3	1:B:231:MET:HB3	1.75	0.45
1:B:231:MET:HE1	1:B:237:LEU:HA	1.99	0.45
1:B:377:GLN:HB2	1:B:396:LEU:HB3	1.98	0.45
1:D:512:ARG:HG2	1:D:513:LEU:O	2.16	0.45
1:A:324:VAL:HG21	2:A:2001:FAD:N3A	2.30	0.45
1:B:335:ILE:HG23	1:B:345:VAL:HG21	1.99	0.45
1:B:458:ARG:HD2	1:B:471:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ILE:HG23	1:B:450:TRP:CD1	2.52	0.45
1:C:518:ARG:HD3	1:C:607:LEU:O	2.17	0.45
1:A:231:MET:HE1	1:A:237:LEU:HA	1.97	0.45
1:B:140:LEU:HD23	1:B:150:LEU:HD12	1.97	0.45
1:B:321:LYS:HB2	2:B:2001:FAD:C5A	2.47	0.45
1:D:716:PHE:HB3	1:D:761:MET:CE	2.47	0.45
1:B:407:ASP:OD1	1:B:407:ASP:N	2.49	0.45
1:B:518:ARG:NH1	1:B:608:ALA:O	2.50	0.45
1:C:377:GLN:HG2	1:C:396:LEU:HD13	1.99	0.45
1:D:923:LEU:HA	1:D:923:LEU:HD23	1.82	0.45
1:C:335:ILE:HG23	1:C:345:VAL:HG21	1.99	0.45
1:D:573:ASN:O	1:D:573:ASN:ND2	2.48	0.45
1:A:640:ASP:OD1	1:A:640:ASP:N	2.48	0.45
1:A:933:THR:HG22	1:A:934:GLU:N	2.31	0.45
1:D:187:LYS:HG2	1:D:230:ASP:HB2	1.98	0.45
1:A:507:LEU:HD23	1:A:507:LEU:HA	1.77	0.45
1:B:513:LEU:HD11	1:B:641:LEU:HD11	1.99	0.45
1:C:290:LYS:HG2	1:C:342:ASN:HA	1.99	0.45
1:B:373:VAL:HG11	1:B:387:VAL:HG11	1.99	0.44
1:C:198:TRP:CE2	1:C:472:PRO:HG3	2.53	0.44
1:B:373:VAL:O	1:B:394:VAL:HA	2.18	0.44
1:B:533:ARG:O	1:B:537:LEU:HG	2.16	0.44
1:D:607:LEU:HD22	1:D:641:LEU:HD22	1.99	0.44
1:D:582:PRO:HB3	1:D:609:ALA:O	2.16	0.44
1:B:263:GLN:NE2	2:B:2001:FAD:O2	2.49	0.44
1:B:526:ALA:HB1	1:B:559:ILE:HG23	1.99	0.44
1:C:8:MET:HB3	1:C:10:TYR:CE2	2.53	0.44
1:D:933:THR:HG21	1:D:983:GLU:OE1	2.18	0.44
1:D:1022:VAL:HB	1:D:1027:TYR:CE2	2.52	0.44
1:A:923:LEU:HA	1:A:923:LEU:HD23	1.88	0.44
1:A:633:ARG:NH1	1:A:637:ILE:O	2.44	0.43
1:B:228:ASN:HD21	1:B:261:VAL:HG23	1.83	0.43
1:B:249:MET:SD	1:B:283:ARG:HG3	2.57	0.43
1:D:933:THR:HG22	1:D:935:PHE:H	1.82	0.43
1:B:1016:ALA:HB3	1:B:1039:ASP:HA	2.01	0.43
1:D:594:PHE:HB2	1:D:598:ILE:HD12	1.99	0.43
1:D:933:THR:HG22	1:D:934:GLU:N	2.33	0.43
1:A:751:VAL:HG21	1:A:800:SER:HA	2.00	0.43
1:C:268:ASP:OD1	1:C:268:ASP:N	2.51	0.43
1:C:775:GLY:HA2	1:C:804:ARG:HH21	1.82	0.43
1:D:532:ILE:CD1	1:D:631:ALA:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:PHE:HZ	1:B:292:LYS:HB3	1.83	0.43
1:D:273:LEU:HD22	1:D:331:MET:HB3	2.00	0.43
1:A:1016:ALA:HB3	1:A:1039:ASP:HA	2.01	0.43
1:C:262:LEU:HA	1:C:262:LEU:HD23	1.87	0.43
1:D:19:GLN:HE21	1:D:443:ARG:HA	1.84	0.43
1:B:406:PHE:O	1:B:410:VAL:HG23	2.19	0.43
1:C:888:TRP:CE3	1:C:1055:LYS:HE3	2.53	0.43
1:D:140:LEU:HD13	1:D:180:ARG:HB2	2.00	0.43
1:D:641:LEU:HD23	1:D:641:LEU:HA	1.73	0.43
1:D:722:LYS:HB2	1:D:725:ALA:HB2	2.01	0.43
1:A:890:ASN:HA	1:A:1011:HIS:NE2	2.34	0.43
1:A:321:LYS:NZ	1:A:325:ASP:OD2	2.48	0.43
1:A:616:LYS:NZ	3:A:2002:NAD:O2B	2.52	0.43
1:B:273:LEU:HB2	1:B:331:MET:HE3	2.00	0.43
1:C:274:GLN:HG2	1:C:334:TYR:CZ	2.53	0.43
1:C:992:ALA:HB1	1:C:997:THR:O	2.19	0.43
1:D:231:MET:HE3	1:D:231:MET:HB3	1.74	0.43
1:C:22:ILE:HD13	1:C:357:SER:HA	2.01	0.42
1:C:541:THR:HA	1:C:546:LYS:O	2.19	0.42
1:D:283:ARG:NH2	1:D:289:ALA:O	2.51	0.42
1:D:521:LEU:HA	1:D:521:LEU:HD23	1.86	0.42
1:B:376:LEU:HD23	1:B:397:TYR:HB3	2.02	0.42
2:A:2001:FAD:H9	2:A:2001:FAD:H1'2	1.78	0.42
1:C:512:ARG:CZ	1:C:512:ARG:HB2	2.49	0.42
1:B:321:LYS:NZ	1:B:325:ASP:OD2	2.44	0.42
1:C:373:VAL:O	1:C:394:VAL:HA	2.19	0.42
1:A:607:LEU:HD22	1:A:641:LEU:HD22	2.01	0.42
1:A:752:GLY:O	1:A:762:ASN:HA	2.19	0.42
1:A:987:ARG:O	1:A:987:ARG:HD3	2.19	0.42
1:C:933:THR:HG22	1:C:934:GLU:N	2.35	0.42
1:B:749:LEU:HD13	1:B:761:MET:CE	2.49	0.42
1:D:705:ASP:OD1	1:D:741:GLN:NE2	2.47	0.42
1:D:794:ASP:OD1	1:D:795:GLU:N	2.52	0.42
1:D:577:HIS:ND1	1:D:916:SER:OG	2.40	0.42
1:B:518:ARG:HD3	1:B:607:LEU:O	2.20	0.42
1:D:533:ARG:O	1:D:537:LEU:HG	2.19	0.42
1:A:222:SER:HA	1:A:223:PRO:HA	1.85	0.42
1:A:335:ILE:HG23	1:A:345:VAL:HG21	2.02	0.42
1:A:387:VAL:O	1:A:391:VAL:HG22	2.19	0.42
1:A:449:ARG:HB3	1:A:449:ARG:HE	1.60	0.42
1:B:616:LYS:O	1:B:616:LYS:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:ALA:HB2	1:C:597:ALA:HA	2.02	0.42
1:C:598:ILE:HD13	1:C:668:THR:HG21	2.02	0.42
1:D:283:ARG:HD3	1:D:289:ALA:O	2.20	0.42
1:D:295:LEU:HA	1:D:295:LEU:HD23	1.57	0.42
1:A:518:ARG:HD3	1:A:607:LEU:O	2.20	0.41
1:B:348:ALA:HA	1:B:374:GLU:O	2.20	0.41
1:D:565:TYR:CE2	1:D:605:ALA:HB2	2.55	0.41
1:D:591:PRO:HD3	1:D:668:THR:HB	2.01	0.41
1:B:330:ARG:HG3	1:B:450:TRP:CZ3	2.55	0.41
1:B:449:ARG:HE	1:B:449:ARG:HB3	1.57	0.41
1:A:295:LEU:HA	1:A:295:LEU:HD23	1.74	0.41
1:B:19:GLN:O	1:B:23:ILE:HG13	2.20	0.41
1:C:195:LEU:HD12	1:C:195:LEU:HA	1.91	0.41
1:D:663:ASP:O	1:D:685:ASN:HB2	2.20	0.41
1:B:641:LEU:HD23	1:B:641:LEU:HA	1.87	0.41
1:C:1016:ALA:HB3	1:C:1039:ASP:HA	2.02	0.41
1:D:884:PRO:HB2	1:D:898:LYS:HD3	2.01	0.41
1:A:16:GLU:CD	1:A:449:ARG:HH22	2.24	0.41
1:B:963:GLU:HG2	1:B:965:ASN:ND2	2.35	0.41
1:A:19:GLN:O	1:A:23:ILE:HG13	2.20	0.41
1:B:148:TYR:CE1	1:B:388:ARG:HD3	2.55	0.41
1:D:536:LEU:HD23	1:D:627:VAL:HG12	2.03	0.41
1:A:492:ARG:O	1:A:646:HIS:HB2	2.21	0.41
1:A:832:GLU:N	1:A:832:GLU:OE2	2.49	0.41
1:C:130:ASP:HB3	1:C:133:GLY:HA3	2.02	0.41
1:A:532:ILE:CD1	1:A:631:ALA:HB2	2.47	0.41
1:C:871:ILE:HB	1:C:1061:THR:HG23	2.01	0.41
1:C:526:ALA:HB1	1:C:559:ILE:HG23	2.01	0.41
1:C:962:CYS:C	1:C:1063:ASN:HB2	2.40	0.41
1:D:455:ASP:HB3	1:D:459:LEU:HD12	2.03	0.41
1:D:12:ASN:H	1:D:12:ASN:HD22	1.69	0.41
1:B:831:LEU:HD23	1:B:859:LEU:HD23	2.02	0.41
1:C:15:LEU:HD12	1:C:449:ARG:HD3	2.03	0.41
1:A:336:LEU:HD23	1:A:336:LEU:HA	1.90	0.40
1:A:526:ALA:HB2	1:A:562:ALA:HB3	2.02	0.40
1:A:693:LYS:HE2	1:A:813:PHE:O	2.21	0.40
1:D:791:LYS:NZ	1:D:794:ASP:O	2.54	0.40
1:A:458:ARG:CB	1:A:474:LEU:HD21	2.51	0.40
1:A:541:THR:HG22	1:A:546:LYS:O	2.21	0.40
1:A:667:LEU:O	1:A:688:ALA:HA	2.21	0.40
1:A:786:LEU:HG	1:A:805:ASP:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:ASP:HB2	1:C:365:ARG:HH21	1.86	0.40
1:D:153:ASN:ND2	1:D:185:SER:O	2.49	0.40
1:D:379:MET:O	1:D:381:PRO:HD3	2.21	0.40
1:D:198:TRP:CE2	1:D:472:PRO:HG3	2.57	0.40
1:C:917:ASP:OD1	1:D:570:ASN:HB3	2.22	0.40
1:A:546:LYS:HG2	1:A:718:HIS:CE1	2.56	0.40
1:A:861:LYS:HE3	1:A:861:LYS:HB3	1.93	0.40
1:D:513:LEU:CD1	1:D:641:LEU:HD11	2.46	0.40
1:A:15:LEU:HA	1:A:15:LEU:HD23	1.90	0.40
1:A:924:PRO:HA	1:A:925:PRO:HD3	1.94	0.40
1:B:674:ALA:O	1:B:678:ARG:HG3	2.20	0.40
1:A:943:ASP:OD1	1:A:1046:GLY:HA3	2.22	0.40
1:B:526:ALA:HB2	1:B:562:ALA:HB3	2.03	0.40
1:C:350:HIS:NE2	1:C:376:LEU:HB2	2.36	0.40
1:D:195:LEU:HA	1:D:195:LEU:HD12	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	957/1076 (89%)	932 (97%)	25 (3%)	0	100	100
1	B	956/1076 (89%)	929 (97%)	27 (3%)	0	100	100
1	C	956/1076 (89%)	929 (97%)	27 (3%)	0	100	100
1	D	956/1076 (89%)	928 (97%)	28 (3%)	0	100	100
All	All	3825/4304 (89%)	3718 (97%)	107 (3%)	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	755/884 (85%)	733 (97%)	22 (3%)	42	71
1	B	739/884 (84%)	718 (97%)	21 (3%)	43	73
1	C	729/884 (82%)	710 (97%)	19 (3%)	46	75
1	D	736/884 (83%)	716 (97%)	20 (3%)	44	74
All	All	2959/3536 (84%)	2877 (97%)	82 (3%)	43	73

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	183	TYR
1	A	220	GLN
1	A	265	TYR
1	A	321	LYS
1	A	404	GLU
1	A	408	VAL
1	A	413	LEU
1	A	449	ARG
1	A	463	GLU
1	A	515	ILE
1	A	612	LYS
1	A	675	SER
1	A	712	TYR
1	A	718	HIS
1	A	727	SER
1	A	781	THR
1	A	800	SER
1	A	819	PHE
1	A	850	HIS
1	A	987	ARG
1	A	1069	ILE
1	B	183	TYR
1	B	206	LEU

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Mol	Chain	Res	Type
1	B	265	TYR
1	B	379	MET
1	B	393	THR
1	B	407	ASP
1	B	411	SER
1	B	420	ASN
1	B	449	ARG
1	B	497	VAL
1	B	515	ILE
1	B	612	LYS
1	B	675	SER
1	B	712	TYR
1	B	718	HIS
1	B	727	SER
1	B	781	THR
1	B	800	SER
1	B	819	PHE
1	B	850	HIS
1	B	987	ARG
1	C	183	TYR
1	C	222	SER
1	C	265	TYR
1	C	295	LEU
1	C	411	SER
1	C	416	ARG
1	C	462	PRO
1	C	497	VAL
1	C	567	ARG
1	C	612	LYS
1	C	675	SER
1	C	712	TYR
1	C	718	HIS
1	C	727	SER
1	C	781	THR
1	C	819	PHE
1	C	850	HIS
1	C	923	LEU
1	C	987	ARG
1	D	12	ASN
1	D	151	ASN
1	D	182	ASP
1	D	183	TYR

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Mol	Chain	Res	Type
1	D	206	LEU
1	D	265	TYR
1	D	338	PRO
1	D	416	ARG
1	D	573	ASN
1	D	612	LYS
1	D	672	GLU
1	D	675	SER
1	D	712	TYR
1	D	718	HIS
1	D	727	SER
1	D	819	PHE
1	D	850	HIS
1	D	923	LEU
1	D	983	GLU
1	D	987	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	228	ASN
1	B	151	ASN
1	B	228	ASN
1	C	151	ASN
1	C	228	ASN
1	D	151	ASN
1	D	228	ASN
1	D	420	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAD	C	2002	-	33,38,48	1.60	7 (21%)	37,58,73	1.30	2 (5%)
2	FAD	D	2001	-	51,58,58	2.45	20 (39%)	60,89,89	1.74	12 (20%)
4	SO4	C	2003	-	4,4,4	0.22	0	6,6,6	0.45	0
4	SO4	A	2003	-	4,4,4	0.17	0	6,6,6	0.49	0
2	FAD	C	2001	-	51,58,58	2.30	20 (39%)	60,89,89	1.72	10 (16%)
3	NAD	B	2002	-	33,38,48	1.60	7 (21%)	37,58,73	1.32	3 (8%)
3	NAD	D	2002	-	33,38,48	1.51	8 (24%)	37,58,73	1.36	4 (10%)
4	SO4	D	2003	-	4,4,4	0.18	0	6,6,6	0.34	0
4	SO4	B	2003	-	4,4,4	0.18	0	6,6,6	0.36	0
2	FAD	A	2001	-	51,58,58	2.39	19 (37%)	60,89,89	2.02	16 (26%)
2	FAD	B	2001	-	51,58,58	2.41	21 (41%)	60,89,89	1.75	14 (23%)
3	NAD	A	2002	-	33,38,48	1.48	5 (15%)	37,58,73	1.58	6 (16%)

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
3	NAD	C	2002	-	-	9/18/51/62	0/4/4/5
2	FAD	D	2001	-	-	8/30/50/50	0/6/6/6
2	FAD	C	2001	-	-	3/30/50/50	0/6/6/6
2	FAD	A	2001	-	-	10/30/50/50	0/6/6/6
3	NAD	D	2002	-	-	7/18/51/62	0/4/4/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	B	2002	-	-	12/18/51/62	0/4/4/5
2	FAD	B	2001	-	-	6/30/50/50	0/6/6/6
3	NAD	A	2002	-	-	5/18/51/62	0/4/4/5

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	FAD	C4X-C10	6.90	1.45	1.38
2	A	2001	FAD	C4X-C10	6.83	1.45	1.38
2	B	2001	FAD	C4X-C10	6.31	1.45	1.38
2	A	2001	FAD	O4-C4	5.70	1.38	1.24
2	C	2001	FAD	C4X-C10	5.60	1.44	1.38
2	D	2001	FAD	O4-C4	5.48	1.38	1.24
2	B	2001	FAD	C4-C4X	5.42	1.50	1.41
2	B	2001	FAD	O4-C4	5.36	1.38	1.24
2	C	2001	FAD	O4-C4	5.22	1.37	1.24
2	A	2001	FAD	C4-C4X	5.20	1.50	1.41
2	D	2001	FAD	C10-N1	5.20	1.39	1.33
2	B	2001	FAD	C10-N1	5.07	1.39	1.33
2	D	2001	FAD	C4-C4X	5.03	1.50	1.41
2	C	2001	FAD	C4-C4X	4.94	1.49	1.41
2	A	2001	FAD	C10-N1	4.78	1.39	1.33
2	C	2001	FAD	C10-N1	4.76	1.39	1.33
2	D	2001	FAD	C4X-N5	4.71	1.40	1.33
2	C	2001	FAD	C4X-N5	4.65	1.40	1.33
2	B	2001	FAD	C4X-N5	4.63	1.39	1.33
2	B	2001	FAD	C9A-N10	4.31	1.44	1.38
2	A	2001	FAD	C4X-N5	4.30	1.39	1.33
2	A	2001	FAD	C4-N3	4.01	1.40	1.33
2	C	2001	FAD	C9A-N10	4.01	1.43	1.38
3	C	2002	NAD	C2D-C3D	-3.96	1.47	1.53
3	B	2002	NAD	C2D-C3D	-3.81	1.47	1.53
2	D	2001	FAD	C2-N1	3.73	1.45	1.38
2	C	2001	FAD	C4-N3	3.53	1.39	1.33
3	D	2002	NAD	C2B-C1B	-3.49	1.48	1.53
2	D	2001	FAD	C5X-N5	3.49	1.41	1.35
2	B	2001	FAD	C2-N1	3.41	1.44	1.38
3	A	2002	NAD	C2D-C3D	-3.40	1.48	1.53
3	C	2002	NAD	C2B-C1B	-3.34	1.48	1.53
2	D	2001	FAD	C2A-N3A	3.33	1.37	1.32
2	A	2001	FAD	C9A-N10	3.33	1.43	1.38
2	A	2001	FAD	C2A-N3A	3.32	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	FAD	C2-N1	3.28	1.44	1.38
2	B	2001	FAD	C4-N3	3.26	1.38	1.33
3	B	2002	NAD	C2B-C1B	-3.23	1.48	1.53
2	D	2001	FAD	C2B-C1B	-3.23	1.48	1.53
2	C	2001	FAD	C2B-C1B	-3.22	1.48	1.53
2	A	2001	FAD	C6A-N6A	3.21	1.45	1.34
2	D	2001	FAD	C4-N3	3.20	1.38	1.33
2	A	2001	FAD	C5X-N5	3.20	1.40	1.35
3	B	2002	NAD	C6A-N6A	3.12	1.45	1.34
2	B	2001	FAD	C2B-C1B	-3.11	1.49	1.53
2	D	2001	FAD	C9A-N10	3.11	1.42	1.38
2	B	2001	FAD	C6A-N6A	3.09	1.45	1.34
2	C	2001	FAD	C2-N1	3.07	1.44	1.38
2	C	2001	FAD	C6A-N6A	3.01	1.45	1.34
3	B	2002	NAD	C2A-N3A	3.00	1.36	1.32
2	D	2001	FAD	O4B-C4B	-2.98	1.38	1.45
2	C	2001	FAD	C2A-N3A	2.98	1.36	1.32
2	D	2001	FAD	C6A-N6A	2.95	1.44	1.34
2	B	2001	FAD	C5X-N5	2.93	1.40	1.35
3	A	2002	NAD	C6A-N6A	2.91	1.44	1.34
3	D	2002	NAD	C2A-N3A	2.89	1.36	1.32
2	B	2001	FAD	O2'-C2'	-2.85	1.37	1.43
2	B	2001	FAD	C2A-N3A	2.84	1.36	1.32
3	C	2002	NAD	C6A-N6A	2.83	1.44	1.34
2	C	2001	FAD	C5X-N5	2.82	1.40	1.35
2	D	2001	FAD	PA-O5B	-2.80	1.47	1.59
3	A	2002	NAD	C2A-N3A	2.80	1.36	1.32
3	D	2002	NAD	C6A-N6A	2.75	1.44	1.34
2	B	2001	FAD	PA-O5B	-2.72	1.48	1.59
2	B	2001	FAD	O4'-C4'	-2.66	1.37	1.43
2	A	2001	FAD	PA-O5B	-2.62	1.48	1.59
2	C	2001	FAD	O2'-C2'	-2.62	1.37	1.43
3	D	2002	NAD	C2D-C3D	-2.59	1.49	1.53
3	C	2002	NAD	O2D-C2D	-2.55	1.38	1.43
3	A	2002	NAD	C2B-C1B	-2.54	1.49	1.53
2	D	2001	FAD	O4'-C4'	-2.53	1.38	1.43
3	D	2002	NAD	O2D-C2D	-2.52	1.38	1.43
2	C	2001	FAD	O4'-C4'	-2.49	1.38	1.43
3	C	2002	NAD	C2A-N3A	2.48	1.36	1.32
3	B	2002	NAD	O2D-C2D	-2.43	1.38	1.43
2	C	2001	FAD	PA-O5B	-2.37	1.49	1.59
2	C	2001	FAD	O4B-C4B	-2.36	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2001	FAD	P-O1P	2.34	1.59	1.50
2	D	2001	FAD	O2'-C2'	-2.32	1.38	1.43
2	B	2001	FAD	O4B-C4B	-2.31	1.39	1.45
3	B	2002	NAD	O2B-C2B	-2.30	1.37	1.43
2	A	2001	FAD	C5'-C4'	2.28	1.55	1.51
2	A	2001	FAD	O4'-C4'	-2.23	1.38	1.43
3	D	2002	NAD	O2B-C2B	-2.22	1.37	1.43
2	C	2001	FAD	O2B-C2B	-2.20	1.37	1.43
2	D	2001	FAD	P-O1P	2.20	1.58	1.50
2	A	2001	FAD	O2'-C2'	-2.20	1.38	1.43
2	D	2001	FAD	O3B-C3B	-2.18	1.37	1.43
2	C	2001	FAD	PA-O2A	-2.18	1.45	1.55
3	D	2002	NAD	O3D-C3D	-2.17	1.37	1.43
2	B	2001	FAD	O3B-C3B	-2.15	1.37	1.43
3	C	2002	NAD	O3D-C3D	-2.14	1.37	1.43
3	A	2002	NAD	O2D-C2D	-2.14	1.38	1.43
2	A	2001	FAD	O3'-C3'	-2.13	1.38	1.43
2	A	2001	FAD	O4B-C4B	-2.12	1.40	1.45
2	B	2001	FAD	PA-O2A	-2.12	1.45	1.55
2	D	2001	FAD	PA-O2A	-2.12	1.45	1.55
2	A	2001	FAD	C2B-C1B	-2.11	1.50	1.53
2	B	2001	FAD	P-O1P	2.09	1.58	1.50
2	D	2001	FAD	O3'-C3'	-2.09	1.38	1.43
2	B	2001	FAD	O3'-C3'	-2.09	1.38	1.43
2	C	2001	FAD	O3'-C3'	-2.08	1.38	1.43
3	B	2002	NAD	C2B-C3B	-2.08	1.47	1.53
2	B	2001	FAD	O2B-C2B	-2.06	1.38	1.43
3	C	2002	NAD	O4D-C4D	-2.06	1.41	1.44
3	D	2002	NAD	C2B-C3B	-2.02	1.47	1.53
2	A	2001	FAD	P-O1P	2.01	1.58	1.50

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	FAD	C4-N3-C2	7.70	121.64	115.14
2	D	2001	FAD	C4-N3-C2	6.75	120.84	115.14
2	B	2001	FAD	C4-N3-C2	6.28	120.44	115.14
2	C	2001	FAD	N3A-C2A-N1A	-5.62	119.89	128.68
3	D	2002	NAD	N3A-C2A-N1A	-5.24	120.49	128.68
2	C	2001	FAD	C4-N3-C2	5.24	119.57	115.14
3	A	2002	NAD	N3A-C2A-N1A	-5.19	120.56	128.68
3	C	2002	NAD	N3A-C2A-N1A	-5.12	120.68	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	FAD	N3A-C2A-N1A	-5.00	120.86	128.68
3	B	2002	NAD	N3A-C2A-N1A	-4.70	121.34	128.68
2	D	2001	FAD	C5X-C9A-N10	4.57	121.03	117.72
2	C	2001	FAD	C4-C4X-C10	-4.50	116.97	119.95
2	B	2001	FAD	C4X-N5-C5X	4.30	121.06	116.77
2	D	2001	FAD	N3A-C2A-N1A	-4.29	121.97	128.68
2	A	2001	FAD	N3A-C2A-N1A	-4.28	121.99	128.68
2	A	2001	FAD	C5X-C9A-N10	4.13	120.71	117.72
2	A	2001	FAD	C4X-N5-C5X	4.10	120.87	116.77
2	A	2001	FAD	C4A-C5A-N7A	-3.96	105.28	109.40
2	A	2001	FAD	C4-C4X-C10	-3.75	117.47	119.95
2	B	2001	FAD	C4-C4X-C10	-3.57	117.59	119.95
2	C	2001	FAD	C4X-N5-C5X	3.53	120.30	116.77
2	C	2001	FAD	C5X-C9A-N10	3.46	120.23	117.72
2	D	2001	FAD	C4-C4X-C10	-3.44	117.67	119.95
2	A	2001	FAD	C4-C4X-N5	3.37	122.45	118.60
2	B	2001	FAD	C4-C4X-N5	3.19	122.24	118.60
2	C	2001	FAD	C4-C4X-N5	3.16	122.21	118.60
2	B	2001	FAD	C5X-C9A-N10	3.15	120.00	117.72
2	D	2001	FAD	C4X-N5-C5X	3.10	119.87	116.77
2	A	2001	FAD	C4X-C4-N3	-3.05	119.25	123.43
3	A	2002	NAD	C1D-O4D-C4D	-2.98	101.21	108.16
3	A	2002	NAD	C4A-C5A-N7A	-2.92	106.35	109.40
2	B	2001	FAD	O5'-P-O1P	2.91	120.43	109.07
2	B	2001	FAD	O5B-PA-O1A	2.70	119.62	109.07
3	B	2002	NAD	C4A-C5A-N7A	-2.64	106.65	109.40
2	C	2001	FAD	O2P-P-O5'	-2.52	96.04	107.75
2	A	2001	FAD	O5'-C5'-C4'	2.51	116.05	109.36
3	A	2002	NAD	O4D-C4D-C3D	-2.42	102.56	104.70
2	D	2001	FAD	C4-C4X-N5	2.41	121.35	118.60
3	B	2002	NAD	PN-O3-PA	-2.39	124.61	132.83
2	B	2001	FAD	C4A-C5A-N7A	-2.38	106.92	109.40
3	A	2002	NAD	O5D-C5D-C4D	2.34	117.05	108.99
2	D	2001	FAD	C1'-N10-C10	2.34	120.50	118.41
2	D	2001	FAD	C6-C5X-N5	2.32	121.61	119.05
3	A	2002	NAD	C2B-C3B-C4B	-2.31	98.16	102.64
3	D	2002	NAD	C4A-C5A-N7A	-2.30	107.00	109.40
2	A	2001	FAD	O5B-PA-O1A	2.29	118.00	109.07
2	A	2001	FAD	C4'-C3'-C2'	2.27	118.07	113.36
2	C	2001	FAD	C1'-N10-C9A	2.26	120.07	118.29
2	A	2001	FAD	O5'-P-O1P	2.25	117.88	109.07
3	D	2002	NAD	O2N-PN-O1N	-2.25	101.11	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	FAD	C4X-C4-N3	-2.22	120.40	123.43
2	D	2001	FAD	C4X-C10-N10	-2.21	118.03	120.30
2	C	2001	FAD	O5B-PA-O1A	2.19	117.63	109.07
2	D	2001	FAD	C4X-C4-N3	-2.18	120.45	123.43
2	B	2001	FAD	O2A-PA-O5B	-2.17	97.67	107.75
2	D	2001	FAD	O2A-PA-O5B	-2.16	97.70	107.75
2	A	2001	FAD	C5A-C6A-N6A	2.13	123.59	120.35
2	C	2001	FAD	C1'-N10-C10	2.13	120.31	118.41
2	B	2001	FAD	O2P-P-O5'	-2.12	97.91	107.75
2	A	2001	FAD	C1'-N10-C10	2.09	120.28	118.41
2	D	2001	FAD	O5B-PA-O1A	2.06	117.14	109.07
2	B	2001	FAD	C1'-N10-C9A	2.06	119.92	118.29
2	B	2001	FAD	C1'-N10-C10	2.04	120.24	118.41
2	A	2001	FAD	C1'-N10-C9A	2.03	119.89	118.29
3	D	2002	NAD	O4D-C4D-C3D	-2.02	102.92	104.70
2	A	2001	FAD	O2P-P-O5'	-2.01	98.40	107.75
3	C	2002	NAD	C4A-C5A-N7A	-2.01	107.30	109.40

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2002	NAD	C5B-O5B-PA-O3
3	C	2002	NAD	C5D-O5D-PN-O3
3	C	2002	NAD	C5D-O5D-PN-O1N
2	D	2001	FAD	C5'-O5'-P-O2P
3	B	2002	NAD	C5B-O5B-PA-O3
3	B	2002	NAD	O4B-C4B-C5B-O5B
3	B	2002	NAD	C5D-O5D-PN-O1N
3	D	2002	NAD	C5B-O5B-PA-O1A
3	D	2002	NAD	C5B-O5B-PA-O2A
3	D	2002	NAD	C5D-O5D-PN-O1N
3	D	2002	NAD	O4D-C4D-C5D-O5D
3	D	2002	NAD	C3D-C4D-C5D-O5D
2	A	2001	FAD	C5'-O5'-P-O1P
2	A	2001	FAD	C5'-O5'-P-O2P
2	B	2001	FAD	P-O3P-PA-O5B
2	B	2001	FAD	C5'-O5'-P-O2P
2	A	2001	FAD	O3'-C3'-C4'-O4'
3	B	2002	NAD	C3B-C4B-C5B-O5B
2	A	2001	FAD	C2'-C3'-C4'-O4'
3	C	2002	NAD	O4B-C4B-C5B-O5B

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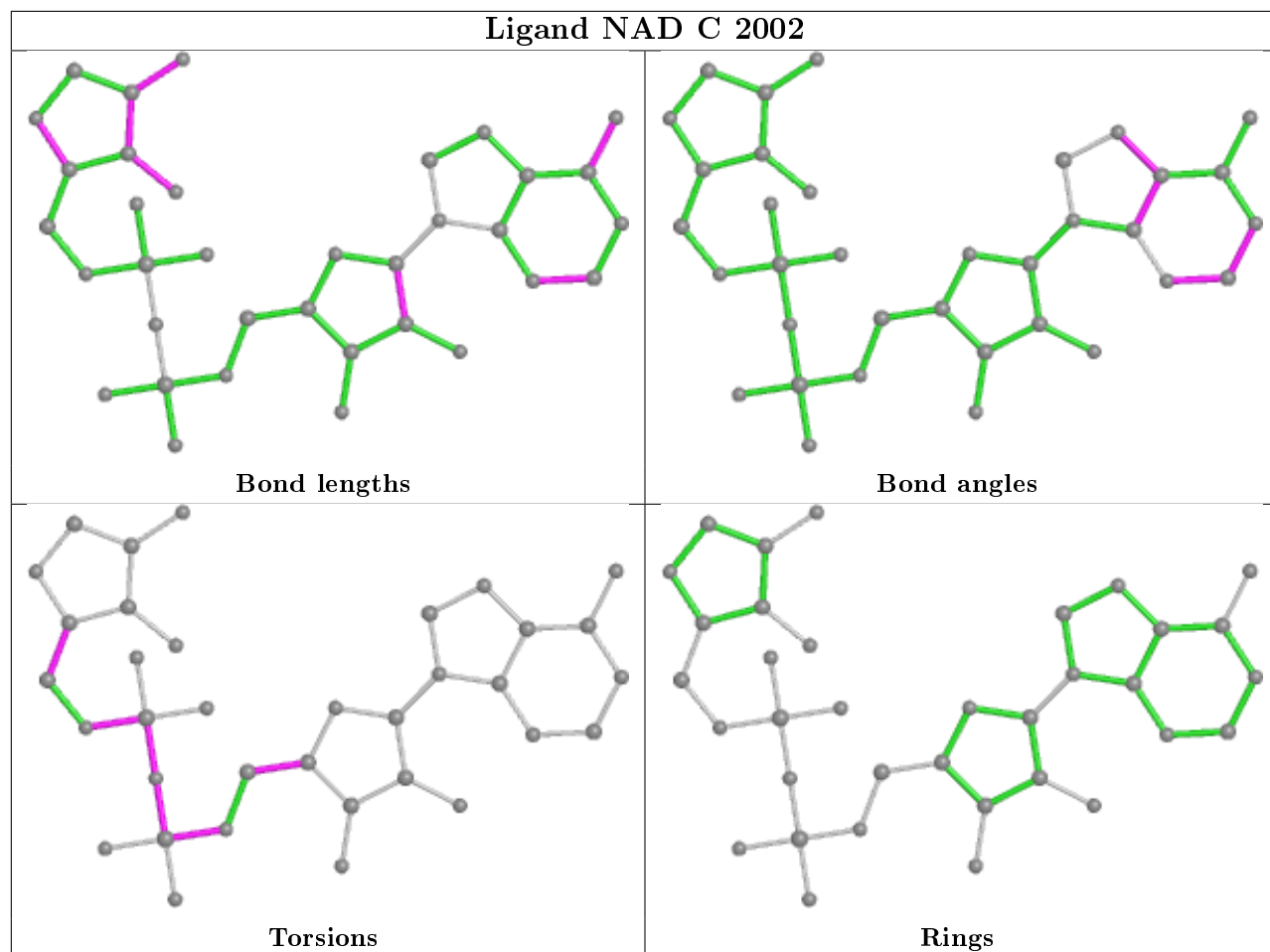
Mol	Chain	Res	Type	Atoms
3	B	2002	NAD	O4D-C4D-C5D-O5D
3	A	2002	NAD	C3B-C4B-C5B-O5B
3	B	2002	NAD	PN-O3-PA-O1A
3	A	2002	NAD	PN-O3-PA-O1A
2	D	2001	FAD	C3B-C4B-C5B-O5B
3	B	2002	NAD	C3D-C4D-C5D-O5D
2	B	2001	FAD	C2'-C3'-C4'-O4'
3	C	2002	NAD	PN-O3-PA-O5B
2	D	2001	FAD	P-O3P-PA-O5B
2	A	2001	FAD	P-O3P-PA-O5B
2	D	2001	FAD	C5B-O5B-PA-O3P
3	B	2002	NAD	C5D-O5D-PN-O3
3	D	2002	NAD	C5B-O5B-PA-O3
2	A	2001	FAD	C5B-O5B-PA-O3P
2	D	2001	FAD	P-O3P-PA-O1A
2	C	2001	FAD	P-O3P-PA-O2A
2	D	2001	FAD	C4'-C5'-O5'-P
3	D	2002	NAD	C4D-C5D-O5D-PN
3	C	2002	NAD	C5B-O5B-PA-O2A
2	D	2001	FAD	C5'-O5'-P-O1P
3	B	2002	NAD	C5B-O5B-PA-O1A
3	B	2002	NAD	C5B-O5B-PA-O2A
2	B	2001	FAD	C5'-O5'-P-O1P
3	A	2002	NAD	O4B-C4B-C5B-O5B
2	A	2001	FAD	C4'-C5'-O5'-P
2	A	2001	FAD	C2'-C3'-C4'-C5'
2	A	2001	FAD	C3B-C4B-C5B-O5B
2	C	2001	FAD	P-O3P-PA-O1A
3	B	2002	NAD	PN-O3-PA-O2A
2	A	2001	FAD	O3'-C3'-C4'-C5'
2	B	2001	FAD	O3'-C3'-C4'-O4'
3	C	2002	NAD	O4D-C4D-C5D-O5D
3	C	2002	NAD	C3B-C4B-C5B-O5B
2	D	2001	FAD	C5'-O5'-P-O3P
2	B	2001	FAD	C4'-C5'-O5'-P
3	C	2002	NAD	PA-O3-PN-O2N
3	B	2002	NAD	PA-O3-PN-O1N
2	C	2001	FAD	C5B-O5B-PA-O1A
3	A	2002	NAD	C5B-O5B-PA-O1A
3	A	2002	NAD	C5D-O5D-PN-O1N

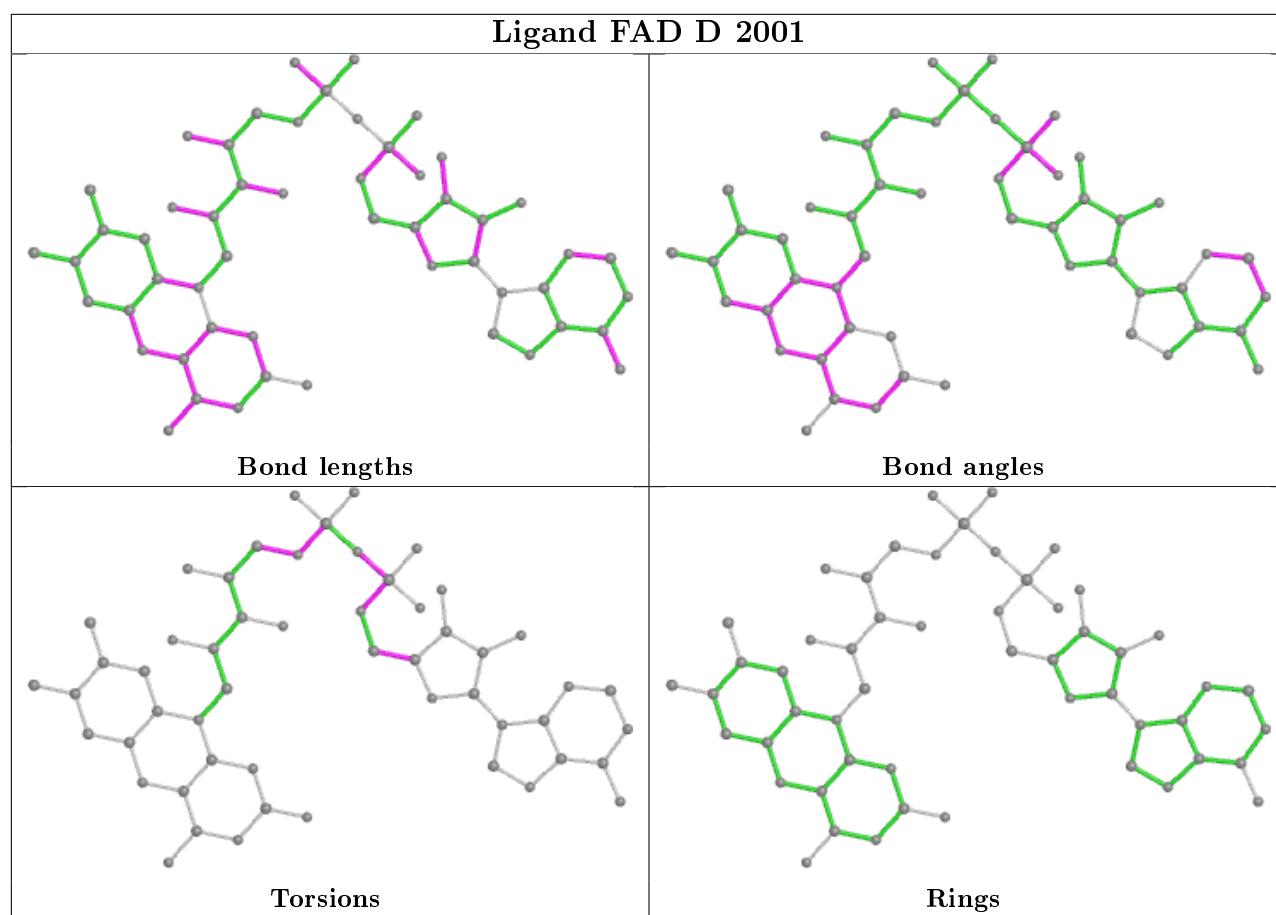
There are no ring outliers.

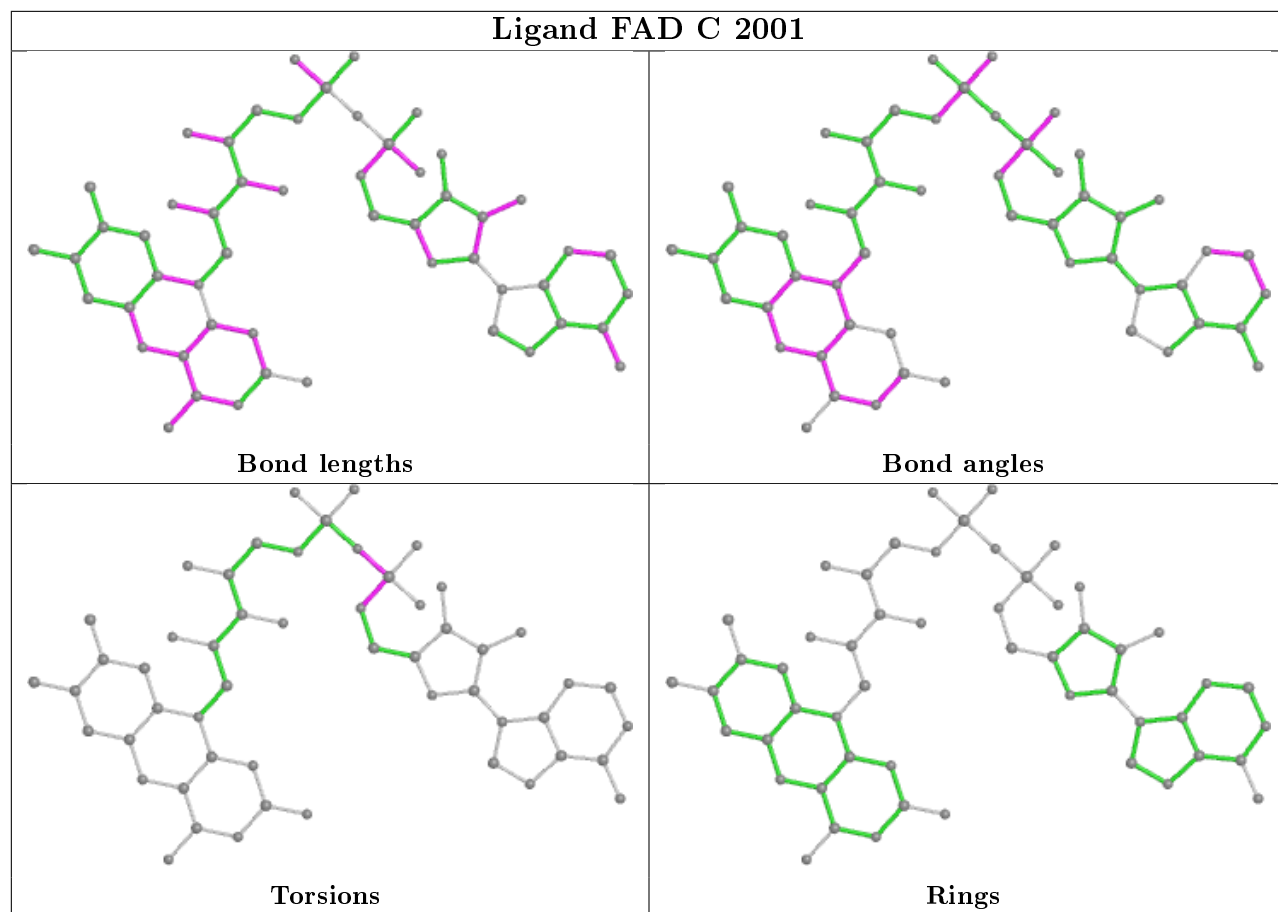
7 monomers are involved in 11 short contacts:

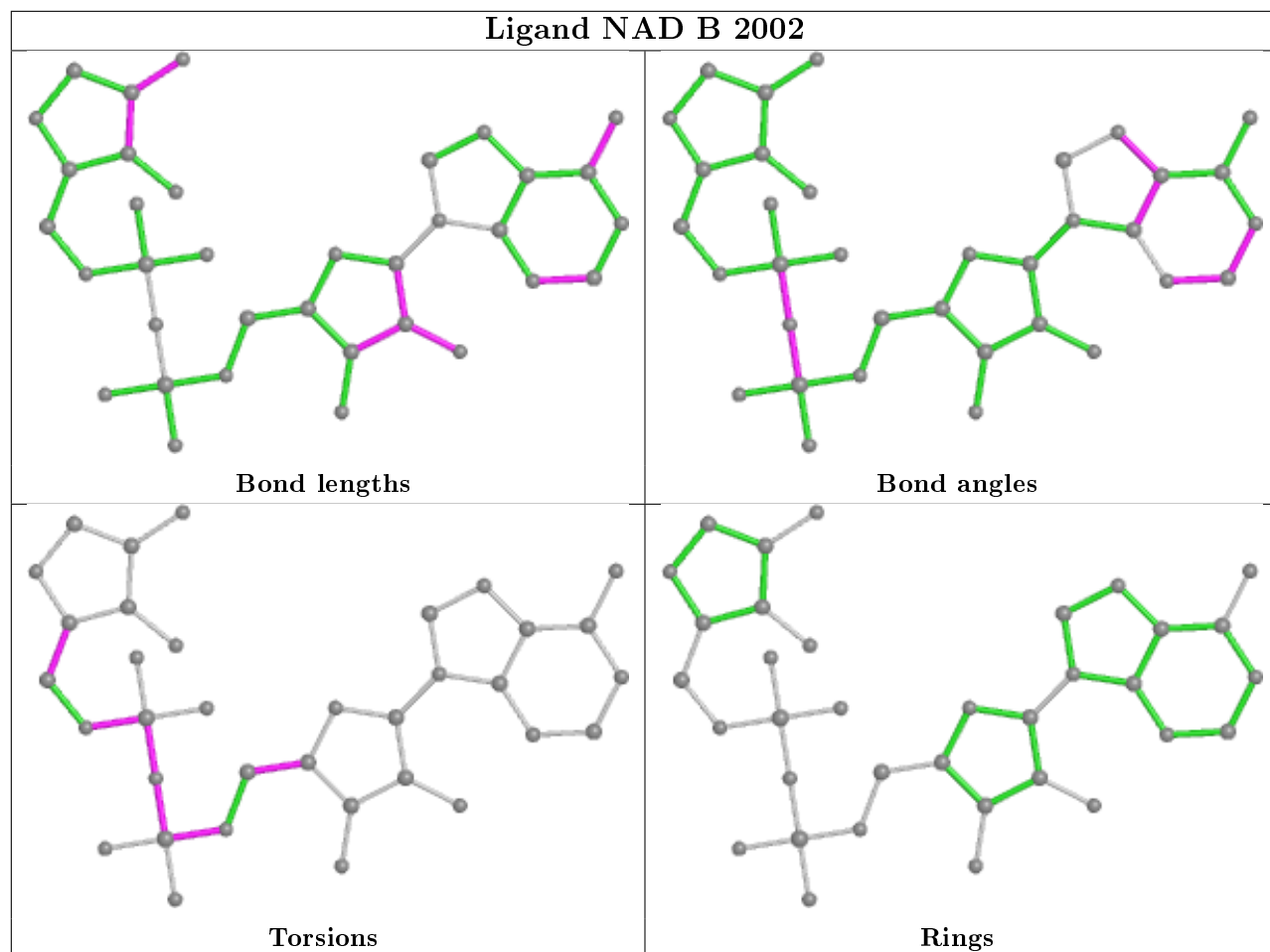
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2002	NAD	2	0
2	C	2001	FAD	1	0
3	B	2002	NAD	1	0
3	D	2002	NAD	1	0
2	A	2001	FAD	3	0
2	B	2001	FAD	2	0
3	A	2002	NAD	1	0

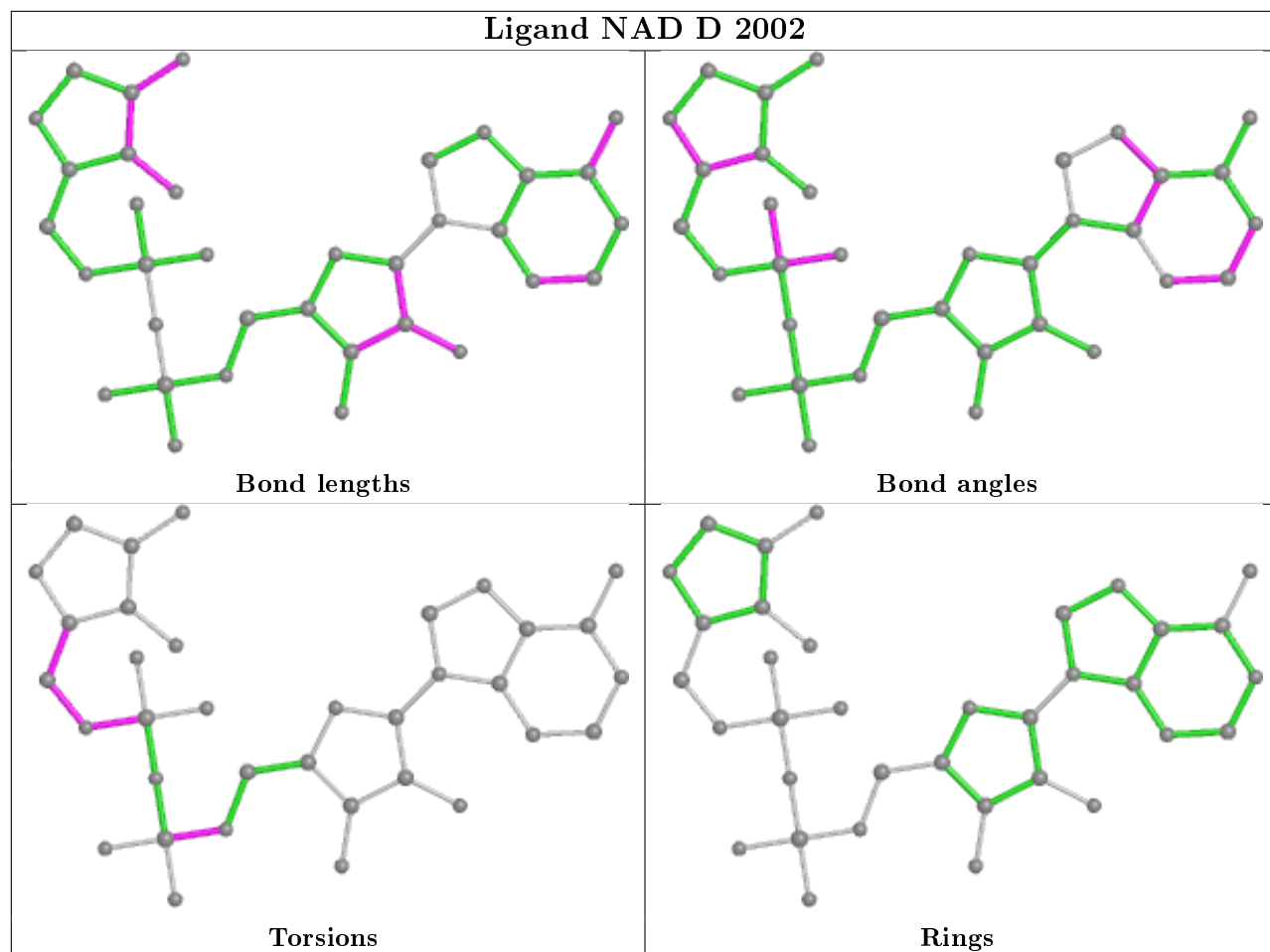
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

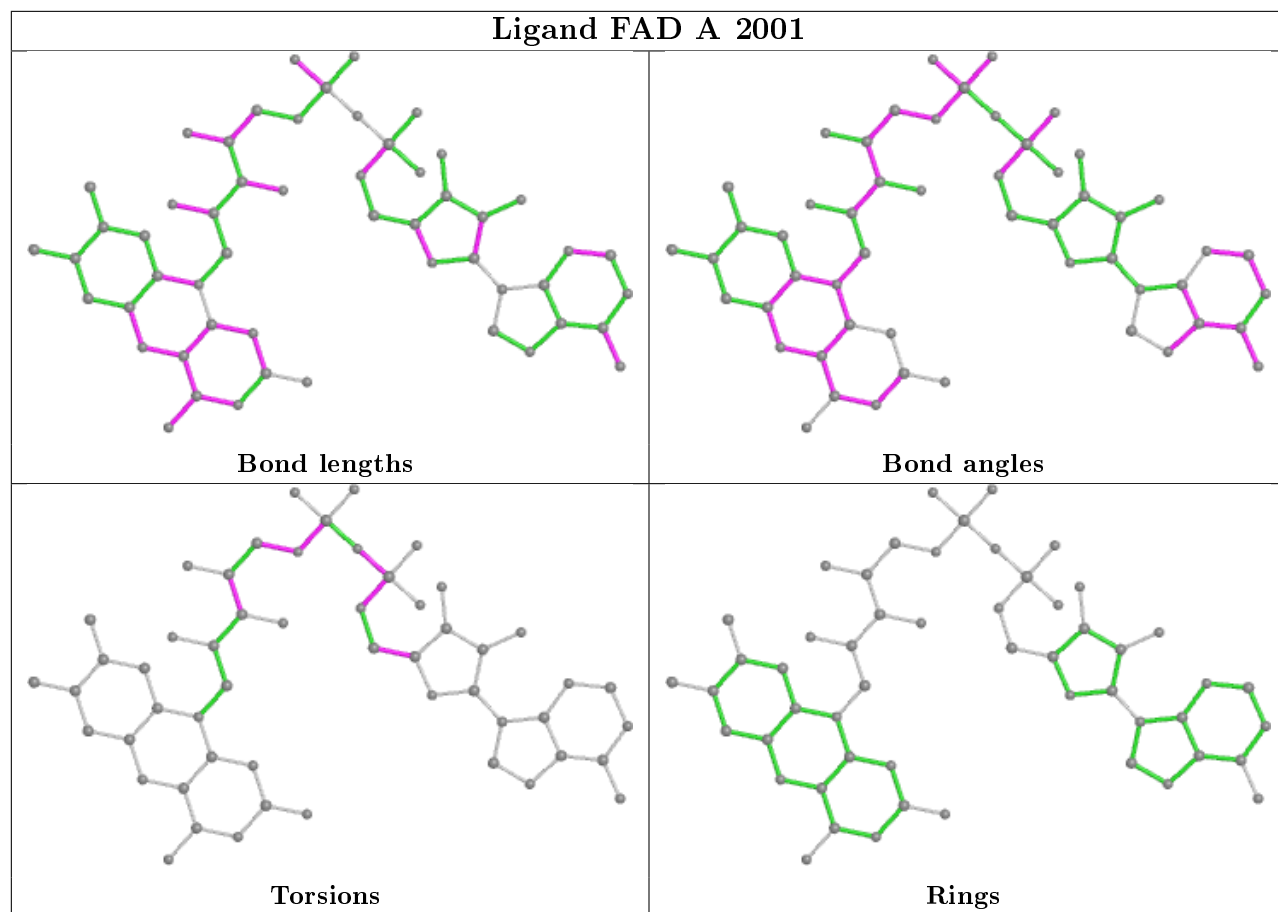


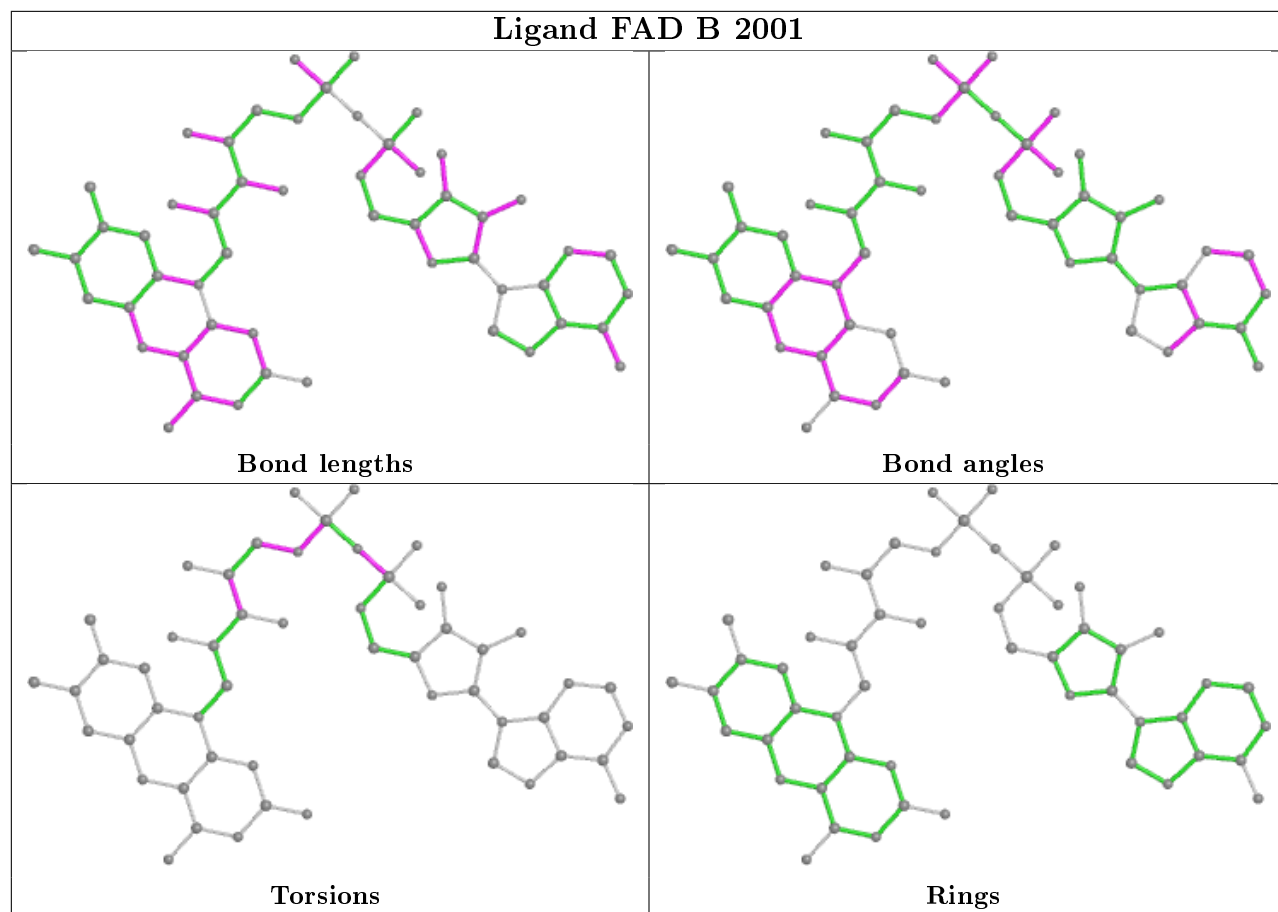


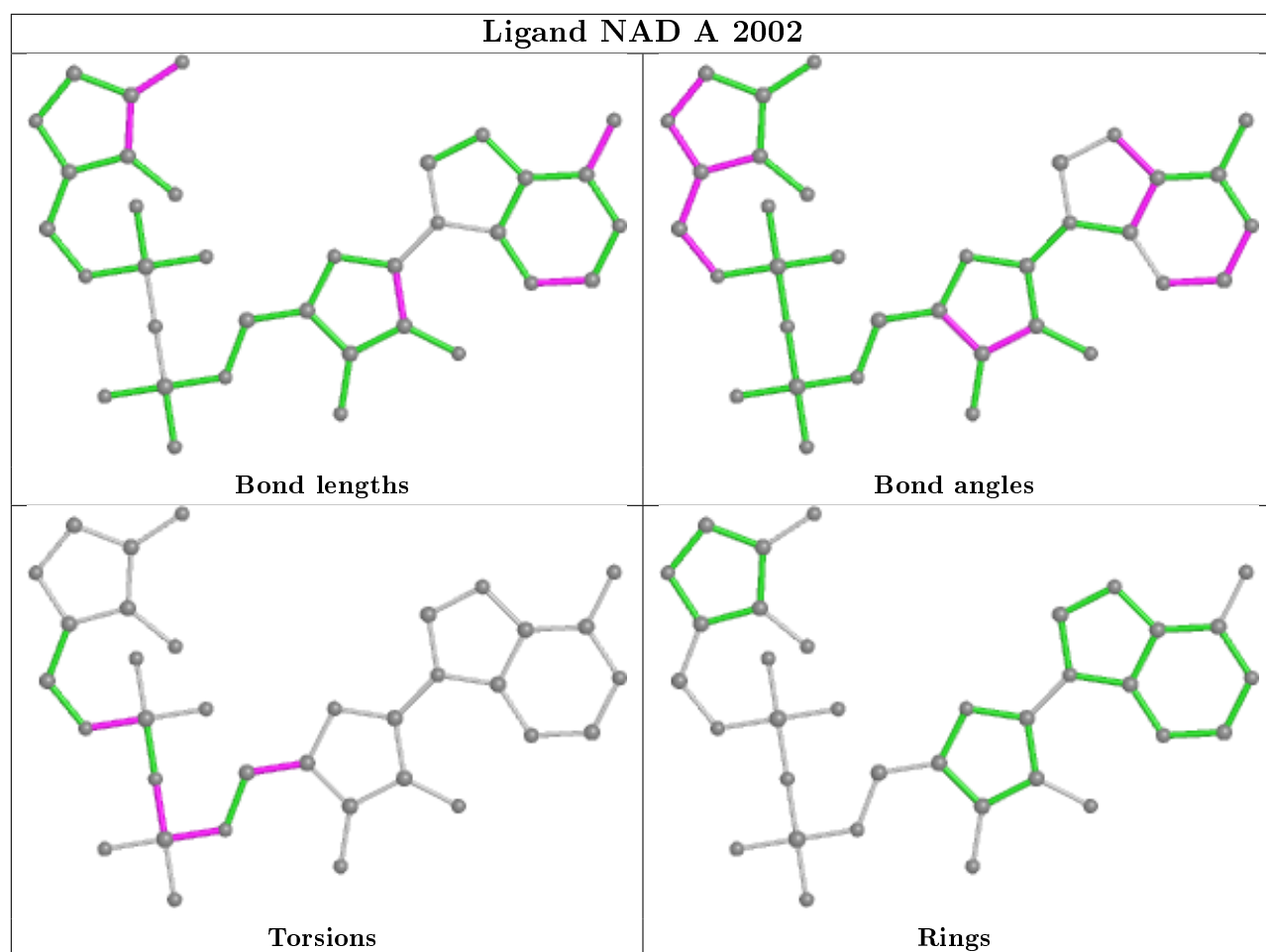












5.7 Other polymers [i](#)

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	963/1076 (89%)	-0.39	1 (0%) 95 96	23, 41, 67, 113	0
1	B	962/1076 (89%)	-0.25	9 (0%) 84 85	26, 51, 83, 110	0
1	C	962/1076 (89%)	-0.23	10 (1%) 82 83	25, 54, 90, 130	0
1	D	962/1076 (89%)	-0.21	10 (1%) 82 83	28, 50, 82, 121	0
All	All	3849/4304 (89%)	-0.27	30 (0%) 86 87	23, 48, 84, 130	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	380	ALA	3.6
1	C	389	GLN	3.3
1	D	380	ALA	3.0
1	B	379	MET	2.8
1	B	384	ALA	2.8
1	D	352	LEU	2.7
1	B	382	ALA	2.7
1	C	390	ALA	2.7
1	D	417	LEU	2.7
1	B	29	TRP	2.6
1	C	377	GLN	2.6
1	B	380	ALA	2.6
1	D	26	ALA	2.6
1	D	379	MET	2.5
1	C	382	ALA	2.4
1	B	387	VAL	2.4
1	D	381	PRO	2.3
1	B	390	ALA	2.3
1	C	1068	TYR	2.3
1	C	29	TRP	2.3
1	C	376	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	24	ALA	2.3
1	B	389	GLN	2.2
1	B	381	PRO	2.2
1	A	31	ALA	2.2
1	D	295	LEU	2.1
1	C	379	MET	2.1
1	C	126	HIS	2.0
1	D	27	ASN	2.0
1	D	29	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

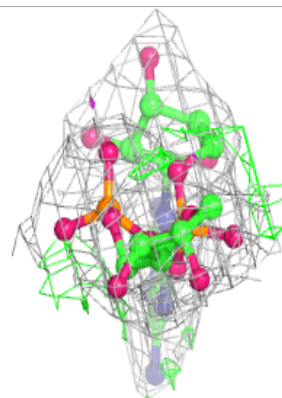
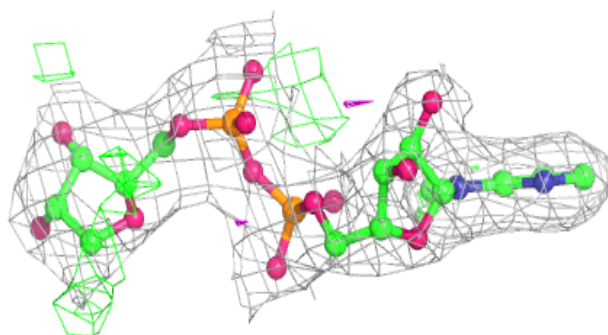
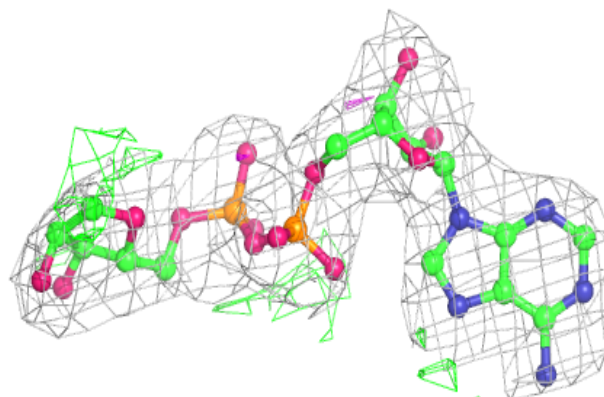
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	C	2003	5/5	0.93	0.13	68,71,78,85	0
3	NAD	C	2002	35/44	0.94	0.15	43,53,90,92	0
4	SO4	A	2003	5/5	0.94	0.16	54,64,66,74	0
3	NAD	B	2002	35/44	0.94	0.13	43,51,79,83	0
3	NAD	D	2002	35/44	0.94	0.15	40,59,89,91	0
3	NAD	A	2002	35/44	0.94	0.15	34,46,77,79	0
4	SO4	B	2003	5/5	0.95	0.16	69,75,80,88	0
2	FAD	D	2001	53/53	0.96	0.19	40,54,69,72	0
4	SO4	D	2003	5/5	0.96	0.19	61,69,83,91	0
2	FAD	C	2001	53/53	0.96	0.16	49,60,77,85	0
2	FAD	B	2001	53/53	0.97	0.18	50,63,74,83	0
2	FAD	A	2001	53/53	0.98	0.15	30,41,58,64	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.

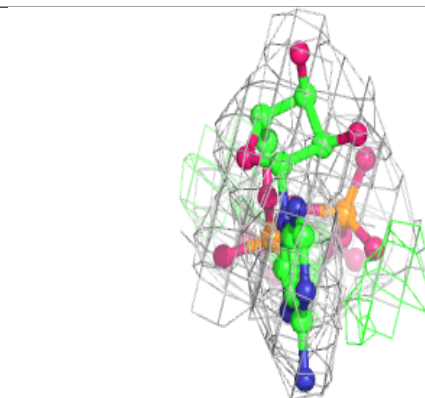
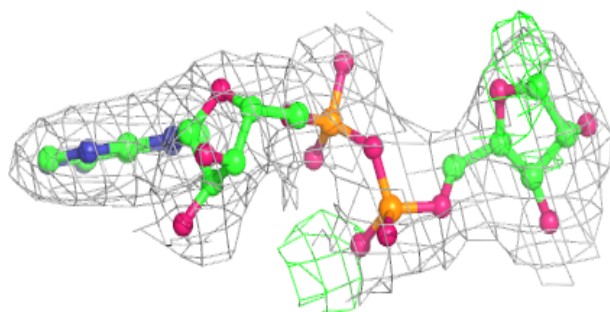
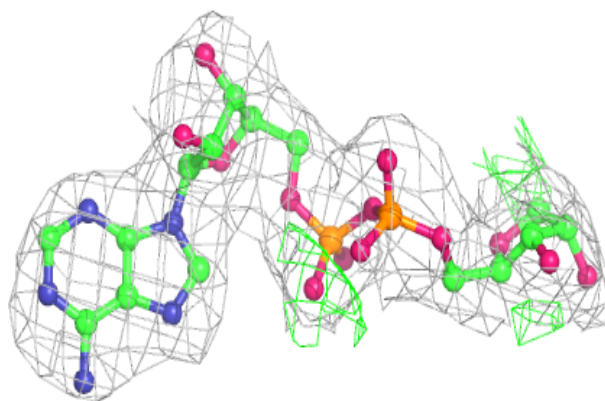
Electron density around NAD C 2002:

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

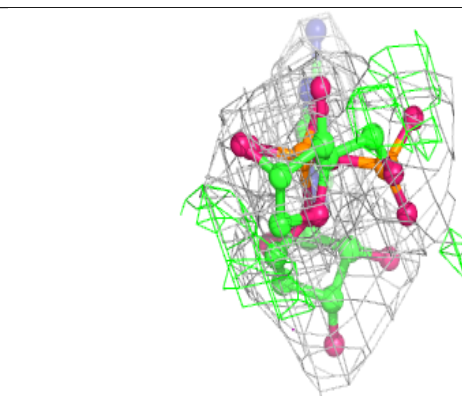
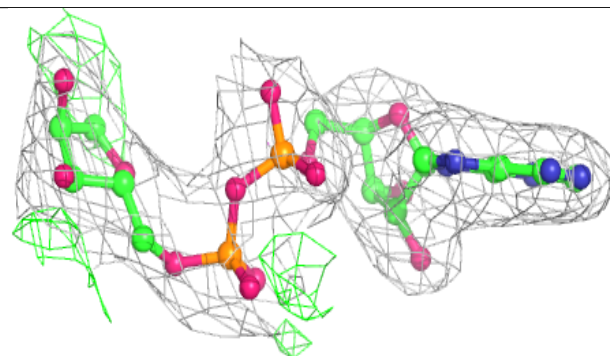
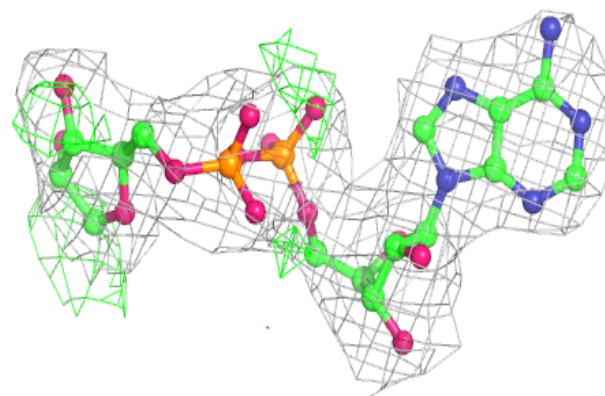


Electron density around NAD B 2002:

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

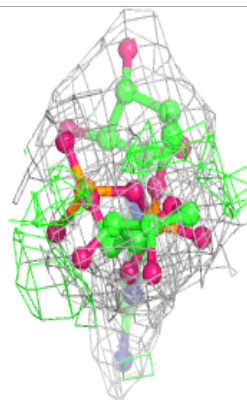
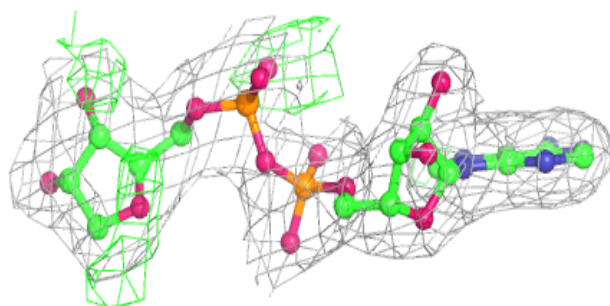
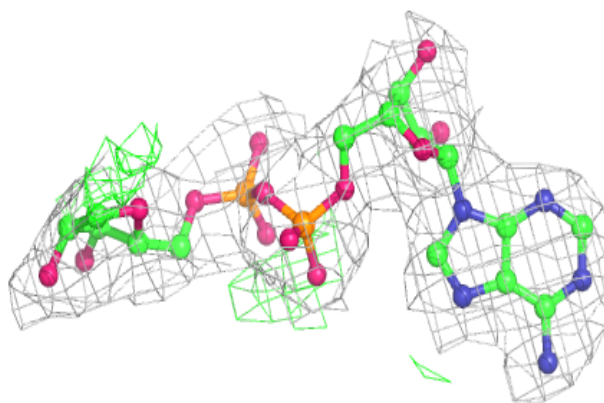
**Electron density around NAD D 2002:**

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

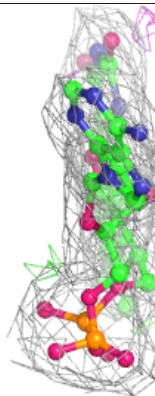
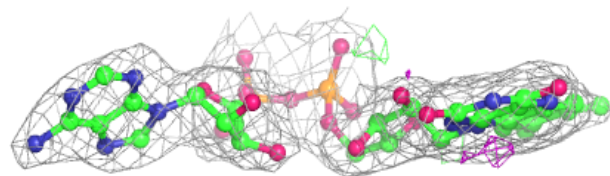
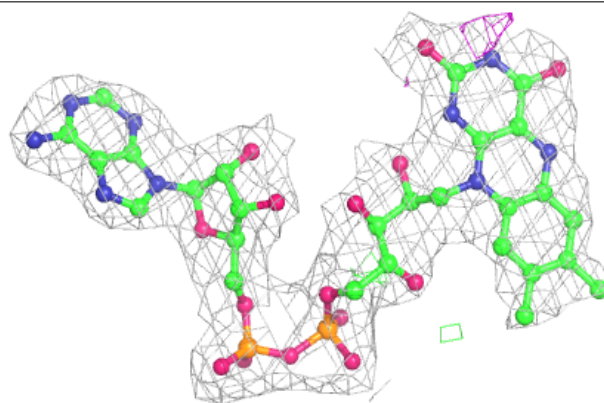


Electron density around NAD A 2002:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

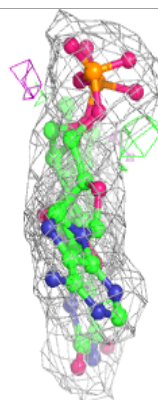
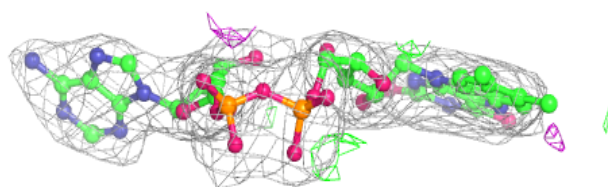
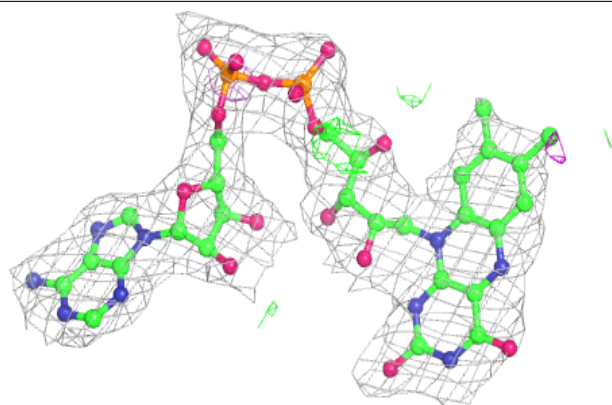
**Electron density around FAD D 2001:**

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

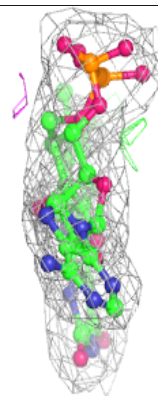
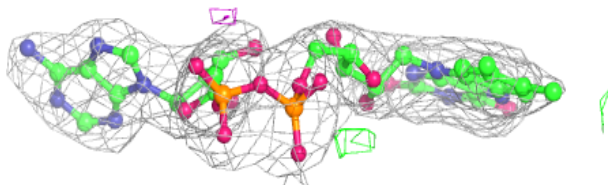
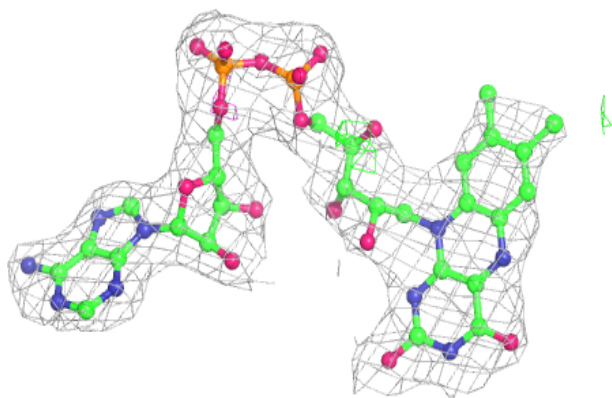


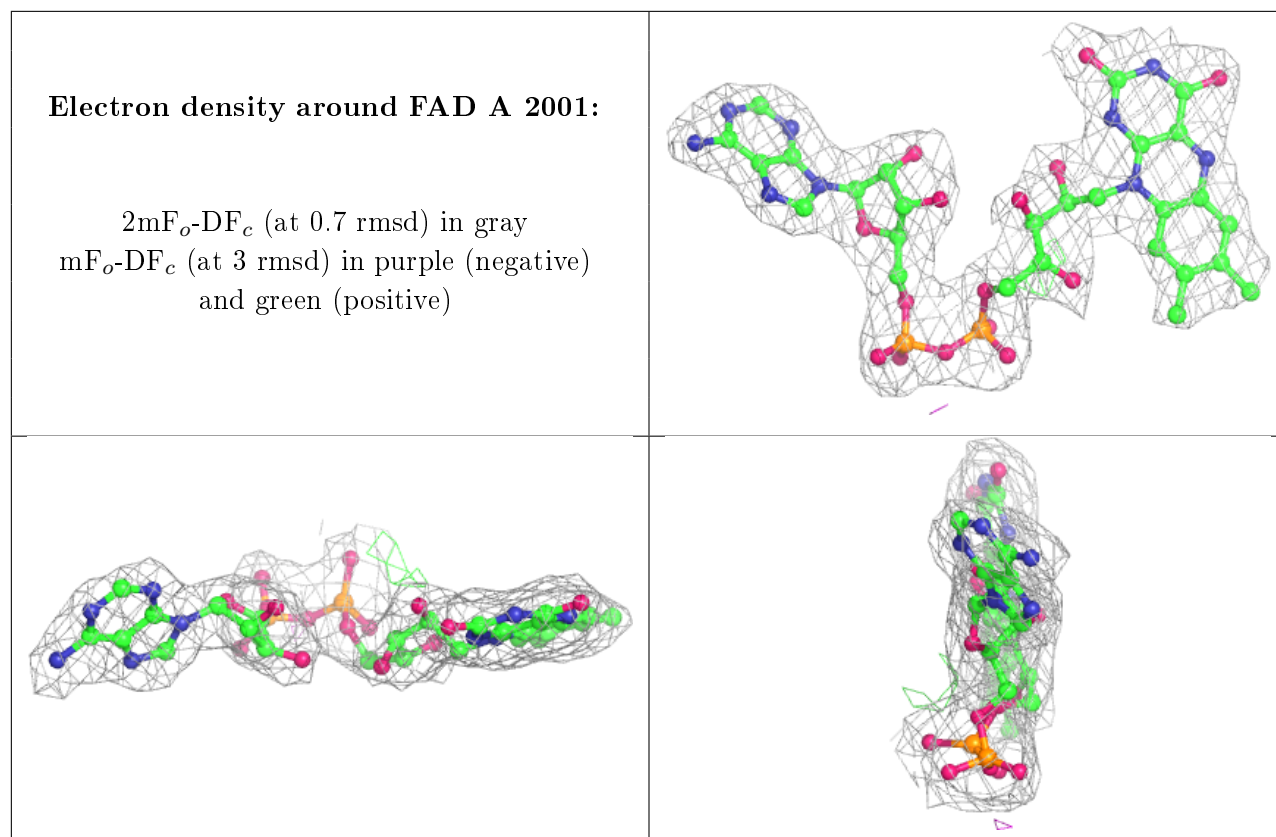
Electron density around FAD C 2001:

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

**Electron density around FAD B 2001:**

$2mF_o-DF_c$ (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.