Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 05:42 AM EST

PDB ID	:	3HAZ
Title	:	Crystal structure of bifunctional proline utilization A (PutA) protein
Authors	:	Tanner, J.J.
Deposited on	:	2009-05-03
Resolution	:	2.10 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:

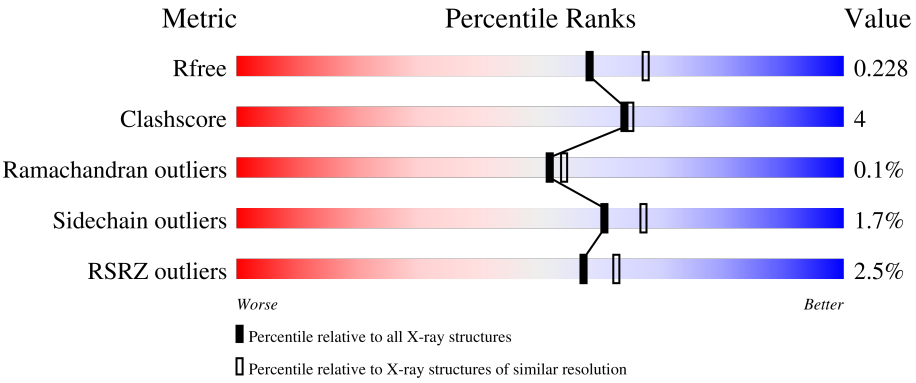
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	1001	2% 89% 9% .
1	B	1001	3% 88% 9% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15737 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.

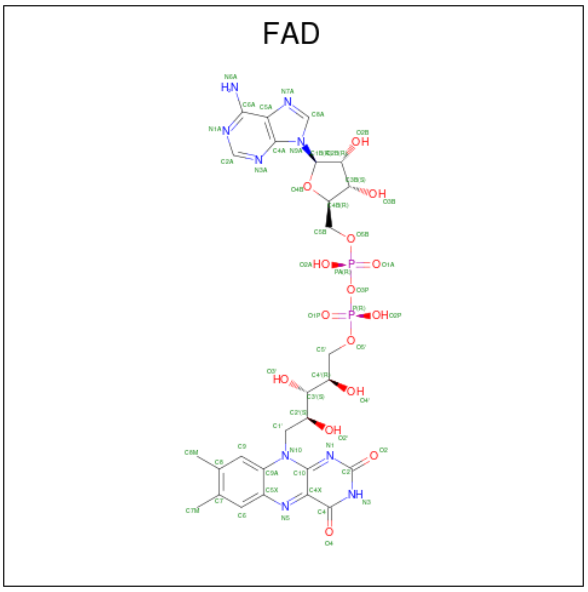
- Molecule 1 is a protein called Proline dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	983	Total	C	N	O	S	0	1	0
			7363	4639	1337	1362	25			
1	B	974	Total	C	N	O	S	0	1	0
			7284	4593	1312	1355	24			

There are 4 discrepancies between the modelled and reference sequences:

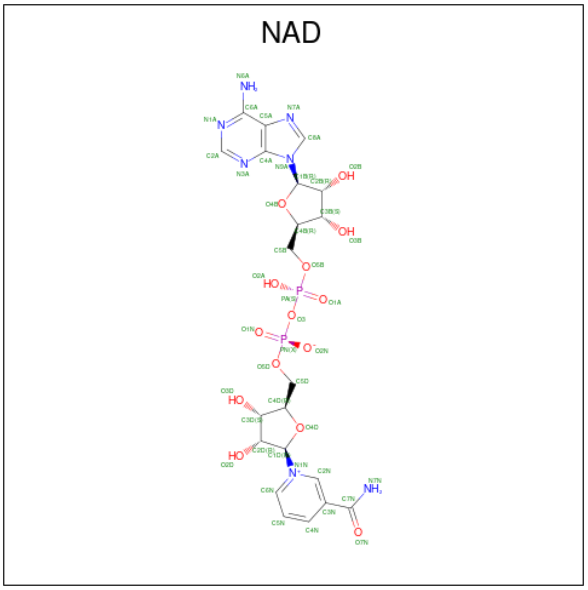
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q89E26
A	0	HIS	-	expression tag	UNP Q89E26
B	-1	GLY	-	expression tag	UNP Q89E26
B	0	HIS	-	expression tag	UNP Q89E26

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



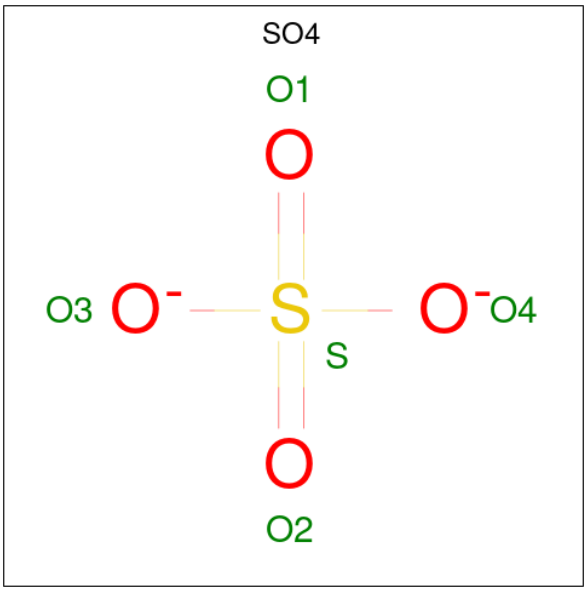
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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



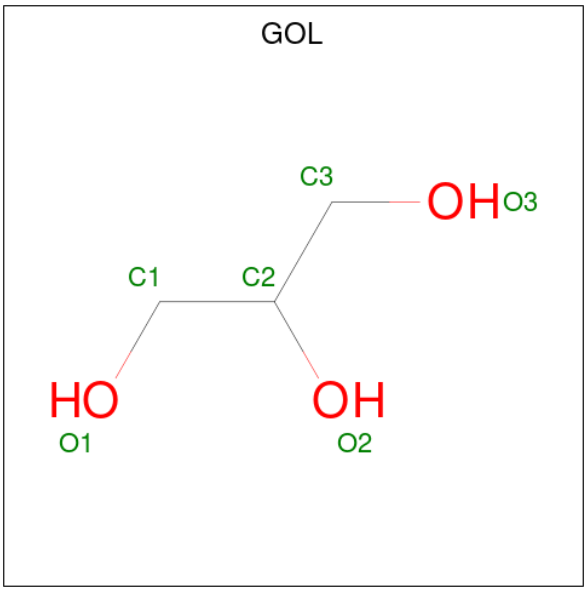
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

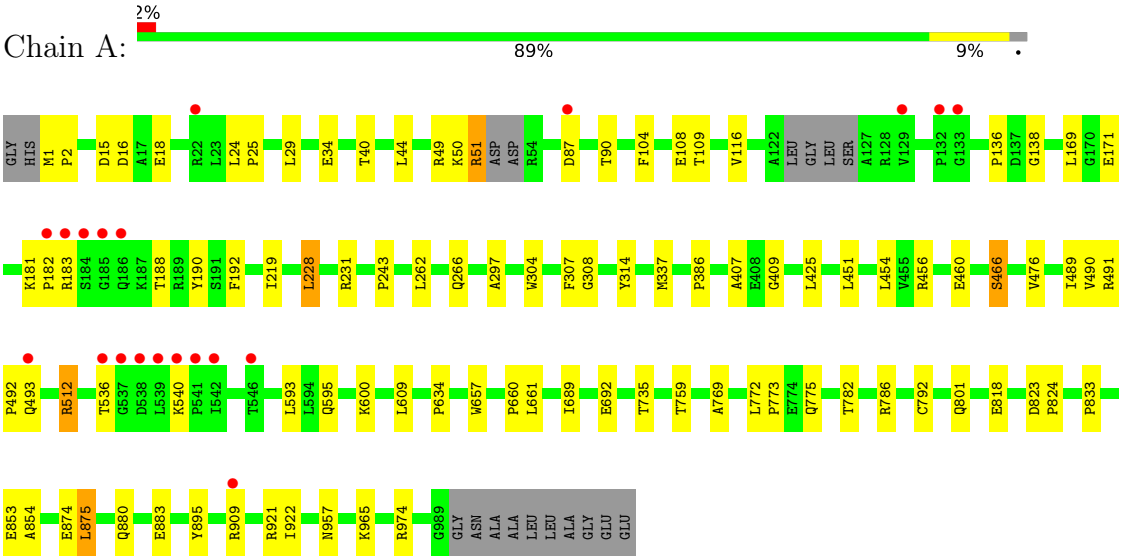
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	442	Total O 442 442	0	0
6	B	353	Total O 353 353	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

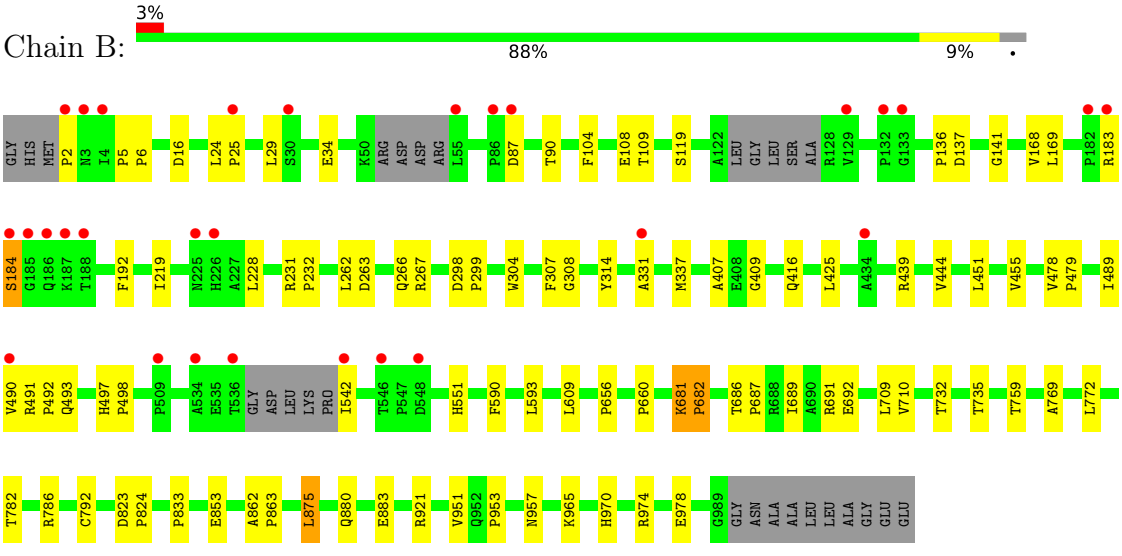
• Molecule 1: Proline dehydrogenase

Chain A:



• Molecule 1: Proline dehydrogenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.76Å 195.85Å 108.68Å 90.00° 121.48° 90.00°	Depositor
Resolution (Å)	42.33 – 2.10 42.32 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.33-2.10) 100.0 (42.32-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.200 , 0.233 0.195 , 0.228	Depositor DCC
R_{free} test set	8703 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15737	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FAD, NAD, GOL, SO4

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	0.28	0/7510	0.45	0/10206
1	B	0.27	0/7429	0.44	0/10101
All	All	0.28	0/14939	0.45	0/20307

There are no bond length outliers.

There are no bond angle outliers.

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	7363	0	7338	64	0
1	B	7284	0	7229	63	0
2	A	53	0	30	0	0
2	B	53	0	31	1	0
3	A	44	0	26	5	0
3	B	44	0	26	5	0
4	A	35	0	0	1	0
4	B	30	0	0	0	0
5	A	18	0	24	1	0
5	B	18	0	24	1	0
6	A	442	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	353	0	0	0	0
All	All	15737	0	14728	124	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 4.

All (124) 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:491:ARG:HD2	1:B:492:PRO:HD2	1.44	1.00
1:A:491:ARG:HD2	1:A:492:PRO:HD2	1.51	0.91
1:B:792[B]:CYS:SG	3:B:2004:NAD:C6N	2.67	0.83
1:A:188:THR:HG22	1:A:190:TYR:H	1.44	0.80
1:A:792[B]:CYS:SG	3:A:2003:NAD:C6N	2.73	0.76
1:B:108:GLU:HG3	1:B:921:ARG:HH11	1.53	0.73
1:B:109:THR:HG23	1:B:769:ALA:HB3	1.73	0.67
1:B:593:LEU:HD21	1:B:692:GLU:HG3	1.78	0.65
1:B:660:PRO:HB2	1:B:689:ILE:HG21	1.78	0.65
1:B:489:ILE:O	1:B:490:VAL:HG22	1.98	0.65
1:A:792[B]:CYS:SG	3:A:2003:NAD:C5N	2.85	0.64
1:A:772:LEU:HD23	1:A:775:GLN:HG2	1.82	0.62
1:B:416:GLN:HG2	1:B:439:ARG:HB3	1.81	0.61
1:A:109:THR:HG22	6:A:1423:HOH:O	2.00	0.61
1:B:792[B]:CYS:SG	3:B:2004:NAD:C5N	2.90	0.60
1:B:29:LEU:HB2	1:B:34:GLU:OE2	2.01	0.60
1:B:686:THR:N	1:B:687:PRO:HD3	2.17	0.60
1:A:108:GLU:HG3	1:A:921:ARG:HH11	1.67	0.59
1:A:489:ILE:O	1:A:490:VAL:HG22	2.04	0.58
1:A:593:LEU:HD21	1:A:692:GLU:HG3	1.85	0.58
1:B:87:ASP:HB3	1:B:90:THR:OG1	2.04	0.58
1:B:792[B]:CYS:SG	3:B:2004:NAD:N1N	2.77	0.57
1:B:656:PRO:HG3	1:B:732:THR:HG22	1.86	0.56
1:B:682:PRO:HG3	1:B:709:LEU:HD11	1.86	0.56
1:B:108:GLU:HG3	1:B:921:ARG:NH1	2.19	0.56
1:A:297:ALA:O	5:A:1009:GOL:H32	2.07	0.55
1:B:451:LEU:HB3	1:B:772:LEU:HD13	1.88	0.55
1:B:425:LEU:C	1:B:425:LEU:HD23	2.26	0.54
1:A:29:LEU:HB2	1:A:34:GLU:OE2	2.06	0.54
1:A:109:THR:HG23	1:A:769:ALA:HB3	1.89	0.54
1:A:735:THR:HA	1:A:759:THR:HG21	1.90	0.53
1:A:875:LEU:HG	1:A:880:GLN:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LEU:HB2	1:B:25:PRO:HD3	1.89	0.52
1:A:660:PRO:HB2	1:A:689:ILE:HG21	1.92	0.52
1:B:491:ARG:HD2	1:B:492:PRO:CD	2.31	0.52
1:B:681:LYS:HG2	1:B:710:VAL:O	2.10	0.52
1:A:824:PRO:HD3	1:A:833:PRO:HD3	1.92	0.51
1:A:308:GLY:HA3	1:A:337:MET:O	2.09	0.51
1:A:634:PRO:O	1:B:951:VAL:HG22	2.11	0.51
1:B:593:LEU:HD23	1:B:689:ILE:HD12	1.93	0.51
1:A:87:ASP:O	1:A:90:THR:HB	2.12	0.50
1:B:262:LEU:O	1:B:266:GLN:HG3	2.11	0.50
1:A:491:ARG:CG	1:A:493:GLN:HG2	2.42	0.50
1:A:965:LYS:HD2	1:B:978:GLU:CB	2.41	0.50
1:A:116:VAL:HG11	1:A:773:PRO:HG2	1.94	0.50
1:A:456:ARG:NH1	4:A:1006:SO4:O2	2.45	0.49
1:A:801:GLN:HG3	1:A:895:TYR:CZ	2.48	0.49
1:A:1:MET:N	1:A:2:PRO:CD	2.75	0.49
1:A:192:PHE:CD2	1:A:219:ILE:HD11	2.48	0.49
1:A:451:LEU:HB3	1:A:772:LEU:HD13	1.95	0.49
1:B:735:THR:HA	1:B:759:THR:HG21	1.94	0.49
1:A:192:PHE:CG	1:A:219:ILE:HD11	2.48	0.48
1:B:228:LEU:CD1	1:B:231:ARG:HD3	2.42	0.48
1:B:824:PRO:HD3	1:B:833:PRO:HD3	1.95	0.48
1:A:792[B]:CYS:SG	3:A:2003:NAD:N1N	2.87	0.48
1:A:657:TRP:O	1:A:660:PRO:HG3	2.13	0.48
1:B:192:PHE:CG	1:B:219:ILE:HD11	2.49	0.48
1:B:407:ALA:C	1:B:409:GLY:H	2.17	0.48
1:A:50:LYS:O	1:A:51:ARG:HG2	2.14	0.47
1:A:460:GLU:OE2	1:A:466:SER:HB2	2.15	0.47
1:A:540:LYS:O	1:A:540:LYS:HG3	2.14	0.47
1:B:590:PHE:HD2	1:B:689:ILE:HD11	1.80	0.47
1:B:792[B]:CYS:SG	3:B:2004:NAD:H2D	2.55	0.47
1:B:782:THR:O	1:B:786:ARG:HB3	2.15	0.46
1:A:425:LEU:C	1:A:425:LEU:HD23	2.35	0.46
1:B:2:PRO:HB2	1:B:331:ALA:HA	1.98	0.46
1:A:304:TRP:CZ3	1:A:307:PHE:HB2	2.51	0.46
1:A:171:GLU:HG3	6:A:1187:HOH:O	2.15	0.46
1:A:491:ARG:HG2	1:A:493:GLN:HG2	1.98	0.46
1:B:970:HIS:CE1	5:B:1008:GOL:H12	2.50	0.46
1:B:29:LEU:HD12	1:B:34:GLU:OE2	2.16	0.45
1:A:24:LEU:HB2	1:A:25:PRO:HD3	1.97	0.45
1:A:595:GLN:HG2	1:A:600:LYS:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:THR:O	1:A:786:ARG:HB3	2.17	0.45
1:A:965:LYS:HD2	1:B:978:GLU:HB2	1.98	0.45
1:B:108:GLU:CG	1:B:921:ARG:HH11	2.25	0.45
1:B:263:ASP:O	1:B:267:ARG:HG3	2.17	0.45
1:B:304:TRP:CZ3	1:B:307:PHE:HB2	2.52	0.45
1:B:491:ARG:HE	1:B:493:GLN:HB3	1.83	0.44
1:B:109:THR:CG2	1:B:769:ALA:HB3	2.44	0.44
1:A:104:PHE:CE2	1:A:136:PRO:HA	2.52	0.44
1:A:823:ASP:HA	1:A:824:PRO:HD2	1.88	0.44
1:B:497:HIS:ND1	1:B:498:PRO:HD2	2.32	0.44
1:A:792[B]:CYS:SG	3:A:2003:NAD:C4N	3.06	0.44
1:B:308:GLY:HA3	1:B:337:MET:O	2.18	0.44
1:B:953:PRO:HB2	1:B:965:LYS:HD3	2.00	0.44
1:A:491:ARG:HE	1:A:493:GLN:HB3	1.82	0.44
1:B:192:PHE:CD2	1:B:219:ILE:HD11	2.53	0.44
1:A:974:ARG:NH2	1:B:974:ARG:NH1	2.66	0.43
1:A:512:ARG:H	1:A:512:ARG:HG2	1.58	0.43
1:A:921:ARG:NH1	6:A:1021:HOH:O	2.50	0.43
1:A:262:LEU:O	1:A:266:GLN:HG3	2.18	0.43
1:A:386:PRO:HD2	6:A:1234:HOH:O	2.17	0.43
1:B:168:VAL:HB	1:B:444:VAL:HG22	2.01	0.43
1:B:451:LEU:O	1:B:455:VAL:HG23	2.19	0.43
1:A:181:LYS:HA	1:A:182:PRO:HD3	1.80	0.43
1:B:691:ARG:HA	1:B:709:LEU:HD22	2.01	0.42
1:B:792[B]:CYS:SG	3:B:2004:NAD:C2N	3.07	0.42
1:B:875:LEU:HG	1:B:880:GLN:HB2	2.01	0.42
1:A:228:LEU:HD13	1:A:231:ARG:HD3	2.00	0.42
1:A:609:LEU:C	1:A:609:LEU:HD13	2.39	0.42
1:A:854:ALA:HB1	1:A:874:GLU:O	2.19	0.42
1:B:298:ASP:HA	1:B:299:PRO:HD3	1.87	0.42
1:A:40:THR:O	1:A:44:LEU:HG	2.19	0.42
1:A:108:GLU:HG3	1:A:921:ARG:NH1	2.34	0.42
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.93	0.42
1:B:823:ASP:HA	1:B:824:PRO:HD2	1.87	0.42
1:A:661:LEU:HB2	1:A:689:ILE:CD1	2.50	0.42
1:B:104:PHE:CE2	1:B:136:PRO:HA	2.54	0.42
1:B:5:PRO:HA	1:B:6:PRO:HD3	1.94	0.41
1:B:609:LEU:HD13	1:B:609:LEU:C	2.41	0.41
1:B:478:VAL:HB	1:B:479:PRO:HD3	2.02	0.41
1:B:542:ILE:HG12	1:B:691:ARG:NH2	2.36	0.41
1:B:862:ALA:HA	1:B:863:PRO:HD3	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASP:O	1:B:141:GLY:HA3	2.21	0.41
1:B:183:ARG:O	1:B:184:SER:HB2	2.21	0.41
1:A:243:PRO:HB2	1:A:818:GLU:HG3	2.01	0.41
1:A:407:ALA:C	1:A:409:GLY:H	2.23	0.41
1:A:792[B]:CYS:SG	3:A:2003:NAD:C2N	3.09	0.40
1:A:15:ASP:OD2	1:A:18:GLU:HG3	2.21	0.40
1:A:138:GLY:HA2	1:A:922:ILE:HG23	2.04	0.40
2:B:2002:FAD:H1'1	2:B:2002:FAD:H4'	1.89	0.40
1:B:219:ILE:CG2	1:B:232:PRO:HB2	2.51	0.40
1:A:49:ARG:NH2	1:A:476:VAL:O	2.49	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	978/1001 (98%)	952 (97%)	25 (3%)	1 (0%)	51	54
1	B	967/1001 (97%)	944 (98%)	22 (2%)	1 (0%)	51	54
All	All	1945/2002 (97%)	1896 (98%)	47 (2%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	ARG
1	B	184	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	725/758 (96%)	712 (98%)	13 (2%)	59	65
1	B	716/758 (94%)	705 (98%)	11 (2%)	65	71
All	All	1441/1516 (95%)	1417 (98%)	24 (2%)	60	67

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	51	ARG
1	A	169	LEU
1	A	228	LEU
1	A	314	TYR
1	A	466	SER
1	A	512	ARG
1	A	536	THR
1	A	853	GLU
1	A	875	LEU
1	A	883	GLU
1	A	909	ARG
1	A	957	ASN
1	B	16	ASP
1	B	119	SER
1	B	169	LEU
1	B	314	TYR
1	B	551	HIS
1	B	681	LYS
1	B	682	PRO
1	B	853	GLU
1	B	875	LEU
1	B	883	GLU
1	B	957	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	A	483	GLN
1	A	551	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	775	GLN
1	B	186	GLN
1	B	419	HIS
1	B	464	ASN
1	B	483	GLN
1	B	934	GLN
1	B	957	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

23 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	$\#\|Z\| > 2$
4	SO4	B	1005	-	4,4,4	0.14	0	6,6,6	0.09	0
5	GOL	B	1008	-	5,5,5	0.38	0	5,5,5	0.35	0
4	SO4	A	1005	-	4,4,4	0.14	0	6,6,6	0.08	0
4	SO4	B	1004	-	4,4,4	0.13	0	6,6,6	0.05	0
5	GOL	A	1007	-	5,5,5	0.37	0	5,5,5	0.37	0
2	FAD	B	2002	-	53,58,58	3.34	24 (45%)	68,89,89	1.59	13 (19%)
4	SO4	B	1001	-	4,4,4	0.15	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	B	1007	-	5,5,5	0.33	0	5,5,5	0.41	0
4	SO4	A	1003	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	A	1000	-	4,4,4	0.17	0	6,6,6	0.18	0
4	SO4	B	1003	-	4,4,4	0.13	0	6,6,6	0.08	0
5	GOL	A	1008	-	5,5,5	0.34	0	5,5,5	0.47	0
5	GOL	A	1009	-	5,5,5	0.39	0	5,5,5	0.28	0
4	SO4	A	1004	-	4,4,4	0.13	0	6,6,6	0.08	0
5	GOL	B	1006	-	5,5,5	0.37	0	5,5,5	0.36	0
2	FAD	A	2001	-	53,58,58	3.30	24 (45%)	68,89,89	1.64	15 (22%)
4	SO4	A	1002	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	B	1000	-	4,4,4	0.15	0	6,6,6	0.12	0
4	SO4	A	1006	-	4,4,4	0.12	0	6,6,6	0.11	0
3	NAD	A	2003	-	42,48,48	2.88	19 (45%)	50,73,73	1.66	11 (22%)
4	SO4	B	1002	-	4,4,4	0.14	0	6,6,6	0.09	0
3	NAD	B	2004	-	42,48,48	2.91	21 (50%)	50,73,73	1.75	14 (28%)
4	SO4	A	1001	-	4,4,4	0.18	0	6,6,6	0.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	1007	-	-	2/4/4/4	-
3	NAD	A	2003	-	-	6/26/62/62	0/5/5/5
5	GOL	A	1009	-	-	4/4/4/4	-
5	GOL	B	1006	-	-	0/4/4/4	-
5	GOL	B	1008	-	-	4/4/4/4	-
2	FAD	A	2001	-	-	6/30/50/50	0/6/6/6
5	GOL	A	1007	-	-	0/4/4/4	-
2	FAD	B	2002	-	-	4/30/50/50	0/6/6/6
5	GOL	A	1008	-	-	2/4/4/4	-
3	NAD	B	2004	-	-	8/26/62/62	0/5/5/5

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	FAD	C4X-N5	10.15	1.50	1.30
2	A	2001	FAD	C4X-N5	9.92	1.50	1.30
2	A	2001	FAD	O4-C4	8.91	1.40	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	FAD	O4-C4	8.80	1.40	1.23
2	A	2001	FAD	C2A-N3A	7.97	1.44	1.32
2	B	2002	FAD	C2A-N3A	7.92	1.44	1.32
2	B	2002	FAD	O2-C2	7.62	1.38	1.24
2	A	2001	FAD	O2-C2	7.54	1.38	1.24
3	B	2004	NAD	C7N-N7N	6.48	1.45	1.33
3	A	2003	NAD	C7N-N7N	6.48	1.45	1.33
3	A	2003	NAD	C4N-C3N	5.58	1.48	1.39
3	B	2004	NAD	C4N-C3N	5.44	1.48	1.39
3	B	2004	NAD	C2N-N1N	5.31	1.41	1.35
3	B	2004	NAD	C2N-C3N	5.14	1.47	1.39
3	A	2003	NAD	C2N-N1N	5.12	1.41	1.35
2	A	2001	FAD	C9-C9A	5.06	1.47	1.39
2	B	2002	FAD	C9-C9A	5.04	1.47	1.39
3	B	2004	NAD	C6N-N1N	4.97	1.47	1.35
3	A	2003	NAD	C6N-N1N	4.95	1.47	1.35
2	A	2001	FAD	C6-C5X	4.79	1.47	1.40
3	A	2003	NAD	C2N-C3N	4.79	1.46	1.39
2	B	2002	FAD	C3B-C4B	-4.76	1.40	1.53
2	B	2002	FAD	C6-C5X	4.76	1.47	1.40
3	A	2003	NAD	C8A-N7A	4.69	1.43	1.34
2	A	2001	FAD	C3B-C4B	-4.68	1.41	1.53
2	A	2001	FAD	C10-N1	4.66	1.42	1.33
3	B	2004	NAD	C8A-N7A	4.64	1.43	1.34
2	B	2002	FAD	C10-N1	4.61	1.42	1.33
2	A	2001	FAD	P-O1P	4.61	1.67	1.50
2	B	2002	FAD	P-O1P	4.59	1.67	1.50
3	A	2003	NAD	PN-O1N	4.55	1.67	1.50
3	B	2004	NAD	C6N-C5N	4.45	1.48	1.38
3	A	2003	NAD	C6N-C5N	4.44	1.48	1.38
3	B	2004	NAD	PN-O1N	4.44	1.66	1.50
3	B	2004	NAD	C2B-C1B	-4.41	1.47	1.53
3	A	2003	NAD	C2B-C1B	-4.37	1.47	1.53
2	B	2002	FAD	O4B-C4B	4.36	1.54	1.45
2	B	2002	FAD	C2A-N1A	4.11	1.41	1.33
2	A	2001	FAD	C2A-N1A	3.99	1.41	1.33
3	B	2004	NAD	C2D-C1D	-3.97	1.47	1.53
3	A	2003	NAD	C2D-C1D	-3.90	1.47	1.53
3	B	2004	NAD	PA-O1A	3.85	1.64	1.50
3	A	2003	NAD	PA-O1A	3.83	1.64	1.50
2	A	2001	FAD	O4B-C4B	3.78	1.53	1.45
2	A	2001	FAD	PA-O1A	3.65	1.63	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	FAD	C10-N10	3.59	1.45	1.37
2	B	2002	FAD	PA-O1A	3.56	1.63	1.50
2	B	2002	FAD	C6A-N6A	3.50	1.46	1.34
2	A	2001	FAD	C10-N10	3.49	1.44	1.37
2	A	2001	FAD	C6A-N6A	3.34	1.46	1.34
2	A	2001	FAD	C9A-N10	3.30	1.46	1.41
3	B	2004	NAD	C6A-N6A	3.25	1.45	1.34
3	A	2003	NAD	C6A-N6A	3.23	1.45	1.34
3	A	2003	NAD	C2A-N3A	3.23	1.37	1.32
2	B	2002	FAD	C9A-N10	3.21	1.46	1.41
3	B	2004	NAD	C2A-N3A	3.17	1.37	1.32
2	A	2001	FAD	C8-C7	3.10	1.48	1.40
2	A	2001	FAD	C2B-C1B	-3.04	1.49	1.53
3	A	2003	NAD	O7N-C7N	-3.04	1.18	1.24
2	B	2002	FAD	C8-C7	3.02	1.48	1.40
3	B	2004	NAD	O7N-C7N	-3.01	1.18	1.24
2	B	2002	FAD	C5'-C4'	2.90	1.55	1.51
2	B	2002	FAD	C2B-C1B	-2.76	1.49	1.53
2	A	2001	FAD	C5'-C4'	2.73	1.55	1.51
3	B	2004	NAD	C2A-N1A	2.71	1.39	1.33
3	A	2003	NAD	C2A-N1A	2.70	1.38	1.33
3	B	2004	NAD	C3N-C7N	2.59	1.54	1.50
3	A	2003	NAD	C3N-C7N	2.52	1.54	1.50
3	A	2003	NAD	C3D-C4D	2.50	1.59	1.53
3	B	2004	NAD	C3D-C4D	2.40	1.59	1.53
3	B	2004	NAD	O4D-C4D	2.34	1.50	1.45
3	B	2004	NAD	C3B-C4B	2.32	1.58	1.53
2	B	2002	FAD	C2-N3	2.30	1.44	1.39
3	A	2003	NAD	C3B-C4B	2.28	1.58	1.53
2	B	2002	FAD	C4'-C3'	2.22	1.57	1.53
2	A	2001	FAD	C2-N3	2.17	1.44	1.39
2	A	2001	FAD	C4'-C3'	2.17	1.57	1.53
3	A	2003	NAD	O4D-C4D	2.13	1.49	1.45
2	B	2002	FAD	C1'-C2'	2.11	1.55	1.52
2	A	2001	FAD	C5A-C4A	-2.11	1.35	1.40
2	B	2002	FAD	C5A-C4A	-2.09	1.35	1.40
3	B	2004	NAD	PA-O5B	2.08	1.67	1.59
3	B	2004	NAD	PN-O5D	2.08	1.67	1.59
2	A	2001	FAD	O4'-C4'	-2.05	1.39	1.43
2	A	2001	FAD	C4X-C10	-2.05	1.38	1.44
2	A	2001	FAD	C6A-C5A	2.04	1.50	1.43
2	B	2002	FAD	C4X-C10	-2.03	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	FAD	C6A-C5A	2.03	1.50	1.43

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	FAD	N3A-C2A-N1A	-5.95	119.38	128.68
2	B	2002	FAD	N3A-C2A-N1A	-5.75	119.70	128.68
3	A	2003	NAD	N3A-C2A-N1A	-5.52	120.04	128.68
3	B	2004	NAD	N3A-C2A-N1A	-5.49	120.09	128.68
3	A	2003	NAD	PN-O3-PA	-3.85	119.60	132.83
3	B	2004	NAD	PN-O3-PA	-3.70	120.14	132.83
2	A	2001	FAD	O4'-C4'-C3'	3.37	117.29	109.10
2	A	2001	FAD	C5B-C4B-C3B	3.31	127.57	115.18
2	A	2001	FAD	O4B-C4B-C5B	3.12	119.64	109.37
3	A	2003	NAD	O3B-C3B-C4B	3.09	120.00	111.05
2	B	2002	FAD	C4-N3-C2	-3.07	119.97	125.64
3	B	2004	NAD	O4D-C4D-C5D	3.05	119.40	109.37
2	A	2001	FAD	O3B-C3B-C2B	2.96	121.38	111.82
3	B	2004	NAD	O3B-C3B-C4B	2.94	119.55	111.05
3	A	2003	NAD	O2D-C2D-C3D	2.93	121.29	111.82
2	A	2001	FAD	C4-N3-C2	-2.91	120.26	125.64
3	A	2003	NAD	O3D-C3D-C4D	2.87	119.34	111.05
2	A	2001	FAD	C3B-C2B-C1B	2.87	105.29	100.98
3	B	2004	NAD	O3D-C3D-C4D	2.82	119.20	111.05
3	B	2004	NAD	O2D-C2D-C3D	2.82	120.94	111.82
2	A	2001	FAD	C4X-C10-N10	2.81	120.59	116.48
2	B	2002	FAD	C4X-C4-N3	2.79	120.27	113.19
2	B	2002	FAD	C4X-C10-N10	2.77	120.53	116.48
2	B	2002	FAD	O4-C4-C4X	-2.74	119.33	126.60
3	A	2003	NAD	O3B-C3B-C2B	2.72	120.61	111.82
2	B	2002	FAD	O4'-C4'-C3'	2.70	115.68	109.10
2	B	2002	FAD	P-O3P-PA	-2.69	123.59	132.83
2	A	2001	FAD	C4X-C4-N3	2.69	120.01	113.19
3	A	2003	NAD	O2D-C2D-C1D	2.68	120.77	110.85
2	B	2002	FAD	O3B-C3B-C2B	2.68	120.49	111.82
2	A	2001	FAD	O3B-C3B-C4B	2.64	118.69	111.05
3	B	2004	NAD	O2D-C2D-C1D	2.63	120.58	110.85
2	A	2001	FAD	O4-C4-C4X	-2.60	119.71	126.60
2	B	2002	FAD	O3B-C3B-C4B	2.60	118.56	111.05
3	B	2004	NAD	O3B-C3B-C2B	2.58	120.17	111.82
3	B	2004	NAD	O2B-C2B-C3B	2.58	120.17	111.82
3	B	2004	NAD	O5D-C5D-C4D	2.52	117.66	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2003	NAD	O2B-C2B-C3B	2.52	119.96	111.82
2	B	2002	FAD	O4B-C4B-C5B	2.48	117.53	109.37
2	A	2001	FAD	P-O3P-PA	-2.48	124.33	132.83
3	B	2004	NAD	O2B-C2B-C1B	2.46	119.93	110.85
3	A	2003	NAD	O2B-C2B-C1B	2.42	119.78	110.85
3	B	2004	NAD	C3N-C7N-N7N	2.41	120.65	117.75
2	B	2002	FAD	C10-C4X-N5	-2.41	119.75	124.86
2	A	2001	FAD	O4B-C4B-C3B	2.40	109.86	105.11
2	B	2002	FAD	C3B-C2B-C1B	2.34	104.49	100.98
3	B	2004	NAD	O3D-C3D-C2D	2.33	119.35	111.82
2	A	2001	FAD	C10-C4X-N5	-2.30	119.98	124.86
2	B	2002	FAD	C9A-C5X-N5	-2.21	120.03	122.43
3	A	2003	NAD	O3D-C3D-C2D	2.20	118.95	111.82
3	A	2003	NAD	O4D-C4D-C5D	2.17	116.51	109.37
2	A	2001	FAD	C9A-C5X-N5	-2.12	120.13	122.43
3	B	2004	NAD	O7N-C7N-N7N	-2.09	119.61	122.58

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	FAD	N10-C1'-C2'-O2'
2	A	2001	FAD	N10-C1'-C2'-C3'
2	A	2001	FAD	C1'-C2'-C3'-C4'
2	B	2002	FAD	N10-C1'-C2'-O2'
2	B	2002	FAD	N10-C1'-C2'-C3'
2	B	2002	FAD	C1'-C2'-C3'-C4'
3	A	2003	NAD	C5B-O5B-PA-O3
3	B	2004	NAD	C5B-O5B-PA-O1A
3	B	2004	NAD	C5B-O5B-PA-O2A
3	B	2004	NAD	C5B-O5B-PA-O3
5	A	1008	GOL	C1-C2-C3-O3
5	A	1009	GOL	O1-C1-C2-C3
5	B	1008	GOL	O1-C1-C2-O2
5	B	1008	GOL	O1-C1-C2-C3
3	B	2004	NAD	O4B-C4B-C5B-O5B
5	A	1009	GOL	O1-C1-C2-O2
3	B	2004	NAD	C3B-C4B-C5B-O5B
5	A	1009	GOL	C1-C2-C3-O3
5	B	1007	GOL	O1-C1-C2-C3
3	B	2004	NAD	C4D-C5D-O5D-PN
5	A	1008	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	2003	NAD	C4D-C5D-O5D-PN
5	B	1007	GOL	O1-C1-C2-O2
5	A	1009	GOL	O2-C2-C3-O3
5	B	1008	GOL	C1-C2-C3-O3
3	A	2003	NAD	C5B-O5B-PA-O1A
3	A	2003	NAD	C5B-O5B-PA-O2A
2	B	2002	FAD	C1'-C2'-C3'-O3'
3	A	2003	NAD	O4D-C4D-C5D-O5D
2	A	2001	FAD	C3B-C4B-C5B-O5B
2	A	2001	FAD	O4B-C4B-C5B-O5B
3	A	2003	NAD	O4B-C4B-C5B-O5B
5	B	1008	GOL	O2-C2-C3-O3
3	B	2004	NAD	O4D-C4D-C5D-O5D
2	A	2001	FAD	C3'-C4'-C5'-O5'
3	B	2004	NAD	C5D-O5D-PN-O1N

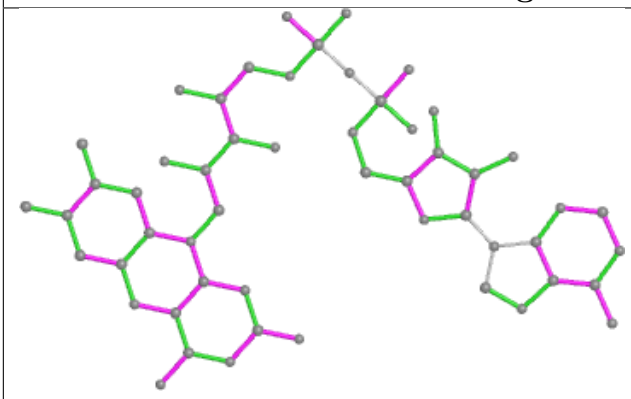
There are no ring outliers.

6 monomers are involved in 14 short contacts:

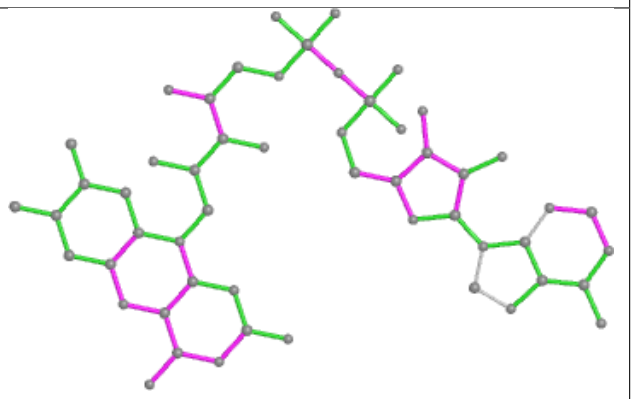
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1008	GOL	1	0
2	B	2002	FAD	1	0
5	A	1009	GOL	1	0
4	A	1006	SO4	1	0
3	A	2003	NAD	5	0
3	B	2004	NAD	5	0

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 then 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.

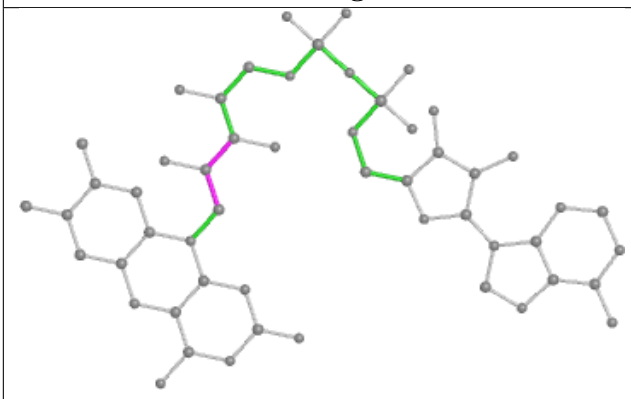
Ligand FAD B 2002



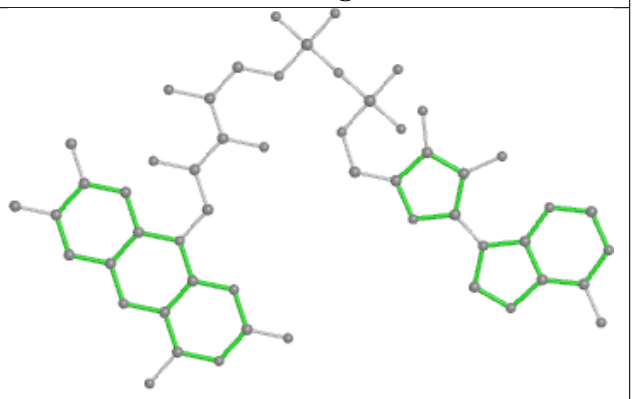
Bond lengths



Bond angles

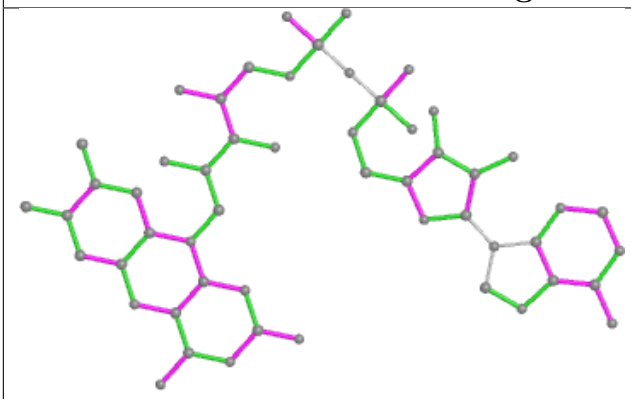


Torsions

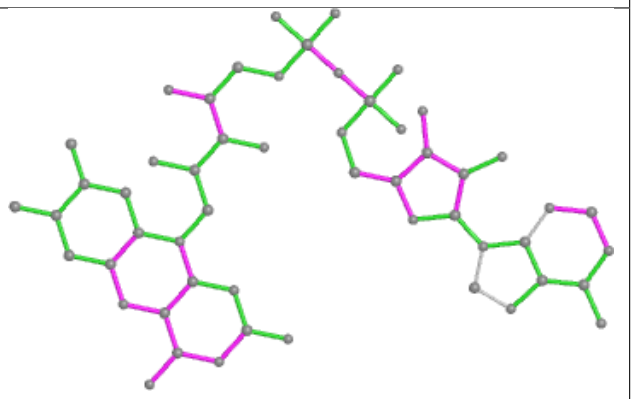


Rings

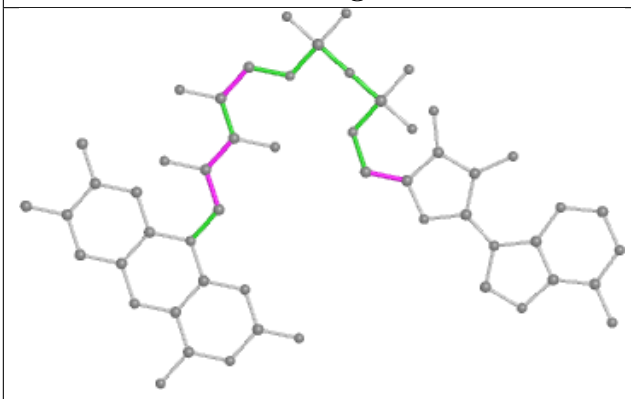
Ligand FAD A 2001



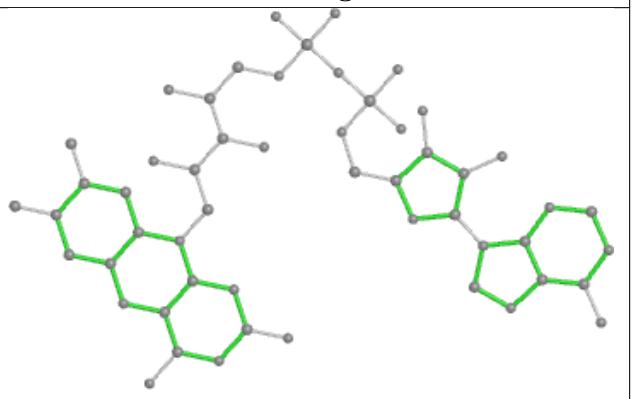
Bond lengths



Bond angles

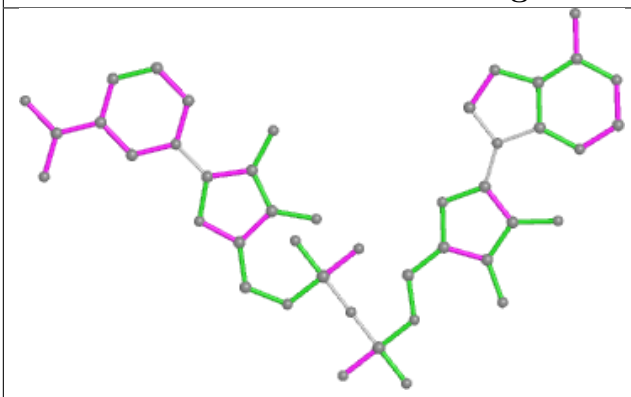


Torsions

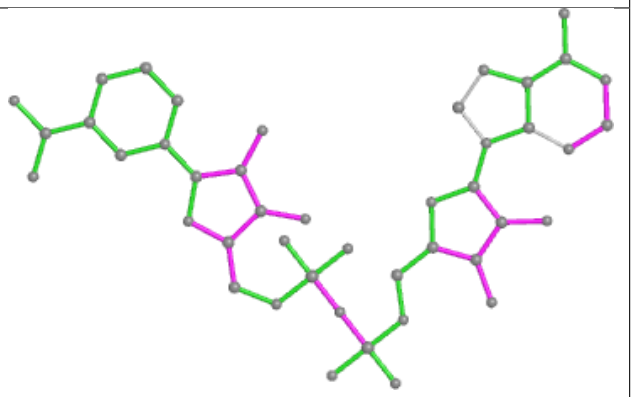


Rings

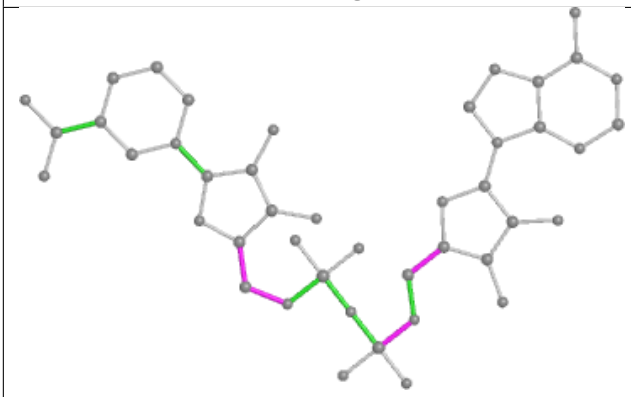
Ligand NAD A 2003



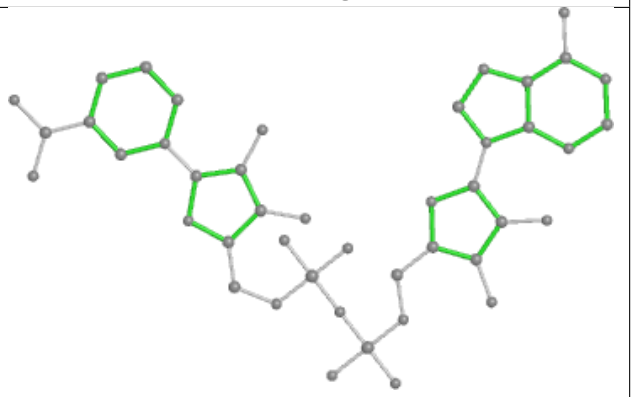
Bond lengths



Bond angles

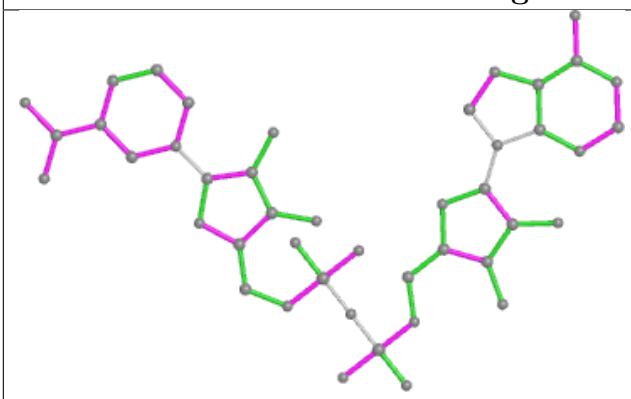


Torsions

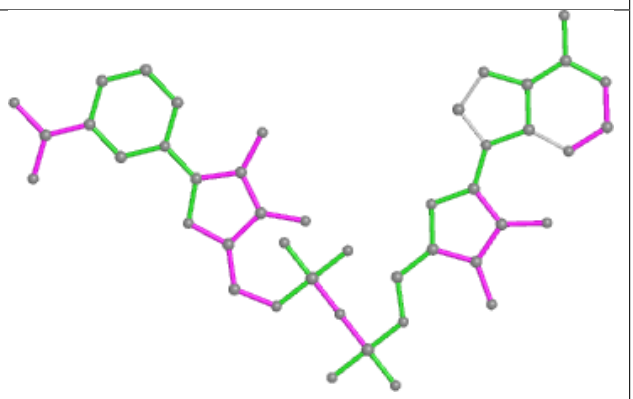


Rings

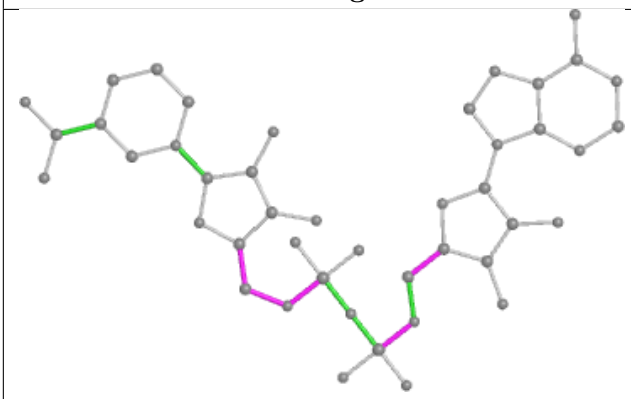
Ligand NAD B 2004



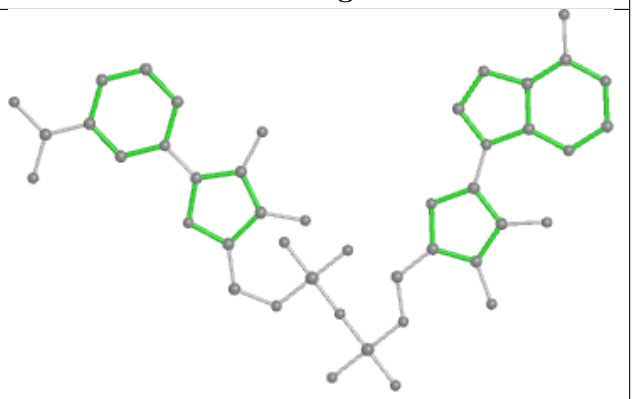
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	983/1001 (98%)	-0.15	20 (2%)	65	69	17, 29, 55, 138	0
1	B	974/1001 (97%)	-0.10	29 (2%)	50	56	18, 34, 60, 111	0
All	All	1957/2002 (97%)	-0.13	49 (2%)	57	62	17, 32, 58, 138	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	539	LEU	8.8
1	B	185	GLY	7.6
1	B	184	SER	5.9
1	A	541	PRO	5.8
1	A	183	ARG	5.8
1	A	184	SER	5.6
1	B	183	ARG	5.5
1	A	537	GLY	5.4
1	A	542	ILE	5.0
1	B	186	GLN	4.9
1	A	129	VAL	4.8
1	B	434	ALA	4.3
1	A	538	ASP	4.3
1	A	536	THR	4.1
1	A	185	GLY	3.9
1	B	129	VAL	3.6
1	B	133	GLY	3.5
1	B	536	THR	3.5
1	B	188	THR	3.4
1	B	542	ILE	3.4
1	B	225	ASN	3.2
1	A	186	GLN	3.2
1	A	133	GLY	3.2
1	B	490	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	55	LEU	3.1
1	B	548	ASP	3.0
1	B	132	PRO	3.0
1	A	132	PRO	3.0
1	B	182	PRO	2.9
1	B	546	THR	2.9
1	B	3	ASN	2.8
1	B	2	PRO	2.6
1	B	509	PRO	2.6
1	A	540	LYS	2.6
1	A	182	PRO	2.5
1	A	493	GLN	2.5
1	B	4	ILE	2.4
1	B	187	LYS	2.4
1	B	331	ALA	2.4
1	B	30	SER	2.3
1	A	22	ARG	2.3
1	B	226	HIS	2.3
1	B	534	ALA	2.3
1	A	909	ARG	2.3
1	B	25	PRO	2.2
1	A	87	ASP	2.1
1	B	86	PRO	2.1
1	A	546	THR	2.0
1	B	87	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

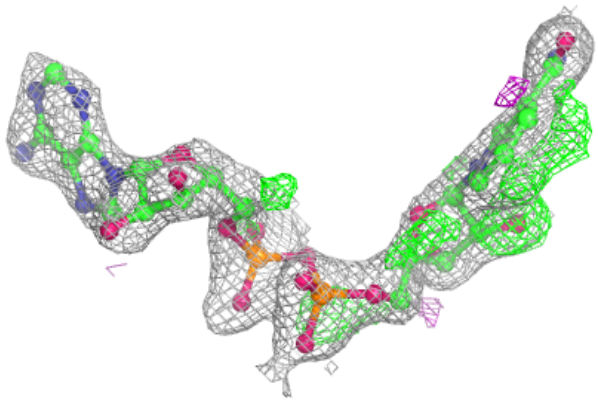
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

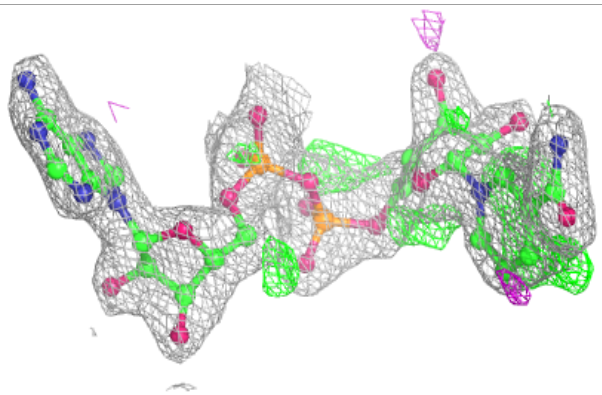
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAD	B	2004	44/44	0.84	0.26	11,33,39,51	44
4	SO4	A	1006	5/5	0.86	0.26	81,87,88,91	0
3	NAD	A	2003	44/44	0.88	0.33	15,33,40,53	44
5	GOL	B	1008	6/6	0.88	0.13	39,49,51,52	0
5	GOL	A	1009	6/6	0.90	0.19	45,49,51,52	0
5	GOL	A	1008	6/6	0.91	0.17	34,46,50,58	0
4	SO4	A	1005	5/5	0.92	0.18	66,74,82,83	0
4	SO4	B	1002	5/5	0.92	0.22	88,89,89,90	0
4	SO4	B	1005	5/5	0.92	0.19	82,83,91,92	0
5	GOL	B	1007	6/6	0.94	0.17	43,52,54,59	0
5	GOL	A	1007	6/6	0.94	0.13	25,34,40,41	0
4	SO4	A	1002	5/5	0.95	0.26	72,73,81,83	0
5	GOL	B	1006	6/6	0.95	0.10	32,37,41,42	0
4	SO4	B	1003	5/5	0.95	0.23	65,70,75,78	0
4	SO4	B	1004	5/5	0.95	0.26	66,69,77,80	0
4	SO4	A	1003	5/5	0.96	0.20	83,84,85,85	0
4	SO4	B	1000	5/5	0.96	0.15	58,61,64,71	0
4	SO4	A	1004	5/5	0.96	0.20	57,70,71,77	0
4	SO4	A	1001	5/5	0.96	0.20	44,44,59,62	0
2	FAD	B	2002	53/53	0.97	0.13	15,26,32,37	0
2	FAD	A	2001	53/53	0.97	0.13	14,20,25,29	0
4	SO4	A	1000	5/5	0.98	0.11	43,44,57,61	0
4	SO4	B	1001	5/5	0.98	0.10	47,54,61,67	0

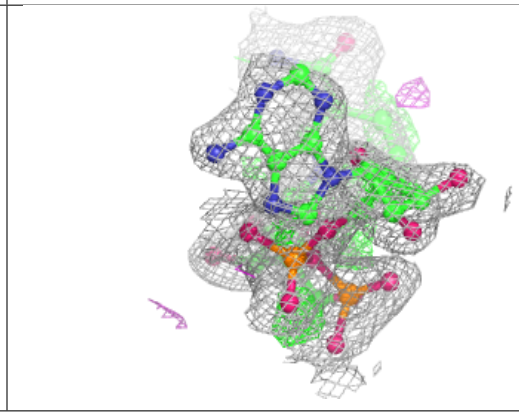
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD B 2004:

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

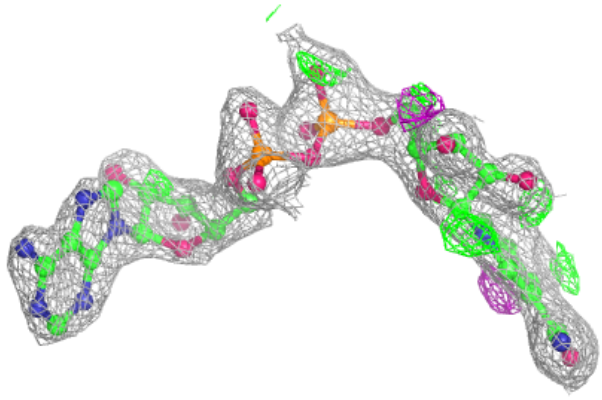


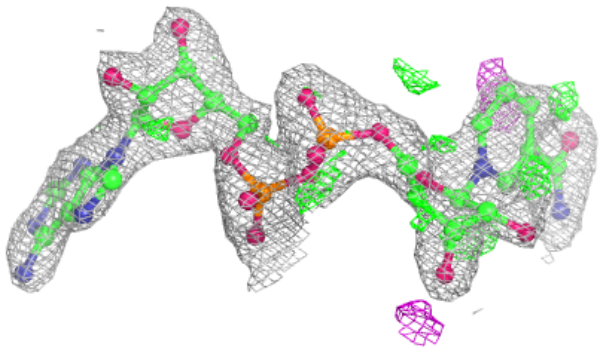


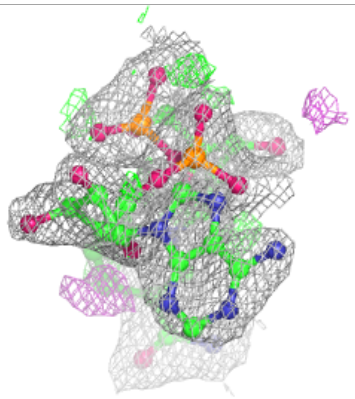


Electron density around NAD A 2003:

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

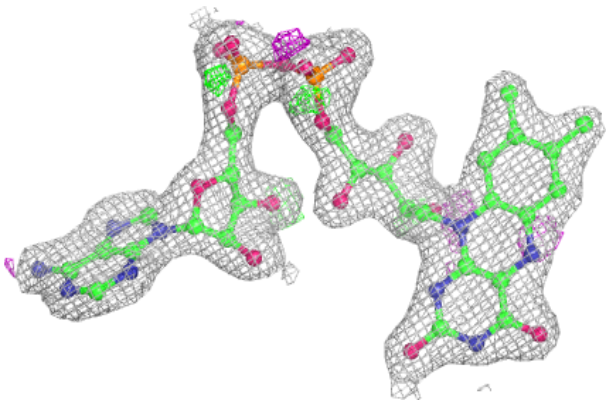


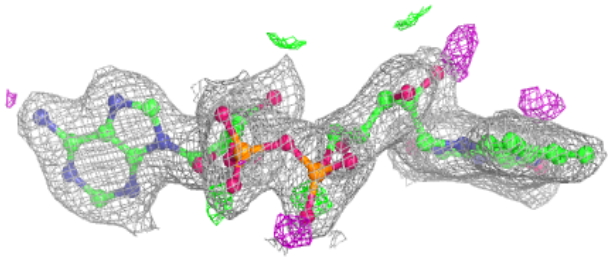




Electron density around FAD B 2002:

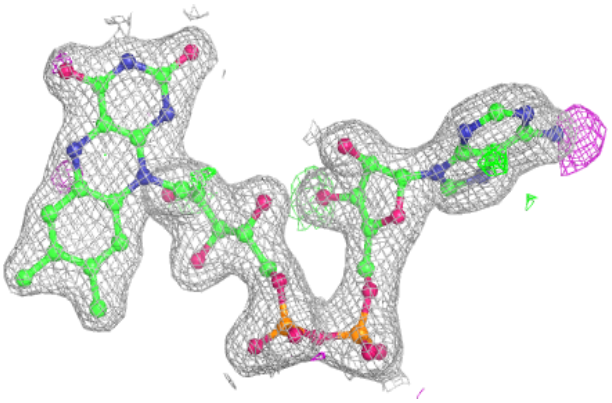
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

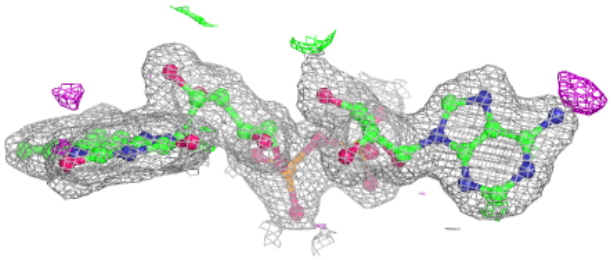


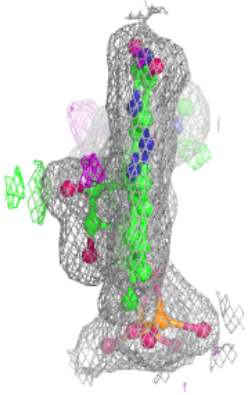


Electron density around FAD A 2001:

$2mF_o$-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.