Full wwPDB X-ray Structure Validation Report ⓘ

Dec 22, 2020 – 03:18 pm GMT

PDB ID	:	7AAU
Title	:	Crystal structure of nitrosoglutathione reductase from Chlamydomonas reinhardtii in complex with NAD+
Authors	:	Fermani, S.; Zaffagnini, M.; Falini, G.; Lemaire, S.D.
Deposited on	:	2020-09-04
Resolution	:	2.30 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:

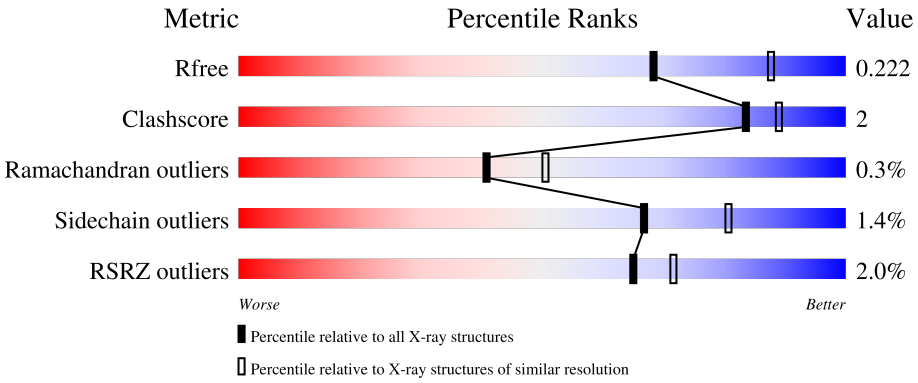
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	378	95% 5%
1	B	378	94% 6%
1	C	378	93% 6%
1	D	378	94% 6%
1	E	378	6% 93% 6%

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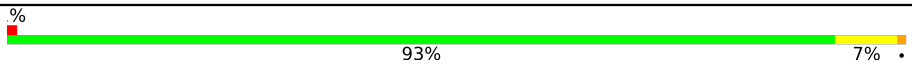
Mol	Chain	Length	Quality of chain
1	F	378	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	F	407	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18798 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.

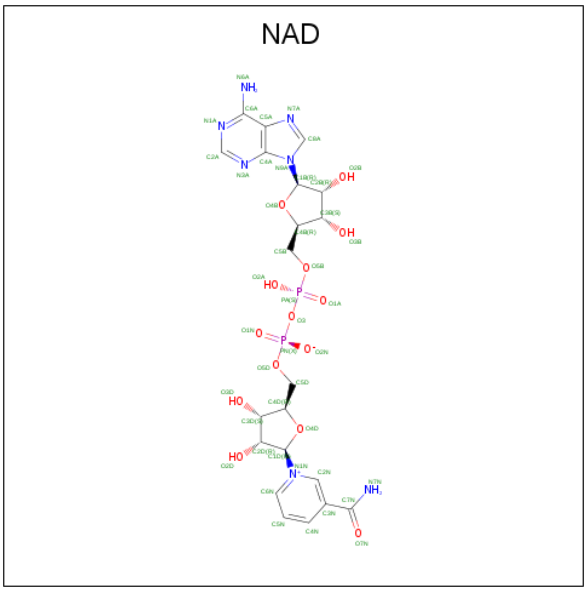
- Molecule 1 is a protein called S-(hydroxymethyl)glutathione dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	2	0
			2835	1796	482	534	23			
1	B	377	Total	C	N	O	S	0	0	0
			2823	1788	482	530	23			
1	C	378	Total	C	N	O	S	0	0	0
			2831	1793	483	531	24			
1	D	378	Total	C	N	O	S	0	0	0
			2831	1793	483	531	24			
1	E	376	Total	C	N	O	S	0	0	0
			2817	1785	481	528	23			
1	F	377	Total	C	N	O	S	0	1	0
			2826	1790	482	530	24			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

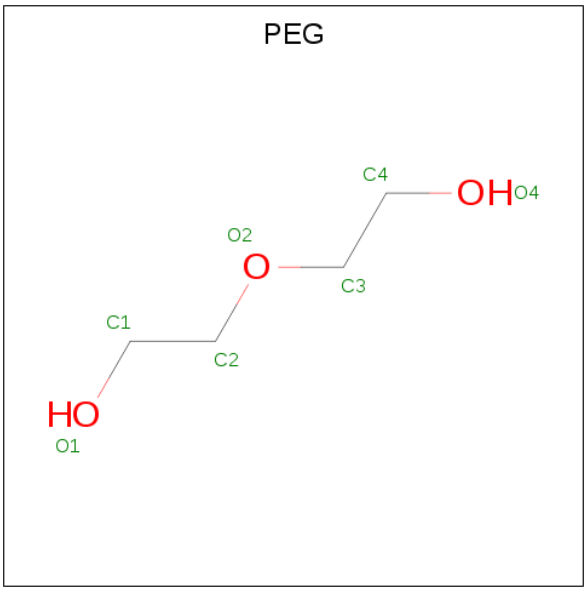
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			6	4	2		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			6	4	2		
4	D	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			6	4	2		
4	F	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C O 7 4 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	2	Total Cl 2 2	0	0
5	F	2	Total Cl 2 2	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

- Molecule 7 is water.

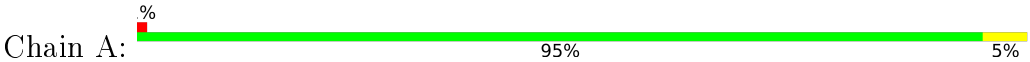
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	265	Total O 265 265	0	0
7	B	283	Total O 283 283	0	0
7	C	260	Total O 260 260	0	0
7	D	258	Total O 258 258	0	0
7	E	169	Total O 169 169	0	0
7	F	218	Total O 218 218	0	0

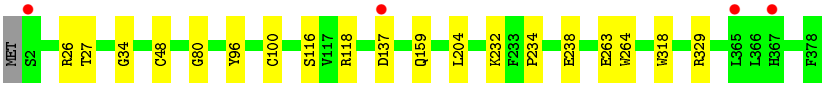
3 Residue-property plots (i)

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: S-(hydroxymethyl)glutathione dehydrogenase

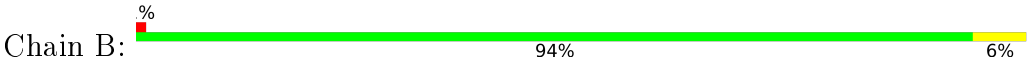
Chain A:

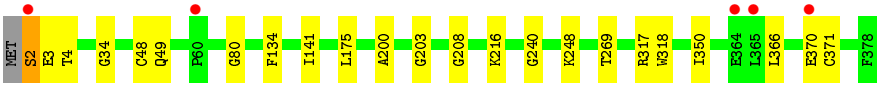




- Molecule 1: S-(hydroxymethyl)glutathione dehydrogenase

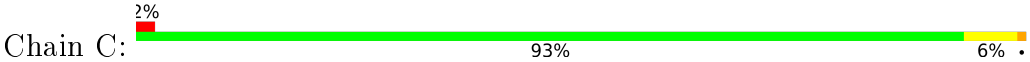
Chain B:





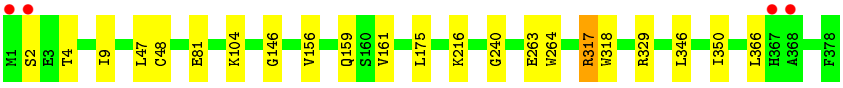
- Molecule 1: S-(hydroxymethyl)glutathione dehydrogenase

Chain C:



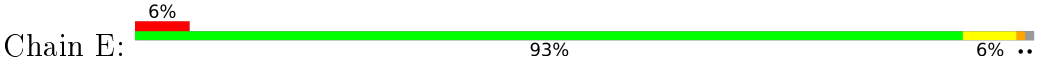
- Molecule 1: S-(hydroxymethyl)glutathione dehydrogenase

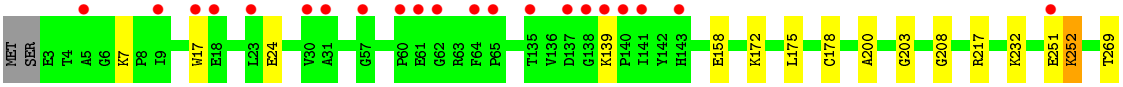
Chain D:

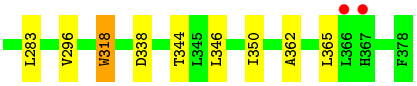


- Molecule 1: S-(hydroxymethyl)glutathione dehydrogenase

Chain E:

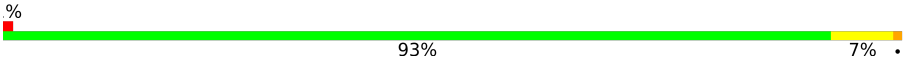


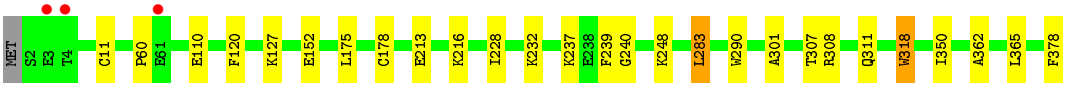




- Molecule 1: S-(hydroxymethyl)glutathione dehydrogenase

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.75Å 142.72Å 206.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 2.30 48.56 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.56-2.30) 99.6 (48.56-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.178 , 0.226 0.171 , 0.222	Depositor DCC
R_{free} test set	5029 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18798	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.05% 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: MG, PEG, ZN, NAD, CL

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	0.29	0/2903	0.49	0/3940
1	B	0.29	0/2885	0.47	0/3916
1	C	0.31	0/2893	0.51	1/3926 (0.0%)
1	D	0.29	0/2893	0.48	0/3926
1	E	0.28	0/2879	0.47	0/3908
1	F	0.29	0/2891	0.50	1/3924 (0.0%)
All	All	0.29	0/17344	0.49	2/23540 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	308	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	C	317	ARG	NE-CZ-NH2	6.55	123.58	120.30

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	2835	0	2812	11	0
1	B	2823	0	2800	9	0
1	C	2831	0	2812	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2831	0	2812	13	0
1	E	2817	0	2795	14	0
1	F	2826	0	2805	14	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	44	0	26	0	0
3	B	44	0	26	1	0
3	C	44	0	26	2	0
3	D	44	0	26	1	0
3	E	44	0	26	2	0
3	F	44	0	26	1	0
4	A	27	0	36	3	0
4	B	13	0	16	0	0
4	C	14	0	20	0	0
4	D	20	0	26	2	0
4	E	13	0	16	0	0
4	F	14	0	20	0	0
5	C	2	0	0	0	0
5	F	2	0	0	2	0
6	F	1	0	0	0	0
7	A	265	0	0	2	0
7	B	283	0	0	0	0
7	C	260	0	0	4	0
7	D	258	0	0	4	0
7	E	169	0	0	2	1
7	F	218	0	0	6	0
All	All	18798	0	17126	84	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (84) 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)
5:F:407:CL:CL	7:F:559:HOH:O	2.26	0.89
1:C:289:GLY:O	7:C:501:HOH:O	1.93	0.86
5:F:407:CL:CL	7:F:643:HOH:O	2.29	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:THR:OG1	7:F:501:HOH:O	1.98	0.81
1:A:96:TYR:HD2	4:A:405:PEG:H41	1.46	0.80
1:E:344:THR:HG22	1:E:346:LEU:H	1.53	0.74
1:A:26:ARG:NH1	1:A:27:THR:O	2.21	0.73
1:E:283:LEU:HD13	1:E:318:TRP:CG	2.27	0.68
1:B:2:SER:O	1:B:4:THR:N	2.27	0.66
1:E:158:GLU:OE2	7:E:501:HOH:O	2.13	0.66
1:D:317:ARG:NH2	7:D:509:HOH:O	2.34	0.61
1:C:1:MET:HE1	1:C:75:VAL:HG12	1.83	0.60
4:D:404:PEG:O1	7:D:502:HOH:O	2.17	0.58
1:E:232:LYS:NZ	7:E:502:HOH:O	2.30	0.55
1:A:96:TYR:CD2	4:A:405:PEG:H41	2.35	0.55
1:C:21:LYS:HG3	1:C:22:PRO:HD2	1.90	0.54
1:D:47:LEU:HD13	1:D:366:LEU:HD11	1.91	0.53
1:F:362:ALA:HA	1:F:365:LEU:HD12	1.91	0.52
1:D:263:GLU:HG2	1:D:264:TRP:CD1	2.45	0.52
1:C:97:GLN:NE2	7:C:509:HOH:O	2.37	0.50
1:D:175:LEU:HD11	1:D:350:ILE:HG13	1.93	0.50
1:A:263[A]:GLU:HG2	1:A:264:TRP:CD1	2.47	0.49
1:D:317:ARG:HD3	1:D:317:ARG:N	2.27	0.49
1:D:159:GLN:O	1:D:329:ARG:HD2	2.12	0.49
1:B:49:GLN:HG2	1:B:366:LEU:HD11	1.94	0.49
1:C:123:LYS:NZ	7:C:512:HOH:O	2.47	0.48
1:F:228:ILE:HB	1:F:248:LYS:HE3	1.95	0.48
1:B:248:LYS:HB3	1:B:248:LYS:HE3	1.66	0.48
1:C:41:GLN:HB2	1:C:153:TYR:CE2	2.48	0.48
1:C:71:GLU:OE2	1:C:178:CYS:HB3	2.14	0.47
1:E:362:ALA:O	1:E:365:LEU:HG	2.14	0.47
1:E:217:ARG:NH1	1:E:338:ASP:OD2	2.34	0.47
1:E:139:LYS:HD3	1:E:139:LYS:HA	1.55	0.47
1:F:378:PHE:OXT	7:F:502:HOH:O	2.21	0.47
1:D:216:LYS:HD2	1:D:240:GLY:HA3	1.97	0.47
1:F:311:GLN:HG3	7:F:501:HOH:O	2.15	0.46
1:C:251:GLU:OE1	7:C:502:HOH:O	2.20	0.46
1:C:159:GLN:O	1:C:329:ARG:HD2	2.15	0.46
3:F:403:NAD:H6N	3:F:403:NAD:H2D	1.70	0.46
1:C:178:CYS:SG	3:C:403:NAD:H5N	2.56	0.46
1:C:296:VAL:O	3:C:403:NAD:H2N	2.16	0.45
1:F:216:LYS:HE2	1:F:240:GLY:HA3	1.99	0.45
1:A:137:ASP:HB3	7:A:645:HOH:O	2.15	0.45
1:F:120:PHE:CE1	1:F:127:LYS:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PRO:O	1:A:238:GLU:HG3	2.17	0.45
1:F:283:LEU:HD13	1:F:318:TRP:CD2	2.52	0.45
3:D:403:NAD:O2A	7:D:503:HOH:O	2.21	0.44
3:E:403:NAD:H2D	3:E:403:NAD:H6N	1.82	0.44
1:B:175:LEU:HD11	1:B:350:ILE:HG13	2.00	0.44
1:B:200:ALA:HB3	1:B:269:THR:HG22	2.00	0.44
1:E:175:LEU:HD11	1:E:350:ILE:HG13	2.00	0.44
1:F:60:PRO:HD3	1:F:301:ALA:HB2	1.98	0.43
1:D:4:THR:HB	1:D:9:ILE:HD11	2.01	0.43
1:E:203:GLY:O	1:E:208:GLY:HA3	2.19	0.43
4:D:405:PEG:H42	4:D:405:PEG:H21	1.78	0.43
1:B:134:PHE:HB2	1:B:141:ILE:HB	2.01	0.43
1:B:34:GLY:O	1:B:80:GLY:HA3	2.19	0.43
1:C:175:LEU:HD11	1:C:350:ILE:HG13	2.00	0.43
1:C:248:LYS:HE3	1:C:248:LYS:HB3	1.66	0.42
1:F:237:LYS:NZ	7:F:509:HOH:O	2.38	0.42
1:D:81:GLU:OE1	7:D:504:HOH:O	2.22	0.42
1:A:204:LEU:O	1:A:232:LYS:HD2	2.20	0.42
1:E:172:LYS:HG2	1:E:350:ILE:HD13	2.02	0.42
1:E:296:VAL:O	3:E:403:NAD:H2N	2.20	0.42
1:A:159:GLN:O	1:A:329:ARG:HD2	2.19	0.42
1:D:161:VAL:O	1:D:329:ARG:HG2	2.19	0.42
4:A:406:PEG:O1	7:A:501:HOH:O	2.18	0.42
1:F:175:LEU:HD11	1:F:350:ILE:HG13	2.01	0.42
1:A:100:CYS:HB3	1:A:116:SER:HB3	2.01	0.41
3:B:403:NAD:H2D	3:B:403:NAD:H6N	1.84	0.41
1:E:252:LYS:H	1:E:252:LYS:HG2	1.46	0.41
1:B:216:LYS:NZ	1:B:240:GLY:O	2.53	0.41
1:C:134:PHE:HB2	1:C:141:ILE:HB	2.02	0.41
1:E:17:TRP:NE1	1:E:24:GLU:OE1	2.49	0.41
1:F:213:GLU:HB2	1:F:239:PHE:HD1	1.85	0.41
1:D:146:GLY:O	1:D:156:VAL:HG12	2.20	0.41
1:A:34:GLY:O	1:A:80:GLY:HA3	2.21	0.41
1:D:175:LEU:HB2	1:D:346:LEU:HD11	2.03	0.41
1:E:200:ALA:HB3	1:E:269:THR:HG22	2.03	0.41
1:F:216:LYS:HD3	1:F:216:LYS:HA	1.66	0.41
1:D:104:LYS:HB3	1:D:104:LYS:HE3	1.68	0.40
1:B:203:GLY:O	1:B:208:GLY:HA3	2.21	0.40
1:A:26:ARG:HH11	1:A:26:ARG:HG3	1.86	0.40
1:F:11:CYS:HB2	1:F:152:GLU:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:559:HOH:O	7:E:644:HOH:O[4_445]	2.18	0.02

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	377/378 (100%)	366 (97%)	11 (3%)	0	100	100
1	B	375/378 (99%)	364 (97%)	10 (3%)	1 (0%)	41	50
1	C	376/378 (100%)	362 (96%)	13 (4%)	1 (0%)	41	50
1	D	376/378 (100%)	364 (97%)	12 (3%)	0	100	100
1	E	374/378 (99%)	360 (96%)	12 (3%)	2 (0%)	29	35
1	F	376/378 (100%)	363 (96%)	11 (3%)	2 (0%)	29	35
All	All	2254/2268 (99%)	2179 (97%)	69 (3%)	6 (0%)	41	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	GLU
1	E	251	GLU
1	E	178	CYS
1	C	178	CYS
1	F	178	CYS
1	F	290	TRP

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	301/300 (100%)	298 (99%)	3 (1%)	76 87
1	B	299/300 (100%)	293 (98%)	6 (2%)	55 72
1	C	300/300 (100%)	295 (98%)	5 (2%)	60 76
1	D	300/300 (100%)	296 (99%)	4 (1%)	69 82
1	E	298/300 (99%)	295 (99%)	3 (1%)	76 87
1	F	300/300 (100%)	296 (99%)	4 (1%)	69 82
All	All	1798/1800 (100%)	1773 (99%)	25 (1%)	67 81

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	CYS
1	A	118	ARG
1	A	318	TRP
1	B	2	SER
1	B	48	CYS
1	B	317	ARG
1	B	318	TRP
1	B	370	GLU
1	B	371	CYS
1	C	137	ASP
1	C	139	LYS
1	C	216	LYS
1	C	248	LYS
1	C	318	TRP
1	D	2	SER
1	D	48	CYS
1	D	317	ARG
1	D	318	TRP
1	E	7	LYS
1	E	252	LYS
1	E	318	TRP
1	F	110	GLU
1	F	232	LYS
1	F	283	LEU
1	F	318	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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

Of 38 ligands modelled in this entry, 17 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
4	PEG	D	405	4	5,5,6	0.52	0	4,4,5	0.31	0
3	NAD	A	403	-	42,48,48	4.81	14 (33%)	50,73,73	1.63	6 (12%)
3	NAD	C	403	-	42,48,48	4.83	15 (35%)	50,73,73	1.70	5 (10%)
4	PEG	A	405	4	6,6,6	0.53	0	5,5,5	1.61	2 (40%)
4	PEG	D	404	4	6,6,6	0.48	0	5,5,5	0.37	0
4	PEG	E	404	4	6,6,6	0.46	0	5,5,5	0.36	0
4	PEG	C	405	-	6,6,6	0.50	0	5,5,5	0.28	0
4	PEG	C	404	-	6,6,6	0.52	0	5,5,5	0.26	0
4	PEG	A	404	4	5,5,6	0.48	0	4,4,5	0.31	0
4	PEG	B	405	4	5,5,6	0.55	0	4,4,5	0.37	0
4	PEG	F	404	-	6,6,6	0.48	0	5,5,5	0.30	0
3	NAD	F	403	-	42,48,48	4.86	12 (28%)	50,73,73	1.66	5 (10%)
4	PEG	B	404	4	6,6,6	0.49	0	5,5,5	0.52	0
3	NAD	B	403	-	42,48,48	4.85	14 (33%)	50,73,73	1.65	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAD	D	403	-	42,48,48	4.89	14 (33%)	50,73,73	1.68	5 (10%)
4	PEG	A	407	-	6,6,6	0.48	0	5,5,5	0.27	0
4	PEG	A	406	-	6,6,6	0.47	0	5,5,5	0.35	0
4	PEG	E	405	4	5,5,6	0.52	0	4,4,5	0.21	0
3	NAD	E	403	-	42,48,48	4.85	15 (35%)	50,73,73	1.75	8 (16%)
4	PEG	D	406	-	6,6,6	0.47	0	5,5,5	0.25	0
4	PEG	F	405	-	6,6,6	0.46	0	5,5,5	0.26	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
4	PEG	D	405	4	-	2/3/3/4	-
3	NAD	A	403	-	-	6/26/62/62	0/5/5/5
3	NAD	C	403	-	-	5/26/62/62	0/5/5/5
4	PEG	A	405	4	-	2/4/4/4	-
4	PEG	D	404	4	-	2/4/4/4	-
4	PEG	E	404	4	-	1/4/4/4	-
4	PEG	C	405	-	-	2/4/4/4	-
4	PEG	C	404	-	-	1/4/4/4	-
4	PEG	A	404	4	-	3/3/3/4	-
4	PEG	B	405	4	-	2/3/3/4	-
4	PEG	F	404	-	-	1/4/4/4	-
3	NAD	F	403	-	-	5/26/62/62	0/5/5/5
4	PEG	B	404	4	-	3/4/4/4	-
3	NAD	B	403	-	-	6/26/62/62	0/5/5/5
3	NAD	D	403	-	-	6/26/62/62	0/5/5/5
4	PEG	A	407	-	-	2/4/4/4	-
4	PEG	A	406	-	-	1/4/4/4	-
4	PEG	E	405	4	-	2/3/3/4	-
3	NAD	E	403	-	-	6/26/62/62	0/5/5/5
4	PEG	D	406	-	-	3/4/4/4	-
4	PEG	F	405	-	-	2/4/4/4	-

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	403	NAD	O4D-C1D	14.80	1.61	1.41
3	F	403	NAD	O4D-C1D	14.76	1.61	1.41
3	C	403	NAD	O4D-C1D	14.60	1.61	1.41
3	B	403	NAD	O4D-C1D	14.51	1.61	1.41
3	E	403	NAD	O4D-C1D	14.49	1.61	1.41
3	A	403	NAD	O4D-C1D	14.46	1.61	1.41
3	D	403	NAD	O4B-C1B	14.33	1.61	1.41
3	B	403	NAD	O4B-C1B	14.21	1.60	1.41
3	E	403	NAD	O4B-C1B	14.15	1.60	1.41
3	F	403	NAD	O4B-C1B	13.91	1.60	1.41
3	C	403	NAD	O4B-C1B	13.79	1.60	1.41
3	A	403	NAD	O4B-C1B	13.71	1.60	1.41
3	A	403	NAD	C2B-C1B	-13.64	1.33	1.53
3	D	403	NAD	C2B-C1B	-13.49	1.33	1.53
3	B	403	NAD	C2B-C1B	-13.46	1.33	1.53
3	E	403	NAD	C2B-C1B	-13.40	1.33	1.53
3	C	403	NAD	C2B-C1B	-13.31	1.33	1.53
3	F	403	NAD	C2B-C1B	-13.25	1.33	1.53
3	C	403	NAD	C2D-C1D	-13.18	1.33	1.53
3	F	403	NAD	C2D-C1D	-13.03	1.34	1.53
3	D	403	NAD	C2D-C1D	-12.99	1.34	1.53
3	E	403	NAD	C2D-C1D	-12.93	1.34	1.53
3	B	403	NAD	C2D-C1D	-12.89	1.34	1.53
3	A	403	NAD	C2D-C1D	-12.80	1.34	1.53
3	F	403	NAD	C7N-N7N	8.04	1.48	1.33
3	B	403	NAD	C7N-N7N	7.96	1.48	1.33
3	A	403	NAD	C7N-N7N	7.89	1.48	1.33
3	D	403	NAD	C7N-N7N	7.87	1.48	1.33
3	E	403	NAD	C7N-N7N	7.85	1.48	1.33
3	C	403	NAD	C7N-N7N	7.72	1.47	1.33
3	F	403	NAD	O4B-C4B	-6.58	1.30	1.45
3	E	403	NAD	O4B-C4B	-6.45	1.30	1.45
3	A	403	NAD	O4B-C4B	-6.37	1.30	1.45
3	C	403	NAD	O4B-C4B	-6.34	1.30	1.45
3	D	403	NAD	O4B-C4B	-6.33	1.30	1.45
3	B	403	NAD	O4B-C4B	-6.27	1.31	1.45
3	D	403	NAD	O4D-C4D	-6.24	1.31	1.45
3	C	403	NAD	O4D-C4D	-6.22	1.31	1.45
3	F	403	NAD	O4D-C4D	-6.22	1.31	1.45
3	E	403	NAD	O4D-C4D	-6.10	1.31	1.45
3	A	403	NAD	O4D-C4D	-6.10	1.31	1.45
3	B	403	NAD	O4D-C4D	-6.03	1.31	1.45
3	E	403	NAD	C4N-C3N	-3.86	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	NAD	C4N-C3N	-3.85	1.32	1.39
3	D	403	NAD	C4N-C3N	-3.81	1.32	1.39
3	F	403	NAD	C4N-C3N	-3.76	1.32	1.39
3	C	403	NAD	C4N-C3N	-3.74	1.32	1.39
3	B	403	NAD	C4N-C3N	-3.59	1.33	1.39
3	F	403	NAD	C2N-C3N	3.23	1.44	1.39
3	E	403	NAD	C2N-C3N	3.21	1.44	1.39
3	D	403	NAD	C2N-C3N	3.09	1.43	1.39
3	C	403	NAD	C2N-C3N	3.03	1.43	1.39
3	A	403	NAD	C2N-C3N	3.00	1.43	1.39
3	B	403	NAD	C2N-C3N	2.97	1.43	1.39
3	D	403	NAD	C5A-C4A	-2.69	1.33	1.40
3	E	403	NAD	C5A-C4A	-2.68	1.33	1.40
3	B	403	NAD	C5A-C4A	-2.68	1.33	1.40
3	C	403	NAD	C5A-C4A	-2.63	1.34	1.40
3	A	403	NAD	C5A-C4A	-2.62	1.34	1.40
3	D	403	NAD	PA-O5B	2.58	1.69	1.59
3	F	403	NAD	C5A-C4A	-2.57	1.34	1.40
3	A	403	NAD	PA-O5B	2.56	1.69	1.59
3	E	403	NAD	PA-O5B	2.56	1.69	1.59
3	B	403	NAD	PA-O5B	2.55	1.69	1.59
3	C	403	NAD	PA-O5B	2.54	1.69	1.59
3	F	403	NAD	PA-O5B	2.53	1.69	1.59
3	F	403	NAD	O2B-C2B	2.32	1.48	1.43
3	C	403	NAD	O2B-C2B	2.31	1.48	1.43
3	B	403	NAD	O3B-C3B	-2.26	1.37	1.43
3	D	403	NAD	O2B-C2B	2.20	1.48	1.43
3	A	403	NAD	O3B-C3B	-2.20	1.37	1.43
3	B	403	NAD	C6N-C5N	2.20	1.43	1.38
3	D	403	NAD	C6N-C5N	2.14	1.43	1.38
3	E	403	NAD	C6N-C5N	2.13	1.43	1.38
3	E	403	NAD	O3B-C3B	-2.13	1.38	1.43
3	D	403	NAD	O3B-C3B	-2.13	1.38	1.43
3	B	403	NAD	O7N-C7N	-2.09	1.20	1.24
3	E	403	NAD	O2B-C2B	2.08	1.47	1.43
3	E	403	NAD	O7N-C7N	-2.08	1.20	1.24
3	A	403	NAD	O2B-C2B	2.05	1.47	1.43
3	A	403	NAD	C6N-C5N	2.05	1.43	1.38
3	C	403	NAD	C6N-C5N	2.03	1.43	1.38
3	C	403	NAD	O3B-C3B	-2.01	1.38	1.43
3	C	403	NAD	O7N-C7N	-2.00	1.20	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	403	NAD	C5A-C6A-N6A	6.95	130.91	120.35
3	C	403	NAD	C5A-C6A-N6A	6.78	130.66	120.35
3	F	403	NAD	C5A-C6A-N6A	6.69	130.52	120.35
3	D	403	NAD	C5A-C6A-N6A	6.46	130.17	120.35
3	A	403	NAD	C5A-C6A-N6A	6.45	130.15	120.35
3	B	403	NAD	C5A-C6A-N6A	6.06	129.56	120.35
3	B	403	NAD	N3A-C2A-N1A	-5.74	119.71	128.68
3	C	403	NAD	N3A-C2A-N1A	-5.69	119.78	128.68
3	D	403	NAD	N3A-C2A-N1A	-5.68	119.80	128.68
3	E	403	NAD	N3A-C2A-N1A	-5.49	120.10	128.68
3	F	403	NAD	N3A-C2A-N1A	-5.35	120.31	128.68
3	A	403	NAD	N3A-C2A-N1A	-5.35	120.32	128.68
3	E	403	NAD	N6A-C6A-N1A	-4.61	109.00	118.57
3	C	403	NAD	N6A-C6A-N1A	-4.58	109.06	118.57
3	F	403	NAD	N6A-C6A-N1A	-4.34	109.57	118.57
3	D	403	NAD	N6A-C6A-N1A	-4.22	109.81	118.57
3	A	403	NAD	N6A-C6A-N1A	-4.20	109.87	118.57
3	B	403	NAD	N6A-C6A-N1A	-4.04	110.20	118.57
3	B	403	NAD	PN-O3-PA	-3.01	122.49	132.83
4	A	405	PEG	C3-O2-C2	2.86	125.67	113.29
3	E	403	NAD	PN-O3-PA	-2.61	123.86	132.83
3	E	403	NAD	C6N-N1N-C2N	-2.61	119.59	121.97
3	D	403	NAD	C6N-N1N-C2N	-2.57	119.63	121.97
3	A	403	NAD	PN-O3-PA	-2.44	124.47	132.83
3	E	403	NAD	C1B-N9A-C4A	-2.43	122.38	126.64
3	F	403	NAD	PN-O3-PA	-2.33	124.83	132.83
3	B	403	NAD	O7N-C7N-N7N	-2.33	119.27	122.58
3	A	403	NAD	C6N-N1N-C2N	-2.31	119.86	121.97
3	E	403	NAD	O7N-C7N-N7N	-2.30	119.31	122.58
3	D	403	NAD	PN-O3-PA	-2.29	124.96	132.83
3	A	403	NAD	O4D-C1D-C2D	-2.07	103.91	106.93
3	E	403	NAD	O4D-C1D-C2D	-2.07	103.91	106.93
4	A	405	PEG	O2-C3-C4	2.06	119.10	110.07
3	C	403	NAD	O7N-C7N-N7N	-2.03	119.69	122.58
3	C	403	NAD	C3B-C2B-C1B	2.02	104.02	100.98
3	F	403	NAD	C6N-N1N-C2N	-2.00	120.15	121.97

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	403	NAD	O4D-C1D-N1N-C2N
3	C	403	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	C	403	NAD	C2D-C1D-N1N-C2N
3	C	403	NAD	C2D-C1D-N1N-C6N
3	D	403	NAD	O4D-C1D-N1N-C2N
3	D	403	NAD	O4D-C1D-N1N-C6N
3	D	403	NAD	C2D-C1D-N1N-C2N
3	D	403	NAD	C2D-C1D-N1N-C6N
3	A	403	NAD	O4D-C1D-N1N-C2N
3	A	403	NAD	O4D-C1D-N1N-C6N
3	A	403	NAD	C2D-C1D-N1N-C2N
3	A	403	NAD	C2D-C1D-N1N-C6N
3	E	403	NAD	O4D-C1D-N1N-C2N
3	E	403	NAD	O4D-C1D-N1N-C6N
3	E	403	NAD	C2D-C1D-N1N-C2N
3	E	403	NAD	C2D-C1D-N1N-C6N
3	F	403	NAD	O4D-C1D-N1N-C2N
3	F	403	NAD	O4D-C1D-N1N-C6N
3	F	403	NAD	C2D-C1D-N1N-C2N
3	F	403	NAD	C2D-C1D-N1N-C6N
3	B	403	NAD	O4D-C1D-N1N-C2N
3	B	403	NAD	O4D-C1D-N1N-C6N
3	B	403	NAD	C2D-C1D-N1N-C2N
3	B	403	NAD	C2D-C1D-N1N-C6N
4	A	405	PEG	C4-C3-O2-C2
4	A	404	PEG	O2-C3-C4-O4
4	C	405	PEG	O1-C1-C2-O2
4	A	405	PEG	O1-C1-C2-O2
4	B	404	PEG	O1-C1-C2-O2
4	A	407	PEG	O1-C1-C2-O2
4	E	404	PEG	O2-C3-C4-O4
4	D	406	PEG	O1-C1-C2-O2
4	E	405	PEG	O2-C3-C4-O4
4	F	405	PEG	O2-C3-C4-O4
4	B	405	PEG	C1-C2-O2-C3
3	D	403	NAD	O4B-C4B-C5B-O5B
3	A	403	NAD	C3B-C4B-C5B-O5B
3	E	403	NAD	O4B-C4B-C5B-O5B
3	E	403	NAD	C3B-C4B-C5B-O5B
3	B	403	NAD	C3B-C4B-C5B-O5B
4	D	404	PEG	O2-C3-C4-O4
4	B	405	PEG	O2-C3-C4-O4
3	D	403	NAD	C3B-C4B-C5B-O5B
3	A	403	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	B	403	NAD	O4B-C4B-C5B-O5B
4	D	405	PEG	C4-C3-O2-C2
4	C	405	PEG	O2-C3-C4-O4
4	A	404	PEG	C1-C2-O2-C3
4	D	404	PEG	C1-C2-O2-C3
4	D	405	PEG	C1-C2-O2-C3
4	A	404	PEG	C4-C3-O2-C2
4	A	406	PEG	O2-C3-C4-O4
4	B	404	PEG	O2-C3-C4-O4
4	F	405	PEG	C1-C2-O2-C3
4	A	407	PEG	C4-C3-O2-C2
4	E	405	PEG	C4-C3-O2-C2
4	D	406	PEG	C1-C2-O2-C3
3	C	403	NAD	O4B-C4B-C5B-O5B
3	F	403	NAD	O4B-C4B-C5B-O5B
4	C	404	PEG	C4-C3-O2-C2
4	B	404	PEG	C1-C2-O2-C3
4	D	406	PEG	C4-C3-O2-C2
4	F	404	PEG	C1-C2-O2-C3

There are no ring outliers.

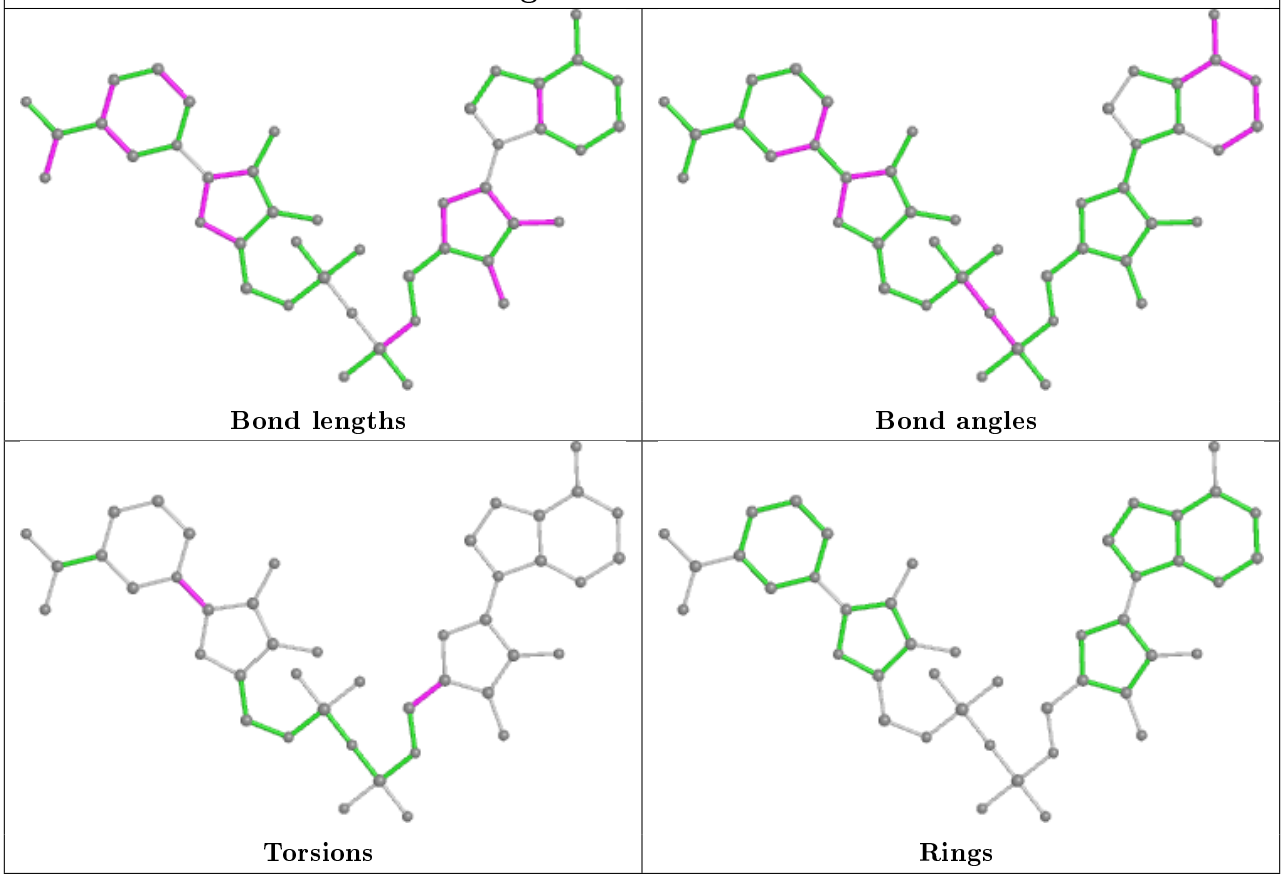
9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	405	PEG	1	0
3	C	403	NAD	2	0
4	A	405	PEG	2	0
4	D	404	PEG	1	0
3	F	403	NAD	1	0
3	B	403	NAD	1	0
3	D	403	NAD	1	0
4	A	406	PEG	1	0
3	E	403	NAD	2	0

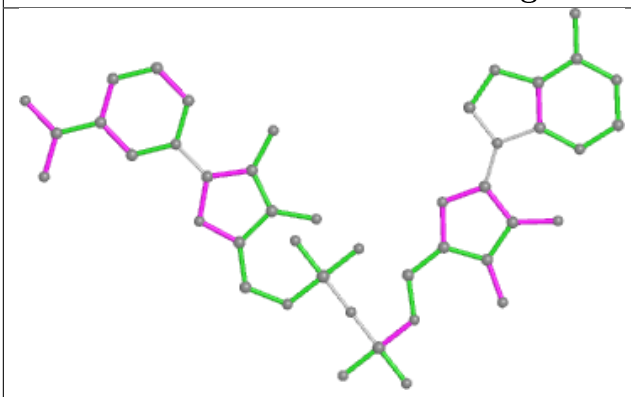
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

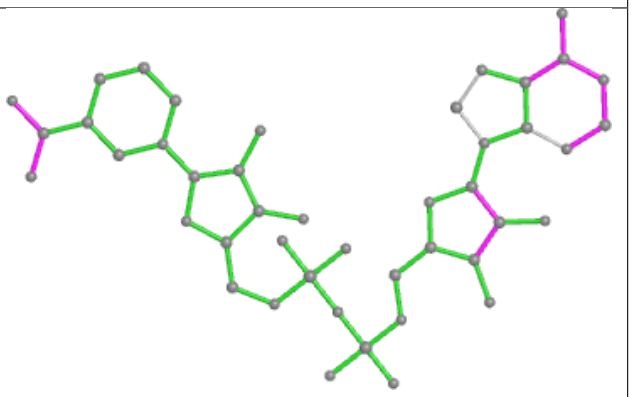
Ligand NAD A 403



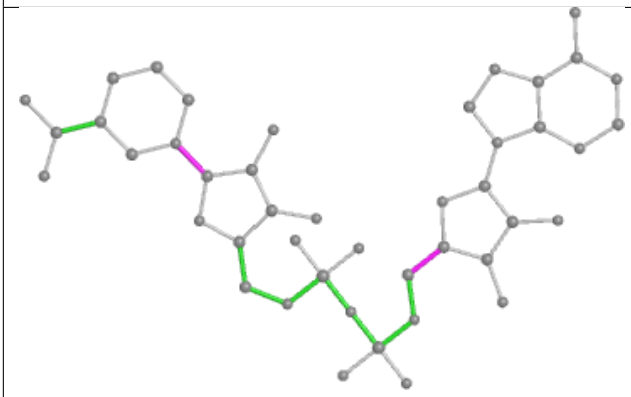
Ligand NAD C 403



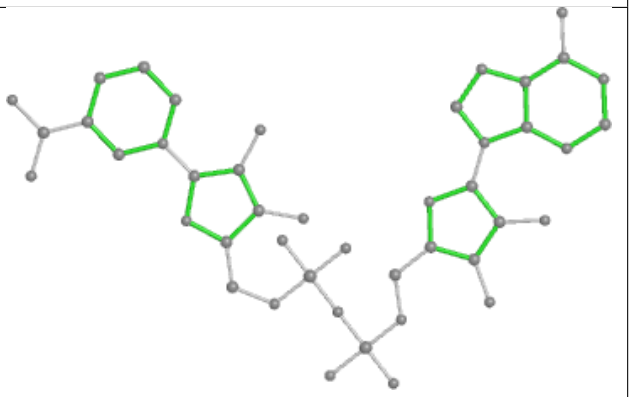
Bond lengths



Bond angles

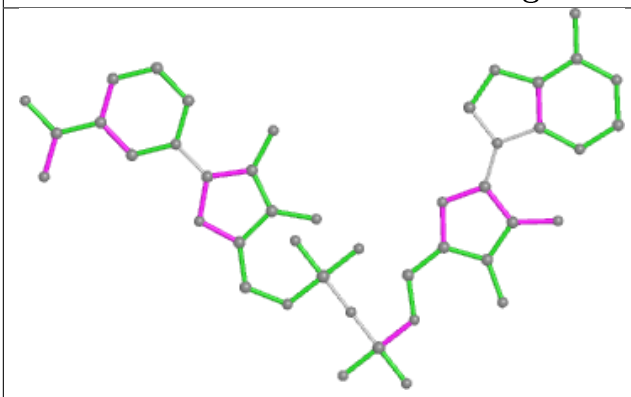


Torsions

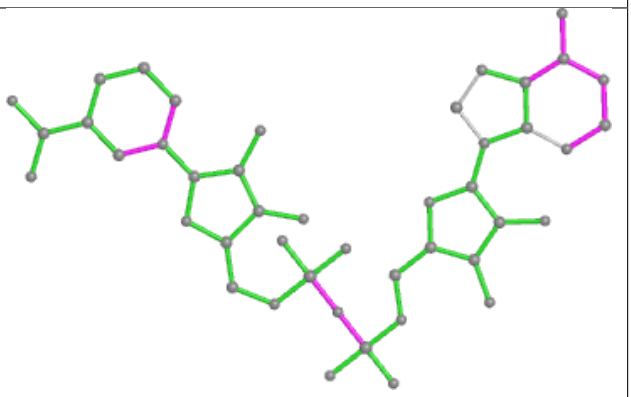


Rings

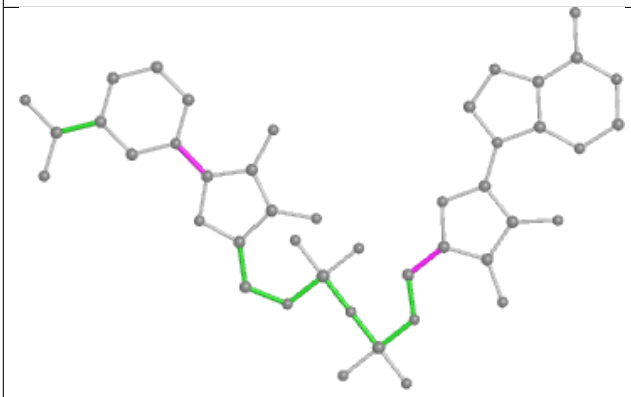
Ligand NAD F 403



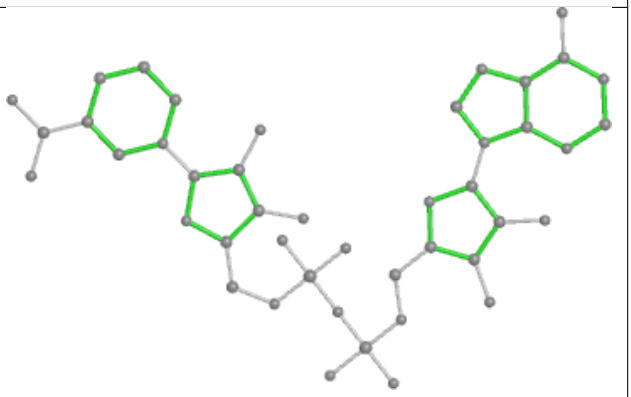
Bond lengths



Bond angles

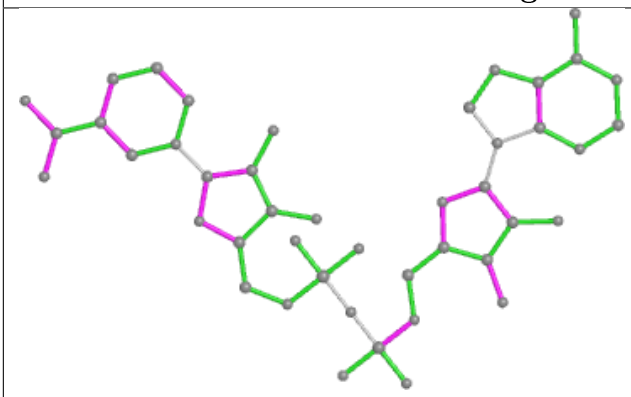


Torsions

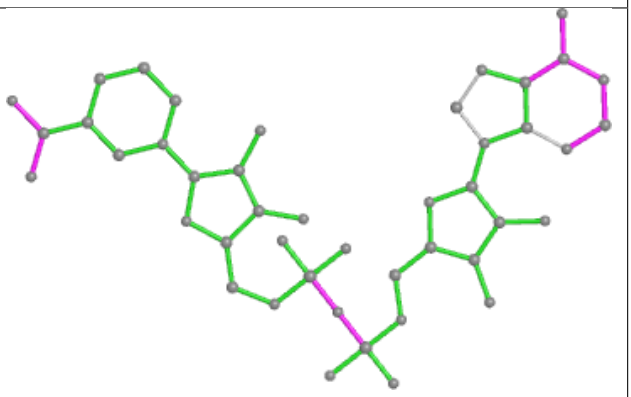


Rings

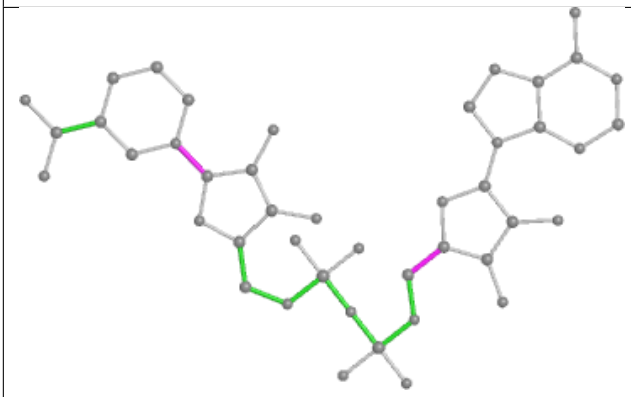
Ligand NAD B 403



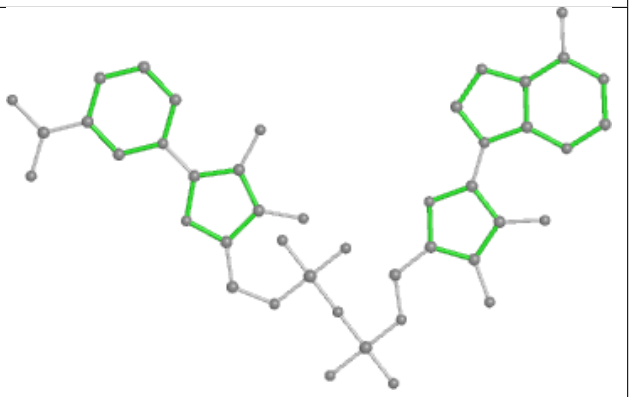
Bond lengths



Bond angles

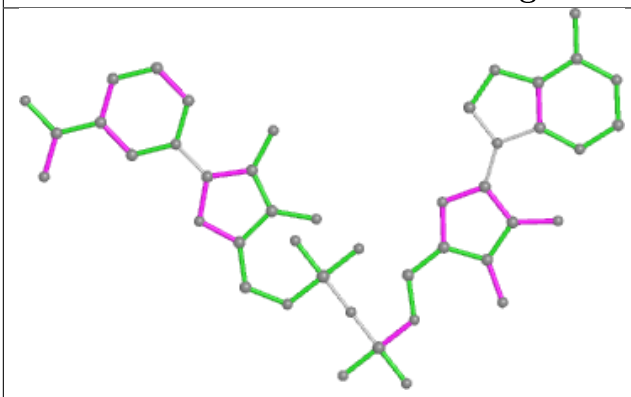


Torsions

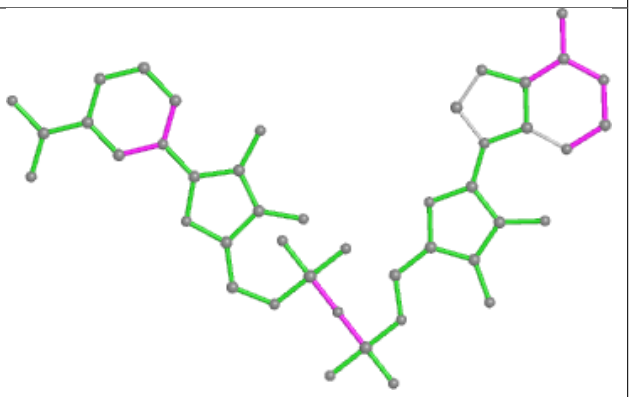


Rings

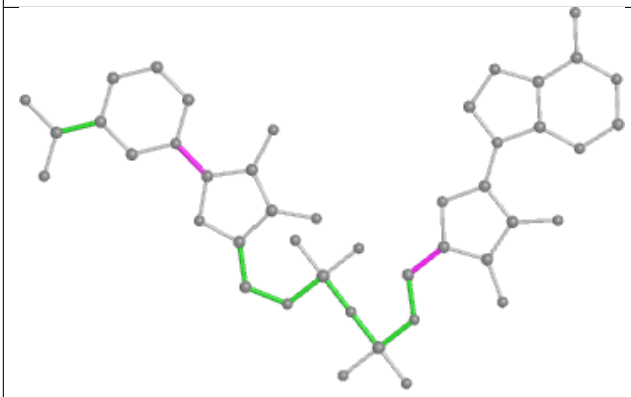
Ligand NAD D 403



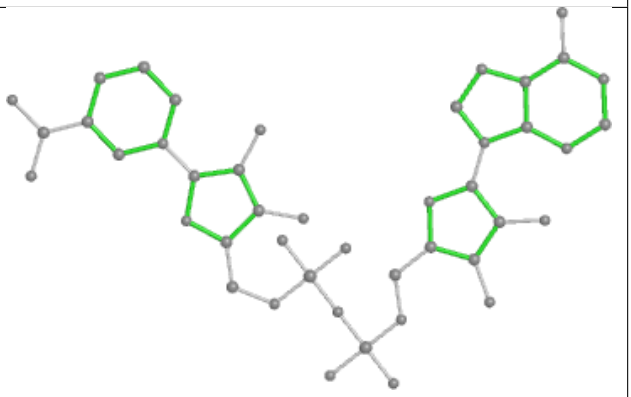
Bond lengths



Bond angles

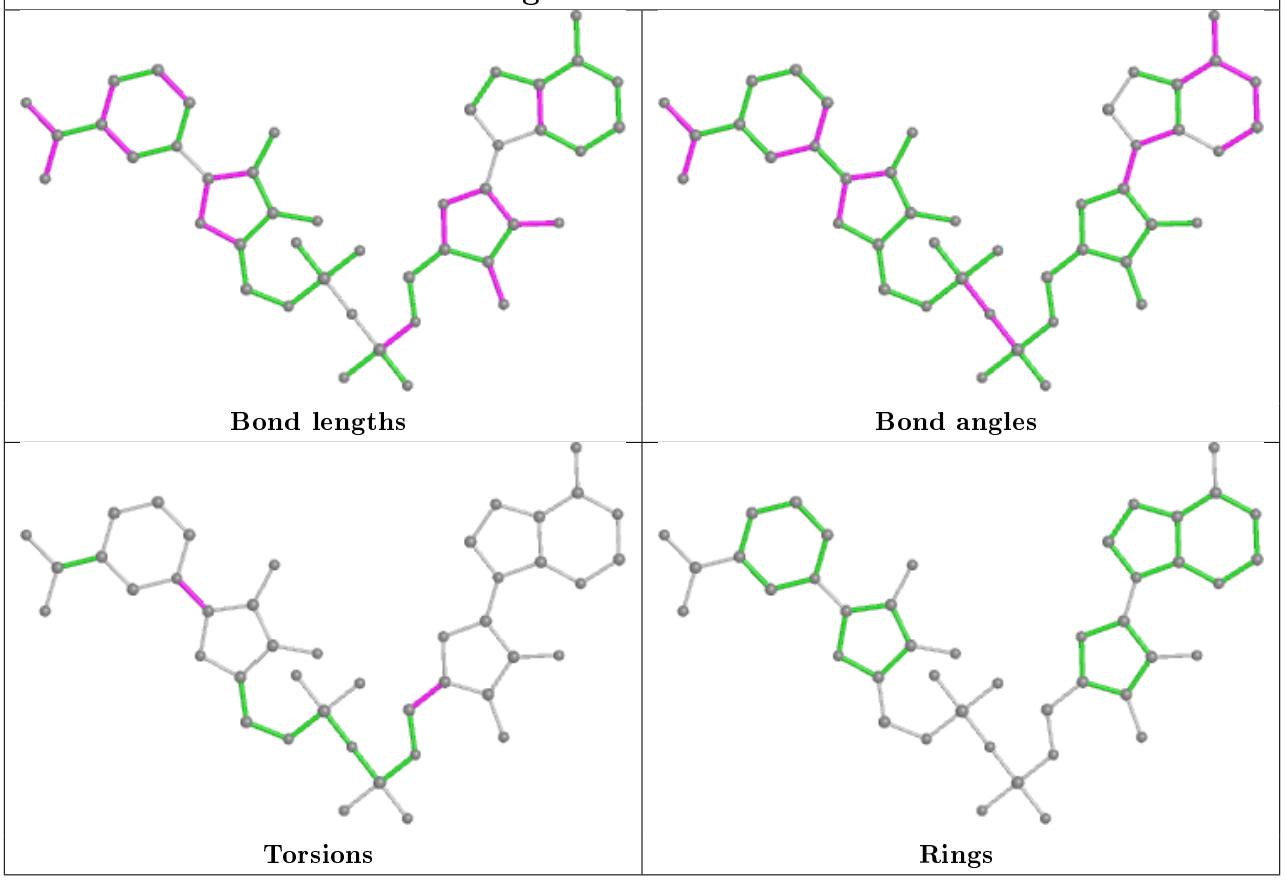


Torsions



Rings

Ligand NAD E 403



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	377/378 (99%)	-0.22	4 (1%) 80 85	18, 26, 48, 75	0
1	B	377/378 (99%)	-0.18	5 (1%) 77 81	18, 26, 48, 74	0
1	C	378/378 (100%)	-0.18	7 (1%) 66 73	18, 27, 53, 68	0
1	D	378/378 (100%)	-0.29	4 (1%) 80 85	18, 27, 45, 67	0
1	E	376/378 (99%)	0.20	23 (6%) 21 27	23, 34, 57, 74	0
1	F	377/378 (99%)	-0.13	3 (0%) 86 89	19, 31, 47, 76	0
All	All	2263/2268 (99%)	-0.13	46 (2%) 65 71	18, 28, 50, 76	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	9.8
1	D	1	MET	8.7
1	B	2	SER	5.9
1	D	2	SER	5.6
1	F	61	GLU	4.8
1	E	138	GLY	3.7
1	C	2	SER	3.5
1	E	57	GLY	3.2
1	A	367	HIS	3.2
1	E	141	ILE	3.1
1	C	56	GLY	3.1
1	F	3	GLU	3.1
1	E	61	GLU	3.0
1	E	23	LEU	2.9
1	E	137	ASP	2.7
1	E	60	PRO	2.7
1	D	368	ALA	2.7
1	E	64	PHE	2.7
1	E	367	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	365	LEU	2.6
1	E	366	LEU	2.6
1	E	31	ALA	2.6
1	C	367	HIS	2.6
1	B	60	PRO	2.5
1	B	364	GLU	2.4
1	C	366	LEU	2.4
1	E	251	GLU	2.4
1	A	137	ASP	2.4
1	A	365	LEU	2.4
1	E	17	TRP	2.3
1	E	143	HIS	2.3
1	E	5	ALA	2.2
1	F	4	THR	2.2
1	E	135	THR	2.2
1	E	18	GLU	2.2
1	E	65	PRO	2.2
1	E	30	VAL	2.2
1	E	62	GLY	2.2
1	E	139	LYS	2.1
1	E	9	ILE	2.1
1	D	367	HIS	2.1
1	E	140	PRO	2.1
1	A	2	SER	2.1
1	C	22	PRO	2.1
1	B	370	GLU	2.0
1	C	21	LYS	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.

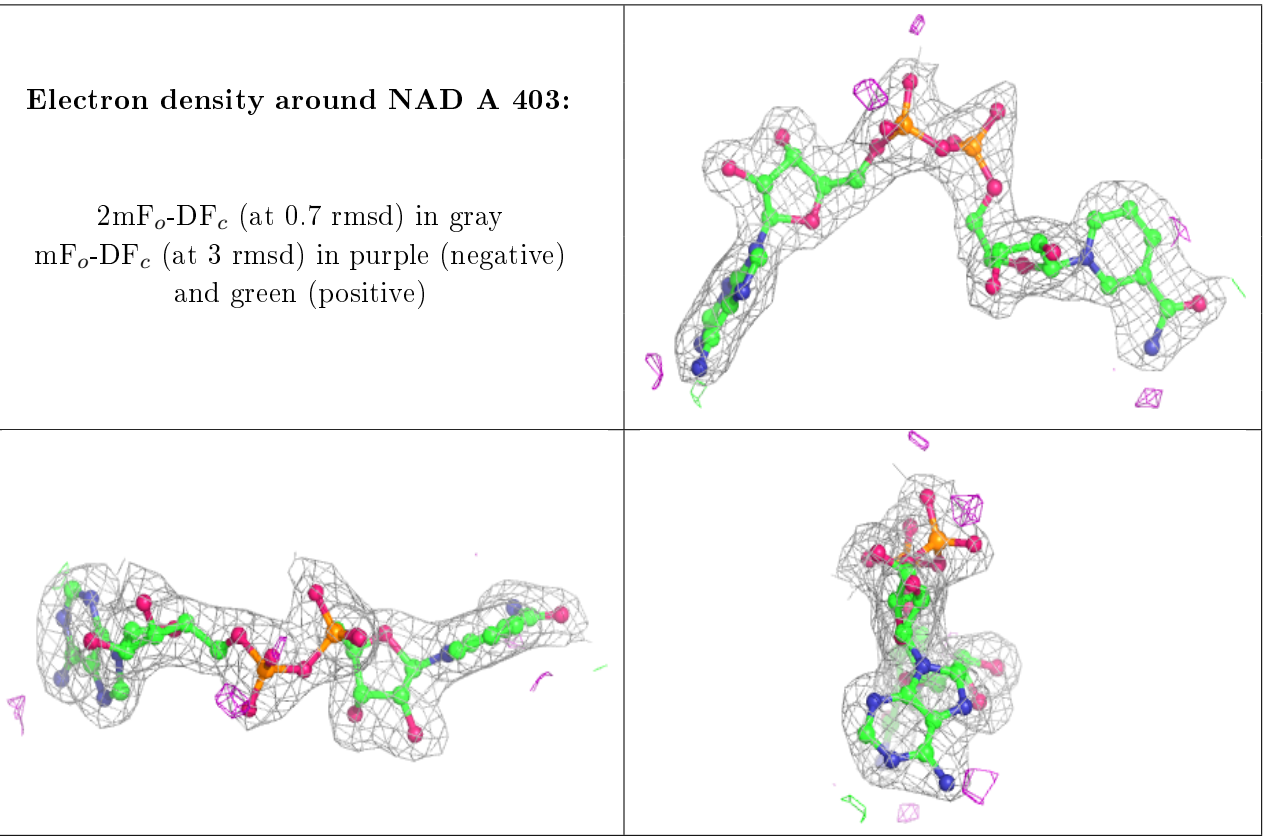
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	C	406	1/1	0.70	0.13	61,61,61,61	0
4	PEG	A	405	7/7	0.77	0.28	27,36,41,46	0
4	PEG	A	407	7/7	0.83	0.16	30,34,37,39	0
4	PEG	C	404	7/7	0.84	0.23	34,38,39,43	0
4	PEG	F	405	7/7	0.86	0.21	36,41,46,49	0
4	PEG	D	406	7/7	0.87	0.16	37,38,45,47	0
4	PEG	E	404	7/7	0.87	0.21	39,40,47,48	0
4	PEG	F	404	7/7	0.89	0.15	30,36,41,43	0
4	PEG	D	405	6/7	0.90	0.19	35,38,42,47	0
4	PEG	E	405	6/7	0.90	0.12	36,38,41,42	0
4	PEG	A	406	7/7	0.91	0.10	29,35,41,44	0
4	PEG	C	405	7/7	0.93	0.11	29,31,38,40	0
4	PEG	B	404	7/7	0.93	0.15	27,29,33,36	0
4	PEG	A	404	6/7	0.93	0.15	31,33,38,47	0
4	PEG	B	405	6/7	0.94	0.17	34,38,40,43	0
5	CL	F	407	1/1	0.94	0.09	51,51,51,51	0
6	MG	F	408	1/1	0.95	0.27	44,44,44,44	0
4	PEG	D	404	7/7	0.95	0.12	36,38,41,46	0
2	ZN	C	401	1/1	0.95	0.08	53,53,53,53	1
2	ZN	F	401	1/1	0.95	0.07	60,60,60,60	1
3	NAD	A	403	44/44	0.96	0.10	22,28,32,37	0
3	NAD	E	403	44/44	0.96	0.11	23,31,38,41	0
3	NAD	F	403	44/44	0.96	0.11	23,30,36,42	0
3	NAD	D	403	44/44	0.96	0.10	21,30,36,39	0
3	NAD	C	403	44/44	0.97	0.10	19,25,30,31	0
3	NAD	B	403	44/44	0.97	0.10	18,26,30,32	0
5	CL	F	406	1/1	0.97	0.10	52,52,52,52	0
2	ZN	D	402	1/1	0.98	0.08	24,24,24,24	0
2	ZN	E	402	1/1	0.98	0.05	28,28,28,28	0
2	ZN	D	401	1/1	0.99	0.05	33,33,33,33	0
5	CL	C	407	1/1	0.99	0.09	40,40,40,40	0
2	ZN	A	401	1/1	0.99	0.05	33,33,33,33	0
2	ZN	B	402	1/1	1.00	0.08	19,19,19,19	0
2	ZN	A	402	1/1	1.00	0.07	25,25,25,25	0
2	ZN	E	401	1/1	1.00	0.04	38,38,38,38	0
2	ZN	C	402	1/1	1.00	0.10	24,24,24,24	0
2	ZN	F	402	1/1	1.00	0.09	25,25,25,25	0
2	ZN	B	401	1/1	1.00	0.06	32,32,32,32	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.

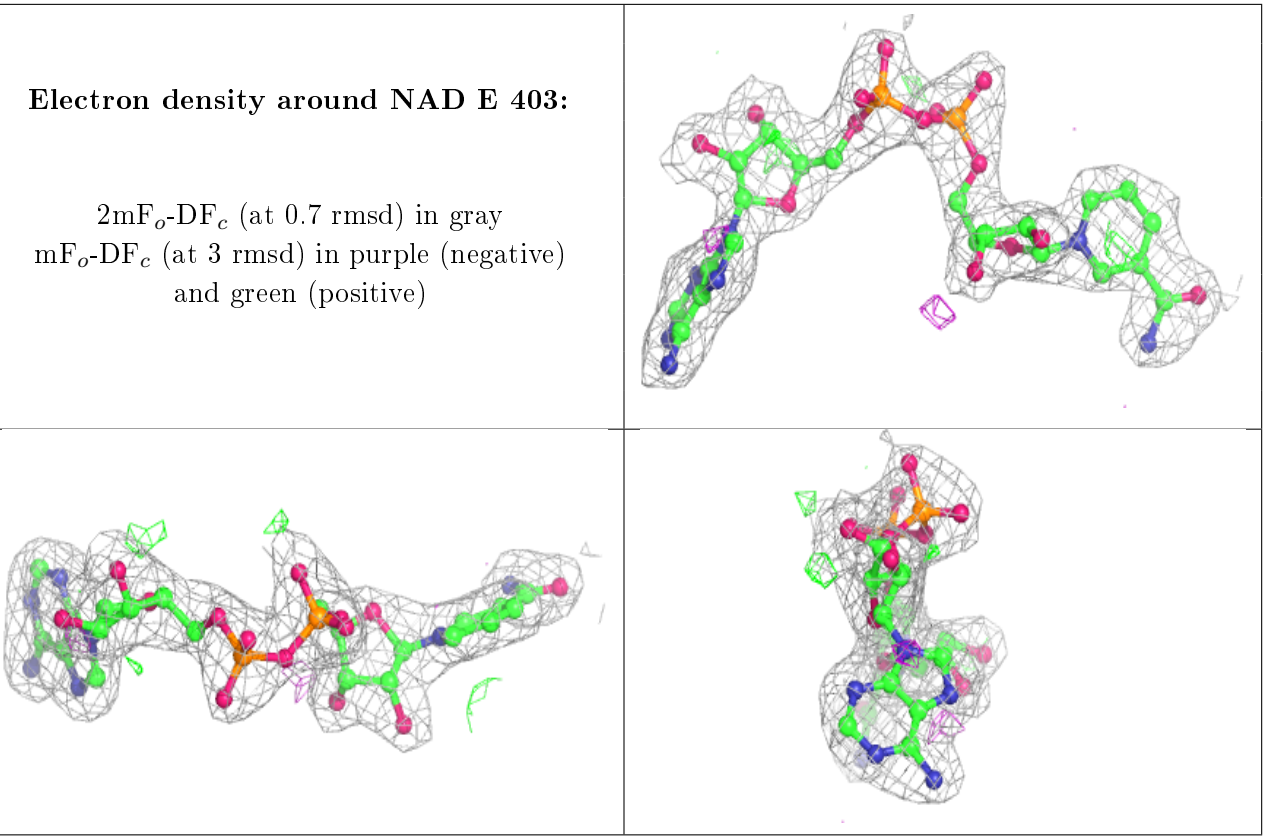
Electron density around NAD A 403:

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



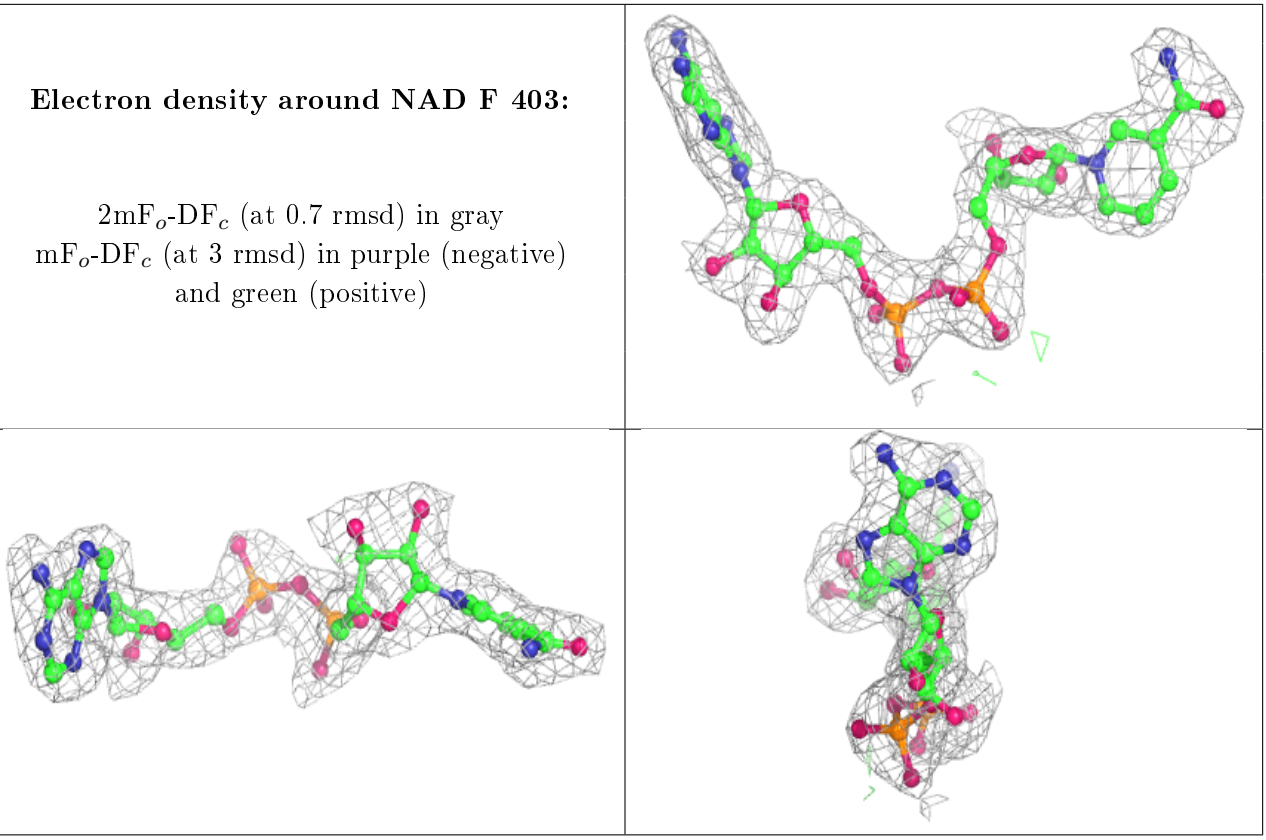
Electron density around NAD E 403:

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



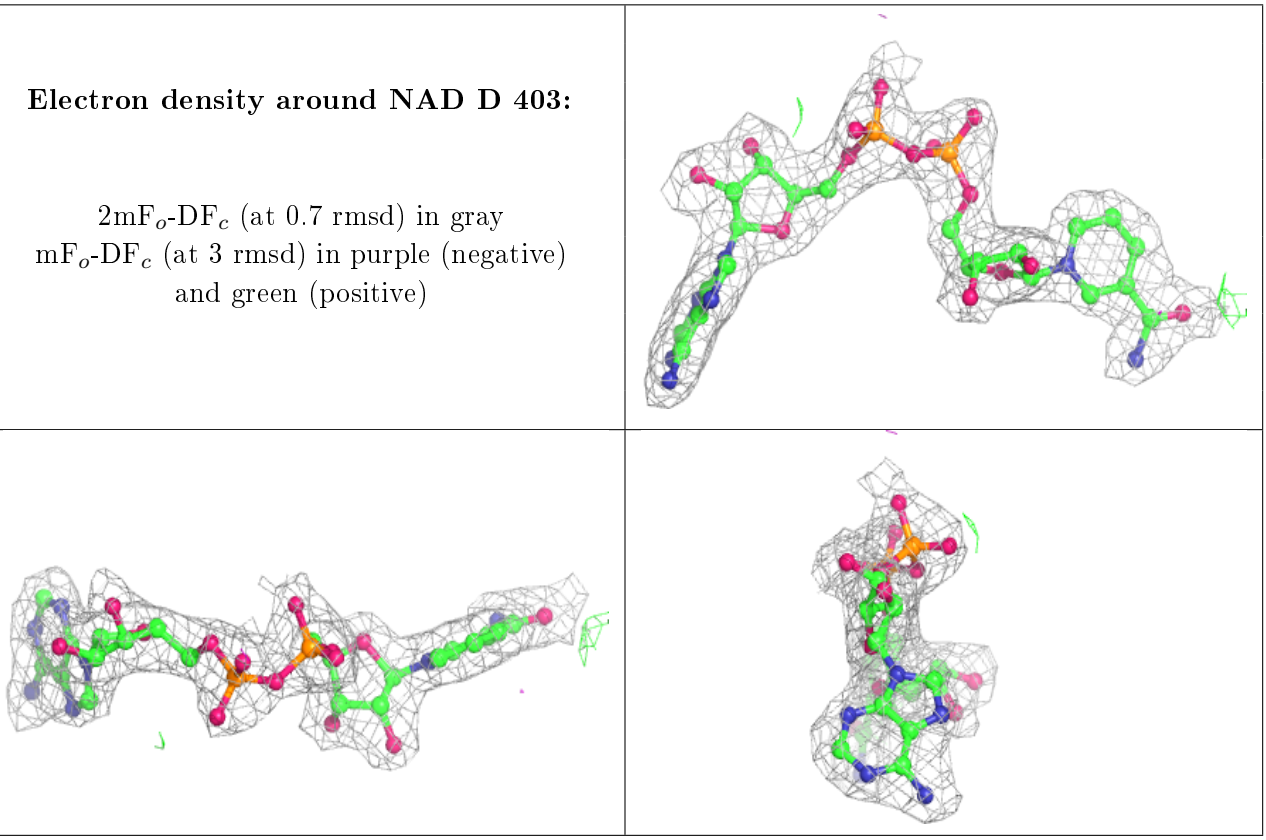
Electron density around NAD F 403:

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



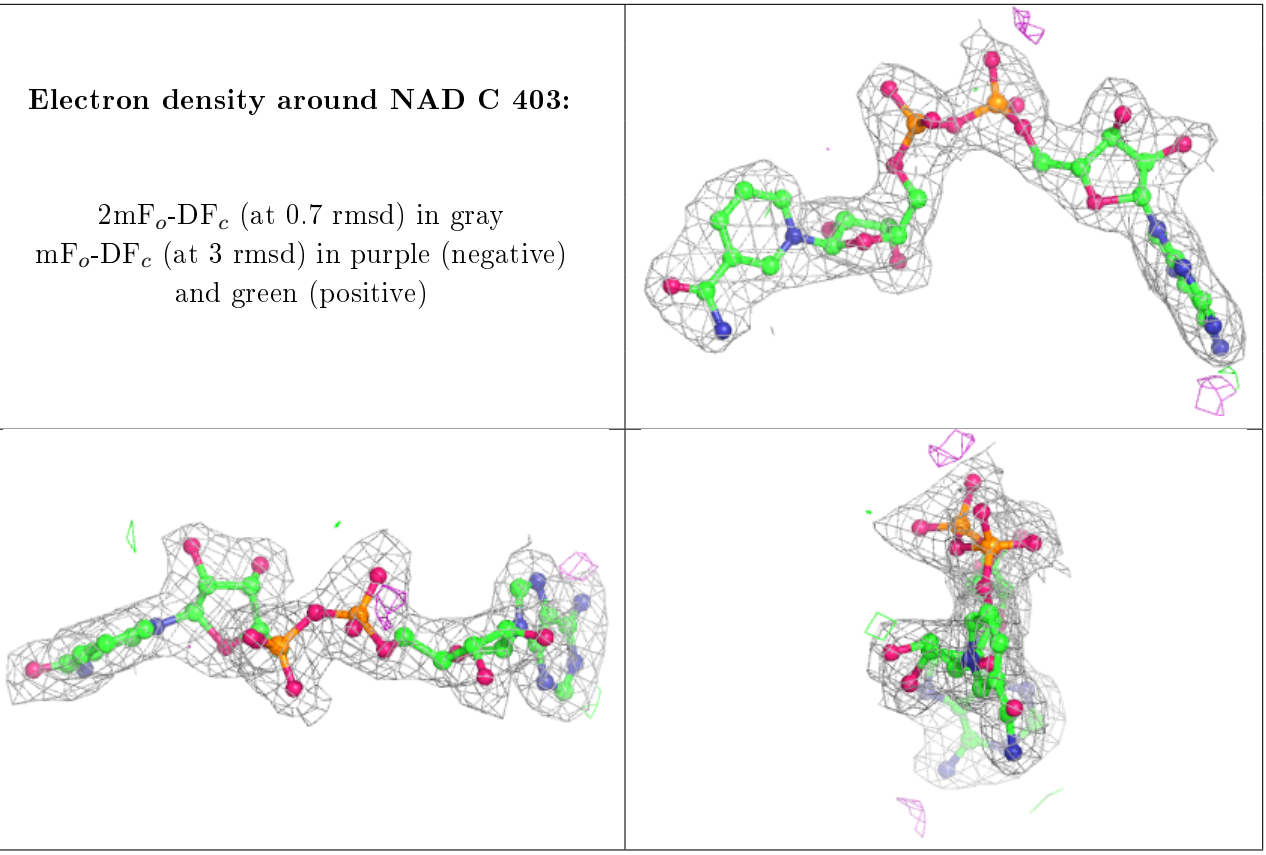
Electron density around NAD D 403:

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



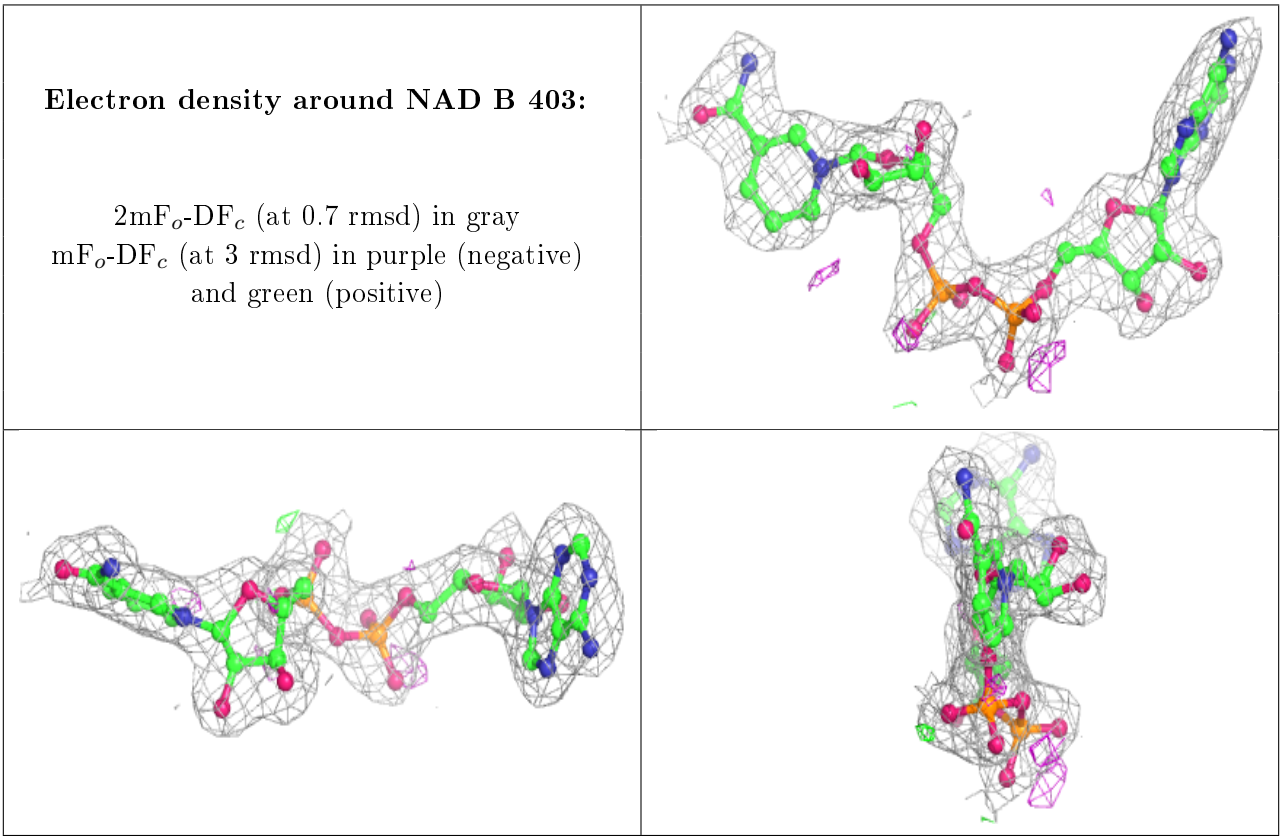
Electron density around NAD C 403:

$2mF_o$-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 403:

$2mF_o$-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.