Full wwPDB X-ray Structure Validation Report (i)

Apr 5, 2026 – 03:57 AM UTC

PDB ID	:	9M3D / pdb_00009m3d
Title	:	Crystal structure of the DgpA1 protein from W974-1 substrate free form
Authors	:	Ma, W.
Deposited on	:	2025-03-01
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

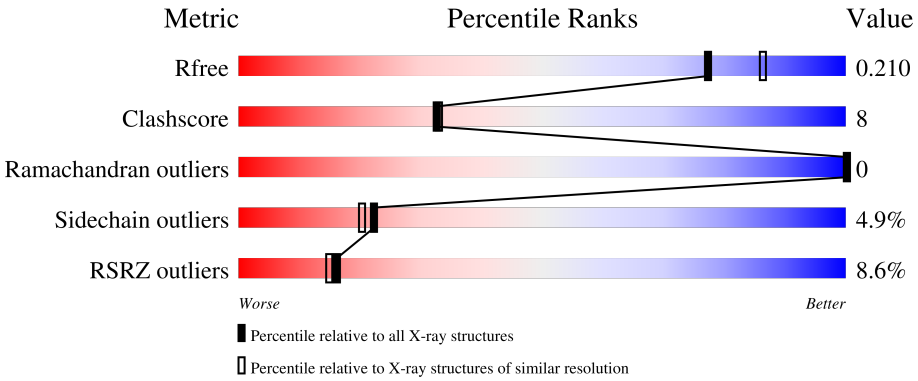
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	366	10% 81% 15%
1	B	366	7% 82% 13%
1	C	366	7% 81% 14%
1	D	366	7% 82% 13%
1	E	366	11% 81% 12%

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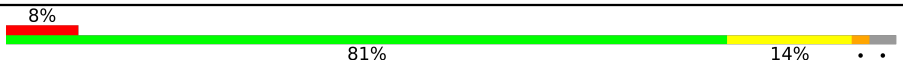
Mol	Chain	Length	Quality of chain
1	F	366	

2 Entry composition

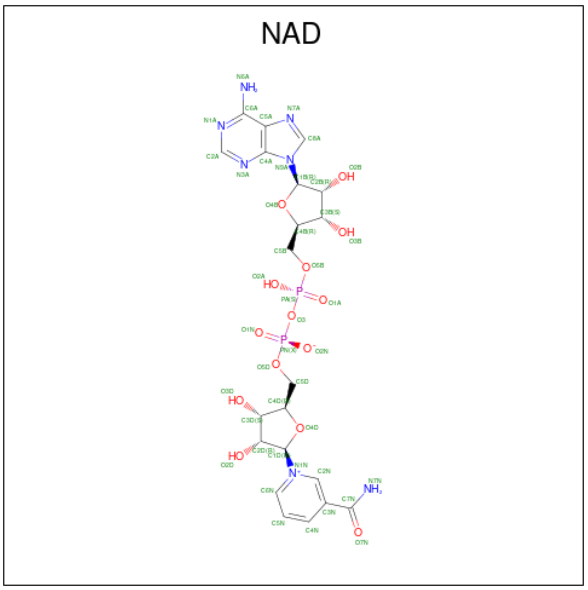
There are 3 unique types of molecules in this entry. The entry contains 17741 atoms, of which 156 are hydrogens and 0 are deuteriums.

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 DgpA1 from W974-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	354	Total	C	N	O	S	0	0	0
			2753	1758	453	527	15			
1	C	355	Total	C	N	O	S	0	0	0
			2755	1759	454	527	15			
1	A	355	Total	C	N	O	S	0	0	0
			2758	1761	453	529	15			
1	D	354	Total	C	N	O	S	0	0	0
			2753	1758	453	527	15			
1	E	352	Total	C	N	O	S	0	0	0
			2732	1747	450	519	16			
1	F	356	Total	C	N	O	S	0	0	0
			2766	1765	455	531	15			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	C	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	E	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	F	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

- Molecule 3 is water.

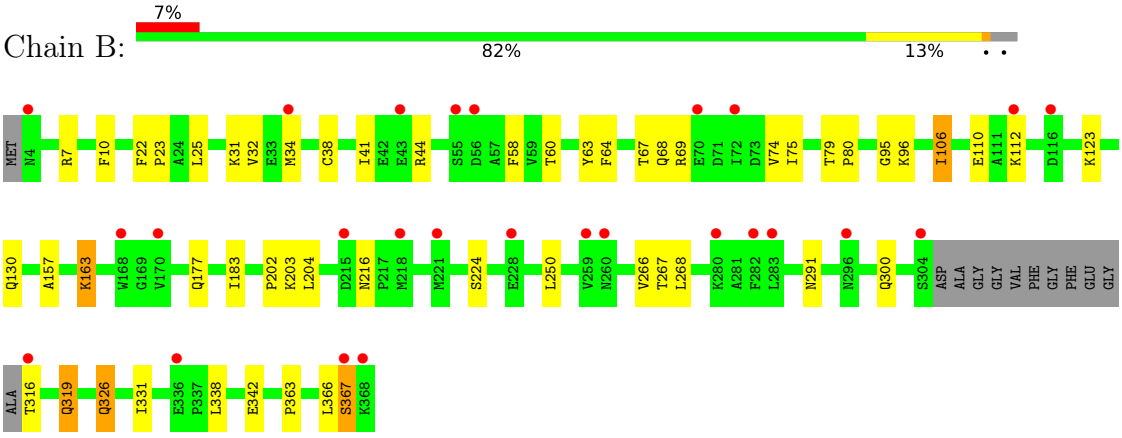
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	147	Total	O	0	0
			147	147		
3	C	143	Total	O	0	0
			143	143		
3	A	100	Total	O	0	0
			100	100		
3	D	177	Total	O	0	0
			177	177		
3	E	103	Total	O	0	0
			103	103		
3	F	134	Total	O	0	0
			134	134		

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.

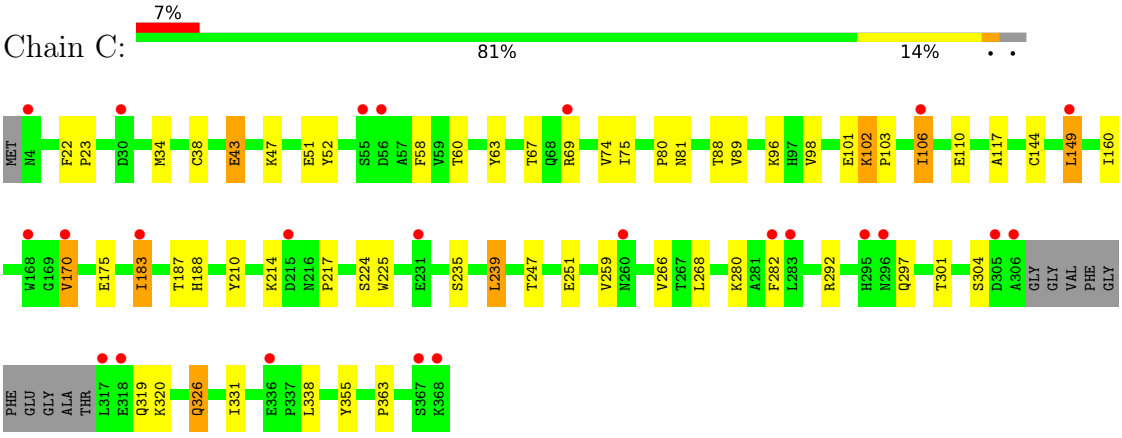
• Molecule 1: DgpA1 from W974-1

Chain B:



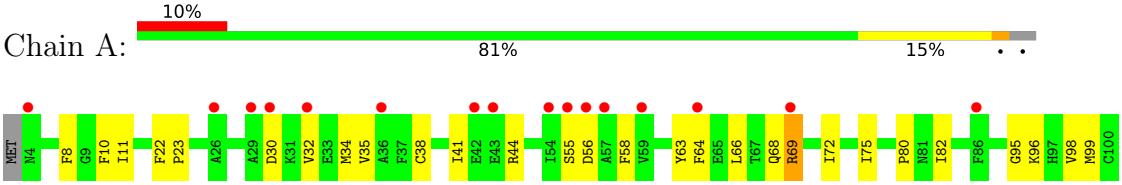
• Molecule 1: DgpA1 from W974-1

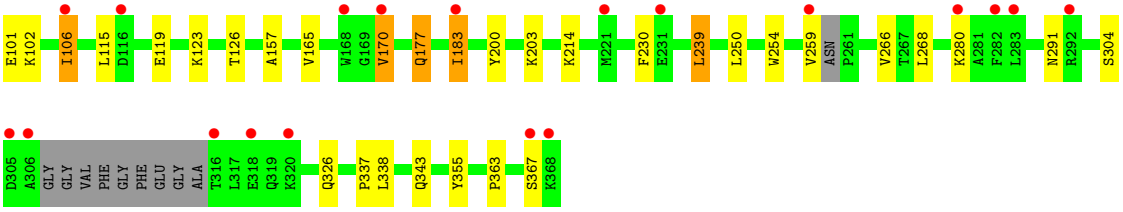
Chain C:



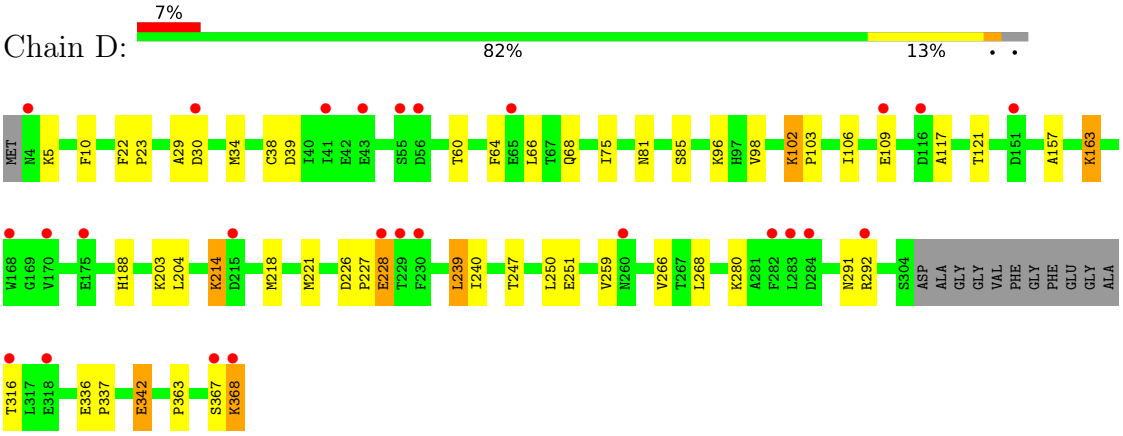
• Molecule 1: DgpA1 from W974-1

Chain A:

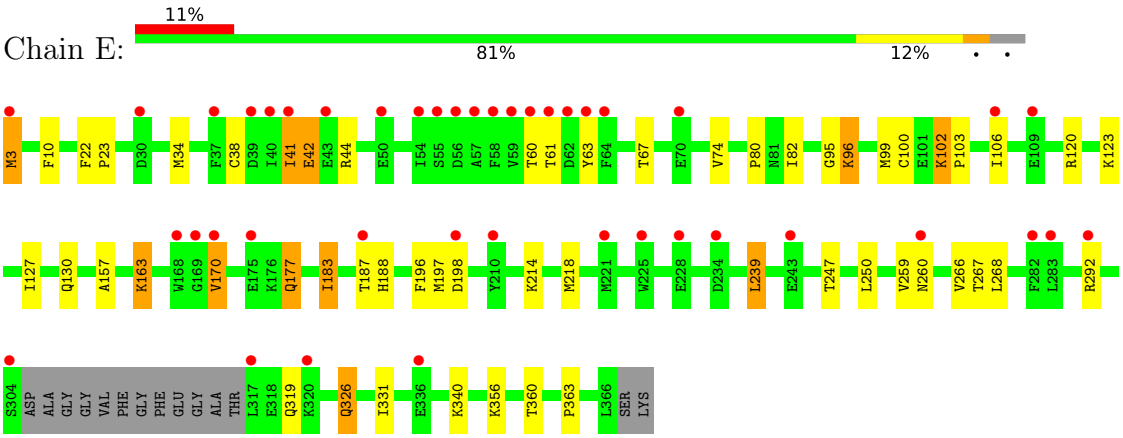




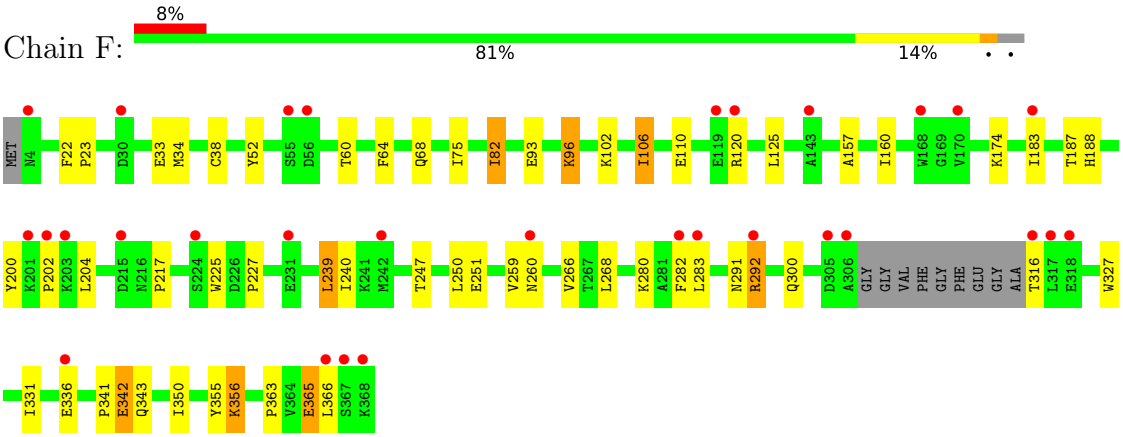
• Molecule 1: DgpA1 from W974-1



• Molecule 1: DgpA1 from W974-1



• Molecule 1: DgpA1 from W974-1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.62Å 161.71Å 201.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.00) 99.9 (50.00-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.202 , 0.211 0.202 , 0.210	Depositor DCC
R_{free} test set	2000 reflections (0.35%)	wwPDB-VP
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 36.9	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	0.96	EDS
Total number of atoms	17741	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: NAD

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	0.32	0/2814	0.51	0/3803
1	B	0.38	0/2810	0.57	0/3800
1	C	0.54	0/2812	0.80	0/3803
1	D	0.35	0/2810	0.55	0/3800
1	E	0.35	0/2789	0.56	0/3772
1	F	0.37	0/2823	0.56	0/3818
All	All	0.39	0/16858	0.60	0/22796

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	2758	0	2718	59	0
1	B	2753	0	2715	41	0
1	C	2755	0	2713	48	0
1	D	2753	0	2715	38	0
1	E	2732	0	2693	43	0
1	F	2766	0	2724	52	0
2	A	44	26	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	26	26	1	0
2	C	44	26	26	1	0
2	D	44	26	26	5	0
2	E	44	26	26	2	0
2	F	44	26	26	0	0
3	A	100	0	0	1	0
3	B	147	0	0	1	0
3	C	143	0	0	1	0
3	D	177	0	0	5	0
3	E	103	0	0	3	0
3	F	134	0	0	3	0
All	All	17585	156	16434	263	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 8.

All (263) 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:363:PRO:HG3	1:C:363:PRO:HG3	1.41	1.03
1:E:363:PRO:HG3	1:F:363:PRO:HG3	1.37	1.02
1:C:34:MET:HE2	1:C:52:TYR:HB3	1.53	0.91
1:B:22:PHE:HA	1:B:34:MET:HE1	1.58	0.85
1:D:239:LEU:HD21	1:D:247:THR:HG23	1.58	0.84
1:F:183:ILE:HD11	1:F:355:TYR:HE2	1.41	0.84
1:F:239:LEU:HD21	1:F:247:THR:HG23	1.62	0.82
1:E:239:LEU:HD21	1:E:247:THR:CG2	2.10	0.81
1:F:183:ILE:HD11	1:F:355:TYR:CE2	2.17	0.79
1:A:157:ALA:HB3	1:A:250:LEU:HD13	1.65	0.79
1:D:39:ASP:HA	2:D:401:NAD:H8A	1.65	0.78
1:F:365:GLU:HG3	3:F:505:HOH:O	1.82	0.78
1:F:75:ILE:HD12	1:F:96:LYS:HG3	1.67	0.77
1:A:64:PHE:O	1:A:68:GLN:HG2	1.86	0.76
1:E:130:GLN:HE22	2:E:401:NAD:H72N	1.34	0.74
1:A:326:GLN:NE2	1:A:338:LEU:H	1.87	0.73
1:B:130:GLN:HE22	2:B:401:NAD:H72N	1.39	0.71
1:A:363:PRO:HG3	1:D:363:PRO:HG3	1.72	0.71
1:A:10:PHE:CZ	1:A:34:MET:HE3	2.26	0.71
1:E:239:LEU:HD21	1:E:247:THR:HG23	1.72	0.70
1:E:319:GLN:HG3	3:E:502:HOH:O	1.91	0.70
1:B:106:ILE:HD11	1:B:110:GLU:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:MET:HE2	1:C:52:TYR:CB	2.23	0.69
1:C:239:LEU:HD21	1:C:247:THR:HG23	1.74	0.69
1:C:106:ILE:HD11	1:C:110:GLU:OE2	1.93	0.68
1:A:99:MET:HE3	1:A:126:THR:HG23	1.75	0.68
1:B:363:PRO:HG3	1:C:363:PRO:CG	2.20	0.68
1:A:82:ILE:HD12	1:A:106:ILE:HD13	1.75	0.68
1:F:75:ILE:CD1	1:F:96:LYS:HG3	2.23	0.67
1:A:22:PHE:CD1	1:A:34:MET:HE1	2.30	0.67
1:C:160:ILE:HD11	1:C:251:GLU:HB2	1.77	0.66
1:A:203:LYS:HG3	1:A:367:SER:OG	1.94	0.66
1:A:326:GLN:HE22	1:A:337:PRO:HA	1.59	0.66
1:B:300:GLN:HE21	1:A:304:SER:CB	2.08	0.66
1:F:82:ILE:HA	1:F:106:ILE:HG12	1.76	0.65
1:A:363:PRO:HG3	1:D:363:PRO:CG	2.26	0.65
1:D:102:LYS:HD3	1:D:188:HIS:CE1	2.31	0.65
1:F:157:ALA:HB3	1:F:250:LEU:HD13	1.77	0.65
1:A:80:PRO:HG3	1:A:170:VAL:HG11	1.78	0.65
1:C:34:MET:CE	1:C:52:TYR:HB3	2.27	0.65
1:D:239:LEU:HD21	1:D:247:THR:CG2	2.28	0.64
1:B:300:GLN:HG3	1:A:304:SER:OG	1.97	0.64
1:E:63:TYR:O	1:E:67:THR:HG23	1.97	0.64
1:F:239:LEU:HD21	1:F:247:THR:CG2	2.28	0.64
1:B:25:LEU:HB2	1:B:34:MET:HE3	1.81	0.63
1:A:22:PHE:HB2	1:A:23:PRO:HD3	1.80	0.63
1:B:75:ILE:HD12	1:B:96:LYS:HG3	1.81	0.63
1:A:326:GLN:NE2	1:A:337:PRO:HA	2.13	0.63
1:C:144:CYS:HA	1:C:149:LEU:CD2	2.28	0.63
1:C:304:SER:OG	1:F:300:GLN:HG3	1.98	0.63
1:A:58:PHE:HB2	1:A:69:ARG:NH1	2.14	0.63
1:C:58:PHE:HB2	1:C:69:ARG:HH21	1.65	0.62
1:E:266:VAL:HG11	1:E:268:LEU:HD21	1.82	0.61
1:E:163:LYS:HE2	1:E:218:MET:O	2.00	0.61
1:A:99:MET:HE3	1:A:126:THR:CG2	2.31	0.60
1:F:106:ILE:CD1	1:F:110:GLU:HG3	2.32	0.60
1:C:149:LEU:H	1:C:149:LEU:HD22	1.66	0.60
1:C:102:LYS:NZ	1:C:187:THR:HG21	2.17	0.60
1:A:99:MET:CE	1:A:126:THR:HG23	2.31	0.60
1:F:106:ILE:HG13	3:F:535:HOH:O	2.02	0.60
1:A:326:GLN:HE22	1:A:338:LEU:H	1.49	0.59
1:E:259:VAL:HG13	1:F:291:ASN:HB3	1.83	0.59
1:F:202:PRO:HG3	1:F:350:ILE:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:LYS:HE2	1:D:218:MET:O	2.02	0.59
1:E:80:PRO:HG3	1:E:170:VAL:HG11	1.84	0.59
1:B:10:PHE:CE1	1:B:34:MET:HG2	2.37	0.58
1:E:42:GLU:HB2	1:E:61:THR:CG2	2.33	0.58
1:B:203:LYS:HG3	1:B:367:SER:HB3	1.85	0.58
1:D:266:VAL:HG11	1:D:268:LEU:HD21	1.85	0.58
1:C:80:PRO:HG3	1:C:170:VAL:HG11	1.85	0.58
1:E:157:ALA:HB3	1:E:250:LEU:HD13	1.85	0.58
1:C:38:CYS:HA	1:C:60:THR:O	2.03	0.57
1:F:183:ILE:CD1	1:F:355:TYR:HE2	2.13	0.57
1:C:266:VAL:HG11	1:C:268:LEU:HD21	1.86	0.57
1:A:101:GLU:OE1	2:A:401:NAD:N3A	2.37	0.57
1:A:115:LEU:O	1:A:119:GLU:HG3	2.05	0.56
1:A:95:GLY:O	1:A:123:LYS:HE2	2.05	0.56
1:F:239:LEU:CD2	1:F:247:THR:HG23	2.34	0.56
1:D:157:ALA:HB3	1:D:250:LEU:HD13	1.88	0.56
1:E:10:PHE:CZ	1:E:34:MET:HE3	2.41	0.56
1:E:22:PHE:CD1	1:E:34:MET:HE1	2.41	0.56
1:A:157:ALA:CB	1:A:250:LEU:HD13	2.33	0.56
1:E:10:PHE:CE1	1:E:34:MET:HE3	2.41	0.56
1:D:64:PHE:O	1:D:68:GLN:HG2	2.05	0.55
1:D:239:LEU:CD2	1:D:247:THR:HG23	2.35	0.55
1:B:22:PHE:HB2	1:B:23:PRO:HD3	1.87	0.55
1:C:144:CYS:HA	1:C:149:LEU:HD23	1.86	0.55
1:A:177:GLN:HE22	2:A:401:NAD:H3B	1.71	0.55
1:E:103:PRO:HG3	1:E:183:ILE:HD13	1.87	0.55
1:C:149:LEU:HD22	1:C:149:LEU:N	2.21	0.55
1:A:8:PHE:CD1	1:A:32:VAL:HG13	2.41	0.55
1:B:106:ILE:HG13	3:B:528:HOH:O	2.07	0.55
1:F:225:TRP:O	1:F:227:PRO:HD3	2.06	0.54
1:B:95:GLY:O	1:B:123:LYS:HE3	2.07	0.54
1:C:47:LYS:HE2	1:C:51:GLU:OE2	2.08	0.54
1:D:214:LYS:HE3	1:D:227:PRO:O	2.07	0.54
1:A:266:VAL:HG11	1:A:268:LEU:HD21	1.90	0.54
1:C:89:VAL:HG13	1:C:117:ALA:HB2	1.88	0.54
1:A:41:ILE:HB	1:A:44:ARG:HD2	1.89	0.54
1:B:41:ILE:HD12	1:B:44:ARG:CZ	2.38	0.54
1:A:75:ILE:HD12	1:A:96:LYS:HG3	1.89	0.54
1:D:10:PHE:CE1	1:D:34:MET:HG2	2.43	0.54
1:E:22:PHE:HB2	1:E:23:PRO:HD3	1.90	0.54
1:B:75:ILE:CD1	1:B:96:LYS:HG3	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:LYS:HD2	1:B:112:LYS:O	2.08	0.53
1:B:266:VAL:HG11	1:B:268:LEU:HD21	1.89	0.53
1:A:239:LEU:HB2	1:D:239:LEU:HD12	1.90	0.53
1:F:64:PHE:O	1:F:68:GLN:HG2	2.08	0.53
1:A:183:ILE:HG13	1:A:355:TYR:HE2	1.74	0.53
1:A:259:VAL:HG13	1:D:291:ASN:HB3	1.91	0.52
1:A:22:PHE:HD1	1:A:34:MET:HE1	1.72	0.52
1:C:239:LEU:CD2	1:C:247:THR:HG23	2.40	0.52
1:E:259:VAL:HG11	1:F:300:GLN:HG2	1.92	0.52
1:A:82:ILE:HD12	1:A:106:ILE:CD1	2.40	0.52
1:E:95:GLY:O	1:E:123:LYS:HE3	2.10	0.52
1:C:106:ILE:HG13	3:C:525:HOH:O	2.10	0.52
1:B:291:ASN:HB3	1:C:259:VAL:HG13	1.92	0.51
1:D:337:PRO:HG2	3:D:547:HOH:O	2.10	0.51
1:B:363:PRO:CG	1:C:363:PRO:HG3	2.29	0.51
1:D:250:LEU:HD12	1:D:251:GLU:N	2.26	0.51
1:B:300:GLN:HE21	1:A:304:SER:HB3	1.73	0.51
1:E:259:VAL:CG1	1:F:300:GLN:HG2	2.40	0.51
1:B:203:LYS:HA	1:B:367:SER:HB3	1.93	0.51
1:F:22:PHE:HB2	1:F:23:PRO:HD3	1.93	0.50
1:C:187:THR:HG23	1:C:188:HIS:H	1.75	0.50
1:D:22:PHE:HB2	1:D:23:PRO:HD3	1.94	0.50
1:D:81:ASN:OD1	1:D:103:PRO:HD2	2.11	0.50
1:C:34:MET:CE	1:C:52:TYR:CB	2.89	0.50
1:A:214:LYS:HG3	1:A:230:PHE:HB3	1.93	0.50
1:C:75:ILE:HD12	1:C:96:LYS:HG3	1.93	0.49
1:D:226:ASP:OD1	1:D:228:GLU:HG2	2.13	0.49
1:C:187:THR:HG23	1:C:188:HIS:N	2.27	0.49
1:C:301:THR:HG21	1:F:292:ARG:HH12	1.78	0.49
1:A:183:ILE:HG22	1:A:183:ILE:O	2.13	0.49
1:A:75:ILE:CD1	1:A:96:LYS:HG3	2.43	0.49
1:F:34:MET:CE	1:F:52:TYR:HB3	2.42	0.49
1:F:106:ILE:HD11	1:F:110:GLU:HG3	1.95	0.48
1:F:157:ALA:CB	1:F:250:LEU:HD13	2.43	0.48
1:F:342:GLU:CD	1:F:342:GLU:H	2.21	0.48
1:A:75:ILE:O	1:A:98:VAL:HA	2.13	0.48
1:F:200:TYR:CZ	1:F:343:GLN:HG2	2.48	0.48
1:A:326:GLN:NE2	1:A:338:LEU:N	2.57	0.48
1:F:82:ILE:O	1:F:82:ILE:HD12	2.13	0.48
1:F:202:PRO:HB2	1:F:366:LEU:HD12	1.96	0.48
1:A:326:GLN:HE22	1:A:337:PRO:CA	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:VAL:HG12	1:E:267:THR:N	2.29	0.47
1:B:300:GLN:CG	1:A:304:SER:OG	2.61	0.47
1:A:165:VAL:HG22	1:A:254:TRP:HB3	1.95	0.47
1:D:102:LYS:C	1:D:102:LYS:HE3	2.39	0.47
1:B:38:CYS:HA	1:B:60:THR:O	2.14	0.47
1:D:203:LYS:HG3	1:D:367:SER:OG	2.14	0.47
1:C:75:ILE:CD1	1:C:96:LYS:HG3	2.44	0.47
1:A:72:ILE:O	1:A:96:LYS:HD2	2.15	0.47
1:D:10:PHE:HE1	1:D:34:MET:HG2	1.80	0.47
1:B:266:VAL:HG12	1:B:267:THR:N	2.30	0.46
1:E:239:LEU:CD2	1:E:247:THR:HG23	2.41	0.46
1:A:214:LYS:HG3	1:A:230:PHE:CB	2.45	0.46
1:B:10:PHE:HE1	1:B:34:MET:HG2	1.79	0.46
1:E:340:LYS:HE3	3:E:546:HOH:O	2.14	0.46
1:F:38:CYS:HA	1:F:60:THR:O	2.16	0.46
1:A:10:PHE:CE1	1:A:34:MET:HE3	2.50	0.46
1:A:72:ILE:HB	1:A:96:LYS:HE3	1.98	0.46
1:D:228:GLU:HG2	1:D:228:GLU:H	1.53	0.46
1:D:342:GLU:CD	1:D:342:GLU:H	2.23	0.46
1:E:67:THR:O	1:E:96:LYS:HE2	2.16	0.46
1:E:356:LYS:O	1:E:360:THR:HG23	2.16	0.46
1:B:58:PHE:CE2	1:B:69:ARG:HD2	2.51	0.45
1:B:163:LYS:HE2	1:B:216:ASN:O	2.16	0.45
1:C:280:LYS:HG2	1:C:282:PHE:CE1	2.51	0.45
1:F:239:LEU:HD23	1:F:240:ILE:N	2.31	0.45
1:A:11:ILE:HD13	1:A:63:TYR:HB2	1.97	0.45
1:D:5:LYS:HE2	1:D:29:ALA:O	2.16	0.45
1:F:266:VAL:HG11	1:F:268:LEU:HD21	1.98	0.45
1:B:326:GLN:OE1	1:B:338:LEU:N	2.38	0.45
1:B:10:PHE:CZ	1:B:34:MET:HE2	2.52	0.45
1:B:157:ALA:HB3	1:B:250:LEU:HD13	1.99	0.45
1:A:266:VAL:HG12	1:A:268:LEU:HG	1.99	0.45
1:F:217:PRO:HA	1:F:225:TRP:CH2	2.51	0.45
1:F:187:THR:HG23	1:F:188:HIS:N	2.32	0.44
2:A:401:NAD:H5N	3:A:557:HOH:O	2.16	0.44
1:F:160:ILE:HD11	1:F:251:GLU:HB2	1.99	0.44
1:C:101:GLU:OE1	2:C:401:NAD:N3A	2.51	0.44
1:F:125:LEU:O	1:F:341:PRO:HD3	2.18	0.44
1:C:102:LYS:HZ2	1:C:187:THR:HG21	1.81	0.44
1:C:106:ILE:HG13	1:C:106:ILE:H	1.43	0.44
2:D:401:NAD:N3A	2:D:401:NAD:H2B	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:TYR:HB2	1:C:235:SER:OG	2.18	0.44
1:E:102:LYS:HD2	1:E:102:LYS:C	2.43	0.44
1:F:204:LEU:HD11	1:F:363:PRO:HB2	1.99	0.44
1:F:356:LYS:HB2	1:F:356:LYS:HE3	1.53	0.44
1:F:75:ILE:HD12	1:F:96:LYS:CG	2.43	0.43
1:F:106:ILE:HG13	1:F:106:ILE:H	1.55	0.43
1:F:187:THR:HG23	1:F:188:HIS:H	1.83	0.43
1:C:102:LYS:HZ3	1:C:187:THR:HG21	1.81	0.43
1:A:56:ASP:OD1	1:A:56:ASP:N	2.48	0.43
1:B:204:LEU:HD21	1:C:363:PRO:HD3	2.00	0.43
1:C:74:VAL:HG21	1:C:331:ILE:HD13	2.01	0.43
1:E:170:VAL:HG13	2:E:401:NAD:O1A	2.18	0.43
1:D:38:CYS:HA	1:D:60:THR:O	2.18	0.43
1:E:187:THR:HG23	1:E:188:HIS:N	2.33	0.43
1:C:239:LEU:HD21	1:C:247:THR:CG2	2.45	0.43
1:A:200:TYR:CZ	1:A:343:GLN:HG2	2.54	0.43
1:F:282:PHE:CD1	1:F:283:LEU:HG	2.54	0.43
1:A:291:ASN:HB3	1:D:259:VAL:CG1	2.48	0.43
1:E:3:MET:HE3	1:E:3:MET:HB3	1.70	0.43
1:B:64:PHE:O	1:B:68:GLN:HG2	2.19	0.43
1:F:93:GLU:OE2	1:F:120:ARG:NH1	2.52	0.43
1:F:250:LEU:HD12	1:F:251:GLU:N	2.34	0.43
1:A:58:PHE:HB2	1:A:69:ARG:CZ	2.49	0.42
1:D:39:ASP:CG	2:D:401:NAD:H1B	2.44	0.42
1:D:292:ARG:HE	1:D:292:ARG:HB3	1.63	0.42
1:E:102:LYS:HE2	1:E:188:HIS:NE2	2.33	0.42
1:F:336:GLU:OE1	1:F:336:GLU:HA	2.19	0.42
1:C:183:ILE:CG1	1:C:355:TYR:HE2	2.32	0.42
1:A:363:PRO:HD3	1:D:204:LEU:HD21	2.01	0.42
1:F:34:MET:HE2	1:F:52:TYR:HB3	2.00	0.42
1:B:300:GLN:NE2	1:A:304:SER:HA	2.35	0.42
1:E:292:ARG:HE	1:E:292:ARG:HB3	1.71	0.42
1:B:79:THR:HB	1:B:80:PRO:CD	2.50	0.42
1:C:67:THR:O	1:C:96:LYS:HE2	2.18	0.42
1:D:239:LEU:HD23	1:D:240:ILE:N	2.34	0.42
1:D:368:LYS:HD2	1:D:368:LYS:H	1.84	0.42
1:A:38:CYS:HB2	1:A:66:LEU:HD12	2.01	0.42
1:D:66:LEU:C	1:D:66:LEU:HD23	2.45	0.42
1:E:198:ASP:CB	3:E:507:HOH:O	2.68	0.42
1:C:63:TYR:O	1:C:67:THR:HG23	2.20	0.42
1:C:326:GLN:OE1	1:C:338:LEU:N	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:MET:HE1	3:D:672:HOH:O	2.20	0.41
1:E:41:ILE:HD12	1:E:44:ARG:CZ	2.50	0.41
1:F:260:ASN:HA	3:F:560:HOH:O	2.20	0.41
1:C:81:ASN:OD1	1:C:103:PRO:HD2	2.20	0.41
1:E:326:GLN:HE21	1:E:326:GLN:HB3	1.52	0.41
1:F:327:TRP:CZ2	1:F:331:ILE:HD11	2.55	0.41
1:E:41:ILE:HB	1:E:44:ARG:HD2	2.01	0.41
1:E:74:VAL:HG21	1:E:331:ILE:HD13	2.01	0.41
1:F:366:LEU:HA	1:F:366:LEU:HD23	1.84	0.41
1:C:22:PHE:HB2	1:C:23:PRO:HD3	2.02	0.41
1:C:88:THR:HG23	1:C:98:VAL:HG11	2.03	0.41
1:E:42:GLU:HB2	1:E:61:THR:HG22	2.03	0.41
1:C:43:GLU:H	1:C:43:GLU:HG3	1.58	0.41
1:F:106:ILE:HD12	1:F:110:GLU:HG3	2.02	0.41
1:B:63:TYR:O	1:B:67:THR:HG23	2.21	0.41
1:B:326:GLN:HE21	1:B:326:GLN:HB3	1.59	0.41
1:C:217:PRO:HA	1:C:225:TRP:CH2	2.56	0.41
1:A:38:CYS:HB2	1:A:66:LEU:CD1	2.50	0.41
1:A:69:ARG:HE	1:A:69:ARG:HB3	1.64	0.41
1:E:100:CYS:O	1:E:127:ILE:HA	2.20	0.41
1:D:85:SER:HB3	3:D:581:HOH:O	2.20	0.41
1:E:259:VAL:O	1:E:260:ASN:HB2	2.20	0.41
1:B:202:PRO:HB2	1:B:366:LEU:HD12	2.04	0.40
1:B:203:LYS:CG	1:B:367:SER:HB3	2.50	0.40
2:D:401:NAD:C2A	3:D:513:HOH:O	2.69	0.40
1:A:326:GLN:HE22	1:A:338:LEU:N	2.15	0.40
1:D:117:ALA:O	1:D:121:THR:HG23	2.21	0.40
2:D:401:NAD:H2A	3:D:513:HOH:O	2.20	0.40
1:E:38:CYS:HA	1:E:60:THR:O	2.21	0.40
1:E:197:MET:O	1:E:198:ASP:HB2	2.21	0.40
1:D:75:ILE:O	1:D:98:VAL:HA	2.21	0.40
1:F:183:ILE:CG1	1:F:355:TYR:HE2	2.35	0.40
1:B:74:VAL:HG21	1:B:331:ILE:HD13	2.03	0.40
1:B:319:GLN:H	1:B:319:GLN:HG2	1.65	0.40
1:E:177:GLN:OE1	1:E:177:GLN:HA	2.21	0.40
1:E:266:VAL:CG1	1:E:267:THR:N	2.85	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	349/366 (95%)	338 (97%)	11 (3%)	0	100	100
1	B	350/366 (96%)	342 (98%)	8 (2%)	0	100	100
1	C	351/366 (96%)	343 (98%)	8 (2%)	0	100	100
1	D	350/366 (96%)	342 (98%)	8 (2%)	0	100	100
1	E	348/366 (95%)	335 (96%)	13 (4%)	0	100	100
1	F	352/366 (96%)	341 (97%)	11 (3%)	0	100	100
All	All	2100/2196 (96%)	2041 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	288/294 (98%)	277 (96%)	11 (4%)	29	29
1	B	288/294 (98%)	275 (96%)	13 (4%)	24	23
1	C	287/294 (98%)	272 (95%)	15 (5%)	21	18
1	D	288/294 (98%)	274 (95%)	14 (5%)	22	20
1	E	284/294 (97%)	267 (94%)	17 (6%)	17	14
1	F	289/294 (98%)	275 (95%)	14 (5%)	23	21
All	All	1724/1764 (98%)	1640 (95%)	84 (5%)	22	20

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	ARG
1	B	31	LYS
1	B	32	VAL
1	B	106	ILE
1	B	163	LYS
1	B	177	GLN
1	B	183	ILE
1	B	224	SER
1	B	316	THR
1	B	319	GLN
1	B	326	GLN
1	B	342	GLU
1	B	367	SER
1	C	43	GLU
1	C	102	LYS
1	C	106	ILE
1	C	149	LEU
1	C	170	VAL
1	C	175	GLU
1	C	183	ILE
1	C	214	LYS
1	C	224	SER
1	C	239	LEU
1	C	292	ARG
1	C	297	GLN
1	C	319	GLN
1	C	320	LYS
1	C	326	GLN
1	A	30	ASP
1	A	35	VAL
1	A	55	SER
1	A	69	ARG
1	A	102	LYS
1	A	106	ILE
1	A	170	VAL
1	A	177	GLN
1	A	183	ILE
1	A	239	LEU
1	A	280	LYS
1	D	30	ASP
1	D	96	LYS
1	D	102	LYS

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Mol	Chain	Res	Type
1	D	106	ILE
1	D	109	GLU
1	D	163	LYS
1	D	214	LYS
1	D	228	GLU
1	D	239	LEU
1	D	280	LYS
1	D	316	THR
1	D	336	GLU
1	D	342	GLU
1	D	368	LYS
1	E	3	MET
1	E	41	ILE
1	E	42	GLU
1	E	82	ILE
1	E	96	LYS
1	E	99	MET
1	E	102	LYS
1	E	106	ILE
1	E	120	ARG
1	E	163	LYS
1	E	170	VAL
1	E	177	GLN
1	E	183	ILE
1	E	196	PHE
1	E	214	LYS
1	E	239	LEU
1	E	326	GLN
1	F	33	GLU
1	F	82	ILE
1	F	96	LYS
1	F	102	LYS
1	F	106	ILE
1	F	174	LYS
1	F	239	LEU
1	F	259	VAL
1	F	280	LYS
1	F	292	ARG
1	F	316	THR
1	F	342	GLU
1	F	356	LYS
1	F	365	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	300	GLN
1	A	177	GLN
1	A	326	GLN
1	D	211	GLN
1	D	216	ASN
1	E	177	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
2	NAD	D	401	-	46,48,48	1.48	7 (15%)	64,73,73	1.97	18 (28%)
2	NAD	B	401	-	46,48,48	1.11	3 (6%)	64,73,73	0.96	2 (3%)
2	NAD	C	401	-	46,48,48	1.05	3 (6%)	64,73,73	1.70	15 (23%)
2	NAD	A	401	-	46,48,48	1.23	3 (6%)	64,73,73	2.05	14 (21%)
2	NAD	F	401	-	46,48,48	1.16	3 (6%)	64,73,73	0.89	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAD	E	401	-	46,48,48	1.25	2 (4%)	64,73,73	1.20	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	401	-	-	4/30/62/62	0/5/5/5
2	NAD	B	401	-	-	2/30/62/62	0/5/5/5
2	NAD	C	401	-	-	9/30/62/62	0/5/5/5
2	NAD	A	401	-	-	8/30/62/62	0/5/5/5
2	NAD	F	401	-	-	2/30/62/62	0/5/5/5
2	NAD	E	401	-	-	7/30/62/62	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	PA-O3	5.91	1.65	1.59
2	E	401	NAD	PA-O3	5.75	1.65	1.59
2	F	401	NAD	PA-O3	5.26	1.65	1.59
2	D	401	NAD	PA-O3	5.25	1.65	1.59
2	B	401	NAD	PA-O3	4.57	1.64	1.59
2	E	401	NAD	PN-O3	4.05	1.63	1.59
2	D	401	NAD	C4A-N9A	-3.59	1.30	1.37
2	C	401	NAD	PA-O3	3.35	1.63	1.59
2	B	401	NAD	PN-O3	3.26	1.63	1.59
2	F	401	NAD	PN-O3	3.20	1.62	1.59
2	D	401	NAD	O4D-C1D	-3.18	1.36	1.40
2	B	401	NAD	O4D-C1D	-2.87	1.37	1.40
2	D	401	NAD	C2A-N3A	-2.81	1.29	1.33
2	F	401	NAD	O4D-C1D	-2.73	1.37	1.40
2	A	401	NAD	PN-O3	2.50	1.62	1.59
2	C	401	NAD	PN-O3	2.29	1.62	1.59
2	D	401	NAD	PN-O3	2.28	1.62	1.59
2	D	401	NAD	C4A-N3A	-2.18	1.30	1.34
2	C	401	NAD	C7N-N7N	2.05	1.36	1.33
2	A	401	NAD	C2N-C3N	-2.04	1.35	1.39
2	D	401	NAD	C5A-C6A	-2.00	1.35	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	NAD	C5A-C4A-N3A	6.33	135.44	126.72
2	A	401	NAD	O4B-C1B-N9A	6.10	119.80	108.09
2	C	401	NAD	C4D-O4D-C1D	5.87	115.30	109.92
2	A	401	NAD	O2B-C2B-C1B	4.93	127.09	110.10
2	D	401	NAD	C2B-C1B-N9A	4.70	124.98	113.30
2	A	401	NAD	O7N-C7N-N7N	4.56	129.20	122.62
2	C	401	NAD	O4D-C4D-C5D	4.31	123.15	109.33
2	A	401	NAD	O4B-C4B-C5B	-4.28	95.62	109.33
2	D	401	NAD	O4B-C4B-C5B	4.20	122.80	109.33
2	D	401	NAD	C4A-C5A-N7A	4.15	115.33	110.58
2	A	401	NAD	O2B-C2B-C3B	-4.01	98.97	111.82
2	A	401	NAD	O3B-C3B-C4B	-3.77	100.26	111.08
2	A	401	NAD	C3B-C2B-C1B	3.68	108.42	101.46
2	A	401	NAD	O7N-C7N-C3N	-3.67	115.11	119.60
2	D	401	NAD	O4B-C4B-C3B	-3.49	98.23	105.15
2	D	401	NAD	O2B-C2B-C1B	3.45	121.98	110.10
2	E	401	NAD	O2N-PN-O3	3.43	116.55	107.27
2	D	401	NAD	C6A-C5A-C4A	-3.36	112.59	117.18
2	D	401	NAD	N3A-C4A-N9A	-3.26	121.63	127.17
2	D	401	NAD	O4B-C1B-C2B	-3.19	99.79	106.62
2	A	401	NAD	C2B-C1B-N9A	-3.17	105.43	113.30
2	A	401	NAD	C1B-N9A-C8A	3.01	133.78	127.09
2	A	401	NAD	C5B-C4B-C3B	3.01	126.03	115.21
2	B	401	NAD	O2A-PA-O1A	2.99	126.36	112.44
2	E	401	NAD	C2B-C3B-C4B	2.99	108.38	102.61
2	C	401	NAD	O4B-C1B-C2B	-2.98	100.23	106.62
2	D	401	NAD	C2A-N3A-C4A	-2.95	104.63	111.83
2	C	401	NAD	O2B-C2B-C1B	2.94	120.22	110.10
2	C	401	NAD	C3B-C2B-C1B	2.91	106.96	101.46
2	C	401	NAD	C6N-N1N-C1D	-2.84	114.16	119.73
2	D	401	NAD	C2B-C3B-C4B	2.83	108.08	102.61
2	D	401	NAD	C5A-N7A-C8A	-2.79	99.06	103.45
2	E	401	NAD	O4B-C4B-C5B	2.79	118.28	109.33
2	D	401	NAD	O2A-PA-O1A	2.76	125.30	112.44
2	C	401	NAD	O2A-PA-O1A	2.72	125.11	112.44
2	C	401	NAD	O7N-C7N-C3N	-2.70	116.30	119.60
2	D	401	NAD	C5A-C4A-N9A	-2.65	102.93	105.81
2	D	401	NAD	C3N-C7N-N7N	-2.58	114.56	117.74
2	C	401	NAD	C6N-N1N-C2N	2.57	124.06	121.88
2	B	401	NAD	O3D-C3D-C4D	-2.53	103.81	111.08
2	E	401	NAD	O3D-C3D-C4D	-2.49	103.93	111.08
2	F	401	NAD	C2B-C1B-N9A	2.49	119.48	113.30
2	C	401	NAD	C4B-O4B-C1B	2.48	114.95	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	NAD	C5D-C4D-C3D	-2.44	106.42	115.21
2	A	401	NAD	C6N-N1N-C2N	2.42	123.93	121.88
2	C	401	NAD	C6N-C5N-C4N	-2.40	115.99	119.45
2	F	401	NAD	C3N-C7N-N7N	-2.38	114.81	117.74
2	C	401	NAD	C5A-C4A-N3A	-2.37	123.45	126.72
2	E	401	NAD	O2A-PA-O1A	2.37	123.47	112.44
2	A	401	NAD	O3D-C3D-C4D	-2.23	104.69	111.08
2	D	401	NAD	O3D-C3D-C4D	-2.21	104.73	111.08
2	A	401	NAD	O2N-PN-O1N	2.13	122.33	112.44
2	D	401	NAD	C4B-O4B-C1B	2.12	114.15	109.47
2	C	401	NAD	O2B-C2B-C3B	-2.05	105.24	111.82
2	C	401	NAD	N3A-C4A-N9A	2.03	130.62	127.17
2	D	401	NAD	O2B-C2B-C3B	-2.01	105.36	111.82

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	C2D-C1D-N1N-C2N
2	C	401	NAD	C2D-C1D-N1N-C6N
2	C	401	NAD	C2N-C3N-C7N-O7N
2	C	401	NAD	C2N-C3N-C7N-N7N
2	A	401	NAD	C5B-O5B-PA-O2A
2	A	401	NAD	C5B-O5B-PA-O3
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	C2D-C1D-N1N-C2N
2	A	401	NAD	C2D-C1D-N1N-C6N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	E	401	NAD	O4D-C1D-N1N-C2N
2	E	401	NAD	O4D-C1D-N1N-C6N
2	F	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	C4N-C3N-C7N-N7N
2	C	401	NAD	C4N-C3N-C7N-O7N
2	A	401	NAD	O4B-C4B-C5B-O5B
2	E	401	NAD	O4B-C4B-C5B-O5B
2	E	401	NAD	PN-O3-PA-O1A
2	E	401	NAD	C3B-C4B-C5B-O5B
2	E	401	NAD	PN-O3-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	E	401	NAD	C2D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C2N
2	D	401	NAD	O4D-C1D-N1N-C2N
2	F	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C4D-C5D-O5D
2	A	401	NAD	O4D-C4D-C5D-O5D
2	D	401	NAD	O4B-C1B-N9A-C8A
2	D	401	NAD	C2B-C1B-N9A-C8A

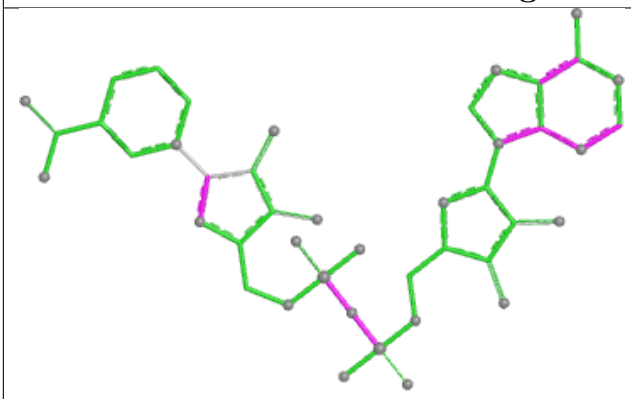
There are no ring outliers.

5 monomers are involved in 12 short contacts:

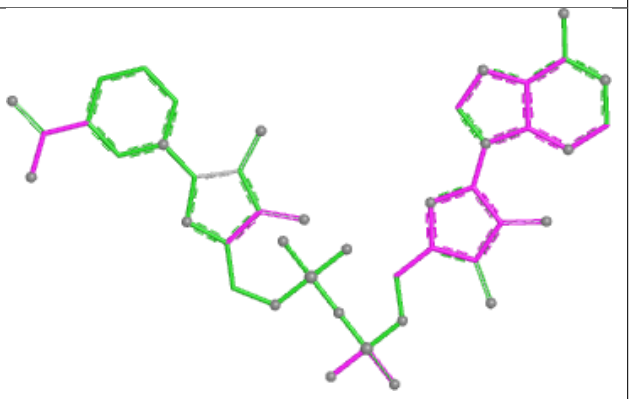
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	NAD	5	0
2	B	401	NAD	1	0
2	C	401	NAD	1	0
2	A	401	NAD	3	0
2	E	401	NAD	2	0

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.

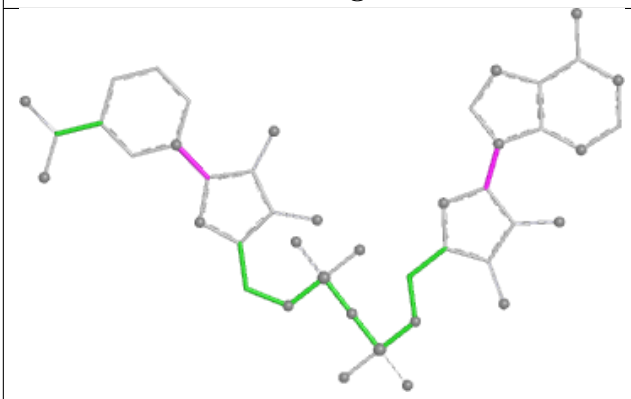
Ligand NAD D 401



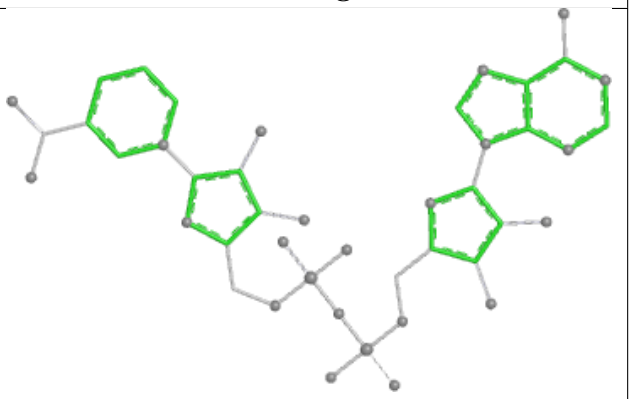
Bond lengths



Bond angles

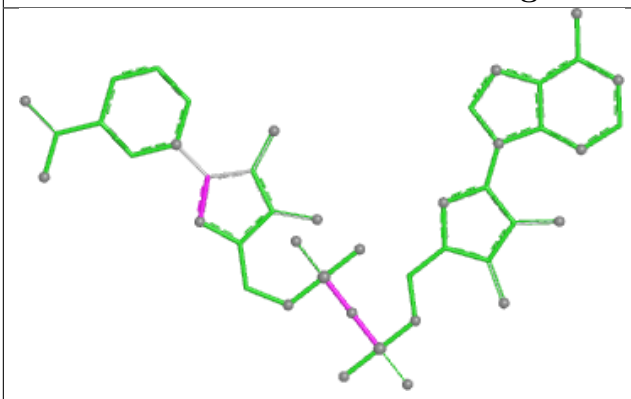


Torsions

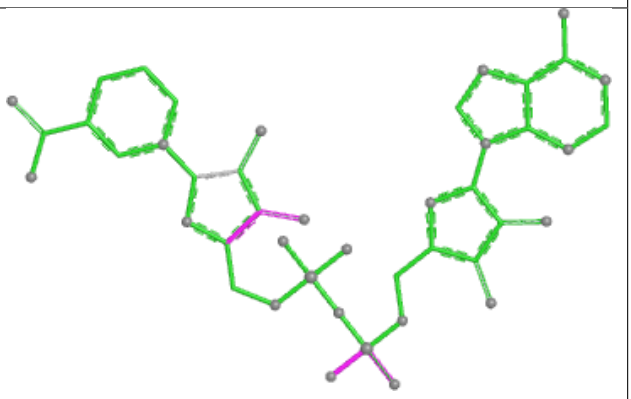


Rings

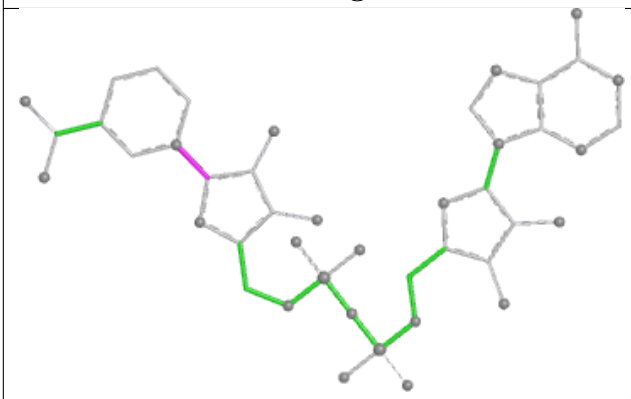
Ligand NAD B 401



Bond lengths



Bond angles



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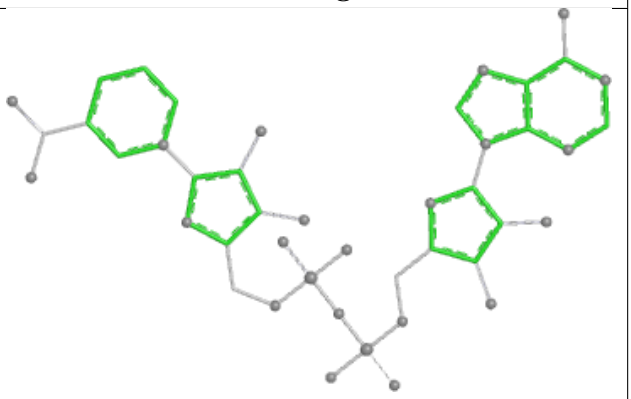
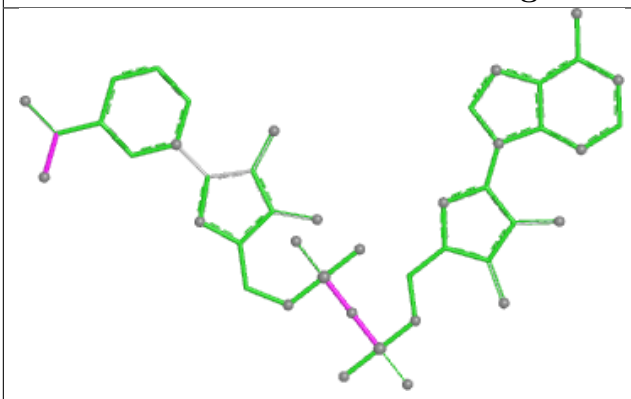
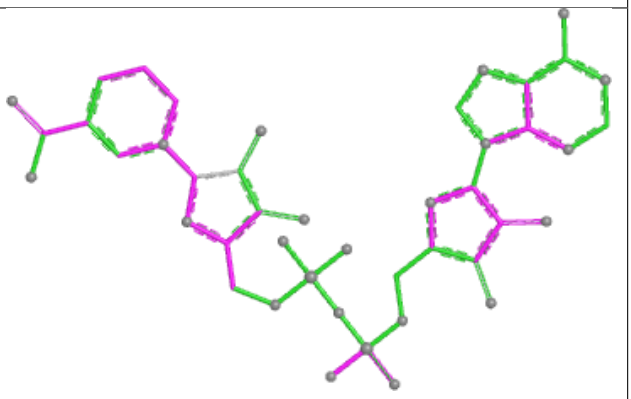


Rings

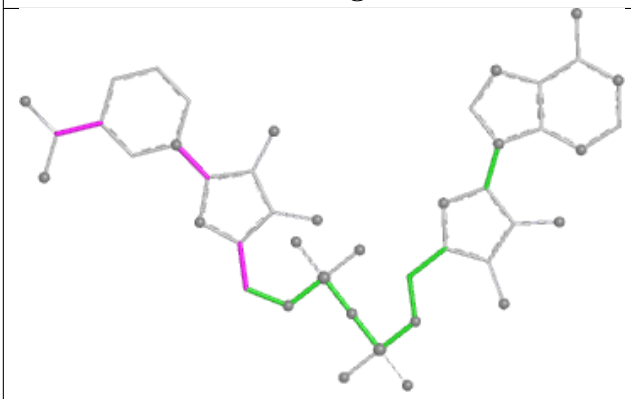
Ligand NAD C 401



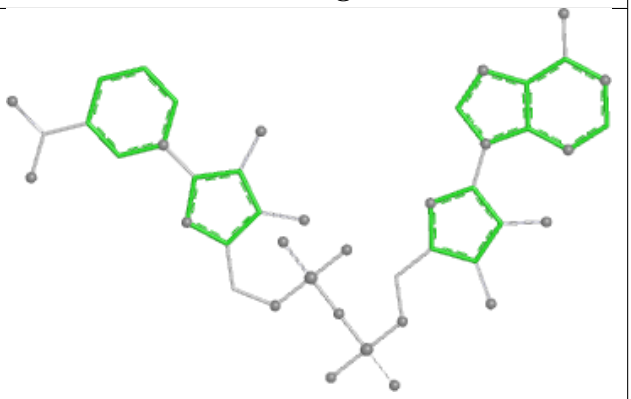
Bond lengths



Bond angles

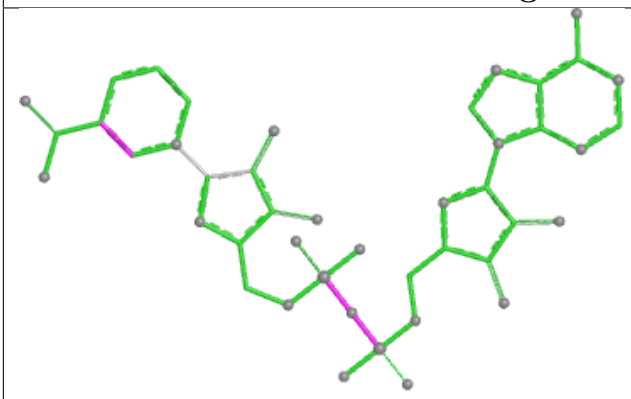


Torsions

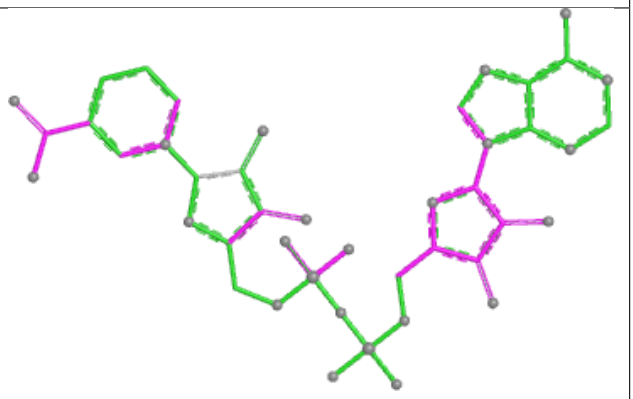


Rings

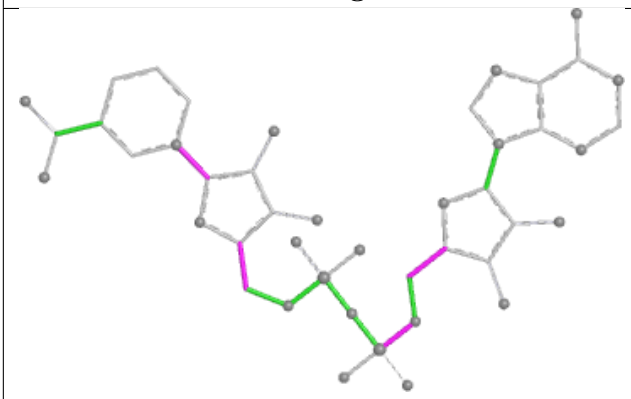
Ligand NAD A 401



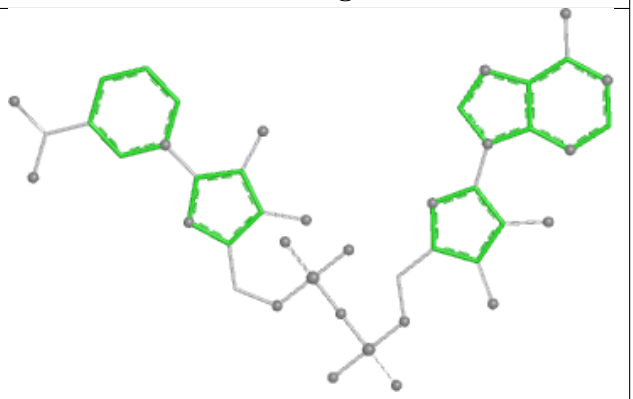
Bond lengths



Bond angles

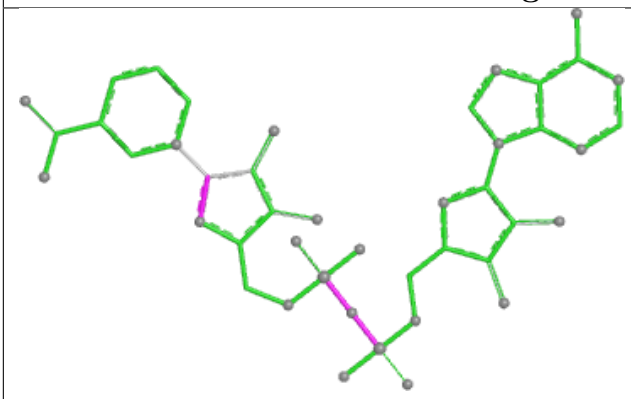


Torsions

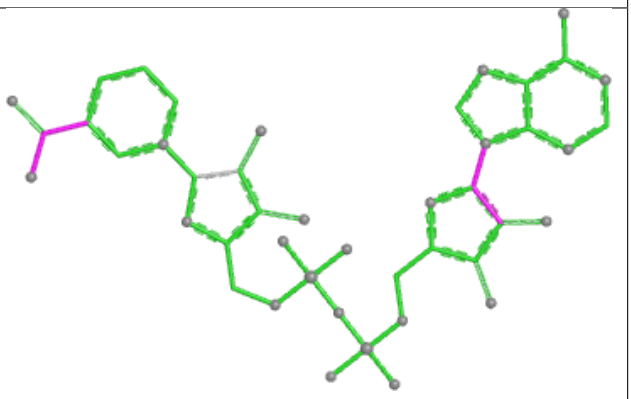


Rings

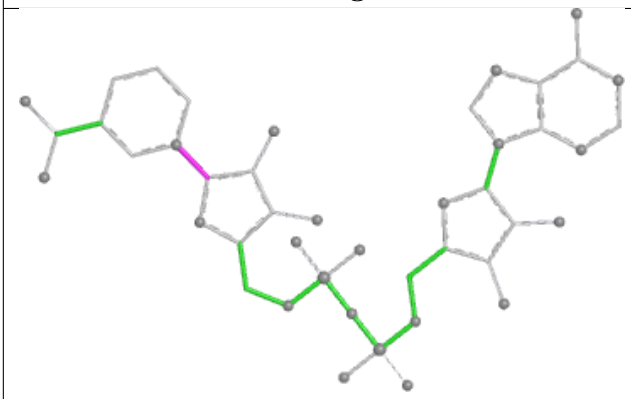
Ligand NAD F 401



Bond lengths



Bond angles



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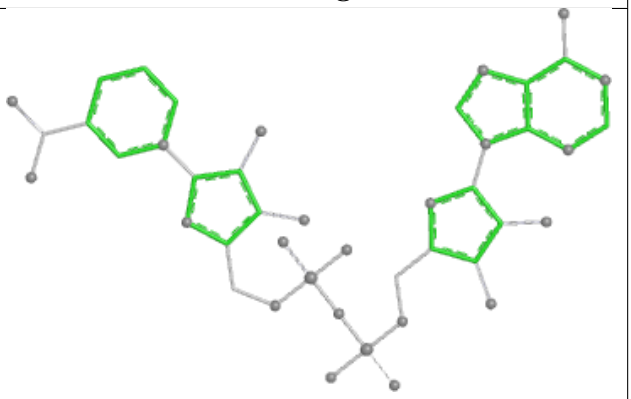
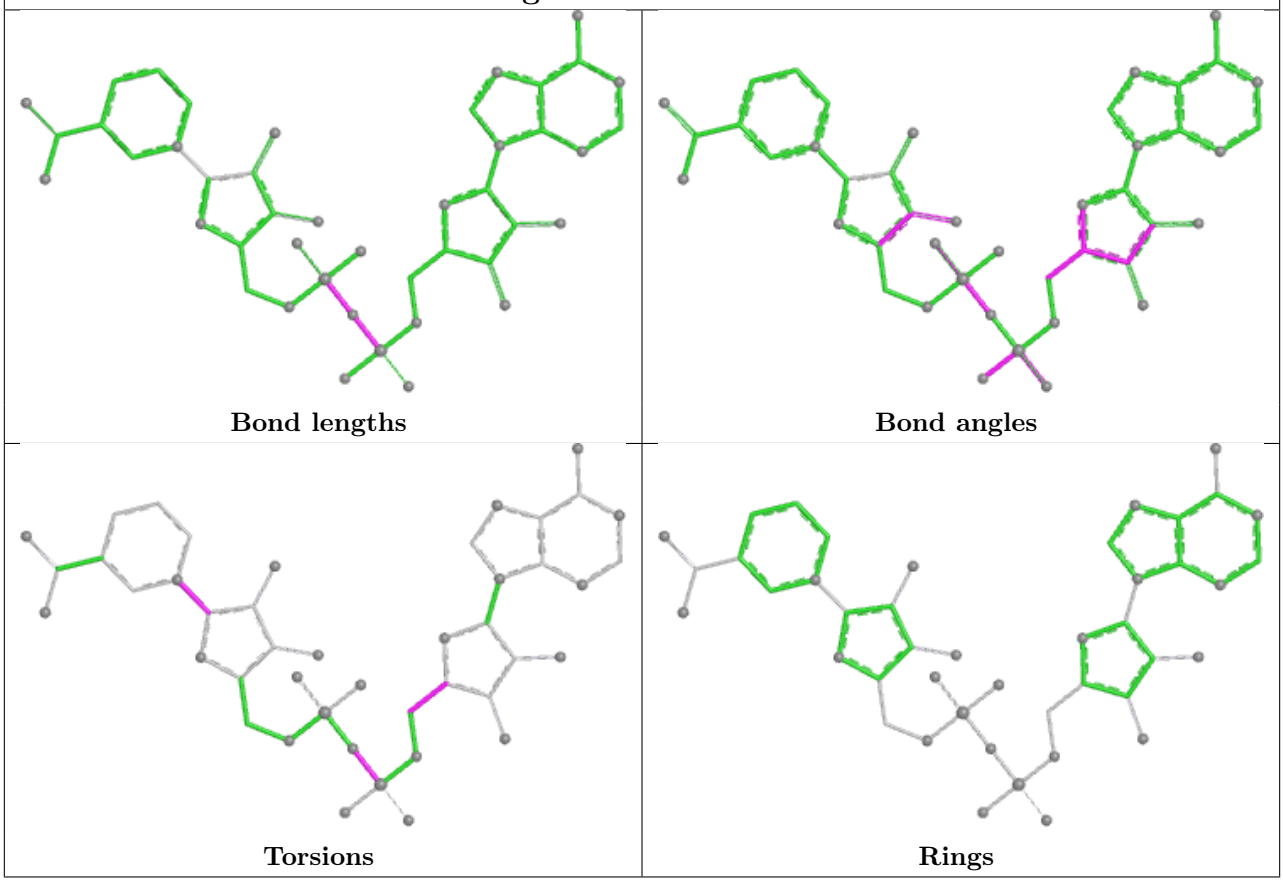


Rings

Ligand NAD E 401



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	355/366 (96%)	0.66	35 (9%)	13	11	31, 46, 66, 94	0
1	B	354/366 (96%)	0.28	26 (7%)	21	19	29, 38, 59, 95	0
1	C	355/366 (96%)	0.42	24 (6%)	23	22	31, 39, 58, 97	0
1	D	354/366 (96%)	0.21	26 (7%)	21	19	30, 37, 58, 103	0
1	E	352/366 (96%)	0.70	42 (11%)	9	8	32, 47, 66, 110	0
1	F	356/366 (97%)	0.35	30 (8%)	17	15	30, 39, 61, 109	0
All	All	2126/2196 (96%)	0.44	183 (8%)	16	15	29, 40, 64, 110	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	367	SER	11.7
1	B	367	SER	9.4
1	C	367	SER	7.1
1	F	367	SER	6.8
1	F	368	LYS	6.5
1	B	170	VAL	6.0
1	A	368	LYS	5.4
1	F	170	VAL	5.4
1	D	367	SER	5.3
1	C	368	LYS	5.3
1	B	218	MET	5.3
1	B	368	LYS	5.0
1	D	368	LYS	5.0
1	B	282	PHE	4.9
1	F	316	THR	4.9
1	C	295	HIS	4.9
1	C	306	ALA	4.8
1	B	283	LEU	4.7
1	F	201	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	306	ALA	4.6
1	E	198	ASP	4.6
1	D	170	VAL	4.5
1	D	316	THR	4.4
1	E	3	MET	4.3
1	F	283	LEU	4.3
1	F	55	SER	4.2
1	C	168	TRP	4.2
1	E	225	TRP	4.2
1	F	30	ASP	4.2
1	D	109	GLU	4.2
1	A	316	THR	4.1
1	E	55	SER	4.1
1	D	56	ASP	4.1
1	E	57	ALA	4.0
1	A	56	ASP	4.0
1	A	282	PHE	4.0
1	E	168	TRP	4.0
1	B	72	ILE	3.9
1	B	316	THR	3.8
1	C	55	SER	3.8
1	A	283	LEU	3.8
1	E	56	ASP	3.7
1	B	168	TRP	3.7
1	F	282	PHE	3.7
1	C	4	ASN	3.6
1	F	306	ALA	3.6
1	E	317	LEU	3.6
1	D	151	ASP	3.6
1	C	183	ILE	3.6
1	F	183	ILE	3.6
1	B	55	SER	3.6
1	E	40	ILE	3.5
1	B	56	ASP	3.4
1	A	55	SER	3.4
1	C	336	GLU	3.4
1	A	69	ARG	3.3
1	E	170	VAL	3.3
1	F	242	MET	3.3
1	A	43	GLU	3.3
1	B	116	ASP	3.3
1	E	210	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	305	ASP	3.2
1	E	282	PHE	3.2
1	C	106	ILE	3.2
1	C	149	LEU	3.2
1	F	56	ASP	3.1
1	A	64	PHE	3.1
1	D	292	ARG	3.1
1	D	228	GLU	3.1
1	C	305	ASP	3.1
1	F	143	ALA	3.1
1	D	168	TRP	3.0
1	E	292	ARG	3.0
1	F	215	ASP	3.0
1	A	320	LYS	3.0
1	A	59	VAL	3.0
1	C	170	VAL	2.9
1	C	56	ASP	2.9
1	C	30	ASP	2.9
1	D	43	GLU	2.9
1	C	260	ASN	2.9
1	F	4	ASN	2.9
1	A	57	ALA	2.9
1	A	4	ASN	2.8
1	D	116	ASP	2.8
1	D	65	GLU	2.8
1	E	41	ILE	2.8
1	D	260	ASN	2.8
1	E	304	SER	2.8
1	B	228	GLU	2.8
1	A	168	TRP	2.8
1	E	30	ASP	2.8
1	E	59	VAL	2.8
1	B	70	GLU	2.7
1	A	36	ALA	2.7
1	A	106	ILE	2.7
1	E	37	PHE	2.7
1	B	259	VAL	2.7
1	E	283	LEU	2.6
1	A	292	ARG	2.6
1	F	336	GLU	2.6
1	C	296	ASN	2.6
1	D	4	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	317	LEU	2.6
1	E	54	ILE	2.6
1	A	86	PHE	2.6
1	F	224	SER	2.6
1	D	175	GLU	2.5
1	A	280	LYS	2.5
1	C	282	PHE	2.5
1	B	34	MET	2.5
1	A	32	VAL	2.5
1	A	259	VAL	2.5
1	B	260	ASN	2.5
1	E	62	ASP	2.5
1	F	168	TRP	2.5
1	E	106	ILE	2.5
1	B	43	GLU	2.5
1	A	42	GLU	2.5
1	B	296	ASN	2.5
1	A	305	ASP	2.4
1	B	280	LYS	2.4
1	D	282	PHE	2.4
1	C	283	LEU	2.4
1	B	336	GLU	2.4
1	A	318	GLU	2.4
1	F	318	GLU	2.4
1	B	304	SER	2.4
1	D	229	THR	2.4
1	A	231	GLU	2.4
1	E	260	ASN	2.4
1	D	215	ASP	2.4
1	E	58	PHE	2.4
1	E	64	PHE	2.4
1	E	60	THR	2.4
1	F	120	ARG	2.3
1	E	175	GLU	2.3
1	F	202	PRO	2.3
1	F	231	GLU	2.3
1	F	260	ASN	2.3
1	A	30	ASP	2.3
1	F	203	LYS	2.3
1	E	61	THR	2.3
1	E	234	ASP	2.3
1	D	55	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	39	ASP	2.3
1	E	320	LYS	2.3
1	D	283	LEU	2.3
1	D	318	GLU	2.2
1	E	43	GLU	2.2
1	A	183	ILE	2.2
1	A	170	VAL	2.2
1	C	231	GLU	2.2
1	A	29	ALA	2.2
1	B	215	ASP	2.2
1	A	54	ILE	2.2
1	E	336	GLU	2.2
1	F	317	LEU	2.2
1	F	292	ARG	2.2
1	B	112	LYS	2.2
1	B	4	ASN	2.2
1	E	221	MET	2.2
1	E	187	THR	2.2
1	E	169	GLY	2.1
1	D	284	ASP	2.1
1	C	69	ARG	2.1
1	E	243	GLU	2.1
1	A	26	ALA	2.1
1	E	50	GLU	2.1
1	A	116	ASP	2.1
1	D	41	ILE	2.1
1	B	221	MET	2.0
1	E	70	GLU	2.0
1	E	63	TYR	2.0
1	C	318	GLU	2.0
1	D	230	PHE	2.0
1	E	109	GLU	2.0
1	E	228	GLU	2.0
1	F	119	GLU	2.0
1	A	221	MET	2.0
1	F	366	LEU	2.0
1	C	215	ASP	2.0
1	D	30	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 oligosaccharides in this entry.

6.4 Ligands (i)

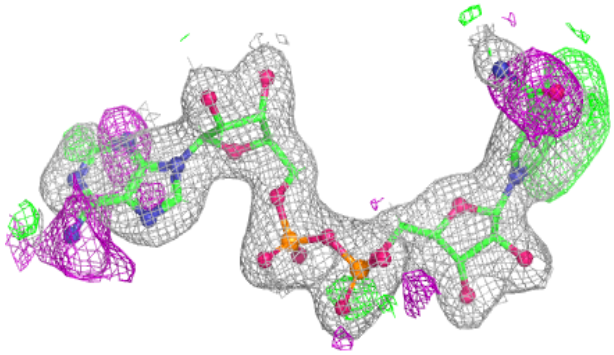
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

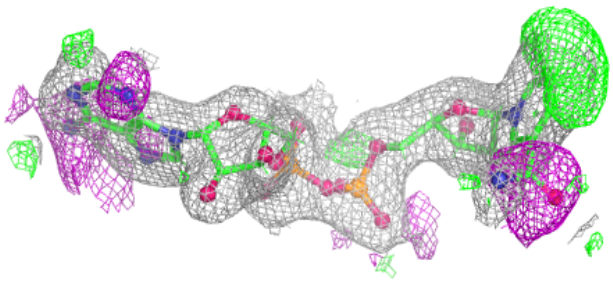
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	C	401	44/44	0.91	0.13	35,43,57,79	0
2	NAD	A	401	44/44	0.92	0.11	44,53,67,78	0
2	NAD	D	401	44/44	0.95	0.09	32,39,50,60	0
2	NAD	E	401	44/44	0.95	0.09	42,52,64,69	0
2	NAD	B	401	44/44	0.98	0.06	30,36,45,47	0
2	NAD	F	401	44/44	0.98	0.06	32,39,48,52	0

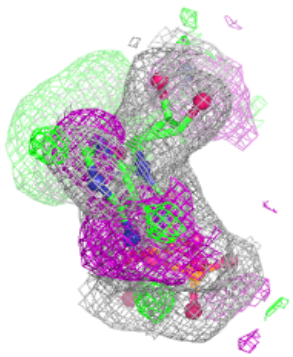
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD C 401:

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

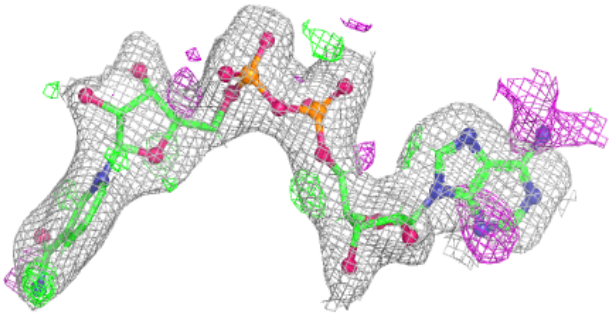


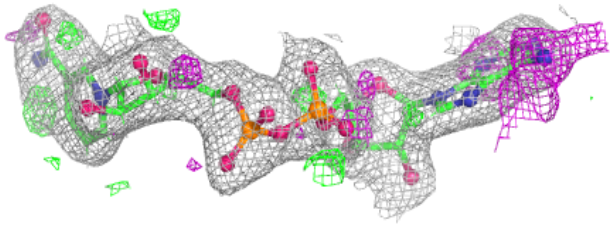


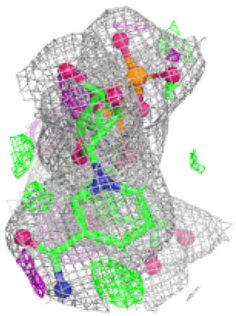


Electron density around NAD A 401:

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

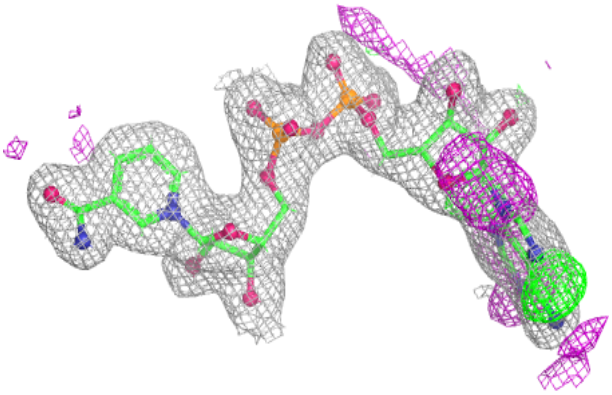


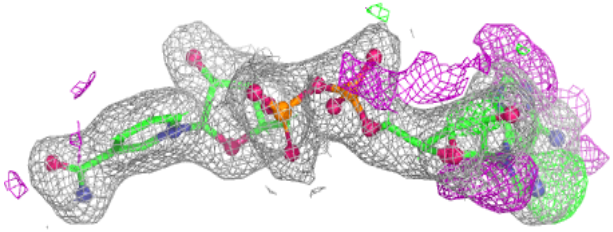


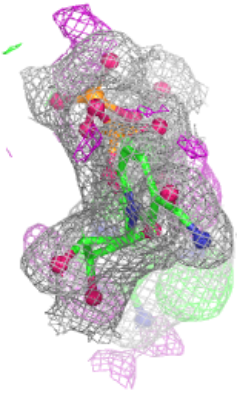


Electron density around NAD D 401:

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

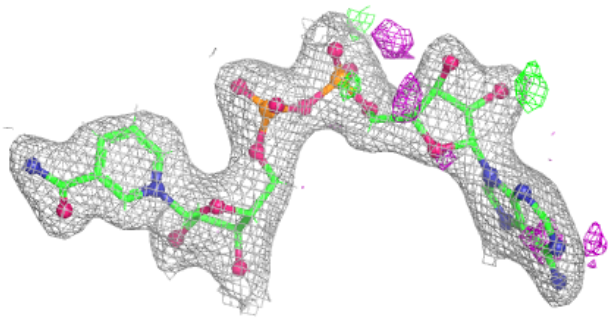


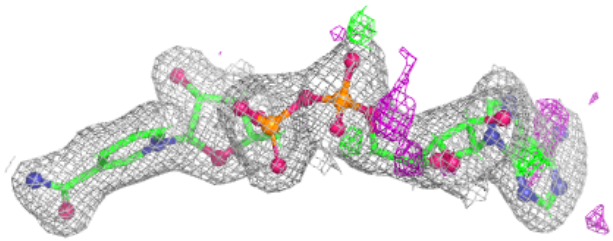


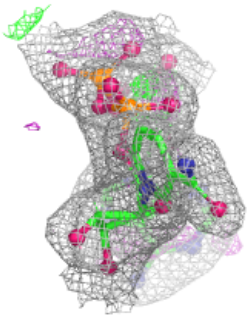


Electron density around NAD E 401:

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

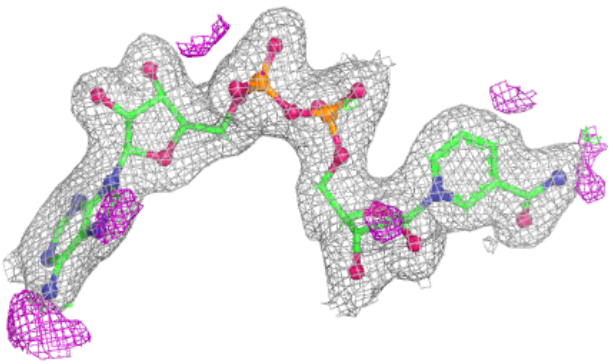


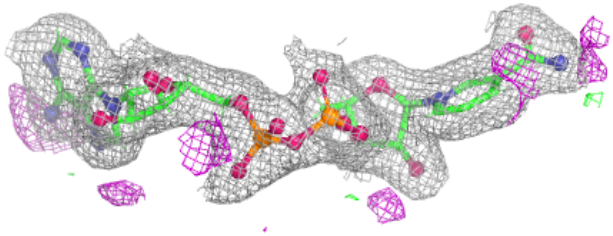


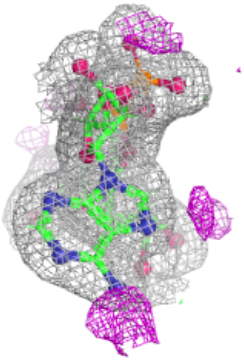


Electron density around NAD B 401:

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

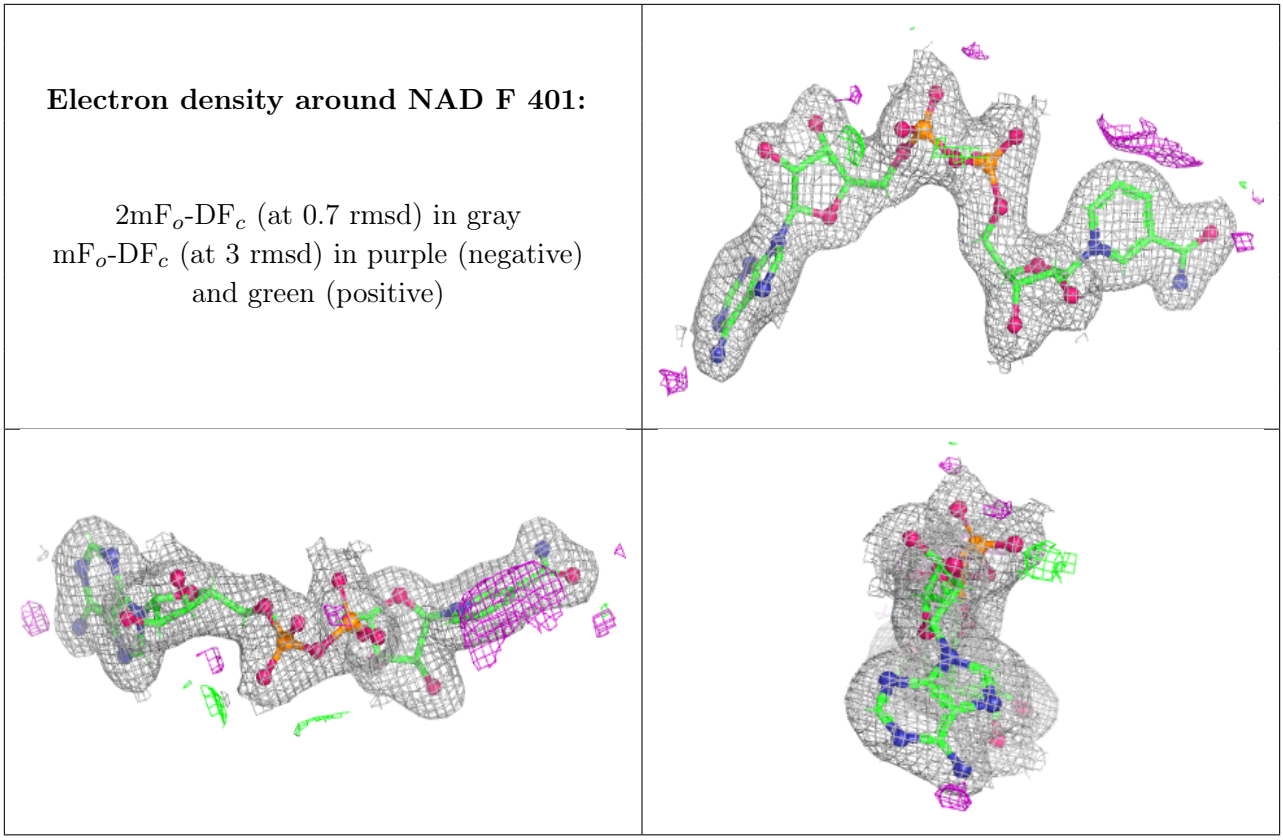






Electron density around NAD F 401:

$2mF_o$-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.