



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:46 am BST

PDB ID : 5GTK
Title : NAD⁺ complex structure of aldehyde dehydrogenase from bacillus cereus
Authors : Ngo, H.P.T.; Hong, S.H.; Ho, T.H.; Oh, D.K.; Kang, L.W.
Deposited on : 2016-08-21
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

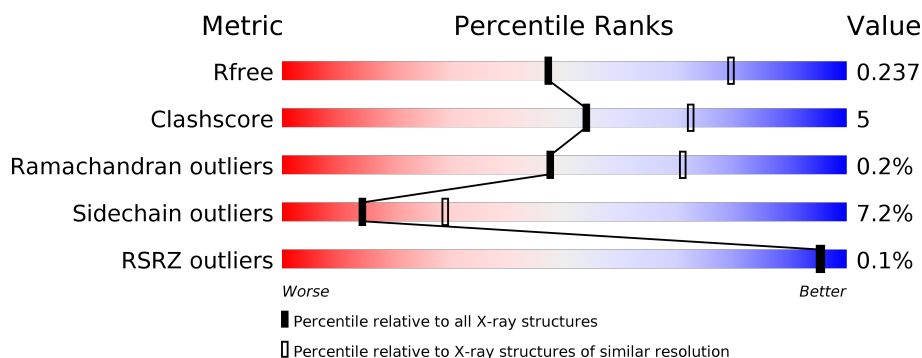
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	494	
1	B	494	
1	C	494	
1	D	494	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15843 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 Betaine-aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3791	2414	630	733	14			
1	B	488	Total	C	N	O	S	0	1	0
			3771	2402	626	728	15			
1	C	489	Total	C	N	O	S	0	0	0
			3776	2406	627	729	14			
1	D	491	Total	C	N	O	S	0	1	0
			3794	2416	630	733	15			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

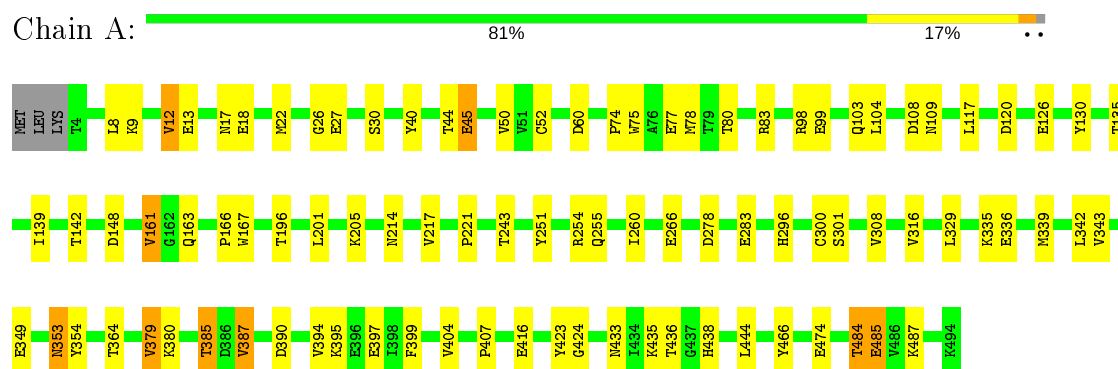
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total	O	0	0
			140	140		
4	B	141	Total	O	0	0
			141	141		
4	C	126	Total	O	0	0
			126	126		
4	D	125	Total	O	0	0
			125	125		

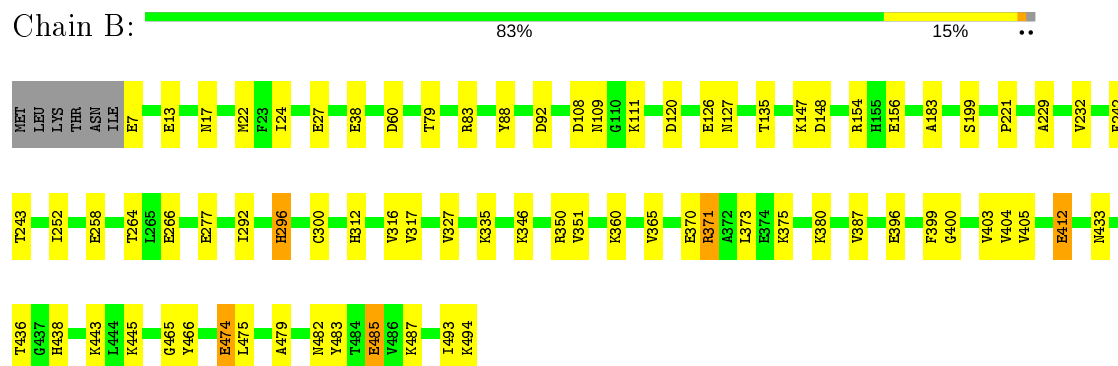
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

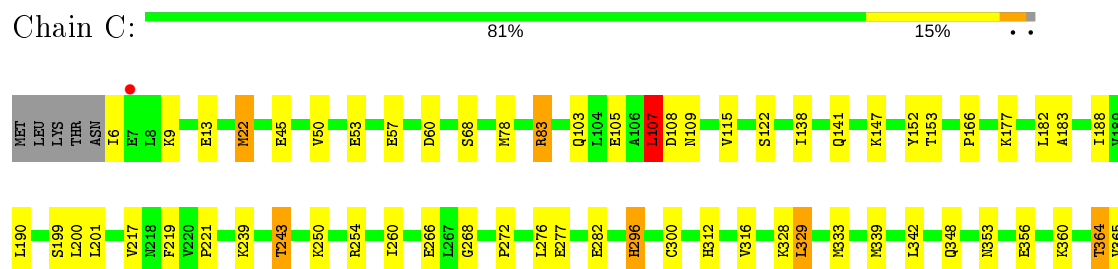
• Molecule 1: Betaine-aldehyde dehydrogenase

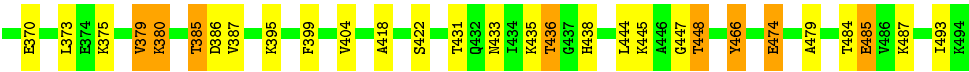


• Molecule 1: Betaine-aldehyde dehydrogenase

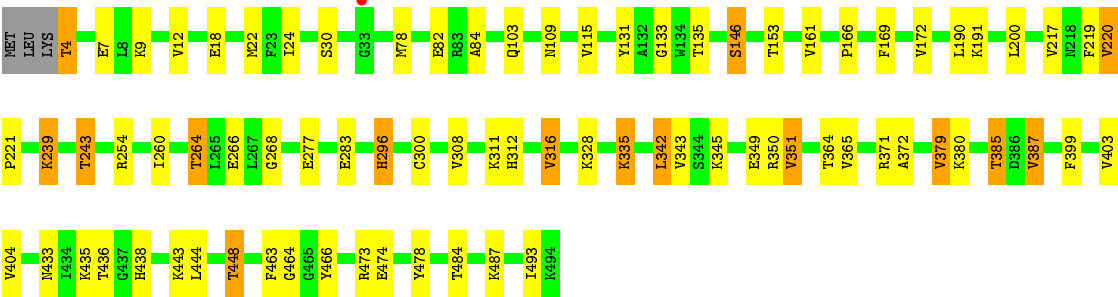
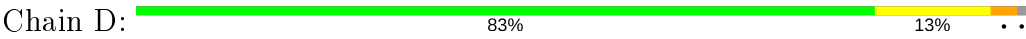


• Molecule 1: Betaine-aldehyde dehydrogenase





● Molecule 1: Betaine-aldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.22Å 93.25Å 145.15Å 90.00° 97.86° 90.00°	Depositor
Resolution (Å)	47.93 – 2.60 47.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.93-2.60) 99.4 (47.93-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	35.35 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.165 , 0.233 0.177 , 0.237	Depositor DCC
R_{free} test set	3414 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15843	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	1.21	9/3870 (0.2%)	0.95	4/5250 (0.1%)
1	B	1.16	10/3853 (0.3%)	0.95	8/5226 (0.2%)
1	C	1.22	6/3855 (0.2%)	0.95	4/5229 (0.1%)
1	D	1.17	6/3876 (0.2%)	0.90	2/5258 (0.0%)
All	All	1.19	31/15454 (0.2%)	0.94	18/20963 (0.1%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	45	GLU	CD-OE1	-7.08	1.17	1.25
1	A	45	GLU	CD-OE1	-6.78	1.18	1.25
1	B	485	GLU	CD-OE2	-6.50	1.18	1.25
1	C	485	GLU	CD-OE2	-6.45	1.18	1.25
1	C	122	SER	CB-OG	-6.22	1.34	1.42
1	A	485	GLU	CD-OE2	-6.11	1.19	1.25
1	B	88	TYR	CG-CD2	5.69	1.46	1.39
1	A	130	TYR	CE1-CZ	-5.65	1.31	1.38
1	D	474	GLU	CD-OE2	-5.60	1.19	1.25
1	A	423	TYR	CE1-CZ	-5.59	1.31	1.38
1	A	474	GLU	CD-OE2	-5.54	1.19	1.25
1	A	354	TYR	CE1-CZ	-5.45	1.31	1.38
1	A	466	TYR	CE1-CZ	-5.39	1.31	1.38
1	B	474	GLU	CD-OE1	-5.36	1.19	1.25
1	D	30	SER	CB-OG	-5.34	1.35	1.42
1	A	485	GLU	CD-OE1	-5.29	1.19	1.25
1	D	133	GLY	C-O	-5.20	1.15	1.23
1	B	126	GLU	CG-CD	5.19	1.59	1.51
1	D	131	TYR	CZ-OH	-5.17	1.29	1.37
1	A	397	GLU	CD-OE1	-5.17	1.20	1.25
1	B	400	GLY	C-O	-5.16	1.15	1.23
1	B	412	GLU	CG-CD	5.16	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	474	GLU	CD-OE1	-5.15	1.20	1.25
1	D	478	TYR	CE1-CZ	-5.13	1.31	1.38
1	C	53	GLU	CD-OE1	-5.09	1.20	1.25
1	B	474	GLU	CD-OE2	-5.04	1.20	1.25
1	B	38	GLU	CD-OE1	-5.04	1.20	1.25
1	C	466	TYR	CE1-CZ	-5.03	1.32	1.38
1	B	483	TYR	CE1-CZ	-5.03	1.32	1.38
1	B	396	GLU	CD-OE2	-5.01	1.20	1.25
1	D	474	GLU	CD-OE1	-5.00	1.20	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ASP	CB-CG-OD1	7.55	125.10	118.30
1	B	108	ASP	CB-CG-OD1	7.36	124.92	118.30
1	C	108	ASP	CB-CG-OD1	7.13	124.72	118.30
1	C	107	LEU	CA-CB-CG	6.80	130.95	115.30
1	D	254	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	278	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	92	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	D	350	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	83	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	A	142	THR	N-CA-CB	5.50	120.75	110.30
1	C	254	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	148	ASP	CB-CG-OD1	5.21	122.98	118.30
1	C	78	MET	N-CA-CB	-5.18	101.28	110.60
1	B	371	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	254	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	60	ASP	CB-CG-OD1	5.14	122.92	118.30
1	B	83	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	B	465	GLY	N-CA-C	5.04	125.69	113.10

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	3791	0	3740	49	0
1	B	3771	0	3721	36	0
1	C	3776	0	3727	57	0
1	D	3794	0	3745	40	0
2	A	44	0	26	1	0
2	B	44	0	26	5	0
2	C	44	0	26	1	0
2	D	44	0	26	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	140	0	0	0	0
4	B	141	0	0	1	0
4	C	126	0	0	4	0
4	D	125	0	0	0	0
All	All	15843	0	15037	162	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (162) 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:C:364:THR:HG21	1:C:386:ASP:OD2	1.44	1.18
1:C:364:THR:CG2	1:C:386:ASP:OD2	2.01	1.08
1:D:364:THR:HB	1:D:385:THR:HG22	1.53	0.88
1:D:387:VAL:HG11	1:D:404:VAL:HG13	1.58	0.86
1:C:433:ASN:HB3	1:C:436:THR:HG23	1.59	0.85
1:D:300[A]:CYS:SG	2:D:501:NAD:C7N	2.69	0.81
1:B:300[B]:CYS:SG	2:B:501:NAD:C7N	2.70	0.80
1:A:387:VAL:HG11	1:A:404:VAL:HG13	1.65	0.78
1:D:243:THR:HB	1:D:266:GLU:HB2	1.68	0.76
1:C:243:THR:HB	1:C:266:GLU:HB2	1.69	0.75
1:A:438:HIS:HE1	1:C:438:HIS:HE1	1.35	0.74
1:D:22:MET:HG2	1:D:221:PRO:HD2	1.71	0.73
1:C:300:CYS:SG	2:C:501:NAD:C7N	2.77	0.72
1:C:435:LYS:HG3	1:D:493:ILE:HA	1.74	0.68
1:A:438:HIS:CE1	1:C:438:HIS:HE1	2.13	0.67
1:A:9:LYS:H	1:A:103:GLN:HE22	1.42	0.66
1:A:349:GLU:O	1:A:353:ASN:HB2	1.96	0.66
1:B:22:MET:HE3	1:B:24:ILE:HD11	1.77	0.66
1:A:300:CYS:SG	2:A:501:NAD:C7N	2.84	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:VAL:HG13	1:A:394:VAL:HG11	1.78	0.65
1:C:342:LEU:HD12	1:C:348:GLN:HA	1.79	0.64
1:D:4:THR:HB	1:D:335:LYS:HB2	1.77	0.64
1:C:356:GLU:O	1:C:360:LYS:HG2	1.99	0.63
1:C:448:THR:CG2	4:C:653:HOH:O	2.47	0.63
1:C:107:LEU:HD13	1:C:333:MET:HG3	1.81	0.62
1:A:166:PRO:HD3	1:A:243:THR:HG23	1.81	0.62
1:A:9:LYS:HB2	1:A:12:VAL:HG13	1.83	0.61
1:A:201:LEU:HD11	1:A:221:PRO:HG3	1.82	0.61
1:D:433:ASN:HD22	1:D:436:THR:H	1.48	0.61
1:B:109:ASN:OD1	1:B:111:LYS:HE2	2.00	0.61
1:B:387:VAL:HG21	1:B:404:VAL:HG13	1.84	0.59
1:C:436:THR:HG21	4:C:613:HOH:O	2.02	0.59
1:B:264:THR:HG21	1:B:482:ASN:CG	2.23	0.58
1:D:9:LYS:H	1:D:103:GLN:HE22	1.49	0.58
1:C:493:ILE:HA	1:D:435:LYS:HG3	1.85	0.58
1:D:372:ALA:HB2	1:D:380:LYS:HG3	1.86	0.57
1:A:487:LYS:NZ	1:D:444:LEU:O	2.38	0.57
1:B:300[B]:CYS:SG	2:B:501:NAD:N7N	2.78	0.57
1:C:22:MET:CG	1:C:221:PRO:HD2	2.36	0.56
1:C:276:LEU:HD12	1:C:431:THR:HB	1.87	0.56
1:A:438:HIS:HE1	1:C:438:HIS:CE1	2.20	0.55
1:D:78:MET:HG2	1:D:82:GLU:HB2	1.88	0.55
1:A:9:LYS:H	1:A:103:GLN:NE2	2.03	0.55
1:A:364:THR:HB	1:A:385:THR:HG22	1.87	0.55
1:C:370:GLU:HG2	1:C:380:LYS:HE2	1.89	0.55
1:B:438:HIS:HE1	1:D:438:HIS:HE1	1.53	0.55
1:A:22:MET:HG2	1:A:221:PRO:HD2	1.89	0.54
1:D:342:LEU:HD22	1:D:379:VAL:CG1	2.38	0.54
1:A:22:MET:HG2	1:A:221:PRO:CD	2.37	0.54
1:A:329:LEU:HD21	1:A:339:MET:HE2	1.90	0.54
1:D:268:GLY:HA2	1:D:300[A]:CYS:SG	2.47	0.54
1:A:201:LEU:HD11	1:A:221:PRO:CG	2.37	0.54
1:D:448:THR:HG21	1:D:463:PHE:CD2	2.43	0.54
1:D:464:GLY:HA3	1:D:473:ARG:HD3	1.91	0.53
1:A:433:ASN:HD22	1:A:436:THR:H	1.56	0.53
1:B:485:GLU:HG3	1:C:466:TYR:CE1	2.44	0.53
1:A:108:ASP:OD2	1:A:196:THR:HA	2.09	0.53
1:C:370:GLU:CG	1:C:380:LYS:HE2	2.39	0.52
1:A:435:LYS:HG2	1:B:493:ILE:HA	1.91	0.52
1:C:277:GLU:O	1:C:312:HIS:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:LEU:HD21	1:D:351:VAL:HG11	1.93	0.51
1:B:438:HIS:HD2	1:C:152:TYR:OH	1.93	0.51
1:A:390:ASP:O	1:A:395:LYS:HE2	2.11	0.51
1:D:22:MET:CE	1:D:24:ILE:HD11	2.40	0.51
1:B:487:LYS:NZ	1:C:444:LEU:O	2.44	0.51
1:A:40:TYR:N	1:A:40:TYR:CD1	2.78	0.51
1:C:260:ILE:O	1:C:260:ILE:HG22	2.11	0.51
1:C:448:THR:HG23	4:C:653:HOH:O	2.10	0.50
1:B:317:VAL:HG22	1:B:405:VAL:HG11	1.94	0.50
1:C:22:MET:HG2	1:C:221:PRO:HD2	1.93	0.50
1:C:342:LEU:HD11	1:C:379:VAL:HG11	1.93	0.50
1:A:387:VAL:HG11	1:A:404:VAL:CG1	2.38	0.50
1:C:138:ILE:O	1:C:138:ILE:HG22	2.11	0.50
1:C:6:ILE:HD12	1:C:333:MET:O	2.10	0.50
1:D:296:HIS:N	1:D:296:HIS:CD2	2.80	0.49
1:A:251:TYR:O	1:A:255:GLN:HG2	2.12	0.49
1:B:258:GLU:O	1:C:250:LYS:HE2	2.13	0.49
1:A:342:LEU:HD22	1:A:379:VAL:CG1	2.43	0.49
1:B:22:MET:HG2	1:B:221:PRO:HD2	1.95	0.48
1:D:277:GLU:O	1:D:312:HIS:HE1	1.96	0.48
1:A:243:THR:HB	1:A:266:GLU:HB2	1.95	0.48
1:C:153:THR:HA	1:C:487:LYS:O	2.14	0.47
1:D:169:PHE:HB3	1:D:172:VAL:CG1	2.43	0.47
1:B:370:GLU:OE2	1:B:380:LYS:NZ	2.38	0.47
1:A:342:LEU:HD22	1:A:379:VAL:HG13	1.97	0.47
1:C:201:LEU:HD11	1:C:221:PRO:HG3	1.96	0.47
1:A:139:ILE:HD12	1:C:141:GLN:HG2	1.97	0.47
1:D:22:MET:HE2	1:D:24:ILE:CD1	2.44	0.47
1:B:433:ASN:HD22	1:B:436:THR:H	1.63	0.46
1:C:83:ARG:NH2	1:C:183:ALA:O	2.47	0.46
1:B:350:ARG:NH1	2:B:501:NAD:O3D	2.48	0.46
1:A:8:LEU:HA	1:A:103:GLN:HE22	1.80	0.46
1:B:292:ILE:HG21	1:B:403:VAL:HB	1.98	0.46
1:D:153:THR:HA	1:D:487:LYS:O	2.15	0.46
1:A:30:SER:HA	1:A:52:CYS:SG	2.55	0.46
1:D:239:LYS:HZ1	1:D:264:THR:CG2	2.30	0.45
1:C:364:THR:HG23	1:C:385:THR:HG22	1.97	0.45
1:D:239:LYS:HZ1	1:D:264:THR:HG23	1.80	0.45
1:C:268:GLY:HA2	1:C:300:CYS:SG	2.57	0.45
1:B:147:LYS:HG2	4:B:709:HOH:O	2.15	0.45
1:B:264:THR:HG21	1:B:482:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ILE:O	1:D:260:ILE:HG22	2.17	0.45
1:D:300[A]:CYS:SG	2:D:501:NAD:N7N	2.90	0.45
1:D:308:VAL:HG11	1:D:316:VAL:HG13	1.99	0.45
1:B:387:VAL:HG21	1:B:404:VAL:CG1	2.47	0.44
1:C:22:MET:HG3	1:C:221:PRO:HD2	1.98	0.44
1:C:375:LYS:HD3	1:C:375:LYS:HA	1.80	0.44
1:C:9:LYS:H	1:C:103:GLN:HE22	1.65	0.44
1:A:44:THR:O	1:A:45:GLU:HB2	2.17	0.44
1:B:79:THR:HG22	1:D:146:SER:HB2	1.99	0.44
1:C:199:SER:HB2	4:C:616:HOH:O	2.18	0.44
1:B:300[B]:CYS:SG	2:B:501:NAD:C2N	3.06	0.44
1:A:80:THR:HB	1:A:135:THR:HG22	1.99	0.43
1:B:135:THR:HG22	1:B:183:ALA:HA	1.99	0.43
1:A:395:LYS:HB2	1:A:395:LYS:HE3	1.71	0.43
1:C:329:LEU:HD12	1:C:339:MET:HB3	1.99	0.43
1:A:444:LEU:O	1:D:487:LYS:NZ	2.50	0.43
1:A:77:GLU:HG2	1:C:147:LYS:HE3	2.00	0.43
1:B:466:TYR:CE1	1:C:485:GLU:HG3	2.53	0.43
1:B:242:PHE:CD1	1:B:252:ILE:CD1	3.01	0.43
1:B:154:ARG:NH2	1:B:156:GLU:OE2	2.48	0.43
1:A:99:GLU:O	1:A:103:GLN:HG3	2.18	0.43
1:B:300[B]:CYS:SG	2:B:501:NAD:C3N	3.07	0.43
1:B:229:ALA:HA	1:B:232:VAL:HG12	2.00	0.42
1:C:190:LEU:HD12	1:C:200:LEU:HD21	2.00	0.42
1:D:22:MET:CE	1:D:220:VAL:HG12	2.48	0.42
1:A:98:ARG:CZ	1:A:117:LEU:HD11	2.49	0.42
1:A:75:TRP:CH2	1:A:83:ARG:HD2	2.54	0.42
1:C:190:LEU:HD12	1:C:200:LEU:CD2	2.50	0.42
1:D:217:VAL:HG13	1:D:219:PHE:CE1	2.55	0.42
1:A:26:GLY:HA3	1:A:214:ASN:HD22	1.85	0.42
1:C:474:GLU:HA	1:C:479:ALA:HB2	2.01	0.42
1:C:272:PRO:HG3	1:C:418:ALA:HB1	2.02	0.42
1:C:296:HIS:CD2	1:C:296:HIS:N	2.88	0.42
1:D:403:VAL:HG22	1:D:404:VAL:N	2.35	0.42
1:A:308:VAL:HG11	1:A:316:VAL:HG13	2.02	0.41
1:B:148:ASP:HB3	1:B:494:LYS:HE2	2.00	0.41
1:D:345:LYS:HE2	1:D:349:GLU:OE2	2.20	0.41
1:A:438:HIS:CE1	1:C:438:HIS:CE1	3.01	0.41
1:B:277:GLU:O	1:B:312:HIS:HE1	2.03	0.41
1:B:296:HIS:CD2	1:B:296:HIS:N	2.88	0.41
1:A:484:THR:CG2	1:A:485:GLU:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:VAL:CG1	1:D:219:PHE:CZ	3.03	0.41
1:A:308:VAL:O	1:A:407:PRO:HA	2.21	0.41
1:C:364:THR:CG2	1:C:386:ASP:CG	2.84	0.41
1:A:260:ILE:HG22	1:A:260:ILE:O	2.20	0.41
1:C:217:VAL:HG13	1:C:219:PHE:CZ	2.56	0.41
1:A:109:ASN:ND2	1:A:167:TRP:O	2.52	0.41
1:A:74:PRO:O	1:A:78:MET:HB2	2.21	0.41
1:C:364:THR:CG2	1:C:386:ASP:HB2	2.50	0.41
1:D:84:ALA:HB2	1:D:135:THR:OG1	2.21	0.41
1:B:243:THR:HA	1:B:266:GLU:O	2.21	0.41
1:B:474:GLU:O	1:B:475:LEU:HB2	2.21	0.41
1:B:475:LEU:N	1:B:479:ALA:HB2	2.36	0.41
1:C:266:GLU:HG3	1:C:474:GLU:OE1	2.21	0.41
1:C:364:THR:HG22	1:C:386:ASP:HB2	2.03	0.41
1:C:177:LYS:NZ	1:C:474:GLU:OE2	2.49	0.41
1:C:182:LEU:HD21	1:C:188:ILE:HD12	2.02	0.40
1:A:485:GLU:HG3	1:D:466:TYR:CE1	2.56	0.40
1:A:161:VAL:HG23	1:A:163:GLN:HG3	2.04	0.40
1:D:190:LEU:HD22	1:D:200:LEU:CD2	2.52	0.40
1:B:487:LYS:HA	1:C:447:GLY:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	489/494 (99%)	472 (96%)	16 (3%)	1 (0%)	47	71
1	B	487/494 (99%)	471 (97%)	16 (3%)	0	100	100
1	C	487/494 (99%)	467 (96%)	19 (4%)	1 (0%)	47	71
1	D	490/494 (99%)	475 (97%)	14 (3%)	1 (0%)	47	71
All	All	1953/1976 (99%)	1885 (96%)	65 (3%)	3 (0%)	47	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	166	PRO
1	A	424	GLY
1	D	166	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/401 (99%)	371 (93%)	27 (7%)	16	32
1	B	396/401 (99%)	374 (94%)	22 (6%)	21	42
1	C	396/401 (99%)	362 (91%)	34 (9%)	10	20
1	D	399/401 (100%)	368 (92%)	31 (8%)	12	25
All	All	1589/1604 (99%)	1475 (93%)	114 (7%)	14	29

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	13	GLU
1	A	17	ASN
1	A	18	GLU
1	A	27	GLU
1	A	50	VAL
1	A	60	ASP
1	A	104	LEU
1	A	120	ASP
1	A	126	GLU
1	A	161	VAL
1	A	205	LYS
1	A	217	VAL
1	A	283	GLU
1	A	296	HIS
1	A	301	SER
1	A	335	LYS

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Mol	Chain	Res	Type
1	A	336	GLU
1	A	343	VAL
1	A	353	ASN
1	A	379	VAL
1	A	380	LYS
1	A	385	THR
1	A	387	VAL
1	A	399	PHE
1	A	416	GLU
1	A	484	THR
1	B	7	GLU
1	B	13	GLU
1	B	17	ASN
1	B	27	GLU
1	B	120	ASP
1	B	127	ASN
1	B	199	SER
1	B	296	HIS
1	B	316	VAL
1	B	327	VAL
1	B	335	LYS
1	B	346	LYS
1	B	351	VAL
1	B	360	LYS
1	B	365	VAL
1	B	371	ARG
1	B	373	LEU
1	B	375	LYS
1	B	399	PHE
1	B	412	GLU
1	B	443	LYS
1	B	445	LYS
1	C	13	GLU
1	C	22	MET
1	C	50	VAL
1	C	57	GLU
1	C	60	ASP
1	C	68	SER
1	C	83	ARG
1	C	105	GLU
1	C	107	LEU
1	C	109	ASN

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Mol	Chain	Res	Type
1	C	115	VAL
1	C	239	LYS
1	C	243	THR
1	C	282	GLU
1	C	296	HIS
1	C	316	VAL
1	C	328	LYS
1	C	329	LEU
1	C	353	ASN
1	C	364	THR
1	C	365	VAL
1	C	373	LEU
1	C	379	VAL
1	C	380	LYS
1	C	385	THR
1	C	387	VAL
1	C	395	LYS
1	C	399	PHE
1	C	404	VAL
1	C	422	SER
1	C	436	THR
1	C	445	LYS
1	C	448	THR
1	C	484	THR
1	D	4	THR
1	D	7	GLU
1	D	12	VAL
1	D	18	GLU
1	D	109	ASN
1	D	115	VAL
1	D	146	SER
1	D	161	VAL
1	D	191	LYS
1	D	220	VAL
1	D	239	LYS
1	D	243	THR
1	D	264	THR
1	D	283	GLU
1	D	296	HIS
1	D	311	LYS
1	D	316	VAL
1	D	328	LYS

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Mol	Chain	Res	Type
1	D	335	LYS
1	D	342	LEU
1	D	343	VAL
1	D	351	VAL
1	D	365	VAL
1	D	371	ARG
1	D	379	VAL
1	D	385	THR
1	D	387	VAL
1	D	399	PHE
1	D	443	LYS
1	D	448	THR
1	D	484	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	214	ASN
1	A	262	HIS
1	A	325	ASN
1	A	326	ASN
1	A	353	ASN
1	A	432	GLN
1	A	433	ASN
1	A	438	HIS
1	B	214	ASN
1	B	312	HIS
1	B	325	ASN
1	B	326	ASN
1	B	357	GLN
1	B	432	GLN
1	B	433	ASN
1	B	438	HIS
1	B	442	ASN
1	B	482	ASN
1	C	103	GLN
1	C	233	ASN
1	C	255	GLN
1	C	290	GLN
1	C	312	HIS
1	C	325	ASN

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Mol	Chain	Res	Type
1	C	326	ASN
1	C	432	GLN
1	C	433	ASN
1	C	438	HIS
1	C	442	ASN
1	D	103	GLN
1	D	214	ASN
1	D	312	HIS
1	D	325	ASN
1	D	326	ASN
1	D	432	GLN
1	D	433	ASN
1	D	438	HIS
1	D	442	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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
2	NAD	C	501	-	42,48,48	0.90	2 (4%)	50,73,73	1.34	7 (14%)
2	NAD	D	501	-	42,48,48	0.90	2 (4%)	50,73,73	1.25	6 (12%)
2	NAD	A	501	-	42,48,48	0.83	1 (2%)	50,73,73	1.14	4 (8%)
2	NAD	B	501	-	42,48,48	0.97	3 (7%)	50,73,73	1.33	9 (18%)

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	C	501	-	-	5/26/62/62	0/5/5/5
2	NAD	D	501	-	-	12/26/62/62	0/5/5/5
2	NAD	A	501	-	-	11/26/62/62	0/5/5/5
2	NAD	B	501	-	-	7/26/62/62	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	NAD	C5A-C4A	2.61	1.47	1.40
2	D	501	NAD	O4D-C1D	2.52	1.44	1.41
2	C	501	NAD	C5A-C4A	2.50	1.47	1.40
2	B	501	NAD	C5A-C4A	2.41	1.47	1.40
2	B	501	NAD	O4D-C1D	2.28	1.44	1.41
2	A	501	NAD	O4D-C1D	2.21	1.44	1.41
2	C	501	NAD	C2A-N3A	2.18	1.35	1.32
2	B	501	NAD	C2A-N3A	2.03	1.35	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	N3A-C2A-N1A	-4.47	121.70	128.68
2	C	501	NAD	C6N-N1N-C2N	-3.83	118.48	121.97
2	D	501	NAD	N3A-C2A-N1A	-3.60	123.05	128.68
2	B	501	NAD	N3A-C2A-N1A	-3.53	123.16	128.68
2	A	501	NAD	PN-O3-PA	-3.09	122.21	132.83
2	B	501	NAD	C1B-N9A-C4A	-3.02	121.33	126.64
2	A	501	NAD	N3A-C2A-N1A	-2.89	124.16	128.68
2	C	501	NAD	C1B-N9A-C4A	-2.64	122.00	126.64
2	D	501	NAD	C2N-C3N-C4N	2.59	121.19	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAD	PN-O3-PA	-2.57	124.00	132.83
2	C	501	NAD	C3N-C2N-N1N	2.54	122.91	120.43
2	B	501	NAD	O5B-PA-O1A	-2.47	99.41	109.07
2	B	501	NAD	PN-O3-PA	-2.46	124.39	132.83
2	D	501	NAD	C3D-C2D-C1D	2.42	104.62	100.98
2	B	501	NAD	O4B-C1B-C2B	-2.40	103.42	106.93
2	A	501	NAD	C4A-C5A-N7A	-2.38	106.92	109.40
2	B	501	NAD	O7N-C7N-N7N	-2.35	119.23	122.58
2	B	501	NAD	C3D-C2D-C1D	2.30	104.44	100.98
2	C	501	NAD	C5A-C6A-N6A	-2.27	116.91	120.35
2	C	501	NAD	C3D-C2D-C1D	2.23	104.34	100.98
2	A	501	NAD	O2N-PN-O5D	2.20	117.95	107.75
2	B	501	NAD	C3N-C7N-N7N	2.18	120.37	117.75
2	D	501	NAD	O2N-PN-O1N	2.17	122.95	112.24
2	C	501	NAD	O3D-C3D-C4D	2.15	117.27	111.05
2	B	501	NAD	C2B-C3B-C4B	-2.14	98.49	102.64
2	D	501	NAD	C2A-N1A-C6A	2.01	122.20	118.75

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	NAD	C5B-O5B-PA-O1A
2	D	501	NAD	C5B-O5B-PA-O2A
2	D	501	NAD	C5B-O5B-PA-O3
2	D	501	NAD	C5D-O5D-PN-O1N
2	B	501	NAD	O4B-C4B-C5B-O5B
2	B	501	NAD	C3B-C4B-C5B-O5B
2	B	501	NAD	C5D-O5D-PN-O1N
2	C	501	NAD	C5D-O5D-PN-O1N
2	C	501	NAD	C5D-O5D-PN-O2N
2	A	501	NAD	C5B-O5B-PA-O1A
2	A	501	NAD	C5D-O5D-PN-O1N
2	A	501	NAD	C5D-O5D-PN-O2N
2	B	501	NAD	C5D-O5D-PN-O3
2	C	501	NAD	C5D-O5D-PN-O3
2	A	501	NAD	C5B-O5B-PA-O3
2	B	501	NAD	C5D-O5D-PN-O2N
2	A	501	NAD	C5B-O5B-PA-O2A
2	D	501	NAD	C4N-C3N-C7N-O7N
2	D	501	NAD	C4N-C3N-C7N-N7N
2	A	501	NAD	C3D-C4D-C5D-O5D

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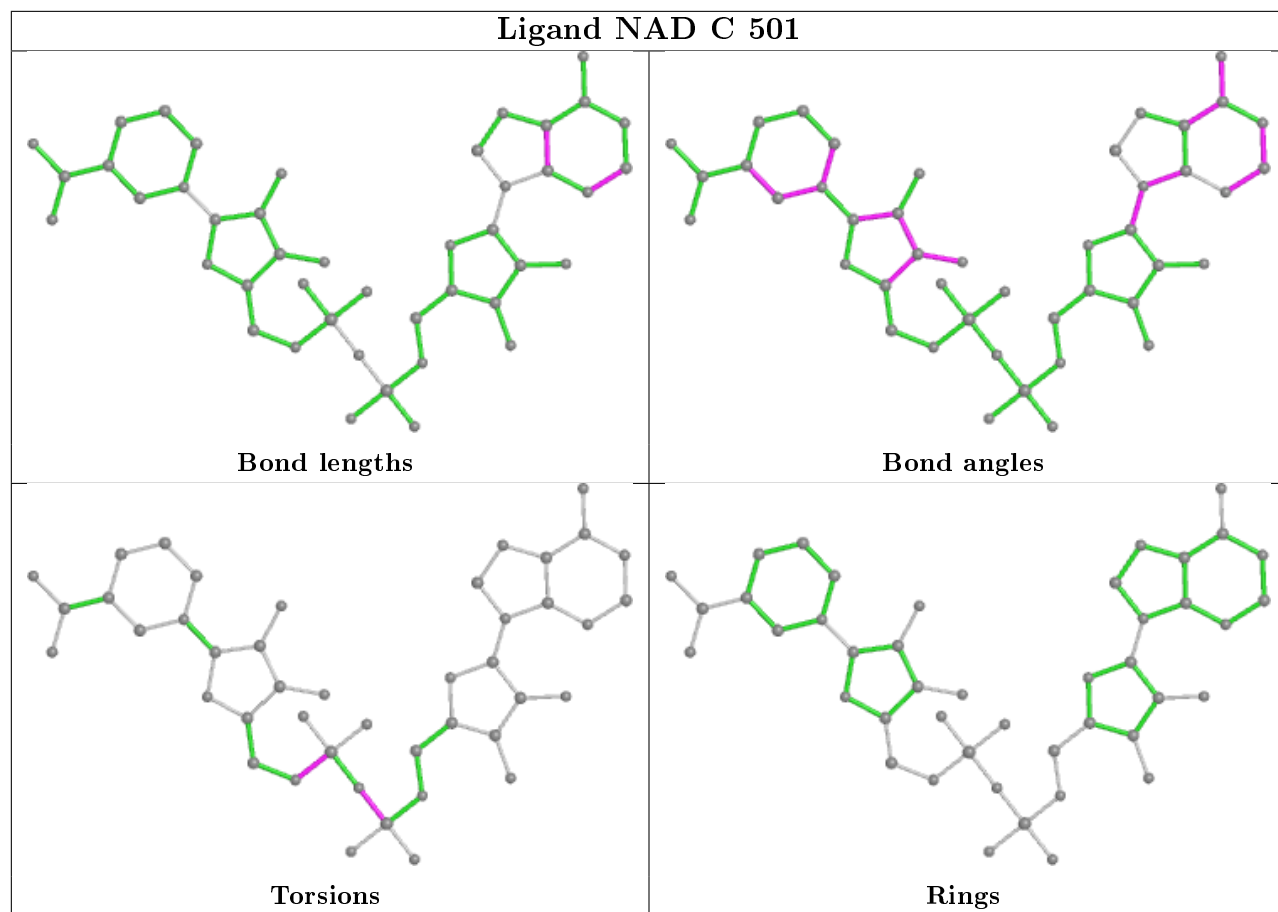
Mol	Chain	Res	Type	Atoms
2	D	501	NAD	PA-O3-PN-O1N
2	C	501	NAD	PN-O3-PA-O1A
2	D	501	NAD	O4D-C4D-C5D-O5D
2	D	501	NAD	C3D-C4D-C5D-O5D
2	A	501	NAD	C4N-C3N-C7N-N7N
2	D	501	NAD	C2N-C3N-C7N-O7N
2	D	501	NAD	C2N-C3N-C7N-N7N
2	A	501	NAD	C4N-C3N-C7N-O7N
2	A	501	NAD	C5D-O5D-PN-O3
2	A	501	NAD	O4D-C4D-C5D-O5D
2	D	501	NAD	PA-O3-PN-O2N
2	B	501	NAD	PN-O3-PA-O1A
2	C	501	NAD	PN-O3-PA-O2A
2	B	501	NAD	O4D-C4D-C5D-O5D
2	A	501	NAD	C4B-C5B-O5B-PA

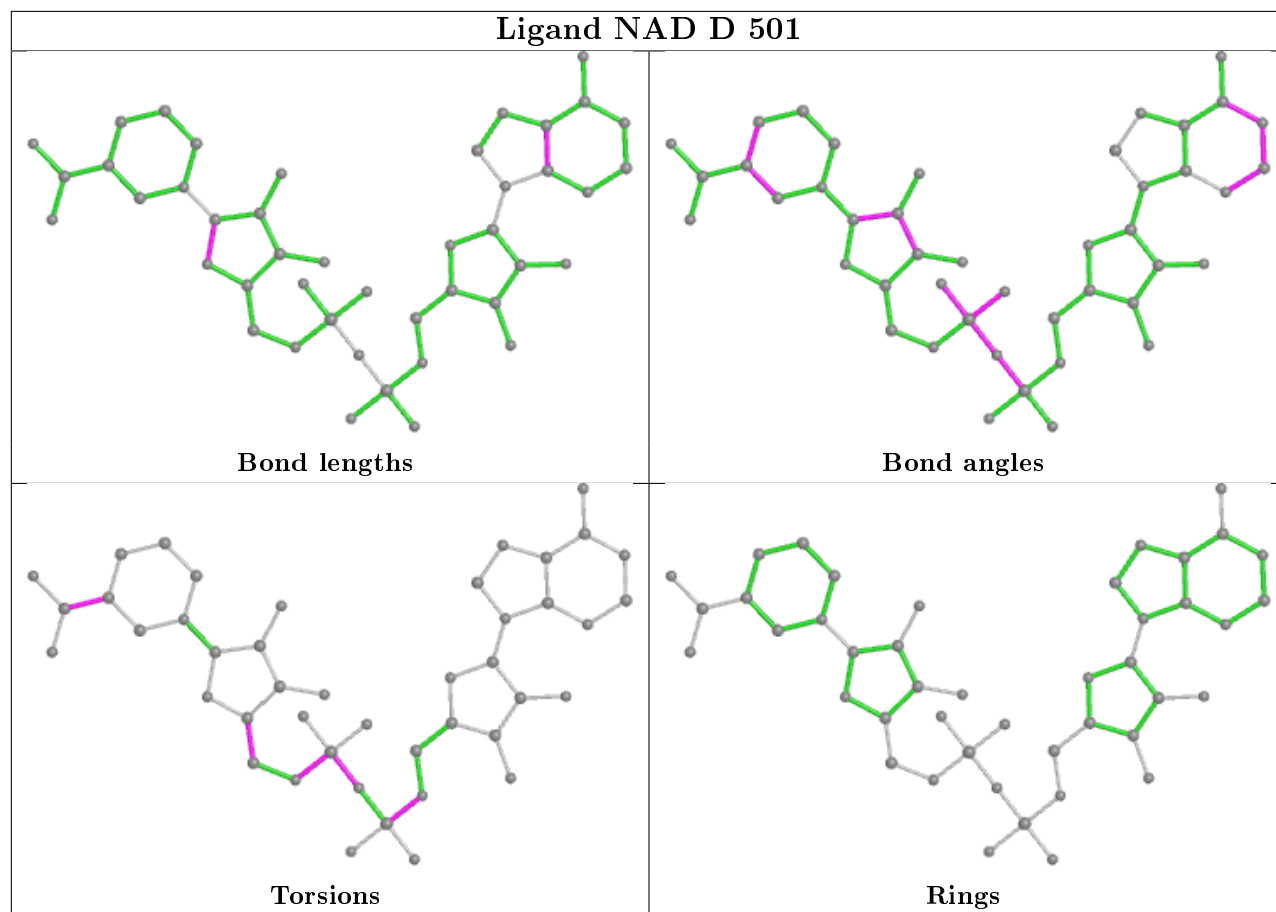
There are no ring outliers.

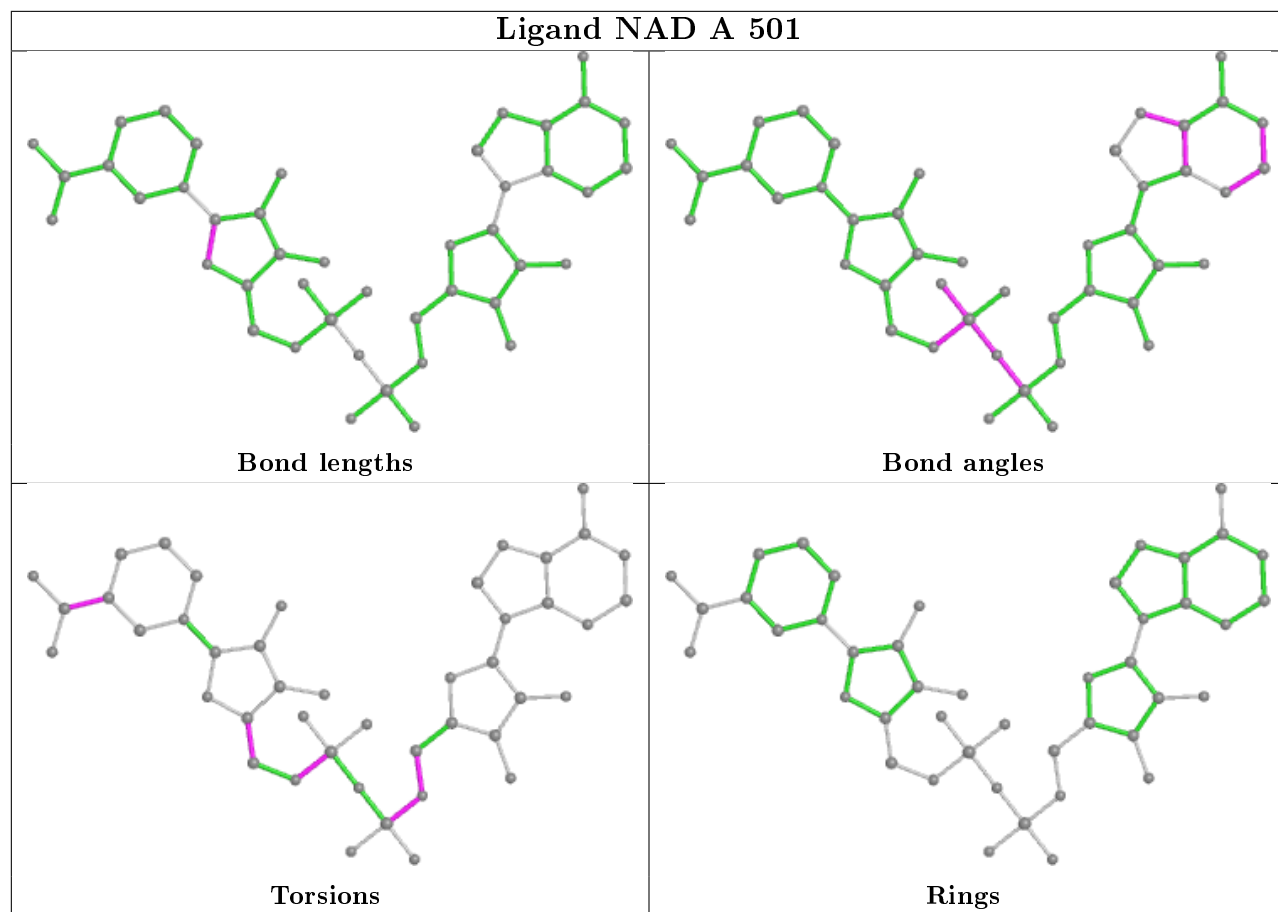
4 monomers are involved in 9 short contacts:

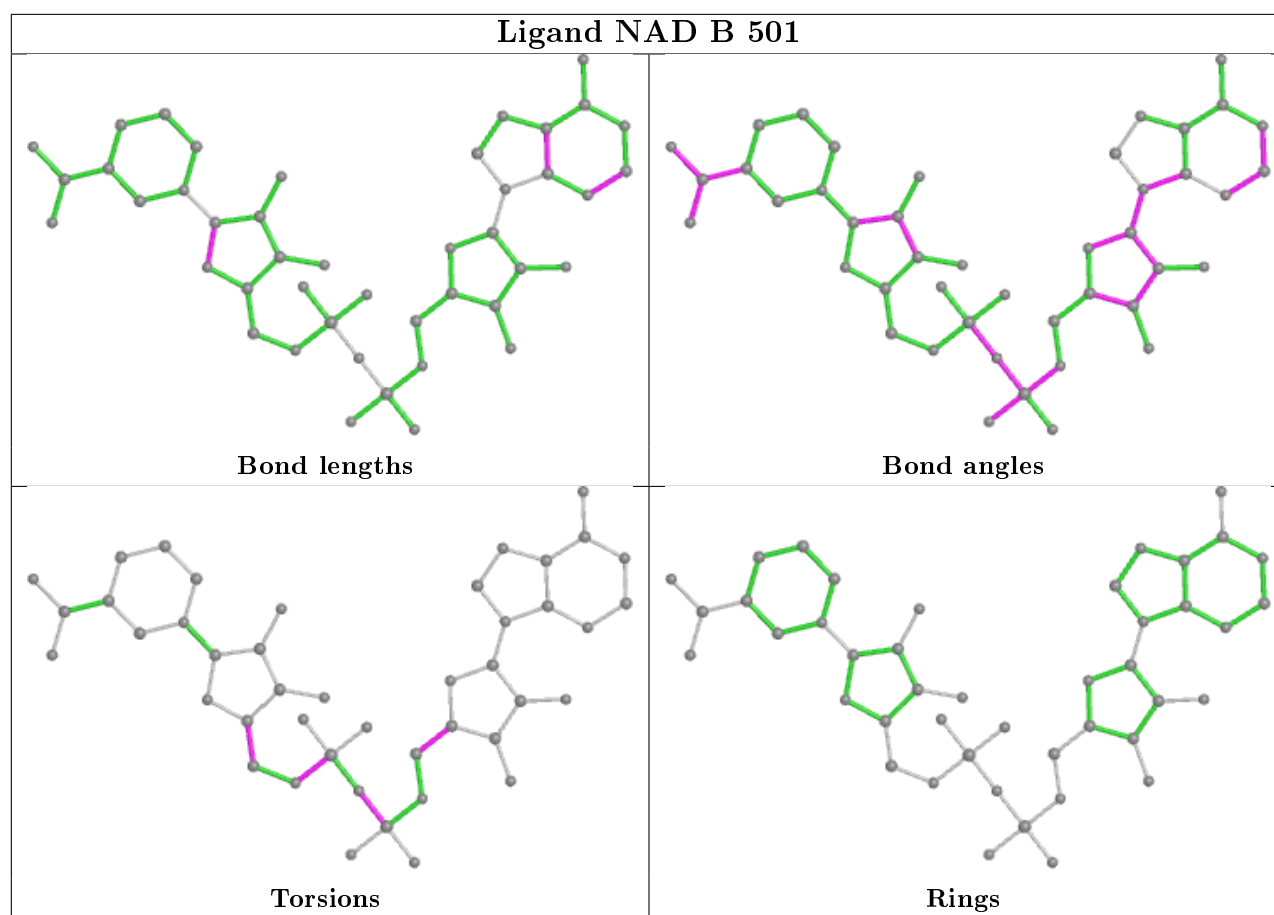
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAD	1	0
2	D	501	NAD	2	0
2	A	501	NAD	1	0
2	B	501	NAD	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	491/494 (99%)	-0.60	0	100 100	8, 14, 26, 42	0
1	B	488/494 (98%)	-0.64	0	100 100	6, 14, 26, 41	0
1	C	489/494 (98%)	-0.61	1 (0%)	95 95	7, 13, 26, 50	0
1	D	491/494 (99%)	-0.52	1 (0%)	95 95	8, 16, 31, 46	0
All	All	1959/1976 (99%)	-0.59	2 (0%)	95 95	6, 14, 27, 50	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	33	GLY	2.6
1	C	7	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

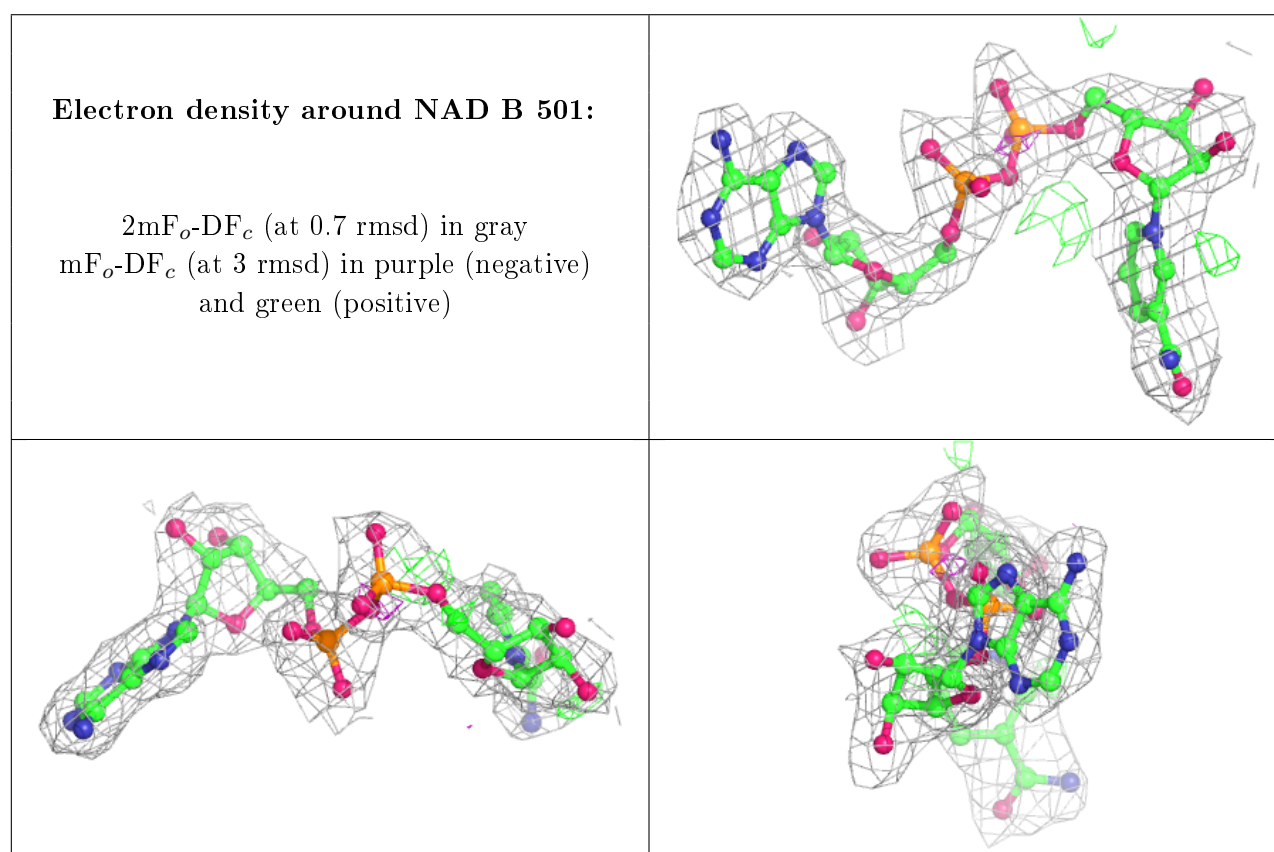
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

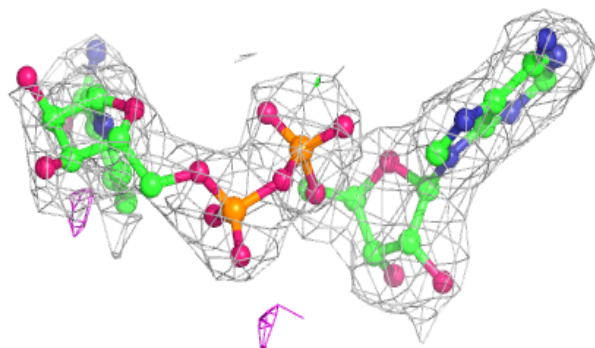
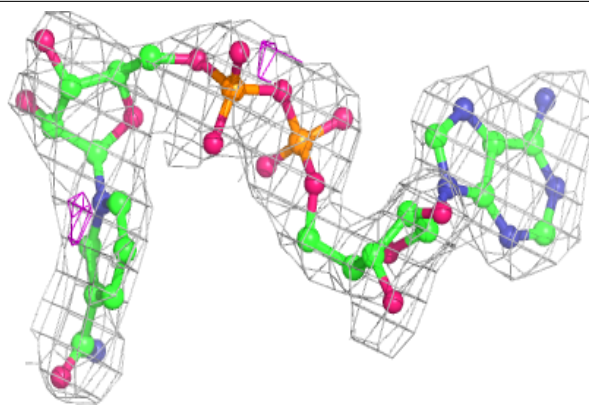
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	B	502	1/1	0.73	0.14	17,17,17,17	0
2	NAD	B	501	44/44	0.94	0.14	17,26,44,48	0
3	NA	D	502	1/1	0.95	0.06	21,21,21,21	0
3	NA	A	502	1/1	0.95	0.11	14,14,14,14	0
2	NAD	D	501	44/44	0.95	0.14	16,27,40,41	0
2	NAD	C	501	44/44	0.96	0.12	18,25,30,33	0
2	NAD	A	501	44/44	0.96	0.12	16,21,30,31	0

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

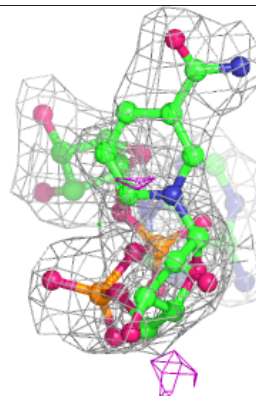
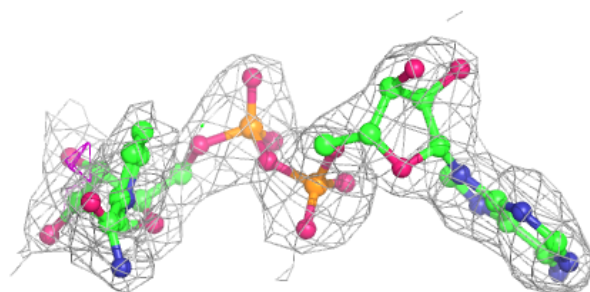
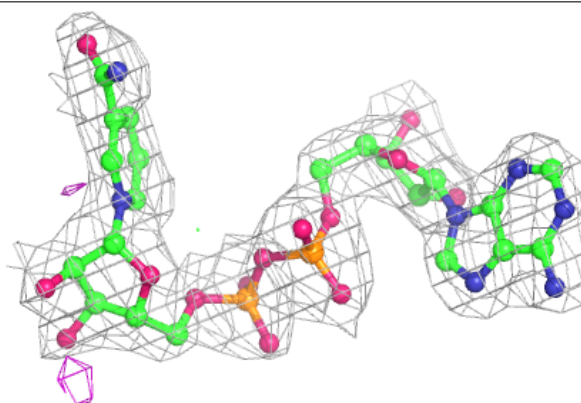


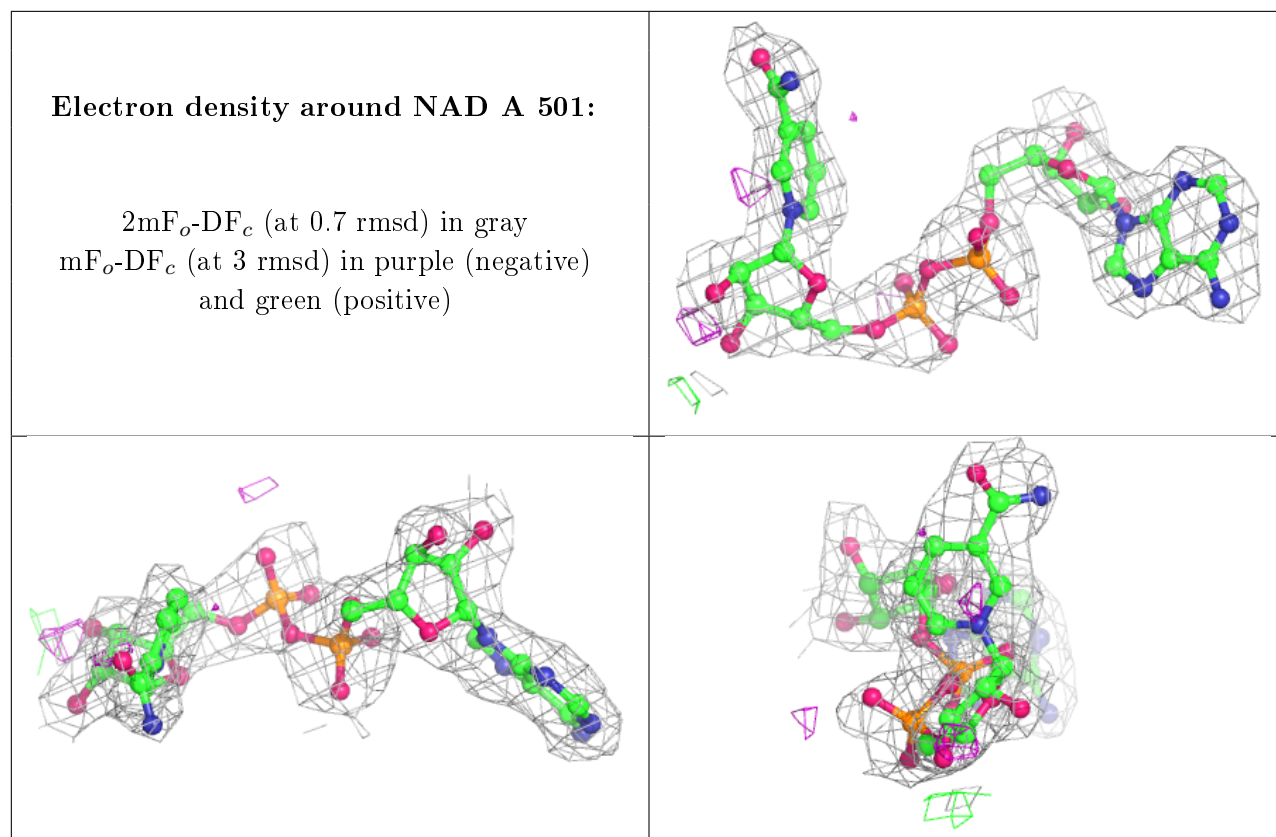
Electron density around NAD D 501:

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

**Electron density around NAD C 501:**

$2mF_o-DF_c$ (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.