



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:48 PM UTC

PDB ID : 2XAA / pdb_00002xaa
Title : Alcohol dehydrogenase ADH-'A' from *Rhodococcus ruber* DSM 44541 at pH 8.5 in complex with NAD and butane-1,4-diol
Authors : Kroutil, W.; Gruber, K.; Grogan, G.
Deposited on : 2010-03-30
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 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

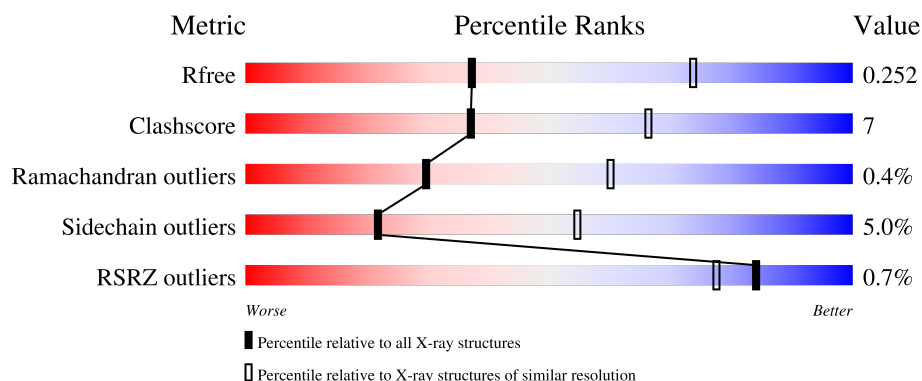
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	345	% 76% 17% • •
1	B	345	% 74% 24% • •
1	C	345	83% 15% •
1	D	345	85% 14% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10078 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 SECONDARY ALCOHOL DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	1	0
			2370	1491	417	449	13			
1	B	342	Total	C	N	O	S	0	0	0
			2434	1533	429	460	12			
1	C	344	Total	C	N	O	S	0	0	0
			2461	1554	431	464	12			
1	D	345	Total	C	N	O	S	0	0	0
			2469	1558	433	466	12			

There are 36 discrepancies between the modelled and reference sequences:

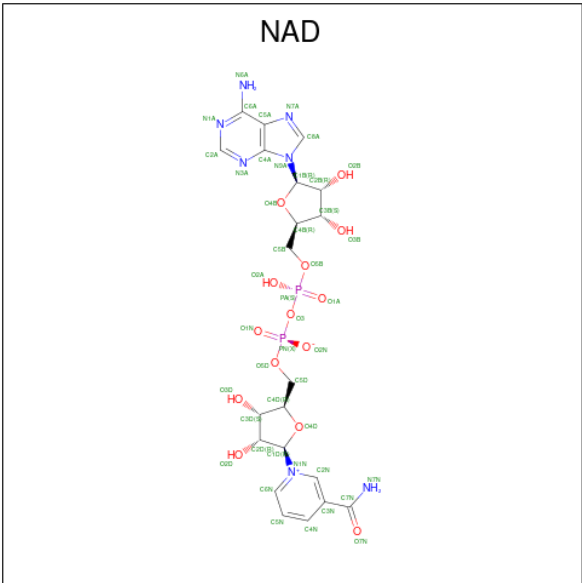
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	VAL	LEU	conflict	UNP Q8KLT9
A	18	ILE	VAL	conflict	UNP Q8KLT9
A	22	THR	ALA	conflict	UNP Q8KLT9
A	73	GLU	ALA	conflict	UNP Q8KLT9
A	80	VAL	THR	conflict	UNP Q8KLT9
A	111	ASP	GLU	conflict	UNP Q8KLT9
A	238	GLN	GLU	conflict	UNP Q8KLT9
A	262	VAL	ILE	conflict	UNP Q8KLT9
A	303	GLU	ASP	conflict	UNP Q8KLT9
B	4	VAL	LEU	conflict	UNP Q8KLT9
B	18	ILE	VAL	conflict	UNP Q8KLT9
B	22	THR	ALA	conflict	UNP Q8KLT9
B	73	GLU	ALA	conflict	UNP Q8KLT9
B	80	VAL	THR	conflict	UNP Q8KLT9
B	111	ASP	GLU	conflict	UNP Q8KLT9
B	238	GLN	GLU	conflict	UNP Q8KLT9
B	262	VAL	ILE	conflict	UNP Q8KLT9
B	303	GLU	ASP	conflict	UNP Q8KLT9
C	4	VAL	LEU	conflict	UNP Q8KLT9
C	18	ILE	VAL	conflict	UNP Q8KLT9
C	22	THR	ALA	conflict	UNP Q8KLT9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	73	GLU	ALA	conflict	UNP Q8KLT9
C	80	VAL	THR	conflict	UNP Q8KLT9
C	111	ASP	GLU	conflict	UNP Q8KLT9
C	238	GLN	GLU	conflict	UNP Q8KLT9
C	262	VAL	ILE	conflict	UNP Q8KLT9
C	303	GLU	ASP	conflict	UNP Q8KLT9
D	4	VAL	LEU	conflict	UNP Q8KLT9
D	18	ILE	VAL	conflict	UNP Q8KLT9
D	22	THR	ALA	conflict	UNP Q8KLT9
D	73	GLU	ALA	conflict	UNP Q8KLT9
D	80	VAL	THR	conflict	UNP Q8KLT9
D	111	ASP	GLU	conflict	UNP Q8KLT9
D	238	GLN	GLU	conflict	UNP Q8KLT9
D	262	VAL	ILE	conflict	UNP Q8KLT9
D	303	GLU	ASP	conflict	UNP Q8KLT9

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

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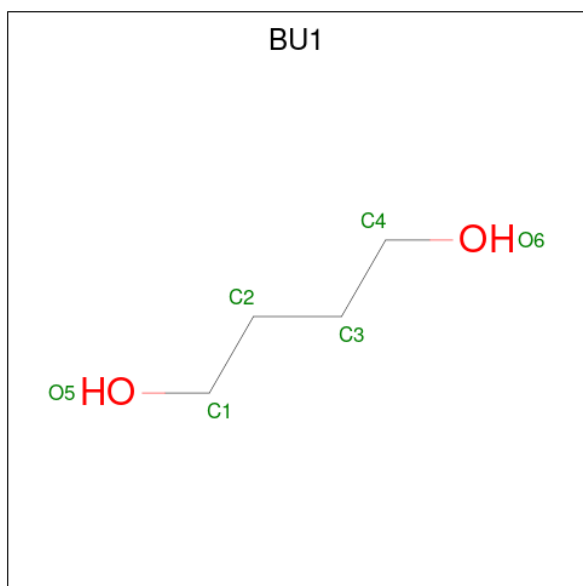
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is 1,4-BUTANEDIOL (CCD ID: BU1) (formula: C₄H₁₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	4	2		
4	C	1	Total	C	O	0	0
			6	4	2		
4	D	1	Total	C	O	0	0
			6	4	2		

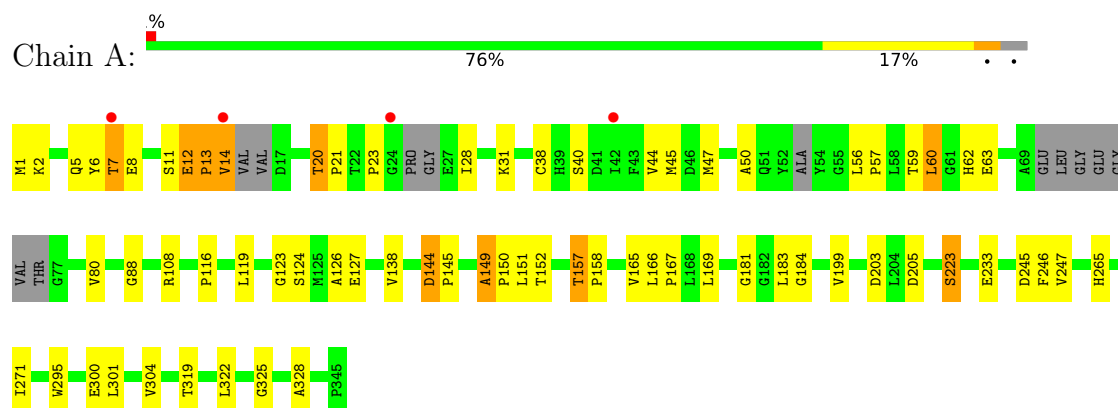
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	28	Total 28	O 28	0	0
5	B	39	Total 39	O 39	0	0
5	C	38	Total 38	O 38	0	0
5	D	37	Total 37	O 37	0	0

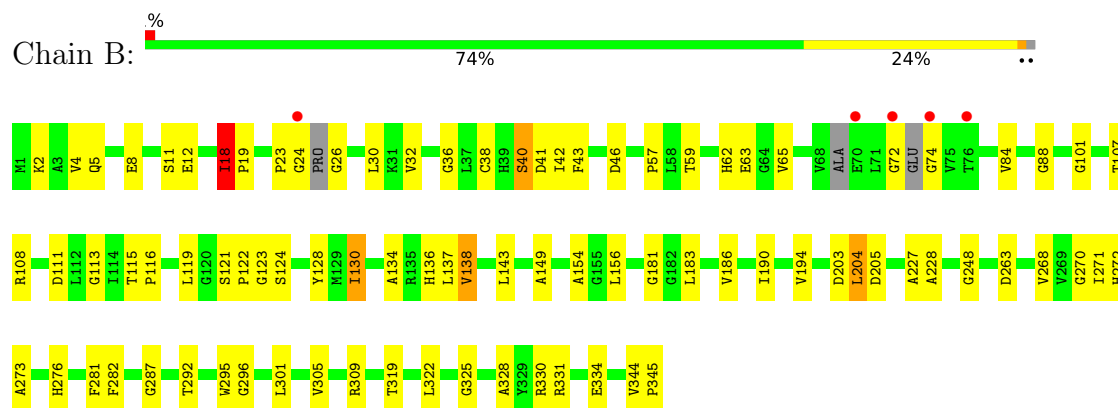
3 Residue-property plots

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.

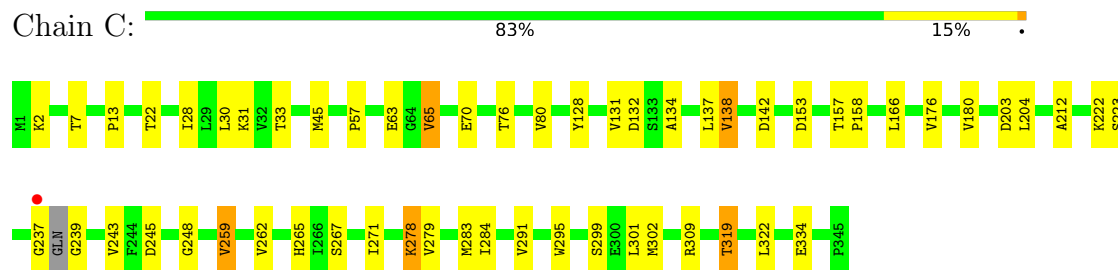
• Molecule 1: SECONDARY ALCOHOL DEHYDROGENASE



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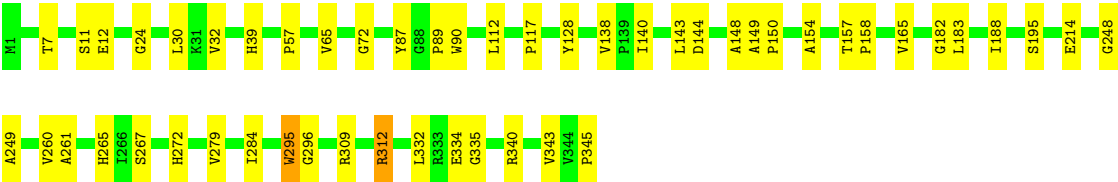
• Molecule 1: SECONDARY ALCOHOL DEHYDROGENASE

Chain D:

85%

14%

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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.67Å 105.10Å 109.18Å 90.00° 91.27° 90.00°	Depositor
Resolution (Å)	109.15 – 2.80 109.15 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (109.15-2.80) 98.7 (109.15-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.188 , 0.258 0.187 , 0.252	Depositor DCC
R_{free} test set	1807 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k 0.018 for -h,-l,-k 0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10078	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: BU1, NAD, ZN

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	0.97	2/2419 (0.1%)	1.16	14/3298 (0.4%)
1	B	0.93	2/2481 (0.1%)	1.11	5/3382 (0.1%)
1	C	0.87	1/2511 (0.0%)	1.05	5/3427 (0.1%)
1	D	0.88	1/2520 (0.0%)	1.06	7/3441 (0.2%)
All	All	0.91	6/9931 (0.1%)	1.09	31/13548 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	138	VAL	CA-CB	6.05	1.59	1.54
1	D	279	VAL	CA-CB	5.73	1.60	1.53
1	B	18	ILE	CA-CB	5.67	1.61	1.54
1	A	7	THR	N-CA	5.26	1.53	1.46
1	B	138	VAL	CA-CB	5.11	1.58	1.54
1	A	13	PRO	CA-C	5.01	1.59	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	VAL	N-CA-C	-7.53	105.08	111.56
1	A	157	THR	CA-C-N	-6.69	112.88	119.64
1	A	157	THR	C-N-CA	-6.69	112.88	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	GLU	N-CA-C	-6.59	105.78	113.88
1	A	12	GLU	CA-C-N	6.33	127.75	119.84
1	A	12	GLU	C-N-CA	6.33	127.75	119.84
1	A	149	ALA	CA-C-N	6.21	126.39	119.32
1	A	149	ALA	C-N-CA	6.21	126.39	119.32
1	A	11	SER	N-CA-C	6.12	114.62	108.75
1	B	186	VAL	N-CA-C	-6.07	105.15	111.58
1	A	199	VAL	N-CA-C	6.01	116.76	107.99
1	B	4	VAL	N-CA-C	5.92	115.26	106.85
1	C	259	VAL	N-CA-C	5.91	119.44	113.47
1	B	115	THR	CA-C-N	5.75	123.80	119.66
1	B	115	THR	C-N-CA	5.75	123.80	119.66
1	D	284	ILE	CA-C-N	-5.75	114.34	120.03
1	D	284	ILE	C-N-CA	-5.75	114.34	120.03
1	D	138	VAL	CA-C-N	5.73	126.06	119.93
1	D	138	VAL	C-N-CA	5.73	126.06	119.93
1	C	134	ALA	N-CA-C	5.65	118.21	111.71
1	A	20	THR	CB-CA-C	5.61	116.61	110.15
1	B	101	GLY	N-CA-C	-5.59	107.39	115.27
1	A	60	LEU	N-CA-C	5.50	117.18	110.41
1	D	144	ASP	CA-C-N	5.44	125.09	119.05
1	D	144	ASP	C-N-CA	5.44	125.09	119.05
1	C	271	ILE	N-CA-C	5.33	115.19	106.72
1	A	8	GLU	N-CA-C	5.31	117.08	108.26
1	A	271	ILE	N-CA-C	5.15	114.99	107.37
1	C	166	LEU	CA-C-N	-5.12	114.80	119.82
1	C	166	LEU	C-N-CA	-5.12	114.80	119.82
1	D	249	ALA	N-CA-C	-5.10	103.20	110.59

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	272	HIS	Peptide

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	2370	0	2314	36	0
1	B	2434	0	2394	50	0
1	C	2461	0	2452	30	0
1	D	2469	0	2456	24	0
2	A	44	0	26	4	0
2	B	44	0	26	1	0
2	C	44	0	26	2	0
2	D	44	0	26	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	B	6	0	10	0	0
4	C	6	0	10	0	0
4	D	6	0	9	0	0
5	A	28	0	0	0	0
5	B	39	0	0	1	0
5	C	38	0	0	4	0
5	D	37	0	0	1	0
All	All	10078	0	9749	139	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 7.

All (139) 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:13:PRO:HD3	1:C:45:MET:HE1	1.44	0.97
1:A:38[A]:CYS:SG	1:A:62:HIS:NE2	2.47	0.86
1:D:312:ARG:HG2	1:D:312:ARG:HH11	1.44	0.83
1:B:116:PRO:HG2	1:B:119:LEU:HB2	1.65	0.77
1:D:312:ARG:HG2	1:D:312:ARG:NH1	2.00	0.72
1:A:5:GLN:O	1:A:13:PRO:HB3	1.90	0.71
1:C:132:ASP:HB3	5:C:2007:HOH:O	1.94	0.68
1:A:38[A]:CYS:HG	1:A:62:HIS:CD2	2.10	0.68
1:B:330:ARG:O	1:B:334:GLU:HG2	1.94	0.67
1:D:182:GLY:HA3	1:D:340:ARG:NH1	2.11	0.66
1:B:301:LEU:O	1:B:305:VAL:HG23	1.96	0.66
1:B:88:GLY:HA3	1:B:295:TRP:CZ2	2.30	0.66
1:D:157:THR:HB	1:D:158:PRO:HD3	1.79	0.65
1:A:116:PRO:HG2	1:A:119:LEU:HB2	1.78	0.65
1:D:143:LEU:HD13	1:D:309:ARG:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HB3	1:A:150:PRO:HD3	1.81	0.63
1:A:59:THR:HB	1:A:123:GLY:H	1.63	0.62
1:A:5:GLN:OE1	1:A:57:PRO:HB2	2.00	0.62
1:B:41:ASP:C	1:B:43:PHE:H	2.08	0.61
1:A:1:MET:HG3	1:A:2:LYS:O	1.99	0.61
1:D:312:ARG:HH11	1:D:312:ARG:CG	2.14	0.60
1:C:204:LEU:O	1:C:222:LYS:HE2	2.02	0.60
1:A:138:VAL:HG21	1:A:301:LEU:HD23	1.84	0.59
1:C:13:PRO:CD	1:C:45:MET:HE1	2.26	0.59
1:B:18:ILE:HB	1:B:19:PRO:HD2	1.84	0.59
1:B:116:PRO:HG2	1:B:119:LEU:CB	2.33	0.58
1:B:203:ASP:OD2	1:B:204:LEU:N	2.36	0.58
1:C:63:GLU:OE2	1:C:153:ASP:HB3	2.04	0.58
1:B:190:ILE:O	1:B:194:VAL:HG22	2.04	0.57
1:B:121:SER:HB3	1:B:122:PRO:CD	2.34	0.57
1:B:8:GLU:HB3	1:B:11:SER:HB2	1.86	0.57
1:B:88:GLY:HA3	1:B:295:TRP:CH2	2.40	0.56
1:C:157:THR:HB	1:C:158:PRO:HD3	1.88	0.55
1:C:237:GLY:O	1:C:239:GLY:N	2.40	0.55
1:A:38[A]:CYS:SG	1:A:63:GLU:HG3	2.47	0.54
1:A:88:GLY:HA3	1:A:295:TRP:CZ2	2.41	0.54
1:B:328:ALA:O	1:B:331:ARG:HB2	2.07	0.54
1:D:32:VAL:HG12	1:D:345:PRO:HG2	1.89	0.54
1:B:38:CYS:HB3	1:B:62:HIS:CE1	2.43	0.54
1:D:39:HIS:HA	1:D:332:LEU:HD21	1.89	0.53
1:A:300:GLU:O	1:A:304:VAL:HG23	2.09	0.53
1:B:156:LEU:HG	1:B:296:GLY:HA3	1.89	0.53
1:A:203:ASP:C	1:A:223:SER:HB2	2.34	0.53
1:B:36:GLY:HA3	1:B:63:GLU:OE1	2.08	0.52
1:D:335:GLY:HA2	5:D:2036:HOH:O	2.08	0.52
1:D:87:TYR:CZ	1:D:89:PRO:HG2	2.44	0.52
1:A:1:MET:SD	1:A:126:ALA:HB1	2.50	0.52
1:A:181:GLY:HA3	2:A:503:NAD:O5B	2.09	0.52
1:A:325:GLY:O	1:A:328:ALA:HB3	2.09	0.52
1:B:5:GLN:OE1	1:B:57:PRO:HB2	2.10	0.51
1:C:299:SER:HB2	5:C:2029:HOH:O	2.10	0.51
1:B:38:CYS:SG	1:B:40:SER:HB2	2.51	0.51
1:B:263:ASP:HA	1:B:287:GLY:O	2.10	0.51
1:C:180:VAL:HG12	1:C:180:VAL:O	2.10	0.51
1:B:41:ASP:C	1:B:43:PHE:N	2.69	0.51
1:D:157:THR:HB	1:D:158:PRO:CD	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ASP:HA	2:A:503:NAD:H2A	1.92	0.50
1:B:30:LEU:O	1:B:128:TYR:HA	2.11	0.50
1:B:111:ASP:C	1:B:113:GLY:H	2.20	0.50
1:B:32:VAL:O	1:B:345:PRO:HG2	2.12	0.50
1:D:154:ALA:HA	1:D:183:LEU:HG	1.93	0.50
1:B:268:VAL:HB	1:B:292:THR:HG22	1.93	0.50
1:A:40:SER:O	1:A:44:VAL:HG23	2.12	0.49
1:C:7:THR:HG22	1:C:57:PRO:HB3	1.94	0.49
1:B:325:GLY:O	1:B:328:ALA:HB3	2.12	0.49
1:B:59:THR:HB	1:B:123:GLY:H	1.77	0.49
1:B:121:SER:HB3	1:B:122:PRO:HD2	1.94	0.49
1:C:204:LEU:HD23	1:C:223:SER:HB3	1.94	0.49
1:C:279:VAL:HG13	1:C:284:ILE:HG21	1.95	0.49
1:C:245:ASP:CG	1:C:248:GLY:H	2.20	0.48
1:D:65:VAL:HG13	1:D:149:ALA:HA	1.95	0.48
1:C:319:THR:HG22	5:C:2009:HOH:O	2.13	0.48
1:A:157:THR:HB	1:A:158:PRO:HD3	1.94	0.48
1:C:2:LYS:HB3	1:C:322:LEU:HD13	1.94	0.48
1:B:84:VAL:HG21	1:B:137:LEU:HD22	1.96	0.47
1:A:44:VAL:O	1:A:47:MET:HB2	2.15	0.47
1:A:203:ASP:HA	2:A:503:NAD:C2A	2.45	0.47
1:B:65:VAL:HG23	1:B:149:ALA:HA	1.96	0.47
1:C:131:VAL:HG21	1:C:137:LEU:HD21	1.96	0.46
1:C:203:ASP:HA	2:C:503:NAD:C2A	2.45	0.46
1:A:60:LEU:O	1:A:124:SER:N	2.48	0.46
1:A:150:PRO:O	1:A:151:LEU:C	2.58	0.46
1:B:134:ALA:O	1:B:136:HIS:N	2.48	0.46
1:A:165:VAL:HG11	1:A:265:HIS:CG	2.51	0.46
1:A:38[A]:CYS:SG	1:A:62:HIS:CD2	3.06	0.46
1:B:319:THR:HG23	1:B:344:VAL:HG23	1.97	0.46
1:C:176:VAL:HB	1:C:243:VAL:HG22	1.98	0.45
1:D:90:TRP:CZ2	1:D:117:PRO:HD3	2.51	0.45
1:B:331:ARG:O	1:B:334:GLU:HG3	2.16	0.45
1:D:165:VAL:HG11	1:D:265:HIS:CG	2.52	0.45
1:B:72:GLY:O	1:B:74:GLY:N	2.49	0.45
1:B:276:HIS:CD2	1:C:278:LYS:HG2	2.52	0.45
1:B:281:PHE:O	1:B:282:PHE:HB2	2.17	0.45
1:C:203:ASP:OD2	2:C:503:NAD:O2B	2.31	0.45
1:C:31:LYS:HD2	1:C:128:TYR:CZ	2.51	0.45
1:A:14:VAL:O	1:A:14:VAL:HG23	2.17	0.45
1:D:7:THR:HG22	1:D:57:PRO:HB3	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:THR:HA	1:A:21:PRO:HD3	1.73	0.44
1:A:6:TYR:CE1	1:A:45:MET:HG2	2.53	0.44
1:B:12:GLU:OE1	1:B:330:ARG:NH2	2.51	0.44
1:B:248:GLY:HA3	1:B:270:GLY:O	2.18	0.44
1:C:33:THR:OG1	1:C:65:VAL:HG12	2.17	0.44
1:D:149:ALA:HB3	1:D:150:PRO:HD3	2.00	0.44
1:B:143:LEU:N	5:B:2014:HOH:O	2.51	0.43
1:C:278:LYS:HB3	1:C:283:MET:HE2	1.99	0.43
1:A:144:ASP:HA	1:A:145:PRO:HD3	1.81	0.43
1:D:148:ALA:O	1:D:149:ALA:C	2.61	0.43
1:B:40:SER:O	1:B:43:PHE:HB3	2.19	0.43
1:B:134:ALA:C	1:B:136:HIS:N	2.76	0.43
1:B:130:ILE:HD13	1:B:130:ILE:HA	1.76	0.43
1:C:180:VAL:HG21	1:C:212:ALA:HB2	2.01	0.43
1:B:38:CYS:C	1:B:40:SER:N	2.77	0.42
1:A:246:PHE:O	2:A:503:NAD:H4D	2.19	0.42
1:C:142:ASP:H	1:C:309:ARG:HH12	1.65	0.42
1:C:319:THR:CG2	5:C:2009:HOH:O	2.67	0.42
1:B:23:PRO:HB2	1:B:72:GLY:HA2	2.02	0.42
1:B:181:GLY:HA3	2:B:503:NAD:O5B	2.20	0.42
1:A:166:LEU:HB3	1:A:167:PRO:HD3	2.00	0.42
1:A:12:GLU:HA	1:A:13:PRO:HD3	1.74	0.42
1:D:30:LEU:O	1:D:128:TYR:HA	2.20	0.42
1:D:140:ILE:O	1:D:143:LEU:HB2	2.19	0.42
1:B:154:ALA:HA	1:B:183:LEU:HG	2.01	0.42
1:B:322:LEU:HD11	1:B:345:PRO:HB3	2.02	0.42
1:A:245:ASP:OD1	1:A:245:ASP:C	2.63	0.41
1:C:265:HIS:CE1	1:C:291:VAL:HG12	2.54	0.41
1:D:260:VAL:HG22	1:D:261:ALA:N	2.34	0.41
1:B:32:VAL:HG11	1:B:124:SER:O	2.20	0.41
1:D:295:TRP:HB3	1:D:296:GLY:H	1.60	0.41
1:A:138:VAL:CG2	1:A:301:LEU:HD23	2.48	0.41
1:B:138:VAL:HG21	1:B:301:LEU:HD23	2.03	0.41
1:B:227:ALA:O	1:B:228:ALA:C	2.64	0.41
1:A:183:LEU:O	1:A:184:GLY:C	2.64	0.41
1:C:28:ILE:HD12	1:C:28:ILE:N	2.36	0.41
1:C:301:LEU:O	1:C:302:MET:C	2.63	0.41
1:B:24:GLY:O	1:B:26:GLY:N	2.53	0.41
1:D:24:GLY:O	1:D:72:GLY:HA3	2.21	0.41
1:C:30:LEU:O	1:C:128:TYR:HA	2.21	0.40
1:D:248:GLY:O	1:D:272:HIS:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLU:HA	1:A:152:THR:OG1	2.21	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	324/345 (94%)	291 (90%)	31 (10%)	2 (1%)	21	51
1	B	334/345 (97%)	310 (93%)	22 (7%)	2 (1%)	21	51
1	C	340/345 (99%)	325 (96%)	15 (4%)	0	100	100
1	D	343/345 (99%)	323 (94%)	19 (6%)	1 (0%)	36	66
All	All	1341/1380 (97%)	1249 (93%)	87 (6%)	5 (0%)	30	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	PRO
1	A	50	ALA
1	B	273	ALA
1	D	188	ILE
1	B	42	ILE

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	232/248 (94%)	218 (94%)	14 (6%)	17	47
1	B	239/248 (96%)	228 (95%)	11 (5%)	24	58
1	C	246/248 (99%)	233 (95%)	13 (5%)	20	52
1	D	246/248 (99%)	236 (96%)	10 (4%)	27	62
All	All	963/992 (97%)	915 (95%)	48 (5%)	22	54

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	14	VAL
1	A	28	ILE
1	A	31	LYS
1	A	56	LEU
1	A	80	VAL
1	A	108	ARG
1	A	144	ASP
1	A	169	LEU
1	A	205	ASP
1	A	223	SER
1	A	233	GLU
1	A	319	THR
1	A	322	LEU
1	B	2	LYS
1	B	18	ILE
1	B	40	SER
1	B	46	ASP
1	B	107	THR
1	B	108	ARG
1	B	130	ILE
1	B	204	LEU
1	B	205	ASP
1	B	271	ILE
1	B	309	ARG
1	C	22	THR
1	C	65	VAL
1	C	70	GLU
1	C	76	THR
1	C	80	VAL
1	C	138	VAL
1	C	259	VAL
1	C	262	VAL

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Mol	Chain	Res	Type
1	C	267	SER
1	C	278	LYS
1	C	295	TRP
1	C	319	THR
1	C	334	GLU
1	D	11	SER
1	D	12	GLU
1	D	112	LEU
1	D	195	SER
1	D	214	GLU
1	D	267	SER
1	D	295	TRP
1	D	312	ARG
1	D	334	GLU
1	D	343	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	316	HIS
1	C	39	HIS
1	C	276	HIS
1	D	39	HIS
1	D	51	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	D	503	-	46,48,48	1.77	5 (10%)	64,73,73	1.69	12 (18%)
2	NAD	C	503	-	46,48,48	1.62	5 (10%)	64,73,73	1.99	14 (21%)
4	BU1	D	1347	3	5,5,5	0.72	0	4,4,4	0.48	0
4	BU1	B	1347	-	5,5,5	0.65	0	4,4,4	0.25	0
4	BU1	C	1348	-	5,5,5	0.53	0	4,4,4	0.37	0
2	NAD	B	503	-	46,48,48	1.68	3 (6%)	64,73,73	1.55	8 (12%)
2	NAD	A	503	-	46,48,48	1.81	6 (13%)	64,73,73	1.75	12 (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	D	503	-	-	9/30/62/62	0/5/5/5
2	NAD	C	503	-	-	8/30/62/62	0/5/5/5
4	BU1	D	1347	3	-	2/3/3/3	-
4	BU1	B	1347	-	-	2/3/3/3	-
4	BU1	C	1348	-	-	0/3/3/3	-
2	NAD	B	503	-	-	8/30/62/62	0/5/5/5
2	NAD	A	503	-	-	7/30/62/62	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	503	NAD	O7N-C7N	9.56	1.41	1.24
2	B	503	NAD	O7N-C7N	9.45	1.41	1.24
2	A	503	NAD	O7N-C7N	9.20	1.41	1.24
2	C	503	NAD	O7N-C7N	8.16	1.39	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	NAD	C8A-N7A	2.85	1.37	1.31
2	B	503	NAD	C8A-N7A	2.77	1.37	1.31
2	C	503	NAD	C8A-N7A	2.77	1.37	1.31
2	A	503	NAD	C2N-N1N	2.75	1.38	1.35
2	D	503	NAD	C2A-N1A	2.71	1.38	1.33
2	D	503	NAD	C8A-N7A	2.66	1.36	1.31
2	D	503	NAD	C2A-N3A	2.52	1.38	1.33
2	A	503	NAD	PN-O3	2.44	1.62	1.59
2	C	503	NAD	C2A-N3A	2.43	1.38	1.33
2	A	503	NAD	C2A-N3A	2.36	1.38	1.33
2	A	503	NAD	PA-O3	2.33	1.62	1.59
2	B	503	NAD	C2A-N3A	2.28	1.38	1.33
2	C	503	NAD	C2A-N1A	2.16	1.37	1.33
2	D	503	NAD	C2N-N1N	2.15	1.37	1.35
2	C	503	NAD	O4D-C1D	2.02	1.43	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	NAD	N3A-C2A-N1A	-6.29	119.05	128.58
2	C	503	NAD	N9A-C8A-N7A	-6.10	105.29	113.94
2	B	503	NAD	N3A-C2A-N1A	-6.01	119.48	128.58
2	A	503	NAD	N3A-C2A-N1A	-5.98	119.53	128.58
2	D	503	NAD	N3A-C2A-N1A	-5.31	120.55	128.58
2	D	503	NAD	N9A-C8A-N7A	-5.11	106.68	113.94
2	A	503	NAD	N9A-C8A-N7A	-5.01	106.82	113.94
2	C	503	NAD	C5A-N7A-C8A	4.72	110.86	103.45
2	B	503	NAD	C5A-C4A-N3A	-4.58	120.41	126.72
2	A	503	NAD	C5A-N7A-C8A	4.03	109.78	103.45
2	A	503	NAD	C5A-C4A-N3A	-3.89	121.36	126.72
2	B	503	NAD	C2A-N3A-C4A	3.81	121.15	111.83
2	A	503	NAD	C6N-N1N-C2N	-3.80	118.65	121.88
2	A	503	NAD	C2A-N3A-C4A	3.71	120.90	111.83
2	D	503	NAD	C4A-N9A-C8A	3.60	109.52	105.74
2	D	503	NAD	C5A-N7A-C8A	3.58	109.08	103.45
2	C	503	NAD	C5A-C4A-N3A	-3.57	121.79	126.72
2	C	503	NAD	C4A-N9A-C8A	3.49	109.40	105.74
2	C	503	NAD	C6N-N1N-C2N	-3.45	118.95	121.88
2	B	503	NAD	N9A-C8A-N7A	-3.44	109.05	113.94
2	C	503	NAD	C4A-C5A-N7A	-3.42	106.67	110.58
2	C	503	NAD	C2A-N3A-C4A	3.31	119.92	111.83
2	C	503	NAD	C6N-N1N-C1D	3.29	126.19	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	503	NAD	C5A-C4A-N3A	-3.19	122.32	126.72
2	D	503	NAD	C2A-N3A-C4A	3.09	119.39	111.83
2	D	503	NAD	O4B-C1B-N9A	3.01	113.86	108.09
2	A	503	NAD	C4A-N9A-C8A	2.82	108.70	105.74
2	D	503	NAD	C6N-N1N-C2N	-2.81	119.49	121.88
2	A	503	NAD	C4A-N9A-C1B	-2.79	120.11	126.63
2	A	503	NAD	C4A-C5A-N7A	-2.74	107.44	110.58
2	B	503	NAD	N3A-C4A-N9A	2.74	131.83	127.17
2	A	503	NAD	C5N-C4N-C3N	-2.73	117.68	120.36
2	C	503	NAD	O4B-C1B-N9A	2.70	113.27	108.09
2	B	503	NAD	C5A-N7A-C8A	2.66	107.63	103.45
2	A	503	NAD	N3A-C4A-N9A	2.49	131.40	127.17
2	C	503	NAD	O7N-C7N-N7N	-2.47	119.04	122.62
2	D	503	NAD	C5B-C4B-C3B	-2.43	106.45	115.21
2	C	503	NAD	C4A-N9A-C1B	-2.38	121.06	126.63
2	D	503	NAD	C4A-N9A-C1B	-2.37	121.09	126.63
2	D	503	NAD	C4A-C5A-N7A	-2.36	107.89	110.58
2	C	503	NAD	O3D-C3D-C4D	-2.34	104.35	111.08
2	B	503	NAD	O4B-C1B-N9A	2.31	112.53	108.09
2	D	503	NAD	N3A-C4A-N9A	2.17	130.85	127.17
2	A	503	NAD	C6N-N1N-C1D	2.11	123.86	119.73
2	B	503	NAD	C4A-C5A-N7A	-2.11	108.17	110.58
2	C	503	NAD	O2A-PA-O3	2.01	112.72	107.27

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	NAD	O4D-C1D-N1N-C2N
2	A	503	NAD	O4D-C1D-N1N-C6N
2	B	503	NAD	O4D-C1D-N1N-C2N
2	B	503	NAD	O4D-C1D-N1N-C6N
2	B	503	NAD	C2D-C1D-N1N-C2N
2	B	503	NAD	C2D-C1D-N1N-C6N
2	C	503	NAD	O4D-C1D-N1N-C2N
2	C	503	NAD	O4D-C1D-N1N-C6N
2	C	503	NAD	C2D-C1D-N1N-C2N
2	C	503	NAD	C2D-C1D-N1N-C6N
2	D	503	NAD	C5B-O5B-PA-O1A
2	D	503	NAD	C5B-O5B-PA-O2A
2	D	503	NAD	C5B-O5B-PA-O3
2	D	503	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	D	503	NAD	O4D-C1D-N1N-C6N
2	D	503	NAD	C2D-C1D-N1N-C2N
2	C	503	NAD	O4B-C4B-C5B-O5B
2	C	503	NAD	C3B-C4B-C5B-O5B
2	D	503	NAD	C3B-C4B-C5B-O5B
2	A	503	NAD	O4B-C4B-C5B-O5B
2	A	503	NAD	C3B-C4B-C5B-O5B
2	B	503	NAD	O4B-C4B-C5B-O5B
2	B	503	NAD	C3B-C4B-C5B-O5B
2	D	503	NAD	O4B-C4B-C5B-O5B
4	B	1347	BU1	C2-C3-C4-O6
4	D	1347	BU1	O5-C1-C2-C3
2	B	503	NAD	PN-O3-PA-O1A
2	A	503	NAD	C5D-O5D-PN-O3
2	C	503	NAD	PN-O3-PA-O1A
2	C	503	NAD	PN-O3-PA-O2A
2	A	503	NAD	C2D-C1D-N1N-C2N
2	D	503	NAD	C2D-C1D-N1N-C6N
4	B	1347	BU1	O5-C1-C2-C3
2	A	503	NAD	PN-O3-PA-O1A
4	D	1347	BU1	C2-C3-C4-O6
2	B	503	NAD	PN-O3-PA-O2A

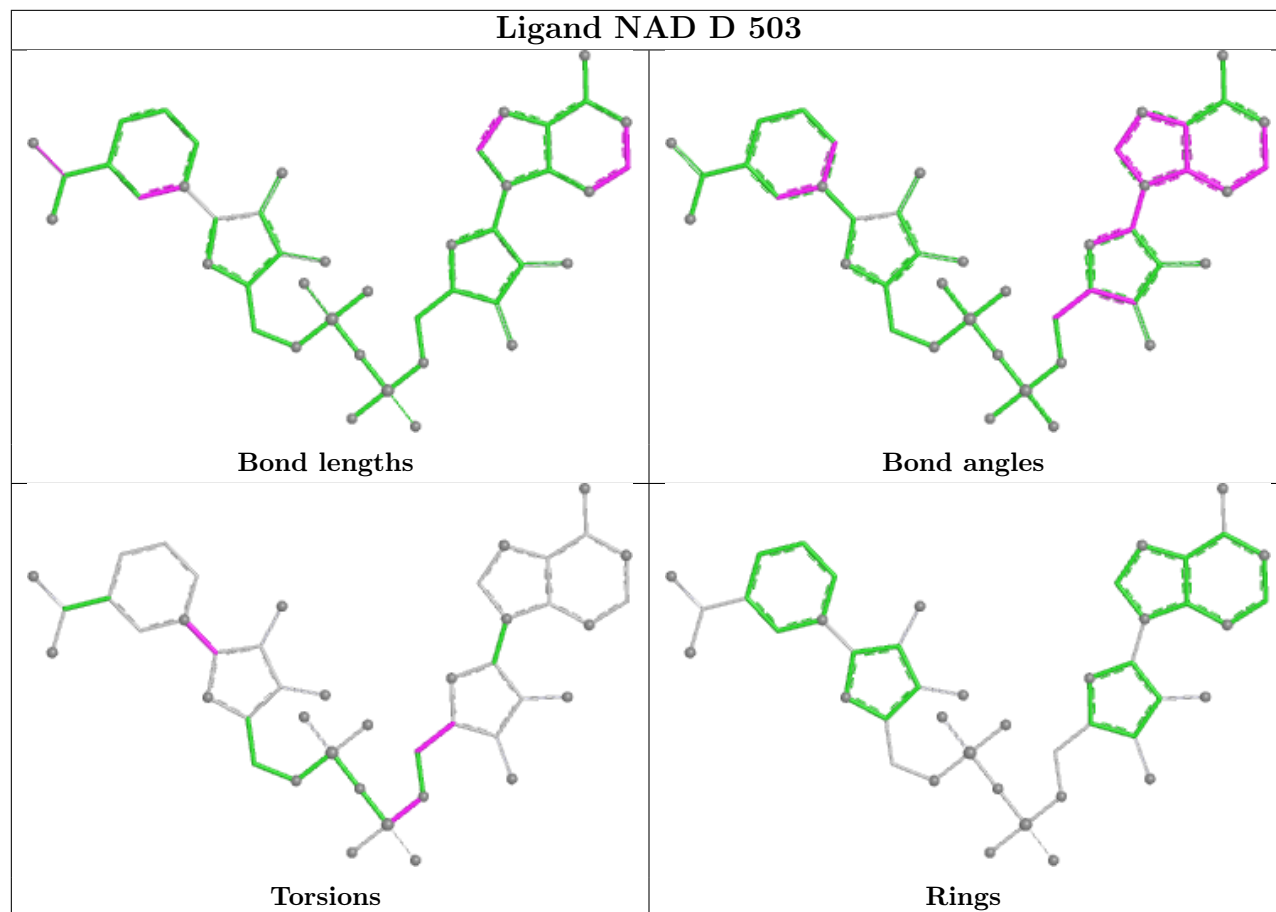
There are no ring outliers.

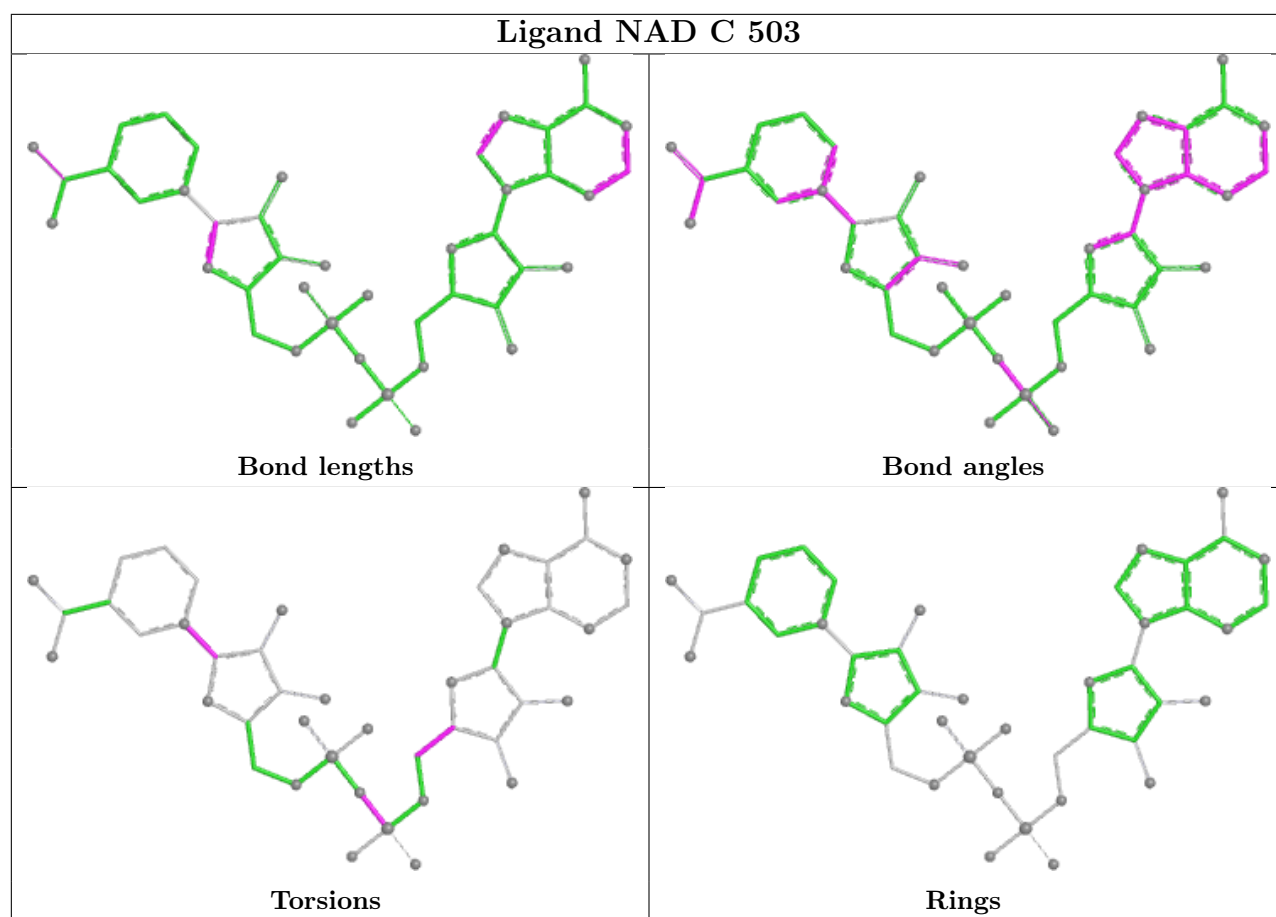
3 monomers are involved in 7 short contacts:

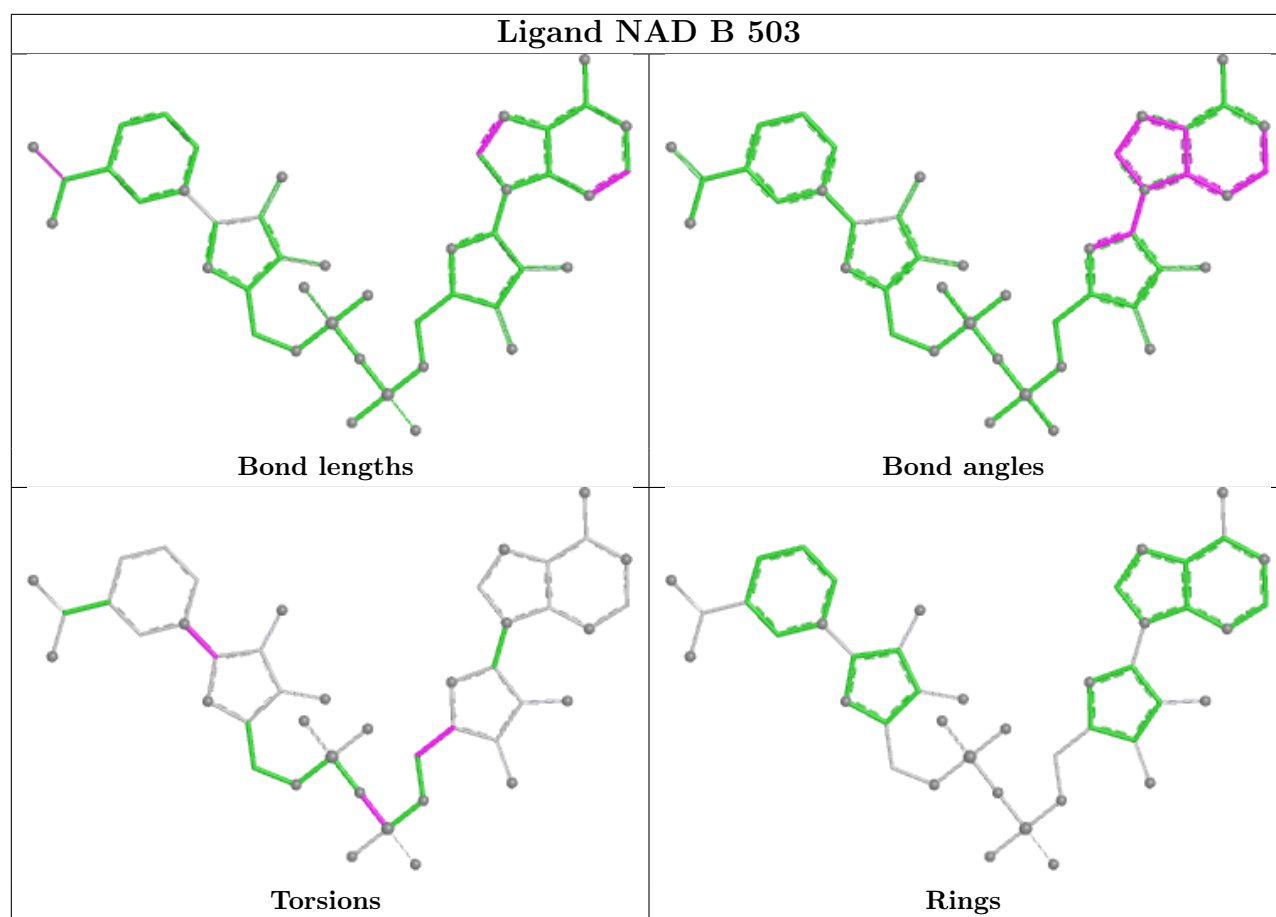
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	503	NAD	2	0
2	B	503	NAD	1	0
2	A	503	NAD	4	0

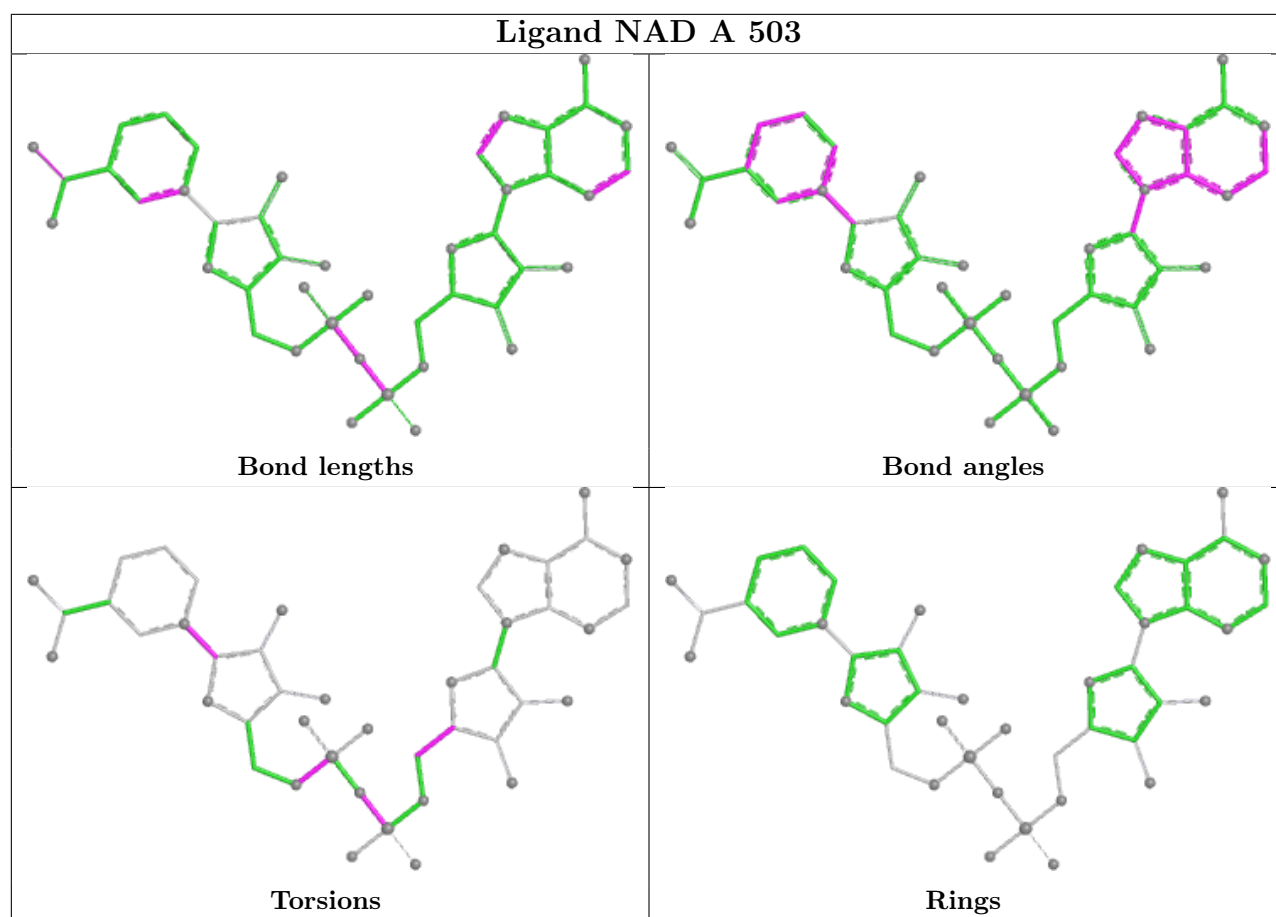
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	333/345 (96%)	-0.26	4 (1%) 76 68	23, 38, 57, 61	1 (0%)
1	B	342/345 (99%)	-0.30	5 (1%) 72 63	23, 39, 58, 71	0
1	C	344/345 (99%)	-0.48	1 (0%) 90 86	23, 38, 54, 60	0
1	D	345/345 (100%)	-0.44	0 100 100	23, 38, 55, 60	0
All	All	1364/1380 (98%)	-0.37	10 (0%) 84 77	23, 38, 57, 71	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	GLY	3.6
1	B	72	GLY	3.3
1	B	70	GLU	3.2
1	A	24	GLY	3.1
1	A	14	VAL	3.0
1	A	42	ILE	2.6
1	B	76	THR	2.6
1	A	7	THR	2.4
1	B	24	GLY	2.3
1	C	237	GLY	2.1

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

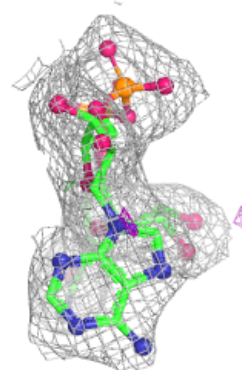
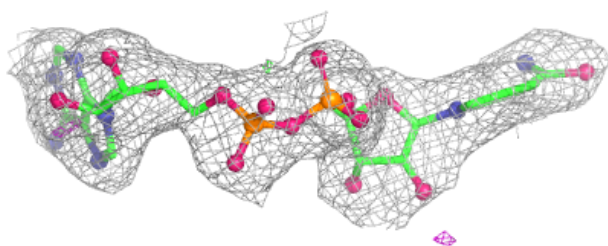
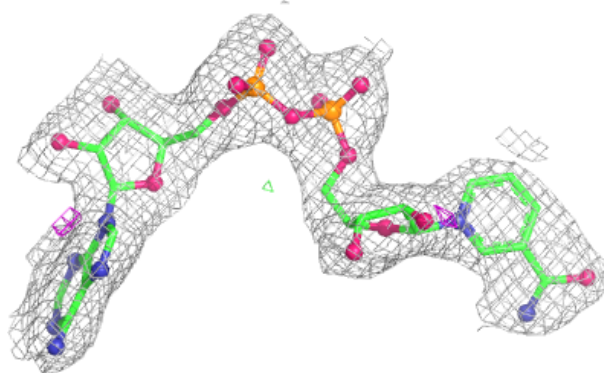
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BU1	B	1347	6/6	0.75	0.30	49,52,53,53	0
4	BU1	C	1348	6/6	0.80	0.26	38,41,44,45	0
4	BU1	D	1347	6/6	0.88	0.20	25,33,33,35	0
2	NAD	A	503	44/44	0.95	0.07	28,37,39,40	0
2	NAD	B	503	44/44	0.96	0.07	34,38,42,43	0
2	NAD	D	503	44/44	0.97	0.06	27,32,36,36	0
2	NAD	C	503	44/44	0.98	0.05	22,29,31,32	0
3	ZN	B	1346	1/1	0.99	0.02	42,42,42,42	0
3	ZN	A	1346	1/1	0.99	0.02	51,51,51,51	0
3	ZN	C	1347	1/1	1.00	0.03	31,31,31,31	0
3	ZN	D	1346	1/1	1.00	0.03	35,35,35,35	0
3	ZN	D	1348	1/1	1.00	0.01	34,34,34,34	0
3	ZN	A	1347	1/1	1.00	0.01	33,33,33,33	0
3	ZN	B	1348	1/1	1.00	0.03	32,32,32,32	0
3	ZN	C	1346	1/1	1.00	0.01	37,37,37,37	0

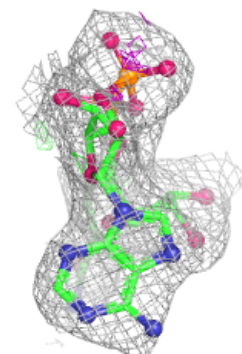
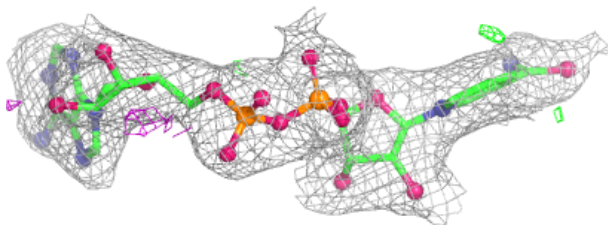
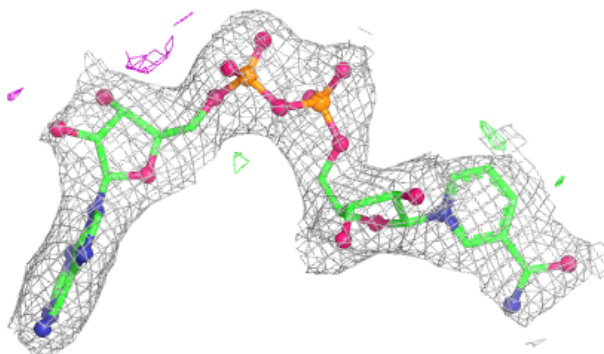
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 503:

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

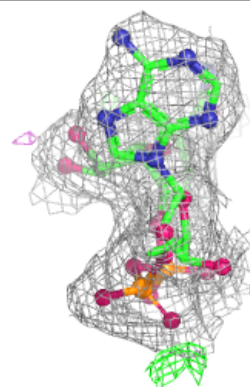
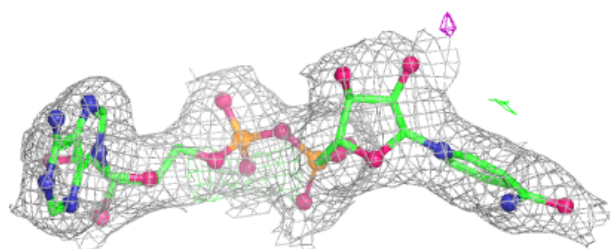
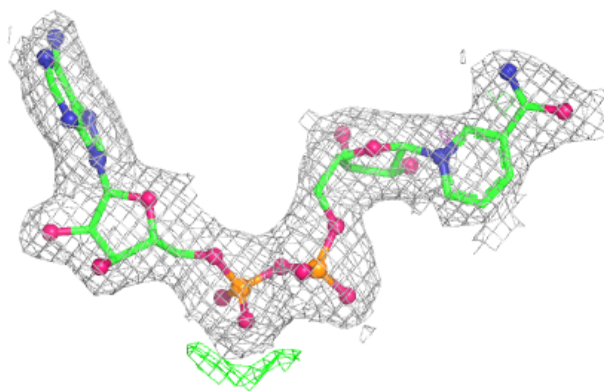
**Electron density around NAD B 503:**

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

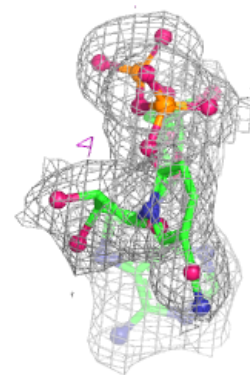
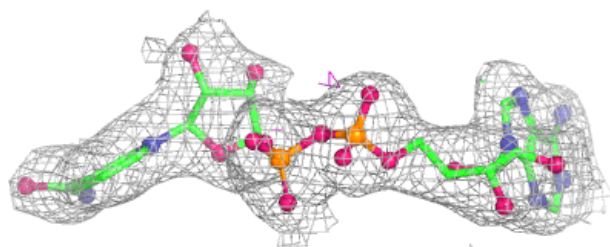
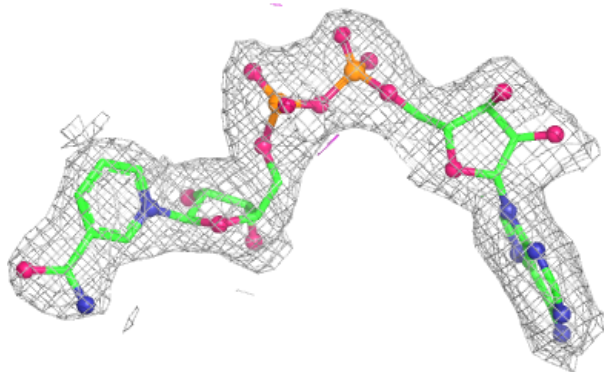


Electron density around NAD D 503:

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

**Electron density around NAD C 503:**

$2mF_o-DF_c$ (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.