



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:38 AM UTC

PDB ID : 1HYH / pdb_00001hyh
Title : CRYSTAL STRUCTURE OF L-2-HYDROXYISOCAPROATE DEHYDROGENASE FROM LACTOBACILLUS CONFUSUS AT 2.2 ANGSTROMS RESOLUTION-AN EXAMPLE OF STRONG ASYMMETRY BETWEEN SUBUNITS
Authors : Niefind, K.; Hecht, H.-J.; Schomburg, D.
Deposited on : 1995-06-05
Resolution : 2.20 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](#) ①) 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

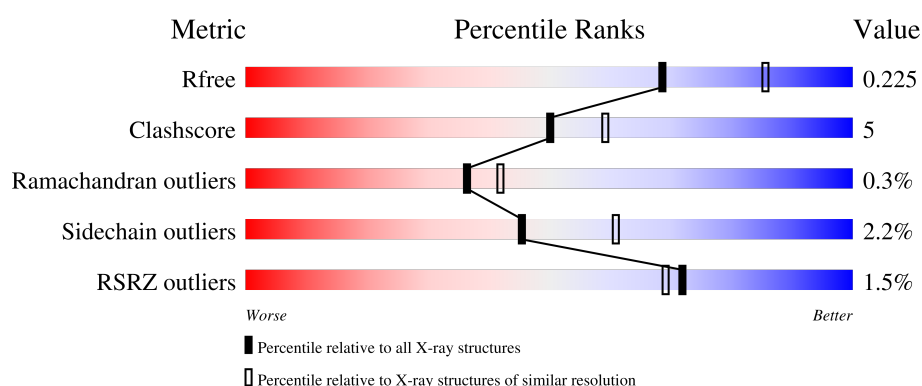
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	309	2% 77% 18% • •
1	B	309	% 73% 20% • 5%
1	C	309	% 78% 17% • •
1	D	309	2% 80% 15% • •

2 Entry composition [i](#)

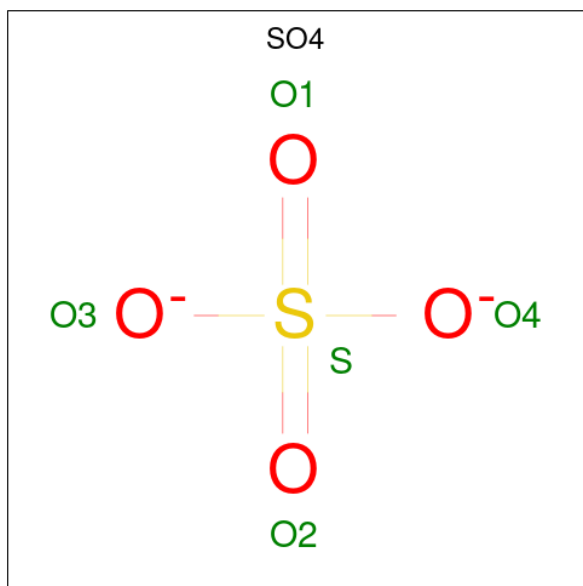
There are 4 unique types of molecules in this entry. The entry contains 9318 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-2-HYDROXYISOCAPROATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	1	0
			2217	1397	381	432	7			
1	B	294	Total	C	N	O	S	0	1	0
			2184	1376	374	427	7			
1	C	297	Total	C	N	O	S	0	0	0
			2207	1389	378	433	7			
1	D	297	Total	C	N	O	S	0	0	0
			2205	1389	376	433	7			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



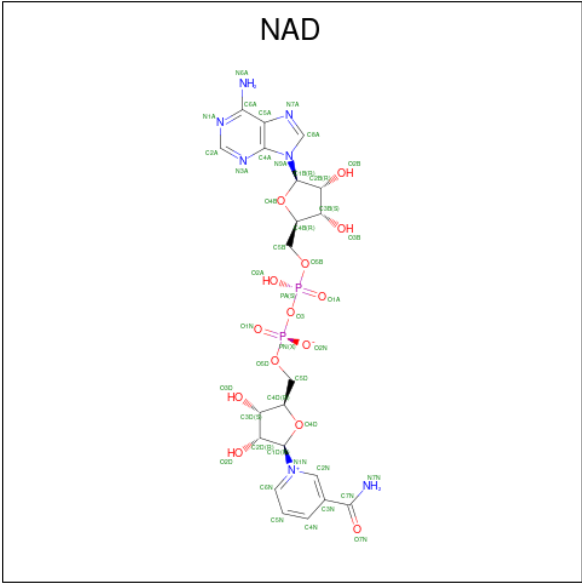
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	70	Total	O	0	0
			70	70		
4	C	79	Total	O	0	0
			79	79		

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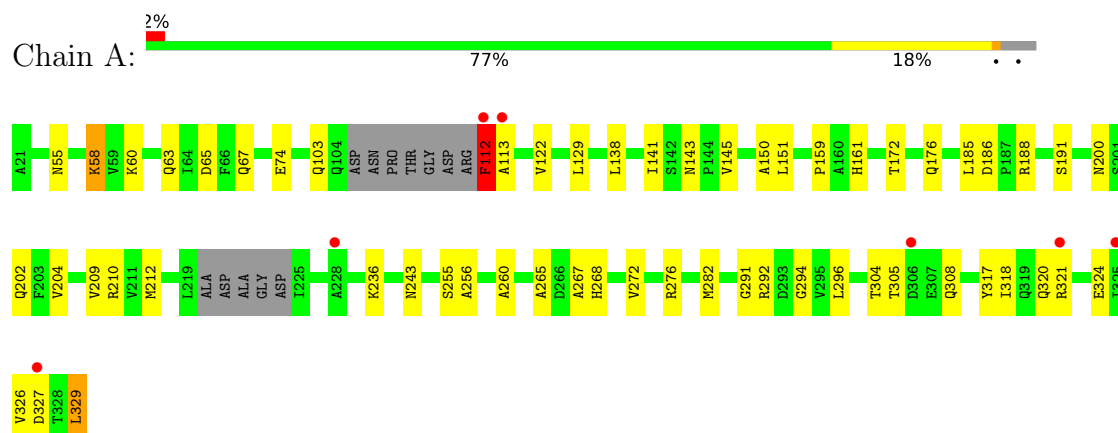
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	73	Total	O	0	0
			73	73		

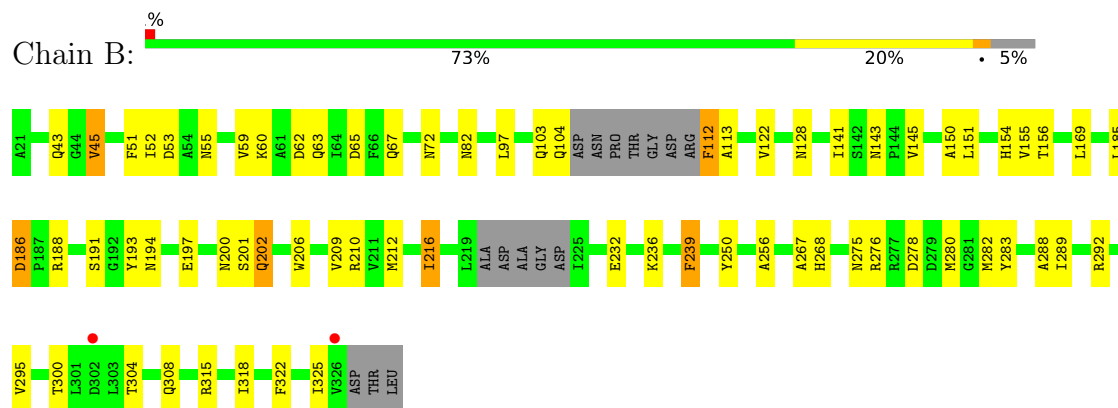
3 Residue-property plots

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.

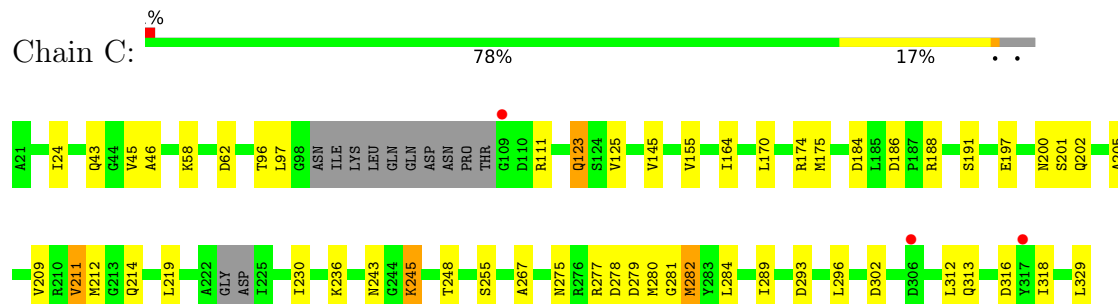
• Molecule 1: L-2-HYDROXYISOCAPROATE DEHYDROGENASE



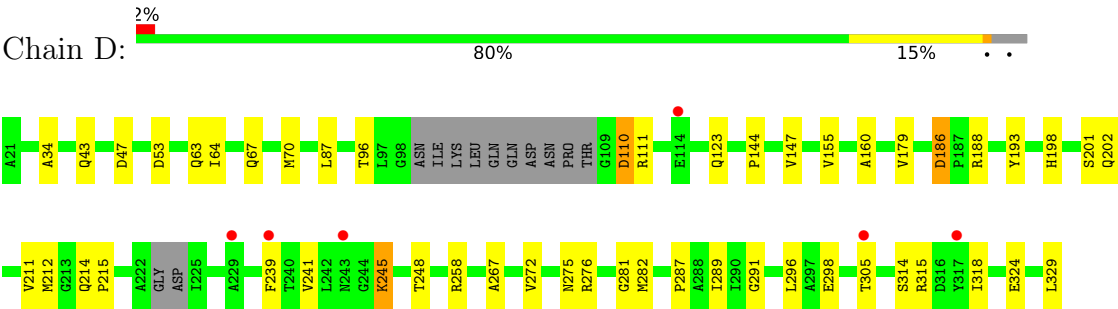
• Molecule 1: L-2-HYDROXYISOCAPROATE DEHYDROGENASE



• Molecule 1: L-2-HYDROXYISOCAPROATE DEHYDROGENASE



● Molecule 1: L-2-HYDROXYISOCAPROATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.90Å 135.90Å 205.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.20 8.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.2 (8.00-2.20) 94.7 (8.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.21Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.210 , 0.250 0.193 , 0.225	Depositor DCC
R_{free} test set	10596 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9318	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: SO4, 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	1.10	4/2253 (0.2%)	1.59	18/3054 (0.6%)
1	B	0.97	4/2220 (0.2%)	1.62	24/3011 (0.8%)
1	C	1.01	3/2238 (0.1%)	1.65	29/3035 (1.0%)
1	D	1.04	3/2236 (0.1%)	1.64	23/3033 (0.8%)
All	All	1.03	14/8947 (0.2%)	1.63	94/12133 (0.8%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	LEU	C-OXT	19.23	1.62	1.23
1	D	329	LEU	C-OXT	12.88	1.49	1.23
1	C	329	LEU	C-OXT	6.08	1.35	1.23
1	A	103	GLN	CD-OE1	5.96	1.34	1.23
1	B	194	ASN	CG-OD1	5.93	1.34	1.23
1	A	243	ASN	CG-OD1	5.89	1.34	1.23
1	B	104	GLN	CD-OE1	5.84	1.34	1.23
1	D	202	GLN	CD-NE2	-5.66	1.21	1.33
1	B	103	GLN	CD-OE1	5.63	1.34	1.23
1	D	202	GLN	CD-OE1	5.49	1.33	1.23
1	A	202	GLN	CD-OE1	5.47	1.33	1.23
1	B	202	GLN	CD-OE1	5.39	1.33	1.23
1	C	202	GLN	CD-OE1	5.29	1.33	1.23
1	C	202	GLN	CD-NE2	-5.23	1.22	1.33

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	PHE	CA-CB-CG	-9.25	104.55	113.80
1	C	186	ASP	CA-CB-CG	8.82	121.42	112.60
1	B	239	PHE	CA-CB-CG	-8.82	104.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	188	ARG	CD-NE-CZ	8.78	136.70	124.40
1	D	239	PHE	CA-CB-CG	-8.67	105.13	113.80
1	D	245	LYS	CA-CB-CG	7.82	129.74	114.10
1	A	327	ASP	CA-C-N	7.80	131.51	120.28
1	A	327	ASP	C-N-CA	7.80	131.51	120.28
1	C	278	ASP	CA-CB-CG	-7.71	104.89	112.60
1	D	188	ARG	CD-NE-CZ	7.36	134.71	124.40
1	B	278	ASP	CA-CB-CG	-7.36	105.25	112.60
1	B	122	VAL	CA-C-O	-7.03	113.74	121.05
1	D	43	GLN	OE1-CD-NE2	6.94	129.54	122.60
1	B	112	PHE	CA-C-N	6.65	129.49	120.38
1	B	112	PHE	C-N-CA	6.65	129.49	120.38
1	A	292	ARG	NE-CZ-NH2	6.64	125.18	119.20
1	C	211	VAL	N-CA-CB	6.59	122.26	111.58
1	D	305	THR	CA-C-O	-6.46	113.70	120.55
1	C	255	SER	CB-CA-C	-6.36	100.89	110.88
1	B	186	ASP	CA-CB-CG	6.28	118.88	112.60
1	C	123	GLN	OE1-CD-NE2	6.27	128.87	122.60
1	C	281	GLY	CA-C-N	6.24	134.19	123.03
1	C	281	GLY	C-N-CA	6.24	134.19	123.03
1	C	282	MET	CA-C-N	6.13	130.84	122.19
1	C	282	MET	C-N-CA	6.13	130.84	122.19
1	A	243	ASN	CB-CG-ND2	6.13	125.59	116.40
1	C	236	LYS	CA-C-N	6.02	126.62	119.94
1	C	236	LYS	C-N-CA	6.02	126.62	119.94
1	A	272	VAL	O-C-N	-5.97	115.65	122.94
1	C	145	VAL	N-CA-C	5.90	116.64	110.62
1	D	267	ALA	N-CA-C	5.89	118.65	111.82
1	C	277	ARG	CD-NE-CZ	5.88	132.63	124.40
1	B	128	ASN	OD1-CG-ND2	5.82	128.42	122.60
1	D	70	MET	CA-C-O	-5.80	114.36	120.63
1	A	113	ALA	CA-C-O	5.77	126.47	119.38
1	C	188	ARG	NE-CZ-NH2	5.75	124.37	119.20
1	A	210	ARG	CB-CG-CD	5.73	124.48	111.30
1	D	64	ILE	CA-C-O	-5.68	114.83	120.85
1	B	169	LEU	N-CA-C	-5.65	105.20	111.36
1	B	276	ARG	CD-NE-CZ	5.65	132.31	124.40
1	C	230	ILE	O-C-N	5.65	127.35	121.87
1	D	179	VAL	CA-C-N	5.64	126.20	119.94
1	D	179	VAL	C-N-CA	5.64	126.20	119.94
1	B	292	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	D	193	TYR	CB-CA-C	-5.59	98.44	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	VAL	N-CA-C	5.59	118.03	111.05
1	B	193	TYR	CA-C-N	5.58	130.70	123.00
1	B	193	TYR	C-N-CA	5.58	130.70	123.00
1	B	154	HIS	O-C-N	-5.50	116.29	122.12
1	A	186	ASP	CA-CB-CG	5.49	118.09	112.60
1	B	128	ASN	CA-CB-CG	-5.48	107.12	112.60
1	B	156	THR	CA-C-O	5.48	126.26	119.79
1	B	60	LYS	CA-C-N	5.47	127.88	120.44
1	B	60	LYS	C-N-CA	5.47	127.88	120.44
1	D	87	LEU	CA-C-N	5.45	127.89	120.54
1	D	87	LEU	C-N-CA	5.45	127.89	120.54
1	A	122	VAL	N-CA-C	5.44	116.17	110.62
1	D	298	GLU	CB-CG-CD	5.44	121.85	112.60
1	C	284	LEU	N-CA-CB	5.43	119.82	111.56
1	D	160	ALA	O-C-N	-5.41	116.38	122.12
1	B	300	THR	N-CA-CB	5.35	119.17	110.77
1	C	245	LYS	CA-CB-CG	5.33	124.77	114.10
1	B	51	PHE	CA-CB-CG	5.33	119.13	113.80
1	C	175	MET	N-CA-C	-5.32	105.40	111.14
1	B	113	ALA	N-CA-C	5.30	117.74	111.33
1	C	186	ASP	CA-C-N	5.29	125.10	119.28
1	C	186	ASP	C-N-CA	5.29	125.10	119.28
1	B	45	VAL	CA-C-O	-5.29	115.57	121.17
1	D	110	ASP	CA-C-N	5.23	127.60	120.54
1	D	110	ASP	C-N-CA	5.23	127.60	120.54
1	B	55	ASN	CA-CB-CG	5.21	117.81	112.60
1	A	255[A]	SER	CA-C-N	5.18	127.65	120.29
1	A	255[A]	SER	C-N-CA	5.18	127.65	120.29
1	A	255[B]	SER	CA-C-N	5.18	127.65	120.29
1	A	255[B]	SER	C-N-CA	5.18	127.65	120.29
1	C	243	ASN	OD1-CG-ND2	5.18	127.78	122.60
1	C	184	ASP	CA-C-N	5.18	130.94	122.81
1	C	184	ASP	C-N-CA	5.18	130.94	122.81
1	C	205	ALA	CA-C-N	5.17	128.88	120.60
1	C	205	ALA	C-N-CA	5.17	128.88	120.60
1	A	276	ARG	CD-NE-CZ	5.17	131.64	124.40
1	D	281	GLY	O-C-N	-5.17	116.42	122.31
1	D	201	SER	N-CA-C	5.16	119.15	113.21
1	D	186	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	281	GLY	CA-C-N	5.15	131.51	121.63
1	D	281	GLY	C-N-CA	5.15	131.51	121.63
1	C	313	GLN	CA-C-N	5.14	127.13	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	313	GLN	C-N-CA	5.14	127.13	120.44
1	B	188	ARG	CD-NE-CZ	5.14	131.59	124.40
1	A	204	VAL	CA-C-O	-5.13	114.92	120.71
1	B	60	LYS	O-C-N	-5.11	116.25	122.22
1	A	260	ALA	O-C-N	-5.09	116.73	122.12
1	C	316	ASP	N-CA-C	-5.05	105.69	111.14
1	D	276	ARG	CA-CB-CG	-5.05	104.00	114.10

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	2217	0	2187	27	0
1	B	2184	0	2139	34	0
1	C	2207	0	2167	22	0
1	D	2205	0	2162	23	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	44	0	26	0	0
3	B	44	0	26	0	0
3	C	44	0	26	2	0
3	D	44	0	26	3	0
4	A	87	0	0	1	0
4	B	70	0	0	0	0
4	C	79	0	0	1	0
4	D	73	0	0	2	0
All	All	9318	0	8759	94	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 (94) 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:62:ASP:OD1	1:D:245:LYS:HE3	1.85	0.74
1:D:282:MET:HE2	1:D:318:ILE:HG22	1.69	0.74
1:B:141:ILE:HD11	1:B:256:ALA:HB2	1.69	0.74
1:D:123:GLN:HA	1:D:155:VAL:HG11	1.71	0.72
1:C:282:MET:HE2	1:C:318:ILE:HG22	1.72	0.72
1:C:123:GLN:HA	1:C:155:VAL:HG11	1.72	0.71
1:A:282:MET:HE2	1:A:318:ILE:HG22	1.76	0.67
1:C:280:MET:HE1	1:C:312:LEU:HD21	1.76	0.67
1:B:150:ALA:HB2	1:B:282:MET:HE1	1.78	0.65
1:A:65:ASP:OD2	1:C:245:LYS:NZ	2.30	0.64
1:A:151:LEU:HD22	1:A:329:LEU:HD11	1.78	0.64
1:B:65:ASP:OD2	1:D:245:LYS:NZ	2.33	0.62
1:C:197:GLU:OE1	1:C:200:ASN:HB3	2.01	0.60
1:B:197:GLU:HB2	1:B:318:ILE:HD11	1.85	0.59
1:B:280:MET:O	1:B:315:ARG:HD2	2.04	0.58
1:D:144:PRO:HG2	1:D:147:VAL:HB	1.84	0.58
1:B:282:MET:HE2	1:B:318:ILE:HG22	1.86	0.57
1:A:141:ILE:HD11	1:A:256:ALA:HB2	1.86	0.57
1:A:112:PHE:HZ	1:A:321:ARG:HG3	1.69	0.57
1:C:96:THR:O	3:C:330:NAD:H4D	2.03	0.57
1:A:150:ALA:CB	1:A:282:MET:HE1	2.35	0.57
1:B:191:SER:OG	1:B:210:ARG:HG3	2.05	0.57
1:C:282:MET:CE	1:C:318:ILE:HG22	2.35	0.56
1:B:150:ALA:CB	1:B:282:MET:HE1	2.35	0.56
1:D:248:THR:HB	4:D:368:HOH:O	2.06	0.55
1:B:52:ILE:HG12	1:B:82:ASN:HA	1.89	0.54
1:B:322:PHE:O	1:B:325:ILE:HG22	2.08	0.54
1:B:143:ASN:HA	1:B:145:VAL:N	2.22	0.53
1:B:191:SER:O	1:B:209:VAL:HA	2.08	0.53
1:B:185:LEU:HD21	1:B:212:MET:HE2	1.91	0.53
1:B:288:ALA:HB1	1:B:295:VAL:HG13	1.91	0.53
1:B:63:GLN:O	1:B:67:GLN:HG3	2.10	0.52
1:B:197:GLU:O	1:B:202:GLN:HB3	2.10	0.52
1:A:188:ARG:HD3	4:C:343:HOH:O	2.10	0.51
1:A:191:SER:O	1:A:209:VAL:HA	2.10	0.51
1:B:197:GLU:HB3	1:B:201:SER:OG	2.10	0.51
1:A:150:ALA:HB2	1:A:282:MET:HE1	1.94	0.50
1:B:267:ALA:O	1:B:268:HIS:HB2	2.13	0.49
1:A:265:ALA:HA	1:D:47:ASP:HB3	1.93	0.49
1:A:317:TYR:O	1:A:321:ARG:HG2	2.13	0.49
1:D:291:GLY:HA3	1:D:296:LEU:HD11	1.93	0.49
1:D:63:GLN:O	1:D:67:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ASP:OD2	3:D:330:NAD:H1B	2.13	0.48
1:A:143:ASN:HA	1:A:145:VAL:N	2.28	0.48
1:A:304:THR:O	1:A:308:GLN:HG3	2.14	0.47
1:A:172:THR:O	1:A:176:GLN:HG3	2.13	0.47
1:A:291:GLY:HA3	1:A:296:LEU:HD11	1.96	0.47
4:A:361:HOH:O	1:C:245:LYS:HE3	2.15	0.46
1:B:151:LEU:O	1:B:155:VAL:HG23	2.16	0.46
1:C:302:ASP:CG	1:D:214:GLN:HE22	2.24	0.45
1:C:58:LYS:NZ	1:C:62:ASP:OD2	2.46	0.45
1:C:191:SER:O	1:C:209:VAL:HA	2.16	0.45
1:C:280:MET:HE1	1:C:312:LEU:CD2	2.46	0.45
1:A:129:LEU:HD21	1:A:138:LEU:HD13	1.99	0.45
1:B:72:ASN:OD1	1:D:258:ARG:NH1	2.42	0.45
1:C:267:ALA:O	1:D:186:ASP:HB2	2.17	0.45
1:B:53:ASP:HB3	1:B:59:VAL:HB	1.99	0.45
1:B:232:GLU:HG3	1:B:236:LYS:NZ	2.32	0.45
1:A:63:GLN:O	1:A:67:GLN:HG3	2.17	0.45
1:A:267:ALA:O	1:B:186:ASP:HB2	2.17	0.45
1:B:282:MET:HE3	1:B:283:TYR:H	1.82	0.44
1:B:206:TRP:HE3	1:B:216:ILE:HG21	1.81	0.44
1:A:55:ASN:ND2	1:A:58:LYS:HB2	2.32	0.44
1:A:212:MET:HE2	1:B:289:ILE:HG13	1.99	0.44
1:B:43:GLN:HB2	1:B:45:VAL:HG23	1.99	0.44
1:A:320:GLN:O	1:A:324:GLU:HG3	2.17	0.43
1:D:96:THR:O	3:D:330:NAD:H4D	2.18	0.43
1:D:248:THR:CB	4:D:368:HOH:O	2.65	0.43
1:B:304:THR:O	1:B:308:GLN:HG3	2.18	0.43
1:C:214:GLN:CB	1:C:219:LEU:HD21	2.49	0.43
1:D:198:HIS:NE2	3:D:330:NAD:O7N	2.51	0.43
1:D:272:VAL:HA	1:D:287:PRO:HA	2.01	0.42
1:A:185:LEU:HD21	1:A:212:MET:HE3	2.01	0.42
1:A:112:PHE:CZ	1:A:321:ARG:HG3	2.51	0.42
1:C:170:LEU:O	1:C:174:ARG:HG3	2.20	0.42
1:B:97:LEU:C	1:B:97:LEU:HD12	2.44	0.42
1:A:321:ARG:HA	1:A:321:ARG:HH11	1.85	0.41
1:D:111:ARG:NH2	1:D:324:GLU:OE1	2.53	0.41
1:B:250:TYR:OH	1:D:34:ALA:HB1	2.20	0.41
1:C:97:LEU:HD21	3:C:330:NAD:C4A	2.50	0.41
1:B:236:LYS:HA	1:B:239:PHE:CD2	2.56	0.41
1:C:24:ILE:HD12	1:C:46:ALA:HB2	2.01	0.41
1:C:97:LEU:CD1	1:C:125:VAL:HG21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:MET:HE3	1:B:283:TYR:HB2	2.02	0.41
1:A:159:PRO:HB2	1:A:161:HIS:CD2	2.56	0.41
1:A:161:HIS:O	1:A:294:GLY:HA3	2.21	0.41
1:B:185:LEU:CD2	1:B:212:MET:HE2	2.51	0.41
1:C:289:ILE:HG13	1:D:212:MET:HE2	2.03	0.41
1:A:267:ALA:O	1:A:268:HIS:HB2	2.20	0.40
1:D:214:GLN:HA	1:D:215:PRO:HD3	1.81	0.40
1:C:43:GLN:HB2	1:C:45:VAL:HG23	2.03	0.40
1:C:293:ASP:HB2	1:C:296:LEU:HD21	2.04	0.40
1:D:241:VAL:CG1	1:D:248:THR:HG22	2.51	0.40
1:C:212:MET:HE2	1:D:289:ILE:HG13	2.04	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	292/309 (94%)	282 (97%)	9 (3%)	1 (0%)	36	42
1	B	289/309 (94%)	280 (97%)	8 (3%)	1 (0%)	36	42
1	C	291/309 (94%)	285 (98%)	5 (2%)	1 (0%)	36	42
1	D	291/309 (94%)	284 (98%)	7 (2%)	0	100	100
All	All	1163/1236 (94%)	1131 (97%)	29 (2%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	200	ASN
1	A	200	ASN
1	C	201	SER

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	229/243 (94%)	223 (97%)	6 (3%)	40	55
1	B	224/243 (92%)	221 (99%)	3 (1%)	61	76
1	C	226/243 (93%)	220 (97%)	6 (3%)	39	53
1	D	225/243 (93%)	220 (98%)	5 (2%)	45	61
All	All	904/972 (93%)	884 (98%)	20 (2%)	45	61

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	60	LYS
1	A	74	GLU
1	A	112	PHE
1	A	236	LYS
1	A	305	THR
1	B	112	PHE
1	B	216	ILE
1	B	275	ASN
1	C	111	ARG
1	C	164	ILE
1	C	211	VAL
1	C	248	THR
1	C	275	ASN
1	C	279	ASP
1	D	110	ASP
1	D	211	VAL
1	D	275	ASN
1	D	314	SER
1	D	315	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	99	ASN
1	B	43	GLN
1	B	243	ASN
1	B	275	ASN
1	C	320	GLN
1	D	123	GLN
1	D	194	ASN
1	D	202	GLN
1	D	214	GLN
1	D	275	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
3	NAD	C	330	-	46,48,48	1.74	10 (21%)	64,73,73	2.48	23 (35%)
2	SO4	D	331	-	4,4,4	0.73	0	6,6,6	0.19	0
3	NAD	D	330	-	46,48,48	2.06	9 (19%)	64,73,73	2.48	18 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	331	-	4,4,4	0.67	0	6,6,6	0.27	0
2	SO4	B	331	-	4,4,4	0.74	0	6,6,6	0.26	0
3	NAD	A	330	-	46,48,48	1.58	7 (15%)	64,73,73	2.05	17 (26%)
2	SO4	A	331	-	4,4,4	0.66	0	6,6,6	0.34	0
3	NAD	B	330	-	46,48,48	1.84	12 (26%)	64,73,73	2.17	17 (26%)

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
3	NAD	C	330	-	-	4/30/62/62	0/5/5/5
3	NAD	A	330	-	-	4/30/62/62	0/5/5/5
3	NAD	B	330	-	-	3/30/62/62	0/5/5/5
3	NAD	D	330	-	-	5/30/62/62	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	330	NAD	PN-O3	7.49	1.67	1.59
3	D	330	NAD	C2N-N1N	5.25	1.40	1.35
3	A	330	NAD	C3N-C7N	5.10	1.58	1.50
3	B	330	NAD	PA-O3	-5.02	1.54	1.59
3	C	330	NAD	C3N-C7N	4.80	1.57	1.50
3	D	330	NAD	C3N-C7N	4.43	1.57	1.50
3	C	330	NAD	PA-O3	-4.37	1.54	1.59
3	B	330	NAD	C3N-C7N	4.34	1.57	1.50
3	B	330	NAD	O4D-C4D	4.01	1.53	1.45
3	D	330	NAD	O4D-C4D	3.98	1.53	1.45
3	A	330	NAD	O4D-C4D	3.79	1.53	1.45
3	C	330	NAD	PN-O3	3.57	1.63	1.59
3	B	330	NAD	C2N-N1N	3.49	1.38	1.35
3	A	330	NAD	C2N-N1N	3.49	1.38	1.35
3	C	330	NAD	C2N-N1N	3.37	1.38	1.35
3	B	330	NAD	PN-O3	3.26	1.63	1.59
3	C	330	NAD	O4D-C4D	3.14	1.52	1.45
3	D	330	NAD	C2A-N3A	3.06	1.39	1.33
3	C	330	NAD	C2A-N3A	2.71	1.38	1.33
3	B	330	NAD	C4A-N3A	2.66	1.39	1.34
3	D	330	NAD	C2N-C3N	-2.59	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	330	NAD	C2A-N3A	2.58	1.38	1.33
3	B	330	NAD	C5N-C4N	2.57	1.43	1.38
3	C	330	NAD	C5D-C4D	-2.53	1.43	1.51
3	D	330	NAD	C5D-C4D	-2.45	1.44	1.51
3	B	330	NAD	C4A-N9A	2.41	1.42	1.37
3	D	330	NAD	PA-O3	-2.38	1.56	1.59
3	A	330	NAD	C7N-N7N	2.37	1.37	1.33
3	B	330	NAD	C5A-N7A	-2.36	1.34	1.39
3	A	330	NAD	O2B-C2B	-2.28	1.37	1.43
3	C	330	NAD	C5N-C4N	2.28	1.42	1.38
3	A	330	NAD	C4A-N3A	2.21	1.38	1.34
3	B	330	NAD	O2B-C2B	-2.17	1.37	1.43
3	D	330	NAD	O2B-C2B	-2.12	1.37	1.43
3	C	330	NAD	O2B-C2B	-2.07	1.37	1.43
3	B	330	NAD	C5A-C6A	2.07	1.46	1.41
3	A	330	NAD	C5N-C4N	2.05	1.42	1.38
3	C	330	NAD	C5A-N7A	-2.01	1.35	1.39

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	330	NAD	C2N-C3N-C4N	8.49	128.14	118.26
3	D	330	NAD	C2N-C3N-C4N	8.46	128.10	118.26
3	C	330	NAD	C5N-C4N-C3N	-8.07	112.44	120.36
3	B	330	NAD	C2N-C3N-C4N	7.71	127.23	118.26
3	B	330	NAD	C5N-C4N-C3N	-7.36	113.13	120.36
3	D	330	NAD	O7N-C7N-C3N	-7.35	110.61	119.60
3	A	330	NAD	C2N-C3N-C4N	6.85	126.22	118.26
3	D	330	NAD	C5N-C4N-C3N	-6.82	113.67	120.36
3	A	330	NAD	C5N-C4N-C3N	-5.90	114.56	120.36
3	D	330	NAD	O7N-C7N-N7N	5.30	130.27	122.62
3	C	330	NAD	C2A-N1A-C6A	5.01	126.96	118.73
3	C	330	NAD	C6N-N1N-C2N	4.96	126.10	121.88
3	D	330	NAD	C6N-N1N-C2N	4.87	126.02	121.88
3	B	330	NAD	O7N-C7N-C3N	-4.54	114.05	119.60
3	C	330	NAD	O7N-C7N-C3N	-4.31	114.33	119.60
3	A	330	NAD	C2A-N1A-C6A	4.21	125.64	118.73
3	C	330	NAD	N3A-C2A-N1A	-4.13	122.33	128.58
3	C	330	NAD	O7N-C7N-N7N	4.12	128.57	122.62
3	B	330	NAD	C2A-N1A-C6A	4.05	125.39	118.73
3	A	330	NAD	C4D-O4D-C1D	-4.05	106.22	109.92
3	D	330	NAD	C2A-N1A-C6A	3.99	125.28	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	330	NAD	C6N-N1N-C2N	3.96	125.24	121.88
3	D	330	NAD	N3A-C2A-N1A	-3.67	123.03	128.58
3	A	330	NAD	C4A-N9A-C8A	-3.64	101.92	105.74
3	B	330	NAD	C2B-C3B-C4B	3.43	109.24	102.61
3	D	330	NAD	C2N-N1N-C1D	-3.42	111.58	119.13
3	C	330	NAD	C4A-N9A-C8A	-3.38	102.19	105.74
3	D	330	NAD	C5A-C4A-N3A	-3.35	122.10	126.72
3	D	330	NAD	C4D-O4D-C1D	-3.24	106.96	109.92
3	B	330	NAD	N3A-C2A-N1A	-3.12	123.86	128.58
3	B	330	NAD	C4A-N9A-C8A	-3.04	102.55	105.74
3	B	330	NAD	O7N-C7N-N7N	3.02	126.99	122.62
3	A	330	NAD	N3A-C2A-N1A	-2.98	124.08	128.58
3	C	330	NAD	O3D-C3D-C4D	-2.94	102.64	111.08
3	C	330	NAD	O2N-PN-O1N	2.87	125.81	112.44
3	B	330	NAD	C6N-N1N-C2N	2.84	124.29	121.88
3	C	330	NAD	C6A-C5A-C4A	2.81	121.01	117.18
3	C	330	NAD	C2N-N1N-C1D	-2.80	112.96	119.13
3	C	330	NAD	C6N-C5N-C4N	2.79	123.47	119.45
3	B	330	NAD	C1B-N9A-C8A	2.72	133.14	127.09
3	C	330	NAD	PA-O5B-C5B	2.71	136.88	121.35
3	C	330	NAD	C2B-C3B-C4B	2.70	107.82	102.61
3	C	330	NAD	C5A-C4A-N3A	-2.70	123.00	126.72
3	D	330	NAD	C4A-N9A-C8A	-2.68	102.93	105.74
3	D	330	NAD	N3A-C4A-N9A	2.57	131.53	127.17
3	B	330	NAD	C4D-O4D-C1D	-2.55	107.59	109.92
3	D	330	NAD	O5D-C5D-C4D	2.53	117.59	108.99
3	C	330	NAD	C5A-C6A-N1A	-2.48	111.21	117.51
3	A	330	NAD	C1B-N9A-C8A	2.47	132.57	127.09
3	A	330	NAD	C5A-C4A-N3A	-2.46	123.33	126.72
3	A	330	NAD	C2N-C3N-C7N	-2.44	112.41	119.46
3	D	330	NAD	C4N-C3N-C7N	-2.44	114.41	121.06
3	A	330	NAD	C6A-C5A-C4A	2.44	120.50	117.18
3	A	330	NAD	C2N-N1N-C1D	-2.43	113.77	119.13
3	D	330	NAD	C6A-C5A-C4A	2.42	120.49	117.18
3	C	330	NAD	O2A-PA-O3	2.41	113.78	107.27
3	D	330	NAD	C2B-C3B-C4B	2.37	107.18	102.61
3	C	330	NAD	C5D-C4D-C3D	2.36	123.71	115.21
3	D	330	NAD	O2N-PN-O1N	2.35	123.36	112.44
3	D	330	NAD	N6A-C6A-N1A	2.34	123.60	118.38
3	C	330	NAD	N6A-C6A-N1A	2.31	123.52	118.38
3	C	330	NAD	C5N-C6N-N1N	-2.31	117.24	120.38
3	C	330	NAD	O2B-C2B-C3B	2.30	119.18	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	330	NAD	O2B-C2B-C1B	2.30	118.01	110.10
3	C	330	NAD	C2N-C3N-C7N	-2.29	112.86	119.46
3	B	330	NAD	C6A-C5A-C4A	2.23	120.22	117.18
3	B	330	NAD	O3D-C3D-C4D	-2.21	104.74	111.08
3	B	330	NAD	C2N-N1N-C1D	-2.18	114.32	119.13
3	A	330	NAD	O4B-C4B-C5B	-2.17	102.39	109.33
3	A	330	NAD	C5N-C6N-N1N	-2.13	117.47	120.38
3	A	330	NAD	O3D-C3D-C4D	-2.13	104.97	111.08
3	A	330	NAD	C2B-C1B-N9A	-2.12	108.04	113.30
3	A	330	NAD	C3B-C2B-C1B	-2.12	97.46	101.46
3	B	330	NAD	C6N-C5N-C4N	2.10	122.48	119.45
3	B	330	NAD	C5A-C4A-N3A	-2.06	123.88	126.72

There are no chirality outliers.

All (16) torsion outliers are listed below:

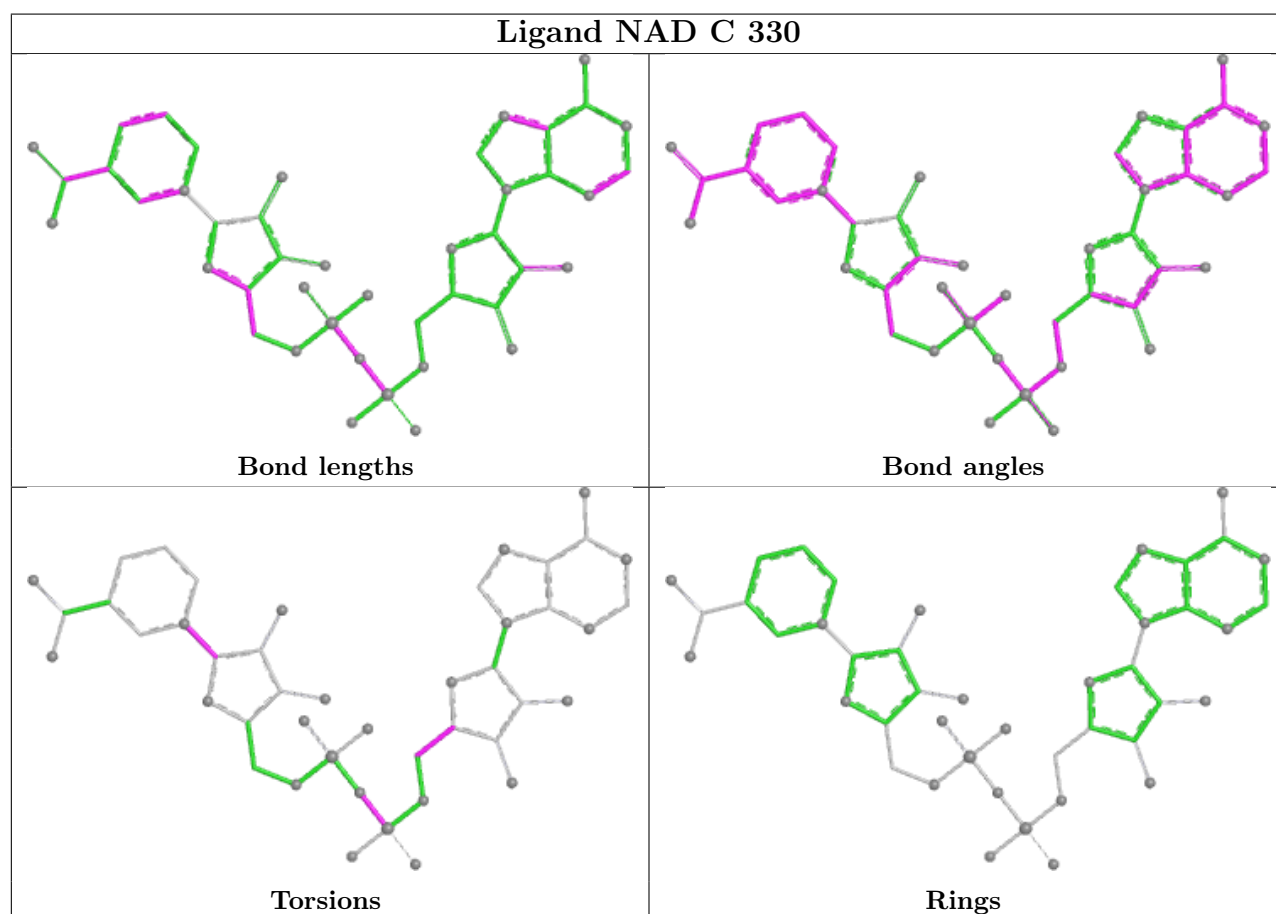
Mol	Chain	Res	Type	Atoms
3	A	330	NAD	O4D-C1D-N1N-C2N
3	A	330	NAD	O4D-C1D-N1N-C6N
3	A	330	NAD	C2D-C1D-N1N-C2N
3	B	330	NAD	O4D-C1D-N1N-C2N
3	B	330	NAD	O4D-C1D-N1N-C6N
3	C	330	NAD	O4D-C1D-N1N-C6N
3	D	330	NAD	O4D-C1D-N1N-C6N
3	D	330	NAD	PN-O3-PA-O1A
3	D	330	NAD	PN-O3-PA-O2A
3	A	330	NAD	C2D-C1D-N1N-C6N
3	C	330	NAD	O4D-C1D-N1N-C2N
3	D	330	NAD	O4D-C1D-N1N-C2N
3	C	330	NAD	PN-O3-PA-O1A
3	D	330	NAD	O4B-C4B-C5B-O5B
3	C	330	NAD	O4B-C4B-C5B-O5B
3	B	330	NAD	O4B-C4B-C5B-O5B

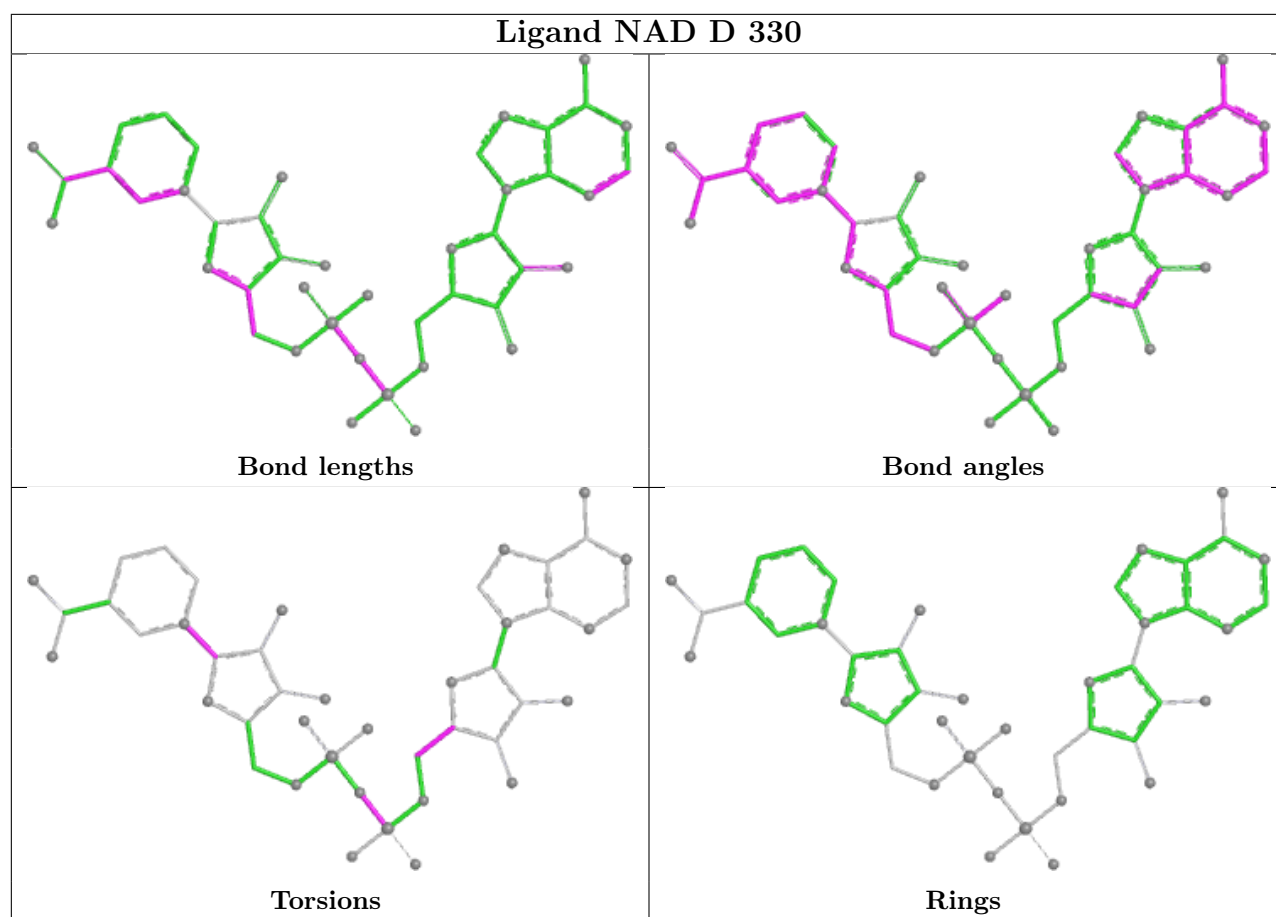
There are no ring outliers.

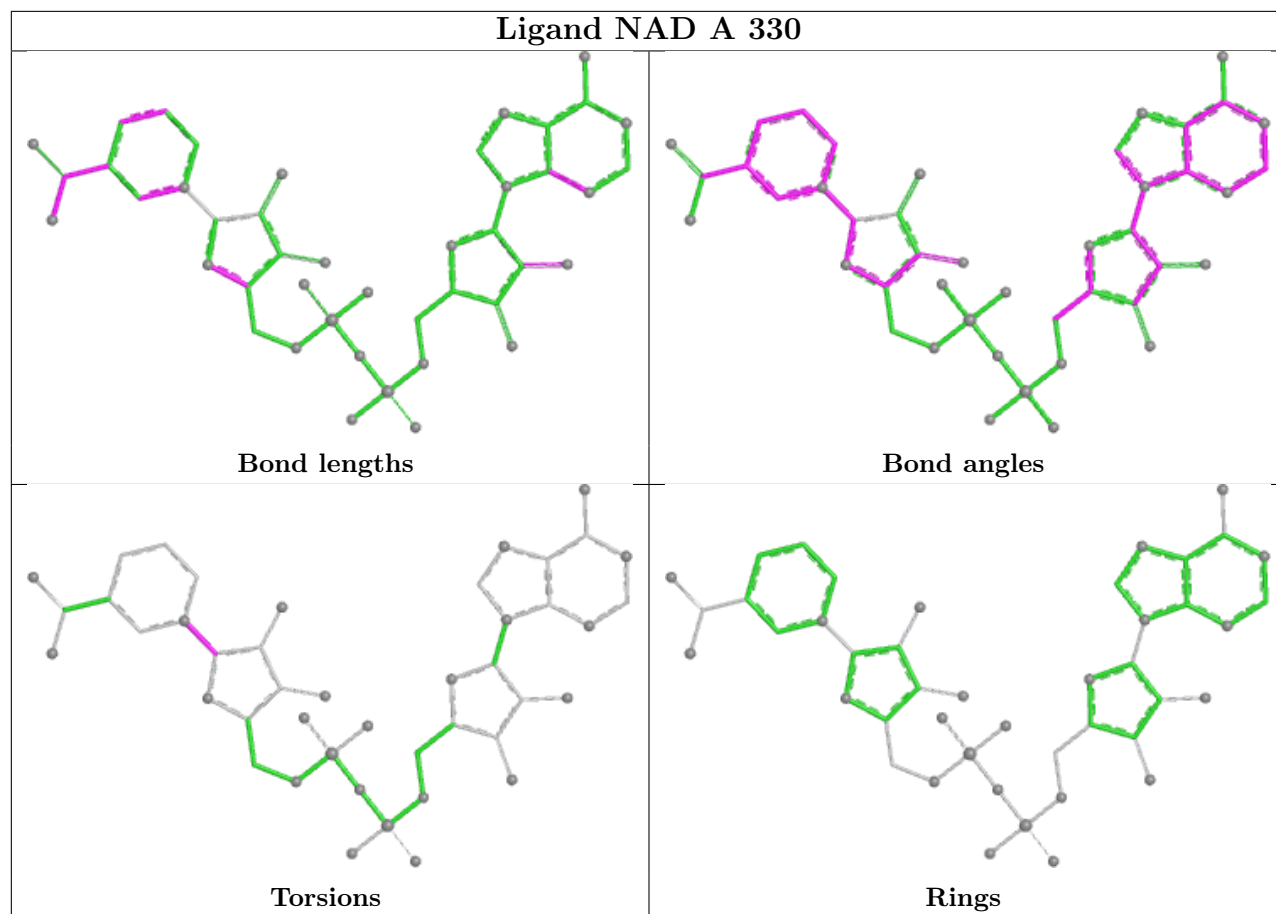
2 monomers are involved in 5 short contacts:

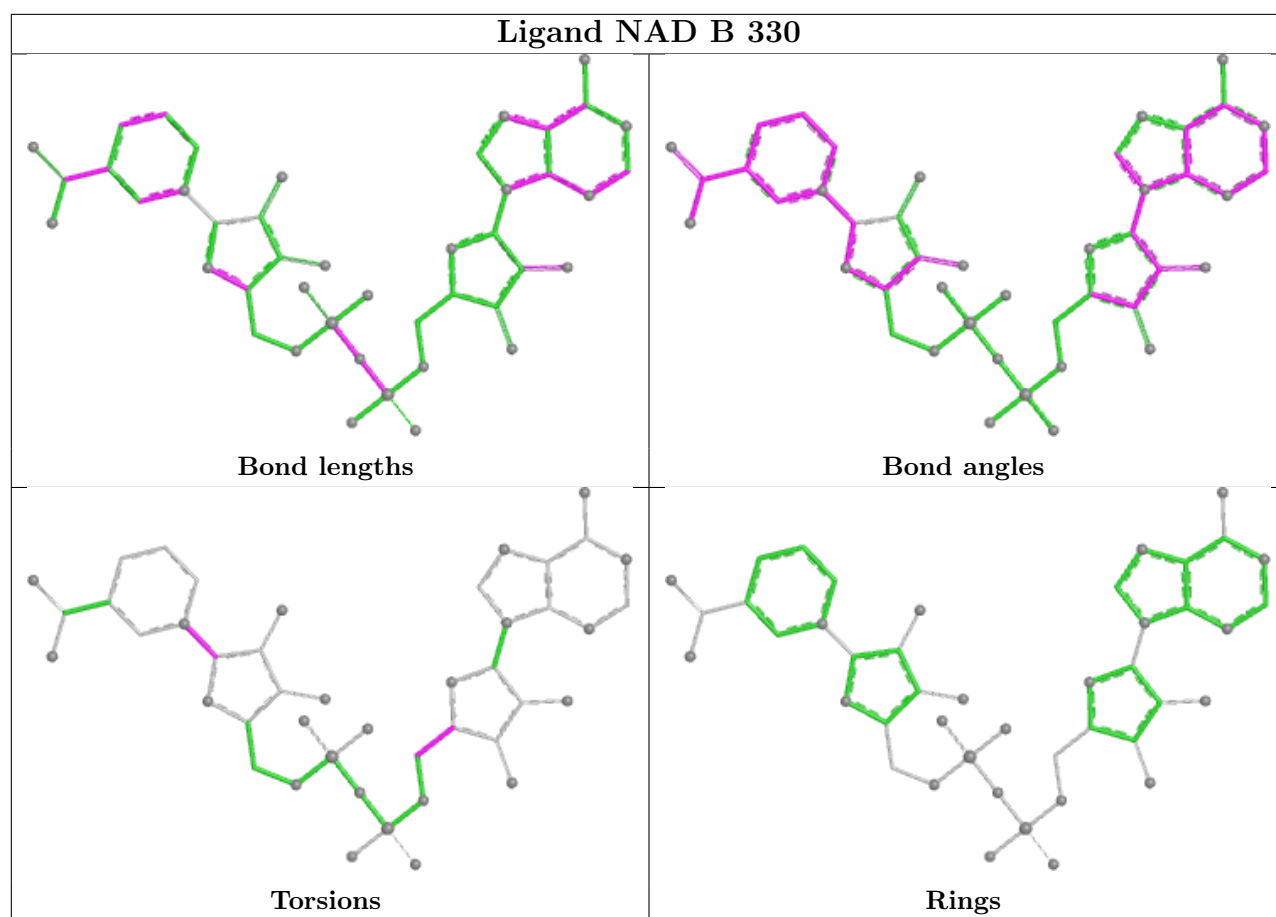
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	330	NAD	2	0
3	D	330	NAD	3	0

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

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	297/309 (96%)	-0.53	7 (2%) 59 56	4, 20, 49, 63	1 (0%)
1	B	294/309 (95%)	-0.20	2 (0%) 84 82	13, 29, 57, 79	1 (0%)
1	C	297/309 (96%)	-0.44	3 (1%) 79 77	11, 21, 46, 65	0
1	D	297/309 (96%)	-0.36	6 (2%) 65 62	10, 22, 49, 64	0
All	All	1185/1236 (95%)	-0.38	18 (1%) 72 69	4, 23, 50, 79	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	109	GLY	3.0
1	C	317	TYR	2.7
1	A	327	ASP	2.6
1	B	326	VAL	2.6
1	D	114	GLU	2.5
1	A	112	PHE	2.3
1	C	306	ASP	2.3
1	A	113	ALA	2.2
1	D	305	THR	2.2
1	D	239	PHE	2.2
1	D	317	TYR	2.2
1	A	306	ASP	2.2
1	D	243	ASN	2.1
1	D	229	ALA	2.1
1	A	228	ALA	2.0
1	A	325	ILE	2.0
1	B	302	ASP	2.0
1	A	321	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

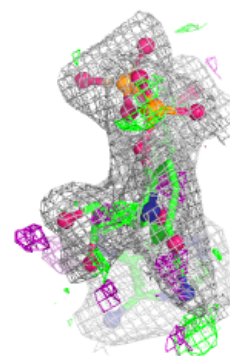
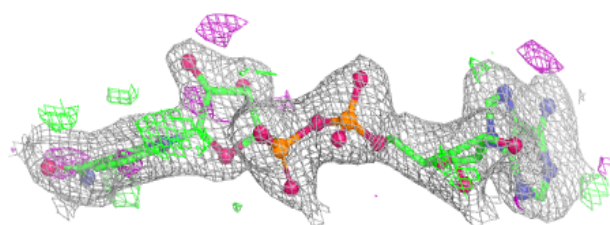
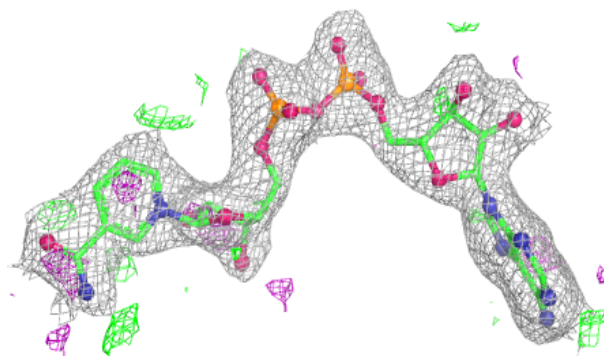
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	331	5/5	0.84	0.12	82,82,82,82	0
2	SO4	D	331	5/5	0.84	0.14	86,86,86,86	0
2	SO4	C	331	5/5	0.88	0.14	78,78,78,78	0
2	SO4	B	331	5/5	0.94	0.07	70,70,70,70	0
3	NAD	D	330	44/44	0.94	0.08	35,35,35,35	0
3	NAD	C	330	44/44	0.95	0.07	32,32,32,32	0
3	NAD	B	330	44/44	0.95	0.08	33,33,33,33	0
3	NAD	A	330	44/44	0.98	0.04	14,14,14,14	0

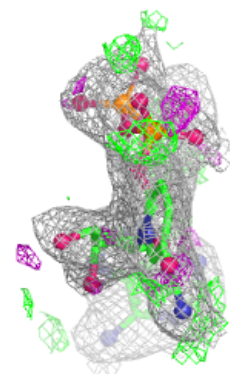
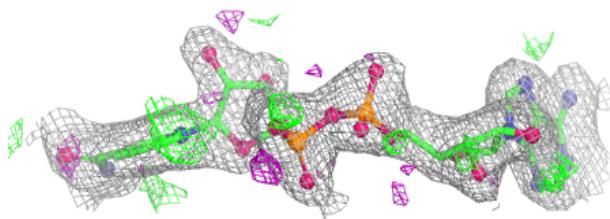
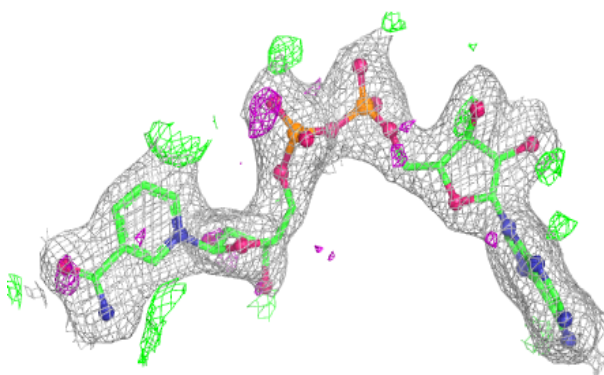
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 330:

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

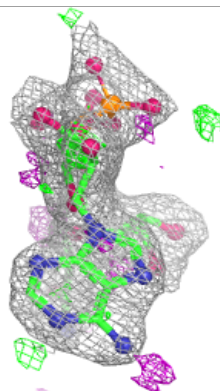
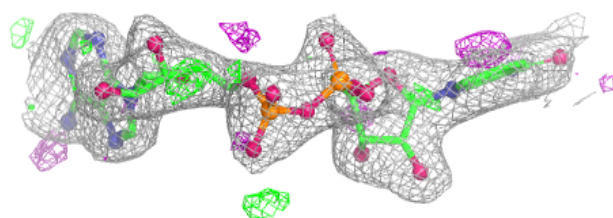
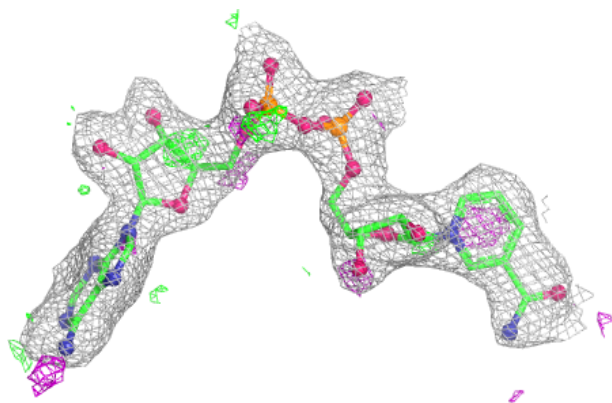
**Electron density around NAD C 330:**

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

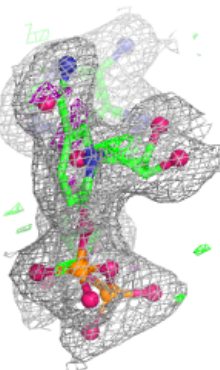
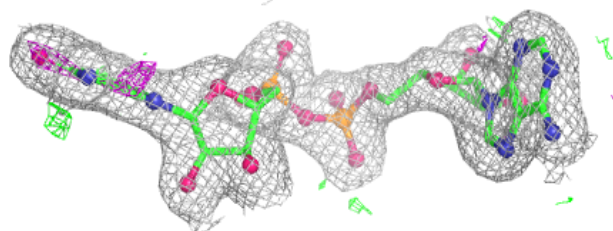
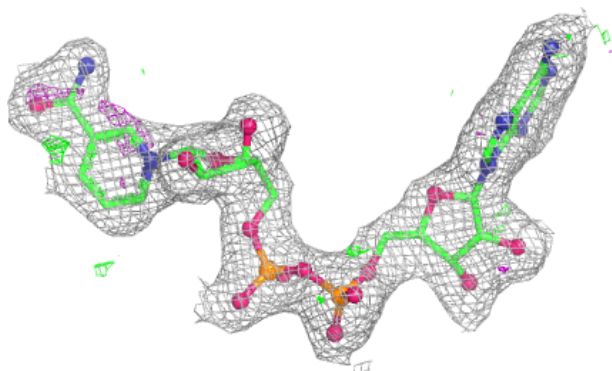


Electron density around NAD B 330:

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

**Electron density around NAD A 330:**

$2mF_o-DF_c$ (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.