



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:12 PM UTC

PDB ID : 5KLO / pdb_00005klo
Title : Crystal structure of thioacyl intermediate in 2-aminomuconate 6-semialdehyde dehydrogenase N169A
Authors : Yang, Y.; Davis, I.; Ha, U.; Wang, Y.; Shin, I.; Liu, A.
Deposited on : 2016-06-24
Resolution : 1.79 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

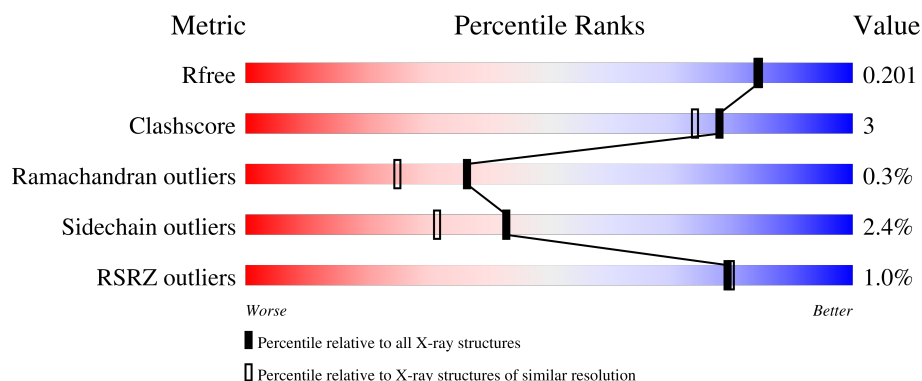
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	520	% 86% 7% 7%
1	B	520	% 86% 6% 7%
1	C	520	% 86% 7% 7%
1	D	520	% 87% 6% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2VS	B	601	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16368 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 2-aminomuconate 6-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3675	2325	637	701	12			
1	B	483	Total	C	N	O	S	0	0	0
			3668	2320	636	700	12			
1	C	483	Total	C	N	O	S	0	0	0
			3668	2320	636	700	12			
1	D	483	Total	C	N	O	S	0	0	0
			3668	2320	636	700	12			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q83V33
A	-18	GLY	-	expression tag	UNP Q83V33
A	-17	SER	-	expression tag	UNP Q83V33
A	-16	SER	-	expression tag	UNP Q83V33
A	-15	HIS	-	expression tag	UNP Q83V33
A	-14	HIS	-	expression tag	UNP Q83V33
A	-13	HIS	-	expression tag	UNP Q83V33
A	-12	HIS	-	expression tag	UNP Q83V33
A	-11	HIS	-	expression tag	UNP Q83V33
A	-10	HIS	-	expression tag	UNP Q83V33
A	-9	SER	-	expression tag	UNP Q83V33
A	-8	SER	-	expression tag	UNP Q83V33
A	-7	GLY	-	expression tag	UNP Q83V33
A	-6	LEU	-	expression tag	UNP Q83V33
A	-5	VAL	-	expression tag	UNP Q83V33
A	-4	PRO	-	expression tag	UNP Q83V33
A	-3	ARG	-	expression tag	UNP Q83V33
A	-2	GLY	-	expression tag	UNP Q83V33
A	-1	SER	-	expression tag	UNP Q83V33
A	0	HIS	-	expression tag	UNP Q83V33
A	169	ALA	ASN	engineered mutation	UNP Q83V33

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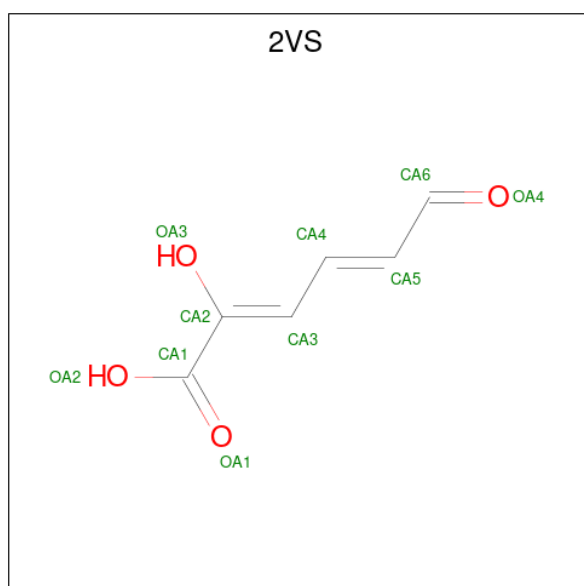
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP Q83V33
B	-18	GLY	-	expression tag	UNP Q83V33
B	-17	SER	-	expression tag	UNP Q83V33
B	-16	SER	-	expression tag	UNP Q83V33
B	-15	HIS	-	expression tag	UNP Q83V33
B	-14	HIS	-	expression tag	UNP Q83V33
B	-13	HIS	-	expression tag	UNP Q83V33
B	-12	HIS	-	expression tag	UNP Q83V33
B	-11	HIS	-	expression tag	UNP Q83V33
B	-10	HIS	-	expression tag	UNP Q83V33
B	-9	SER	-	expression tag	UNP Q83V33
B	-8	SER	-	expression tag	UNP Q83V33
B	-7	GLY	-	expression tag	UNP Q83V33
B	-6	LEU	-	expression tag	UNP Q83V33
B	-5	VAL	-	expression tag	UNP Q83V33
B	-4	PRO	-	expression tag	UNP Q83V33
B	-3	ARG	-	expression tag	UNP Q83V33
B	-2	GLY	-	expression tag	UNP Q83V33
B	-1	SER	-	expression tag	UNP Q83V33
B	0	HIS	-	expression tag	UNP Q83V33
B	169	ALA	ASN	engineered mutation	UNP Q83V33
C	-19	MET	-	initiating methionine	UNP Q83V33
C	-18	GLY	-	expression tag	UNP Q83V33
C	-17	SER	-	expression tag	UNP Q83V33
C	-16	SER	-	expression tag	UNP Q83V33
C	-15	HIS	-	expression tag	UNP Q83V33
C	-14	HIS	-	expression tag	UNP Q83V33
C	-13	HIS	-	expression tag	UNP Q83V33
C	-12	HIS	-	expression tag	UNP Q83V33
C	-11	HIS	-	expression tag	UNP Q83V33
C	-10	HIS	-	expression tag	UNP Q83V33
C	-9	SER	-	expression tag	UNP Q83V33
C	-8	SER	-	expression tag	UNP Q83V33
C	-7	GLY	-	expression tag	UNP Q83V33
C	-6	LEU	-	expression tag	UNP Q83V33
C	-5	VAL	-	expression tag	UNP Q83V33
C	-4	PRO	-	expression tag	UNP Q83V33
C	-3	ARG	-	expression tag	UNP Q83V33
C	-2	GLY	-	expression tag	UNP Q83V33
C	-1	SER	-	expression tag	UNP Q83V33
C	0	HIS	-	expression tag	UNP Q83V33
C	169	ALA	ASN	engineered mutation	UNP Q83V33

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	initiating methionine	UNP Q83V33
D	-18	GLY	-	expression tag	UNP Q83V33
D	-17	SER	-	expression tag	UNP Q83V33
D	-16	SER	-	expression tag	UNP Q83V33
D	-15	HIS	-	expression tag	UNP Q83V33
D	-14	HIS	-	expression tag	UNP Q83V33
D	-13	HIS	-	expression tag	UNP Q83V33
D	-12	HIS	-	expression tag	UNP Q83V33
D	-11	HIS	-	expression tag	UNP Q83V33
D	-10	HIS	-	expression tag	UNP Q83V33
D	-9	SER	-	expression tag	UNP Q83V33
D	-8	SER	-	expression tag	UNP Q83V33
D	-7	GLY	-	expression tag	UNP Q83V33
D	-6	LEU	-	expression tag	UNP Q83V33
D	-5	VAL	-	expression tag	UNP Q83V33
D	-4	PRO	-	expression tag	UNP Q83V33
D	-3	ARG	-	expression tag	UNP Q83V33
D	-2	GLY	-	expression tag	UNP Q83V33
D	-1	SER	-	expression tag	UNP Q83V33
D	0	HIS	-	expression tag	UNP Q83V33
D	169	ALA	ASN	engineered mutation	UNP Q83V33

- Molecule 2 is (2Z,4E)-2-hydroxy-6-oxohexa-2,4-dienoic acid (CCD ID: 2VS) (formula: C₆H₆O₄).

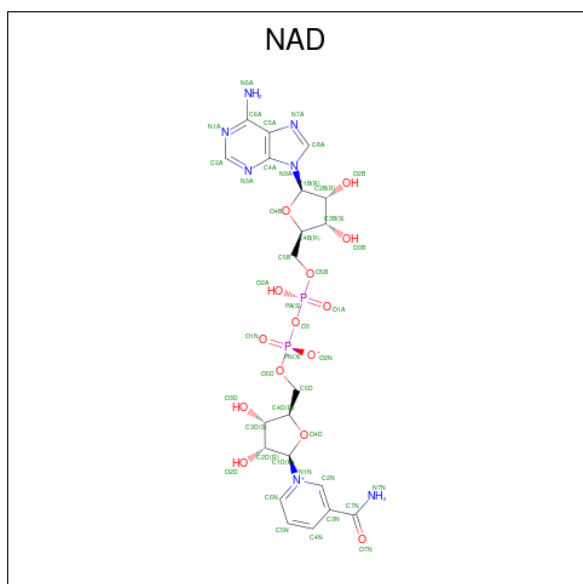


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 10	C 6	O 4	0	0
2	B	1	Total 10	C 6	O 4	0	0
2	C	1	Total 10	C 6	O 4	0	0
2	D	1	Total 10	C 6	O 4	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



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

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

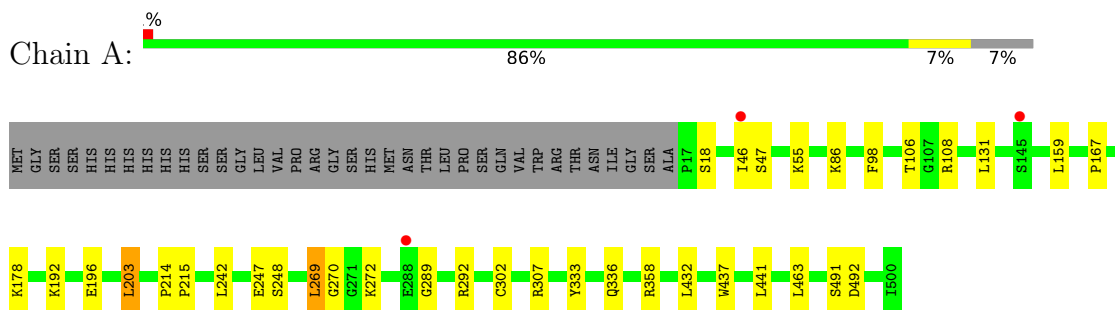
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	410	Total	O	0	0
			410	410		
5	B	364	Total	O	0	0
			364	364		
5	C	370	Total	O	0	0
			370	370		
5	D	325	Total	O	0	0
			325	325		

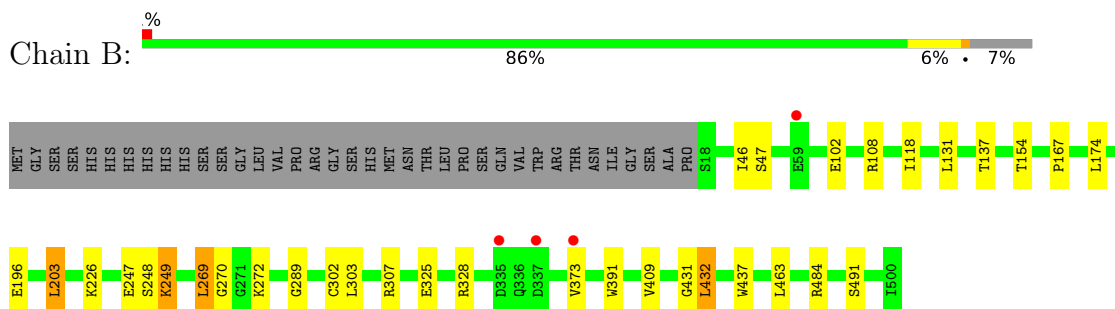
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

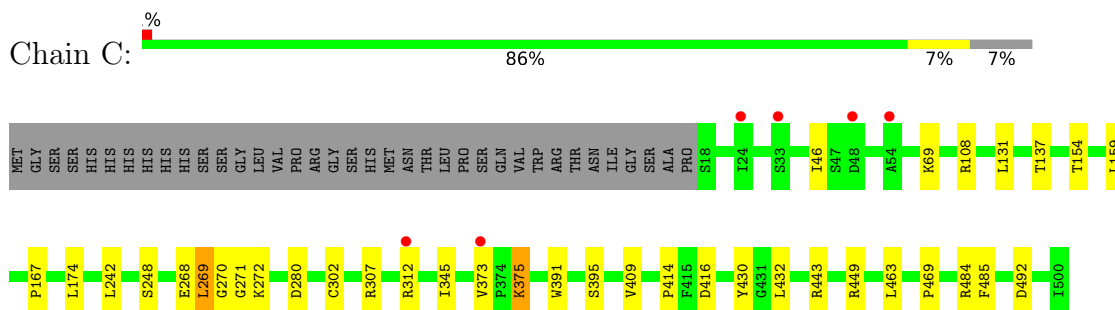
- Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase



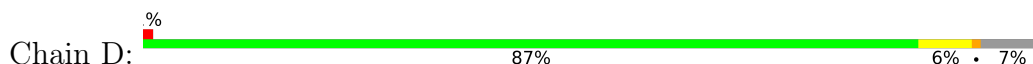
- Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase

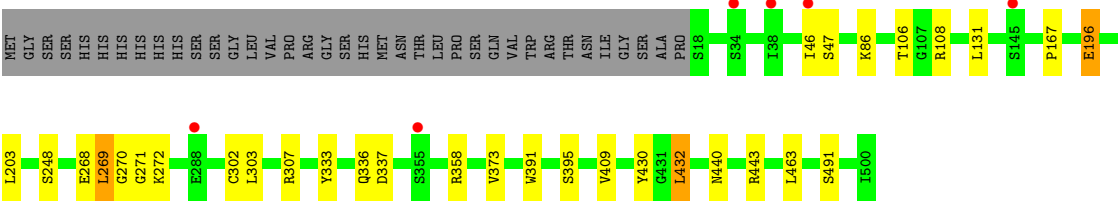


- Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase



- Molecule 1: 2-aminomuconate 6-semialdehyde dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.11Å 141.72Å 171.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.90 – 1.79 34.90 – 1.79	Depositor EDS
% Data completeness (in resolution range)	95.0 (34.90-1.79) 92.7 (34.90-1.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.78Å)	Xtriage
Refinement program	PHENIX phenix.refine: 1.7.3_928	Depositor
R, R_{free}	0.179 , 0.203 0.176 , 0.201	Depositor DCC
R_{free} test set	2000 reflections (1.03%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16368	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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: NAD, 2VS, NA

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	0.47	0/3755	0.77	3/5105 (0.1%)
1	B	0.45	0/3747	0.77	3/5094 (0.1%)
1	C	0.46	0/3747	0.76	1/5094 (0.0%)
1	D	0.42	0/3747	0.76	3/5094 (0.1%)
All	All	0.45	0/14996	0.76	10/20387 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	ILE	CB-CA-C	-7.37	103.08	111.55
1	B	46	ILE	CB-CA-C	-6.35	104.24	111.55
1	A	46	ILE	CB-CA-C	-6.30	104.31	111.55
1	D	46	ILE	CB-CA-C	-5.67	105.11	111.80
1	D	196	GLU	CA-C-N	-5.35	117.39	122.37
1	D	196	GLU	C-N-CA	-5.35	117.39	122.37
1	B	196	GLU	CA-C-N	-5.11	117.23	122.85
1	B	196	GLU	C-N-CA	-5.11	117.23	122.85
1	A	196	GLU	CA-C-N	-5.02	117.33	122.85
1	A	196	GLU	C-N-CA	-5.02	117.33	122.85

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	3675	0	3612	22	0
1	B	3668	0	3603	20	0
1	C	3668	0	3604	19	0
1	D	3668	0	3604	16	0
2	A	10	0	4	3	0
2	B	10	0	3	5	0
2	C	10	0	4	2	0
2	D	10	0	4	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	44	0	26	1	0
4	B	44	0	26	2	0
4	C	44	0	26	2	0
4	D	44	0	26	2	0
5	A	410	0	0	7	0
5	B	364	0	0	3	0
5	C	370	0	0	5	0
5	D	325	0	0	4	0
All	All	16368	0	14542	83	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 3.

All (83) 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:302:CYS:SG	2:B:601:2VS:CA6	2.03	1.46
1:C:302:CYS:SG	2:C:601:2VS:H1	1.55	1.44
1:D:302:CYS:SG	2:D:601:2VS:CA6	2.06	1.43
1:A:302:CYS:SG	2:A:601:2VS:CA6	2.14	1.36
1:C:302:CYS:SG	2:C:601:2VS:CA6	2.15	1.34
1:D:302:CYS:SG	2:D:601:2VS:H1	1.64	1.33
1:A:302:CYS:SG	2:A:601:2VS:H1	1.71	1.30
1:B:302:CYS:SG	2:B:601:2VS:CA5	2.46	1.04
1:C:248:SER:HA	1:C:269:LEU:HG	1.58	0.85
1:D:248:SER:HA	1:D:269:LEU:HG	1.62	0.80
1:B:248:SER:HA	1:B:269:LEU:HG	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:CYS:SG	2:D:601:2VS:CA5	2.71	0.77
4:B:603:NAD:H52N	4:B:603:NAD:H6N	1.67	0.77
1:B:174:LEU:HD21	2:B:601:2VS:H5	1.67	0.77
1:A:248:SER:HA	1:A:269:LEU:HG	1.68	0.76
4:C:603:NAD:H6N	4:C:603:NAD:H52N	1.67	0.76
1:C:272:LYS:HG3	1:C:307:ARG:HD2	1.69	0.74
1:A:292:ARG:NH2	5:A:703:HOH:O	2.19	0.74
1:C:108:ARG:NH2	5:C:702:HOH:O	2.22	0.71
4:D:603:NAD:H6N	4:D:603:NAD:H52N	1.74	0.69
1:A:272:LYS:HG3	1:A:307:ARG:HD2	1.73	0.69
1:A:302:CYS:SG	2:A:601:2VS:CA5	2.80	0.68
1:B:108:ARG:NH2	5:B:704:HOH:O	2.28	0.67
1:D:196:GLU:OE1	5:D:701:HOH:O	2.12	0.66
1:C:312:ARG:HG2	1:C:414:PRO:HB2	1.77	0.65
1:D:272:LYS:HG3	1:D:307:ARG:HD2	1.79	0.65
1:C:375:LYS:NZ	5:C:707:HOH:O	2.30	0.64
1:D:358:ARG:NH2	5:D:705:HOH:O	2.30	0.64
1:B:272:LYS:HG3	1:B:307:ARG:HD2	1.81	0.63
1:C:69:LYS:NZ	5:C:710:HOH:O	2.34	0.61
1:A:270:GLY:HA2	1:A:302:CYS:HB2	1.83	0.59
1:A:358:ARG:NH2	5:A:701:HOH:O	2.15	0.59
1:A:491:SER:O	5:A:702:HOH:O	2.17	0.57
1:B:391:TRP:CH2	1:B:409:VAL:HG21	2.42	0.55
1:A:108:ARG:NH2	5:A:711:HOH:O	2.40	0.54
1:C:280:ASP:OD2	1:C:443:ARG:NH1	2.40	0.54
4:D:603:NAD:H6N	4:D:603:NAD:C5D	2.38	0.53
1:D:491:SER:O	5:D:702:HOH:O	2.19	0.53
4:C:603:NAD:H6N	4:C:603:NAD:C5D	2.39	0.53
1:C:270:GLY:HA2	1:C:302:CYS:HB2	1.91	0.52
1:B:270:GLY:HA2	1:B:302:CYS:HB2	1.92	0.51
4:B:603:NAD:H6N	4:B:603:NAD:C5D	2.39	0.51
1:D:333:TYR:HB2	1:D:336:GLN:HB2	1.93	0.50
1:D:270:GLY:HA2	1:D:302:CYS:HB2	1.93	0.50
1:D:108:ARG:NH2	5:D:713:HOH:O	2.45	0.49
1:D:271:GLY:HA2	1:D:430:TYR:CD1	2.48	0.49
1:C:484:ARG:NH2	5:C:712:HOH:O	2.35	0.48
1:A:86:LYS:HE3	5:A:1046:HOH:O	2.13	0.48
1:A:333:TYR:HB2	1:A:336:GLN:HB2	1.96	0.48
1:B:303:LEU:HD23	1:B:432:LEU:HD13	1.96	0.47
1:C:345:ILE:O	5:C:701:HOH:O	2.20	0.47
1:B:491:SER:O	5:B:702:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD21	2:B:601:2VS:CA4	2.40	0.46
1:A:178:LYS:NZ	5:A:717:HOH:O	2.46	0.46
1:D:391:TRP:CH2	1:D:409:VAL:HG21	2.51	0.45
1:A:86:LYS:HB3	1:A:86:LYS:HE2	1.66	0.45
1:B:247:GLU:HG2	1:B:249:LYS:HG2	1.98	0.45
1:D:303:LEU:HD23	1:D:432:LEU:HD13	1.98	0.45
1:C:159:LEU:HD12	1:C:492:ASP:OD1	2.15	0.45
1:B:289:GLY:HA3	1:B:437:TRP:CZ2	2.52	0.44
1:A:289:GLY:HA3	1:A:437:TRP:CZ2	2.53	0.44
1:B:102:GLU:HG3	1:B:118:ILE:HD11	1.99	0.44
1:C:174:LEU:HD23	1:C:174:LEU:HA	1.88	0.44
1:B:137:THR:HB	1:B:154:THR:OG1	2.19	0.43
1:D:106:THR:HG21	1:D:108:ARG:HH21	1.83	0.43
1:A:98:PHE:CE1	1:A:203:LEU:HB3	2.54	0.43
1:B:302:CYS:SG	2:B:601:2VS:H4	2.50	0.43
1:A:247:GLU:HB2	4:A:603:NAD:O4D	2.18	0.43
1:A:106:THR:HG21	1:A:108:ARG:HH21	1.84	0.42
1:C:137:THR:HB	1:C:154:THR:OG1	2.19	0.42
1:C:391:TRP:CH2	1:C:409:VAL:HG21	2.54	0.42
1:D:440:ASN:HB3	1:D:443:ARG:HB3	2.01	0.42
1:A:55:LYS:HD3	5:A:1003:HOH:O	2.20	0.42
1:C:469:PRO:HB3	1:C:485:PHE:CE1	2.55	0.42
1:C:312:ARG:HG3	1:C:416:ASP:OD1	2.20	0.42
1:A:18:SER:OG	1:A:47:SER:HB3	2.19	0.42
1:B:484:ARG:NH2	5:B:722:HOH:O	2.51	0.42
1:A:159:LEU:HD12	1:A:492:ASP:OD1	2.19	0.41
1:C:271:GLY:HA2	1:C:430:TYR:CD1	2.54	0.41
1:B:203:LEU:HD12	1:B:203:LEU:HA	1.91	0.41
1:B:325:GLU:OE2	1:B:328:ARG:NH1	2.54	0.41
1:B:174:LEU:HD23	1:B:174:LEU:HA	1.91	0.40
1:A:214:PRO:HA	1:A:215:PRO:HD3	1.94	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	482/520 (93%)	469 (97%)	12 (2%)	1 (0%)	43	31
1	B	481/520 (92%)	467 (97%)	12 (2%)	2 (0%)	30	19
1	C	481/520 (92%)	466 (97%)	14 (3%)	1 (0%)	43	31
1	D	481/520 (92%)	467 (97%)	13 (3%)	1 (0%)	43	31
All	All	1925/2080 (92%)	1869 (97%)	51 (3%)	5 (0%)	36	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	167	PRO
1	A	167	PRO
1	D	167	PRO
1	B	431	GLY
1	C	167	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	392/423 (93%)	384 (98%)	8 (2%)	48	38
1	B	391/423 (92%)	382 (98%)	9 (2%)	44	33
1	C	391/423 (92%)	381 (97%)	10 (3%)	40	28
1	D	391/423 (92%)	380 (97%)	11 (3%)	38	26
All	All	1565/1692 (92%)	1527 (98%)	38 (2%)	43	31

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LEU
1	A	192	LYS
1	A	203	LEU

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Mol	Chain	Res	Type
1	A	242	LEU
1	A	269	LEU
1	A	432	LEU
1	A	441	LEU
1	A	463	LEU
1	B	47	SER
1	B	131	LEU
1	B	203	LEU
1	B	226	LYS
1	B	249	LYS
1	B	269	LEU
1	B	373	VAL
1	B	432	LEU
1	B	463	LEU
1	C	131	LEU
1	C	242	LEU
1	C	268	GLU
1	C	269	LEU
1	C	373	VAL
1	C	375	LYS
1	C	395	SER
1	C	432	LEU
1	C	449	ARG
1	C	463	LEU
1	D	47	SER
1	D	86	LYS
1	D	131	LEU
1	D	203	LEU
1	D	268	GLU
1	D	269	LEU
1	D	337	ASP
1	D	373	VAL
1	D	395	SER
1	D	432	LEU
1	D	463	LEU

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

Mol	Chain	Res	Type
1	A	112	GLN
1	B	382	GLN
1	C	27	ASN

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Mol	Chain	Res	Type
1	C	112	GLN
1	C	136	HIS
1	C	235	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAD	D	603	-	46,48,48	1.95	10 (21%)	64,73,73	1.69	12 (18%)
4	NAD	A	603	-	46,48,48	1.93	9 (19%)	64,73,73	1.72	13 (20%)
4	NAD	C	603	-	46,48,48	1.91	10 (21%)	64,73,73	1.71	10 (15%)
2	2VS	C	601	-	9,9,9	3.00	4 (44%)	9,10,10	2.51	4 (44%)
2	2VS	B	601	-	9,9,9	2.95	4 (44%)	9,10,10	2.90	5 (55%)
2	2VS	A	601	-	9,9,9	2.95	3 (33%)	9,10,10	2.44	4 (44%)
4	NAD	B	603	-	46,48,48	1.98	9 (19%)	64,73,73	1.71	12 (18%)
2	2VS	D	601	-	9,9,9	2.95	4 (44%)	9,10,10	2.85	6 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	D	603	-	-	6/30/62/62	0/5/5/5
4	NAD	A	603	-	-	4/30/62/62	0/5/5/5
4	NAD	C	603	-	-	5/30/62/62	0/5/5/5
2	2VS	C	601	-	-	1/9/9/9	-
2	2VS	B	601	-	-	1/9/9/9	-
2	2VS	A	601	-	-	1/9/9/9	-
4	NAD	B	603	-	-	6/30/62/62	0/5/5/5
2	2VS	D	601	-	-	1/9/9/9	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	NAD	O4D-C1D	7.40	1.50	1.40
4	D	603	NAD	O4D-C1D	7.27	1.50	1.40
4	C	603	NAD	O4D-C1D	7.22	1.50	1.40
4	A	603	NAD	O4D-C1D	7.15	1.50	1.40
4	A	603	NAD	C7N-N7N	6.04	1.44	1.33
2	B	601	2VS	OA4-CA6	5.81	1.39	1.22
4	B	603	NAD	C7N-N7N	5.75	1.43	1.33
2	A	601	2VS	OA4-CA6	5.72	1.39	1.22
2	C	601	2VS	OA4-CA6	5.69	1.39	1.22
2	D	601	2VS	OA4-CA6	5.63	1.39	1.22
4	D	603	NAD	C7N-N7N	5.57	1.43	1.33
4	C	603	NAD	C7N-N7N	5.27	1.42	1.33
2	D	601	2VS	CA3-CA2	4.35	1.49	1.39
2	B	601	2VS	CA3-CA2	4.24	1.49	1.39
2	C	601	2VS	CA3-CA2	4.19	1.49	1.39
2	A	601	2VS	OA3-CA2	-4.09	1.23	1.33
2	C	601	2VS	OA3-CA2	-4.07	1.23	1.33
2	D	601	2VS	OA3-CA2	-4.01	1.23	1.33
2	A	601	2VS	CA3-CA2	3.90	1.48	1.39
2	B	601	2VS	OA3-CA2	-3.87	1.23	1.33
4	B	603	NAD	C6A-N6A	3.77	1.43	1.34
4	A	603	NAD	C6A-N6A	3.75	1.43	1.34
4	D	603	NAD	C6A-N6A	3.71	1.43	1.34
4	D	603	NAD	C2B-C3B	-3.56	1.43	1.53
4	C	603	NAD	C6A-N6A	3.48	1.43	1.34
4	B	603	NAD	C2B-C3B	-3.44	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	NAD	C2B-C3B	-3.35	1.44	1.53
4	A	603	NAD	C2B-C3B	-3.31	1.44	1.53
4	B	603	NAD	PA-O3	-3.11	1.56	1.59
4	C	603	NAD	PA-O3	-2.93	1.56	1.59
4	D	603	NAD	PA-O3	-2.78	1.56	1.59
4	D	603	NAD	O4B-C4B	-2.54	1.39	1.45
4	D	603	NAD	C2B-C1B	-2.38	1.46	1.53
4	C	603	NAD	O4B-C4B	-2.34	1.39	1.45
4	A	603	NAD	C2B-C1B	-2.29	1.46	1.53
4	C	603	NAD	O2D-C2D	-2.28	1.37	1.43
4	B	603	NAD	O4B-C4B	-2.27	1.39	1.45
4	C	603	NAD	O5D-C5D	-2.27	1.36	1.44
4	B	603	NAD	C2B-C1B	-2.22	1.46	1.53
4	A	603	NAD	O3D-C3D	-2.21	1.37	1.43
4	A	603	NAD	O4B-C4B	-2.21	1.40	1.45
4	A	603	NAD	PA-O3	-2.16	1.57	1.59
4	B	603	NAD	O3D-C3D	-2.15	1.37	1.43
4	D	603	NAD	O2D-C2D	-2.15	1.37	1.43
4	B	603	NAD	O5D-C5D	-2.06	1.36	1.44
2	D	601	2VS	CA4-CA3	2.06	1.49	1.43
4	D	603	NAD	O5D-C5D	-2.06	1.36	1.44
4	C	603	NAD	C2B-C1B	-2.05	1.47	1.53
2	C	601	2VS	CA4-CA3	2.03	1.49	1.43
2	B	601	2VS	CA4-CA3	2.03	1.49	1.43
4	C	603	NAD	O3D-C3D	-2.02	1.38	1.43
4	D	603	NAD	O3D-C3D	-2.01	1.38	1.43
4	A	603	NAD	C8A-N7A	2.00	1.35	1.31

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	NAD	C5A-C4A-N3A	-5.59	119.02	126.72
4	A	603	NAD	N3A-C2A-N1A	-5.58	120.14	128.58
4	D	603	NAD	N3A-C2A-N1A	-5.46	120.32	128.58
4	C	603	NAD	N3A-C2A-N1A	-5.41	120.39	128.58
2	C	601	2VS	OA3-CA2-CA1	5.41	119.29	114.17
4	B	603	NAD	N3A-C2A-N1A	-5.36	120.47	128.58
2	B	601	2VS	OA2-CA1-CA2	5.25	121.63	115.78
4	A	603	NAD	C5A-C4A-N3A	-5.24	119.50	126.72
2	A	601	2VS	OA3-CA2-CA1	5.11	119.01	114.17
2	B	601	2VS	OA3-CA2-CA1	5.11	119.01	114.17
2	D	601	2VS	OA3-CA2-CA1	5.08	118.99	114.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	NAD	C5A-C4A-N3A	-4.99	119.84	126.72
4	D	603	NAD	C5A-C4A-N3A	-4.97	119.88	126.72
2	D	601	2VS	OA2-CA1-CA2	4.91	121.25	115.78
4	C	603	NAD	C2A-N3A-C4A	4.00	121.60	111.83
4	C	603	NAD	N3A-C4A-N9A	3.96	133.91	127.17
4	A	603	NAD	C2A-N3A-C4A	3.95	121.49	111.83
4	D	603	NAD	C2A-N3A-C4A	3.80	121.12	111.83
4	B	603	NAD	C2A-N3A-C4A	3.71	120.88	111.83
4	B	603	NAD	O5D-C5D-C4D	3.65	121.41	108.99
4	A	603	NAD	N3A-C4A-N9A	3.56	133.22	127.17
4	B	603	NAD	N3A-C4A-N9A	3.51	133.14	127.17
4	A	603	NAD	C3N-C7N-N7N	3.48	122.02	117.74
4	D	603	NAD	N3A-C4A-N9A	3.44	133.03	127.17
4	D	603	NAD	O5D-C5D-C4D	3.26	120.08	108.99
4	A	603	NAD	O7N-C7N-C3N	-3.13	115.77	119.60
4	A	603	NAD	O5D-C5D-C4D	3.13	119.63	108.99
4	D	603	NAD	C3N-C7N-N7N	3.12	121.59	117.74
4	B	603	NAD	C3N-C7N-N7N	2.95	121.37	117.74
4	C	603	NAD	O5D-C5D-C4D	2.94	118.99	108.99
2	A	601	2VS	OA4-CA6-CA5	-2.92	116.29	125.61
4	B	603	NAD	N9A-C8A-N7A	-2.91	109.81	113.94
2	C	601	2VS	OA4-CA6-CA5	-2.80	116.67	125.61
4	C	603	NAD	C3N-C7N-N7N	2.75	121.13	117.74
2	C	601	2VS	CA3-CA2-CA1	-2.73	118.52	122.51
2	C	601	2VS	CA5-CA4-CA3	-2.73	117.94	123.52
4	A	603	NAD	N9A-C8A-N7A	-2.68	110.14	113.94
2	A	601	2VS	CA5-CA4-CA3	-2.65	118.09	123.52
4	B	603	NAD	C4A-C5A-N7A	-2.63	107.57	110.58
2	A	601	2VS	CA3-CA2-CA1	-2.63	118.67	122.51
4	B	603	NAD	C5A-N7A-C8A	2.60	107.54	103.45
4	C	603	NAD	C4A-C5A-N7A	-2.59	107.62	110.58
4	D	603	NAD	N9A-C8A-N7A	-2.58	110.28	113.94
4	C	603	NAD	N9A-C8A-N7A	-2.56	110.31	113.94
4	C	603	NAD	C5A-N7A-C8A	2.54	107.44	103.45
4	D	603	NAD	C4A-C5A-N7A	-2.48	107.75	110.58
4	A	603	NAD	C4A-C5A-N7A	-2.44	107.79	110.58
2	B	601	2VS	CA3-CA2-CA1	-2.44	118.94	122.51
2	D	601	2VS	CA3-CA2-CA1	-2.41	118.99	122.51
2	B	601	2VS	OA4-CA6-CA5	-2.37	118.04	125.61
4	B	603	NAD	C2D-C3D-C4D	2.33	107.11	102.61
4	D	603	NAD	C2D-C3D-C4D	2.28	107.02	102.61
4	A	603	NAD	C5A-N7A-C8A	2.28	107.03	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	2VS	OA1-CA1-CA2	-2.26	117.53	120.12
4	D	603	NAD	C5A-N7A-C8A	2.23	106.96	103.45
4	B	603	NAD	C4A-N9A-C8A	2.22	108.07	105.74
2	D	601	2VS	CA5-CA4-CA3	-2.21	119.00	123.52
4	D	603	NAD	O5B-C5B-C4B	2.21	116.52	108.99
4	A	603	NAD	O5B-C5B-C4B	2.19	116.44	108.99
2	D	601	2VS	OA1-CA1-CA2	-2.12	117.69	120.12
4	C	603	NAD	C2N-C3N-C4N	2.10	120.70	118.26
4	D	603	NAD	C4A-N9A-C8A	2.08	107.92	105.74
4	A	603	NAD	C2N-C3N-C4N	2.08	120.68	118.26
4	B	603	NAD	O5B-C5B-C4B	2.05	115.98	108.99
4	A	603	NAD	C4D-O4D-C1D	-2.03	108.06	109.92
2	D	601	2VS	OA4-CA6-CA5	-2.01	119.19	125.61

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	2VS	CA4-CA5-CA6-OA4
2	B	601	2VS	CA4-CA5-CA6-OA4
2	D	601	2VS	CA4-CA5-CA6-OA4
4	A	603	NAD	C5B-O5B-PA-O1A
4	A	603	NAD	C5B-O5B-PA-O3
4	B	603	NAD	C5B-O5B-PA-O1A
4	B	603	NAD	C5B-O5B-PA-O2A
4	B	603	NAD	C5B-O5B-PA-O3
4	C	603	NAD	C5B-O5B-PA-O1A
4	D	603	NAD	C5B-O5B-PA-O1A
4	D	603	NAD	C5B-O5B-PA-O3
4	C	603	NAD	C3D-C4D-C5D-O5D
4	D	603	NAD	C3D-C4D-C5D-O5D
4	B	603	NAD	C3D-C4D-C5D-O5D
4	D	603	NAD	O4D-C4D-C5D-O5D
4	B	603	NAD	O4D-C4D-C5D-O5D
4	C	603	NAD	O4D-C4D-C5D-O5D
4	A	603	NAD	C5B-O5B-PA-O2A
4	C	603	NAD	C5B-O5B-PA-O2A
4	D	603	NAD	C5B-O5B-PA-O2A
4	B	603	NAD	C2B-C1B-N9A-C8A
4	A	603	NAD	C2B-C1B-N9A-C8A
4	C	603	NAD	C2B-C1B-N9A-C8A
2	C	601	2VS	CA2-CA3-CA4-CA5

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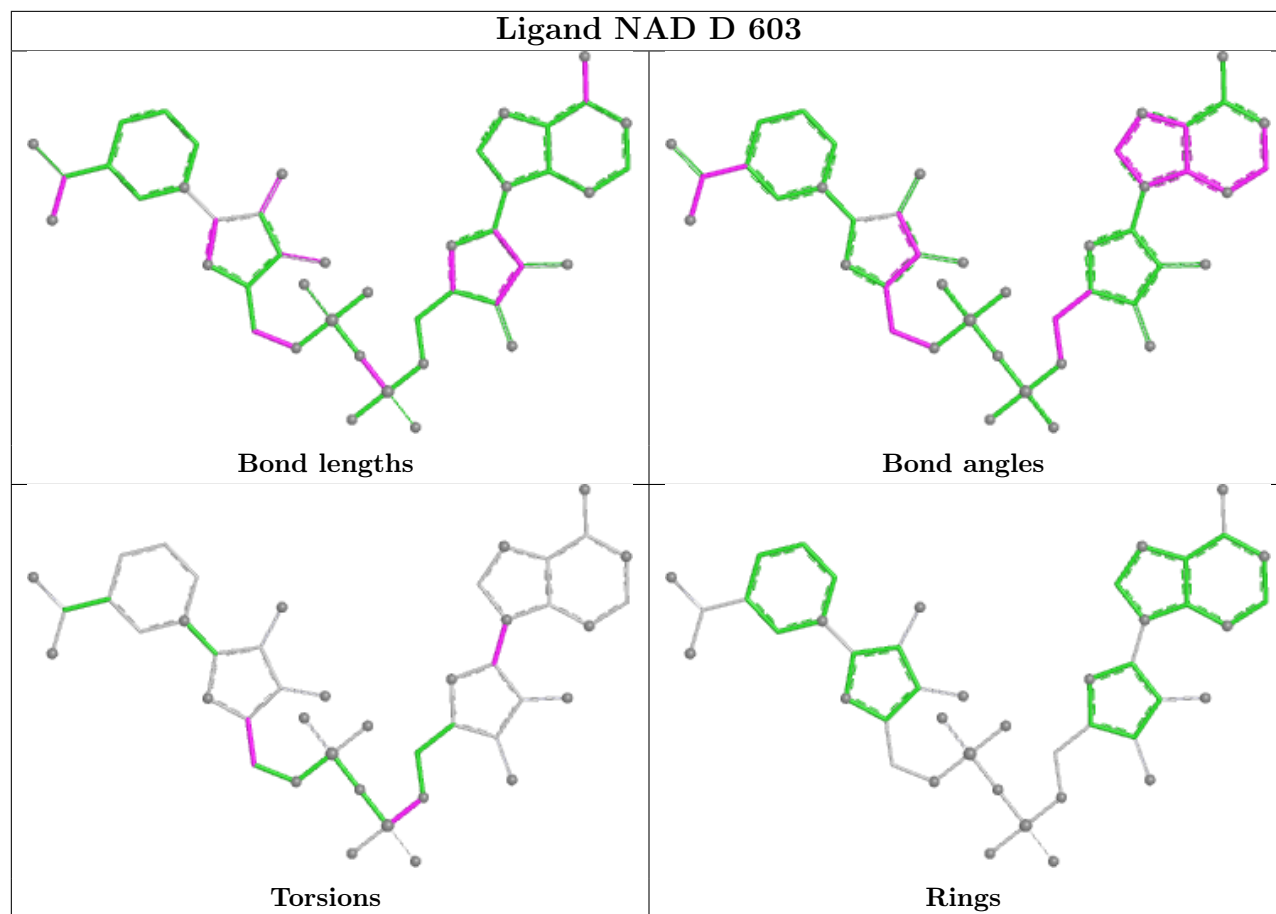
Mol	Chain	Res	Type	Atoms
4	D	603	NAD	C2B-C1B-N9A-C8A

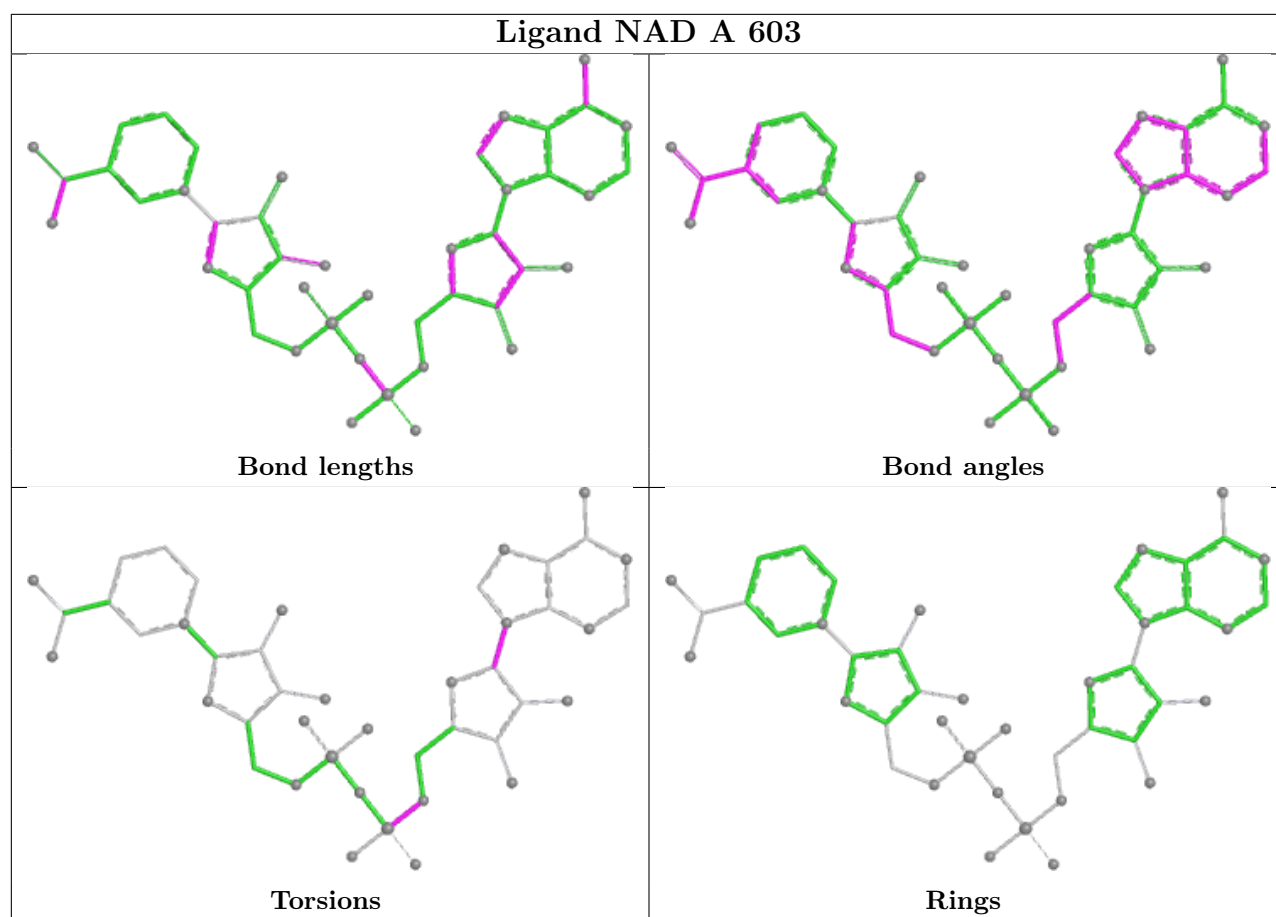
There are no ring outliers.

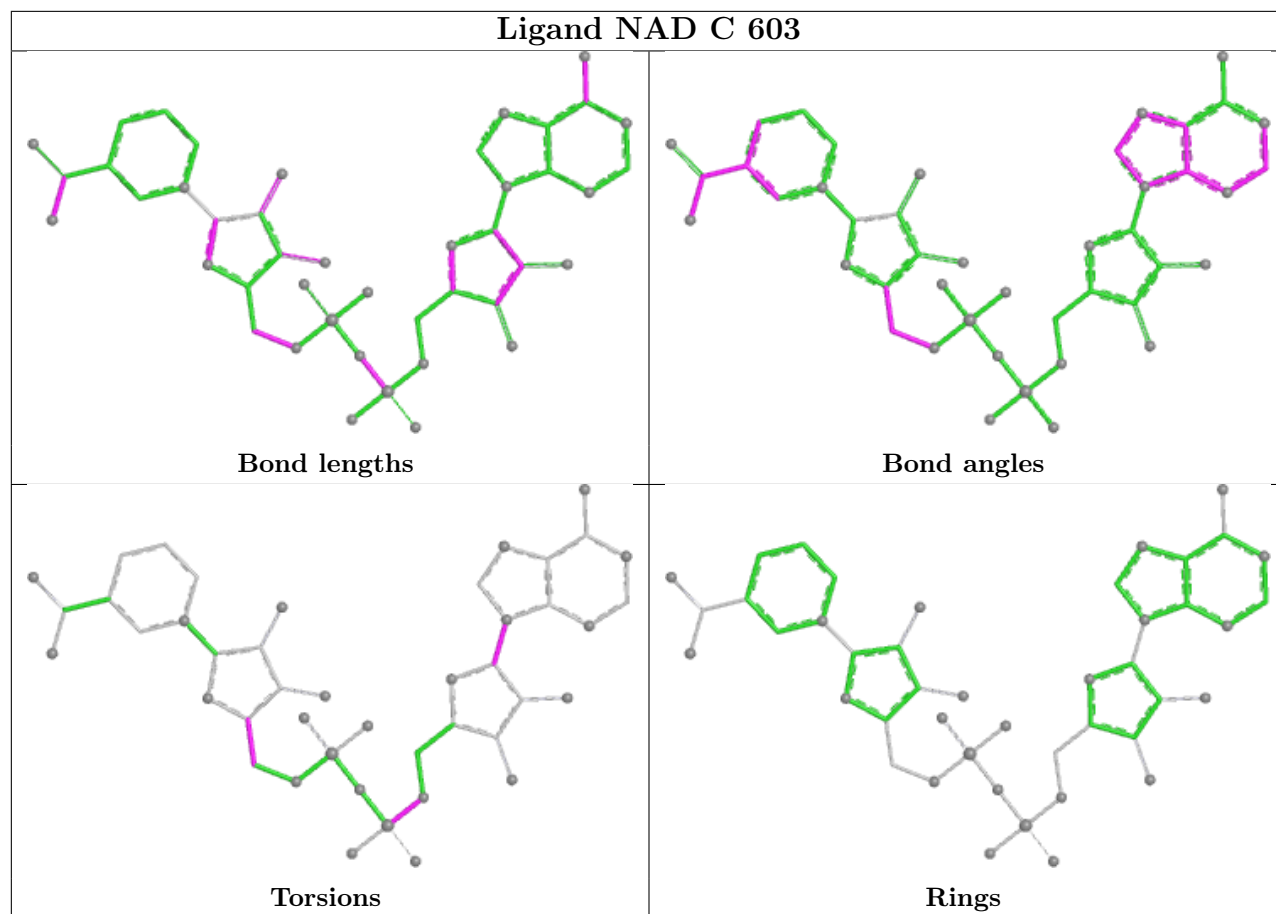
8 monomers are involved in 20 short contacts:

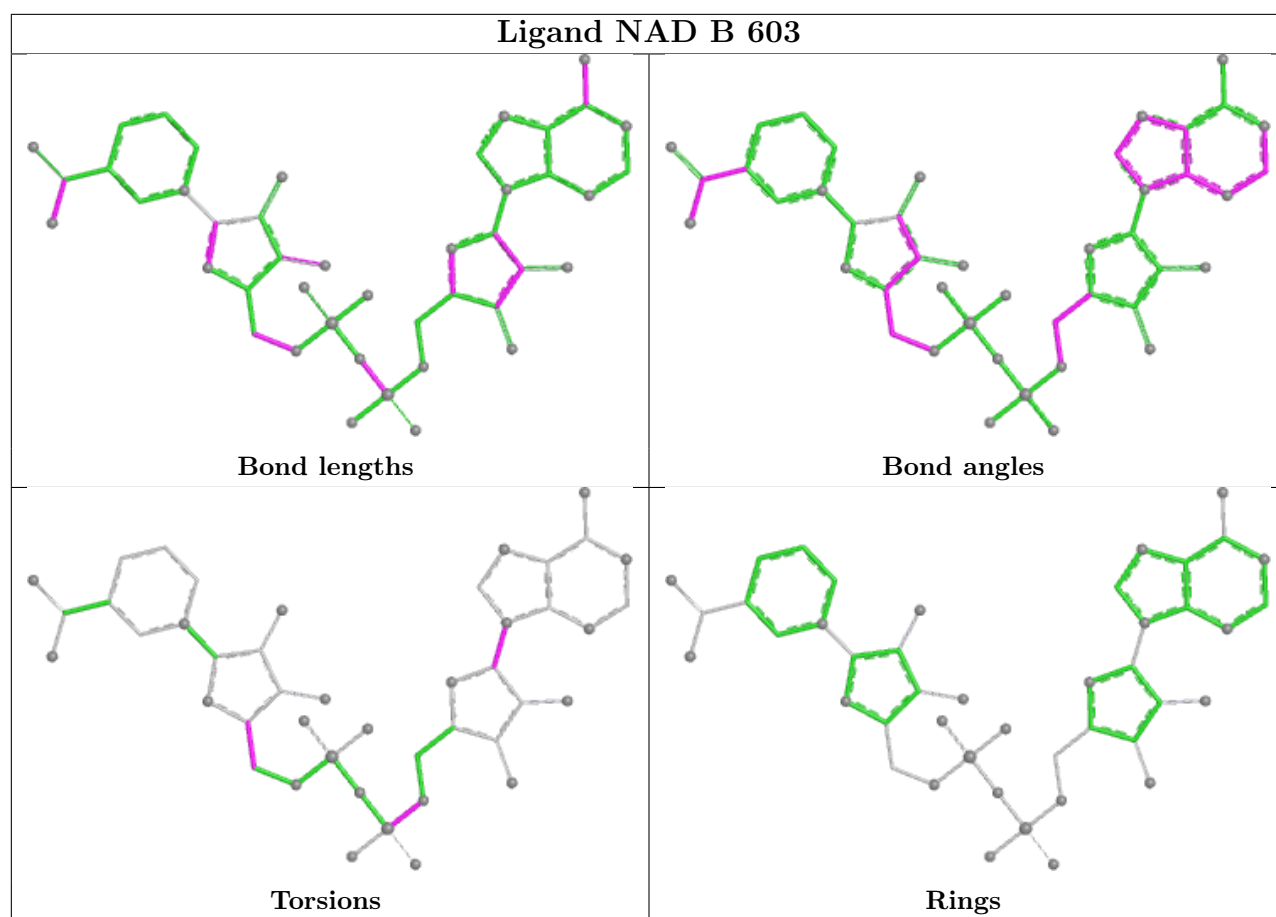
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	603	NAD	2	0
4	A	603	NAD	1	0
4	C	603	NAD	2	0
2	C	601	2VS	2	0
2	B	601	2VS	5	0
2	A	601	2VS	3	0
4	B	603	NAD	2	0
2	D	601	2VS	3	0

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	484/520 (93%)	0.04	3 (0%) 85 86	23, 30, 40, 58	0
1	B	483/520 (92%)	0.16	4 (0%) 82 83	24, 32, 42, 51	0
1	C	483/520 (92%)	0.22	6 (1%) 76 77	23, 32, 43, 55	0
1	D	483/520 (92%)	0.40	6 (1%) 76 77	23, 35, 47, 61	0
All	All	1933/2080 (92%)	0.21	19 (0%) 79 80	23, 32, 44, 61	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	ASP	3.0
1	C	54	ALA	2.8
1	D	38	ILE	2.6
1	C	373	VAL	2.5
1	D	46	ILE	2.5
1	C	24	ILE	2.4
1	D	288	GLU	2.4
1	C	33	SER	2.3
1	B	373	VAL	2.2
1	D	355	SER	2.2
1	D	145	SER	2.2
1	A	145	SER	2.1
1	C	312	ARG	2.1
1	A	46	ILE	2.1
1	B	59	GLU	2.1
1	D	34	SER	2.1
1	A	288	GLU	2.0
1	B	335	ASP	2.0
1	C	48	ASP	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 ⓘ

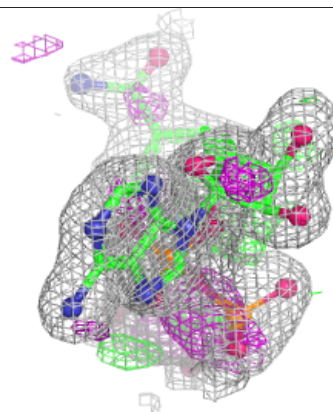
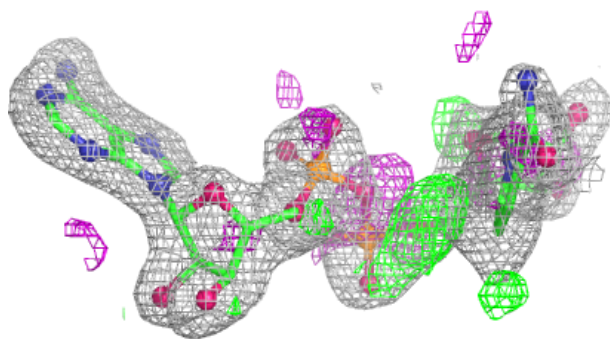
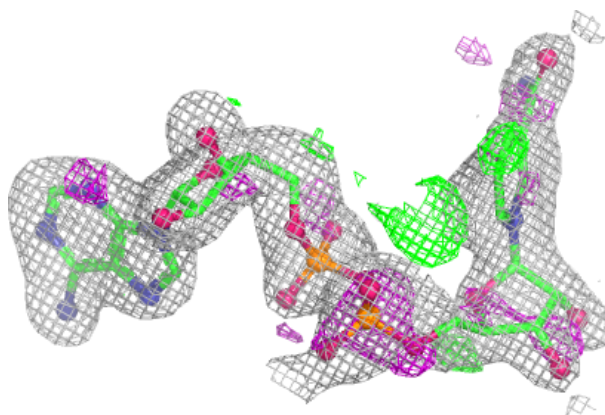
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAD	D	603	44/44	0.88	0.10	33,40,48,57	0
4	NAD	B	603	44/44	0.89	0.10	31,39,48,57	0
4	NAD	A	603	44/44	0.89	0.10	31,38,47,51	0
4	NAD	C	603	44/44	0.91	0.09	29,36,45,56	0
3	NA	D	602	1/1	0.91	0.15	37,37,37,37	0
3	NA	C	602	1/1	0.93	0.09	33,33,33,33	0
2	2VS	D	601	10/10	0.94	0.07	33,34,40,40	0
2	2VS	B	601	10/10	0.95	0.07	30,32,37,38	0
3	NA	A	602	1/1	0.97	0.06	27,27,27,27	0
3	NA	B	602	1/1	0.97	0.07	30,30,30,30	0
2	2VS	C	601	10/10	0.97	0.05	28,32,36,37	0
2	2VS	A	601	10/10	0.97	0.06	27,30,34,35	0

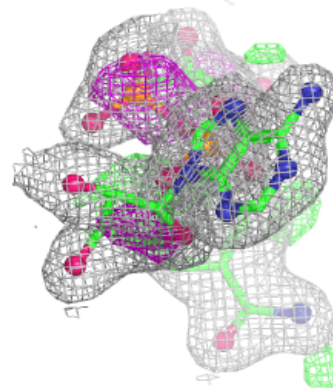
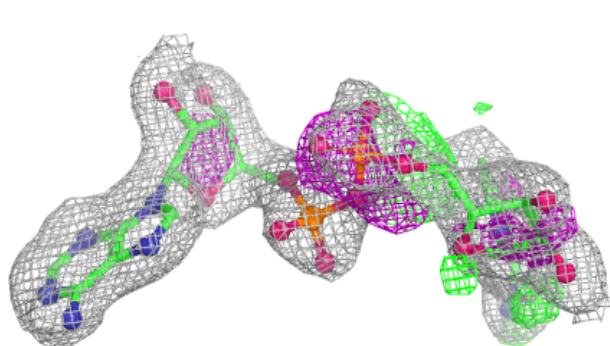
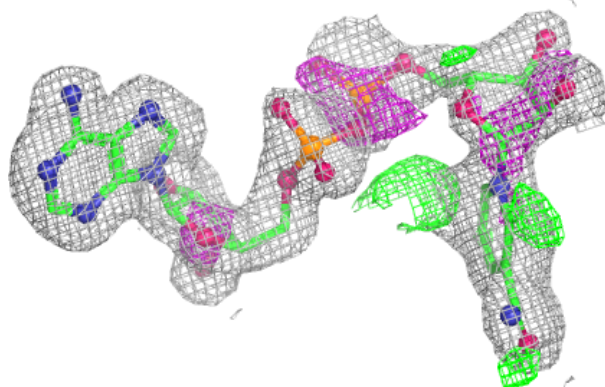
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD D 603:

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

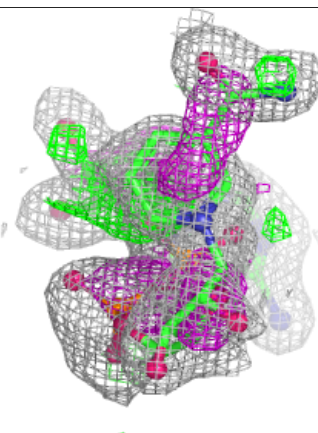
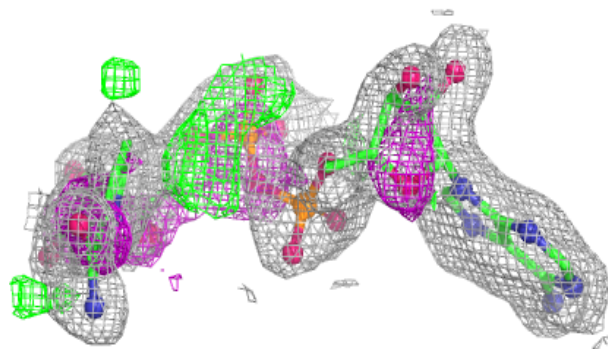
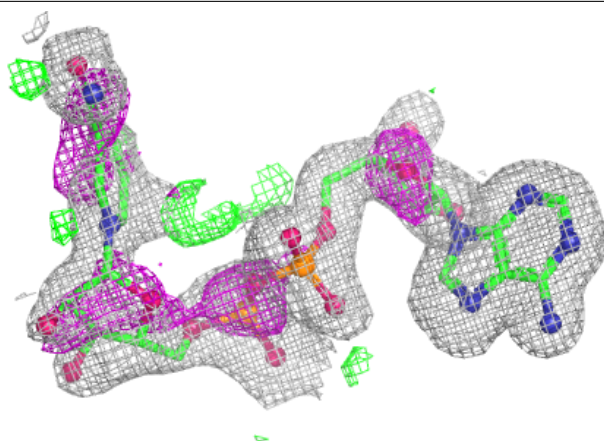
**Electron density around NAD B 603:**

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

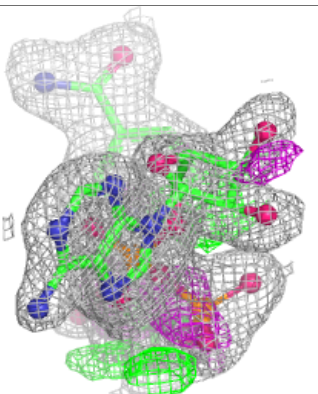
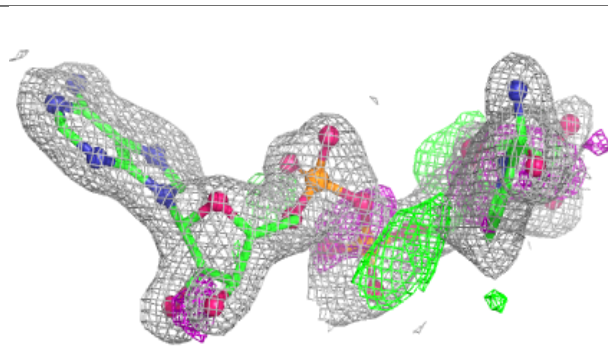
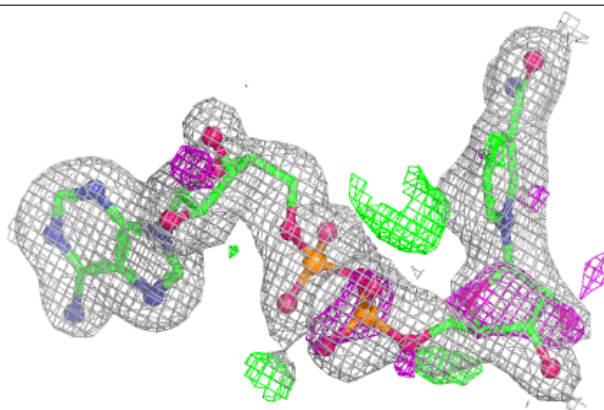


Electron density around NAD A 603:

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

**Electron density around NAD C 603:**

$2mF_o-DF_c$ (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.