



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 06:13 PM EDT

PDB ID : 5KLO
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

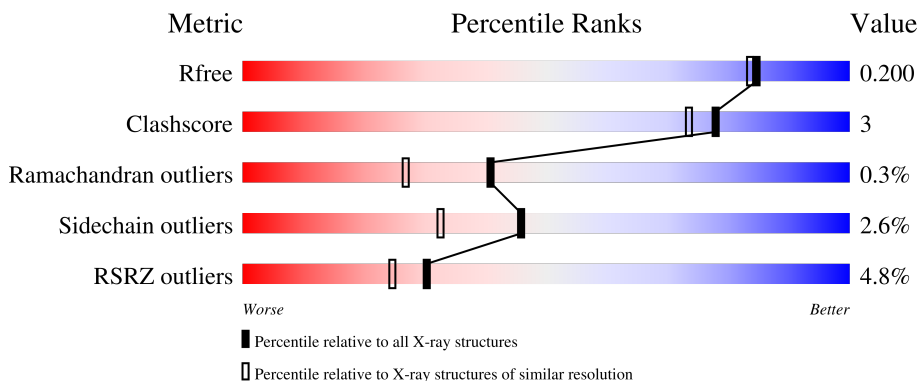
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

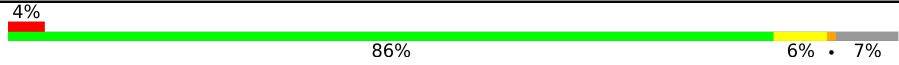



The reported resolution of this entry is 1.79 Å.

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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	 4% 86% 6% • 7%
1	B	520	 4% 87% 5% • 7%
1	C	520	 4% 86% 7% 7%
1	D	520	 6% 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	A	601	-	-	X	-
2	2VS	B	601	-	-	X	-
2	2VS	D	601	-	-	X	-

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	484	3675	2325	637	701	12	0	0	0
1	B	483	3668	2320	636	700	12	0	0	0
1	C	483	3668	2320	636	700	12	0	0	0
1	D	483	3668	2320	636	700	12	0	0	0

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

Continued on next page...

Continued from previous page...

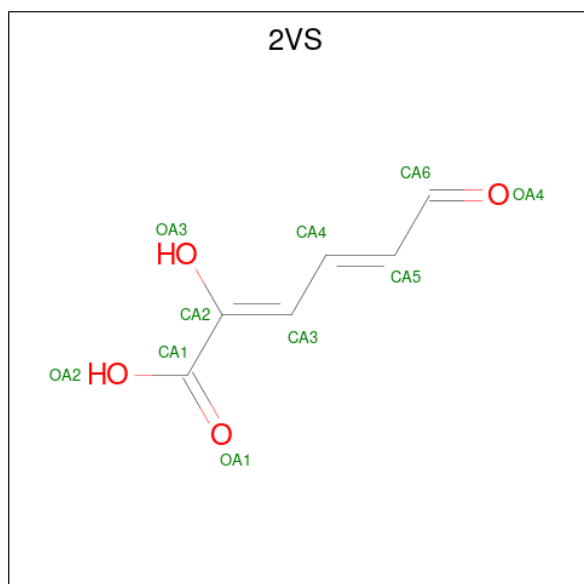
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP Q83V33
B	-18	GLY	-	expression tag	UNP Q83V33
B	-17	SER	-	expression tag	UNP Q83V33
B	-16	SER	-	expression tag	UNP Q83V33
B	-15	HIS	-	expression tag	UNP Q83V33
B	-14	HIS	-	expression tag	UNP Q83V33
B	-13	HIS	-	expression 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

Continued on next page...

Continued from previous page...

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 (three-letter code: 2VS) (formula: C₆H₆O₄).



Continued from previous page...

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		

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) 92.4 (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)	Xtrriage
Refinement program	PHENIX phenix.refine: 1.7.3_928	Depositor
R, R_{free}	0.179 , 0.203 0.175 , 0.200	Depositor DCC
R_{free} test set	2000 reflections (1.03%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtrriage
Anisotropy	0.337	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: NA, NAD, 2VS

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	0.38	0/3755	0.61	3/5105 (0.1%)
1	B	0.36	0/3747	0.57	2/5094 (0.0%)
1	C	0.38	0/3747	0.59	2/5094 (0.0%)
1	D	0.34	0/3747	0.54	1/5094 (0.0%)
All	All	0.36	0/14996	0.58	8/20387 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	A	307	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	C	307	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	C	307	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	B	307	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	D	307	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	307	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	108	ARG	NE-CZ-NH2	-5.10	117.75	120.30

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	20	0
1	D	3668	0	3604	17	0
2	A	10	0	4	4	0
2	B	10	0	3	5	0
2	C	10	0	4	3	0
2	D	10	0	4	4	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	6	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	85	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 (85) 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:D:302:CYS:HG	2:D:601:2VS:H1	1.24	1.00
1:C:302:CYS:HG	2:C:601:2VS:H1	1.15	0.95
1:A:302:CYS:HG	2:A:601:2VS:H1	1.32	0.90
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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: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%)	47	33
1	B	481/520 (92%)	467 (97%)	12 (2%)	2 (0%)	34	21
1	C	481/520 (92%)	466 (97%)	14 (3%)	1 (0%)	47	33
1	D	481/520 (92%)	467 (97%)	13 (3%)	1 (0%)	47	33
All	All	1925/2080 (92%)	1869 (97%)	51 (3%)	5 (0%)	41	27

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 [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	392/423 (93%)	383 (98%)	9 (2%)	50	37
1	B	391/423 (92%)	383 (98%)	8 (2%)	55	44
1	C	391/423 (92%)	380 (97%)	11 (3%)	43	30
1	D	391/423 (92%)	378 (97%)	13 (3%)	38	23
All	All	1565/1692 (92%)	1524 (97%)	41 (3%)	46	32

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LYS
1	A	131	LEU
1	A	192	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	242	LEU
1	A	269	LEU
1	A	406	PHE
1	A	432	LEU
1	A	441	LEU
1	A	463	LEU
1	B	47	SER
1	B	131	LEU
1	B	192	LYS
1	B	203	LEU
1	B	269	LEU
1	B	406	PHE
1	B	432	LEU
1	B	463	LEU
1	C	131	LEU
1	C	192	LYS
1	C	242	LEU
1	C	268	GLU
1	C	269	LEU
1	C	373	VAL
1	C	395	SER
1	C	406	PHE
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	192	LYS
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	406	PHE
1	D	432	LEU
1	D	463	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	A	603	-	42,48,48	2.03	8 (19%)	50,73,73	1.45	6 (12%)
2	2VS	C	601	-	9,9,9	2.90	3 (33%)	9,10,10	3.45	4 (44%)
4	NAD	C	603	-	42,48,48	1.98	10 (23%)	50,73,73	1.49	6 (12%)
2	2VS	A	601	-	9,9,9	2.85	3 (33%)	9,10,10	3.31	4 (44%)
2	2VS	D	601	-	9,9,9	2.86	3 (33%)	9,10,10	3.71	5 (55%)
4	NAD	D	603	-	42,48,48	2.05	10 (23%)	50,73,73	1.51	8 (16%)
4	NAD	B	603	-	42,48,48	2.04	9 (21%)	50,73,73	1.52	8 (16%)
2	2VS	B	601	-	9,9,9	2.86	3 (33%)	9,10,10	3.77	5 (55%)

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	A	603	-	-	3/26/62/62	0/5/5/5
2	2VS	C	601	-	-	0/8/9/9	-
4	NAD	C	603	-	-	5/26/62/62	0/5/5/5
2	2VS	A	601	-	-	1/8/9/9	-
2	2VS	D	601	-	-	1/8/9/9	-
4	NAD	D	603	-	-	5/26/62/62	0/5/5/5
4	NAD	B	603	-	-	5/26/62/62	0/5/5/5
2	2VS	B	601	-	-	1/8/9/9	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	NAD	O4D-C1D	6.83	1.50	1.41
4	D	603	NAD	O4D-C1D	6.70	1.50	1.41
4	C	603	NAD	O4D-C1D	6.65	1.50	1.41
4	A	603	NAD	O4D-C1D	6.59	1.50	1.41
4	A	603	NAD	C7N-N7N	5.83	1.44	1.33
4	B	603	NAD	C7N-N7N	5.54	1.43	1.33
2	B	601	2VS	OA4-CA6	5.49	1.39	1.22
2	A	601	2VS	OA4-CA6	5.40	1.39	1.22
2	C	601	2VS	OA4-CA6	5.38	1.39	1.22
4	D	603	NAD	C7N-N7N	5.37	1.43	1.33
2	D	601	2VS	OA4-CA6	5.32	1.39	1.22
4	D	603	NAD	C2B-C1B	-5.11	1.46	1.53
4	C	603	NAD	C7N-N7N	5.08	1.42	1.33
4	A	603	NAD	C2B-C1B	-4.93	1.46	1.53
4	B	603	NAD	C2B-C1B	-4.77	1.46	1.53
4	C	603	NAD	C2B-C1B	-4.43	1.47	1.53
2	D	601	2VS	CA3-CA2	4.29	1.49	1.39
2	B	601	2VS	CA3-CA2	4.19	1.49	1.39
2	C	601	2VS	CA3-CA2	4.14	1.49	1.39
2	A	601	2VS	OA3-CA2	-4.10	1.23	1.34
2	C	601	2VS	OA3-CA2	-4.08	1.23	1.34
2	D	601	2VS	OA3-CA2	-4.02	1.23	1.34
2	B	601	2VS	OA3-CA2	-3.88	1.23	1.34
2	A	601	2VS	CA3-CA2	3.86	1.48	1.39
4	D	603	NAD	C2B-C3B	-3.51	1.43	1.53
4	B	603	NAD	C2B-C3B	-3.40	1.44	1.53
4	C	603	NAD	C2B-C3B	-3.31	1.44	1.53
4	A	603	NAD	C2B-C3B	-3.26	1.44	1.53
4	D	603	NAD	C2D-C1D	-3.19	1.48	1.53
4	C	603	NAD	C2D-C1D	-2.92	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	NAD	C2D-C1D	-2.86	1.49	1.53
4	A	603	NAD	C2D-C1D	-2.75	1.49	1.53
4	B	603	NAD	C6A-N6A	2.69	1.43	1.34
4	A	603	NAD	C6A-N6A	2.68	1.43	1.34
4	D	603	NAD	C6A-N6A	2.64	1.43	1.34
4	D	603	NAD	O4B-C4B	-2.53	1.39	1.45
4	C	603	NAD	C6A-N6A	2.49	1.43	1.34
4	C	603	NAD	O2D-C2D	-2.41	1.37	1.43
4	A	603	NAD	O3D-C3D	-2.33	1.37	1.43
4	C	603	NAD	O4B-C4B	-2.33	1.39	1.45
4	C	603	NAD	O5D-C5D	-2.27	1.36	1.44
4	B	603	NAD	O3D-C3D	-2.27	1.37	1.43
4	D	603	NAD	O2D-C2D	-2.27	1.37	1.43
4	B	603	NAD	O4B-C4B	-2.26	1.39	1.45
4	A	603	NAD	O4B-C4B	-2.20	1.40	1.45
4	C	603	NAD	O3D-C3D	-2.13	1.38	1.43
4	D	603	NAD	O3D-C3D	-2.12	1.38	1.43
4	B	603	NAD	O5D-C5D	-2.07	1.36	1.44
4	D	603	NAD	O5D-C5D	-2.07	1.36	1.44

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	2VS	OA3-CA2-CA1	8.72	119.29	114.01
2	A	601	2VS	OA3-CA2-CA1	8.26	119.01	114.01
2	B	601	2VS	OA3-CA2-CA1	8.25	119.01	114.01
2	D	601	2VS	OA3-CA2-CA1	8.22	118.99	114.01
2	B	601	2VS	OA2-CA1-CA2	5.92	121.63	115.91
2	D	601	2VS	OA2-CA1-CA2	5.53	121.25	115.91
4	A	603	NAD	N3A-C2A-N1A	-5.46	120.14	128.68
4	D	603	NAD	N3A-C2A-N1A	-5.35	120.32	128.68
4	C	603	NAD	N3A-C2A-N1A	-5.31	120.39	128.68
4	B	603	NAD	N3A-C2A-N1A	-5.25	120.47	128.68
4	B	603	NAD	O5D-C5D-C4D	3.61	121.41	108.99
4	A	603	NAD	C3N-C7N-N7N	3.56	122.02	117.75
2	C	601	2VS	CA3-CA2-CA1	-3.46	118.52	122.69
2	A	601	2VS	CA3-CA2-CA1	-3.34	118.67	122.69
4	A	603	NAD	O7N-C7N-C3N	-3.23	115.77	119.63
4	D	603	NAD	O5D-C5D-C4D	3.22	120.08	108.99
4	D	603	NAD	C3N-C7N-N7N	3.20	121.59	117.75
2	B	601	2VS	CA3-CA2-CA1	-3.12	118.94	122.69
4	A	603	NAD	O5D-C5D-C4D	3.09	119.63	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	2VS	CA3-CA2-CA1	-3.07	118.99	122.69
4	B	603	NAD	C3N-C7N-N7N	3.01	121.37	117.75
4	C	603	NAD	O5D-C5D-C4D	2.90	118.99	108.99
4	C	603	NAD	C3N-C7N-N7N	2.81	121.13	117.75
2	A	601	2VS	OA4-CA6-CA5	-2.75	116.29	125.67
2	C	601	2VS	CA5-CA4-CA3	-2.70	117.94	123.47
2	C	601	2VS	OA4-CA6-CA5	-2.64	116.67	125.67
2	A	601	2VS	CA5-CA4-CA3	-2.63	118.09	123.47
4	C	603	NAD	C3D-C2D-C1D	2.52	104.78	100.98
4	B	603	NAD	C2D-C3D-C4D	2.30	107.11	102.64
4	D	603	NAD	C2D-C3D-C4D	2.25	107.02	102.64
4	B	603	NAD	PN-O3-PA	-2.25	125.11	132.83
2	B	601	2VS	OA4-CA6-CA5	-2.23	118.04	125.67
4	D	603	NAD	C3D-C2D-C1D	2.22	104.31	100.98
2	B	601	2VS	OA1-CA1-CA2	-2.21	117.53	120.08
4	B	603	NAD	C3D-C2D-C1D	2.19	104.28	100.98
4	D	603	NAD	O5B-C5B-C4B	2.19	116.52	108.99
2	D	601	2VS	CA5-CA4-CA3	-2.19	119.00	123.47
4	B	603	NAD	C1B-N9A-C4A	-2.18	122.81	126.64
4	A	603	NAD	O5B-C5B-C4B	2.16	116.44	108.99
4	D	603	NAD	PN-O3-PA	-2.16	125.43	132.83
4	C	603	NAD	C2N-C3N-C4N	2.15	120.70	118.26
4	A	603	NAD	C2N-C3N-C4N	2.13	120.68	118.26
4	D	603	NAD	C1B-N9A-C4A	-2.12	122.92	126.64
4	C	603	NAD	PN-O3-PA	-2.11	125.59	132.83
2	D	601	2VS	OA1-CA1-CA2	-2.07	117.69	120.08
4	B	603	NAD	O5B-C5B-C4B	2.03	115.98	108.99

There are no chirality outliers.

All (21) 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	B	603	NAD	C5B-O5B-PA-O1A
4	B	603	NAD	C5B-O5B-PA-O2A
4	C	603	NAD	C5B-O5B-PA-O1A
4	D	603	NAD	C5B-O5B-PA-O1A
4	D	603	NAD	C3D-C4D-C5D-O5D
4	B	603	NAD	C3D-C4D-C5D-O5D

Continued on next page...

Continued from previous page...

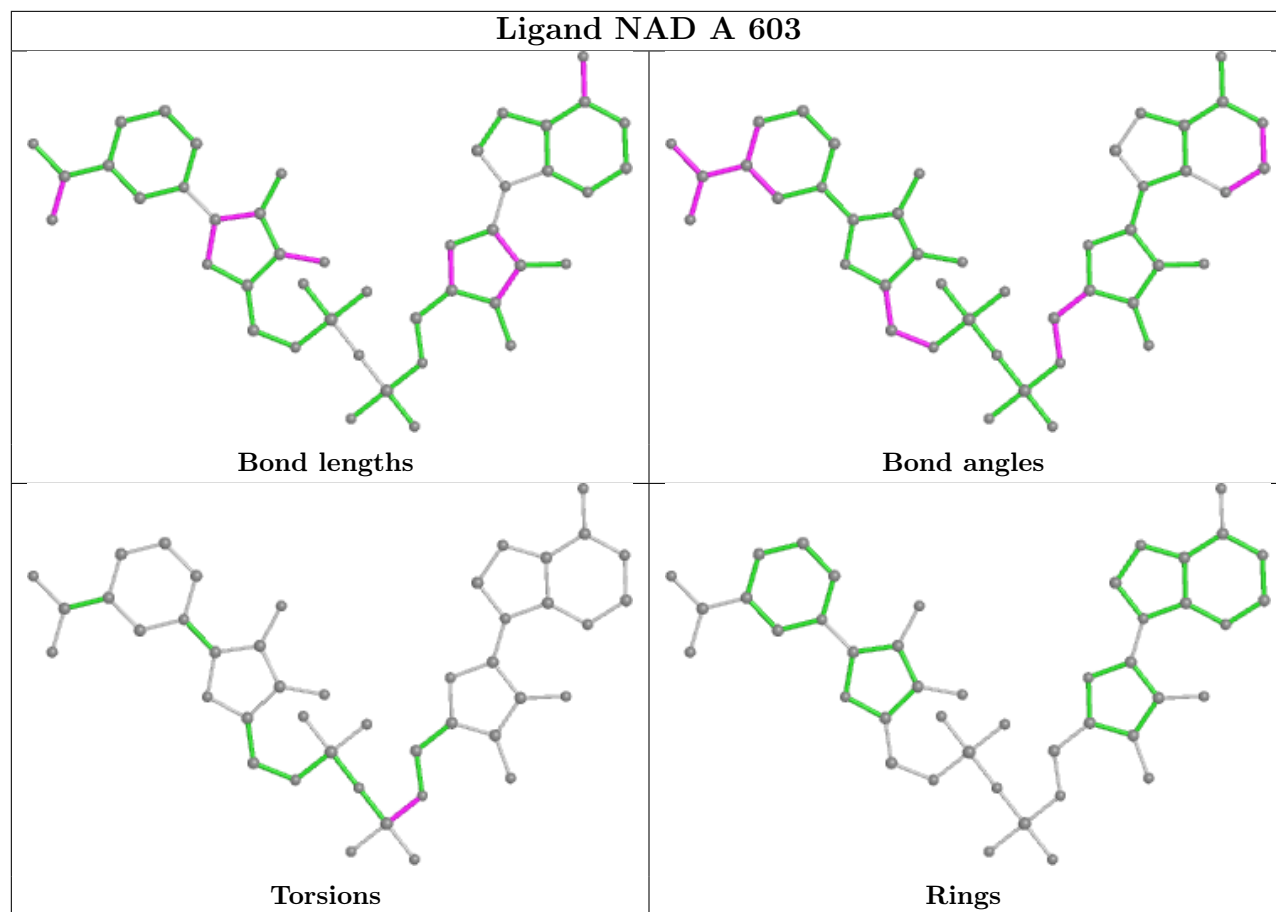
Mol	Chain	Res	Type	Atoms
4	C	603	NAD	C3D-C4D-C5D-O5D
4	B	603	NAD	O4D-C4D-C5D-O5D
4	C	603	NAD	O4D-C4D-C5D-O5D
4	D	603	NAD	O4D-C4D-C5D-O5D
4	A	603	NAD	C5B-O5B-PA-O3
4	B	603	NAD	C5B-O5B-PA-O3
4	D	603	NAD	C5B-O5B-PA-O3
4	A	603	NAD	C5B-O5B-PA-O2A
4	C	603	NAD	C5B-O5B-PA-O2A
4	D	603	NAD	C5B-O5B-PA-O2A
4	C	603	NAD	C5B-O5B-PA-O3

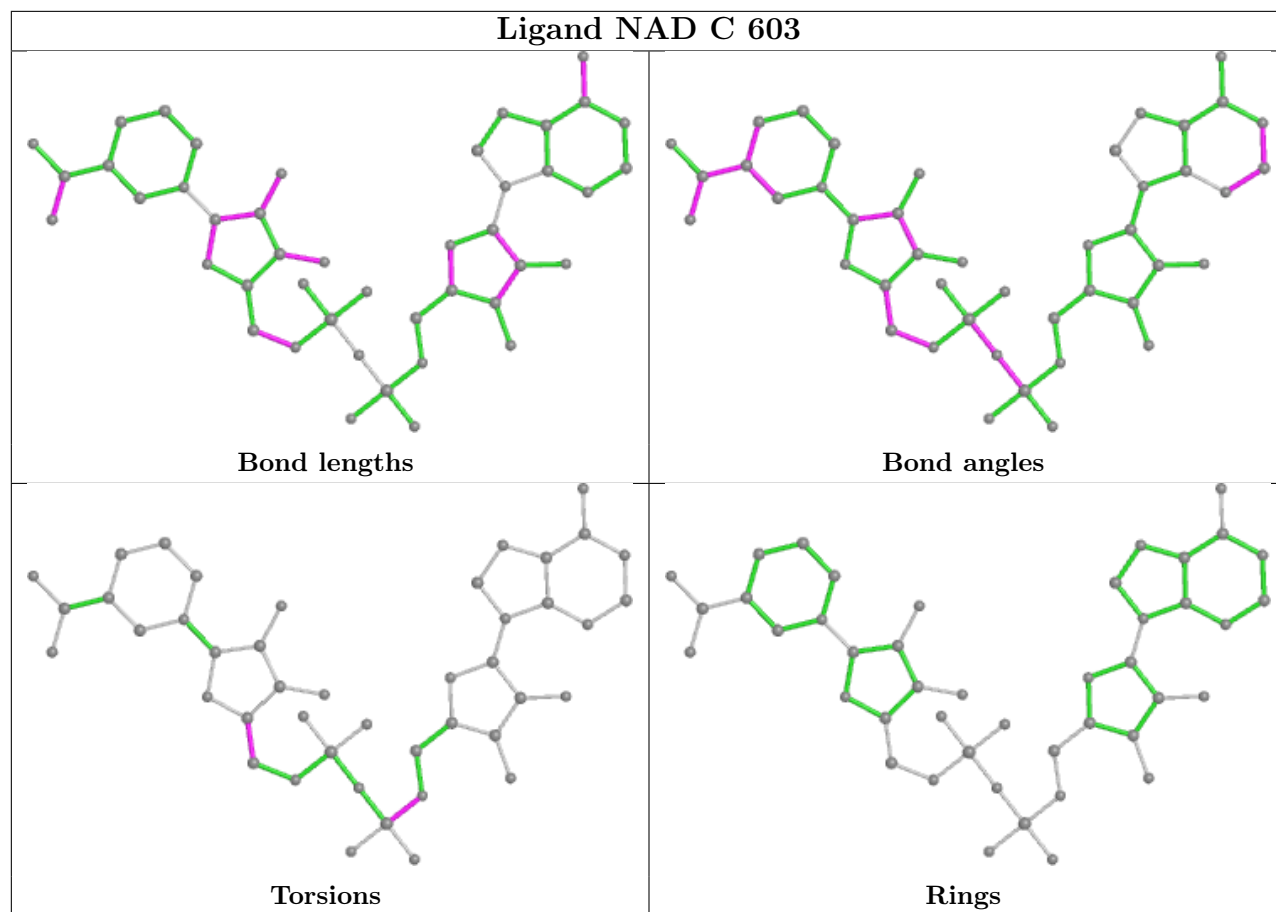
There are no ring outliers.

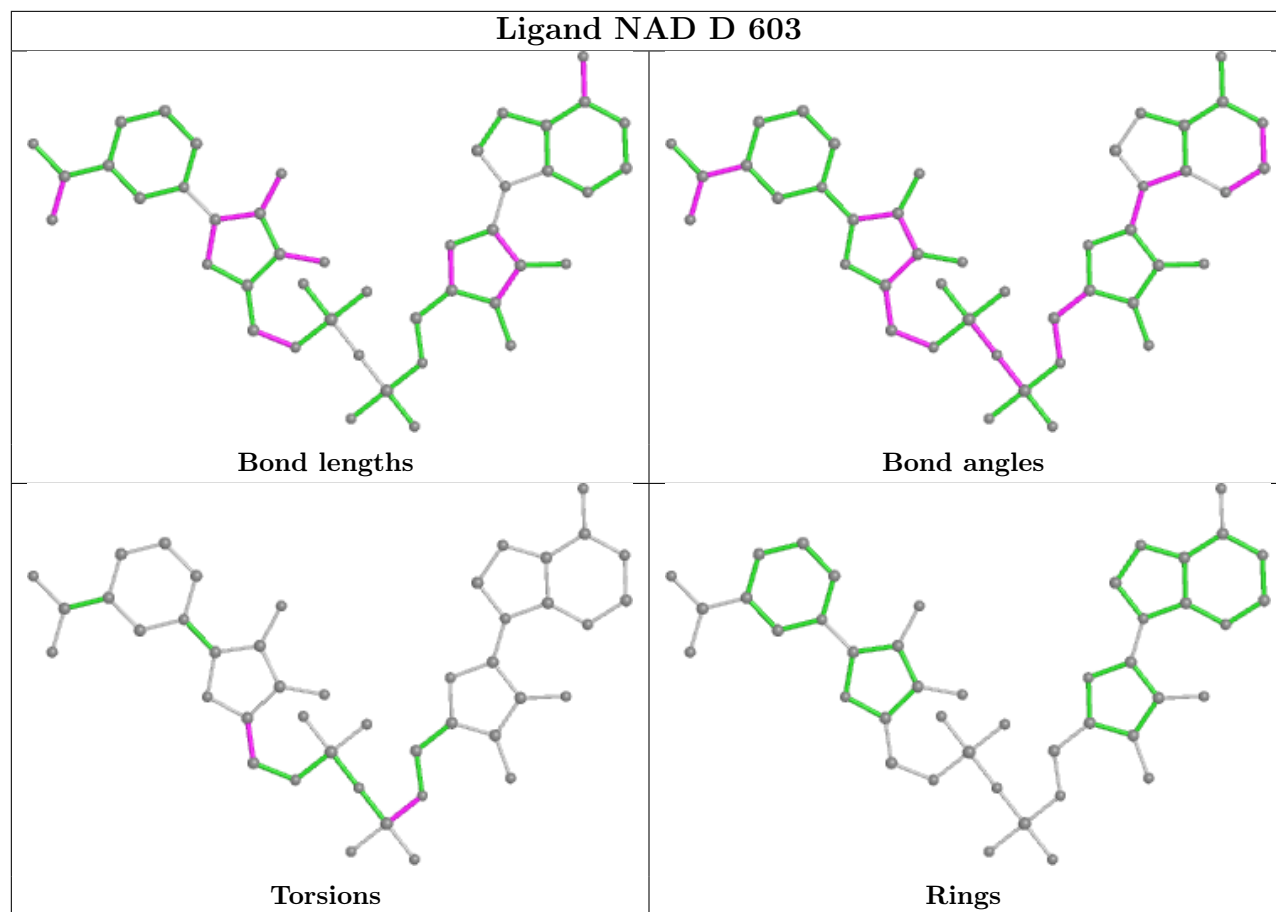
8 monomers are involved in 23 short contacts:

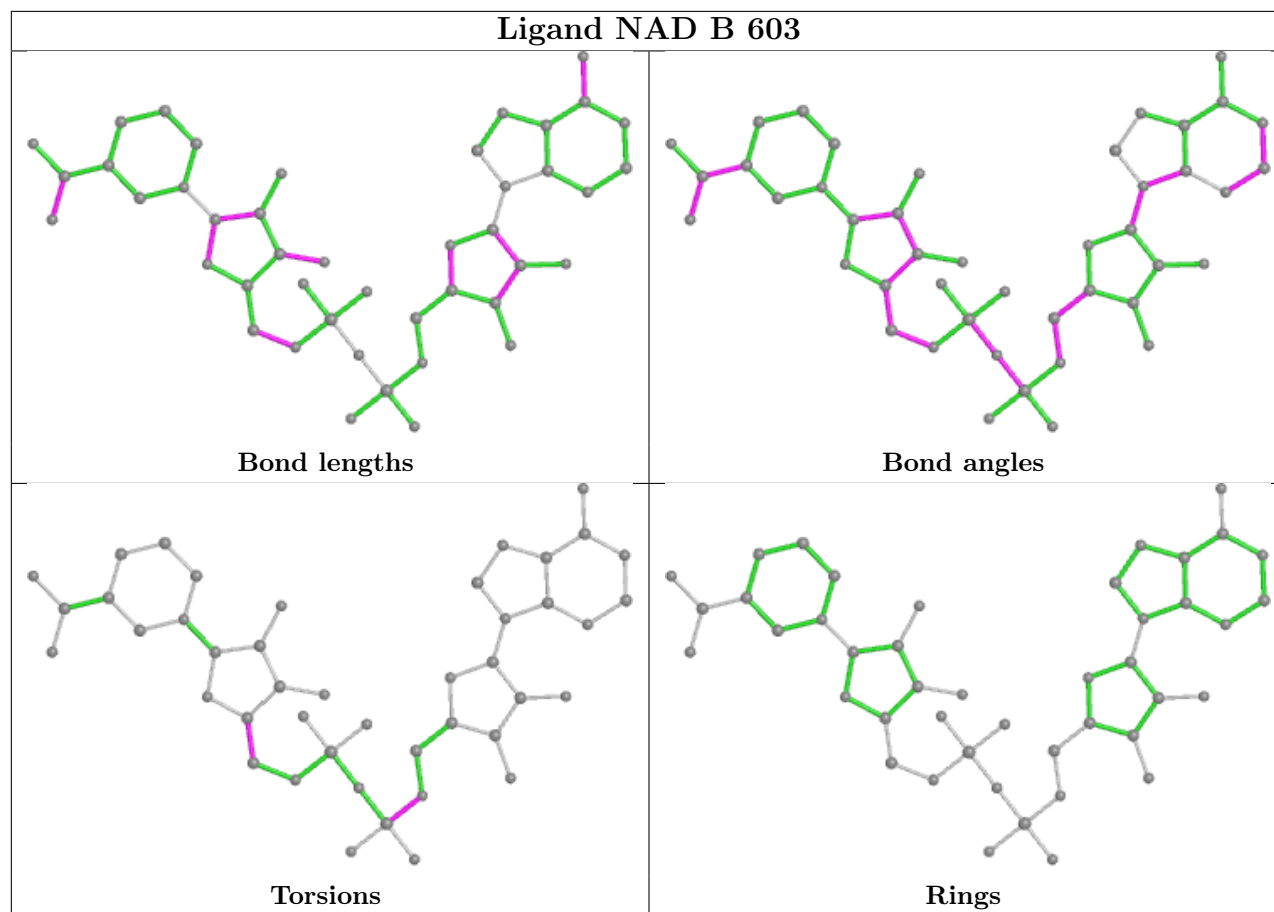
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	NAD	1	0
2	C	601	2VS	3	0
4	C	603	NAD	2	0
2	A	601	2VS	4	0
2	D	601	2VS	4	0
4	D	603	NAD	2	0
4	B	603	NAD	2	0
2	B	601	2VS	5	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.12	19 (3%) 39 33	23, 30, 40, 58	0
1	B	483/520 (92%)	0.16	20 (4%) 37 31	24, 32, 42, 51	0
1	C	483/520 (92%)	0.24	21 (4%) 35 29	23, 32, 43, 55	0
1	D	483/520 (92%)	0.30	32 (6%) 18 14	23, 35, 47, 61	0
All	All	1933/2080 (92%)	0.21	92 (4%) 30 25	23, 32, 44, 61	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	PRO	5.0
1	B	174	LEU	4.9
1	D	45	LEU	4.8
1	D	174	LEU	4.3
1	A	164	VAL	4.3
1	B	169	ALA	4.3
1	C	170	LEU	4.2
1	B	337	ASP	4.1
1	A	174	LEU	4.0
1	B	168	TRP	3.7
1	D	324	VAL	3.6
1	D	382	GLN	3.5
1	D	337	ASP	3.4
1	B	303	LEU	3.2
1	C	169	ALA	3.2
1	D	333	TYR	3.2
1	B	173	LEU	3.2
1	C	164	VAL	3.2
1	A	179	VAL	3.1
1	A	175	PHE	3.0
1	C	174	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	170	LEU	3.0
1	D	339	VAL	2.9
1	C	168	TRP	2.9
1	D	376	PHE	2.9
1	C	433	ALA	2.9
1	A	176	THR	2.8
1	C	175	PHE	2.8
1	A	165	ILE	2.8
1	C	146	ASP	2.8
1	D	301	VAL	2.8
1	D	303	LEU	2.8
1	D	328	ARG	2.7
1	B	165	ILE	2.7
1	A	193	PRO	2.7
1	C	434	CYS	2.7
1	D	93	ALA	2.7
1	D	18	SER	2.7
1	A	167	PRO	2.7
1	A	191	ALA	2.6
1	C	19	GLN	2.6
1	B	175	PHE	2.6
1	D	44	LYS	2.6
1	D	362	ASP	2.6
1	B	32	ALA	2.5
1	C	191	ALA	2.5
1	B	170	LEU	2.5
1	D	175	PHE	2.5
1	D	335	ASP	2.5
1	B	177	TRP	2.5
1	C	358	ARG	2.4
1	C	312	ARG	2.4
1	D	38	ILE	2.4
1	C	303	LEU	2.4
1	D	50	PHE	2.4
1	D	166	SER	2.4
1	C	301	VAL	2.3
1	D	170	LEU	2.3
1	B	301	VAL	2.3
1	B	45	LEU	2.3
1	A	180	ALA	2.3
1	C	93	ALA	2.3
1	A	18	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	173	LEU	2.2
1	D	375	LYS	2.2
1	B	179	VAL	2.2
1	C	147	GLY	2.2
1	B	167	PRO	2.2
1	A	358	ARG	2.2
1	D	46	ILE	2.2
1	D	364	GLY	2.2
1	A	183	LEU	2.2
1	C	45	LEU	2.2
1	D	147	GLY	2.2
1	C	173	LEU	2.1
1	A	177	TRP	2.1
1	B	358	ARG	2.1
1	D	358	ARG	2.1
1	A	220	LEU	2.1
1	C	165	ILE	2.1
1	D	378	ASP	2.1
1	D	168	TRP	2.1
1	D	249	LYS	2.1
1	B	284	ASP	2.1
1	C	148	SER	2.1
1	D	111	HIS	2.1
1	B	245	THR	2.0
1	A	260	ASP	2.0
1	B	164	VAL	2.0
1	B	19	GLN	2.0
1	D	226	LYS	2.0
1	D	329	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

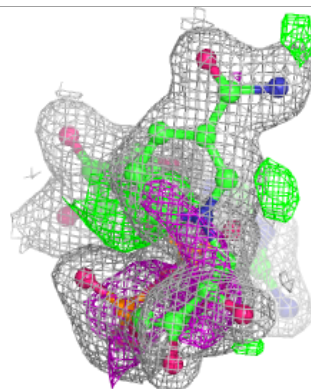
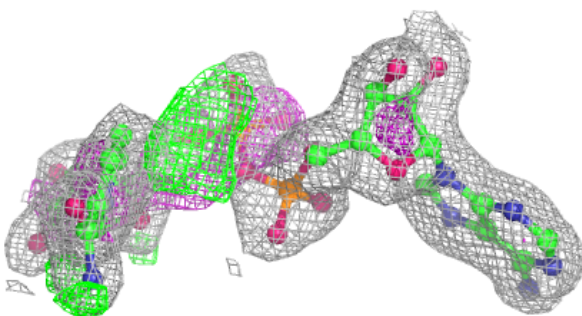
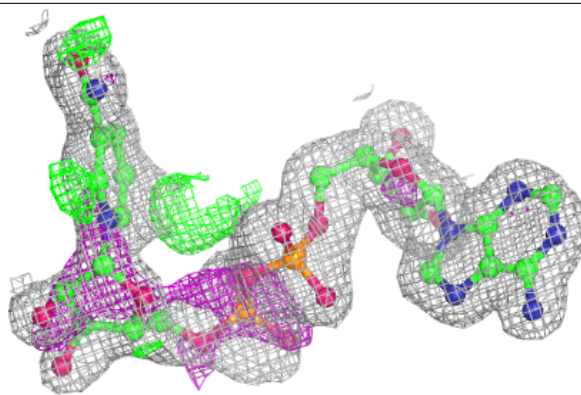
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAD	B	603	44/44	0.91	0.11	31,39,48,57	0
4	NAD	A	603	44/44	0.92	0.11	31,38,47,51	0
3	NA	D	602	1/1	0.92	0.24	37,37,37,37	0
4	NAD	D	603	44/44	0.93	0.10	33,40,48,57	0
4	NAD	C	603	44/44	0.94	0.10	29,36,45,56	0
3	NA	C	602	1/1	0.94	0.08	33,33,33,33	0
2	2VS	D	601	10/10	0.95	0.20	33,34,40,40	0
3	NA	A	602	1/1	0.96	0.10	27,27,27,27	0
3	NA	B	602	1/1	0.96	0.14	30,30,30,30	0
2	2VS	C	601	10/10	0.97	0.15	28,32,36,37	0
2	2VS	B	601	10/10	0.97	0.14	30,32,37,38	0
2	2VS	A	601	10/10	0.98	0.15	27,30,34,35	0

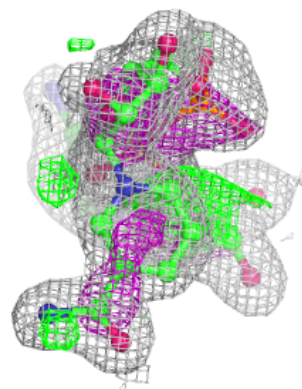
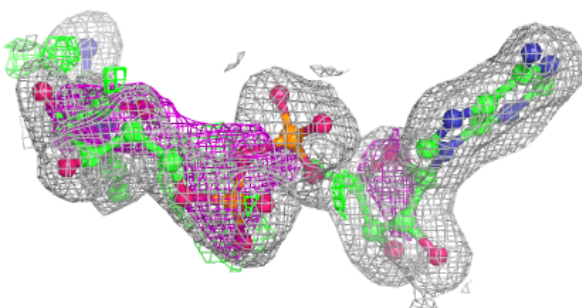
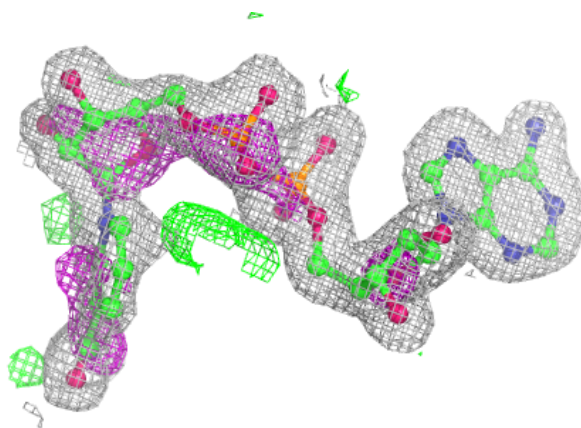
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD 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)

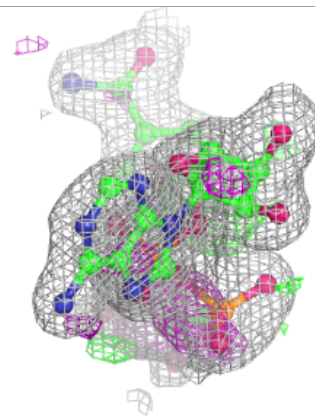
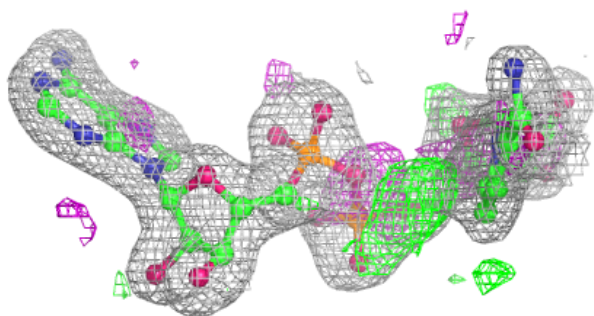
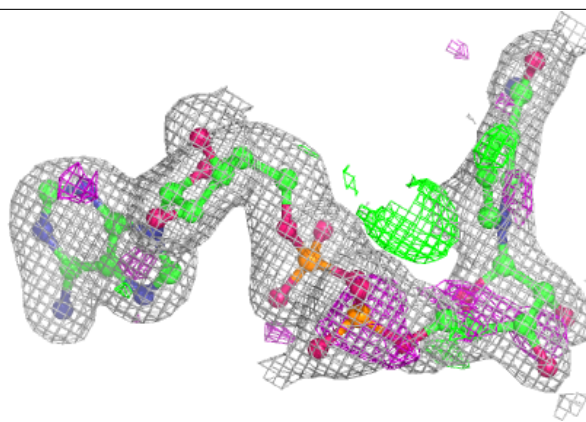
**Electron density around NAD A 603:**

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

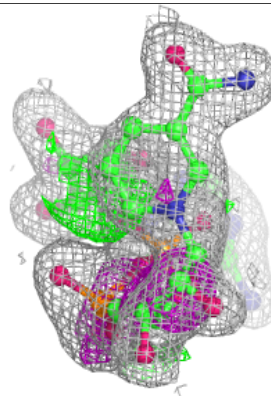
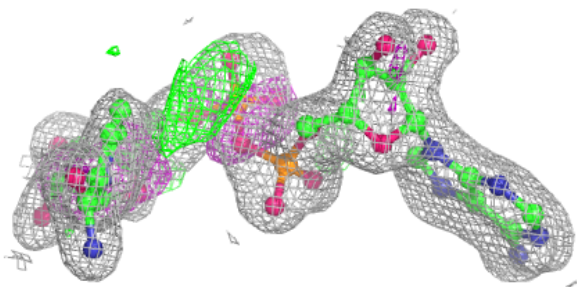
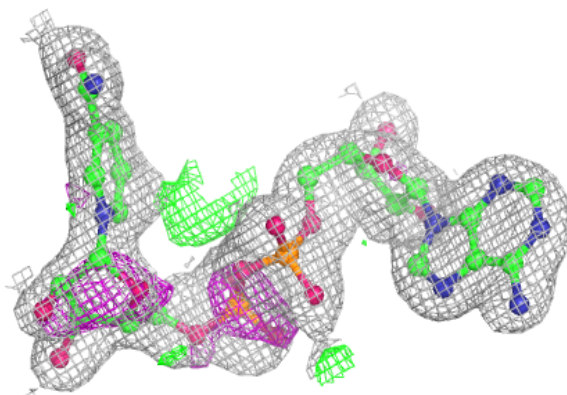


Electron density around NAD D 603:

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

**Electron density around NAD 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.