



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 05:01 PM BST

PDB ID : 6BAZ
Title : Lactate Dehydrogenase in complex with inhibitor (S)-5-((2-chlorophenyl)thio)-6'-((4-fluorophenyl)amino)-4-hydroxy-2-(thiophen-3-yl)-2,3-dihydro-[2,2'-bipyridin]-6(1H)-one
Authors : Ultsch, M.; Eigenbrot, C.
Deposited on : 2017-10-16
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

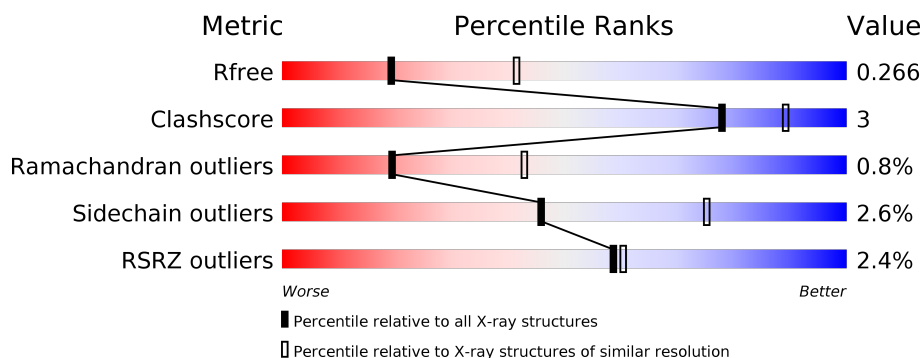
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	331	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	331	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>.</div> </div> </div>
1	C	331	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>..</div> </div> </div>
1	D	331	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>

2 Entry composition [i](#)

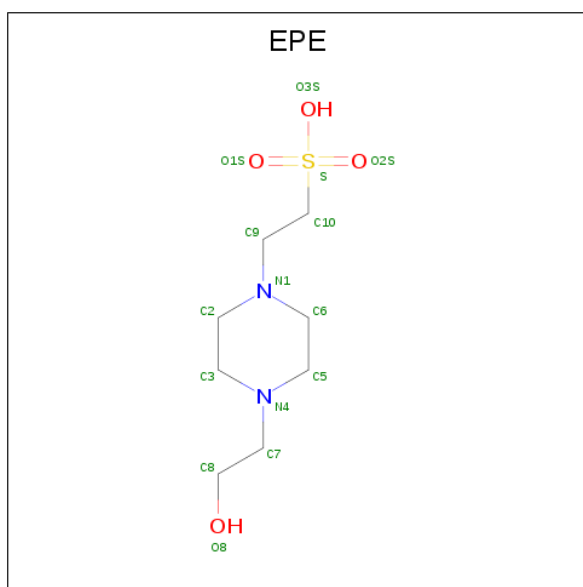
There are 7 unique types of molecules in this entry. The entry contains 10512 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	4	0
			2539	1626	429	470	14			
1	B	323	Total	C	N	O	S	0	3	0
			2524	1620	429	462	13			
1	C	328	Total	C	N	O	S	0	2	0
			2552	1632	435	472	13			
1	D	331	Total	C	N	O	S	0	3	0
			2581	1650	439	478	14			

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



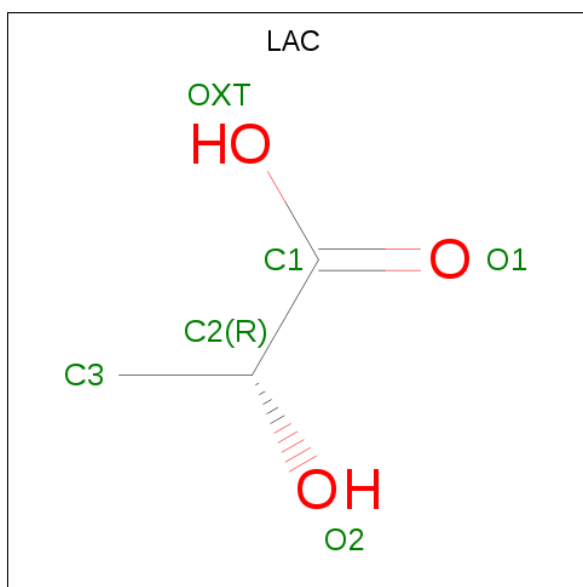
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

-
- The chemical structure of NADH (Nicotinamide Adenine Dinucleotide) is shown. It consists of a nicotinamide ring (top) linked to a ribose sugar (middle), which is connected via a pyrophosphate bridge to another ribose sugar (bottom), which is in turn linked to an adenine ring (bottom). The structure is color-coded: the nicotinamide ring is blue, the ribose sugar is red, the pyrophosphate bridge is purple, and the adenine ring is green. The structure is labeled with various atoms and groups, including NGA, NTA, C5A, C6A, C7A, C8A, C9A, C10A, C11A, C12A, C13A, C14A, C15A, C16A, C17A, C18A, C19A, C20A, C21A, C22A, C23A, C24A, C25A, C26A, C27A, C28A, C29A, C30A, C31A, C32A, C33A, C34A, C35A, C36A, C37A, C38A, C39A, C40A, C41A, C42A, C43A, C44A, C45A, C46A, C47A, C48A, C49A, C50A, C51A, C52A, C53A, C54A, C55A, C56A, C57A, C58A, C59A, C60A, C61A, C62A, C63A, C64A, C65A, C66A, C67A, C68A, C69A, C70A, C71A, C72A, C73A, C74A, C75A, C76A, C77A, C78A, C79A, C80A, C81A, C82A, C83A, C84A, C85A, C86A, C87A, C88A, C89A, C90A, C91A, C92A, C93A, C94A, C95A, C96A, C97A, C98A, C99A, C100A, C101A, C102A, C103A, C104A, C105A, C106A, C107A, C108A, C109A, C110A, C111A, C112A, C113A, C114A, C115A, C116A, C117A, C118A, C119A, C120A, C121A, C122A, C123A, C124A, C125A, C126A, C127A, C128A, C129A, C130A, C131A, C132A, C133A, C134A, C135A, C136A, C137A, C138A, C139A, C140A, C141A, C142A, C143A, C144A, C145A, C146A, C147A, C148A, C149A, C150A, C151A, C152A, C153A, C154A, C155A, C156A, C157A, C158A, C159A, C160A, C161A, C162A, C163A, C164A, C165A, C166A, C167A, C168A, C169A, C170A, C171A, C172A, C173A, C174A, C175A, C176A, C177A, C178A, C179A, C180A, C181A, C182A, C183A, C184A, C185A, C186A, C187A, C188A, C189A, C190A, C191A, C192A, C193A, C194A, C195A, C196A, C197A, C198A, C199A, C200A, C201A, C202A, C203A, C204A, C205A, C206A, C207A, C208A, C209A, C210A, C211A, C212A, C213A, C214A, C215A, C216A, C217A, C218A, C219A, C220A, C221A, C222A, C223A, C224A, C225A, C226A, C227A, C228A, C229A, C230A, C231A, C232A, C233A, C234A, C235A, C236A, C237A, C238A, C239A, C240A, C241A, C242A, C243A, C244A, C245A, C246A, C247A, C248A, C249A, C250A, C251A, C252A, C253A, C254A, C255A, C256A, C257A, C258A, C259A, C260A, C261A, C262A, C263A, C264A, C265A, C266A, C267A, C268A, C269A, C270A, C271A, C272A, C273A, C274A, C275A, C276A, C277A, C278A, C279A, C280A, C281A, C282A, C283A, C284A, C285A, C286A, C287A, C288A, C289A, C290A, C291A, C292A, C293A, C294A, C295A, C296A, C297A, C298A, C299A, C300A, C301A, C302A, C303A, C304A, C305A, C306A, C307A, C308A, C309A, C310A, C311A, C312A, C313A, C314A, C315A, C316A, C317A, C318A, C319A, C320A, C321A, C322A, C323A, C324A, C325A, C326A, C327A, C328A, C329A, C330A, C331A, C332A, C333A, C334A, C335A, C336A, C337A, C338A, C339A, C340A, C341A, C342A, C343A, C344A, C345A, C346A, C347A, C348A, C349A, C350A, C351A, C352A, C353A, C354A, C355A, C356A, C357A, C358A, C359A, C360A, C361A, C362A, C363A, C364A, C365A, C366A, C367A, C368A, C369A, C370A, C371A, C372A, C373A, C374A, C375A, C376A, C377A, C378A, C379A, C380A, C381A, C382A, C383A, C384A, C385A, C386A, C387A, C388A, C389A, C390A, C391A, C392A, C393A, C394A, C395A, C396A, C397A, C398A, C399A, C400A, C401A, C402A, C403A, C404A, C405A, C406A, C407A, C408A, C409A, C410A, C411A, C412A, C413A, C414A, C415A, C416A, C417A, C418A, C419A, C420A, C421A, C422A, C423A, C424A, C425A, C426A, C427A, C428A, C429A, C430A, C431A, C432A, C433A, C434A, C435A, C436A, C437A, C438A, C439A, C440A, C441A, C442A, C443A, C444A, C445A, C446A, C447A, C448A, C449A, C450A, C451A, C452A, C453A, C454A, C455A, C456A, C457A, C458A, C459A, C460A, C461A, C462A, C463A, C464A, C465A, C466A, C467A, C468A, C469A, C470A, C471A, C472A, C473A, C474A, C475A, C476A, C477A, C478A, C479A, C480A, C481A, C482A, C483A, C484A, C485A, C486A, C487A, C488A, C489A, C490A, C491A, C492A, C493A, C494A, C495A, C496A, C497A, C498A, C499A, C500A, C501A, C502A, C503A, C504A, C505A, C506A, C507A, C508A, C509A, C510A, C511A, C512A, C513A, C514A, C515A, C516A, C517A, C518A, C519A, C520A, C521A, C522A, C523A, C524A, C525A, C526A, C527A, C528A, C529A, C530A, C531A, C532A, C533A, C534A, C535A, C536A, C537A, C538A, C539A, C540A, C541A, C542A, C543A, C544A, C545A, C546A, C547A, C548A, C549A, C550A, C551A, C552A, C553A, C554A, C555A, C556A, C557A, C558A, C559A, C560A, C561A, C562A, C563A, C564A, C565A, C566A, C567A, C568A, C569A, C570A, C571A, C572A, C573A, C574A, C575A, C576A, C577A, C578A, C579A, C580A, C581A, C582A, C583A, C584A, C585A, C586A, C587A, C588A, C589A, C590A, C591A, C592A, C593A, C594A, C595A, C596A, C597A, C598A, C599A, C600A, C601A, C602A, C603A, C604A, C605A, C606A, C607A, C608A, C609A, C610A, C611A, C612A, C613A, C614A, C615A, C616A, C617A, C618A, C619A, C620A, C621A, C622A, C623A, C624A, C625A, C626A, C627A, C628A, C629A, C630A, C631A, C632A, C633A, C634A, C635A, C636A, C637A, C638A, C639A, C640A, C641A, C642A, C643A, C644A, C645A, C646A, C647A, C648A, C649A, C650A, C651A, C652A, C653A, C654A, C655A, C656A, C657A, C658A, C659A, C660A, C661A, C662A, C663A, C664A, C665A, C666A, C667A, C668A, C669A, C670A, C671A, C672A, C673A, C674A, C675A,

- Molecule 4 is LACTIC ACID (three-letter code: LAC) (formula: $C_3H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

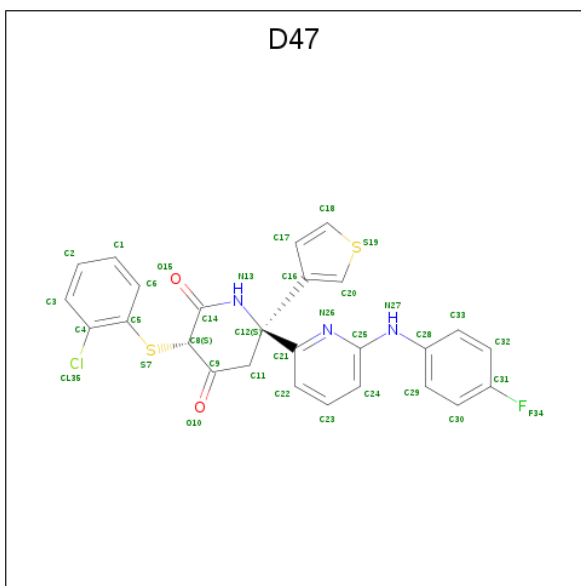
- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

- Molecule 6 is (3S,6S)-3-[(2-chlorophenyl)sulfanyl]-6-{6-[(4-fluorophenyl)amino]pyridin-2-yl}-

6-(thiophen-3-yl)piperidine-2,4-dione (three-letter code: D47) (formula: C₂₆H₁₉ClFN₃O₂S₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	C	1	Total	C	Cl	F	N	O	S	0	0
			35	26	1	1	3	2	2		
6	D	1	Total	C	Cl	F	N	O	S	0	0
			35	26	1	1	3	2	2		

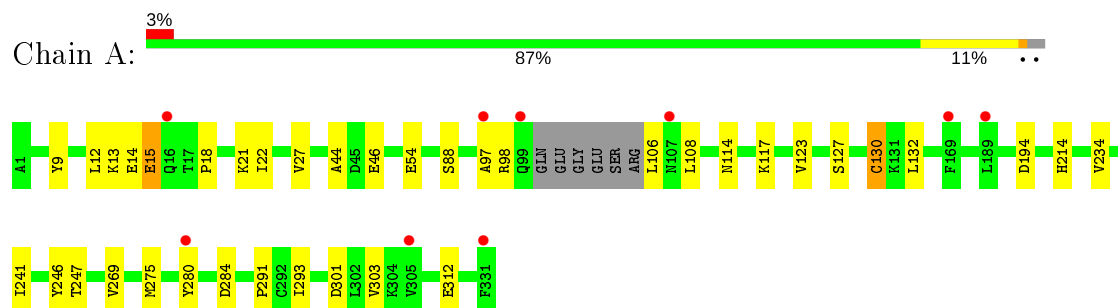
- Molecule 7 is water.

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

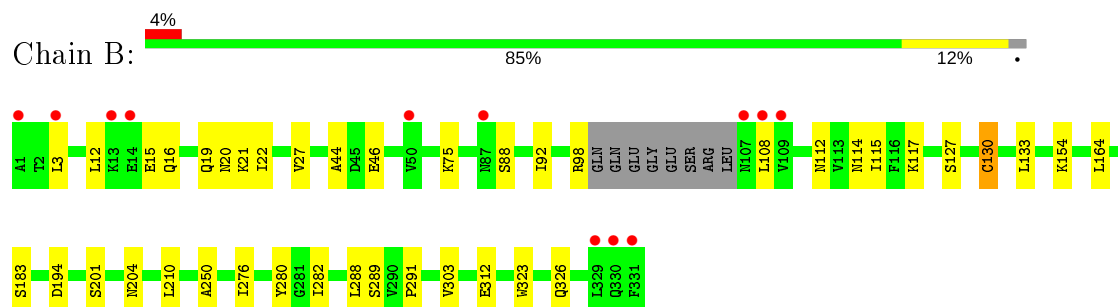
3 Residue-property plots [i](#)

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.

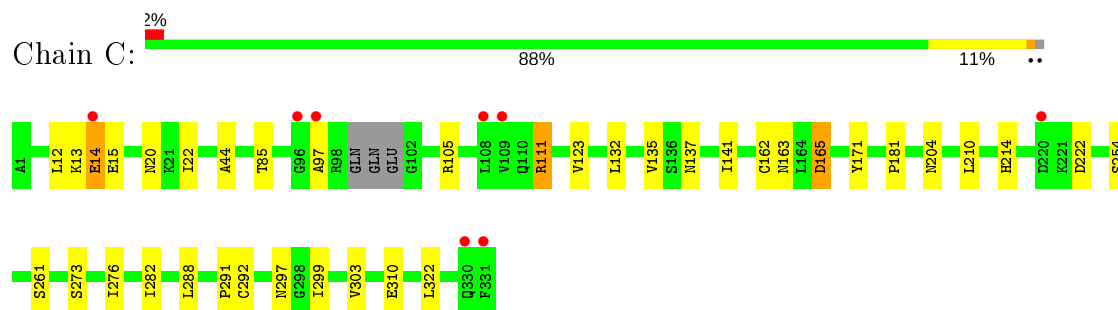
• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.70 Å 80.08 Å 103.67 Å 90.00° 97.37° 90.00°	Depositor
Resolution (Å)	46.30 – 2.70 43.26 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.30-2.70) 98.7 (43.26-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.69 Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.213 , 0.261 0.212 , 0.266	Depositor DCC
R_{free} test set	703 reflections (2.12%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10512	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, D47, SO4, NAD, LAC

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	0.40	0/2594	0.61	0/3507
1	B	0.39	0/2577	0.61	0/3484
1	C	0.41	0/2601	0.61	0/3515
1	D	0.39	0/2634	0.61	0/3561
All	All	0.40	0/10406	0.61	0/14067

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2539	0	2638	18	0
1	B	2524	0	2628	18	0
1	C	2552	0	2650	18	0
1	D	2581	0	2681	14	0
2	A	15	0	17	0	0
2	B	15	0	17	0	0
2	C	15	0	17	0	0
3	A	44	0	25	1	0
3	B	44	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	44	0	25	1	0
3	D	44	0	25	0	0
4	A	6	0	5	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	C	35	0	0	0	0
6	D	35	0	0	0	0
7	A	3	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
All	All	10512	0	10753	62	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 (62) 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:A:14:GLU:HB3	1:A:15:GLU:HA	1.31	1.09
1:A:14:GLU:HB3	1:A:15:GLU:CA	2.13	0.78
1:B:276:ILE:HG12	1:B:288:LEU:HB2	1.82	0.61
1:C:276:ILE:HG12	1:C:288:LEU:HB2	1.86	0.58
1:A:9:TYR:HB2	1:D:304:LYS:HE2	1.89	0.55
1:D:293[A]:ILE:HD12	1:D:301:ASP:HB2	1.88	0.55
1:A:18:PRO:HB2	1:A:21:LYS:HB2	1.87	0.54
1:A:269:VAL:HG22	1:A:293:ILE:HD13	1.88	0.54
1:B:21:LYS:HB3	1:B:88:SER:HA	1.89	0.54
1:A:293:ILE:HG13	1:A:301:ASP:HB2	1.90	0.53
1:A:123:VAL:HG11	1:A:132:LEU:HD21	1.89	0.53
1:C:214:HIS:HB2	1:D:3:LEU:HD13	1.89	0.53
1:B:46:GLU:HG3	1:B:75:LYS:HB3	1.91	0.52
1:D:127:SER:HB3	1:D:130:CYS:HB3	1.92	0.52
1:C:135:VAL:O	3:C:402:NAD:H2N	2.10	0.51
1:A:21:LYS:HB3	1:A:88:SER:HA	1.91	0.51
1:A:291:PRO:HB2	1:A:303:VAL:HB	1.92	0.50
1:A:22:ILE:HD12	1:A:44:ALA:HB2	1.92	0.50
1:A:114:ASN:HA	1:A:117:LYS:HD3	1.93	0.50
1:C:276:ILE:HD13	1:C:282:ILE:HD13	1.94	0.48
1:D:236:SER:O	1:D:240:VAL:HG23	2.12	0.48
1:B:291:PRO:HB2	1:B:303:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:VAL:HG11	1:C:132:LEU:HD21	1.96	0.47
1:B:16:GLN:HE21	1:C:297:ASN:HD22	1.62	0.47
1:A:280:TYR:HB3	1:A:312[B]:GLU:HG3	1.94	0.47
1:B:114:ASN:HA	1:B:117:LYS:HD2	1.98	0.46
1:B:127:SER:HB3	1:B:130:CYS:HB3	1.96	0.46
1:B:20:ASN:HD21	1:C:20:ASN:HD21	1.63	0.46
1:C:171:TYR:HA	1:C:181:PRO:HG3	1.98	0.46
1:D:123:VAL:HG11	1:D:132:LEU:HD21	1.98	0.45
1:C:97:ALA:HB3	1:C:111:ARG:HH22	1.80	0.45
1:B:92:ILE:HG12	1:B:133:LEU:HD23	1.99	0.45
1:A:241:ILE:HD13	1:A:246:TYR:HA	1.98	0.45
1:B:22:ILE:HD12	1:B:44:ALA:HB2	1.98	0.45
1:A:214:HIS:HB2	1:B:3:LEU:HD13	1.99	0.44
1:A:127:SER:HB3	1:A:130:CYS:HB3	1.98	0.44
1:B:183:SER:HB3	1:D:269:VAL:HG23	1.99	0.44
1:A:194:ASP:HA	1:A:234:VAL:HG21	2.00	0.43
1:D:293[B]:ILE:HD13	1:D:301:ASP:HB2	1.99	0.43
1:A:21:LYS:HG3	1:A:46:GLU:HB3	2.00	0.43
1:C:12:LEU:HD13	1:C:14:GLU:HB2	2.00	0.43
1:B:164:LEU:HD11	1:B:250:ALA:HB1	2.00	0.43
1:B:112:ASN:HA	1:B:115:ILE:HD12	1.99	0.43
1:C:163:ASN:HD22	1:C:254:SER:HB2	1.84	0.42
1:D:105:ARG:O	1:D:109:VAL:HG23	2.19	0.42
1:D:22:ILE:HD12	1:D:44:ALA:HB2	2.01	0.42
1:C:291:PRO:HG2	1:C:303:VAL:HB	2.01	0.42
1:B:204:ASN:HA	1:B:210:LEU:HD13	2.01	0.42
1:B:280:TYR:HB3	1:B:312:GLU:HG3	2.02	0.42
1:C:204:ASN:HA	1:C:210:LEU:HD13	2.01	0.42
1:B:323:TRP:HA	1:B:326:GLN:HB2	2.02	0.41
1:C:22:ILE:HD12	1:C:44:ALA:HB2	2.02	0.41
1:D:104:SER:H	1:D:107:ASN:HD22	1.68	0.41
1:C:105:ARG:HH22	1:C:137:ASN:HB3	1.86	0.41
1:D:92:ILE:HG12	1:D:133:LEU:HD23	2.02	0.41
1:C:292:CYS:HB3	1:C:299:ILE:HG23	2.02	0.41
1:D:292:CYS:HB3	1:D:299:ILE:HG23	2.02	0.41
1:C:141:ILE:HG13	1:C:322:LEU:HD22	2.04	0.40
1:A:247:THR:OG1	3:A:402:NAD:H5N	2.21	0.40
1:B:280:TYR:HB2	1:B:282:ILE:HD12	2.04	0.40
1:C:162:CYS:HA	1:C:165:ASP:OD2	2.21	0.40
1:D:189:LEU:HD22	1:D:290:VAL:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	325/331 (98%)	308 (95%)	14 (4%)	3 (1%)	17	40
1	B	322/331 (97%)	305 (95%)	14 (4%)	3 (1%)	17	40
1	C	326/331 (98%)	312 (96%)	12 (4%)	2 (1%)	25	50
1	D	332/331 (100%)	316 (95%)	14 (4%)	2 (1%)	25	50
All	All	1305/1324 (99%)	1241 (95%)	54 (4%)	10 (1%)	19	43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ARG
1	C	14	GLU
1	B	15	GLU
1	C	222	ASP
1	D	15	GLU
1	A	97	ALA
1	B	154	LYS
1	A	27	VAL
1	D	27	VAL
1	B	27	VAL

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	286/287 (100%)	277 (97%)	9 (3%)	40	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	283/287 (99%)	275 (97%)	8 (3%)	43	73
1	C	286/287 (100%)	278 (97%)	8 (3%)	43	73
1	D	290/287 (101%)	286 (99%)	4 (1%)	67	86
All	All	1145/1148 (100%)	1116 (98%)	29 (2%)	46	76

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	13	LYS
1	A	15	GLU
1	A	54	GLU
1	A	106	LEU
1	A	108	LEU
1	A	130	CYS
1	A	275	MET
1	A	284	ASP
1	B	12	LEU
1	B	19	GLN
1	B	98	ARG
1	B	108	LEU
1	B	130	CYS
1	B	194	ASP
1	B	201	SER
1	B	289	SER
1	C	13	LYS
1	C	15	GLU
1	C	85	THR
1	C	111	ARG
1	C	165	ASP
1	C	261	SER
1	C	273	SER
1	C	310	GLU
1	D	8	ILE
1	D	14	GLU
1	D	165	ASP
1	D	315	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	16	GLN
1	C	20	ASN
1	C	296	GLN
1	D	107	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	$\# Z > 2$
6	D47	C	403	-	32,39,39	1.30	2 (6%)	37,56,56	1.62	7 (18%)
5	SO4	A	404	-	4,4,4	0.15	0	6,6,6	0.08	0
2	EPE	C	401	-	15,15,15	1.15	1 (6%)	18,20,20	0.38	0
2	EPE	B	401	-	15,15,15	1.09	1 (6%)	18,20,20	0.29	0
3	NAD	A	402	-	42,48,48	1.87	8 (19%)	50,73,73	1.41	9 (18%)
3	NAD	B	402	-	42,48,48	1.86	10 (23%)	50,73,73	1.28	6 (12%)
6	D47	D	802	-	32,39,39	1.26	2 (6%)	37,56,56	1.60	7 (18%)
4	LAC	A	403	-	2,5,5	0.46	0	3,6,6	0.71	0
2	EPE	A	401	-	15,15,15	1.19	1 (6%)	18,20,20	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	B	403	-	4,4,4	0.18	0	6,6,6	0.08	0
3	NAD	D	801	-	42,48,48	1.89	11 (26%)	50,73,73	1.37	9 (18%)
3	NAD	C	402	-	42,48,48	1.88	9 (21%)	50,73,73	1.38	8 (16%)

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
6	D47	C	403	-	-	3/12/38/38	0/5/5/5
2	EPE	C	401	-	-	0/9/19/19	0/1/1/1
2	EPE	B	401	-	-	2/9/19/19	0/1/1/1
3	NAD	A	402	-	-	10/26/62/62	0/5/5/5
6	D47	D	802	-	-	1/12/38/38	0/5/5/5
4	LAC	A	403	-	-	0/0/4/4	-
2	EPE	A	401	-	-	5/9/19/19	0/1/1/1
3	NAD	B	402	-	-	7/26/62/62	0/5/5/5
3	NAD	D	801	-	-	6/26/62/62	0/5/5/5
3	NAD	C	402	-	-	3/26/62/62	0/5/5/5

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	801	NAD	C7N-N7N	5.18	1.42	1.33
6	C	403	D47	C20-C16	-5.15	1.33	1.37
3	B	402	NAD	C7N-N7N	5.11	1.42	1.33
3	C	402	NAD	C7N-N7N	5.08	1.42	1.33
3	A	402	NAD	C7N-N7N	5.04	1.42	1.33
6	D	802	D47	C20-C16	-5.02	1.34	1.37
3	A	402	NAD	C2B-C3B	-4.61	1.40	1.53
3	C	402	NAD	C2B-C3B	-4.53	1.40	1.53
3	D	801	NAD	C2B-C3B	-4.48	1.41	1.53
3	B	402	NAD	C2B-C3B	-4.46	1.41	1.53
2	A	401	EPE	C10-S	-4.42	1.71	1.77
2	C	401	EPE	C10-S	-4.30	1.71	1.77
2	B	401	EPE	C10-S	-4.17	1.71	1.77
3	B	402	NAD	O2D-C2D	-3.55	1.34	1.43
3	D	801	NAD	O2D-C2D	-3.55	1.34	1.43
6	C	403	D47	C20-S19	3.54	1.75	1.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	801	NAD	C2B-C1B	-3.45	1.48	1.53
3	C	402	NAD	C6A-N6A	3.42	1.46	1.34
3	C	402	NAD	O2D-C2D	-3.42	1.34	1.43
3	A	402	NAD	O2D-C2D	-3.40	1.35	1.43
3	B	402	NAD	C6A-N6A	3.39	1.46	1.34
3	A	402	NAD	C6A-N6A	3.31	1.46	1.34
3	D	801	NAD	C6A-N6A	3.23	1.45	1.34
6	D	802	D47	C20-S19	3.08	1.74	1.70
3	A	402	NAD	C2B-C1B	-2.86	1.49	1.53
3	C	402	NAD	C2B-C1B	-2.85	1.49	1.53
3	B	402	NAD	C2B-C1B	-2.70	1.49	1.53
3	C	402	NAD	C5D-C4D	-2.50	1.43	1.51
3	A	402	NAD	C5D-C4D	-2.50	1.43	1.51
3	B	402	NAD	C2D-C1D	-2.49	1.50	1.53
3	C	402	NAD	C2D-C1D	-2.45	1.50	1.53
3	D	801	NAD	C5D-C4D	-2.44	1.44	1.51
3	D	801	NAD	C2D-C1D	-2.32	1.50	1.53
3	B	402	NAD	C5D-C4D	-2.30	1.44	1.51
3	D	801	NAD	O4B-C4B	-2.25	1.40	1.45
3	D	801	NAD	C5B-C4B	-2.18	1.44	1.51
3	A	402	NAD	C2D-C1D	-2.18	1.50	1.53
3	A	402	NAD	C5B-C4B	-2.15	1.44	1.51
3	C	402	NAD	C2N-N1N	2.15	1.37	1.35
3	D	801	NAD	O2B-C2B	-2.14	1.37	1.43
3	B	402	NAD	C5B-C4B	-2.13	1.45	1.51
3	C	402	NAD	C5B-C4B	-2.11	1.45	1.51
3	B	402	NAD	C3D-C4D	-2.05	1.47	1.53
3	D	801	NAD	C2N-N1N	2.03	1.37	1.35
3	B	402	NAD	O4B-C4B	-2.00	1.40	1.45

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	802	D47	C16-C20-S19	-4.89	109.14	112.29
3	B	402	NAD	N3A-C2A-N1A	-4.72	121.31	128.68
3	D	801	NAD	N3A-C2A-N1A	-4.60	121.50	128.68
3	A	402	NAD	N3A-C2A-N1A	-4.44	121.75	128.68
6	C	403	D47	C16-C20-S19	-4.40	109.45	112.29
3	C	402	NAD	N3A-C2A-N1A	-4.35	121.88	128.68
6	C	403	D47	C12-N13-C14	4.02	125.69	117.58
6	D	802	D47	C25-N26-C21	4.02	123.87	118.17
6	D	802	D47	C12-N13-C14	3.88	125.40	117.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	403	D47	C25-N26-C21	3.64	123.32	118.17
3	D	801	NAD	PN-O3-PA	-3.63	120.38	132.83
3	A	402	NAD	PN-O3-PA	-3.31	121.48	132.83
3	C	402	NAD	PN-O3-PA	-3.08	122.26	132.83
3	C	402	NAD	O5D-C5D-C4D	3.04	119.46	108.99
6	C	403	D47	O15-C14-N13	-2.83	118.77	123.07
6	D	802	D47	O15-C14-N13	-2.71	118.95	123.07
3	A	402	NAD	O7N-C7N-N7N	-2.71	118.73	122.58
3	A	402	NAD	C6N-N1N-C2N	-2.69	119.53	121.97
3	B	402	NAD	PN-O3-PA	-2.67	123.67	132.83
3	A	402	NAD	C3N-C7N-N7N	2.65	120.93	117.75
3	C	402	NAD	O4B-C1B-C2B	-2.63	103.08	106.93
3	B	402	NAD	O5D-C5D-C4D	2.63	118.04	108.99
3	C	402	NAD	O7N-C7N-N7N	-2.57	118.92	122.58
3	A	402	NAD	O5D-C5D-C4D	2.57	117.83	108.99
3	D	801	NAD	O7N-C7N-N7N	-2.56	118.94	122.58
3	D	801	NAD	C3N-C7N-N7N	2.52	120.78	117.75
6	D	802	D47	C24-C25-N26	-2.44	119.05	123.16
3	D	801	NAD	O4B-C1B-C2B	-2.40	103.41	106.93
3	D	801	NAD	O4D-C1D-C2D	-2.40	103.42	106.93
3	D	801	NAD	C4A-C5A-N7A	-2.38	106.92	109.40
6	C	403	D47	C24-C25-N26	-2.36	119.18	123.16
3	A	402	NAD	C4A-C5A-N7A	-2.34	106.96	109.40
3	D	801	NAD	O5D-C5D-C4D	2.31	116.94	108.99
3	C	402	NAD	C3N-C7N-N7N	2.26	120.46	117.75
3	C	402	NAD	C4A-C5A-N7A	-2.24	107.06	109.40
3	B	402	NAD	O4B-C1B-C2B	-2.22	103.69	106.93
3	C	402	NAD	C6N-N1N-C2N	-2.21	119.96	121.97
3	A	402	NAD	C3D-C2D-C1D	2.18	104.26	100.98
6	D	802	D47	C12-C21-N26	2.15	119.41	116.12
3	B	402	NAD	O7N-C7N-N7N	-2.14	119.53	122.58
3	A	402	NAD	O4B-C1B-C2B	-2.11	103.85	106.93
6	D	802	D47	C22-C21-N26	-2.10	119.44	122.20
6	C	403	D47	C12-C21-N26	2.09	119.31	116.12
3	D	801	NAD	C6N-N1N-C2N	-2.08	120.08	121.97
3	B	402	NAD	C6N-N1N-C2N	-2.06	120.09	121.97
6	C	403	D47	C22-C21-N26	-2.04	119.52	122.20

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	NAD	C5B-O5B-PA-O3
3	A	402	NAD	O4D-C1D-N1N-C2N
3	A	402	NAD	O4D-C1D-N1N-C6N
3	A	402	NAD	C2D-C1D-N1N-C2N
3	B	402	NAD	C5D-O5D-PN-O1N
3	B	402	NAD	O4D-C1D-N1N-C2N
3	B	402	NAD	O4D-C1D-N1N-C6N
3	B	402	NAD	C2D-C1D-N1N-C2N
3	B	402	NAD	C2D-C1D-N1N-C6N
3	D	801	NAD	C5D-O5D-PN-O1N
3	D	801	NAD	O4D-C1D-N1N-C2N
3	D	801	NAD	O4D-C1D-N1N-C6N
3	D	801	NAD	C2D-C1D-N1N-C2N
2	A	401	EPE	C10-C9-N1-C2
2	A	401	EPE	C9-C10-S-O1S
2	A	401	EPE	C9-C10-S-O3S
3	C	402	NAD	O4D-C1D-N1N-C2N
3	C	402	NAD	O4D-C1D-N1N-C6N
2	B	401	EPE	C8-C7-N4-C5
3	A	402	NAD	PN-O3-PA-O1A
2	B	401	EPE	C8-C7-N4-C3
3	A	402	NAD	O4B-C4B-C5B-O5B
3	B	402	NAD	C5D-O5D-PN-O3
3	A	402	NAD	C5B-O5B-PA-O1A
2	A	401	EPE	C9-C10-S-O2S
6	D	802	D47	C11-C12-C21-C22
3	B	402	NAD	O4B-C4B-C5B-O5B
2	A	401	EPE	C10-C9-N1-C6
3	D	801	NAD	O4B-C4B-C5B-O5B
6	C	403	D47	C29-C28-N27-C25
6	C	403	D47	C33-C28-N27-C25
3	A	402	NAD	C2D-C1D-N1N-C6N
3	D	801	NAD	C5D-O5D-PN-O3
3	C	402	NAD	O4B-C4B-C5B-O5B
3	A	402	NAD	C5B-O5B-PA-O2A
3	A	402	NAD	C5D-O5D-PN-O1N
6	C	403	D47	C11-C12-C21-C22

There are no ring outliers.

2 monomers are involved in 2 short contacts:

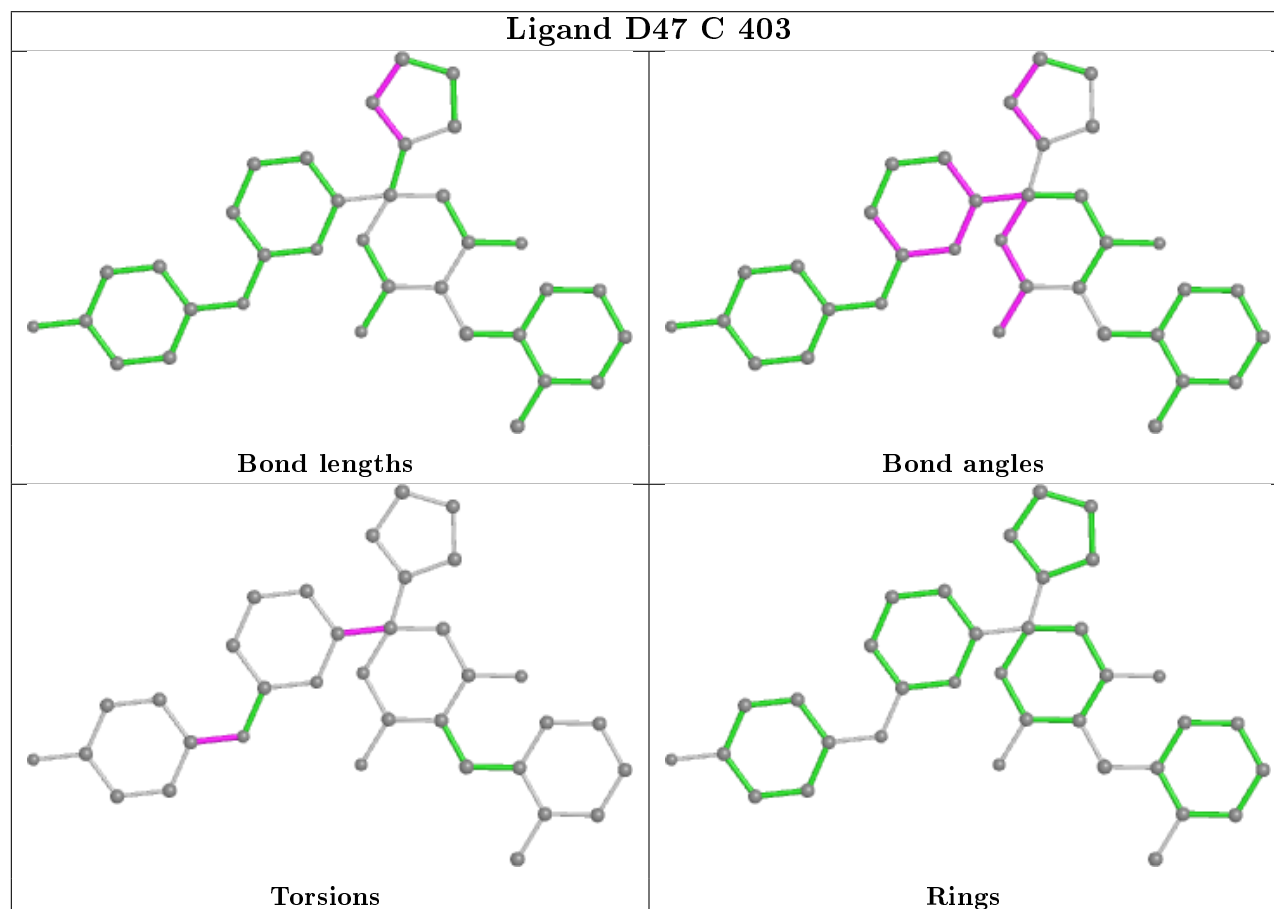
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	NAD	1	0

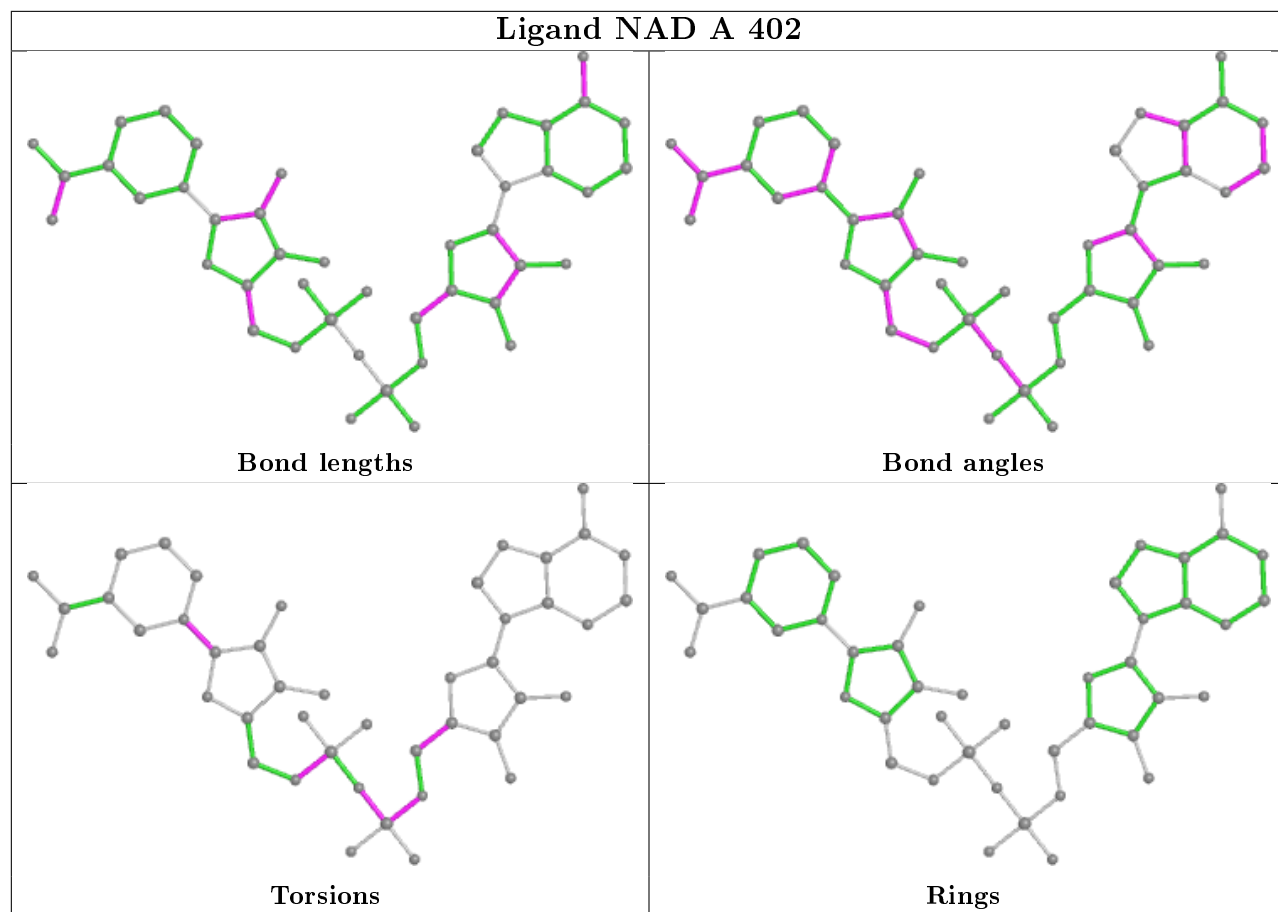
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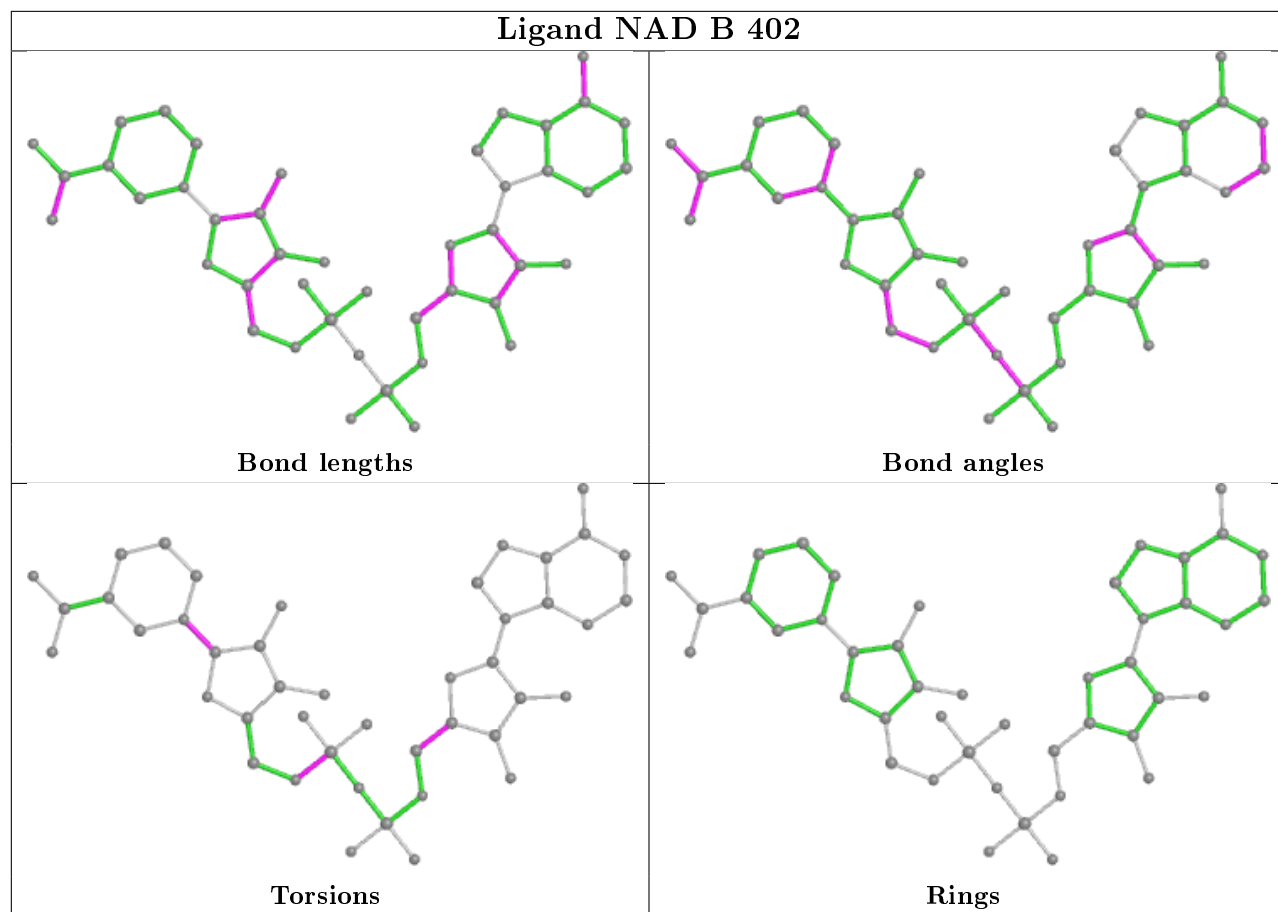
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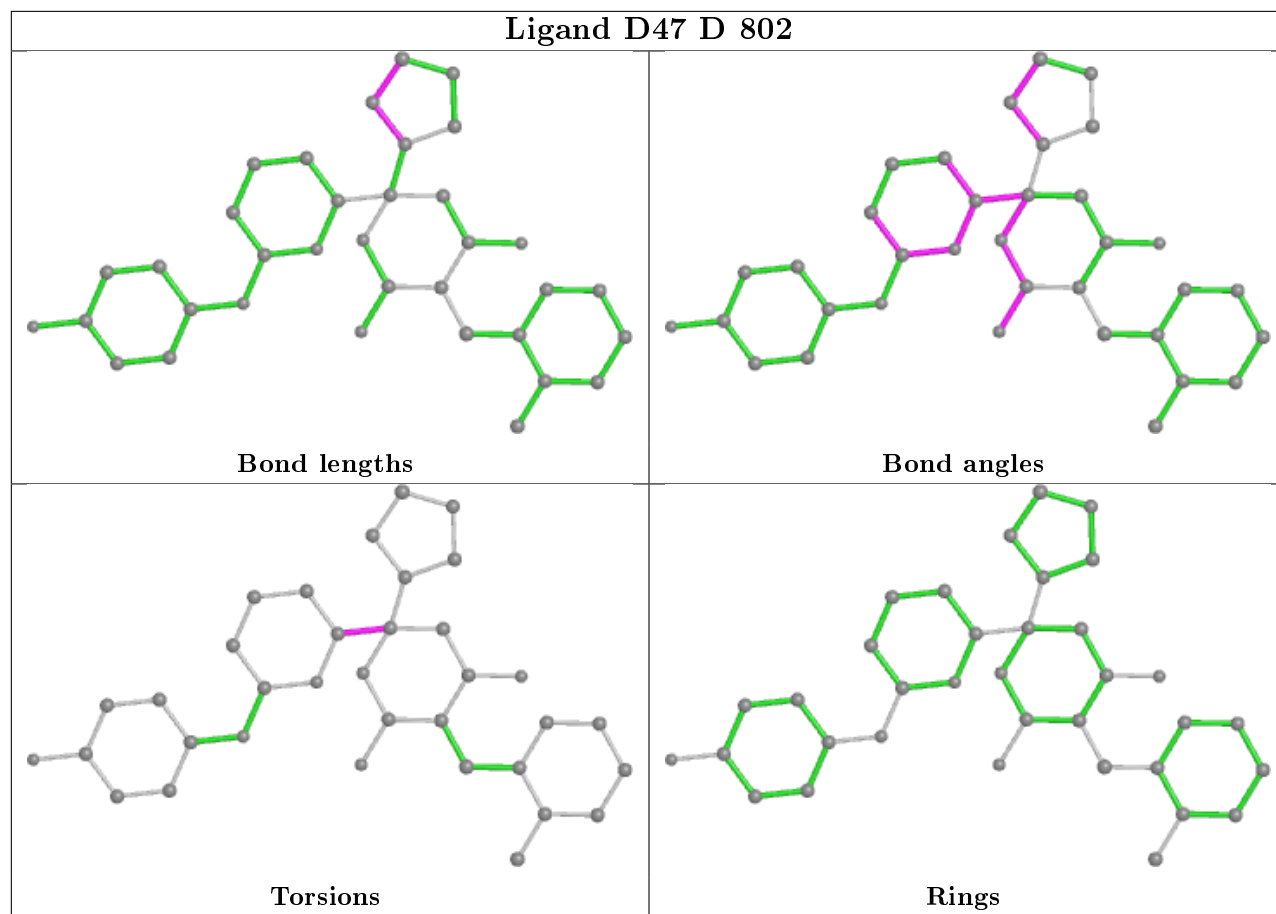
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	NAD	1	0

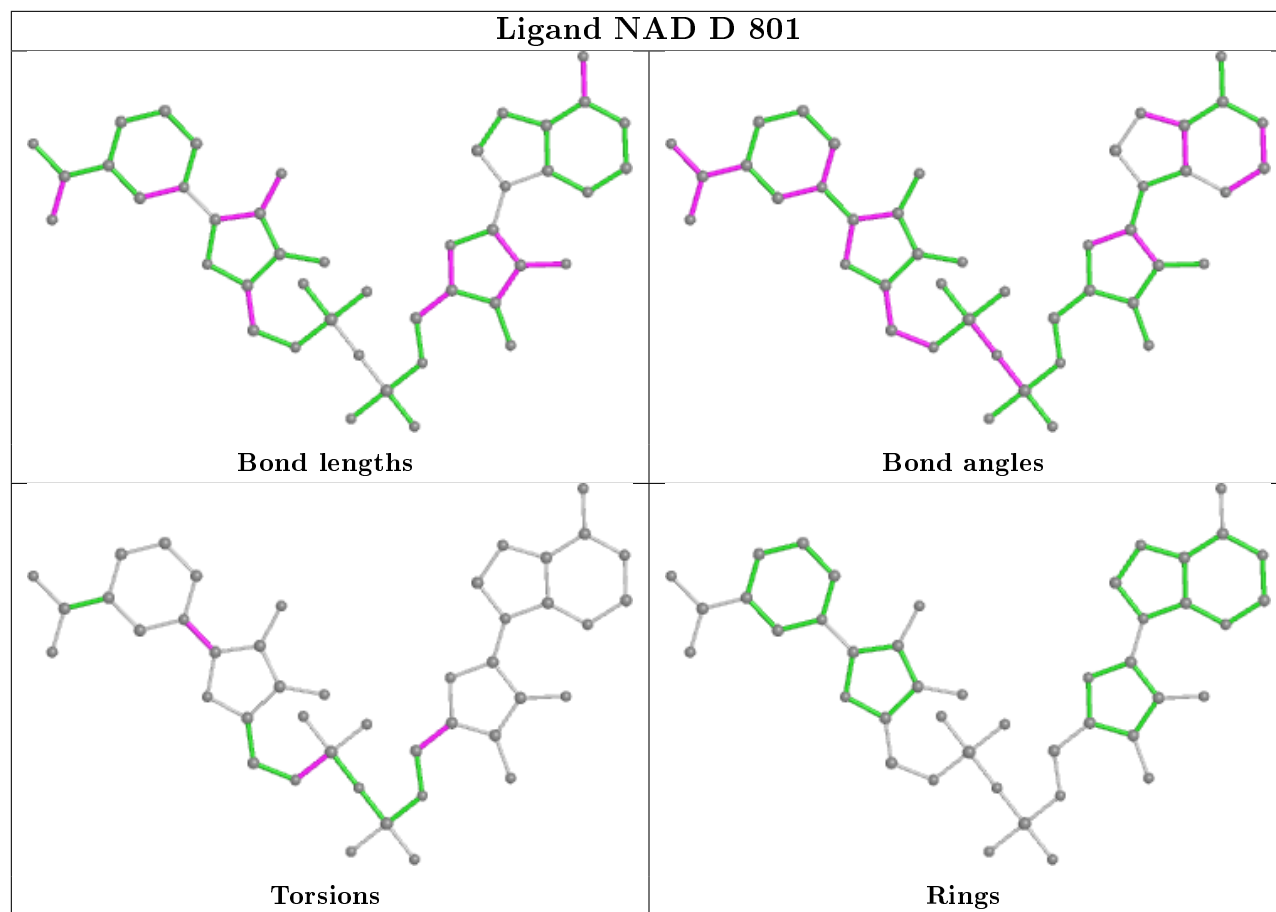
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

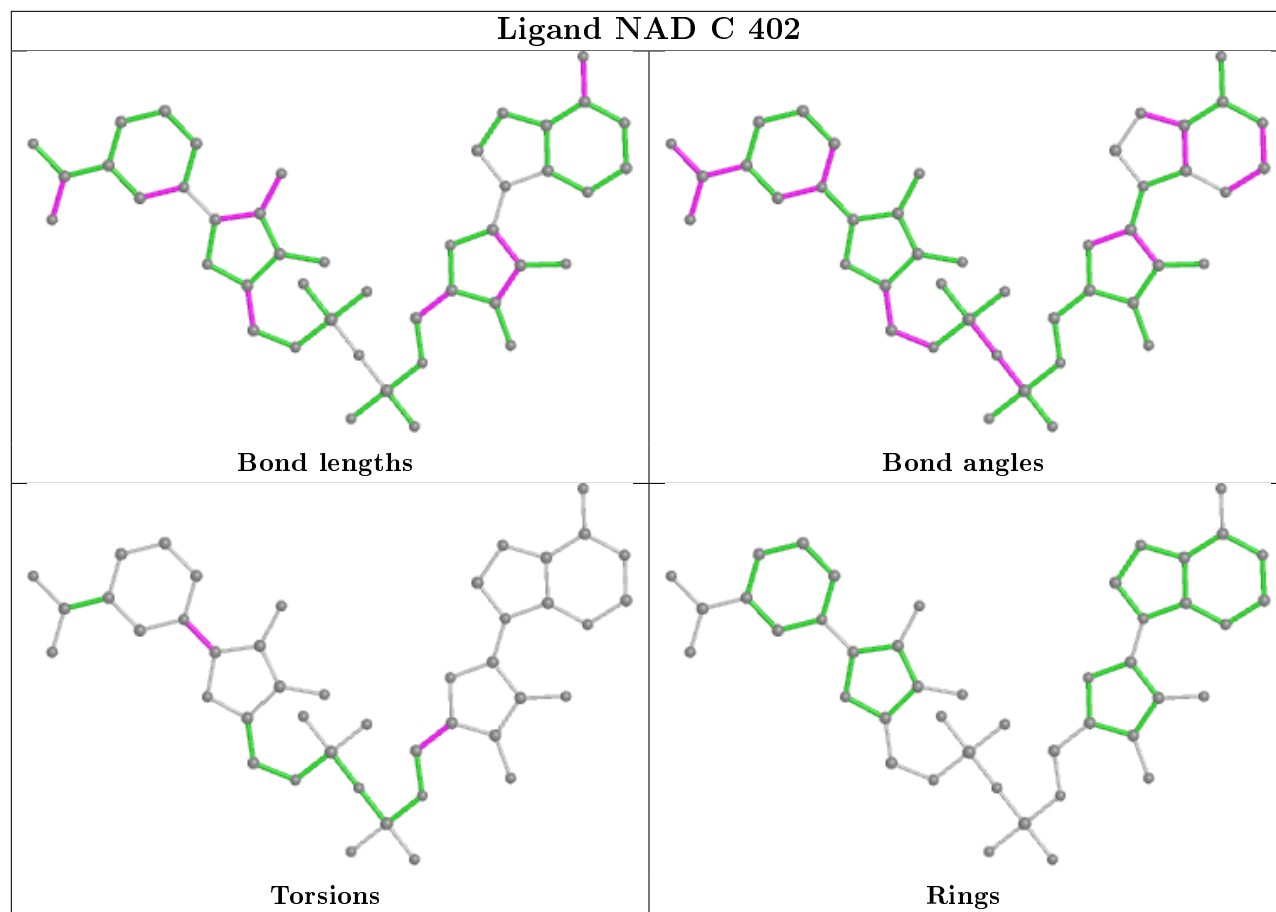












5.7 Other polymers [i](#)

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	325/331 (98%)	-0.10	9 (2%) 53 54	44, 61, 93, 133	0
1	B	323/331 (97%)	-0.23	12 (3%) 41 41	45, 63, 91, 120	0
1	C	328/331 (99%)	-0.01	8 (2%) 59 60	43, 64, 103, 134	0
1	D	331/331 (100%)	-0.25	3 (0%) 84 85	43, 57, 89, 108	0
All	All	1307/1324 (98%)	-0.15	32 (2%) 59 60	43, 62, 93, 134	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	GLN	5.2
1	B	331	PHE	4.8
1	B	1	ALA	4.2
1	B	50	VAL	3.8
1	C	97	ALA	3.7
1	D	1	ALA	3.3
1	A	99	GLN	3.1
1	B	87	ASN	3.1
1	B	108	LEU	2.9
1	A	305	VAL	2.9
1	B	107	ASN	2.9
1	B	13	LYS	2.8
1	A	97	ALA	2.8
1	A	331	PHE	2.8
1	D	3	LEU	2.7
1	A	107	ASN	2.7
1	C	331	PHE	2.7
1	D	15	GLU	2.6
1	A	280	TYR	2.6
1	A	16	GLN	2.5
1	B	14	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	3	LEU	2.4
1	C	220	ASP	2.4
1	C	96	GLY	2.4
1	A	169	PHE	2.4
1	B	109	VAL	2.3
1	C	14	GLU	2.2
1	C	109	VAL	2.2
1	B	329	LEU	2.2
1	C	330	GLN	2.0
1	A	189	LEU	2.0
1	C	108	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 [i](#)

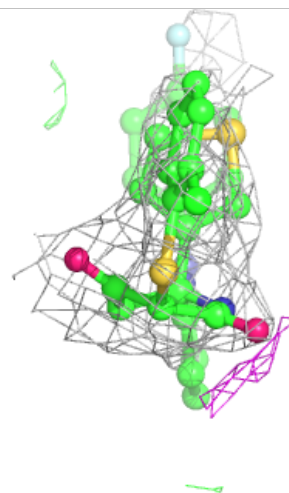
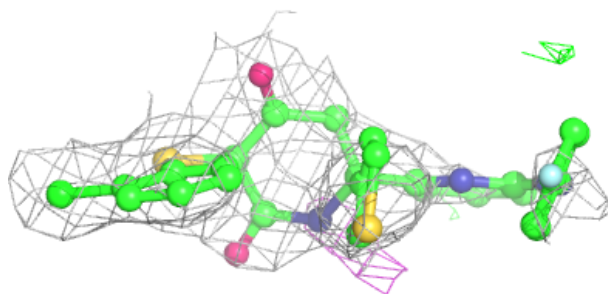
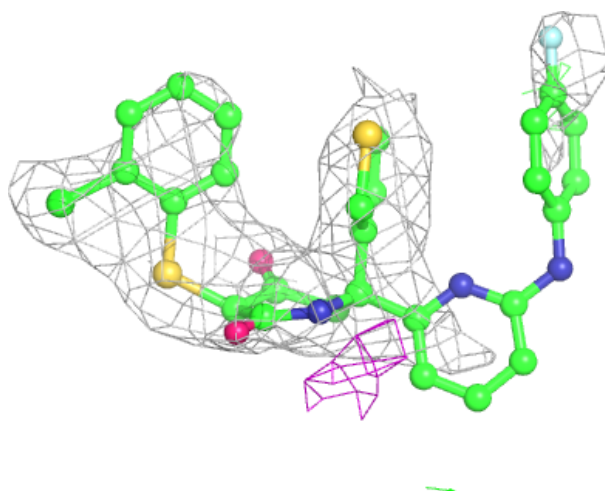
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	D47	C	403	35/35	0.78	0.35	105,119,124,124	0
2	EPE	C	401	15/15	0.78	0.27	103,108,110,110	15
2	EPE	A	401	15/15	0.79	0.37	75,77,81,81	15
5	SO4	B	403	5/5	0.81	0.47	68,69,69,69	5
2	EPE	B	401	15/15	0.82	0.27	112,113,115,115	15
5	SO4	A	404	5/5	0.84	0.51	83,83,84,84	5
4	LAC	A	403	6/6	0.85	0.14	60,61,62,62	0
3	NAD	C	402	44/44	0.91	0.20	81,85,93,93	0
6	D47	D	802	35/35	0.93	0.23	62,77,85,86	0
3	NAD	A	402	44/44	0.94	0.14	61,65,68,70	0
3	NAD	B	402	44/44	0.95	0.16	60,64,66,67	0
3	NAD	D	801	44/44	0.97	0.13	47,53,60,64	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.

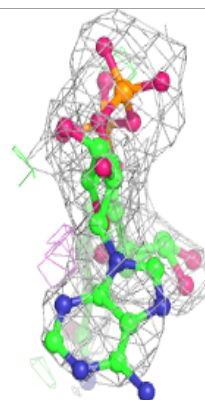
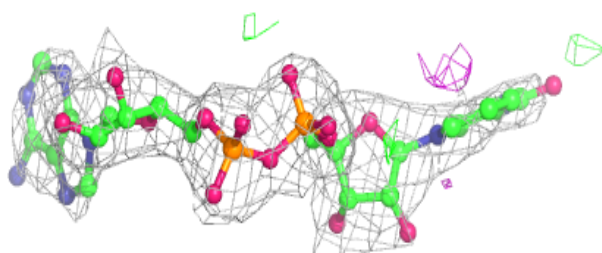
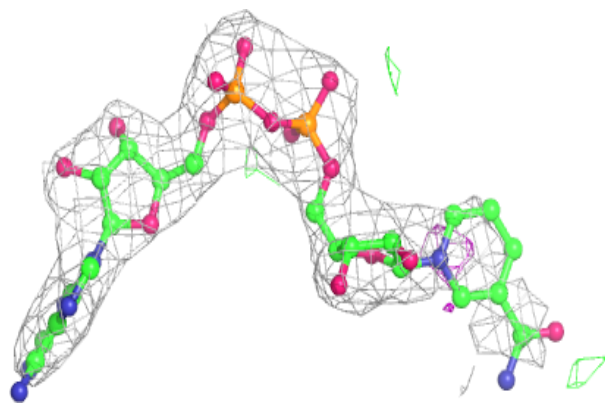
Electron density around D47 C 403:

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

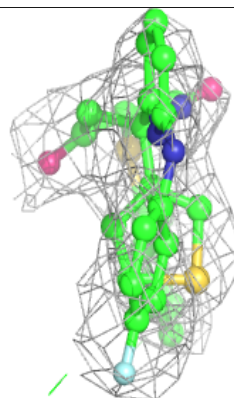
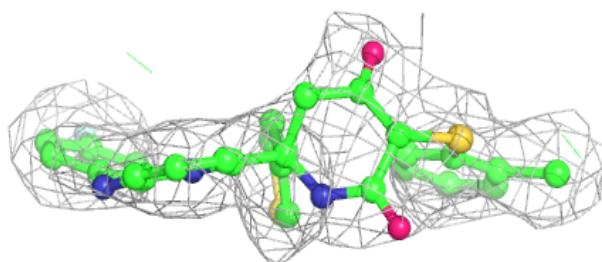
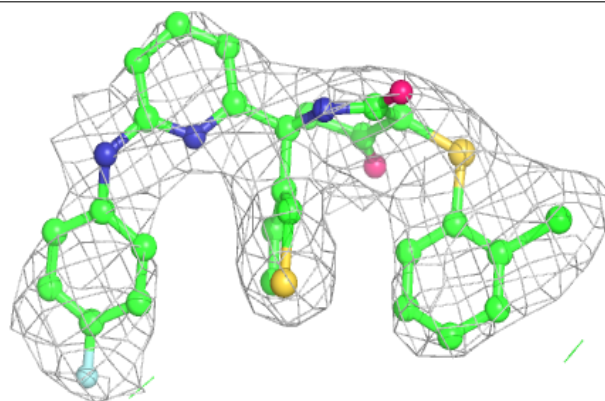


Electron density around NAD C 402:

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

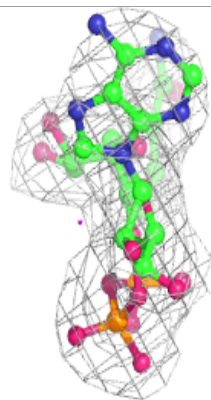
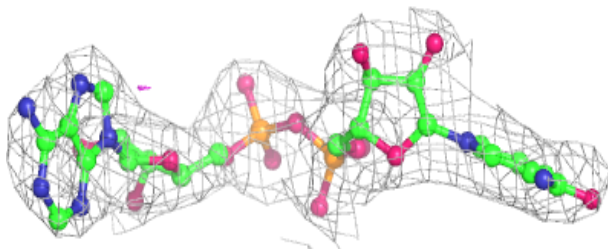
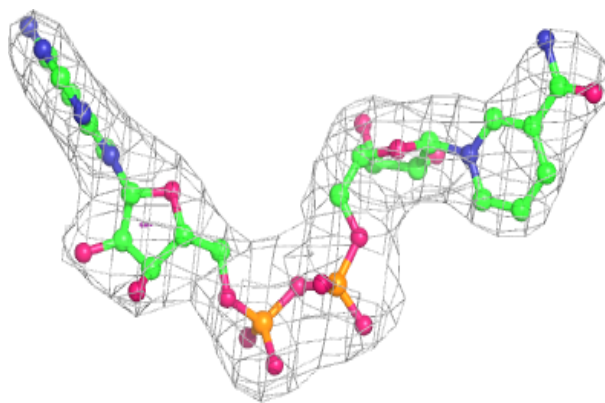
**Electron density around D47 D 802:**

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

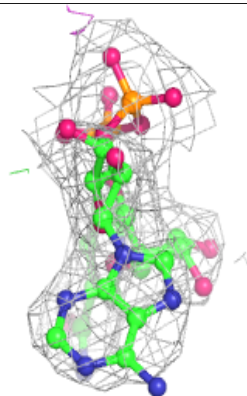
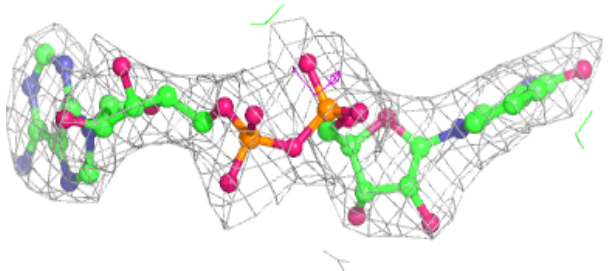
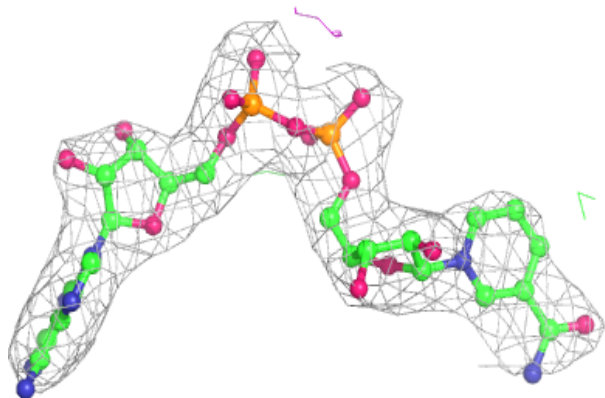


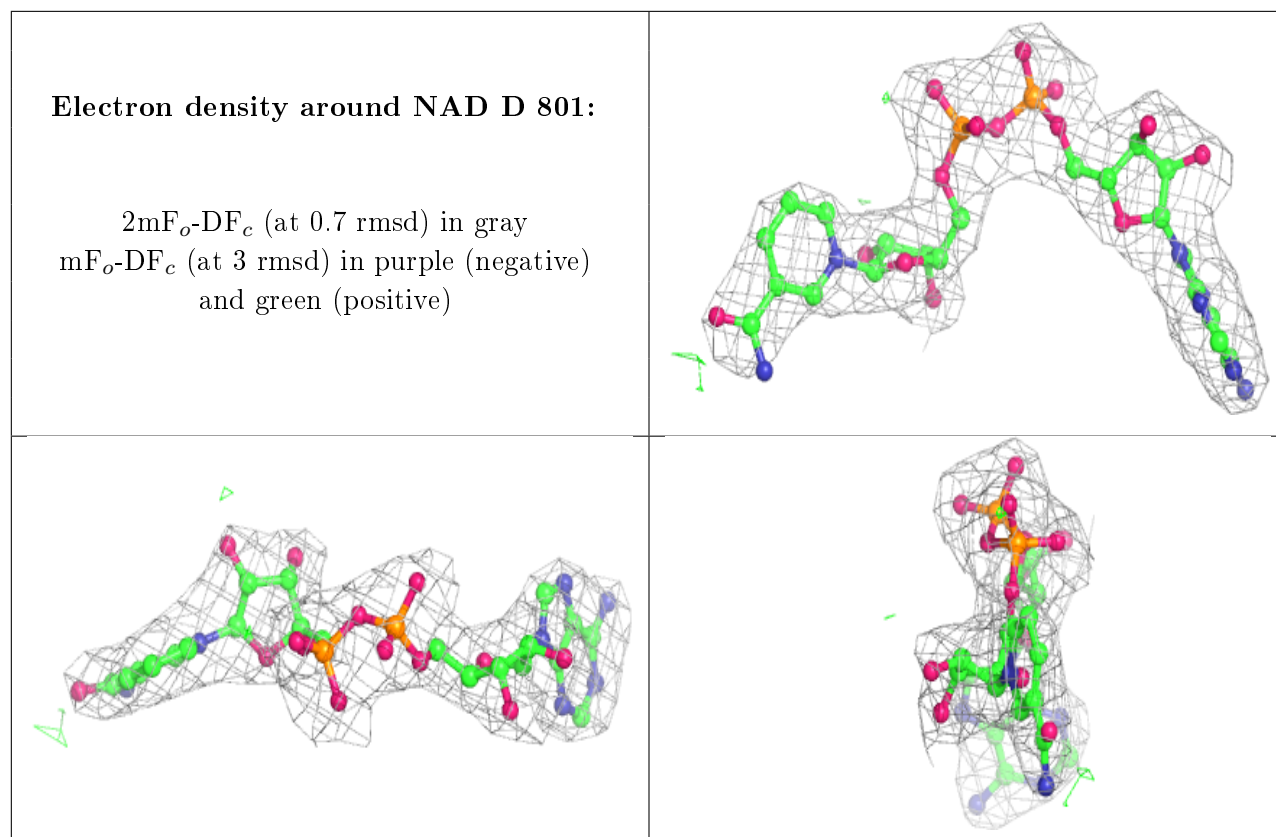
Electron density around NAD A 402:

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

**Electron density around NAD B 402:**

$2mF_o-DF_c$ (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.