Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 09:51 PM JST

PDB ID	:	5YAQ
Title	:	Crystal structure of scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity complexed with scyllo-inosose
Authors	:	Fukano, K.; Shimizu, T.; Sasaki, Y.; Nakamura, A.; Yajima, S.
Deposited on	:	2017-09-01
Resolution	:	1.99 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 (i) 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 (i)) were used in the production of this report:

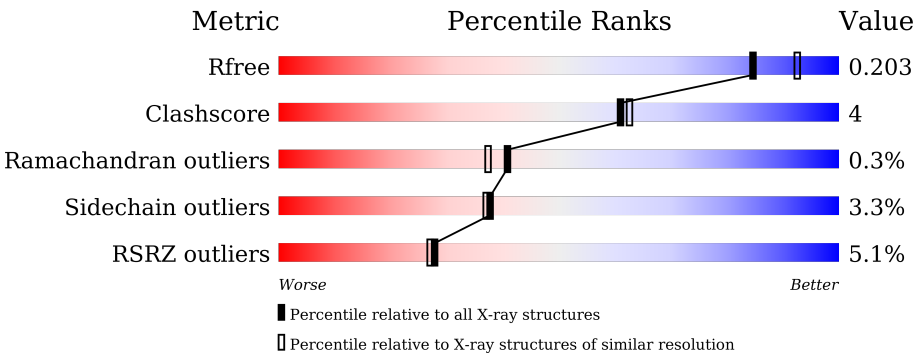
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	380	5% 88% 8% •
1	B	380	4% 84% 11% • • •
1	C	380	8% 86% 10% • •
1	D	380	3% 88% 7% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11787 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 Scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	366	2785	1744	510	513	18	0	0	0
1	B	366	2785	1744	510	513	18	0	0	0
1	C	366	2785	1744	510	513	18	0	0	0
1	D	362	2755	1724	506	507	18	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	SER	ASN	engineered mutation	UNP K7ZP76
A	373	LEU	-	expression tag	UNP K7ZP76
A	374	GLU	-	expression tag	UNP K7ZP76
A	375	HIS	-	expression tag	UNP K7ZP76
A	376	HIS	-	expression tag	UNP K7ZP76
A	377	HIS	-	expression tag	UNP K7ZP76
A	378	HIS	-	expression tag	UNP K7ZP76
A	379	HIS	-	expression tag	UNP K7ZP76
A	380	HIS	-	expression tag	UNP K7ZP76
B	72	SER	ASN	engineered mutation	UNP K7ZP76
B	373	LEU	-	expression tag	UNP K7ZP76
B	374	GLU	-	expression tag	UNP K7ZP76
B	375	HIS	-	expression tag	UNP K7ZP76
B	376	HIS	-	expression tag	UNP K7ZP76
B	377	HIS	-	expression tag	UNP K7ZP76
B	378	HIS	-	expression tag	UNP K7ZP76
B	379	HIS	-	expression tag	UNP K7ZP76
B	380	HIS	-	expression tag	UNP K7ZP76
C	72	SER	ASN	engineered mutation	UNP K7ZP76
C	373	LEU	-	expression tag	UNP K7ZP76

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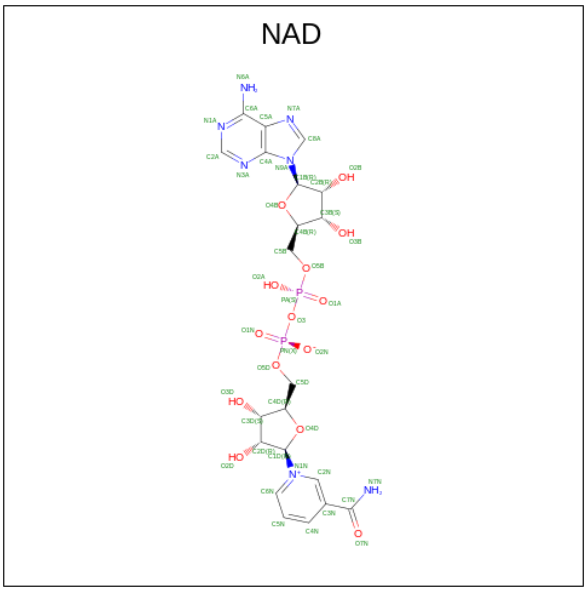
Chain	Residue	Modelled	Actual	Comment	Reference
C	374	GLU	-	expression tag	UNP K7ZP76
C	375	HIS	-	expression tag	UNP K7ZP76
C	376	HIS	-	expression tag	UNP K7ZP76
C	377	HIS	-	expression tag	UNP K7ZP76
C	378	HIS	-	expression tag	UNP K7ZP76
C	379	HIS	-	expression tag	UNP K7ZP76
C	380	HIS	-	expression tag	UNP K7ZP76
D	72	SER	ASN	engineered mutation	UNP K7ZP76
D	373	LEU	-	expression tag	UNP K7ZP76
D	374	GLU	-	expression tag	UNP K7ZP76
D	375	HIS	-	expression tag	UNP K7ZP76
D	376	HIS	-	expression tag	UNP K7ZP76
D	377	HIS	-	expression tag	UNP K7ZP76
D	378	HIS	-	expression tag	UNP K7ZP76
D	379	HIS	-	expression tag	UNP K7ZP76
D	380	HIS	-	expression tag	UNP K7ZP76

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

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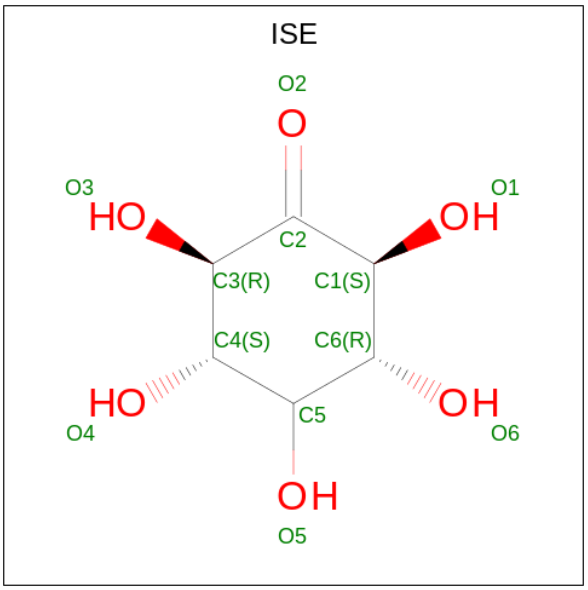
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	D	1	44	21	7	14	2	0	0

- Molecule 3 is (2R,3S,4s,5R,6S)-2,3,4,5,6-pentahydroxycyclohexanone (three-letter code: ISE) (formula: $C_6H_{10}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	12	6	6	0	0
3	C	1	12	6	6	0	0
3	D	1	12	6	6	0	0

- Molecule 4 is water.

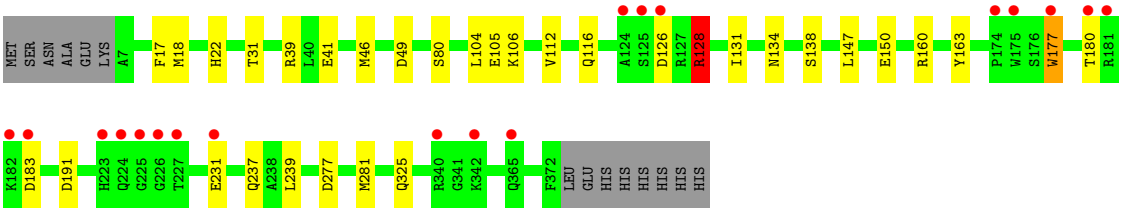
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	122	122	122	0	0
4	B	124	124	124	0	0
4	C	94	94	94	0	0
4	D	125	125	125	0	0

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.

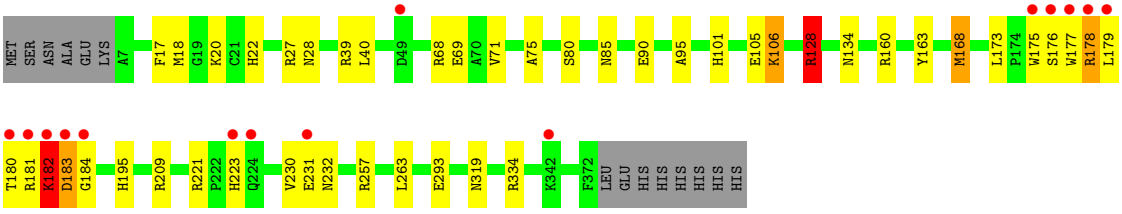
• Molecule 1: Scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity

Chain A:



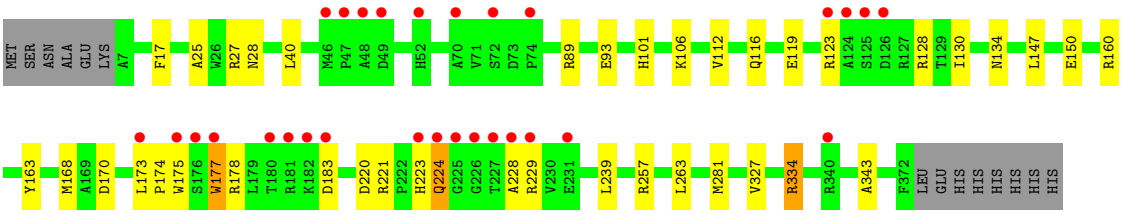
• Molecule 1: Scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity

Chain B:



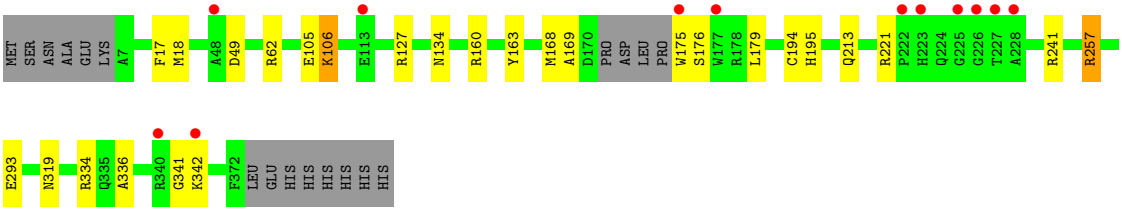
• Molecule 1: Scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity

Chain C:



• Molecule 1: Scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity

Chain D:


MET
SER
ASN
ALA
GLU
LYS
A7
F17
M18
A48
D49
R62
E105
K106
E113
R127
N134
R160
Y163
M168
A169
D170
PRO
ASP
LEU
PRO
W175
S176
W177
R178
L179
C194
H195
Q213
R221
P222
H223
Q224
G225
G226
T227
A228
R241
R257

E293
N319
R334
Q335
A336
R340
G341
K342
F372
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.55Å 121.24Å 140.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 1.99 38.98 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.00-1.99) 99.6 (38.98-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.69 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.180 , 0.194 0.189 , 0.203	Depositor DCC
R_{free} test set	5054 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11787	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ISE, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.51	0/2851	0.80	4/3865 (0.1%)
1	B	0.51	0/2851	0.87	8/3865 (0.2%)
1	C	0.49	0/2851	0.80	6/3865 (0.2%)
1	D	0.50	0/2818	0.82	8/3816 (0.2%)
All	All	0.50	0/11371	0.82	26/15411 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	128	ARG	NE-CZ-NH2	-13.11	113.74	120.30
1	B	128	ARG	NE-CZ-NH1	8.97	124.79	120.30
1	C	257	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	160	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	A	160	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	C	334	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	B	160	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	D	257	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	C	257	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	C	160	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	D	257	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	B	160	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	D	160	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	334	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	D	334	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	128	ARG	CG-CD-NE	-5.90	99.41	111.80
1	D	127	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	B	334	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	257	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	160	ARG	NE-CZ-NH2	-5.45	117.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	168	MET	CG-SD-CE	5.36	108.77	100.20
1	D	241	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	334	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	277	ASP	CB-CG-OD1	5.25	123.02	118.30
1	D	241	ARG	NE-CZ-NH1	5.10	122.85	120.30

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	2785	0	2702	16	0
1	B	2785	0	2702	52	0
1	C	2785	0	2702	20	0
1	D	2755	0	2672	18	0
2	A	44	0	26	1	0
2	B	44	0	26	3	0
2	C	44	0	26	1	0
2	D	44	0	26	3	0
3	B	12	0	10	1	0
3	C	12	0	10	1	0
3	D	12	0	10	1	0
4	A	122	0	0	1	0
4	B	124	0	0	5	0
4	C	94	0	0	0	0
4	D	125	0	0	2	0
All	All	11787	0	10912	100	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 4.

All (100) 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:177:TRP:CE2	1:B:178:ARG:HG3	1.55	1.39
1:B:177:TRP:CZ2	1:B:178:ARG:HG3	1.96	1.01
1:B:177:TRP:HE1	1:B:178:ARG:NH1	1.63	0.96
1:B:177:TRP:CE2	1:B:178:ARG:CG	2.48	0.95
1:B:177:TRP:CZ2	1:B:178:ARG:CG	2.50	0.95
1:B:177:TRP:HE1	1:B:178:ARG:HH11	1.02	0.94
1:C:89:ARG:NH1	1:C:93:GLU:OE2	2.04	0.91
1:B:177:TRP:CG	1:B:178:ARG:N	2.42	0.87
1:B:177:TRP:O	1:B:179:LEU:N	2.08	0.86
1:D:49:ASP:HB2	4:D:620:HOH:O	1.76	0.85
1:A:191:ASP:HB2	4:A:638:HOH:O	1.82	0.80
1:B:177:TRP:NE1	1:B:178:ARG:HG3	1.96	0.80
1:B:175:TRP:CZ3	1:B:223:HIS:CE1	2.71	0.78
1:B:177:TRP:HZ2	1:B:178:ARG:CZ	1.98	0.76
1:B:177:TRP:NE1	1:B:178:ARG:NH1	2.37	0.71
1:B:106:LYS:HD3	1:B:195:HIS:NE2	2.07	0.70
1:A:39:ARG:NH1	1:A:41:GLU:OE2	2.25	0.69
1:B:209:ARG:HG3	4:B:618:HOH:O	1.94	0.68
1:B:101:HIS:HD2	1:B:128:ARG:H	1.39	0.68
2:D:401:NAD:C3N	3:D:402:ISE:O2	2.43	0.67
1:B:168:MET:HE2	1:B:221:ARG:CZ	2.26	0.65
1:B:177:TRP:CZ2	1:B:178:ARG:CZ	2.80	0.65
1:C:101:HIS:HD2	1:C:128:ARG:H	1.44	0.64
1:C:112:VAL:O	1:C:116:GLN:HG3	1.99	0.63
1:B:177:TRP:CZ2	1:B:178:ARG:HG2	2.34	0.62
1:D:106:LYS:HD3	1:D:194:CYS:SG	2.40	0.61
1:C:173:LEU:O	1:C:221:ARG:HD3	2.02	0.60
1:B:177:TRP:CD2	1:B:178:ARG:N	2.68	0.59
1:D:342:LYS:HE2	4:D:501:HOH:O	2.02	0.58
1:B:175:TRP:CE3	1:B:223:HIS:CE1	2.91	0.58
1:B:182:LYS:O	1:B:184:GLY:N	2.37	0.57
1:A:150:GLU:OE1	1:D:293:GLU:OE1	2.22	0.57
1:B:71:VAL:CG1	1:B:95:ALA:HA	2.34	0.57
1:C:168:MET:O	1:C:221:ARG:NH2	2.38	0.56
1:B:177:TRP:HZ2	1:B:178:ARG:NE	2.03	0.56
1:B:71:VAL:HG13	1:B:95:ALA:HA	1.89	0.55
1:D:175:TRP:CE3	1:D:221:ARG:HG3	2.41	0.54
1:B:22:HIS:HE1	1:B:105:GLU:OE2	1.90	0.54
1:B:175:TRP:CE3	1:B:175:TRP:O	2.61	0.54
1:A:177:TRP:HD1	1:A:183:ASP:HB2	1.73	0.53
1:B:177:TRP:CZ2	1:B:178:ARG:NE	2.77	0.53
1:B:231:GLU:C	4:B:501:HOH:O	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:MET:HG2	1:B:319:ASN:HD22	1.72	0.53
1:B:179:LEU:HD11	1:B:221:ARG:HD2	1.92	0.52
1:A:22:HIS:HE1	1:A:105:GLU:OE2	1.93	0.51
2:B:401:NAD:C3N	3:B:402:ISE:O2	2.58	0.51
1:A:31:THR:O	1:B:20:LYS:HE3	2.11	0.51
1:C:220:ASP:HA	1:C:228:ALA:O	2.11	0.51
1:D:179:LEU:CD1	1:D:221:ARG:HD2	2.41	0.51
1:A:138:SER:HB3	1:A:325:GLN:HE21	1.75	0.50
1:C:175:TRP:HH2	1:C:177:TRP:CD1	2.30	0.49
1:B:105:GLU:OE1	2:B:401:NAD:H2N	2.13	0.48
1:B:22:HIS:HD2	1:B:80:SER:OG	1.96	0.48
1:B:85:ASN:HB2	1:B:183:ASP:O	2.14	0.48
1:B:223:HIS:CE1	4:B:510:HOH:O	2.68	0.47
1:C:223:HIS:CE1	1:C:224:GLN:OE1	2.68	0.47
1:C:281:MET:HG2	1:D:319:ASN:HD22	1.79	0.47
1:A:126:ASP:O	1:A:128:ARG:NH2	2.47	0.47
1:D:106:LYS:HE2	1:D:195:HIS:NE2	2.30	0.47
1:A:22:HIS:HD2	1:A:80:SER:OG	1.97	0.47
1:A:147:LEU:HD21	1:D:293:GLU:HG2	1.97	0.47
1:B:209:ARG:HH22	1:D:213:GLN:HE21	1.63	0.47
1:C:223:HIS:O	1:C:224:GLN:HG2	2.16	0.46
1:D:105:GLU:OE1	2:D:401:NAD:H2N	2.16	0.46
1:B:177:TRP:CD2	1:B:178:ARG:HG3	2.36	0.45
1:B:293:GLU:HG2	1:C:147:LEU:HD21	1.98	0.45
1:A:239:LEU:HG	1:C:239:LEU:HG	1.98	0.45
1:B:177:TRP:C	1:B:179:LEU:N	2.69	0.45
1:C:119:GLU:OE2	1:C:123:ARG:NH1	2.50	0.45
1:B:175:TRP:CE3	1:B:223:HIS:ND1	2.84	0.45
1:D:18:MET:HG3	2:D:401:NAD:C2N	2.48	0.44
1:D:179:LEU:HD11	1:D:221:ARG:HD2	2.00	0.44
1:B:68:ARG:NH2	1:B:90:GLU:OE2	2.51	0.44
1:B:177:TRP:C	1:B:179:LEU:H	2.21	0.44
1:B:177:TRP:O	1:B:178:ARG:C	2.57	0.43
1:B:293:GLU:OE2	1:C:150:GLU:OE1	2.36	0.43
1:C:170:ASP:O	1:C:221:ARG:NH1	2.35	0.43
1:A:180:THR:HA	1:A:231:GLU:HB2	2.01	0.42
1:B:39:ARG:NH2	1:B:75:ALA:O	2.52	0.42
1:B:180:THR:O	1:B:232:ASN:ND2	2.52	0.42
1:B:179:LEU:HD13	1:B:230:VAL:HG22	2.02	0.42
1:D:336:ALA:HA	1:D:341:GLY:O	2.19	0.42
1:D:106:LYS:HD2	1:D:106:LYS:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:MET:CE	1:D:179:LEU:HD21	2.50	0.42
1:A:18:MET:HG3	2:A:500:NAD:C2N	2.50	0.42
1:B:181:ARG:C	1:B:182:LYS:O	2.58	0.42
1:C:175:TRP:NE1	1:C:229:ARG:O	2.50	0.42
1:D:169:ALA:HB1	1:D:257:ARG:HD3	2.02	0.42
1:B:18:MET:HG3	2:B:401:NAD:C2N	2.49	0.41
1:B:27:ARG:HD2	1:B:40:LEU:HD11	2.01	0.41
1:C:173:LEU:HA	1:C:174:PRO:HD3	1.94	0.41
1:C:25:ALA:HA	1:C:327:VAL:HG22	2.03	0.41
1:C:130:ILE:HD12	1:C:343:ALA:HB1	2.03	0.41
1:B:293:GLU:HB2	4:B:606:HOH:O	2.19	0.41
1:A:112:VAL:O	1:A:116:GLN:HG3	2.21	0.41
2:C:401:NAD:C3N	3:C:402:ISE:O2	2.69	0.40
1:A:104:LEU:O	1:A:131:ILE:HA	2.21	0.40
1:B:232:ASN:N	4:B:501:HOH:O	2.55	0.40
1:C:27:ARG:HG2	1:C:40:LEU:HD11	2.04	0.40
1:D:169:ALA:CB	1:D:257:ARG:HD3	2.52	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	364/380 (96%)	357 (98%)	7 (2%)	0	100	100
1	B	364/380 (96%)	349 (96%)	12 (3%)	3 (1%)	19	13
1	C	364/380 (96%)	354 (97%)	9 (2%)	1 (0%)	41	37
1	D	358/380 (94%)	351 (98%)	7 (2%)	0	100	100
All	All	1450/1520 (95%)	1411 (97%)	35 (2%)	4 (0%)	41	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	ARG
1	B	183	ASP
1	C	224	GLN
1	B	182	LYS

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	275/288 (96%)	266 (97%)	9 (3%)	38	37
1	B	275/288 (96%)	264 (96%)	11 (4%)	31	29
1	C	275/288 (96%)	265 (96%)	10 (4%)	35	34
1	D	271/288 (94%)	265 (98%)	6 (2%)	52	55
All	All	1096/1152 (95%)	1060 (97%)	36 (3%)	38	37

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	A	46	MET
1	A	49	ASP
1	A	106	LYS
1	A	128	ARG
1	A	134	ASN
1	A	163	TYR
1	A	177	TRP
1	A	237	GLN
1	B	17	PHE
1	B	28	ASN
1	B	69	GLU
1	B	106	LYS
1	B	128	ARG
1	B	134	ASN
1	B	163	TYR
1	B	173	LEU
1	B	176	SER

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Mol	Chain	Res	Type
1	B	182	LYS
1	B	263	LEU
1	C	17	PHE
1	C	28	ASN
1	C	106	LYS
1	C	134	ASN
1	C	163	TYR
1	C	177	TRP
1	C	178	ARG
1	C	183	ASP
1	C	263	LEU
1	C	334	ARG
1	D	17	PHE
1	D	62	ARG
1	D	106	LYS
1	D	134	ASN
1	D	163	TYR
1	D	176	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	28	ASN
1	A	52	HIS
1	A	237	GLN
1	A	278	GLN
1	A	306	GLN
1	A	325	GLN
1	A	358	HIS
1	B	22	HIS
1	B	28	ASN
1	B	52	HIS
1	B	101	HIS
1	B	223	HIS
1	B	306	GLN
1	B	319	ASN
1	B	358	HIS
1	C	28	ASN
1	C	101	HIS
1	C	116	GLN
1	C	223	HIS

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Mol	Chain	Res	Type
1	C	306	GLN
1	C	358	HIS
1	C	365	GLN
1	D	28	ASN
1	D	213	GLN
1	D	278	GLN
1	D	319	ASN
1	D	325	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
2	NAD	C	401	-	42,48,48	1.07	3 (7%)	50,73,73	1.24	5 (10%)
3	ISE	D	402	-	12,12,12	0.97	0	16,18,18	1.47	2 (12%)
2	NAD	A	500	-	42,48,48	1.05	4 (9%)	50,73,73	1.34	6 (12%)
2	NAD	B	401	-	42,48,48	1.13	5 (11%)	50,73,73	1.40	9 (18%)
3	ISE	B	402	-	12,12,12	0.89	0	16,18,18	1.69	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	D	401	-	42,48,48	1.06	4 (9%)	50,73,73	1.32	5 (10%)
3	ISE	C	402	-	12,12,12	0.80	0	16,18,18	1.60	2 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	C	401	-	-	4/26/62/62	0/5/5/5
3	ISE	D	402	-	-	-	0/1/1/1
2	NAD	A	500	-	-	4/26/62/62	0/5/5/5
2	NAD	B	401	-	-	3/26/62/62	0/5/5/5
3	ISE	B	402	-	-	-	0/1/1/1
2	NAD	D	401	-	-	4/26/62/62	0/5/5/5
3	ISE	C	402	-	-	-	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NAD	O4D-C1D	3.17	1.45	1.41
2	B	401	NAD	O4D-C1D	3.08	1.45	1.41
2	B	401	NAD	C5A-C4A	2.73	1.48	1.40
2	A	500	NAD	O4D-C1D	2.72	1.44	1.41
2	D	401	NAD	C2A-N3A	2.62	1.36	1.32
2	B	401	NAD	C2A-N3A	2.62	1.36	1.32
2	C	401	NAD	C5A-C4A	2.59	1.47	1.40
2	D	401	NAD	C5A-C4A	2.48	1.47	1.40
2	A	500	NAD	C5A-C4A	2.28	1.46	1.40
2	B	401	NAD	O4B-C1B	2.26	1.44	1.41
2	C	401	NAD	C2A-N3A	2.21	1.35	1.32
2	D	401	NAD	C7N-N7N	2.19	1.37	1.33
2	B	401	NAD	C7N-N7N	2.16	1.37	1.33
2	A	500	NAD	C7N-N7N	2.13	1.37	1.33
2	A	500	NAD	C2A-N3A	2.12	1.35	1.32
2	D	401	NAD	O4B-C1B	2.09	1.44	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	ISE	O1-C1-C6	-4.92	100.37	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	NAD	N3A-C2A-N1A	-4.57	121.54	128.68
2	C	401	NAD	N3A-C2A-N1A	-4.22	122.09	128.68
2	D	401	NAD	N3A-C2A-N1A	-4.17	122.17	128.68
3	C	402	ISE	O1-C1-C6	-4.10	102.07	110.53
2	B	401	NAD	N3A-C2A-N1A	-3.88	122.61	128.68
3	D	402	ISE	O1-C1-C6	-3.31	103.70	110.53
2	D	401	NAD	C4A-C5A-N7A	-3.14	106.13	109.40
2	B	401	NAD	C1B-N9A-C4A	-3.03	121.31	126.64
2	A	500	NAD	C1B-N9A-C4A	-2.86	121.62	126.64
2	A	500	NAD	O2A-PA-O1A	2.73	125.72	112.24
2	B	401	NAD	C3N-C2N-N1N	2.69	123.06	120.43
2	D	401	NAD	C1B-N9A-C4A	-2.53	122.19	126.64
2	C	401	NAD	C1B-N9A-C4A	-2.52	122.21	126.64
2	B	401	NAD	C3B-C2B-C1B	-2.51	97.19	100.98
2	B	401	NAD	C4A-C5A-N7A	-2.49	106.81	109.40
2	D	401	NAD	PN-O3-PA	-2.46	124.38	132.83
2	C	401	NAD	O2A-PA-O1A	2.43	124.27	112.24
2	C	401	NAD	C3N-C2N-N1N	2.40	122.77	120.43
2	B	401	NAD	C2A-N1A-C6A	2.37	122.81	118.75
2	A	500	NAD	PN-O3-PA	-2.35	124.75	132.83
2	B	401	NAD	PN-O3-PA	-2.35	124.75	132.83
3	B	402	ISE	C6-C5-C4	-2.32	106.77	110.82
2	B	401	NAD	O2A-PA-O1A	2.22	123.21	112.24
2	D	401	NAD	C3B-C2B-C1B	-2.21	97.65	100.98
2	C	401	NAD	C2A-N1A-C6A	2.19	122.50	118.75
3	D	402	ISE	O3-C3-C2	2.16	116.04	109.94
2	A	500	NAD	C3N-C2N-N1N	2.16	122.54	120.43
2	A	500	NAD	C2A-N1A-C6A	2.15	122.43	118.75
2	B	401	NAD	O2N-PN-O1N	2.13	122.77	112.24
3	C	402	ISE	C5-C4-C3	2.10	113.52	110.18

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	NAD	O4D-C1D-N1N-C2N
2	A	500	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	O4D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	D	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	O4B-C4B-C5B-O5B
2	A	500	NAD	C2D-C1D-N1N-C2N
2	C	401	NAD	C2D-C1D-N1N-C2N
2	A	500	NAD	O4B-C4B-C5B-O5B
2	C	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	O4B-C4B-C5B-O5B

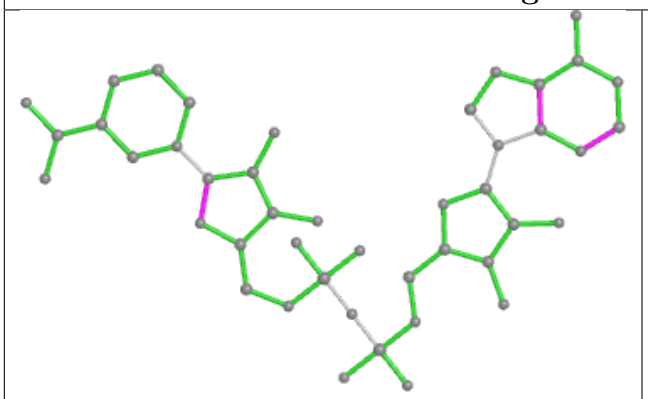
There are no ring outliers.

7 monomers are involved in 8 short contacts:

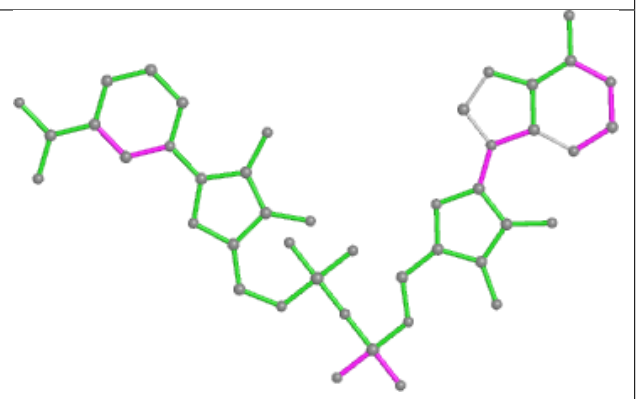
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	NAD	1	0
3	D	402	ISE	1	0
2	A	500	NAD	1	0
2	B	401	NAD	3	0
3	B	402	ISE	1	0
2	D	401	NAD	3	0
3	C	402	ISE	1	0

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 then 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.

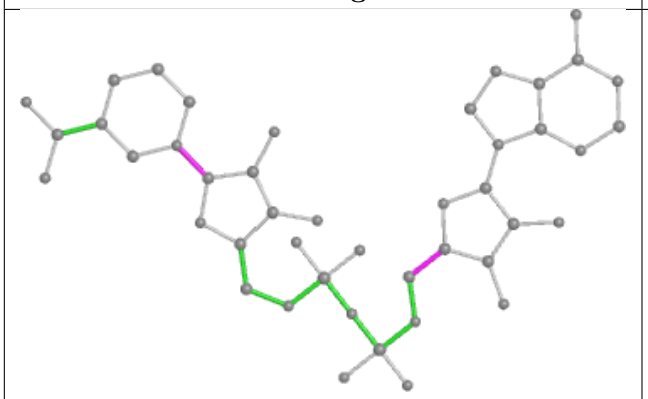
Ligand NAD C 401



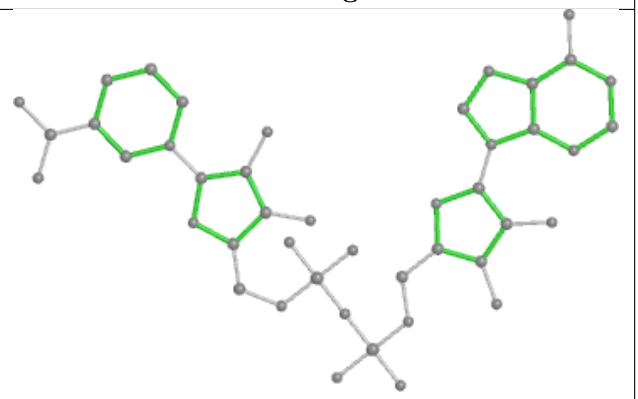
Bond lengths



Bond angles

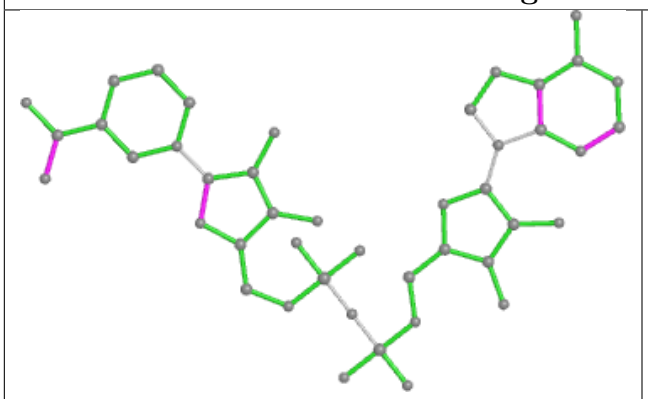


Torsions

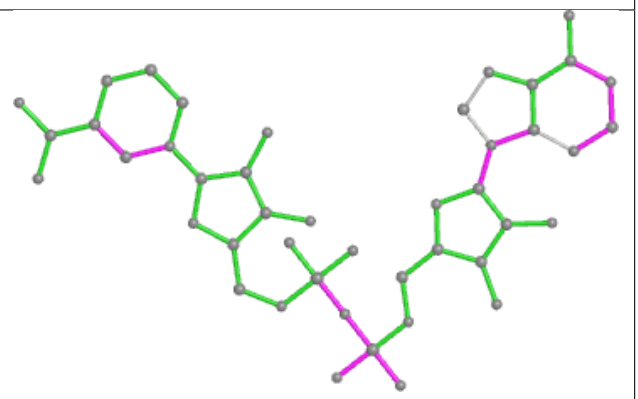


Rings

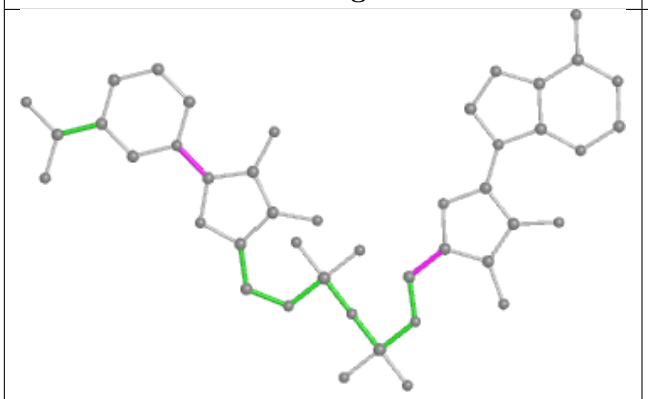
Ligand NAD A 500



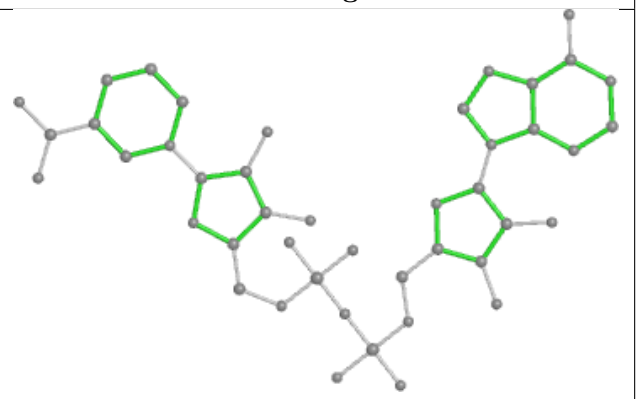
Bond lengths



Bond angles

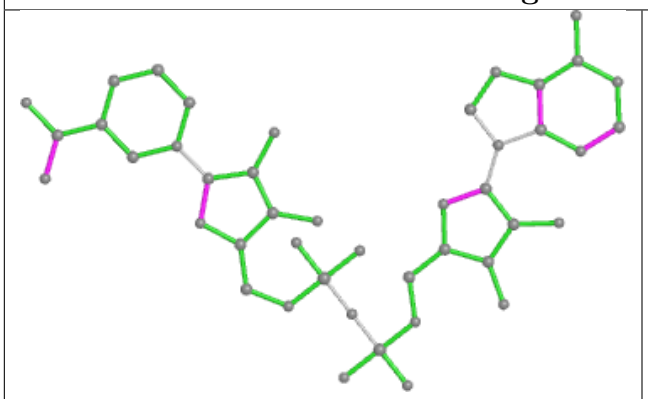


Torsions

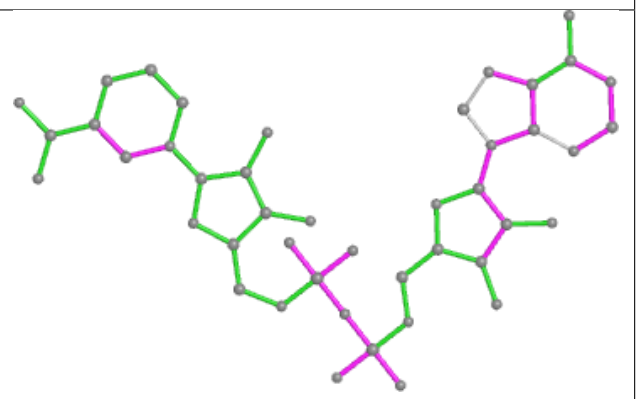


Rings

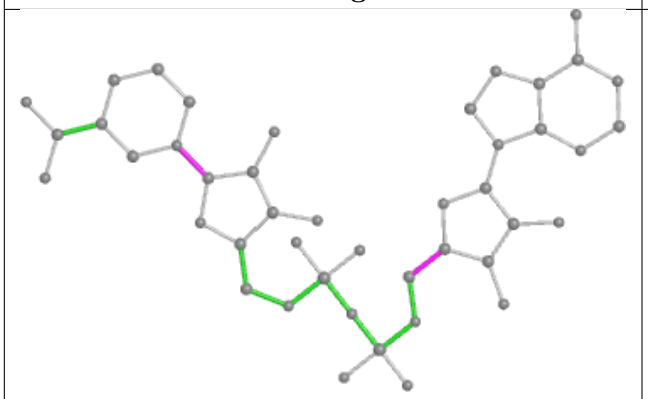
Ligand NAD B 401



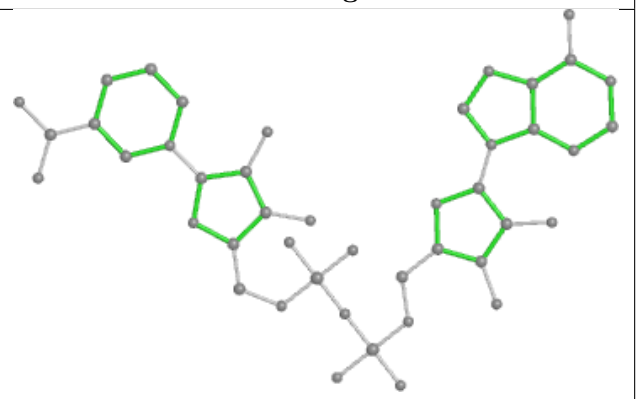
Bond lengths



Bond angles

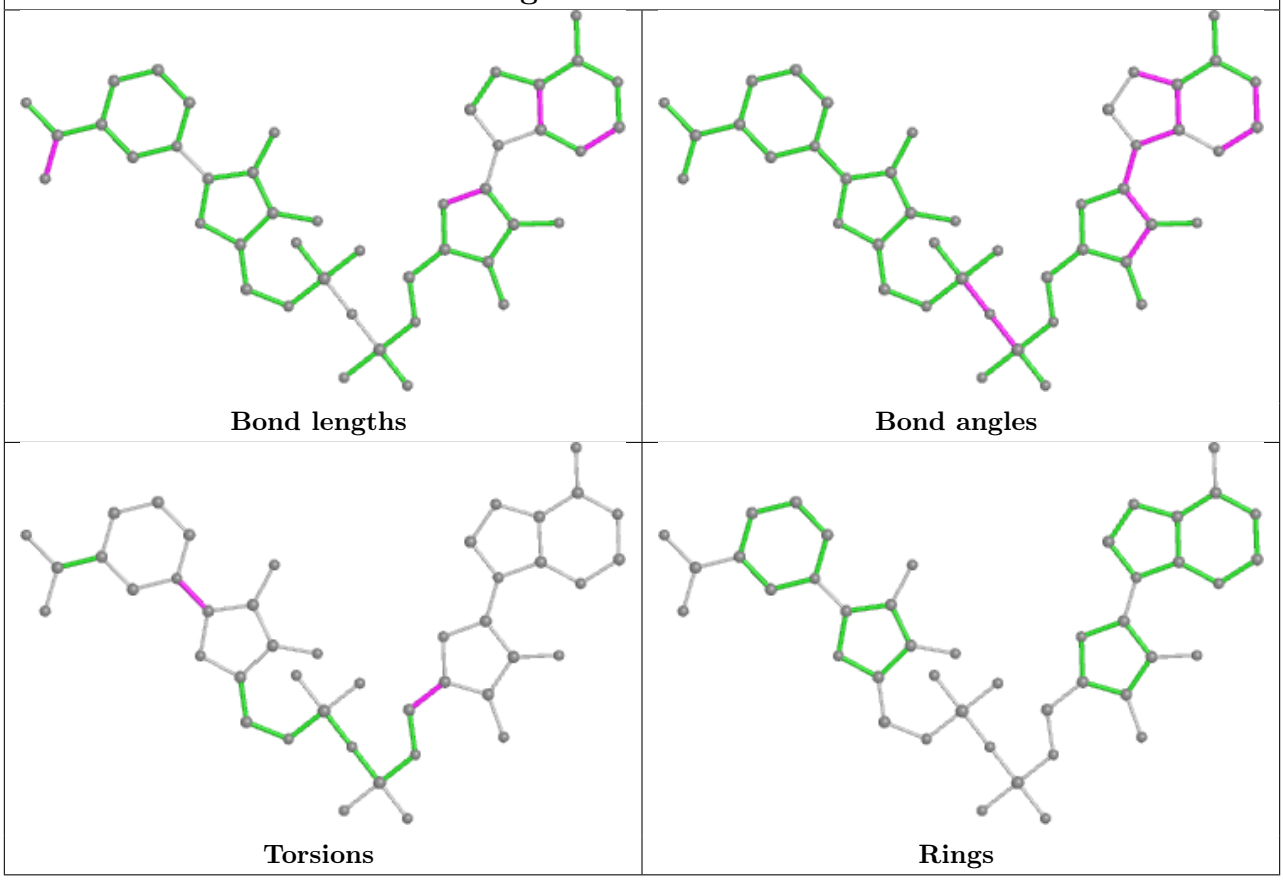


Torsions



Rings

Ligand NAD D 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	366/380 (96%)	0.23	19 (5%)	27	26	15, 21, 35, 52	0
1	B	366/380 (96%)	0.14	15 (4%)	37	36	15, 21, 37, 51	0
1	C	366/380 (96%)	0.40	29 (7%)	12	11	15, 22, 41, 58	0
1	D	362/380 (95%)	0.14	12 (3%)	46	45	15, 21, 33, 50	0
All	All	1460/1520 (96%)	0.23	75 (5%)	28	27	15, 21, 37, 58	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	THR	10.0
1	C	177	TRP	9.6
1	B	177	TRP	9.5
1	B	175	TRP	8.7
1	A	177	TRP	8.5
1	C	224	GLN	7.7
1	C	223	HIS	7.4
1	B	176	SER	7.3
1	C	182	LYS	6.7
1	D	225	GLY	6.2
1	C	228	ALA	6.1
1	D	223	HIS	5.0
1	C	226	GLY	4.9
1	A	225	GLY	4.8
1	D	340	ARG	4.8
1	C	175	TRP	4.6
1	D	175	TRP	4.6
1	A	182	LYS	4.6
1	A	181	ARG	4.2
1	C	225	GLY	4.2
1	C	227	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	224	GLN	4.2
1	A	124	ALA	4.1
1	C	229	ARG	4.1
1	B	183	ASP	4.0
1	A	126	ASP	3.9
1	C	49	ASP	3.9
1	A	175	TRP	3.9
1	B	49	ASP	3.7
1	C	52	HIS	3.6
1	A	223	HIS	3.3
1	C	176	SER	3.2
1	C	126	ASP	3.1
1	C	183	ASP	3.1
1	A	231	GLU	3.1
1	C	173	LEU	3.1
1	A	125	SER	3.0
1	B	223	HIS	3.0
1	B	181	ARG	2.9
1	A	226	GLY	2.9
1	A	342	LYS	2.9
1	C	48	ALA	2.9
1	C	125	SER	2.9
1	C	46	MET	2.8
1	C	124	ALA	2.7
1	B	231	GLU	2.7
1	B	179	LEU	2.6
1	D	227	THR	2.6
1	A	340	ARG	2.5
1	D	226	GLY	2.5
1	C	181	ARG	2.5
1	C	72	SER	2.5
1	C	74	PRO	2.5
1	A	227	THR	2.4
1	C	340	ARG	2.4
1	C	70	ALA	2.4
1	D	113	GLU	2.4
1	D	177	TRP	2.4
1	A	183	ASP	2.3
1	D	222	PRO	2.3
1	B	184	GLY	2.2
1	A	174	PRO	2.2
1	A	365	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	228	ALA	2.2
1	B	178	ARG	2.2
1	B	182	LYS	2.2
1	C	180	THR	2.2
1	B	342	LYS	2.2
1	D	342	LYS	2.1
1	A	180	THR	2.1
1	C	123	ARG	2.1
1	B	224	GLN	2.1
1	C	231	GLU	2.0
1	D	48	ALA	2.0
1	C	47	PRO	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)

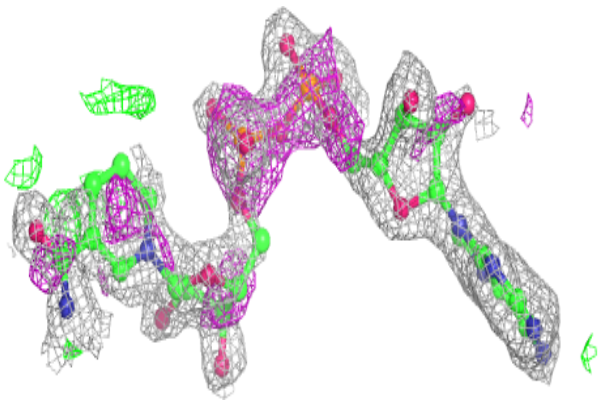
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

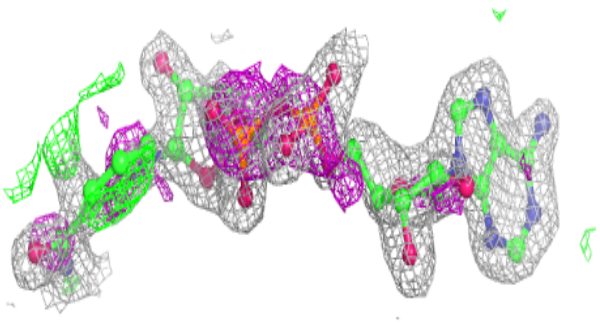
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	A	500	44/44	0.82	0.28	31,34,40,44	0
2	NAD	C	401	44/44	0.83	0.30	33,37,44,47	0
2	NAD	B	401	44/44	0.88	0.27	25,33,35,37	0
3	ISE	B	402	12/12	0.90	0.12	21,22,23,23	0
3	ISE	C	402	12/12	0.90	0.17	22,22,24,24	0
2	NAD	D	401	44/44	0.93	0.22	25,29,33,35	0
3	ISE	D	402	12/12	0.94	0.12	21,22,23,23	0

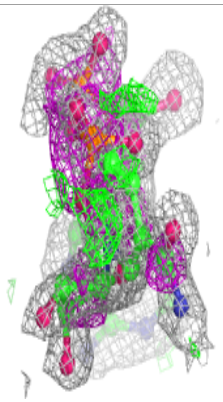
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 500:

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

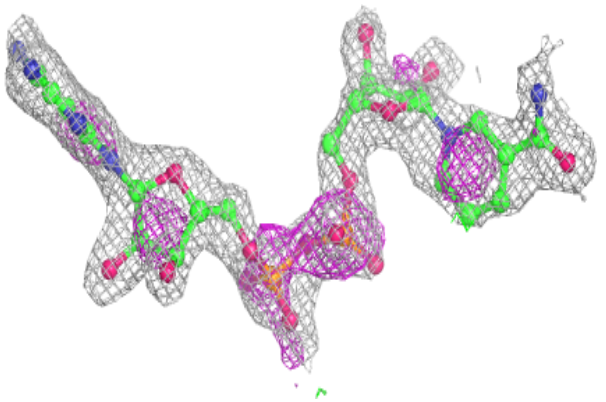


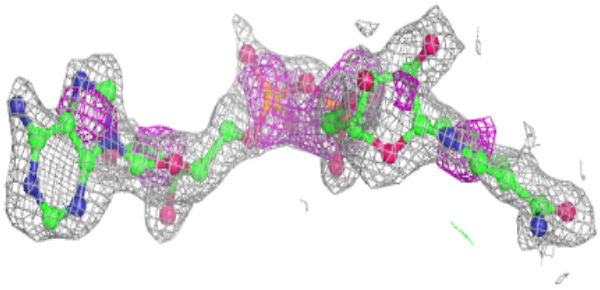


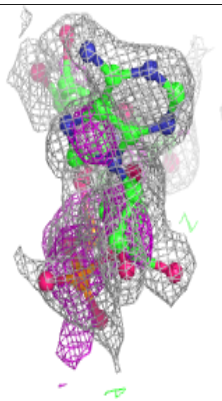


Electron density around NAD C 401:

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

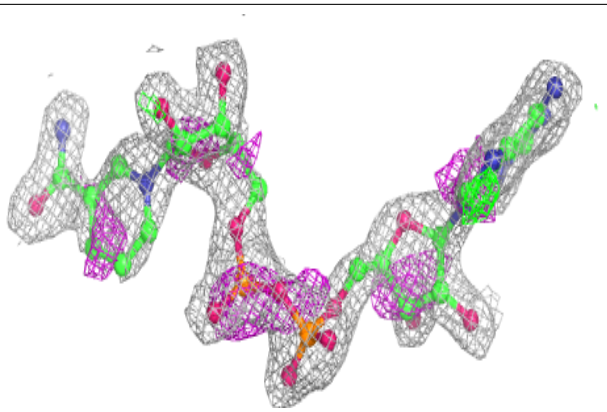


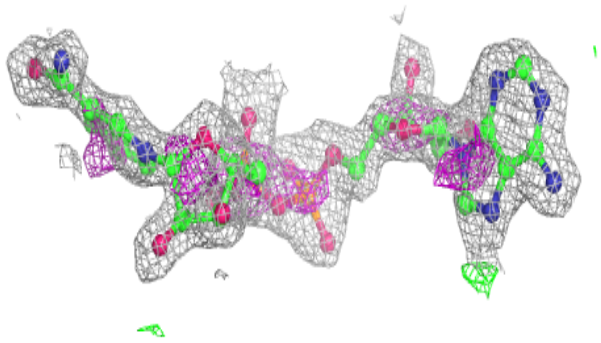


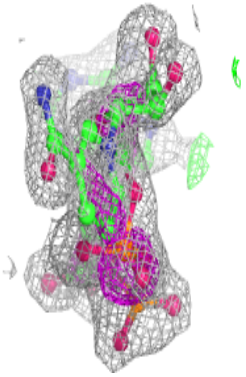


Electron density around NAD B 401:

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

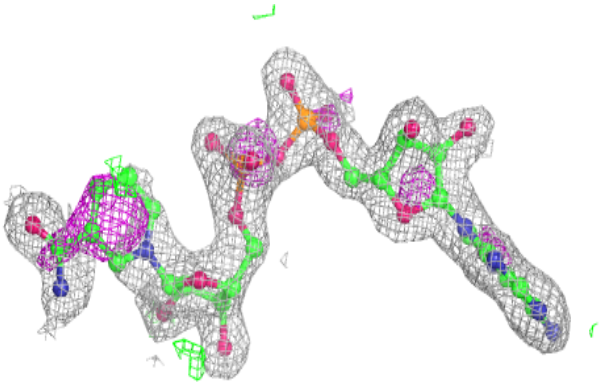


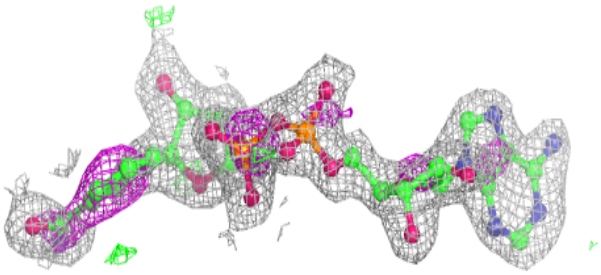


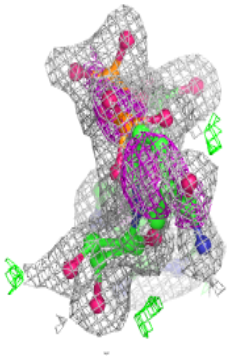


Electron density around NAD D 401:

$2mF_o$-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.