



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:36 AM UTC

PDB ID : 5YA8 / pdb_00005ya8
Title : Crystal structure of scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity complexed with myo-inositol
Authors : Fukano, K.; Shimizu, T.; Sasaki, Y.; Nakamura, A.; Yajima, S.
Deposited on : 2017-08-31
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

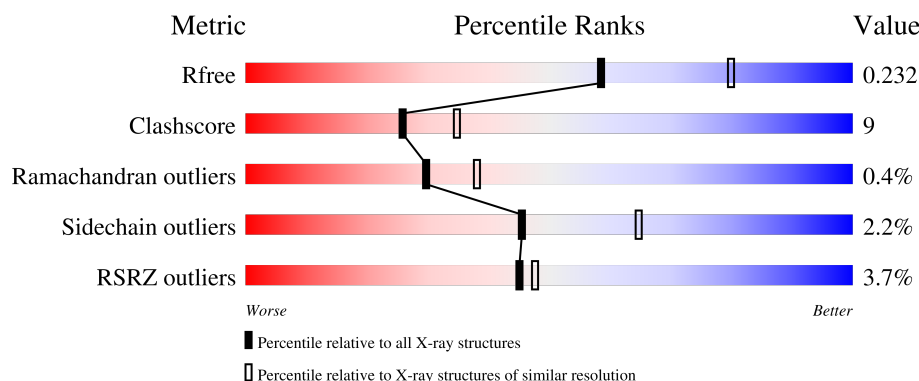
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	380	4% 82% 13% ..
1	B	380	3% 82% 14% .
1	C	380	5% 82% 13% ..
1	D	380	2% 81% 14% ..

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
3	INS	B	402	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11763 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
1	A	366	Total	C	N	O	S	0	0	0
			2785	1744	510	513	18			
1	B	366	Total	C	N	O	S	0	0	0
			2785	1744	510	513	18			
1	C	366	Total	C	N	O	S	0	0	0
			2785	1744	510	513	18			
1	D	365	Total	C	N	O	S	0	0	0
			2777	1738	509	512	18			

There are 36 discrepancies between the modelled and reference sequences:

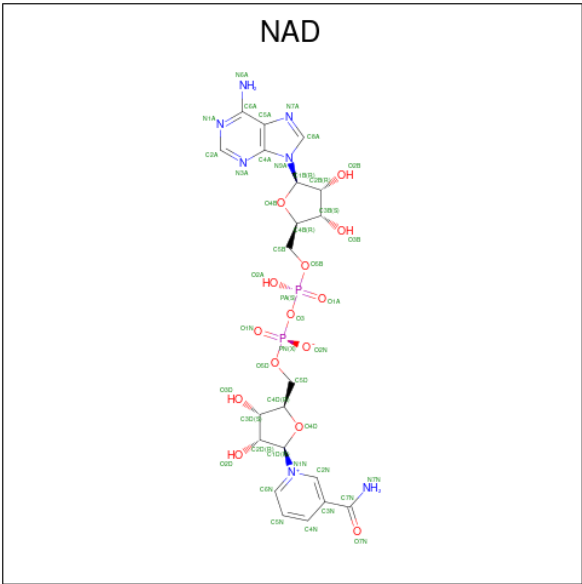
Chain	Residue	Modelled	Actual	Comment	Reference
A	72	SER	ASN	engineered mutation	UNP K7ZP76
A	373	LEU	-	expression tag	UNP K7ZP76
A	374	GLU	-	expression tag	UNP K7ZP76
A	375	HIS	-	expression tag	UNP K7ZP76
A	376	HIS	-	expression tag	UNP K7ZP76
A	377	HIS	-	expression tag	UNP K7ZP76
A	378	HIS	-	expression 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 (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



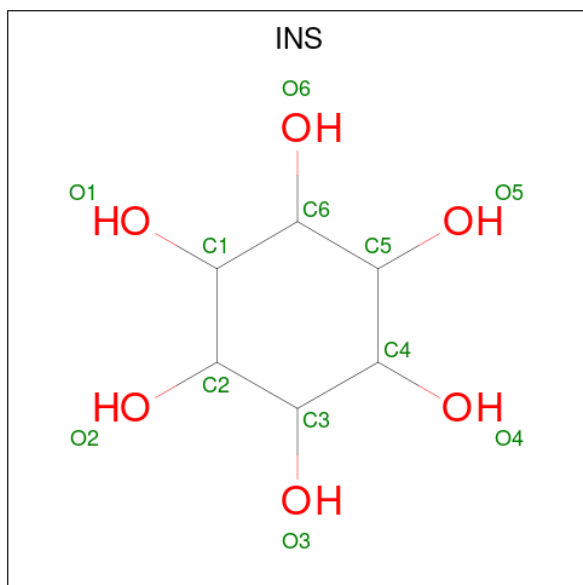
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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

- Molecule 3 is 1,2,3,4,5,6-HEXAHYDROXY-CYCLOHEXANE (CCD ID: INS) (formula: $C_6H_{12}O_6$).



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

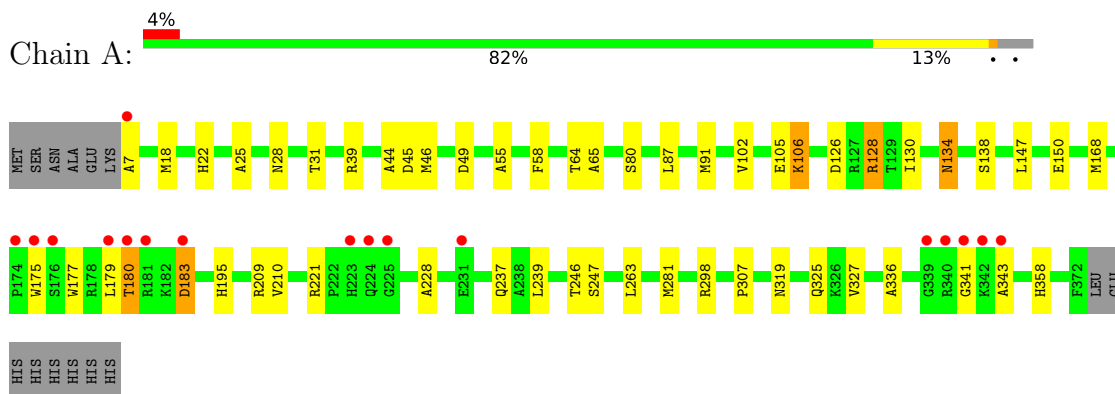
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	104	Total	O		
			104	104	0	0
4	B	116	Total	O		
			116	116	0	0
4	C	84	Total	O		
			84	84	0	0
4	D	115	Total	O		
			115	115	0	0

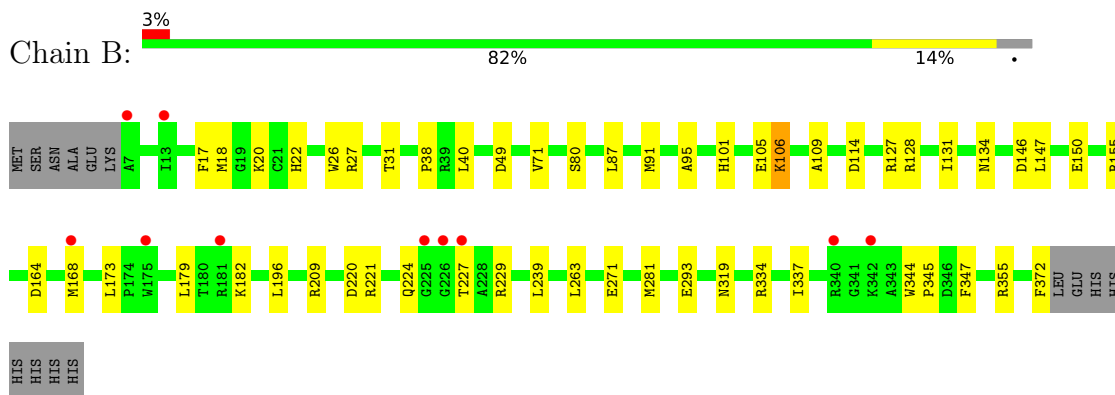
3 Residue-property plots [i](#)

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.

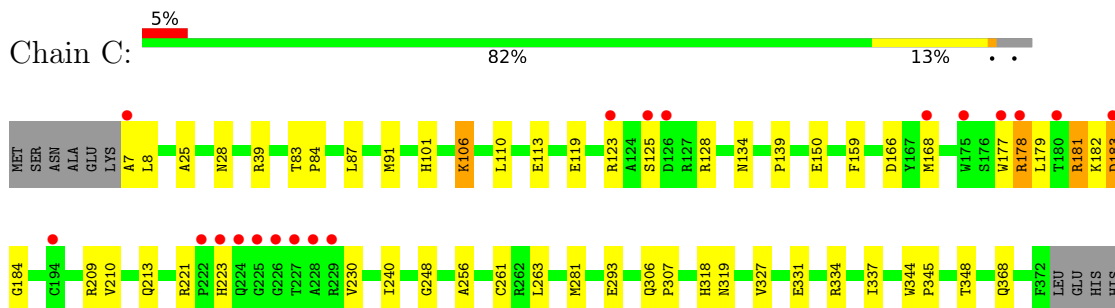
- Molecule 1: Scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity



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

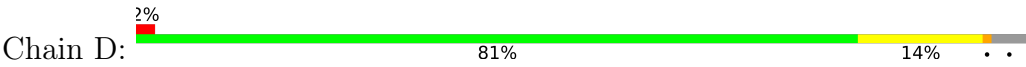


- Molecule 1: Scyllo-inositol dehydrogenase with L-glucose dehydrogenase activity



HIS
HIS
HIS
HIS

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



HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.21Å 120.15Å 140.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.30 – 2.30 49.30 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.30-2.30) 98.0 (49.30-2.30)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.192 , 0.224 0.198 , 0.232	Depositor DCC
R_{free} test set	3214 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11763	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, INS

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	0.94	0/2851	1.01	4/3865 (0.1%)
1	B	0.95	0/2851	0.98	1/3865 (0.0%)
1	C	0.94	0/2851	1.02	1/3865 (0.0%)
1	D	0.94	0/2842	1.00	3/3850 (0.1%)
All	All	0.94	0/11395	1.00	9/15445 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ASP	N-CA-C	-8.67	97.40	110.14
1	D	170	ASP	CA-C-N	6.71	126.67	119.28
1	D	170	ASP	C-N-CA	6.71	126.67	119.28
1	A	177	TRP	N-CA-C	6.41	118.26	111.28
1	C	125	SER	N-CA-C	5.82	119.20	111.75
1	A	102	VAL	N-CA-C	5.50	115.92	107.77
1	B	334	ARG	CB-CA-C	-5.28	102.59	110.88
1	A	55	ALA	N-CA-C	-5.24	105.65	111.36
1	D	309	PHE	N-CA-C	5.13	116.56	111.07

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	2785	0	2702	48	0
1	B	2785	0	2702	46	1
1	C	2785	0	2702	52	1
1	D	2777	0	2691	62	0
2	A	44	0	26	8	0
2	B	44	0	26	7	0
2	C	44	0	26	3	0
2	D	44	0	26	12	0
3	A	12	0	12	4	0
3	B	12	0	12	6	0
3	D	12	0	12	5	0
4	A	104	0	0	15	0
4	B	116	0	0	12	0
4	C	84	0	0	21	0
4	D	115	0	0	16	0
All	All	11763	0	10937	211	1

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 9.

All (211) 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:195:HIS:HB3	4:A:578:HOH:O	1.33	1.29
1:C:83:THR:OG1	1:C:91:MET:HE1	1.47	1.15
4:A:537:HOH:O	1:D:294:ILE:HB	1.49	1.09
1:B:196:LEU:HA	4:B:558:HOH:O	1.56	1.05
1:C:181:ARG:HD3	4:C:606:HOH:O	1.56	1.04
1:C:178:ARG:HB3	4:C:649:HOH:O	1.59	1.03
1:B:196:LEU:HD12	4:B:558:HOH:O	1.60	1.01
1:A:58:PHE:HA	4:B:502:HOH:O	1.61	1.00
1:C:178:ARG:CB	4:C:649:HOH:O	2.13	0.96
1:D:191:ASP:HB3	4:D:518:HOH:O	1.67	0.95
2:B:401:NAD:C4N	3:B:402:INS:H4	1.99	0.93
1:D:46:MET:SD	4:D:507:HOH:O	2.27	0.92
2:C:500:NAD:H2B	4:C:638:HOH:O	1.69	0.91
1:D:113:GLU:HG3	4:D:596:HOH:O	1.71	0.90
2:A:401:NAD:C4N	3:A:402:INS:H4	2.03	0.88
1:B:155:ARG:HD3	4:B:512:HOH:O	1.75	0.87
1:B:372:PHE:C	4:B:505:HOH:O	2.16	0.87
1:A:18:MET:HE2	2:A:401:NAD:N7N	1.91	0.86
1:A:18:MET:HE2	2:A:401:NAD:C7N	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:LYS:O	1:C:184:GLY:N	2.13	0.82
1:C:223:HIS:HD2	4:C:678:HOH:O	1.63	0.81
1:D:162:MET:SD	4:D:611:HOH:O	2.40	0.80
1:B:101:HIS:HD2	1:B:128:ARG:H	1.31	0.79
1:D:276:PHE:CD2	4:D:506:HOH:O	2.37	0.77
1:A:263:LEU:HD11	4:A:578:HOH:O	1.87	0.75
2:D:401:NAD:C4N	3:D:402:INS:H4	2.17	0.74
2:D:401:NAD:C3N	3:D:402:INS:O4	2.37	0.73
1:C:306:GLN:HB3	4:C:603:HOH:O	1.90	0.72
1:A:18:MET:HE3	1:A:105:GLU:OE2	1.90	0.71
1:D:209:ARG:HG2	4:D:529:HOH:O	1.90	0.71
1:B:146:ASP:O	1:B:150:GLU:HG3	1.91	0.70
1:C:139:PRO:CA	4:C:603:HOH:O	2.40	0.70
2:B:401:NAD:C3N	3:B:402:INS:O4	2.39	0.70
2:B:401:NAD:C4N	3:B:402:INS:C4	2.70	0.70
1:C:182:LYS:C	1:C:184:GLY:H	1.99	0.70
1:D:175:TRP:HE3	1:D:221:ARG:HG3	1.58	0.69
1:D:276:PHE:CG	4:D:506:HOH:O	2.45	0.69
1:A:87:LEU:HB3	1:A:91:MET:HE3	1.75	0.68
1:D:126:ASP:O	1:D:127:ARG:NH1	2.28	0.66
1:D:106:LYS:HD2	1:D:106:LYS:C	2.20	0.66
1:A:180:THR:O	1:A:183:ASP:O	2.13	0.66
1:B:106:LYS:HE2	3:B:402:INS:HO4	1.61	0.66
1:B:106:LYS:HE2	3:B:402:INS:O4	1.96	0.65
1:C:139:PRO:HB3	4:C:603:HOH:O	1.96	0.64
1:A:147:LEU:HD21	1:D:293:GLU:HG2	1.80	0.64
1:C:139:PRO:HA	4:C:603:HOH:O	1.98	0.64
1:D:265:TRP:CZ2	4:D:506:HOH:O	2.50	0.64
1:A:263:LEU:CD1	4:A:578:HOH:O	2.45	0.63
1:C:183:ASP:HB2	4:C:656:HOH:O	1.98	0.63
1:C:83:THR:OG1	1:C:91:MET:CE	2.38	0.63
1:A:307:PRO:HA	4:A:600:HOH:O	1.99	0.62
1:D:175:TRP:CE3	1:D:221:ARG:HG3	2.34	0.62
1:A:175:TRP:CD1	4:A:561:HOH:O	2.53	0.62
1:B:71:VAL:CG1	1:B:95:ALA:HA	2.30	0.61
1:A:175:TRP:CG	4:A:561:HOH:O	2.54	0.61
1:C:177:TRP:CE3	1:C:183:ASP:HB3	2.36	0.61
1:A:18:MET:HE2	2:A:401:NAD:C3N	2.30	0.61
2:A:401:NAD:C3N	3:A:402:INS:O4	2.48	0.61
1:C:83:THR:HB	1:C:84:PRO:HD2	1.83	0.60
1:B:31:THR:HG23	4:B:502:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:LEU:HD21	1:C:337:ILE:HG21	1.83	0.60
2:D:401:NAD:C6A	4:D:507:HOH:O	2.49	0.60
1:B:271:GLU:HG3	4:B:611:HOH:O	2.02	0.59
1:D:18:MET:HG2	2:D:401:NAD:C5N	2.32	0.59
1:D:209:ARG:HD2	1:D:371:ASN:OD1	2.02	0.59
1:C:177:TRP:CD1	1:C:177:TRP:H	2.20	0.58
2:A:401:NAD:C4N	3:A:402:INS:C4	2.81	0.58
1:C:178:ARG:HB2	4:C:649:HOH:O	1.93	0.58
2:D:401:NAD:C4N	3:D:402:INS:C4	2.82	0.57
1:A:18:MET:HE1	1:A:134:ASN:OD1	2.05	0.57
2:B:401:NAD:C5N	3:B:402:INS:H4	2.34	0.57
1:A:298:ARG:CD	4:A:537:HOH:O	2.53	0.57
1:B:229:ARG:HD3	4:B:587:HOH:O	2.04	0.56
1:C:182:LYS:C	1:C:184:GLY:N	2.62	0.56
1:A:31:THR:O	1:B:20:LYS:HE3	2.06	0.56
1:A:138:SER:HB3	1:A:325:GLN:HE21	1.70	0.55
1:B:22:HIS:HE1	1:B:105:GLU:OE2	1.89	0.55
1:C:281:MET:HG2	1:D:319:ASN:HD22	1.71	0.55
1:A:106:LYS:HE2	3:A:402:INS:O4	2.07	0.54
1:D:172:ASP:C	1:D:174:PRO:HG3	2.33	0.54
1:C:139:PRO:CB	4:C:603:HOH:O	2.53	0.54
1:D:106:LYS:HD3	1:D:194:CYS:SG	2.47	0.54
1:A:281:MET:HG2	1:B:319:ASN:HD22	1.72	0.54
1:D:172:ASP:HA	1:D:223:HIS:HD2	1.73	0.53
1:A:22:HIS:HE1	1:A:105:GLU:OE2	1.92	0.53
1:C:166:ASP:HB3	1:C:256:ALA:O	2.09	0.53
2:D:401:NAD:O5D	2:D:401:NAD:H6N	2.09	0.53
2:C:500:NAD:C8A	4:C:638:HOH:O	2.57	0.53
1:D:170:ASP:CG	4:D:547:HOH:O	2.52	0.53
1:D:168:MET:SD	1:D:179:LEU:HD21	2.48	0.52
1:D:265:TRP:CE2	4:D:506:HOH:O	2.62	0.52
1:C:344:TRP:CE3	1:C:345:PRO:HD3	2.45	0.52
1:A:25:ALA:HA	1:A:327:VAL:HG22	1.91	0.52
1:D:27:ARG:HG2	1:D:40:LEU:HD11	1.91	0.52
1:B:372:PHE:N	4:B:505:HOH:O	2.42	0.52
1:D:168:MET:HG3	1:D:254:ARG:HD2	1.91	0.52
1:B:196:LEU:CD1	4:B:558:HOH:O	2.36	0.51
1:A:209:ARG:NE	4:A:501:HOH:O	2.32	0.51
1:A:7:ALA:O	1:A:39:ARG:NH1	2.44	0.51
1:A:168:MET:HE3	1:A:221:ARG:CZ	2.41	0.51
1:C:318:HIS:NE2	3:D:402:INS:O2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LYS:HB2	4:B:541:HOH:O	2.10	0.50
1:D:265:TRP:NE1	4:D:506:HOH:O	2.44	0.50
1:A:18:MET:HE3	1:A:105:GLU:CD	2.37	0.50
1:C:83:THR:HG1	1:C:91:MET:HE1	1.71	0.50
1:B:71:VAL:HG13	1:B:95:ALA:HA	1.94	0.50
1:A:106:LYS:HD2	1:A:106:LYS:C	2.37	0.49
1:A:336:ALA:HA	1:A:341:GLY:O	2.13	0.49
1:B:18:MET:HE3	2:B:401:NAD:C4N	2.42	0.49
1:D:167:TYR:CE1	1:D:168:MET:HG2	2.47	0.49
1:A:18:MET:CE	2:A:401:NAD:C7N	2.87	0.49
1:C:368:GLN:CD	4:C:648:HOH:O	2.56	0.49
4:A:537:HOH:O	1:D:294:ILE:HD12	2.13	0.49
1:B:27:ARG:HD2	1:B:40:LEU:HD11	1.93	0.49
1:A:18:MET:CE	2:A:401:NAD:N7N	2.68	0.49
1:A:319:ASN:HD22	1:B:281:MET:HG2	1.77	0.49
1:A:126:ASP:O	1:A:128:ARG:NH2	2.45	0.48
1:C:101:HIS:CD2	1:C:337:ILE:HG12	2.48	0.48
2:C:500:NAD:H8A	4:C:638:HOH:O	2.13	0.48
1:C:209:ARG:CZ	4:C:618:HOH:O	2.61	0.48
1:D:217:VAL:HG21	1:D:255:VAL:HG21	1.95	0.48
1:D:126:ASP:C	1:D:127:ARG:HH11	2.21	0.48
1:A:228:ALA:CB	4:A:561:HOH:O	2.62	0.47
1:C:319:ASN:OD1	1:D:281:MET:HG2	2.14	0.47
1:D:25:ALA:HA	1:D:327:VAL:HG22	1.96	0.47
1:C:209:ARG:HG2	1:C:210:VAL:N	2.27	0.47
1:D:46:MET:CG	4:D:507:HOH:O	2.59	0.47
1:A:130:ILE:HD12	1:A:343:ALA:HB1	1.95	0.47
1:B:127:ARG:C	1:B:128:ARG:HH11	2.21	0.47
1:C:110:LEU:HD11	1:C:183:ASP:HA	1.95	0.47
1:B:105:GLU:OE1	2:B:401:NAD:H2N	2.15	0.47
1:A:22:HIS:HD2	1:A:80:SER:OG	1.98	0.46
1:B:18:MET:HG3	2:B:401:NAD:C2N	2.45	0.46
1:B:22:HIS:HD2	1:B:80:SER:OG	1.99	0.46
1:C:106:LYS:O	1:C:106:LYS:HE3	2.15	0.46
1:C:123:ARG:HD2	4:C:674:HOH:O	2.15	0.46
1:C:210:VAL:HG12	1:C:240:ILE:HD12	1.97	0.46
1:C:179:LEU:HD13	1:C:230:VAL:HG22	1.95	0.46
1:C:7:ALA:O	1:C:39:ARG:NH1	2.49	0.46
1:C:331:GLU:OE1	1:C:334:ARG:NH1	2.47	0.46
1:D:105:GLU:OE1	2:D:401:NAD:H2N	2.16	0.46
1:B:179:LEU:HD13	1:B:221:ARG:HD2	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ALA:HB3	4:A:561:HOH:O	2.15	0.45
1:D:18:MET:HG2	2:D:401:NAD:C6N	2.47	0.45
1:C:306:GLN:CB	4:C:603:HOH:O	2.56	0.45
1:B:168:MET:HE2	1:B:173:LEU:HD23	1.98	0.45
1:D:17:PHE:C	1:D:17:PHE:CD1	2.95	0.45
1:A:209:ARG:NH2	4:A:501:HOH:O	2.50	0.44
1:C:25:ALA:HA	1:C:327:VAL:HG22	1.99	0.44
1:D:138:SER:HB3	1:D:325:GLN:HE21	1.82	0.44
1:C:87:LEU:HB3	1:C:91:MET:HE2	1.98	0.44
1:C:368:GLN:HG3	4:C:648:HOH:O	2.17	0.44
1:D:18:MET:CE	1:D:326:LYS:HE2	2.47	0.44
1:D:46:MET:HG3	4:D:507:HOH:O	2.18	0.44
1:B:101:HIS:CE1	1:B:337:ILE:HG23	2.53	0.44
1:C:307:PRO:N	4:C:603:HOH:O	2.51	0.44
1:D:218:ILE:HG21	1:D:221:ARG:HH21	1.82	0.44
1:A:44:ALA:HA	1:A:64:THR:O	2.17	0.44
1:A:298:ARG:HD2	4:A:537:HOH:O	2.15	0.44
1:D:18:MET:HG2	2:D:401:NAD:C4N	2.47	0.44
1:B:147:LEU:HD21	1:C:293:GLU:HG2	2.00	0.44
1:D:179:LEU:CD1	1:D:221:ARG:HD2	2.48	0.44
1:D:106:LYS:HE2	1:D:195:HIS:NE2	2.33	0.43
1:A:168:MET:HE2	1:A:179:LEU:HD21	2.00	0.43
2:D:401:NAD:C7N	3:D:402:INS:O4	2.65	0.43
1:A:209:ARG:HD2	1:A:210:VAL:N	2.33	0.43
1:D:106:LYS:HE3	2:D:401:NAD:C2N	2.49	0.43
1:A:106:LYS:HE2	1:A:195:HIS:NE2	2.34	0.43
1:D:17:PHE:C	1:D:17:PHE:HD1	2.27	0.43
1:D:168:MET:CE	1:D:179:LEU:HD21	2.49	0.43
1:B:127:ARG:HA	1:B:127:ARG:HE	1.83	0.43
1:D:155:ARG:HD2	4:D:545:HOH:O	2.19	0.43
1:C:179:LEU:HD23	4:C:649:HOH:O	2.19	0.42
1:A:45:ASP:O	1:A:65:ALA:HA	2.19	0.42
1:D:44:ALA:HA	1:D:64:THR:O	2.18	0.42
1:B:293:GLU:OE2	1:C:150:GLU:OE1	2.36	0.42
1:C:119:GLU:OE2	1:C:348:THR:OG1	2.36	0.42
1:B:344:TRP:HA	1:B:345:PRO:HA	1.82	0.42
1:C:101:HIS:CD2	1:C:128:ARG:H	2.38	0.42
1:B:131:ILE:HG12	1:B:345:PRO:O	2.20	0.42
1:B:263:LEU:HD21	4:B:558:HOH:O	2.19	0.42
1:B:131:ILE:HD11	1:B:347:PHE:CD1	2.55	0.42
1:C:210:VAL:HG12	1:C:240:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:ARG:HB3	1:D:340:ARG:CZ	2.50	0.42
1:A:239:LEU:HD13	1:C:213:GLN:HG2	2.02	0.41
1:B:179:LEU:CD1	1:B:221:ARG:HD2	2.50	0.41
1:B:239:LEU:HD11	1:D:238:ALA:HA	2.02	0.41
1:C:159:PHE:O	1:C:248:GLY:HA2	2.19	0.41
1:B:26:TRP:HE3	1:B:38:PRO:HG2	1.84	0.41
1:B:87:LEU:HB3	1:B:91:MET:HE3	2.03	0.41
1:D:175:TRP:CZ3	1:D:228:ALA:HB1	2.55	0.41
1:D:344:TRP:HA	1:D:345:PRO:HA	1.86	0.41
1:A:150:GLU:HG2	1:A:150:GLU:O	2.19	0.41
1:B:209:ARG:HH22	1:D:213:GLN:NE2	2.18	0.41
1:B:109:ALA:HB3	1:B:114:ASP:HB3	2.02	0.41
1:D:18:MET:HE2	1:D:326:LYS:HZ3	1.86	0.41
1:D:177:TRP:HB2	1:D:183:ASP:HB3	2.01	0.41
1:B:17:PHE:CD1	1:B:17:PHE:C	2.99	0.41
1:D:27:ARG:HG3	4:D:604:HOH:O	2.20	0.41
1:D:167:TYR:CD1	1:D:168:MET:HG2	2.56	0.41
1:B:164:ASP:OD2	1:D:160:ARG:NH2	2.54	0.41
1:D:175:TRP:CD1	1:D:175:TRP:C	2.97	0.41
1:A:358:HIS:HE1	4:A:523:HOH:O	2.04	0.41
1:C:168:MET:HE3	1:C:221:ARG:CZ	2.51	0.41
1:C:223:HIS:O	1:C:223:HIS:CG	2.71	0.41
1:D:18:MET:HG3	2:D:401:NAD:C2N	2.51	0.40
1:D:27:ARG:CG	1:D:40:LEU:HD11	2.52	0.40
1:A:246:THR:HG22	1:A:247:SER:N	2.37	0.40
1:B:128:ARG:HH11	1:B:128:ARG:N	2.19	0.40
1:A:150:GLU:OE2	1:D:293:GLU:OE1	2.40	0.40
1:B:101:HIS:CD2	1:B:128:ARG:H	2.23	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ARG:NH1	1:C:113:GLU:OE2[1_655]	2.18	0.02

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	364/380 (96%)	351 (96%)	13 (4%)	0	100	100
1	B	364/380 (96%)	352 (97%)	10 (3%)	2 (0%)	24	31
1	C	364/380 (96%)	346 (95%)	16 (4%)	2 (0%)	24	31
1	D	361/380 (95%)	348 (96%)	11 (3%)	2 (1%)	21	27
All	All	1453/1520 (96%)	1397 (96%)	50 (3%)	6 (0%)	30	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	227	THR
1	B	224	GLN
1	C	183	ASP
1	D	175	TRP
1	D	225	GLY
1	C	261	CYS

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	275/288 (96%)	267 (97%)	8 (3%)	37	55
1	B	275/288 (96%)	271 (98%)	4 (2%)	57	75
1	C	275/288 (96%)	269 (98%)	6 (2%)	45	65
1	D	274/288 (95%)	268 (98%)	6 (2%)	45	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1099/1152 (95%)	1075 (98%)	24 (2%)	45 65

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	46	MET
1	A	49	ASP
1	A	106	LYS
1	A	128	ARG
1	A	134	ASN
1	A	180	THR
1	A	237	GLN
1	B	49	ASP
1	B	106	LYS
1	B	134	ASN
1	B	220	ASP
1	C	28	ASN
1	C	106	LYS
1	C	134	ASN
1	C	178	ARG
1	C	181	ARG
1	C	263	LEU
1	D	17	PHE
1	D	62	ARG
1	D	71	VAL
1	D	134	ASN
1	D	263	LEU
1	D	340	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	28	ASN
1	A	319	ASN
1	A	323	ASN
1	A	325	GLN
1	A	358	HIS
1	B	22	HIS
1	B	28	ASN

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Mol	Chain	Res	Type
1	B	101	HIS
1	B	319	ASN
1	B	323	ASN
1	B	358	HIS
1	C	28	ASN
1	C	101	HIS
1	C	223	HIS
1	C	335	GLN
1	C	358	HIS
1	D	28	ASN
1	D	213	GLN
1	D	223	HIS
1	D	278	GLN
1	D	319	ASN
1	D	325	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	401	-	46,48,48	1.53	9 (19%)	64,73,73	1.70	9 (14%)
3	INS	D	402	-	12,12,12	0.83	0	18,18,18	2.27	5 (27%)
2	NAD	B	401	-	46,48,48	1.48	6 (13%)	64,73,73	2.02	20 (31%)
3	INS	A	402	-	12,12,12	0.99	0	18,18,18	2.35	6 (33%)
2	NAD	D	401	-	46,48,48	1.61	8 (17%)	64,73,73	1.80	12 (18%)
3	INS	B	402	-	12,12,12	0.84	0	18,18,18	2.58	8 (44%)
2	NAD	C	500	-	46,48,48	1.80	7 (15%)	64,73,73	1.71	14 (21%)

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	A	401	-	-	4/30/62/62	0/5/5/5
3	INS	D	402	-	-	-	0/1/1/1
2	NAD	B	401	-	-	5/30/62/62	0/5/5/5
3	INS	A	402	-	-	-	0/1/1/1
2	NAD	D	401	-	-	4/30/62/62	0/5/5/5
3	INS	B	402	-	-	-	0/1/1/1
2	NAD	C	500	-	-	4/30/62/62	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	NAD	PN-O3	7.19	1.67	1.59
2	C	500	NAD	PA-O3	5.27	1.65	1.59
2	A	401	NAD	C5A-C4A	4.85	1.47	1.39
2	B	401	NAD	C2N-N1N	-4.44	1.30	1.35
2	D	401	NAD	C5A-C4A	4.29	1.46	1.39
2	D	401	NAD	C2N-N1N	-4.26	1.30	1.35
2	B	401	NAD	C5A-C4A	4.16	1.46	1.39
2	C	500	NAD	C5A-C4A	3.98	1.46	1.39
2	D	401	NAD	PA-O3	3.88	1.63	1.59
2	D	401	NAD	C4N-C3N	3.82	1.45	1.39
2	A	401	NAD	C8A-N7A	3.29	1.38	1.31
2	C	500	NAD	C4A-N9A	-3.12	1.31	1.37
2	B	401	NAD	O4D-C1D	3.02	1.44	1.40
2	A	401	NAD	O4D-C1D	2.98	1.44	1.40
2	A	401	NAD	C3N-C7N	2.80	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C5A-C6A	2.71	1.48	1.41
2	C	500	NAD	C8A-N7A	2.63	1.36	1.31
2	A	401	NAD	C4A-N9A	-2.60	1.32	1.37
2	B	401	NAD	C5A-C6A	2.60	1.48	1.41
2	A	401	NAD	C5A-N7A	-2.58	1.34	1.39
2	D	401	NAD	C5A-N7A	-2.56	1.34	1.39
2	D	401	NAD	C8A-N7A	2.34	1.36	1.31
2	A	401	NAD	C5N-C4N	2.32	1.42	1.38
2	A	401	NAD	C7N-N7N	2.30	1.37	1.33
2	B	401	NAD	PN-O3	2.25	1.61	1.59
2	B	401	NAD	C4A-N3A	2.24	1.38	1.34
2	D	401	NAD	C5A-C6A	2.18	1.47	1.41
2	C	500	NAD	C5A-C6A	2.15	1.47	1.41
2	C	500	NAD	O4D-C1D	2.11	1.43	1.40
2	D	401	NAD	C4A-N9A	-2.09	1.33	1.37

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAD	C4A-N9A-C8A	6.86	112.94	105.74
3	B	402	INS	C3-C2-C1	6.22	121.74	110.83
3	A	402	INS	C3-C2-C1	5.93	121.24	110.83
2	A	401	NAD	C5A-C4A-N3A	-5.75	118.80	126.72
2	D	401	NAD	C5A-C4A-N3A	-5.67	118.91	126.72
2	D	401	NAD	N3A-C4A-N9A	5.54	136.59	127.17
3	B	402	INS	C6-C5-C4	-5.16	101.76	110.83
2	B	401	NAD	N3A-C4A-N9A	4.90	135.50	127.17
3	D	402	INS	C3-C2-C1	4.68	119.04	110.83
3	A	402	INS	O6-C6-C5	-4.54	99.68	110.38
3	D	402	INS	C6-C5-C4	-4.41	103.10	110.83
2	C	500	NAD	C4A-N9A-C8A	4.40	110.36	105.74
2	C	500	NAD	C5A-C4A-N3A	-4.26	120.85	126.72
2	B	401	NAD	N3A-C2A-N1A	-4.17	122.27	128.58
2	A	401	NAD	C2A-N3A-C4A	4.11	121.88	111.83
2	B	401	NAD	N9A-C8A-N7A	-4.08	108.15	113.94
3	B	402	INS	O6-C6-C5	-3.94	101.08	110.38
2	A	401	NAD	N3A-C2A-N1A	-3.92	122.65	128.58
2	D	401	NAD	C4A-N9A-C8A	3.90	109.83	105.74
3	D	402	INS	O6-C6-C5	-3.89	101.21	110.38
2	C	500	NAD	N3A-C4A-N9A	3.84	133.71	127.17
2	C	500	NAD	N3A-C2A-N1A	-3.79	122.84	128.58
2	A	401	NAD	N3A-C4A-N9A	3.78	133.60	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	INS	C6-C1-C2	3.78	117.46	110.83
2	B	401	NAD	C5A-C4A-N3A	-3.61	121.74	126.72
2	B	401	NAD	C3B-C2B-C1B	-3.61	94.63	101.46
2	D	401	NAD	C2A-N3A-C4A	3.57	120.55	111.83
2	A	401	NAD	C4A-C5A-N7A	-3.45	106.64	110.58
2	C	500	NAD	C2A-N3A-C4A	3.22	119.70	111.83
2	D	401	NAD	C6N-C5N-C4N	-3.18	114.86	119.45
2	B	401	NAD	C2A-N3A-C4A	3.16	119.55	111.83
3	A	402	INS	C6-C5-C4	-3.12	105.35	110.83
2	B	401	NAD	C5A-N7A-C8A	3.11	108.34	103.45
2	A	401	NAD	O2N-PN-O3	2.99	115.36	107.27
2	C	500	NAD	O2N-PN-O3	2.92	115.17	107.27
2	A	401	NAD	O4B-C1B-N9A	2.89	113.64	108.09
2	C	500	NAD	N9A-C8A-N7A	-2.86	109.89	113.94
2	D	401	NAD	O4B-C1B-N9A	2.83	113.52	108.09
2	B	401	NAD	C5A-C4A-N9A	-2.80	102.75	105.81
3	B	402	INS	O2-C2-C1	-2.80	103.77	110.38
3	A	402	INS	O2-C2-C3	-2.75	103.89	110.38
2	B	401	NAD	C4A-N9A-C1B	-2.73	120.25	126.63
2	A	401	NAD	O2A-PA-O1A	2.71	125.07	112.44
2	D	401	NAD	N3A-C2A-N1A	-2.71	124.48	128.58
3	A	402	INS	O3-C3-C4	-2.69	104.03	110.38
2	A	401	NAD	C6A-C5A-N7A	2.69	137.28	132.09
3	B	402	INS	O5-C5-C4	2.67	116.68	110.38
2	D	401	NAD	N6A-C6A-N1A	2.57	124.10	118.38
2	C	500	NAD	C3N-C7N-N7N	2.48	120.80	117.74
2	B	401	NAD	C6N-N1N-C1D	2.45	124.54	119.73
2	B	401	NAD	C4A-C5A-N7A	-2.43	107.81	110.58
2	D	401	NAD	C5A-C6A-N6A	-2.41	117.32	123.29
3	D	402	INS	O5-C5-C4	2.41	116.06	110.38
2	D	401	NAD	C2N-N1N-C1D	-2.38	113.88	119.13
2	B	401	NAD	C5N-C4N-C3N	-2.37	118.03	120.36
2	B	401	NAD	C6A-C5A-N7A	2.36	136.64	132.09
2	D	401	NAD	O2A-PA-O3	2.33	113.58	107.27
2	C	500	NAD	C3B-C2B-C1B	-2.33	97.05	101.46
2	D	401	NAD	N9A-C8A-N7A	-2.33	110.63	113.94
2	B	401	NAD	C5A-C6A-N6A	-2.28	117.65	123.29
2	C	500	NAD	C4A-C5A-N7A	-2.27	107.99	110.58
3	B	402	INS	O2-C2-C3	-2.27	105.04	110.38
2	C	500	NAD	O3D-C3D-C4D	-2.26	104.59	111.08
2	B	401	NAD	O2A-PA-O1A	2.25	122.90	112.44
2	B	401	NAD	N6A-C6A-N1A	2.23	123.34	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	NAD	C4A-N9A-C1B	-2.17	121.55	126.63
3	B	402	INS	O3-C3-C4	-2.16	105.29	110.38
2	C	500	NAD	C4D-O4D-C1D	-2.15	107.95	109.92
2	B	401	NAD	C6N-N1N-C2N	-2.13	120.07	121.88
2	C	500	NAD	C5N-C6N-N1N	-2.09	117.53	120.38
3	A	402	INS	C5-C6-C1	-2.07	107.19	110.83
2	B	401	NAD	O2N-PN-O1N	2.05	121.97	112.44
2	B	401	NAD	O2N-PN-O3	2.04	112.80	107.27
3	B	402	INS	C6-C1-C2	2.01	114.35	110.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	C2D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	C2D-C1D-N1N-C2N
2	C	500	NAD	O4D-C1D-N1N-C2N
2	C	500	NAD	O4D-C1D-N1N-C6N
2	C	500	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	O4D-C1D-N1N-C2N
2	D	401	NAD	O4D-C1D-N1N-C6N
2	D	401	NAD	C2D-C1D-N1N-C2N
2	D	401	NAD	C2D-C1D-N1N-C6N
2	B	401	NAD	PN-O3-PA-O1A
2	B	401	NAD	PN-O3-PA-O2A
2	C	500	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	PN-O3-PA-O2A

There are no ring outliers.

7 monomers are involved in 34 short contacts:

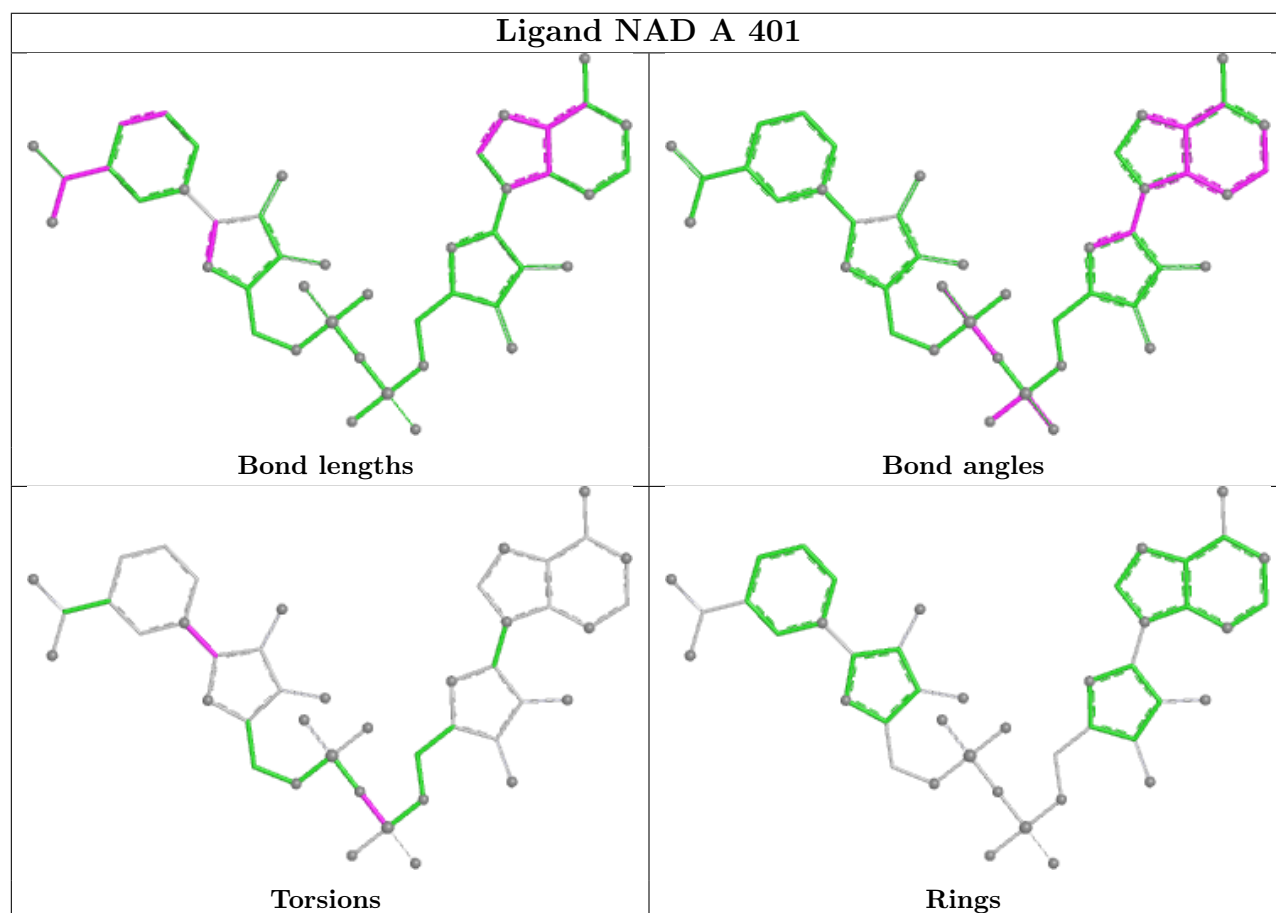
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAD	8	0
3	D	402	INS	5	0
2	B	401	NAD	7	0
3	A	402	INS	4	0
2	D	401	NAD	12	0

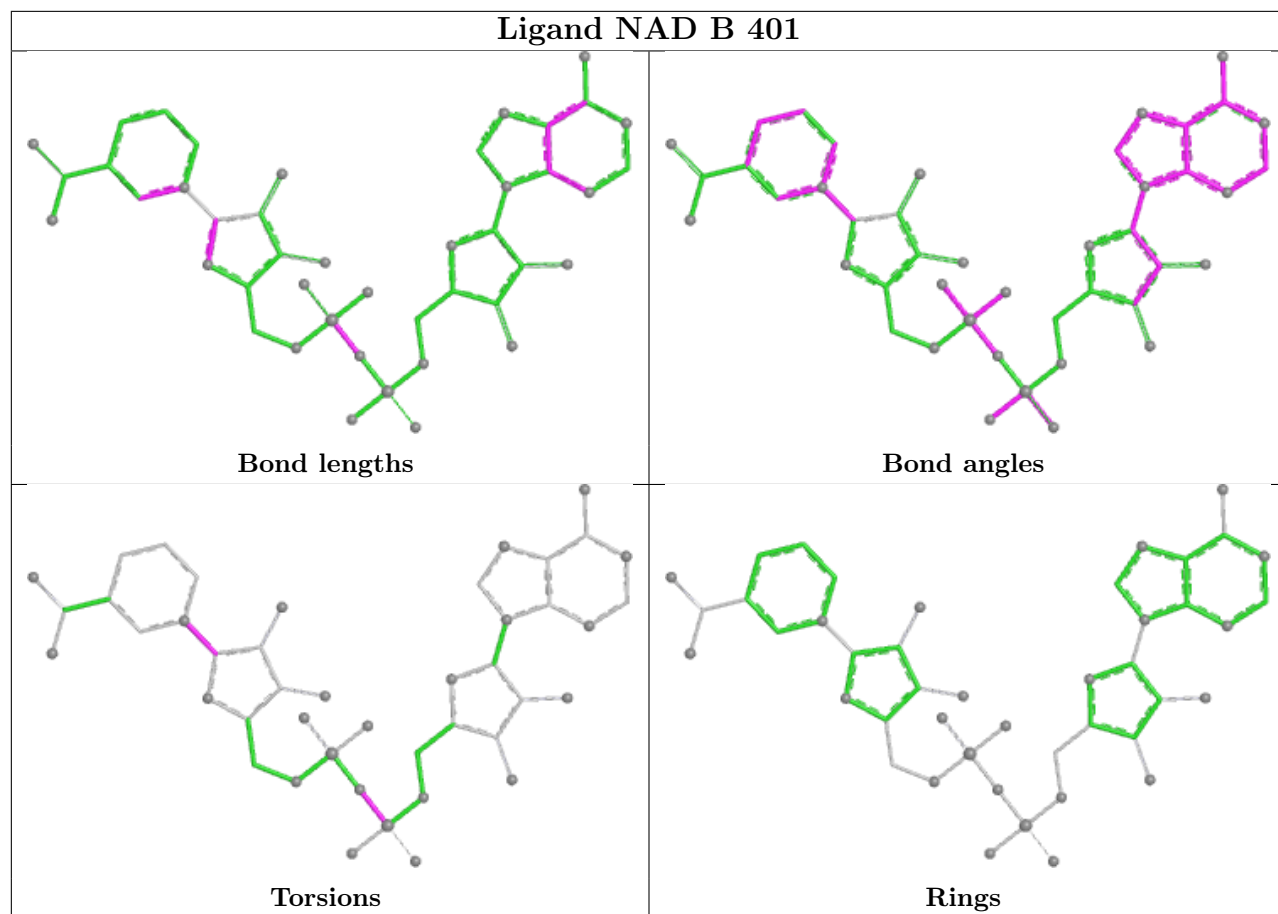
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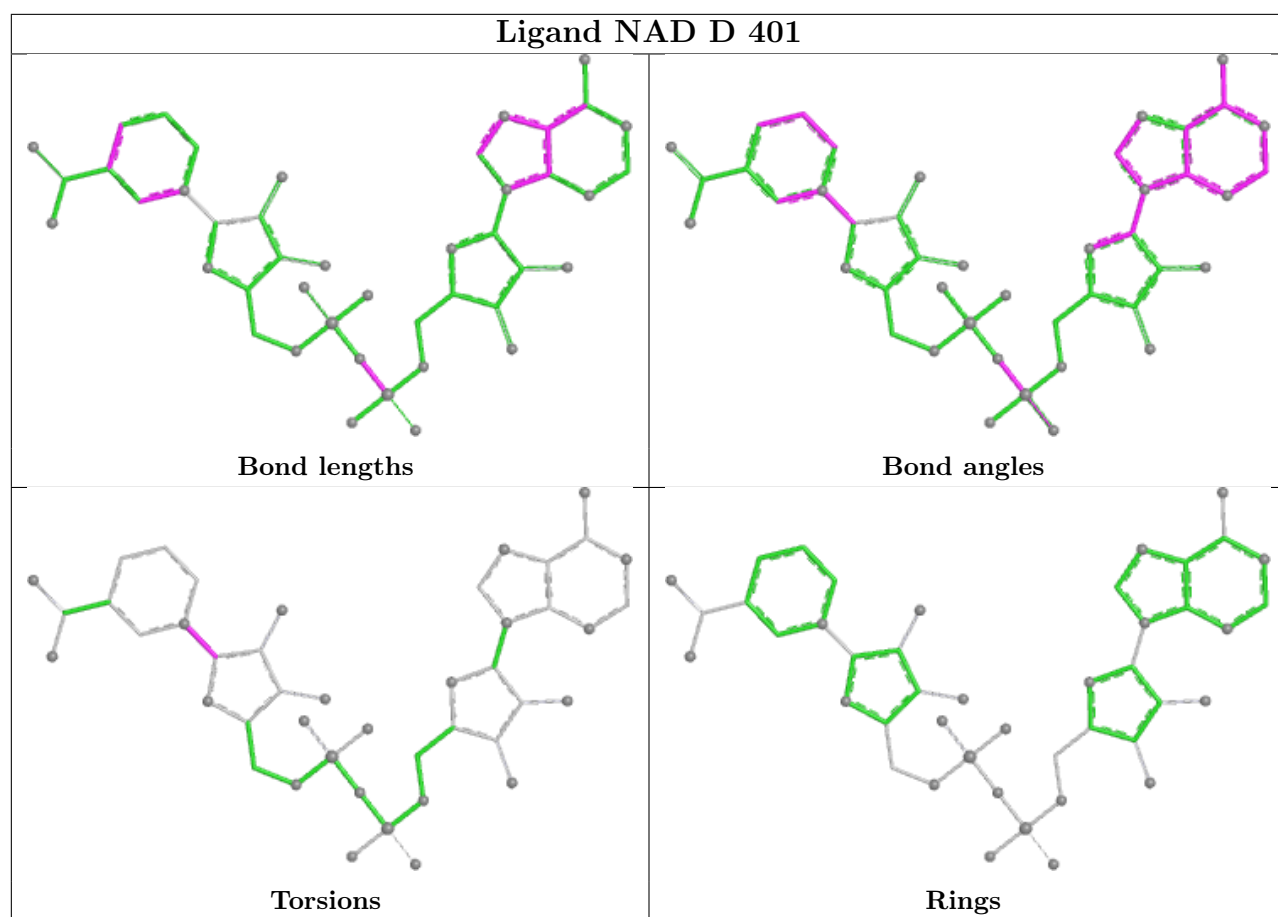
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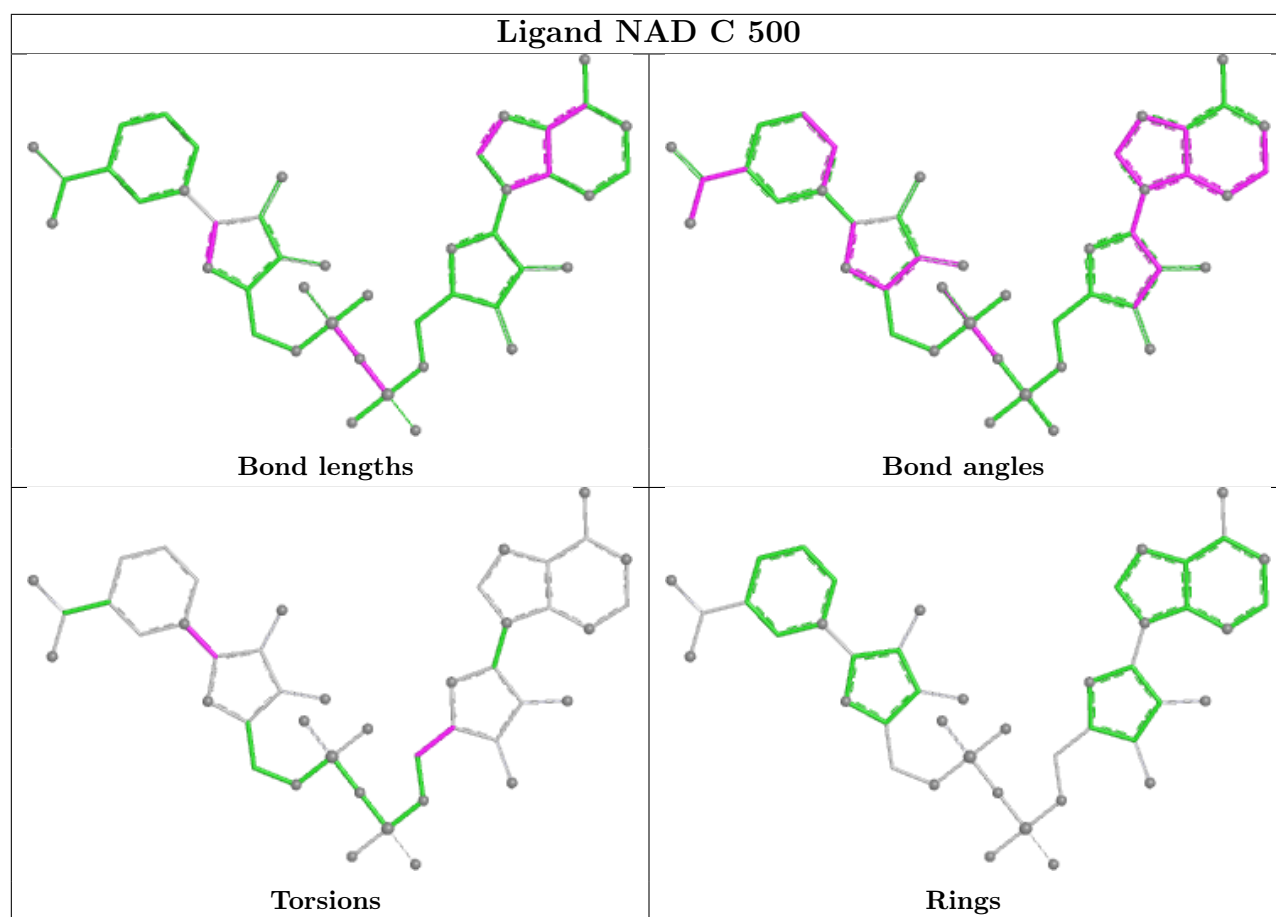
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	INS	6	0
2	C	500	NAD	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	366/380 (96%)	0.01	17 (4%) 37 39	16, 25, 46, 87	0
1	B	366/380 (96%)	-0.03	10 (2%) 56 58	10, 24, 45, 66	4 (1%)
1	C	366/380 (96%)	0.12	19 (5%) 33 34	12, 26, 58, 103	2 (0%)
1	D	365/380 (96%)	-0.08	8 (2%) 62 64	9, 24, 41, 71	1 (0%)
All	All	1463/1520 (96%)	0.01	54 (3%) 45 48	9, 25, 48, 103	7 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	TRP	6.3
1	C	183	ASP	5.0
1	B	227	THR	4.1
1	D	171	PRO	3.9
1	D	174	PRO	3.9
1	B	13	ILE	3.8
1	B	175	TRP	3.7
1	C	177	TRP	3.7
1	A	342	LYS	3.6
1	A	176	SER	3.4
1	B	7	ALA	3.3
1	C	223	HIS	3.3
1	D	172	ASP	3.3
1	C	224	GLN	3.2
1	A	180	THR	3.1
1	A	343	ALA	3.1
1	D	227	THR	3.0
1	C	229	ARG	3.0
1	C	125	SER	3.0
1	A	183	ASP	2.9
1	D	175	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	168	MET	2.8
1	A	7	ALA	2.7
1	C	227	THR	2.7
1	C	225	GLY	2.6
1	C	194	CYS	2.6
1	A	223	HIS	2.5
1	C	222	PRO	2.5
1	C	175	TRP	2.4
1	C	226	GLY	2.4
1	A	181	ARG	2.4
1	A	224	GLN	2.4
1	C	178	ARG	2.4
1	B	168	MET	2.3
1	B	181	ARG	2.3
1	C	7	ALA	2.3
1	A	341	GLY	2.3
1	C	126	ASP	2.3
1	B	226	GLY	2.3
1	C	228	ALA	2.3
1	A	179	LEU	2.2
1	C	180	THR	2.2
1	D	225	GLY	2.2
1	B	340	ARG	2.2
1	C	123	ARG	2.2
1	A	174	PRO	2.2
1	A	225	GLY	2.2
1	B	225	GLY	2.2
1	D	213	GLN	2.2
1	B	342	LYS	2.1
1	D	223	HIS	2.1
1	A	340	ARG	2.1
1	A	339	GLY	2.1
1	A	231	GLU	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](#)

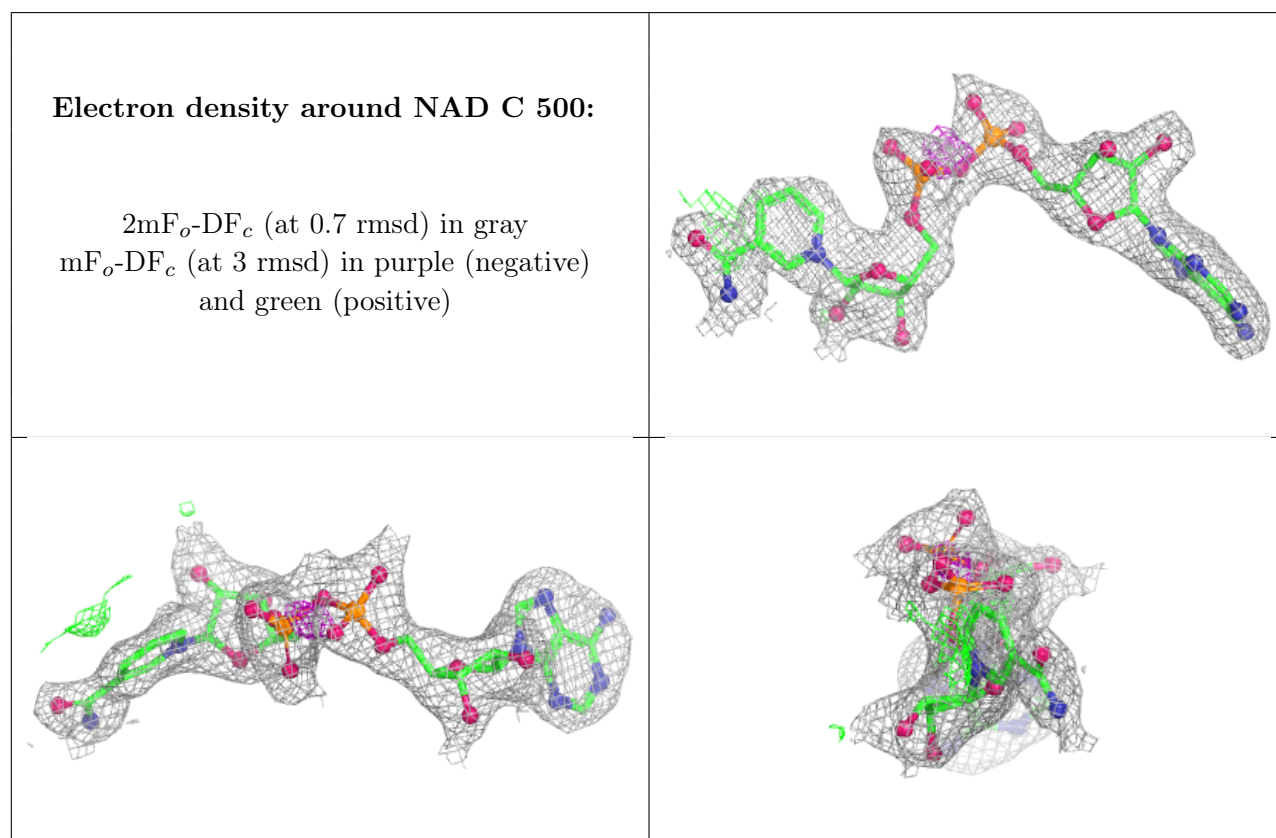
There are no oligosaccharides in this entry.

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.

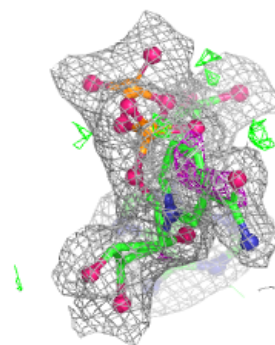
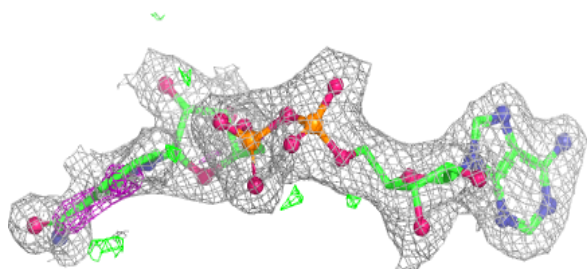
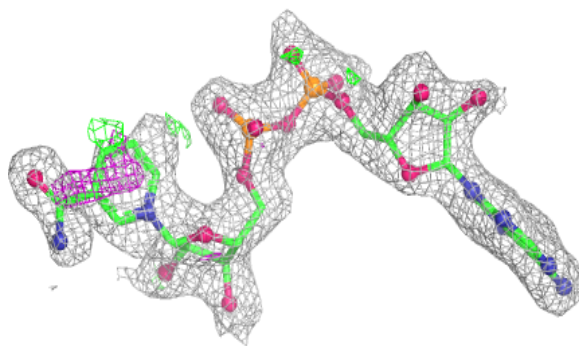
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	INS	A	402	12/12	0.88	0.14	23,24,26,26	0
3	INS	B	402	12/12	0.89	0.11	23,23,23,26	0
3	INS	D	402	12/12	0.89	0.13	22,23,24,24	0
2	NAD	C	500	44/44	0.92	0.09	26,30,36,38	0
2	NAD	A	401	44/44	0.93	0.09	23,27,32,34	0
2	NAD	D	401	44/44	0.94	0.09	18,25,33,35	0
2	NAD	B	401	44/44	0.94	0.09	23,28,32,35	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.

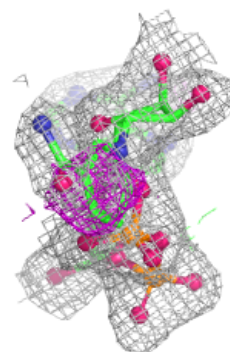
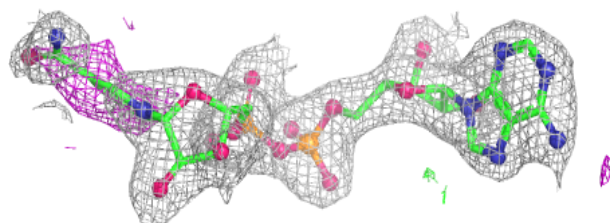
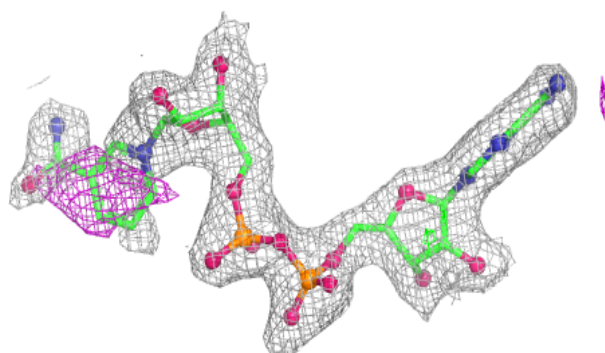


Electron density around NAD A 401:

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

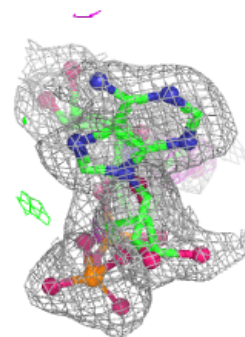
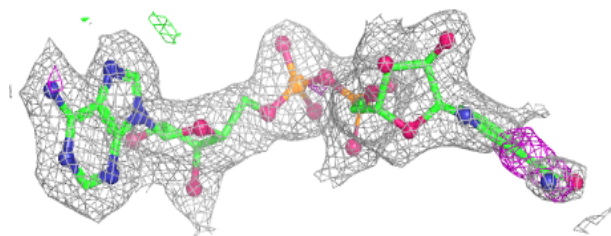
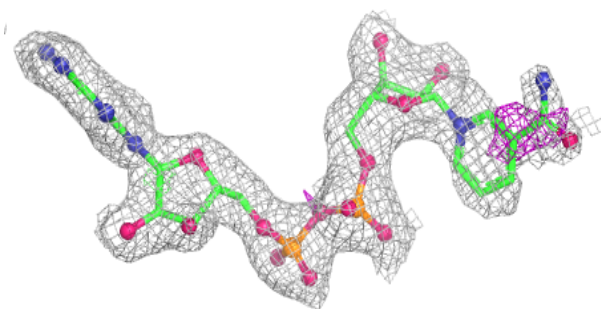
**Electron density around NAD D 401:**

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.