



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:15 PM UTC

PDB ID : 6AJB / pdb_00006ajb
Title : Crystal structure of Trypanosoma brucei glycosomal isocitrate dehydrogenase in complex with NADH, alpha-ketoglutarate and ca2+
Authors : Wang, X.; Inaoka, D.K.; Shiba, T.; Balogun, E.O.; Ziebart, N.; Allman, S.; Watanabe, Y.; Nozaki, T.; Boshart, M.; Bringaud, F.; Harada, S.; Kita, K.
Deposited on : 2018-08-27
Resolution : 2.90 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

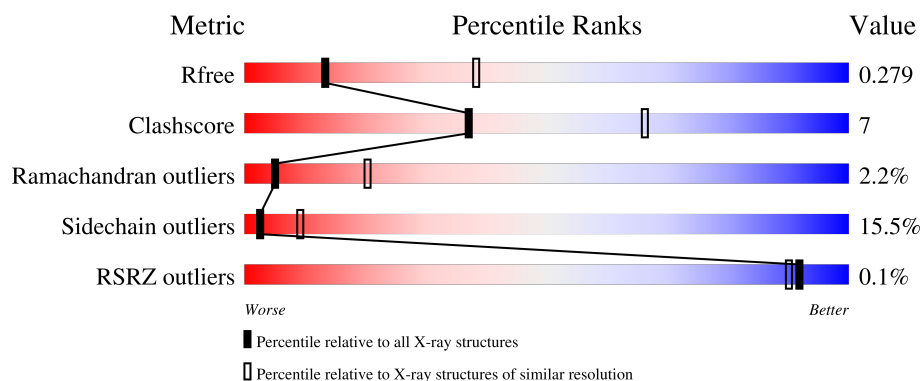
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	413	70% 25% .
1	B	413	70% 23% 6%
1	C	413	70% 23% 5%
1	D	413	68% 27% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13236 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.

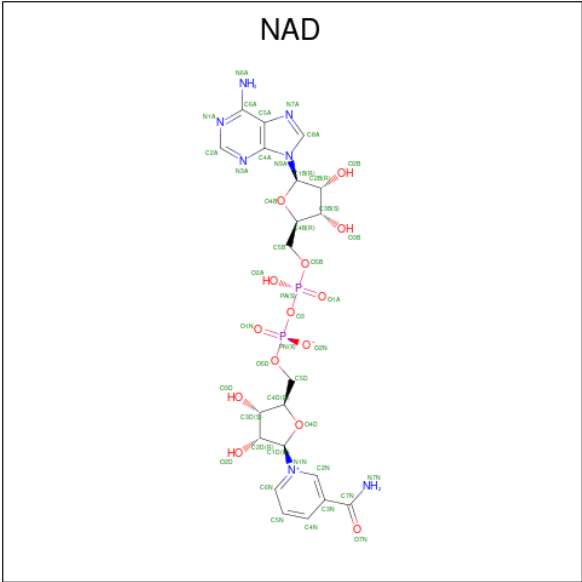
- Molecule 1 is a protein called Isocitrate dehydrogenase [NADP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3259	2070	559	608	22			
1	B	411	Total	C	N	O	S	0	0	0
			3265	2073	560	610	22			
1	C	407	Total	C	N	O	S	0	0	0
			3240	2059	555	604	22			
1	D	413	Total	C	N	O	S	0	0	0
			3282	2084	563	613	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	MET	engineered mutation	UNP Q387G0
B	1	SER	MET	engineered mutation	UNP Q387G0
C	1	SER	MET	engineered mutation	UNP Q387G0
D	1	SER	MET	engineered mutation	UNP Q387G0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).

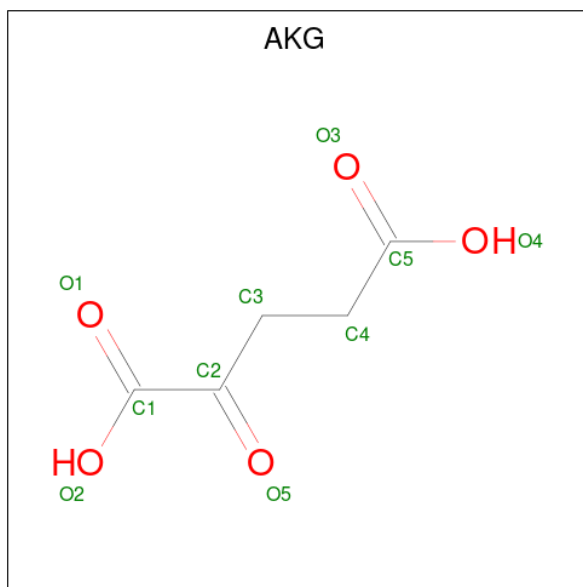


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).

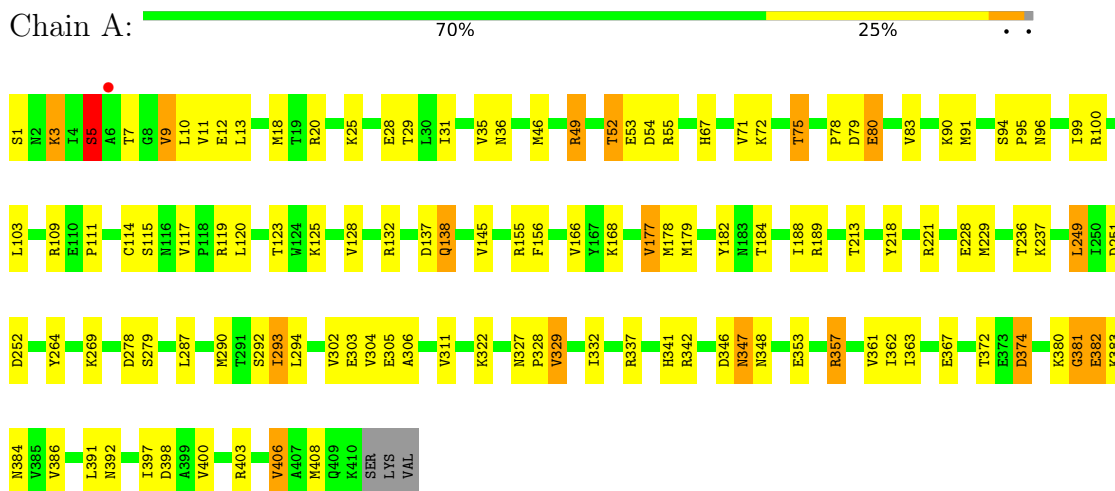


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			10	5	5		

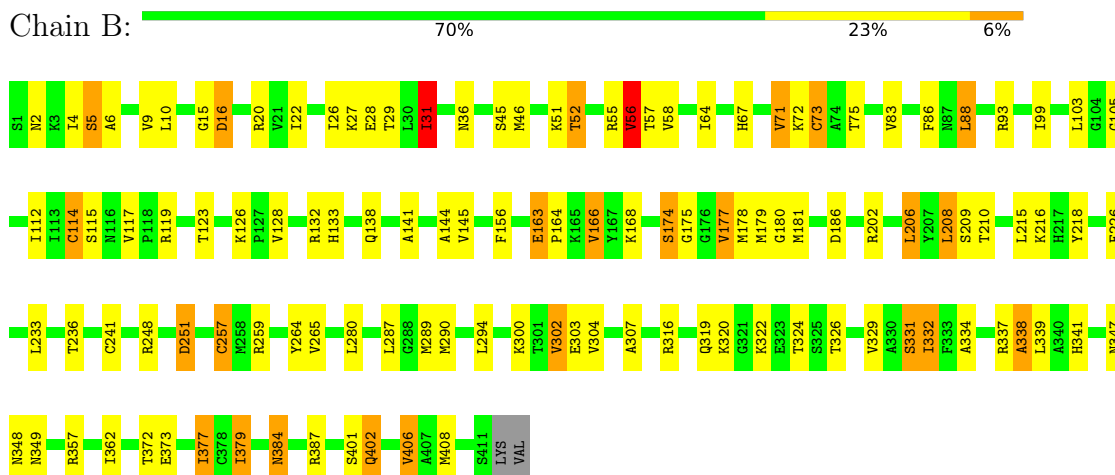
3 Residue-property plots

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: Isocitrate dehydrogenase [NADP]

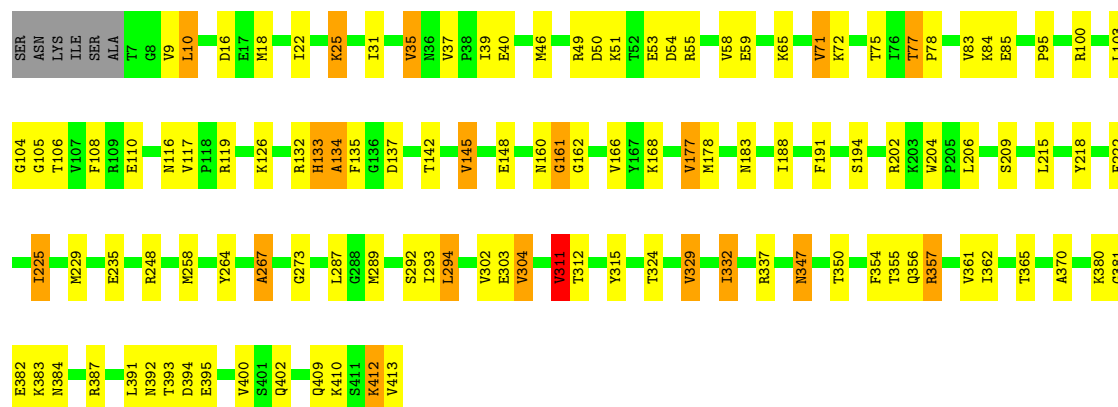


• Molecule 1: Isocitrate dehydrogenase [NADP]



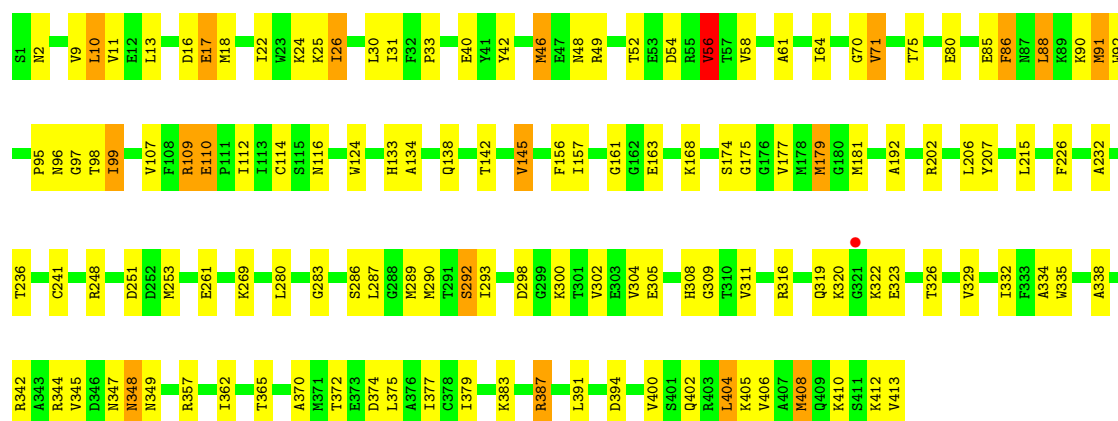
• Molecule 1: Isocitrate dehydrogenase [NADP]





● Molecule 1: Isocitrate dehydrogenase [NADP]

Chain D: 68% 27% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.52Å 70.46Å 121.93Å 90.00° 113.42° 90.00°	Depositor
Resolution (Å)	19.98 – 2.90 19.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	81.9 (19.98-2.90) 81.9 (19.98-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.192 , 0.284 0.193 , 0.279	Depositor DCC
R_{free} test set	1741 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 6.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13236	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: NAD, CA, AKG

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	1.01	1/3327 (0.0%)	1.20	8/4493 (0.2%)
1	B	0.99	2/3333 (0.1%)	1.20	16/4501 (0.4%)
1	C	0.99	1/3308 (0.0%)	1.20	10/4466 (0.2%)
1	D	1.01	1/3350 (0.0%)	1.22	9/4522 (0.2%)
All	All	1.00	5/13318 (0.0%)	1.20	43/17982 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	267	ALA	CA-C	5.69	1.60	1.52
1	B	208	LEU	CA-C	-5.66	1.45	1.52
1	A	252	ASP	CA-C	-5.50	1.46	1.52
1	D	145	VAL	CA-CB	5.43	1.60	1.54
1	B	166	VAL	N-CA	5.07	1.51	1.46

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	320	LYS	N-CA-C	8.74	121.61	110.33
1	C	77	THR	CB-CA-C	8.60	118.68	110.17
1	C	58	VAL	N-CA-C	-8.36	102.19	110.30
1	B	379	ILE	N-CA-CB	8.07	119.77	110.65
1	D	56	VAL	N-CA-CB	7.07	118.36	110.51
1	B	56	VAL	N-CA-C	-7.01	104.93	111.45
1	B	4	ILE	N-CA-C	6.77	117.63	111.81
1	B	16	ASP	N-CA-C	6.52	118.05	108.86
1	B	332	ILE	CB-CA-C	-6.50	103.64	111.97
1	B	67	HIS	N-CA-C	6.47	120.39	112.23
1	C	116	ASN	N-CA-C	6.47	120.77	113.01
1	C	16	ASP	N-CA-C	6.42	119.99	109.85
1	A	329	VAL	N-CA-CB	6.39	118.03	110.55
1	C	304	VAL	CB-CA-C	6.32	120.81	110.69
1	D	322	LYS	N-CA-C	5.99	116.46	108.38
1	C	311	VAL	CB-CA-C	5.98	121.10	111.29
1	C	37	VAL	CB-CA-C	-5.97	104.34	110.13
1	A	182	TYR	N-CA-C	5.96	118.02	109.14
1	A	228	GLU	N-CA-C	-5.91	104.53	110.97
1	B	257	CYS	CA-C-N	5.90	128.50	120.54
1	B	257	CYS	C-N-CA	5.90	128.50	120.54
1	A	383	LYS	N-CA-C	-5.88	101.49	109.95
1	D	56	VAL	CB-CA-C	-5.87	104.37	111.88
1	B	163	GLU	CA-C-N	-5.72	113.80	119.93
1	B	163	GLU	C-N-CA	-5.72	113.80	119.93
1	D	86	PHE	N-CA-C	-5.67	101.24	110.20
1	B	31	ILE	CB-CA-C	5.56	116.00	111.05
1	A	166	VAL	N-CA-C	5.55	116.10	110.05
1	A	188	ILE	CB-CA-C	-5.47	104.67	112.22
1	B	322	LYS	N-CA-C	5.40	117.66	110.53
1	D	30	LEU	N-CA-C	5.40	117.98	111.40
1	B	9	VAL	N-CA-C	5.36	116.00	108.17
1	B	384	ASN	N-CA-C	5.34	118.81	112.72
1	C	168	LYS	N-CA-C	-5.28	101.84	109.59
1	C	264	TYR	N-CA-C	5.26	116.52	108.42
1	C	332	ILE	CB-CA-C	-5.22	105.19	112.04
1	A	99	ILE	N-CA-C	5.22	115.43	110.42
1	B	73	CYS	N-CA-C	-5.21	103.52	110.55
1	B	132	ARG	N-CA-C	5.18	117.41	109.07
1	D	48	ASN	N-CA-C	5.10	119.51	113.28
1	D	157	ILE	CB-CA-C	-5.09	105.33	111.18
1	D	370	ALA	N-CA-C	5.06	118.13	110.64
1	A	251	ASP	N-CA-C	5.04	116.46	111.07

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ASP	Peptide
1	A	3	LYS	Peptide
1	B	105	GLY	Peptide
1	C	135	PHE	Peptide
1	D	112	ILE	Peptide
1	D	319	GLN	Peptide

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	3259	0	3247	44	0
1	B	3265	0	3252	53	0
1	C	3240	0	3226	45	0
1	D	3282	0	3274	54	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	D	10	0	4	3	0
All	All	13236	0	13107	186	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 7.

All (186) 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:179:MET:HE1	1:B:181:MET:HE2	1.36	1.05
1:A:179:MET:HE3	1:B:181:MET:HE3	1.43	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:LYS:HE3	1:C:394:ASP:HA	1.64	0.80
1:B:289:MET:SD	1:B:329:VAL:HG11	2.26	0.76
1:C:218:TYR:HA	1:D:177:VAL:HG21	1.76	0.67
1:D:25:LYS:NZ	1:D:394:ASP:OD1	2.26	0.65
1:A:46:MET:HE1	1:A:78:PRO:HG3	1.79	0.64
1:C:22:ILE:HD12	1:C:393:THR:HG21	1.81	0.63
1:B:141:ALA:HB1	1:B:180:GLY:O	1.99	0.62
1:A:332:ILE:HG21	1:A:362:ILE:HD11	1.81	0.62
1:C:294:LEU:C	1:C:294:LEU:HD12	2.25	0.62
1:D:16:ASP:OD2	1:D:46:MET:N	2.34	0.60
1:C:218:TYR:HA	1:D:177:VAL:CG2	2.32	0.60
1:D:22:ILE:HD11	1:D:326:THR:HG23	1.82	0.59
1:A:178:MET:HE1	1:B:156:PHE:HB2	1.84	0.59
1:B:329:VAL:HG23	1:B:362:ILE:HG21	1.84	0.59
1:B:408:MET:HA	1:B:408:MET:HE2	1.85	0.59
1:C:365:THR:HG22	1:C:370:ALA:HB3	1.85	0.59
1:D:179:MET:HE1	1:D:181:MET:HE3	1.84	0.59
1:A:79:ASP:C	1:A:91:MET:HE2	2.28	0.58
1:B:331:SER:O	1:B:334:ALA:HB3	2.03	0.58
1:D:365:THR:HG21	1:D:400:VAL:HG22	1.85	0.58
1:A:80:GLU:O	1:A:83:VAL:HG22	2.04	0.58
1:B:316:ARG:HA	1:B:319:GLN:HE21	1.69	0.58
1:C:357:ARG:O	1:C:361:VAL:HG23	2.03	0.58
1:B:206:LEU:HD23	1:B:265:VAL:HB	1.87	0.56
1:A:156:PHE:HB2	1:B:178:MET:HE1	1.86	0.56
1:B:338:ALA:O	1:B:341:HIS:N	2.39	0.56
1:C:133:HIS:O	1:C:134:ALA:HB3	2.06	0.56
1:A:72:LYS:NZ	1:A:75:THR:OG1	2.33	0.56
1:B:26:ILE:HD12	1:B:332:ILE:HG12	1.88	0.56
1:B:99:ILE:HG22	1:B:103:LEU:HD23	1.88	0.56
1:C:106:THR:HG22	1:C:108:PHE:CE1	2.41	0.55
1:D:71:VAL:HG22	1:D:338:ALA:CB	2.36	0.55
1:D:174:SER:OG	1:D:175:GLY:N	2.40	0.55
1:D:95:PRO:O	1:D:99:ILE:HG23	2.07	0.55
1:B:128:VAL:HG13	1:B:264:TYR:CE1	2.42	0.54
1:C:100:ARG:NH2	1:C:105:GLY:O	2.41	0.54
1:C:329:VAL:HA	1:C:332:ILE:HD12	1.90	0.54
1:D:374:ASP:HA	1:D:377:ILE:HG12	1.90	0.54
1:C:55:ARG:NH2	1:C:59:GLU:OE1	2.41	0.53
1:B:114:CYS:HB2	1:B:117:VAL:HG12	1.89	0.53
1:D:133:HIS:O	1:D:134:ALA:HB3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TYR:HA	1:B:177:VAL:HG21	1.90	0.53
1:C:191:PHE:CZ	1:C:267:ALA:HB1	2.44	0.53
1:B:15:GLY:HA2	1:B:75:THR:HG22	1.90	0.52
1:D:192:ALA:HB2	1:D:226:PHE:CE1	2.44	0.52
1:D:332:ILE:HG21	1:D:362:ILE:HD11	1.91	0.52
1:B:251:ASP:OD1	1:B:251:ASP:N	2.37	0.52
1:C:75:THR:HG21	1:C:95:PRO:HG2	1.90	0.52
1:A:55:ARG:CZ	1:A:55:ARG:HA	2.39	0.52
1:C:132:ARG:HG3	1:C:273:GLY:HA3	1.91	0.52
1:C:209:SER:HA	1:C:248:ARG:O	2.10	0.52
1:B:179:MET:CE	1:B:181:MET:HE2	2.25	0.52
1:C:391:LEU:HB3	1:C:395:GLU:HG3	1.93	0.51
1:A:11:VAL:HG12	1:A:13:LEU:CD1	2.40	0.51
1:D:22:ILE:O	1:D:26:ILE:HG23	2.10	0.51
1:D:26:ILE:HD11	1:D:335:TRP:CD1	2.46	0.50
1:B:304:VAL:CG1	1:B:338:ALA:HB2	2.41	0.50
1:B:209:SER:HA	1:B:248:ARG:O	2.11	0.50
1:D:90:LYS:O	1:D:91:MET:CB	2.59	0.50
1:C:10:LEU:HD21	1:C:71:VAL:HG22	1.94	0.50
1:C:381:GLY:O	1:C:382:GLU:C	2.55	0.50
1:D:46:MET:HE3	1:D:49:ARG:NH1	2.26	0.49
1:B:174:SER:OG	1:B:175:GLY:N	2.44	0.49
1:D:286:SER:OG	1:D:287:LEU:N	2.46	0.49
2:D:501:NAD:C4N	4:D:502:AKG:H41	2.42	0.49
1:A:52:THR:HB	1:A:55:ARG:HB3	1.94	0.49
1:A:9:VAL:CG2	1:A:67:HIS:CG	2.95	0.49
1:B:294:LEU:O	1:B:302:VAL:HA	2.13	0.49
1:A:177:VAL:CG1	1:B:218:TYR:CD2	2.96	0.48
1:D:304:VAL:CG1	1:D:338:ALA:HB2	2.43	0.48
1:B:332:ILE:HG21	1:B:362:ILE:HD11	1.95	0.48
1:D:10:LEU:HD21	1:D:71:VAL:HG23	1.94	0.48
1:B:52:THR:HG21	1:B:56:VAL:HG23	1.95	0.48
1:A:213:THR:HG23	1:A:249:LEU:HD11	1.95	0.48
1:A:403:ARG:O	1:A:406:VAL:HG12	2.14	0.48
1:D:107:VAL:HG23	1:D:134:ALA:HB2	1.95	0.48
1:C:18:MET:HB2	1:C:315:TYR:HB2	1.96	0.48
1:C:178:MET:HE1	1:D:156:PHE:HB2	1.96	0.47
1:B:64:ILE:HD13	1:B:303:GLU:HG3	1.97	0.47
1:C:46:MET:HE1	1:C:78:PRO:HB3	1.95	0.47
1:A:218:TYR:HA	1:B:177:VAL:CG2	2.44	0.47
1:C:145:VAL:HA	1:C:177:VAL:HG23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:VAL:O	1:D:70:GLY:HA2	2.14	0.47
1:C:117:VAL:HG23	1:C:117:VAL:O	2.14	0.47
1:B:83:VAL:HG12	1:B:88:LEU:HD12	1.97	0.47
1:A:363:ILE:HG22	1:A:367:GLU:HG3	1.98	0.46
1:C:22:ILE:CD1	1:C:393:THR:HG21	2.44	0.46
1:D:86:PHE:HB2	1:D:88:LEU:HD13	1.98	0.46
1:A:12:GLU:C	1:A:13:LEU:HD12	2.41	0.46
1:A:79:ASP:C	1:A:79:ASP:OD1	2.59	0.46
1:A:120:LEU:HD22	1:B:123:THR:HG23	1.98	0.46
1:A:177:VAL:HG13	1:B:218:TYR:CD2	2.50	0.46
1:B:10:LEU:HD22	1:B:71:VAL:HG22	1.98	0.46
1:C:133:HIS:O	1:C:134:ALA:CB	2.64	0.46
1:B:83:VAL:CG1	1:B:88:LEU:HD12	2.45	0.46
1:A:218:TYR:CD1	1:B:177:VAL:HG13	2.51	0.46
1:B:22:ILE:HD11	1:B:326:THR:HB	1.98	0.46
1:A:128:VAL:HG13	1:A:264:TYR:CE1	2.51	0.46
1:A:374:ASP:OD1	1:A:374:ASP:N	2.49	0.46
1:D:109:ARG:NH2	4:D:502:AKG:O2	2.46	0.45
1:B:117:VAL:HG13	1:B:117:VAL:O	2.17	0.45
1:D:298:ASP:O	1:D:300:LYS:N	2.47	0.45
1:A:381:GLY:O	1:A:382:GLU:HB2	2.17	0.45
1:B:144:ALA:HB3	1:B:178:MET:HG3	1.99	0.45
1:C:289:MET:SD	1:C:329:VAL:HG21	2.57	0.45
1:C:35:VAL:HG11	1:C:354:PHE:CD2	2.53	0.44
1:D:323:GLU:OE1	1:D:387:ARG:NH1	2.49	0.44
1:A:29:THR:HG21	1:A:397:ILE:HG22	1.99	0.44
1:B:208:LEU:HD22	1:B:226:PHE:CD1	2.52	0.44
1:B:257:CYS:HA	1:B:264:TYR:OH	2.16	0.44
1:D:207:TYR:CD1	1:D:253:MET:HE1	2.52	0.44
1:D:292:SER:O	1:D:304:VAL:HG23	2.18	0.44
1:B:6:ALA:HB2	1:B:348:ASN:OD1	2.17	0.44
1:C:412:LYS:HG2	1:C:413:VAL:HG12	1.99	0.44
1:D:18:MET:HG2	1:D:326:THR:HG21	1.99	0.44
2:D:501:NAD:C5N	4:D:502:AKG:H42	2.48	0.44
1:A:341:HIS:O	1:A:342:ARG:C	2.61	0.44
1:C:311:VAL:O	1:C:312:THR:C	2.59	0.44
1:D:22:ILE:HD11	1:D:326:THR:CG2	2.47	0.44
1:D:289:MET:HG3	1:D:375:LEU:HD21	1.99	0.43
1:B:133:HIS:CD2	1:B:133:HIS:O	2.71	0.43
1:B:27:LYS:HA	1:B:31:ILE:HG13	1.99	0.43
1:A:117:VAL:O	1:A:117:VAL:HG13	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ILE:HG22	1:C:225:ILE:HG21	2.00	0.43
1:A:49:ARG:NH1	1:A:95:PRO:HG3	2.34	0.43
1:B:20:ARG:NH1	1:B:45:SER:HB3	2.32	0.43
1:B:72:LYS:HG2	1:B:73:CYS:O	2.18	0.43
1:D:61:ALA:HB2	1:D:99:ILE:HB	2.00	0.43
1:C:25:LYS:HE3	1:C:394:ASP:CA	2.42	0.43
1:C:202:ARG:HG2	1:C:204:TRP:CZ3	2.54	0.43
1:A:114:CYS:O	1:A:115:SER:C	2.62	0.43
1:A:229:MET:HE3	1:A:229:MET:HB2	1.82	0.43
1:A:357:ARG:O	1:A:361:VAL:HG23	2.18	0.43
1:B:16:ASP:HA	1:B:20:ARG:HB2	2.00	0.43
1:C:332:ILE:HG21	1:C:362:ILE:HD11	2.01	0.43
1:D:90:LYS:HD3	1:D:92:TRP:CZ3	2.54	0.43
1:D:96:ASN:ND2	2:D:501:NAD:O7N	2.49	0.43
1:A:346:ASP:O	1:A:347:ASN:C	2.62	0.42
1:B:290:MET:HB3	1:B:307:ALA:HB3	2.00	0.42
1:D:241:CYS:O	1:D:241:CYS:SG	2.77	0.42
1:C:188:ILE:HD11	1:C:222:PHE:CZ	2.55	0.42
1:A:294:LEU:C	1:A:294:LEU:HD23	2.45	0.42
1:D:90:LYS:O	1:D:91:MET:HB3	2.20	0.42
1:A:75:THR:O	2:A:501:NAD:H2N	2.20	0.42
1:D:110:GLU:OE2	1:D:202:ARG:NH1	2.53	0.42
1:A:305:GLU:HG3	1:A:306:ALA:O	2.20	0.42
1:C:72:LYS:NZ	1:C:75:THR:HG22	2.34	0.42
1:D:80:GLU:N	1:D:80:GLU:OE2	2.53	0.42
1:A:96:ASN:O	1:A:100:ARG:HG3	2.20	0.42
1:B:163:GLU:O	1:B:164:PRO:C	2.61	0.42
1:D:357:ARG:HD3	1:D:408:MET:HA	2.02	0.42
1:A:189:ARG:HG2	1:A:229:MET:HE1	2.01	0.42
1:A:348:ASN:OD1	1:A:348:ASN:C	2.63	0.42
1:C:354:PHE:O	1:C:355:THR:C	2.63	0.42
1:D:304:VAL:HG22	1:D:334:ALA:HA	2.00	0.42
1:D:116:ASN:HD22	1:D:116:ASN:HA	1.71	0.41
1:B:357:ARG:HA	1:B:357:ARG:HD3	1.87	0.41
1:B:373:GLU:O	1:B:377:ILE:HG23	2.20	0.41
1:A:111:PRO:HB3	1:A:290:MET:HE3	2.02	0.41
1:C:160:ASN:O	1:C:161:GLY:C	2.63	0.41
1:B:26:ILE:HD12	1:B:332:ILE:CG1	2.50	0.41
1:D:124:TRP:CZ3	1:D:283:GLY:HA3	2.56	0.41
1:C:100:ARG:O	1:C:104:GLY:N	2.47	0.41
1:A:5:SER:HA	1:A:36:ASN:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:MET:HB3	1:A:311:VAL:HG13	2.03	0.41
1:D:13:LEU:HA	1:D:42:TYR:O	2.20	0.41
1:C:361:VAL:O	1:C:365:THR:OG1	2.36	0.41
1:D:387:ARG:HA	1:D:387:ARG:HD2	1.92	0.41
1:B:402:GLN:O	1:B:406:VAL:HG12	2.21	0.41
1:D:64:ILE:HG12	1:D:70:GLY:HA3	2.03	0.41
1:D:308:HIS:HD2	1:D:309:GLY:O	2.04	0.41
1:C:49:ARG:NH2	1:C:75:THR:OG1	2.54	0.40
1:C:294:LEU:C	1:C:294:LEU:CD1	2.91	0.40
1:D:18:MET:CG	1:D:326:THR:HG21	2.51	0.40
1:C:50:ASP:O	1:C:51:LYS:C	2.64	0.40
1:D:52:THR:OG1	1:D:56:VAL:HG22	2.21	0.40
1:D:75:THR:O	2:D:501:NAD:H2N	2.21	0.40
1:B:52:THR:HG23	1:B:55:ARG:H	1.86	0.40
1:C:108:PHE:CD1	1:C:108:PHE:N	2.90	0.40
1:C:381:GLY:O	1:C:383:LYS:N	2.54	0.40
1:D:25:LYS:CE	1:D:394:ASP:OD1	2.69	0.40
1:D:97:GLY:O	1:D:98:THR:C	2.64	0.40
1:D:404:LEU:O	1:D:408:MET:N	2.55	0.40
1:A:327:ASN:HA	1:A:328:PRO:HD3	1.86	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	408/413 (99%)	364 (89%)	34 (8%)	10 (2%)	4	17
1	B	409/413 (99%)	366 (90%)	38 (9%)	5 (1%)	10	34
1	C	405/413 (98%)	356 (88%)	39 (10%)	10 (2%)	4	17
1	D	411/413 (100%)	357 (87%)	43 (10%)	11 (3%)	4	16
All	All	1633/1652 (99%)	1443 (88%)	154 (9%)	36 (2%)	5	20

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	384	ASN
1	D	91	MET
1	D	348	ASN
1	A	347	ASN
1	A	382	GLU
1	C	54	ASP
1	C	133	HIS
1	C	235	GLU
1	D	17	GLU
1	D	412	LYS
1	A	80	GLU
1	A	138	GLN
1	B	5	SER
1	C	134	ALA
1	C	162	GLY
1	D	2	ASN
1	D	85	GLU
1	A	5	SER
1	A	53	GLU
1	A	90	LYS
1	B	88	LEU
1	B	338	ALA
1	C	137	ASP
1	C	347	ASN
1	D	232	ALA
1	D	293	ILE
1	D	347	ASN
1	A	3	LYS
1	B	57	THR
1	B	339	LEU
1	C	53	GLU
1	A	381	GLY
1	C	161	GLY
1	D	161	GLY
1	A	293	ILE
1	D	311	VAL

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	350/353 (99%)	293 (84%)	57 (16%)	2	8
1	B	351/353 (99%)	297 (85%)	54 (15%)	2	9
1	C	348/353 (99%)	296 (85%)	52 (15%)	3	10
1	D	353/353 (100%)	298 (84%)	55 (16%)	2	9
All	All	1402/1412 (99%)	1184 (84%)	218 (16%)	2	9

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	5	SER
1	A	7	THR
1	A	9	VAL
1	A	10	LEU
1	A	20	ARG
1	A	25	LYS
1	A	28	GLU
1	A	31	ILE
1	A	35	VAL
1	A	49	ARG
1	A	52	THR
1	A	54	ASP
1	A	71	VAL
1	A	75	THR
1	A	94	SER
1	A	103	LEU
1	A	109	ARG
1	A	119	ARG
1	A	123	THR
1	A	125	LYS
1	A	132	ARG
1	A	138	GLN
1	A	145	VAL
1	A	155	ARG
1	A	168	LYS
1	A	177	VAL
1	A	184	THR
1	A	221	ARG
1	A	236	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	237	LYS
1	A	249	LEU
1	A	269	LYS
1	A	278	ASP
1	A	279	SER
1	A	287	LEU
1	A	292	SER
1	A	293	ILE
1	A	302	VAL
1	A	303	GLU
1	A	304	VAL
1	A	322	LYS
1	A	329	VAL
1	A	337	ARG
1	A	353	GLU
1	A	357	ARG
1	A	372	THR
1	A	374	ASP
1	A	380	LYS
1	A	384	ASN
1	A	386	VAL
1	A	391	LEU
1	A	392	ASN
1	A	398	ASP
1	A	400	VAL
1	A	406	VAL
1	A	408	MET
1	B	2	ASN
1	B	5	SER
1	B	28	GLU
1	B	29	THR
1	B	31	ILE
1	B	36	ASN
1	B	46	MET
1	B	51	LYS
1	B	52	THR
1	B	56	VAL
1	B	58	VAL
1	B	71	VAL
1	B	86	PHE
1	B	93	ARG
1	B	112	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	114	CYS
1	B	115	SER
1	B	119	ARG
1	B	126	LYS
1	B	138	GLN
1	B	145	VAL
1	B	166	VAL
1	B	168	LYS
1	B	174	SER
1	B	177	VAL
1	B	186	ASP
1	B	202	ARG
1	B	206	LEU
1	B	210	THR
1	B	215	LEU
1	B	216	LYS
1	B	233	LEU
1	B	236	THR
1	B	241	CYS
1	B	251	ASP
1	B	259	ARG
1	B	280	LEU
1	B	287	LEU
1	B	300	LYS
1	B	302	VAL
1	B	320	LYS
1	B	324	THR
1	B	331	SER
1	B	337	ARG
1	B	347	ASN
1	B	349	ASN
1	B	372	THR
1	B	377	ILE
1	B	379	ILE
1	B	384	ASN
1	B	387	ARG
1	B	401	SER
1	B	402	GLN
1	B	406	VAL
1	C	9	VAL
1	C	10	LEU
1	C	25	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	31	ILE
1	C	35	VAL
1	C	39	ILE
1	C	40	GLU
1	C	65	LYS
1	C	71	VAL
1	C	77	THR
1	C	83	VAL
1	C	84	LYS
1	C	85	GLU
1	C	103	LEU
1	C	110	GLU
1	C	119	ARG
1	C	126	LYS
1	C	142	THR
1	C	145	VAL
1	C	148	GLU
1	C	166	VAL
1	C	177	VAL
1	C	183	ASN
1	C	194	SER
1	C	206	LEU
1	C	215	LEU
1	C	225	ILE
1	C	229	MET
1	C	258	MET
1	C	287	LEU
1	C	292	SER
1	C	293	ILE
1	C	294	LEU
1	C	302	VAL
1	C	303	GLU
1	C	304	VAL
1	C	311	VAL
1	C	324	THR
1	C	329	VAL
1	C	337	ARG
1	C	347	ASN
1	C	350	THR
1	C	356	GLN
1	C	357	ARG
1	C	380	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	387	ARG
1	C	392	ASN
1	C	400	VAL
1	C	402	GLN
1	C	409	GLN
1	C	410	LYS
1	C	412	LYS
1	D	9	VAL
1	D	10	LEU
1	D	17	GLU
1	D	24	LYS
1	D	26	ILE
1	D	31	ILE
1	D	33	PRO
1	D	40	GLU
1	D	46	MET
1	D	54	ASP
1	D	56	VAL
1	D	58	VAL
1	D	71	VAL
1	D	88	LEU
1	D	99	ILE
1	D	109	ARG
1	D	110	GLU
1	D	114	CYS
1	D	138	GLN
1	D	142	THR
1	D	145	VAL
1	D	163	GLU
1	D	168	LYS
1	D	179	MET
1	D	206	LEU
1	D	215	LEU
1	D	236	THR
1	D	248	ARG
1	D	251	ASP
1	D	261	GLU
1	D	269	LYS
1	D	280	LEU
1	D	290	MET
1	D	292	SER
1	D	302	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	305	GLU
1	D	316	ARG
1	D	329	VAL
1	D	342	ARG
1	D	344	ARG
1	D	345	VAL
1	D	348	ASN
1	D	349	ASN
1	D	372	THR
1	D	379	ILE
1	D	383	LYS
1	D	387	ARG
1	D	391	LEU
1	D	402	GLN
1	D	404	LEU
1	D	405	LYS
1	D	406	VAL
1	D	408	MET
1	D	410	LYS
1	D	413	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	HIS
1	A	138	GLN
1	A	347	ASN
1	B	133	HIS
1	B	270	ASN
1	B	319	GLN
1	B	347	ASN
1	B	409	GLN
1	C	36	ASN
1	C	48	ASN
1	C	67	HIS
1	C	87	ASN
1	C	183	ASN
1	C	256	HIS
1	C	282	GLN
1	D	116	ASN
1	D	133	HIS
1	D	270	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	308	HIS
1	D	347	ASN
1	D	384	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	A	501	-	46,48,48	1.38	8 (17%)	64,73,73	1.81	18 (28%)
2	NAD	C	501	-	46,48,48	1.47	6 (13%)	64,73,73	2.05	16 (25%)
2	NAD	B	501	-	46,48,48	1.52	9 (19%)	64,73,73	2.07	16 (25%)
4	AKG	D	502	3	9,9,9	1.51	2 (22%)	11,11,11	2.56	4 (36%)
2	NAD	D	501	-	46,48,48	1.49	7 (15%)	64,73,73	1.79	17 (26%)

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	501	-	-	8/30/62/62	0/5/5/5
2	NAD	C	501	-	-	13/30/62/62	0/5/5/5
2	NAD	B	501	-	-	11/30/62/62	0/5/5/5
4	AKG	D	502	3	-	1/9/9/9	-
2	NAD	D	501	-	-	12/30/62/62	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NAD	C5A-C4A	5.48	1.48	1.39
2	A	501	NAD	C5A-C4A	4.47	1.47	1.39
2	B	501	NAD	C5A-C4A	4.43	1.47	1.39
2	D	501	NAD	PN-O3	4.22	1.64	1.59
2	D	501	NAD	PA-O3	4.10	1.63	1.59
2	D	501	NAD	C5A-C4A	3.95	1.46	1.39
2	B	501	NAD	PN-O3	3.78	1.63	1.59
2	D	501	NAD	C5A-N7A	-3.34	1.33	1.39
2	C	501	NAD	C5A-C6A	3.30	1.50	1.41
2	B	501	NAD	O4D-C1D	3.20	1.45	1.40
4	D	502	AKG	C2-C1	-2.96	1.49	1.53
2	B	501	NAD	C5A-N7A	-2.91	1.33	1.39
2	A	501	NAD	PA-O3	2.89	1.62	1.59
2	C	501	NAD	O4D-C1D	2.64	1.44	1.40
2	B	501	NAD	PA-O3	2.62	1.62	1.59
2	C	501	NAD	PN-O3	2.62	1.62	1.59
2	B	501	NAD	C8A-N7A	2.59	1.36	1.31
2	D	501	NAD	C4A-N9A	-2.58	1.32	1.37
2	A	501	NAD	C4A-N9A	-2.55	1.32	1.37
2	B	501	NAD	C5A-C6A	2.54	1.48	1.41
2	A	501	NAD	C5A-N7A	-2.54	1.34	1.39
2	D	501	NAD	O4D-C1D	2.52	1.44	1.40
2	A	501	NAD	C8A-N7A	2.47	1.36	1.31
2	C	501	NAD	C8A-N7A	2.42	1.36	1.31
2	A	501	NAD	O4D-C1D	2.40	1.44	1.40
2	C	501	NAD	C1B-N9A	2.27	1.52	1.46
2	B	501	NAD	C3N-C7N	2.22	1.53	1.50
2	A	501	NAD	C5A-C6A	2.20	1.47	1.41
2	A	501	NAD	PN-O3	2.12	1.61	1.59
4	D	502	AKG	O2-C1	-2.08	1.24	1.30
2	B	501	NAD	C2N-C3N	2.06	1.42	1.39
2	D	501	NAD	C5A-C6A	2.06	1.46	1.41

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	C5A-C4A-N3A	-7.13	116.89	126.72
2	B	501	NAD	C5A-C4A-N3A	-6.85	117.28	126.72
4	D	502	AKG	C4-C3-C2	-6.00	101.65	112.91
2	C	501	NAD	N3A-C4A-N9A	5.75	136.94	127.17
2	B	501	NAD	C3N-C7N-N7N	5.74	124.81	117.74
2	D	501	NAD	C5A-C4A-N3A	-5.30	119.42	126.72
2	C	501	NAD	C3N-C7N-N7N	5.18	124.11	117.74
2	D	501	NAD	N3A-C4A-N9A	4.95	135.58	127.17
2	B	501	NAD	N3A-C4A-N9A	4.70	135.16	127.17
2	A	501	NAD	C5A-C4A-N3A	-4.57	120.43	126.72
2	A	501	NAD	C3N-C7N-N7N	4.33	123.07	117.74
2	B	501	NAD	C6N-N1N-C2N	-4.27	118.24	121.88
2	A	501	NAD	O7N-C7N-N7N	-4.26	116.46	122.62
2	D	501	NAD	N3A-C2A-N1A	-4.24	122.17	128.58
2	C	501	NAD	C2A-N3A-C4A	4.23	122.16	111.83
2	B	501	NAD	C4D-O4D-C1D	4.06	113.64	109.92
2	B	501	NAD	C2A-N3A-C4A	4.00	121.59	111.83
2	C	501	NAD	O4B-C1B-N9A	3.88	115.54	108.09
4	D	502	AKG	C3-C2-C1	3.76	122.25	115.86
2	D	501	NAD	C2A-N3A-C4A	3.74	120.97	111.83
2	B	501	NAD	C4A-C5A-N7A	-3.74	106.31	110.58
2	D	501	NAD	C4A-N9A-C8A	3.60	109.52	105.74
2	A	501	NAD	N3A-C4A-N9A	3.56	133.22	127.17
2	C	501	NAD	C4A-C5A-N7A	-3.50	106.58	110.58
2	A	501	NAD	N3A-C2A-N1A	-3.46	123.34	128.58
2	C	501	NAD	O7N-C7N-N7N	-3.33	117.81	122.62
2	D	501	NAD	C3N-C7N-N7N	3.32	121.83	117.74
2	D	501	NAD	C6N-N1N-C2N	-3.25	119.11	121.88
2	C	501	NAD	N3A-C2A-N1A	-3.12	123.86	128.58
2	B	501	NAD	C3B-C2B-C1B	3.04	107.22	101.46
2	A	501	NAD	C2A-N3A-C4A	3.00	119.15	111.83
2	A	501	NAD	C4A-C5A-N7A	-2.99	107.16	110.58
2	C	501	NAD	O3B-C3B-C4B	2.94	119.54	111.08
2	C	501	NAD	C6N-N1N-C2N	-2.94	119.37	121.88
2	A	501	NAD	C6A-C5A-N7A	2.87	137.62	132.09
2	D	501	NAD	O2N-PN-O1N	2.87	125.78	112.44
2	A	501	NAD	C6N-N1N-C2N	-2.83	119.47	121.88
2	A	501	NAD	C4A-N9A-C1B	-2.80	120.08	126.63
2	C	501	NAD	C5A-N7A-C8A	2.78	107.83	103.45
2	B	501	NAD	O2N-PN-O3	2.76	114.74	107.27
2	B	501	NAD	O2A-PA-O3	2.75	114.70	107.27
2	A	501	NAD	C4A-N9A-C8A	2.72	108.60	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAD	O7N-C7N-C3N	-2.66	116.35	119.60
2	C	501	NAD	O2A-PA-O1A	2.65	124.78	112.44
2	D	501	NAD	N6A-C6A-N1A	2.63	124.24	118.38
2	B	501	NAD	C5A-N7A-C8A	2.63	107.58	103.45
2	B	501	NAD	O7N-C7N-N7N	-2.63	118.82	122.62
2	A	501	NAD	C3B-C2B-C1B	2.61	106.41	101.46
2	B	501	NAD	N3A-C2A-N1A	-2.55	124.72	128.58
2	A	501	NAD	O4B-C1B-N9A	2.55	112.98	108.09
2	C	501	NAD	O2N-PN-O1N	2.50	124.09	112.44
2	A	501	NAD	O4B-C4B-C3B	2.47	110.06	105.15
2	D	501	NAD	N9A-C8A-N7A	-2.45	110.45	113.94
2	D	501	NAD	C4A-C5A-N7A	-2.42	107.81	110.58
2	D	501	NAD	C5A-N7A-C8A	2.39	107.21	103.45
2	B	501	NAD	C6A-C5A-N7A	2.32	136.56	132.09
4	D	502	AKG	O2-C1-O1	-2.31	118.41	123.90
2	A	501	NAD	O2N-PN-O1N	2.29	123.10	112.44
2	D	501	NAD	O2D-C2D-C3D	2.23	118.98	111.82
2	C	501	NAD	N6A-C6A-N1A	2.20	123.28	118.38
2	D	501	NAD	C2A-N1A-C6A	2.17	122.30	118.73
2	A	501	NAD	O2A-PA-O1A	2.16	122.52	112.44
2	D	501	NAD	O7N-C7N-N7N	-2.15	119.51	122.62
2	C	501	NAD	C2B-C1B-N9A	-2.15	107.97	113.30
2	B	501	NAD	O4B-C1B-N9A	2.14	112.20	108.09
2	D	501	NAD	C6N-N1N-C1D	2.09	123.83	119.73
2	A	501	NAD	C2D-C3D-C4D	2.08	106.62	102.61
2	A	501	NAD	C2A-N1A-C6A	2.07	122.13	118.73
2	D	501	NAD	C5A-C6A-N6A	-2.04	118.24	123.29
2	C	501	NAD	O2A-PA-O3	-2.02	101.80	107.27
4	D	502	AKG	O3-C5-C4	-2.00	116.74	123.09

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	C5B-O5B-PA-O1A
2	A	501	NAD	C5B-O5B-PA-O2A
2	A	501	NAD	C5D-O5D-PN-O3
2	A	501	NAD	C5D-O5D-PN-O1N
2	A	501	NAD	C5D-O5D-PN-O2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N

Continued on next page...

Continued from previous page...

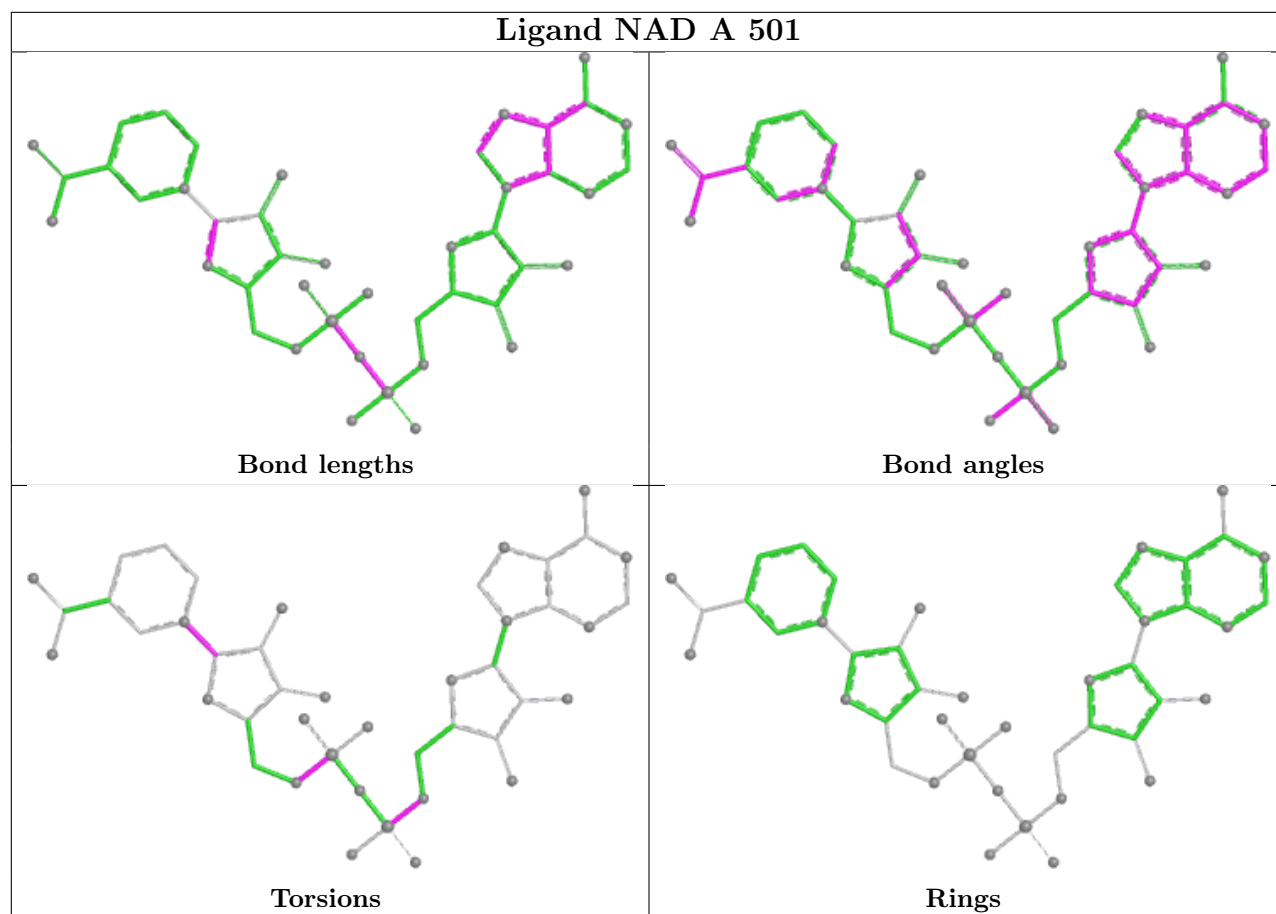
Mol	Chain	Res	Type	Atoms
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	C	501	NAD	C5B-O5B-PA-O1A
2	C	501	NAD	C5B-O5B-PA-O3
2	C	501	NAD	C5D-O5D-PN-O3
2	C	501	NAD	C5D-O5D-PN-O1N
2	C	501	NAD	C5D-O5D-PN-O2N
2	C	501	NAD	O4D-C1D-N1N-C2N
2	C	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C5B-O5B-PA-O3
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C2D-C1D-N1N-C2N
2	D	501	NAD	C2D-C1D-N1N-C6N
2	D	501	NAD	C2N-C3N-C7N-O7N
2	D	501	NAD	C2N-C3N-C7N-N7N
4	D	502	AKG	C1-C2-C3-C4
2	D	501	NAD	C4N-C3N-C7N-O7N
2	D	501	NAD	C4N-C3N-C7N-N7N
2	C	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	C3B-C4B-C5B-O5B
2	B	501	NAD	PA-O3-PN-O1N
2	C	501	NAD	PN-O3-PA-O5B
2	D	501	NAD	C3B-C4B-C5B-O5B
2	B	501	NAD	PN-O3-PA-O2A
2	D	501	NAD	O4B-C4B-C5B-O5B
2	A	501	NAD	C5B-O5B-PA-O3
2	B	501	NAD	C5D-O5D-PN-O3
2	B	501	NAD	C5D-O5D-PN-O1N
2	B	501	NAD	C5D-O5D-PN-O2N
2	C	501	NAD	C5B-O5B-PA-O2A
2	B	501	NAD	PA-O3-PN-O2N
2	C	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	PN-O3-PA-O1A
2	C	501	NAD	PA-O3-PN-O2N
2	D	501	NAD	PA-O3-PN-O2N

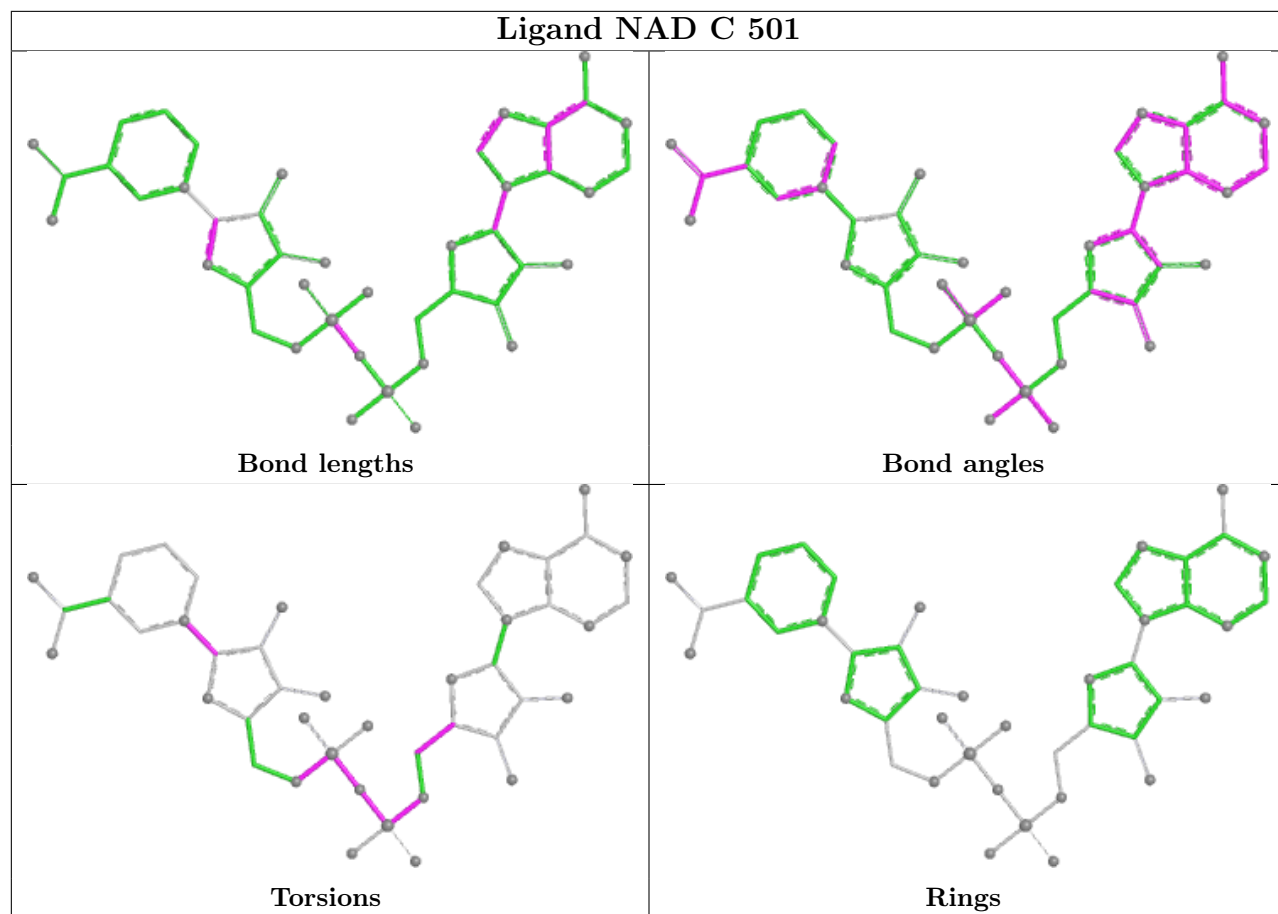
There are no ring outliers.

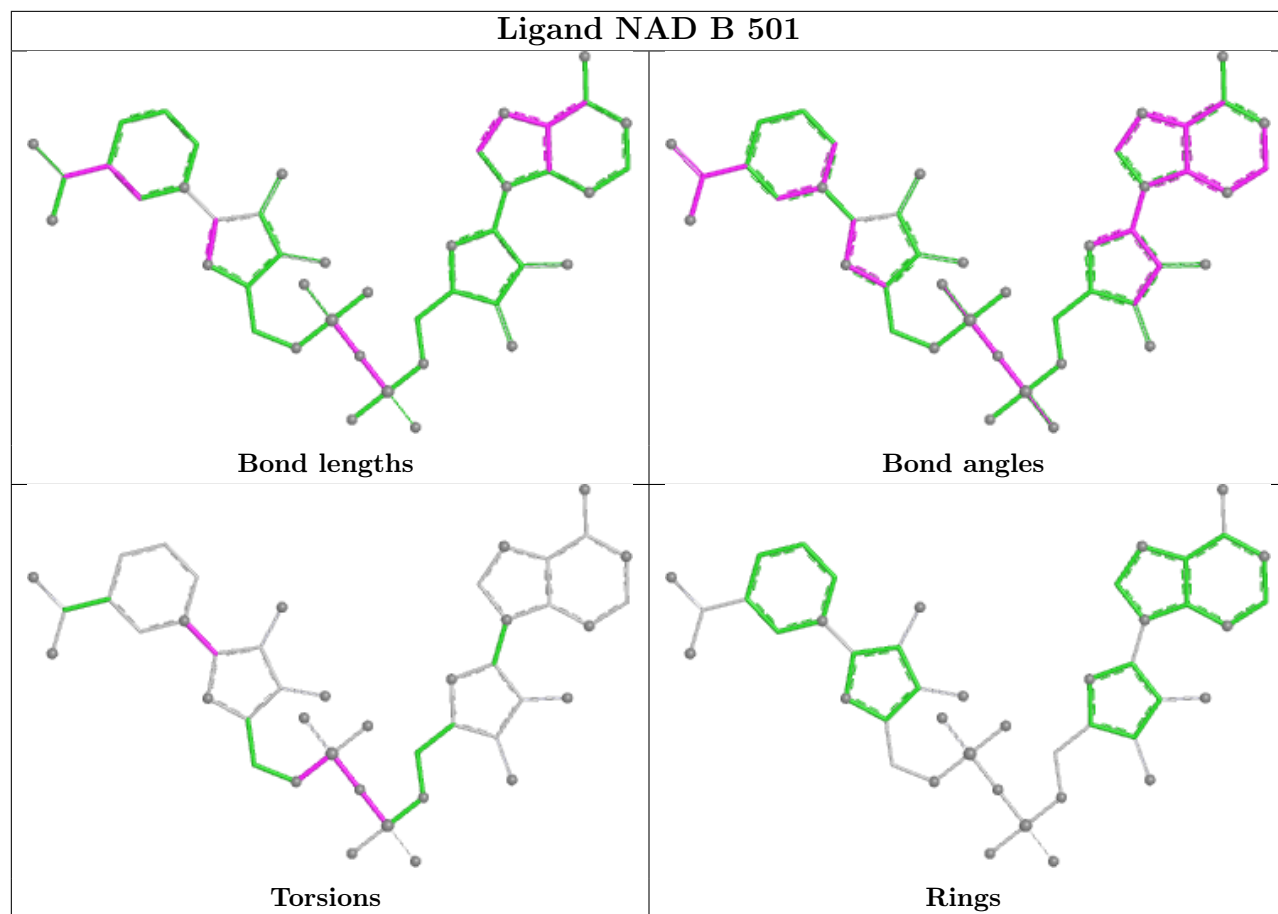
3 monomers are involved in 6 short contacts:

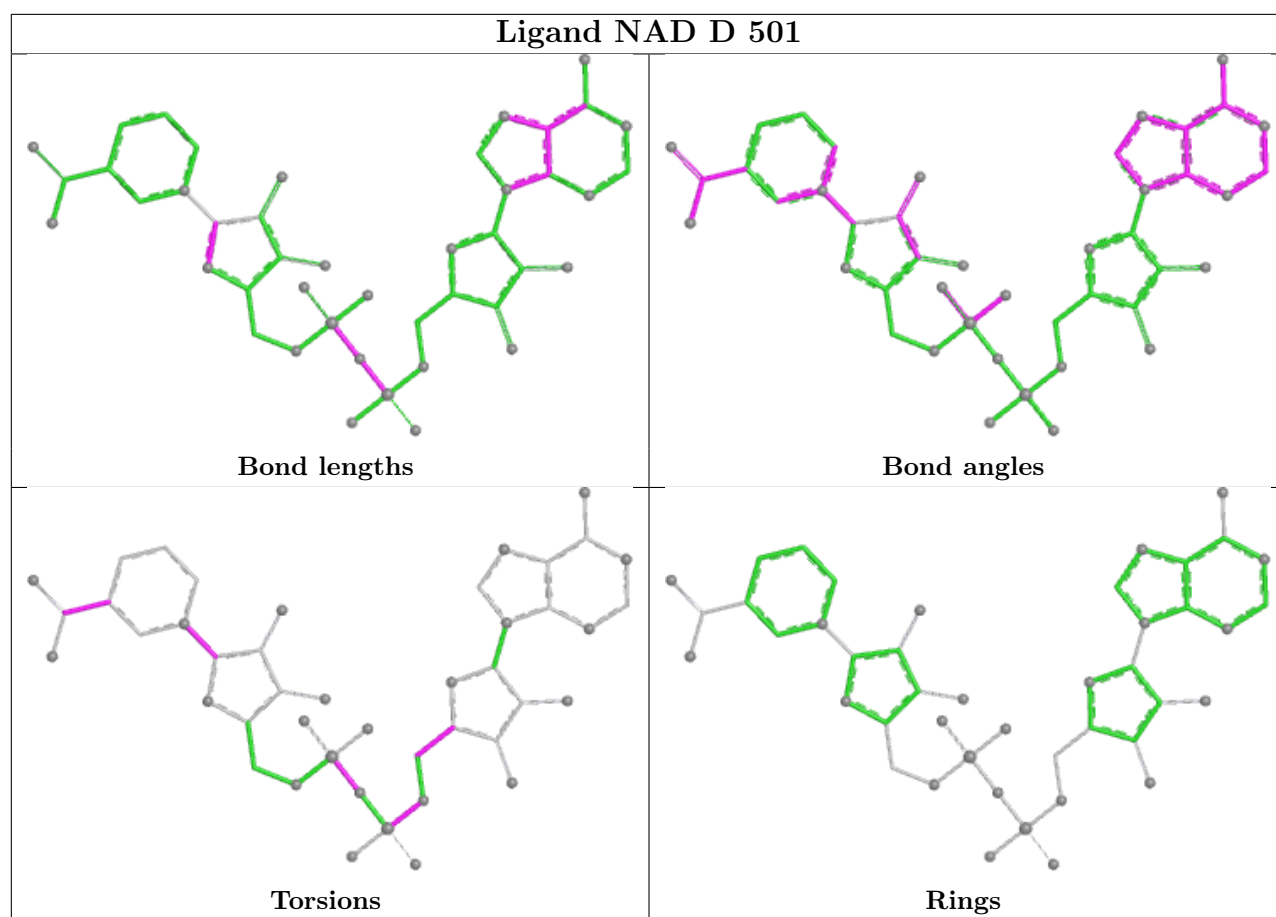
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAD	1	0
4	D	502	AKG	3	0
2	D	501	NAD	4	0

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 [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	410/413 (99%)	-0.58	1 (0%) 91 89	30, 47, 73, 131	0
1	B	411/413 (99%)	-0.51	0 100 100	37, 55, 88, 116	0
1	C	407/413 (98%)	-0.50	0 100 100	34, 53, 78, 148	0
1	D	413/413 (100%)	-0.36	1 (0%) 91 89	37, 61, 87, 117	0
All	All	1641/1652 (99%)	-0.49	2 (0%) 92 90	30, 54, 84, 148	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	321	GLY	2.2
1	A	6	ALA	2.1

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](#)

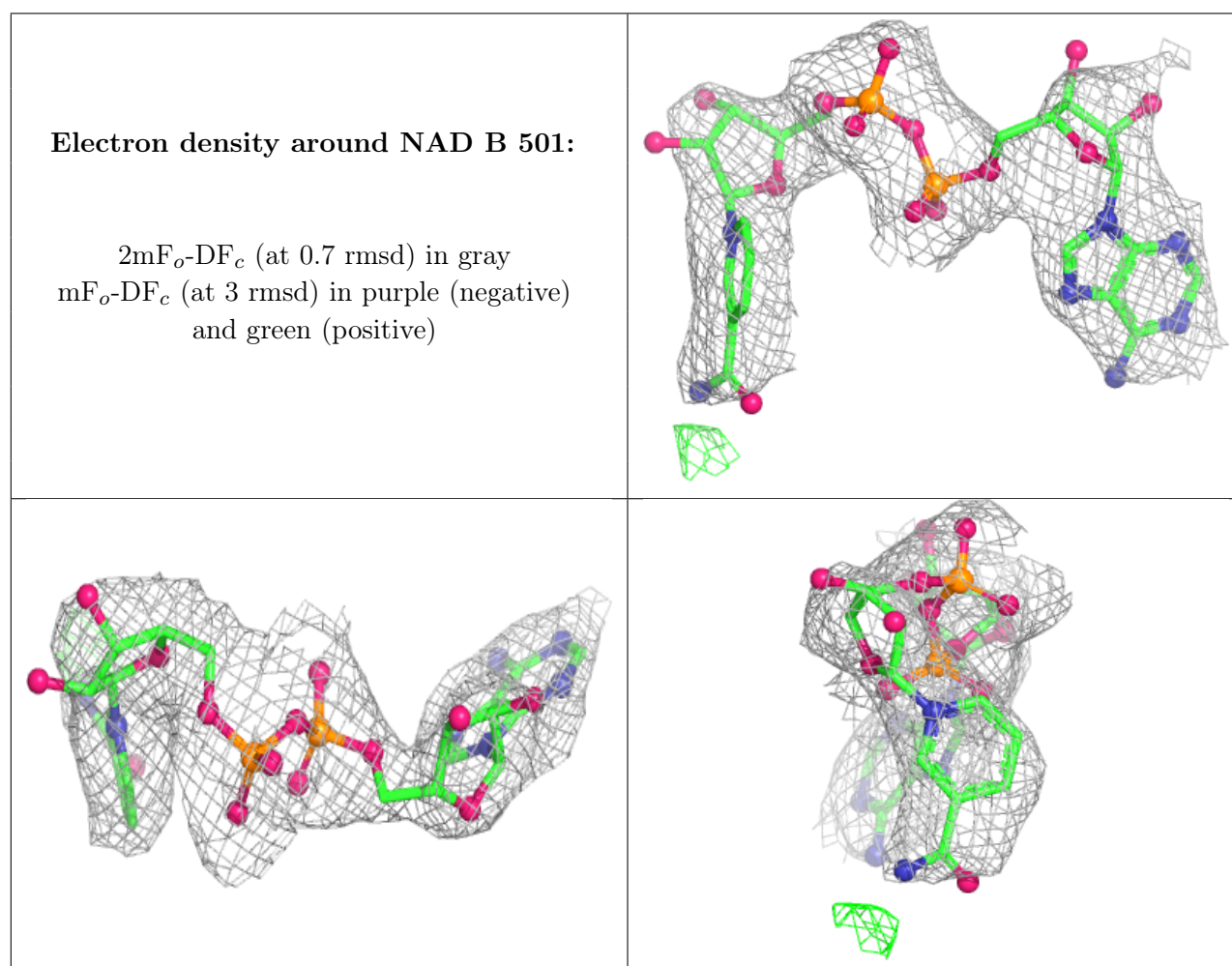
There are no oligosaccharides in this entry.

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.

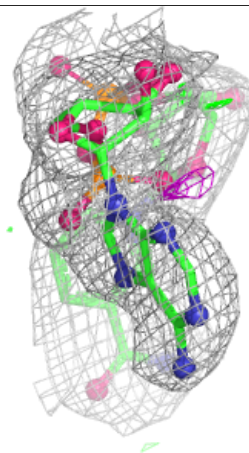
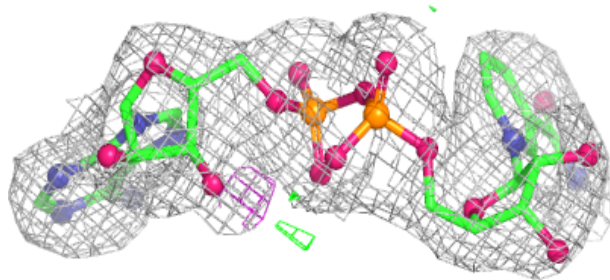
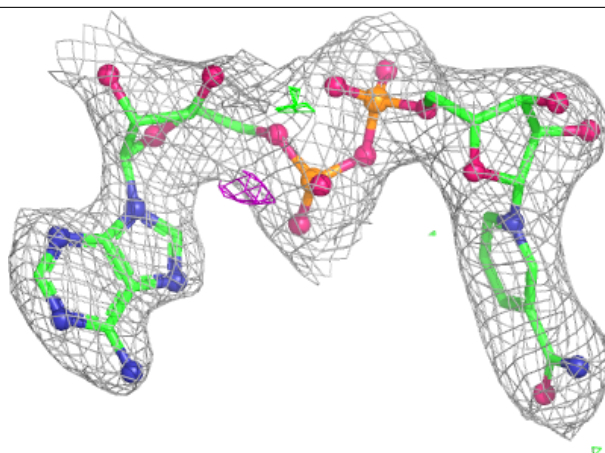
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AKG	D	502	10/10	0.83	0.10	59,61,62,62	0
2	NAD	B	501	44/44	0.91	0.08	56,73,77,81	0
3	CA	B	502	1/1	0.92	0.05	94,94,94,94	0
3	CA	A	502	1/1	0.94	0.08	64,64,64,64	0
2	NAD	C	501	44/44	0.94	0.07	45,49,55,57	0
2	NAD	D	501	44/44	0.94	0.07	50,58,61,63	0
2	NAD	A	501	44/44	0.96	0.05	40,44,51,54	0
3	CA	D	503	1/1	0.98	0.04	59,59,59,59	0
3	CA	C	502	1/1	0.98	0.03	69,69,69,69	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.



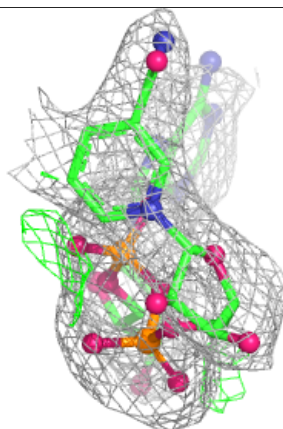
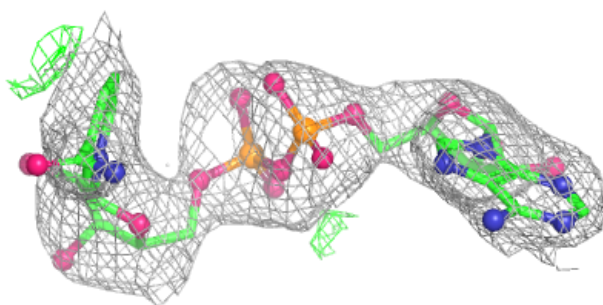
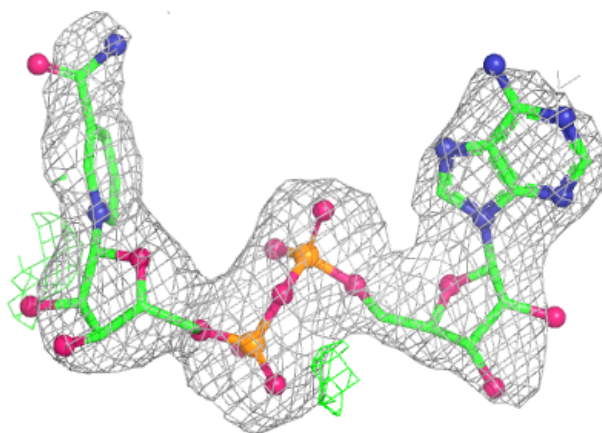
Electron density around NAD C 501:

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

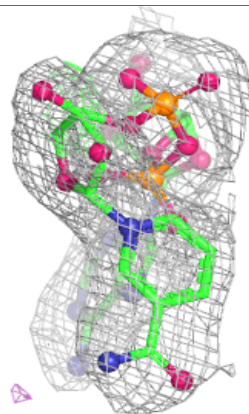
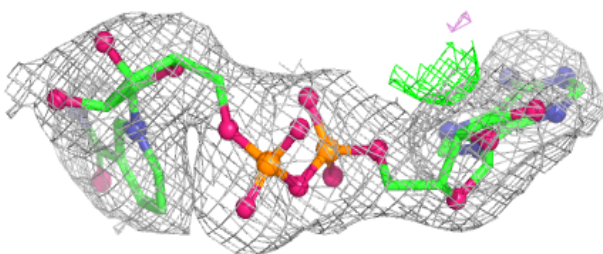
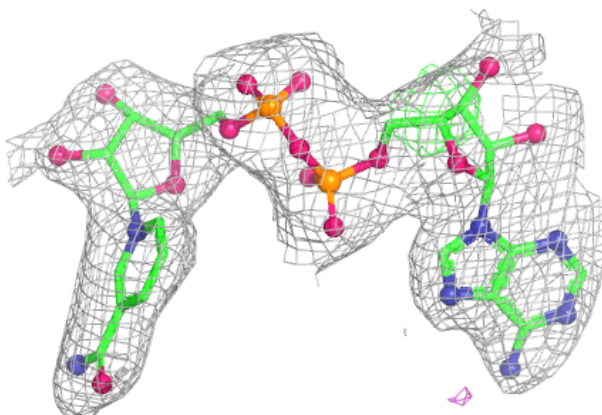


Electron density around NAD D 501:

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

**Electron density around NAD A 501:**

$2mF_o-DF_c$ (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.