



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:40 am BST

PDB ID : 3O9Z
Title : Crystal structure of the WlbA (WbpB) dehydrogenase from *Thermus thermophilus* in complex with NAD and alpha-ketoglutarate at 1.45 angstrom resolution
Authors : Holden, H.M.; Thoden, J.B.
Deposited on : 2010-08-04
Resolution : 1.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

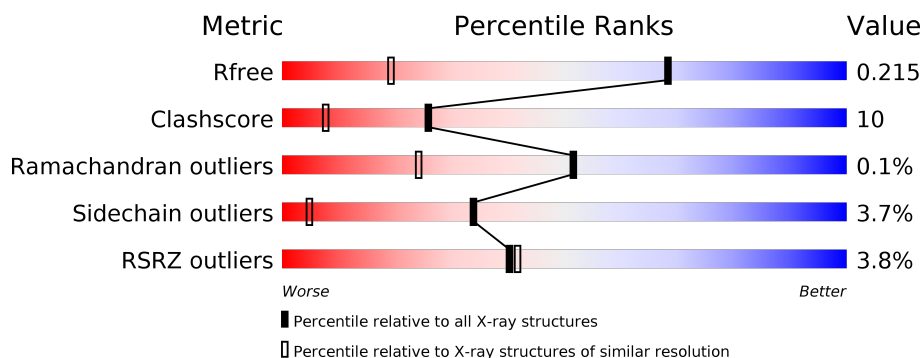
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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

Mol	Chain	Length	Quality of chain
1	A	312	<div> <div>2%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	B	312	<div> <div>2%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
1	C	312	<div> <div>2%</div> <div>89%</div> <div>7%</div> <div>...</div> </div>
1	D	312	<div> <div>9%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AKG	D	312	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11324 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 Lipopolysaccharide biosynthesis protein wbpB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	4	0
			2475	1589	438	445	3			
1	B	310	Total	C	N	O	S	0	3	0
			2470	1587	436	444	3			
1	C	310	Total	C	N	O	S	0	1	0
			2459	1578	435	444	2			
1	D	309	Total	C	N	O	S	0	4	0
			2472	1590	436	444	2			

There are 8 discrepancies between the modelled and reference sequences:

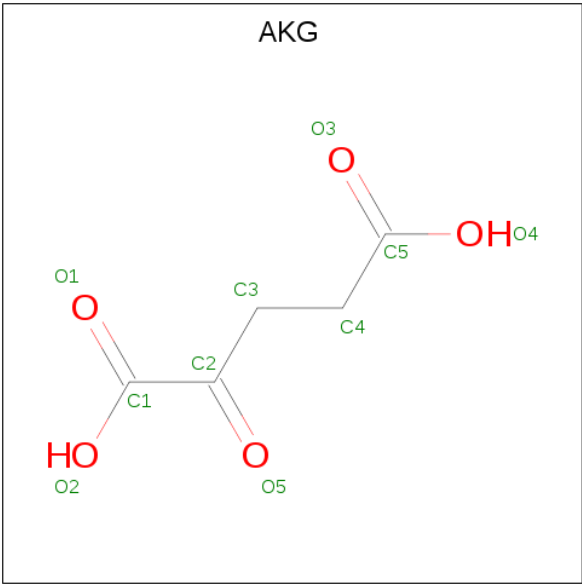
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q72KX8
A	0	HIS	-	EXPRESSION TAG	UNP Q72KX8
B	-1	GLY	-	EXPRESSION TAG	UNP Q72KX8
B	0	HIS	-	EXPRESSION TAG	UNP Q72KX8
C	-1	GLY	-	EXPRESSION TAG	UNP Q72KX8
C	0	HIS	-	EXPRESSION TAG	UNP Q72KX8
D	-1	GLY	-	EXPRESSION TAG	UNP Q72KX8
D	0	HIS	-	EXPRESSION TAG	UNP Q72KX8

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: 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 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C₅H₆O₅).

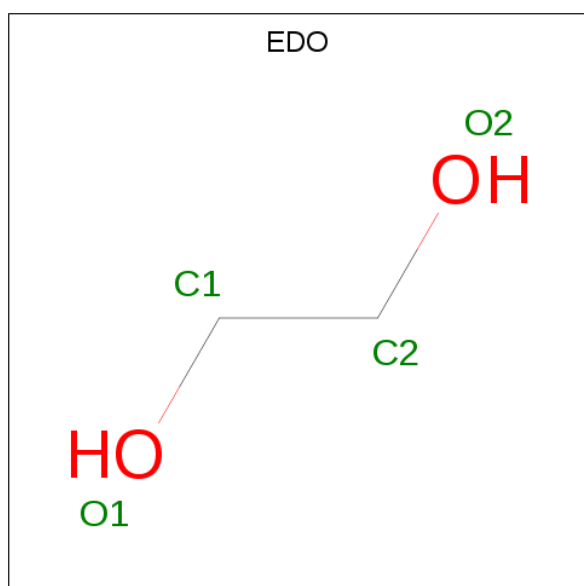


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		

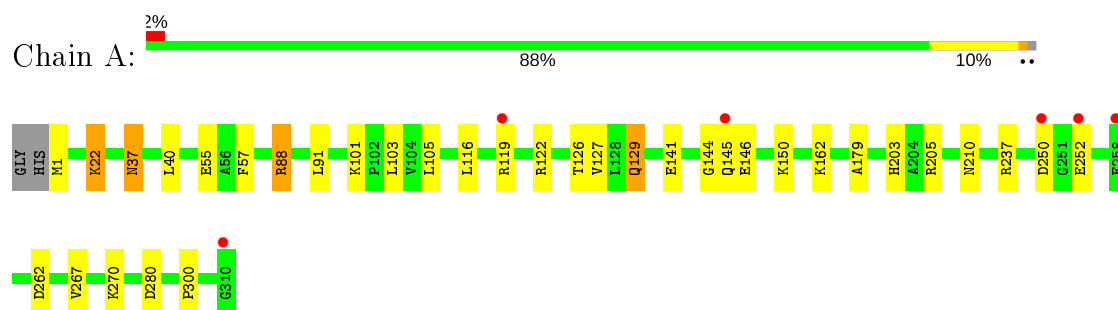
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	337	Total	O	0	0
			337	337		
6	B	351	Total	O	0	0
			351	351		
6	C	287	Total	O	0	0
			287	287		
6	D	241	Total	O	0	0
			241	241		

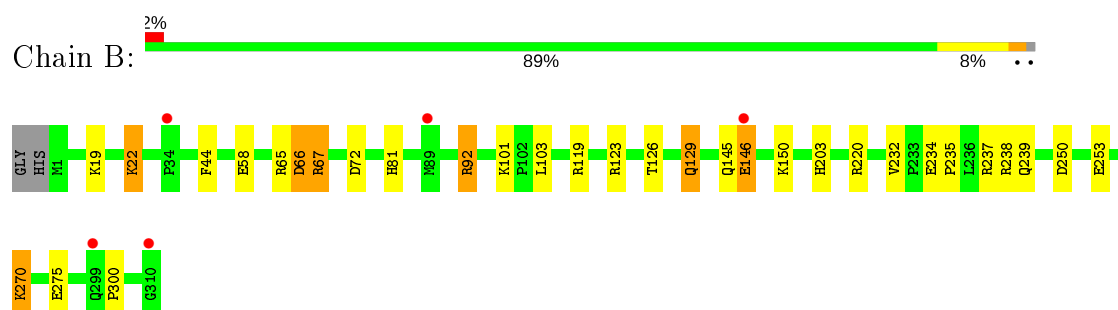
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

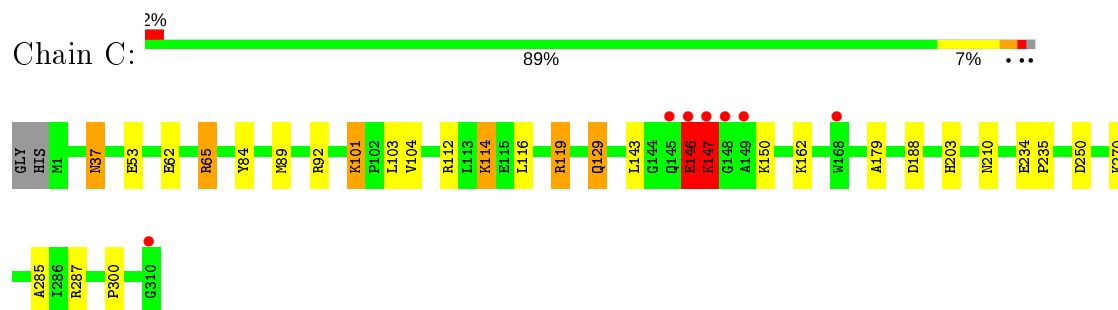
- Molecule 1: Lipopolysaccharide biosynthesis protein wbpB



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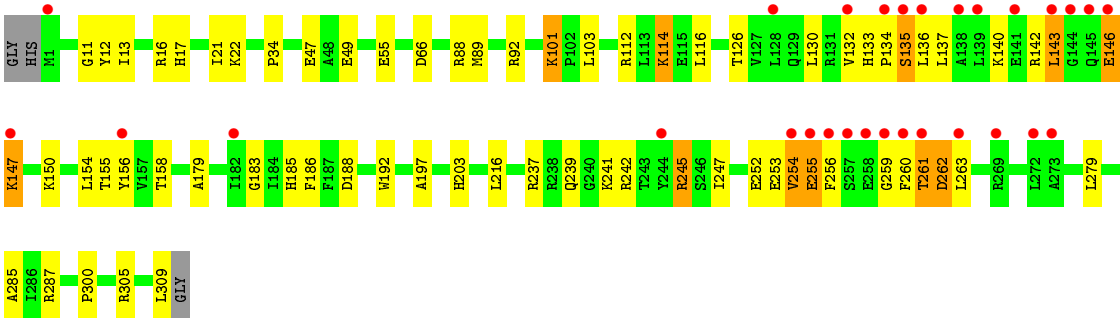


- Molecule 1: Lipopolysaccharide biosynthesis protein wbpB



- Molecule 1: Lipopolysaccharide biosynthesis protein wbpB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.78 Å 68.20 Å 164.05 Å 90.00° 94.66° 90.00°	Depositor
Resolution (Å)	30.00 – 1.45 48.01 – 1.45	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.00-1.45) 96.7 (48.01-1.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 1.45 Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.194 , 0.226 0.187 , 0.215	Depositor DCC
R_{free} test set	13629 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11324	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: AKG, EDO, NAD, CL

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	0.61	0/2547	0.96	3/3451 (0.1%)
1	B	0.62	0/2539	0.99	5/3440 (0.1%)
1	C	0.73	4/2522 (0.2%)	0.95	7/3419 (0.2%)
1	D	0.69	3/2545 (0.1%)	0.88	4/3453 (0.1%)
All	All	0.67	7/10153 (0.1%)	0.94	19/13763 (0.1%)

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	D	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	146	GLU	CG-CD	17.66	1.78	1.51
1	D	147	LYS	CD-CE	-16.48	1.10	1.51
1	D	147	LYS	CE-NZ	15.45	1.87	1.49
1	C	146	GLU	CD-OE1	-15.12	1.09	1.25
1	C	146	GLU	CD-OE2	-8.38	1.16	1.25
1	C	89	MET	SD-CE	-5.67	1.46	1.77
1	D	89	MET	SD-CE	-5.57	1.46	1.77

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	GLU	CG-CD-OE1	11.11	140.52	118.30
1	C	92	ARG	NE-CZ-NH1	10.54	125.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	GLU	CG-CD-OE2	-9.97	98.36	118.30
1	C	92	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	D	92	ARG	NE-CZ-NH1	-7.57	116.51	120.30
1	D	55	GLU	OE1-CD-OE2	7.21	131.96	123.30
1	D	287	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	57	PHE	CB-CG-CD1	6.64	125.45	120.80
1	C	287	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	88	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	C	287	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	B	220	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	B	66	ASP	CB-CG-OD1	5.42	123.17	118.30
1	B	123	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	B	220	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	205	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	72	ASP	CB-CG-OD1	-5.05	113.75	118.30
1	D	88	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	C	146	GLU	OE1-CD-OE2	-5.01	117.29	123.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	253	GLU	Peptide
1	D	255	GLU	Peptide
1	D	261	THR	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	2475	0	2495	28	0
1	B	2470	0	2490	28	0
1	C	2459	0	2468	30	0
1	D	2472	0	2489	127	1
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	44	0	26	9	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	1	0
3	D	10	0	4	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	8	0	12	0	0
5	C	4	0	6	0	0
6	A	337	0	0	8	1
6	B	351	0	0	5	0
6	C	287	0	0	3	1
6	D	241	0	0	9	1
All	All	11324	0	10080	211	2

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 10.

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:D:136:LEU:CG	1:D:256:PHE:CE1	1.91	1.53
1:D:136:LEU:HD11	1:D:256:PHE:CE1	1.44	1.51
1:C:146:GLU:CG	1:C:146:GLU:CD	1.78	1.51
1:D:136:LEU:CG	1:D:256:PHE:HE1	1.21	1.47
1:D:136:LEU:CD1	1:D:256:PHE:CE1	1.95	1.46
1:D:156:TYR:CE1	1:D:245:ARG:HD3	1.52	1.43
1:D:136:LEU:CD2	1:D:256:PHE:CE1	2.03	1.41
1:D:136:LEU:HD21	1:D:256:PHE:CE1	1.54	1.40
1:D:147:LYS:CE	1:D:147:LYS:NZ	1.87	1.37
1:D:136:LEU:CD1	1:D:256:PHE:HE1	1.30	1.32
1:D:136:LEU:HG	1:D:256:PHE:CZ	1.63	1.31
1:D:133:HIS:O	1:D:137:LEU:HD12	1.32	1.24
1:D:16:ARG:NH2	1:D:261:THR:HG23	1.57	1.18
1:D:16:ARG:CZ	1:D:261:THR:HG23	1.73	1.17
1:D:156:TYR:OH	1:D:245:ARG:NH1	1.77	1.15
1:D:133:HIS:CD2	1:D:134:PRO:HD2	1.82	1.15
1:D:156:TYR:CE1	1:D:245:ARG:CD	2.31	1.14
1:D:136:LEU:CD2	1:D:256:PHE:HE1	1.50	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:LEU:HD11	1:D:256:PHE:CD1	1.83	1.12
1:D:133:HIS:HD2	1:D:134:PRO:N	1.49	1.09
1:B:67:ARG:O	1:B:67:ARG:HG2	1.32	1.06
1:D:133:HIS:CD2	1:D:134:PRO:CD	2.40	1.04
1:D:247[A]:ILE:HD12	1:D:256:PHE:CE2	1.95	1.01
1:A:146:GLU:OE1	1:A:150:LYS:HE3	1.59	1.01
1:D:133:HIS:CD2	1:D:135:SER:H	1.78	1.01
1:D:156:TYR:CD1	1:D:245:ARG:HD3	1.96	1.00
1:D:133:HIS:O	1:D:137:LEU:CD1	2.11	0.99
1:D:133:HIS:CD2	1:D:134:PRO:N	2.33	0.96
1:D:133:HIS:C	1:D:137:LEU:HD12	1.86	0.95
1:D:237:ARG:HG3	6:D:860:HOH:O	1.66	0.94
1:D:179:ALA:O	1:D:183:GLY:HA3	1.67	0.94
1:B:65:ARG:NH2	1:B:66:ASP:OD1	2.01	0.94
1:C:116:LEU:HG	6:C:780:HOH:O	1.65	0.93
1:D:136:LEU:HG	1:D:256:PHE:HZ	1.23	0.93
1:A:103:LEU:HD13	1:A:126:THR:HB	1.49	0.93
1:D:156:TYR:HH	1:D:245:ARG:NH1	1.55	0.92
1:C:143:LEU:O	1:C:146:GLU:HG3	1.71	0.91
1:D:34:PRO:HG2	2:D:311:NAD:O2B	1.69	0.90
1:D:136:LEU:CG	1:D:256:PHE:CZ	2.34	0.89
1:D:156:TYR:CZ	1:D:245:ARG:HD3	2.07	0.89
1:B:146:GLU:OE1	1:B:250:ASP:OD1	1.92	0.86
1:D:147:LYS:CD	1:D:147:LYS:NZ	2.38	0.86
1:D:179:ALA:O	1:D:183:GLY:CA	2.24	0.85
1:D:133:HIS:O	1:D:137:LEU:HB2	1.76	0.84
1:D:156:TYR:OH	3:D:312:AKG:O4	1.95	0.84
1:D:16:ARG:CZ	1:D:261:THR:CG2	2.53	0.84
1:C:146:GLU:CG	1:C:146:GLU:OE2	2.26	0.83
1:B:67:ARG:O	1:B:67:ARG:CG	2.22	0.83
1:D:154:LEU:HD22	1:D:247[A]:ILE:HG12	1.61	0.83
1:B:146:GLU:HB2	1:B:150:LYS:NZ	1.93	0.82
1:D:132:VAL:C	1:D:137:LEU:HD11	2.00	0.81
1:D:136:LEU:CD2	1:D:256:PHE:CZ	2.63	0.80
1:D:136:LEU:N	1:D:136:LEU:HD12	1.97	0.79
1:A:162:LYS:NZ	6:A:896:HOH:O	2.13	0.79
1:A:37:ASN:H	1:A:37:ASN:HD22	1.32	0.77
1:D:247[A]:ILE:HD12	1:D:256:PHE:HE2	1.43	0.77
1:D:101:LYS:HD3	1:D:101:LYS:O	1.85	0.76
1:D:133:HIS:CD2	1:D:135:SER:N	2.54	0.76
1:A:237:ARG:NH1	6:A:786:HOH:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:HIS:HD2	1:D:134:PRO:CD	1.85	0.74
1:A:280:ASP:OD2	6:A:977:HOH:O	2.07	0.72
1:D:156:TYR:CZ	1:D:245:ARG:NH1	2.57	0.72
1:D:137:LEU:O	6:D:770:HOH:O	2.07	0.72
1:D:132:VAL:C	1:D:137:LEU:CD1	2.59	0.71
1:B:129:GLN:H	1:B:129:GLN:HE21	1.40	0.70
1:D:156:TYR:CE1	1:D:245:ARG:NE	2.59	0.70
1:D:254:VAL:HG12	6:D:752:HOH:O	1.92	0.70
1:D:133:HIS:O	1:D:137:LEU:CB	2.40	0.70
1:D:247[B]:ILE:HG22	1:D:256:PHE:HE2	1.57	0.69
1:D:146:GLU:OE1	1:D:150:LYS:HE3	1.93	0.69
1:D:156:TYR:HH	1:D:245:ARG:HH11	1.38	0.68
1:D:154:LEU:CD2	1:D:247[A]:ILE:HG12	2.23	0.68
1:A:88:ARG:HD2	1:A:116:LEU:HD13	1.76	0.67
1:D:179:ALA:O	1:D:183:GLY:N	2.27	0.67
1:D:11:GLY:HA3	6:D:356:HOH:O	1.94	0.67
1:D:259:GLY:O	1:D:263:LEU:HD11	1.94	0.67
1:D:156:TYR:HH	3:D:312:AKG:C5	2.04	0.67
1:B:146:GLU:HB2	1:B:150:LYS:HZ1	1.61	0.66
1:D:247[A]:ILE:CD1	1:D:256:PHE:CE2	2.77	0.66
1:B:270:LYS:HE2	1:B:275:GLU:OE1	1.96	0.65
1:A:22:LYS:HA	1:A:22:LYS:HE3	1.79	0.65
1:A:252:GLU:O	6:A:938:HOH:O	2.15	0.65
1:A:129:GLN:HE21	1:A:129:GLN:H	1.44	0.65
1:D:136:LEU:HD21	1:D:256:PHE:CD1	2.26	0.63
1:B:146:GLU:HB2	1:B:150:LYS:HZ2	1.59	0.63
1:D:16:ARG:NH1	1:D:261:THR:HA	2.14	0.63
1:D:133:HIS:O	1:D:137:LEU:CG	2.47	0.62
2:D:311:NAD:N6A	6:D:374:HOH:O	2.26	0.62
1:D:147:LYS:HD3	1:D:147:LYS:NZ	2.15	0.62
1:A:145:GLN:NE2	6:A:908:HOH:O	2.25	0.62
1:D:132:VAL:CA	1:D:137:LEU:HD11	2.30	0.61
1:D:156:TYR:CZ	3:D:312:AKG:O4	2.54	0.61
1:D:136:LEU:N	1:D:136:LEU:CD1	2.64	0.61
1:A:88:ARG:CD	1:A:116:LEU:CD1	2.79	0.60
1:B:203:HIS:CE1	1:B:300:PRO:HB3	2.37	0.60
1:A:88:ARG:HD2	1:A:116:LEU:CD1	2.31	0.59
1:C:146:GLU:HB2	1:C:150:LYS:NZ	2.17	0.59
1:B:103:LEU:HD13	1:B:126:THR:HB	1.84	0.59
1:D:156:TYR:CD1	1:D:245:ARG:CD	2.75	0.59
1:C:129:GLN:H	1:C:129:GLN:HE21	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247[B]:ILE:CG2	1:D:256:PHE:HE2	2.17	0.58
1:D:114:LYS:HG2	1:D:279:LEU:HD13	1.84	0.58
1:D:132:VAL:HA	1:D:137:LEU:HD11	1.86	0.58
1:C:146:GLU:HB2	1:C:150:LYS:HZ2	1.68	0.58
1:A:141:GLU:OE1	6:A:962:HOH:O	2.17	0.57
1:D:156:TYR:CE2	3:D:312:AKG:O4	2.57	0.56
1:B:119:ARG:HG2	1:B:119:ARG:HH11	1.71	0.56
1:D:34:PRO:CG	2:D:311:NAD:O2B	2.50	0.56
1:D:133:HIS:HD2	1:D:134:PRO:CA	2.19	0.55
1:C:101:LYS:HZ2	3:C:312:AKG:C1	2.20	0.55
1:D:11:GLY:CA	6:D:356:HOH:O	2.53	0.55
1:C:179:ALA:HB2	1:C:210:ASN:HD22	1.72	0.54
1:B:22:LYS:HE2	1:B:44:PHE:CD1	2.42	0.54
1:A:141:GLU:O	6:A:1009:HOH:O	2.18	0.54
1:C:114:LYS:HB2	1:C:114:LYS:HZ2	1.73	0.54
1:C:162:LYS:HD3	1:D:49:GLU:OE2	2.07	0.54
1:D:186:PHE:HZ	1:D:245:ARG:CG	2.21	0.54
1:C:119:ARG:NH1	6:C:1052:HOH:O	2.40	0.53
1:D:156:TYR:HE1	1:D:245:ARG:NE	2.06	0.53
1:B:22:LYS:HE2	1:B:44:PHE:HD1	1.73	0.53
1:A:203:HIS:CE1	1:A:300:PRO:HB3	2.43	0.53
1:D:142:ARG:O	1:D:143:LEU:C	2.46	0.53
1:D:133:HIS:CD2	1:D:133:HIS:C	2.82	0.53
1:C:37:ASN:ND2	1:C:37:ASN:H	2.07	0.52
1:C:62:GLU:HG3	1:C:65:ARG:NH2	2.24	0.52
1:D:13:ILE:HG13	1:D:13:ILE:O	2.09	0.52
1:B:232:VAL:O	1:B:237:ARG:HD3	2.10	0.52
1:B:237:ARG:NH1	6:B:650:HOH:O	2.42	0.52
1:D:112:ARG:HH22	1:D:116:LEU:HD21	1.74	0.51
1:D:103:LEU:HD13	1:D:126:THR:HB	1.93	0.51
1:B:145:GLN:HE21	1:B:145:GLN:HA	1.75	0.51
1:D:136:LEU:CD1	1:D:136:LEU:H	2.25	0.50
1:D:247[B]:ILE:HG22	1:D:256:PHE:CE2	2.42	0.50
1:C:112:ARG:NH1	6:C:552:HOH:O	2.28	0.50
1:A:37:ASN:HD22	1:A:37:ASN:N	2.06	0.49
1:A:88:ARG:CD	1:A:116:LEU:HD13	2.40	0.49
1:D:136:LEU:HG	1:D:256:PHE:CE1	1.80	0.49
1:B:19:LYS:HE2	6:B:692:HOH:O	2.12	0.49
1:D:259:GLY:O	1:D:263:LEU:CD1	2.61	0.49
1:A:91:LEU:HD22	1:A:122[A]:ARG:HB2	1.95	0.49
1:D:245:ARG:O	1:D:256:PHE:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ALA:HB2	1:A:210:ASN:HD22	1.76	0.48
1:A:91:LEU:HD22	1:A:122[B]:ARG:HB2	1.95	0.48
1:D:186:PHE:CZ	1:D:245:ARG:CG	2.96	0.48
1:B:146:GLU:CD	1:B:250:ASP:OD1	2.50	0.48
1:D:245:ARG:NH1	3:D:312:AKG:O4	2.47	0.48
1:C:146:GLU:CB	1:C:150:LYS:HZ2	2.27	0.47
1:D:156:TYR:CZ	1:D:158:THR:HB	2.49	0.47
1:D:156:TYR:CE1	1:D:245:ARG:CZ	2.96	0.47
1:D:261:THR:O	1:D:261:THR:HG22	2.15	0.47
1:B:145:GLN:HG3	6:B:1047:HOH:O	2.14	0.47
1:D:136:LEU:H	1:D:136:LEU:HD12	1.73	0.47
1:C:162:LYS:HE3	1:D:49:GLU:OE1	2.15	0.47
1:D:156:TYR:OH	1:D:245:ARG:CZ	2.55	0.47
1:A:150:LYS:HD2	1:A:250:ASP:OD2	2.15	0.47
1:C:103:LEU:HD23	1:C:104:VAL:HG13	1.97	0.47
1:D:101:LYS:HG3	6:D:351:HOH:O	2.13	0.47
1:D:133:HIS:HA	1:D:134:PRO:HD3	1.76	0.47
1:D:17:HIS:O	1:D:21:ILE:HG13	2.15	0.46
1:D:112:ARG:NH2	1:D:116:LEU:HD21	2.30	0.46
1:D:34:PRO:CD	2:D:311:NAD:C4A	2.94	0.46
1:D:185[B]:HIS:CD2	1:D:260:PHE:CE1	3.04	0.45
1:D:11:GLY:O	1:D:12:TYR:C	2.54	0.45
1:B:81:HIS:HE1	1:C:53:GLU:OE1	1.99	0.45
1:D:156:TYR:CD1	1:D:245:ARG:CG	3.00	0.45
2:D:311:NAD:C5B	6:D:332:HOH:O	2.64	0.45
1:D:16:ARG:NE	1:D:261:THR:CG2	2.80	0.45
1:C:146:GLU:HB2	1:C:147:LYS:H	1.50	0.45
1:C:162:LYS:HD2	1:D:49:GLU:HA	1.97	0.45
1:C:84:TYR:OH	1:C:112:ARG:HD2	2.17	0.45
1:D:203:HIS:CE1	1:D:300:PRO:HB3	2.52	0.45
1:C:203:HIS:CE1	1:C:300:PRO:HB3	2.53	0.44
1:B:270:LYS:HE3	6:B:550:HOH:O	2.17	0.44
1:D:185[B]:HIS:CE1	1:D:186:PHE:CE2	3.05	0.44
1:D:130:LEU:HD22	1:D:136:LEU:HD22	1.99	0.44
1:C:146:GLU:CB	1:C:146:GLU:CD	2.72	0.44
1:B:234:GLU:N	1:B:235:PRO:CD	2.81	0.43
1:B:58:GLU:OE1	1:B:92:ARG:NH1	2.40	0.43
1:C:234:GLU:N	1:C:235:PRO:HD2	2.33	0.43
1:D:262:ASP:HB3	1:D:263:LEU:HG	1.99	0.43
1:A:127:VAL:HA	1:A:267:VAL:HG11	2.01	0.43
1:B:145:GLN:HB2	6:B:975:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HA	1:A:105:LEU:HD23	1.84	0.43
1:D:197:ALA:HA	1:D:216:LEU:HD22	2.00	0.43
1:C:188:ASP:HA	1:C:285:ALA:HB2	2.01	0.42
1:C:114:LYS:CB	1:C:114:LYS:HZ2	2.33	0.42
1:D:154:LEU:HD13	1:D:154:LEU:C	2.39	0.42
1:D:140:LYS:HE2	1:D:192:TRP:NE1	2.33	0.42
1:B:22:LYS:HB3	1:B:22:LYS:HE3	1.38	0.42
1:A:144:GLY:HA3	6:A:1009:HOH:O	2.20	0.42
1:B:234:GLU:O	1:B:238:ARG:HG3	2.20	0.42
1:D:132:VAL:C	1:D:137:LEU:HD12	2.37	0.42
1:D:154:LEU:HD13	1:D:155:THR:N	2.35	0.42
1:D:156:TYR:HH	1:D:245:ARG:HH12	1.55	0.42
1:D:143:LEU:HA	1:D:143:LEU:HD12	1.92	0.41
2:D:311:NAD:C4B	6:D:332:HOH:O	2.67	0.41
1:C:114:LYS:CB	1:C:114:LYS:NZ	2.83	0.41
1:C:146:GLU:OE1	1:C:250:ASP:CG	2.58	0.41
1:C:270:LYS:HE3	1:C:270:LYS:HB3	1.83	0.41
1:D:156:TYR:CZ	1:D:245:ARG:CD	2.89	0.41
1:D:309:LEU:HA	1:D:309:LEU:HD23	1.82	0.41
1:A:119:ARG:HH12	1:D:66:ASP:CG	2.22	0.41
1:D:260:PHE:CD2	1:D:260:PHE:O	2.74	0.41
1:D:300:PRO:HG2	1:D:305:ARG:NH2	2.36	0.41
1:D:188:ASP:HA	1:D:285:ALA:HB2	2.03	0.41
1:B:119:ARG:HG2	1:B:119:ARG:NH1	2.35	0.40
1:A:55:GLU:OE1	2:D:311:NAD:N6A	2.46	0.40
1:A:270:LYS:HB3	1:A:270:LYS:HE3	1.75	0.40
1:D:239:GLN:OE1	1:D:241:LYS:CE	2.69	0.40
1:D:34:PRO:HD2	2:D:311:NAD:H1B	2.04	0.40
1:D:34:PRO:HD3	2:D:311:NAD:C4A	2.52	0.40

All (2) 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:D:147:LYS:NZ	6:D:1057:HOH:O[2_746]	1.82	0.38
6:A:1207:HOH:O	6:C:829:HOH:O[2_645]	2.15	0.05

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	312/312 (100%)	308 (99%)	4 (1%)	0	100	100
1	B	311/312 (100%)	309 (99%)	2 (1%)	0	100	100
1	C	309/312 (99%)	303 (98%)	5 (2%)	1 (0%)	41	19
1	D	311/312 (100%)	297 (96%)	14 (4%)	0	100	100
All	All	1243/1248 (100%)	1217 (98%)	25 (2%)	1 (0%)	51	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	147	LYS

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	256/253 (101%)	249 (97%)	7 (3%)	44	11
1	B	255/253 (101%)	246 (96%)	9 (4%)	36	6
1	C	253/253 (100%)	245 (97%)	8 (3%)	39	8
1	D	256/253 (101%)	242 (94%)	14 (6%)	21	2
All	All	1020/1012 (101%)	982 (96%)	38 (4%)	34	5

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	22	LYS
1	A	37	ASN
1	A	40	LEU
1	A	101	LYS
1	A	129	GLN
1	A	262	ASP
1	B	22	LYS
1	B	67	ARG
1	B	92	ARG
1	B	101	LYS
1	B	129	GLN
1	B	146	GLU
1	B	239	GLN
1	B	253	GLU
1	B	270	LYS
1	C	37	ASN
1	C	65	ARG
1	C	101	LYS
1	C	114	LYS
1	C	119	ARG
1	C	129	GLN
1	C	146	GLU
1	C	147	LYS
1	D	22	LYS
1	D	47	GLU
1	D	101	LYS
1	D	114	LYS
1	D	135	SER
1	D	143	LEU
1	D	146	GLU
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	245	ARG
1	D	252	GLU
1	D	254	VAL
1	D	255	GLU
1	D	262	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN

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Mol	Chain	Res	Type
1	A	210	ASN
1	B	81	HIS
1	B	145	GLN
1	B	210	ASN
1	C	37	ASN
1	C	210	ASN
1	D	81	HIS
1	D	133	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	D	311	-	42,48,48	1.05	3 (7%)	50,73,73	2.10	13 (26%)
2	NAD	B	311	-	42,48,48	1.10	2 (4%)	50,73,73	2.14	14 (28%)
5	EDO	C	313	-	3,3,3	0.55	0	2,2,2	0.37	0
2	NAD	C	311	-	42,48,48	1.10	4 (9%)	50,73,73	1.89	13 (26%)
2	NAD	A	311	-	42,48,48	1.03	3 (7%)	50,73,73	2.34	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	313	-	3,3,3	0.52	0	2,2,2	0.27	0
5	EDO	B	314	-	3,3,3	0.60	0	2,2,2	0.39	0
3	AKG	A	312	-	3,9,9	0.38	0	4,11,11	1.31	1 (25%)
3	AKG	D	312	-	3,9,9	1.15	0	4,11,11	1.59	1 (25%)
3	AKG	B	312	-	3,9,9	1.16	0	4,11,11	1.81	1 (25%)
3	AKG	C	312	-	3,9,9	0.59	0	4,11,11	4.90	3 (75%)

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	D	311	-	-	14/26/62/62	0/5/5/5
2	NAD	B	311	-	-	5/26/62/62	0/5/5/5
5	EDO	C	313	-	-	0/1/1/1	-
2	NAD	C	311	-	-	7/26/62/62	0/5/5/5
2	NAD	A	311	-	-	4/26/62/62	0/5/5/5
5	EDO	B	313	-	-	0/1/1/1	-
5	EDO	B	314	-	-	0/1/1/1	-
3	AKG	A	312	-	-	2/3/9/9	-
3	AKG	D	312	-	-	2/3/9/9	-
3	AKG	B	312	-	-	2/3/9/9	-
3	AKG	C	312	-	-	3/3/9/9	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	311	NAD	C2N-N1N	-4.25	1.29	1.35
2	C	311	NAD	C2N-N1N	-3.49	1.30	1.35
2	D	311	NAD	O4B-C1B	3.14	1.45	1.41
2	C	311	NAD	O4D-C1D	2.77	1.44	1.41
2	D	311	NAD	O4D-C1D	2.63	1.44	1.41
2	A	311	NAD	C2A-N3A	2.58	1.36	1.32
2	C	311	NAD	C8A-N7A	-2.56	1.30	1.34
2	A	311	NAD	C2N-N1N	-2.40	1.32	1.35
2	A	311	NAD	O4D-C1D	2.37	1.44	1.41
2	B	311	NAD	O4D-C1D	2.16	1.44	1.41
2	D	311	NAD	C2N-N1N	-2.03	1.32	1.35
2	C	311	NAD	C3N-C7N	-2.02	1.47	1.50

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	311	NAD	C5B-C4B-C3B	-8.90	81.83	115.18
3	C	312	AKG	O5-C2-C3	8.35	134.63	120.38
2	A	311	NAD	N3A-C2A-N1A	-7.29	117.28	128.68
2	A	311	NAD	C2A-N1A-C6A	7.03	130.78	118.75
2	B	311	NAD	C1B-N9A-C4A	-5.49	117.00	126.64
2	B	311	NAD	N3A-C2A-N1A	-4.99	120.88	128.68
2	B	311	NAD	C2A-N1A-C6A	4.97	127.26	118.75
2	A	311	NAD	C1B-N9A-C4A	-4.96	117.92	126.64
2	C	311	NAD	O7N-C7N-C3N	4.68	125.24	119.63
2	B	311	NAD	O7N-C7N-C3N	4.57	125.10	119.63
2	A	311	NAD	C3N-C2N-N1N	4.34	124.67	120.43
2	B	311	NAD	C3N-C2N-N1N	4.23	124.56	120.43
2	C	311	NAD	C1B-N9A-C4A	-4.15	119.36	126.64
2	A	311	NAD	N6A-C6A-N1A	3.98	126.83	118.57
3	C	312	AKG	C3-C2-C1	-3.92	111.55	121.32
2	C	311	NAD	C2A-N1A-C6A	3.87	125.37	118.75
2	C	311	NAD	C5N-C4N-C3N	-3.73	115.93	120.34
2	C	311	NAD	O4B-C1B-C2B	-3.58	101.69	106.93
2	D	311	NAD	PN-O3-PA	-3.54	120.68	132.83
2	B	311	NAD	O4B-C1B-C2B	-3.48	101.84	106.93
2	D	311	NAD	N3A-C2A-N1A	-3.36	123.43	128.68
2	D	311	NAD	C2B-C3B-C4B	3.35	109.14	102.64
2	C	311	NAD	C3N-C7N-N7N	-3.32	113.77	117.75
3	B	312	AKG	C4-C3-C2	-3.28	106.06	113.14
2	D	311	NAD	O5D-PN-O1N	-3.28	96.25	109.07
2	A	311	NAD	C5A-C6A-N1A	-3.25	112.98	120.35
2	B	311	NAD	C5N-C4N-C3N	-3.25	116.50	120.34
2	C	311	NAD	C5B-C4B-C3B	-3.23	103.07	115.18
2	A	311	NAD	C3D-C2D-C1D	3.11	105.65	100.98
2	D	311	NAD	C4A-C5A-N7A	-3.10	106.16	109.40
2	B	311	NAD	C5N-C6N-N1N	-3.08	115.99	120.40
2	A	311	NAD	C3N-C7N-N7N	-2.99	114.17	117.75
2	A	311	NAD	O4B-C1B-C2B	-2.95	102.61	106.93
2	C	311	NAD	O5D-PN-O1N	-2.94	97.58	109.07
2	B	311	NAD	C6N-C5N-C4N	2.93	123.69	119.44
2	A	311	NAD	C5N-C4N-C3N	-2.86	116.96	120.34
2	D	311	NAD	O5B-PA-O1A	-2.84	97.97	109.07
2	C	311	NAD	N3A-C2A-N1A	-2.84	124.25	128.68
3	C	312	AKG	C4-C3-C2	-2.76	107.18	113.14
2	D	311	NAD	O3B-C3B-C2B	-2.63	103.30	111.82
2	D	311	NAD	O2B-C2B-C3B	-2.60	103.41	111.82
2	B	311	NAD	C5A-C6A-N1A	-2.59	114.48	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	311	NAD	O4D-C4D-C5D	-2.58	100.88	109.37
2	C	311	NAD	C5A-C6A-N1A	-2.58	114.51	120.35
3	A	312	AKG	C4-C3-C2	-2.53	107.68	113.14
2	C	311	NAD	O5B-PA-O1A	-2.50	99.30	109.07
2	D	311	NAD	PN-O5D-C5D	-2.49	107.10	121.68
2	D	311	NAD	PA-O5B-C5B	-2.42	107.47	121.68
2	A	311	NAD	C6N-C5N-C4N	2.33	122.83	119.44
3	D	312	AKG	C3-C4-C5	-2.29	108.83	112.67
2	B	311	NAD	O7N-C7N-N7N	-2.28	119.34	122.58
2	B	311	NAD	N6A-C6A-N1A	2.26	123.27	118.57
2	C	311	NAD	N6A-C6A-N1A	2.18	123.10	118.57
2	A	311	NAD	O4D-C1D-C2D	-2.14	103.80	106.93
2	B	311	NAD	O5B-PA-O1A	-2.08	100.95	109.07
2	D	311	NAD	O4D-C4D-C5D	-2.06	102.60	109.37
2	A	311	NAD	C3B-C2B-C1B	-2.05	97.89	100.98
2	B	311	NAD	O4D-C4D-C5D	-2.04	102.65	109.37
2	A	311	NAD	O2A-PA-O1A	2.03	122.28	112.24
2	D	311	NAD	C1B-N9A-C4A	-2.02	123.10	126.64

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	311	NAD	C5B-O5B-PA-O1A
2	D	311	NAD	C5B-O5B-PA-O2A
2	D	311	NAD	PN-O3-PA-O5B
2	D	311	NAD	O4B-C4B-C5B-O5B
2	D	311	NAD	C3B-C4B-C5B-O5B
2	D	311	NAD	C5D-O5D-PN-O1N
2	D	311	NAD	C5D-O5D-PN-O2N
2	D	311	NAD	O4D-C1D-N1N-C2N
2	D	311	NAD	O4D-C1D-N1N-C6N
2	D	311	NAD	C2D-C1D-N1N-C2N
2	B	311	NAD	O4D-C1D-N1N-C2N
2	B	311	NAD	O4D-C1D-N1N-C6N
2	C	311	NAD	O4D-C1D-N1N-C2N
2	C	311	NAD	O4D-C1D-N1N-C6N
2	A	311	NAD	O4D-C1D-N1N-C2N
2	A	311	NAD	O4D-C1D-N1N-C6N
3	C	312	AKG	C2-C3-C4-C5
3	B	312	AKG	C1-C2-C3-C4
3	A	312	AKG	C1-C2-C3-C4

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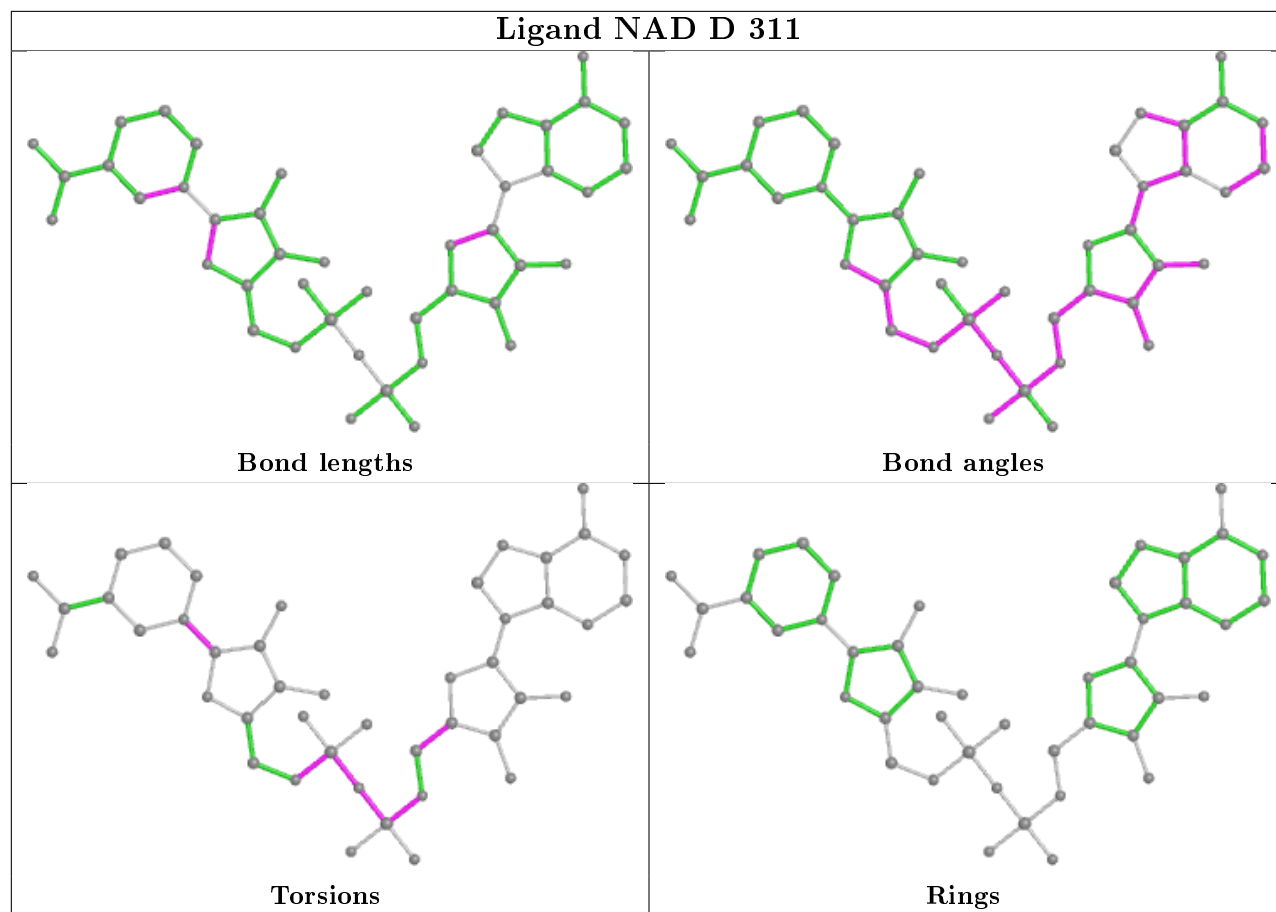
Mol	Chain	Res	Type	Atoms
3	D	312	AKG	C1-C2-C3-C4
3	B	312	AKG	O5-C2-C3-C4
2	D	311	NAD	C5B-O5B-PA-O3
2	C	311	NAD	C5D-O5D-PN-O3
3	A	312	AKG	O5-C2-C3-C4
2	D	311	NAD	PA-O3-PN-O2N
3	D	312	AKG	O5-C2-C3-C4
3	C	312	AKG	C1-C2-C3-C4
3	C	312	AKG	O5-C2-C3-C4
2	D	311	NAD	C5D-O5D-PN-O3
2	D	311	NAD	C2D-C1D-N1N-C6N
2	B	311	NAD	C5D-O5D-PN-O3
2	B	311	NAD	C2D-C1D-N1N-C2N
2	C	311	NAD	C2D-C1D-N1N-C2N
2	A	311	NAD	C2D-C1D-N1N-C2N
2	B	311	NAD	O4B-C4B-C5B-O5B
2	C	311	NAD	O4B-C4B-C5B-O5B
2	C	311	NAD	C3B-C4B-C5B-O5B
2	C	311	NAD	PA-O3-PN-O1N
2	A	311	NAD	O4B-C4B-C5B-O5B

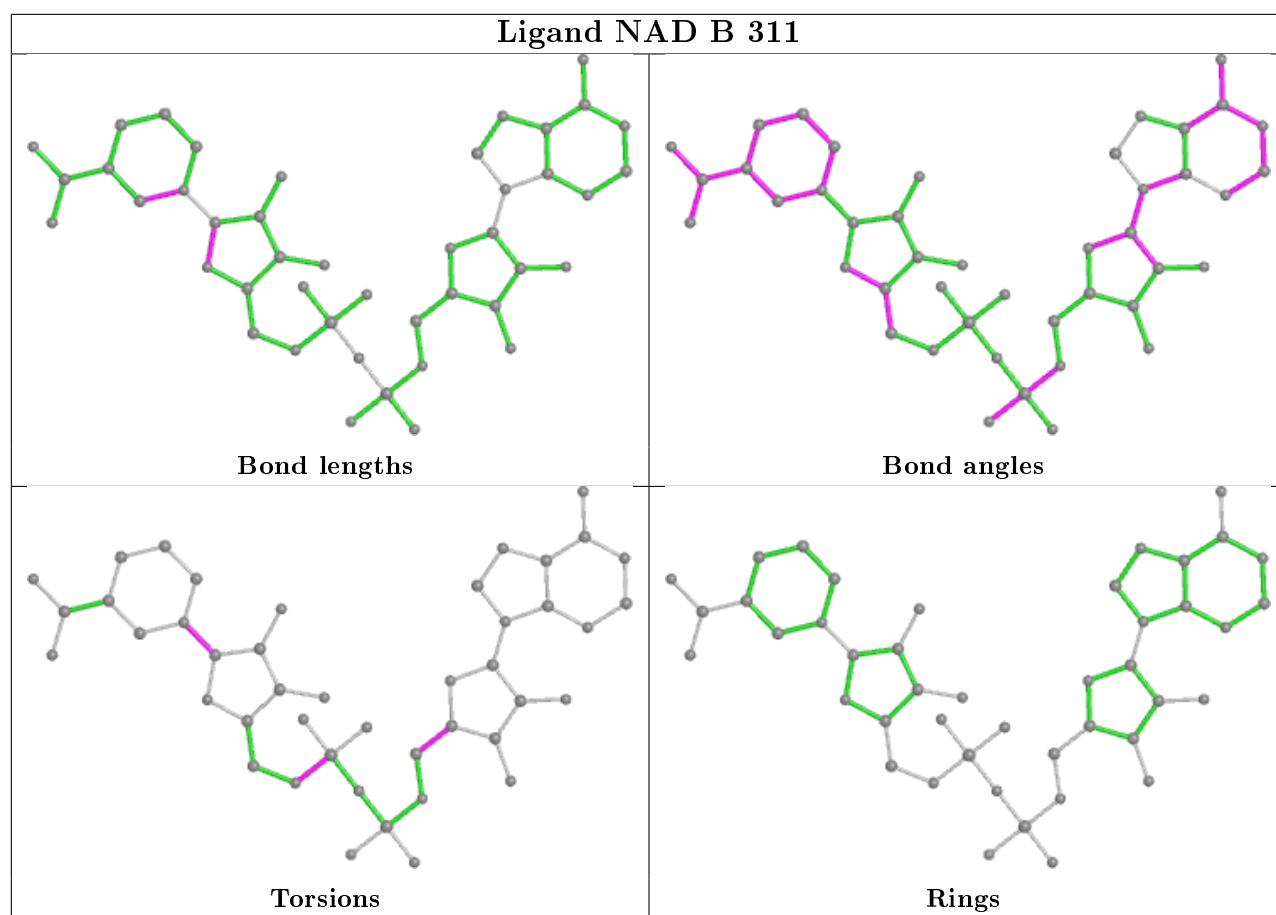
There are no ring outliers.

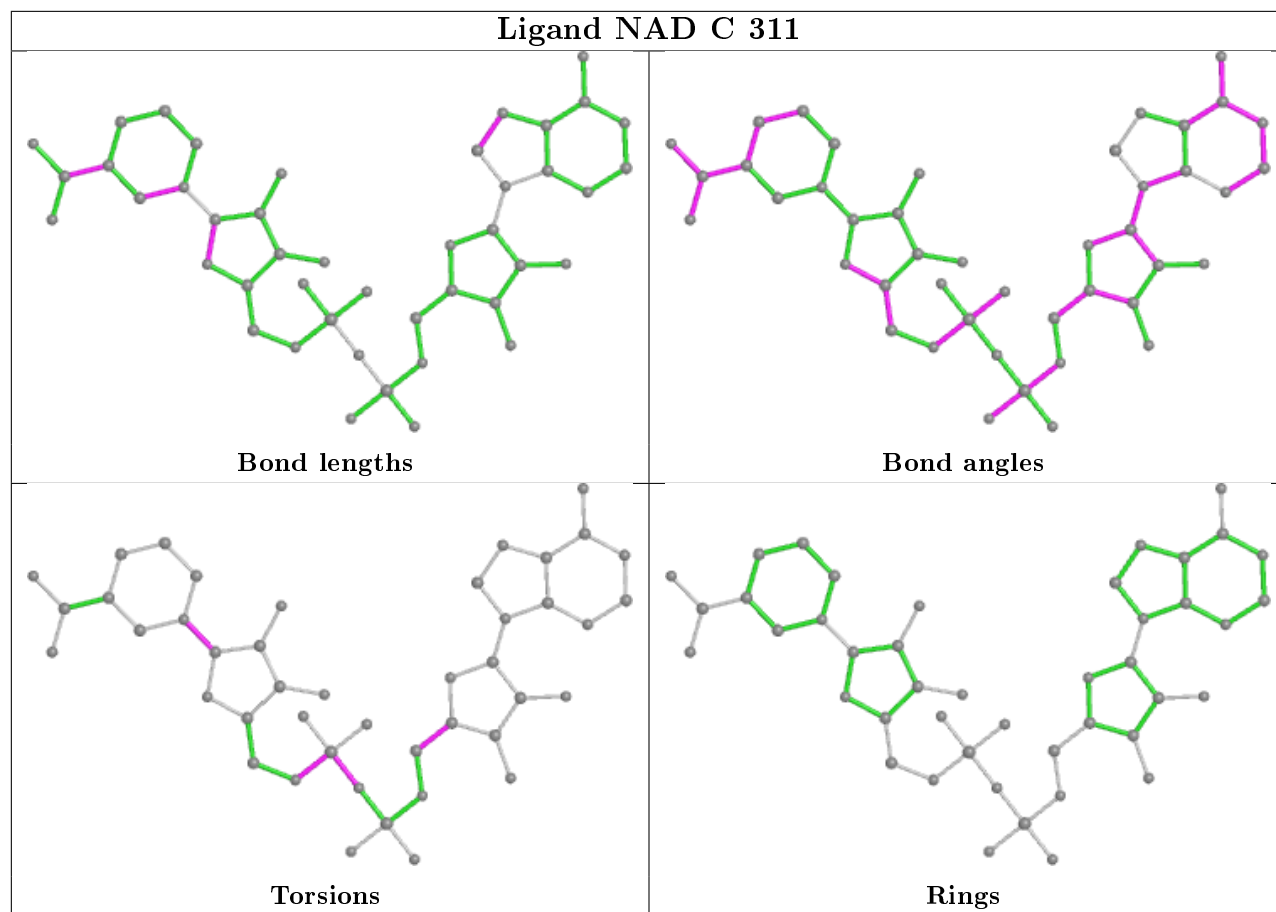
3 monomers are involved in 15 short contacts:

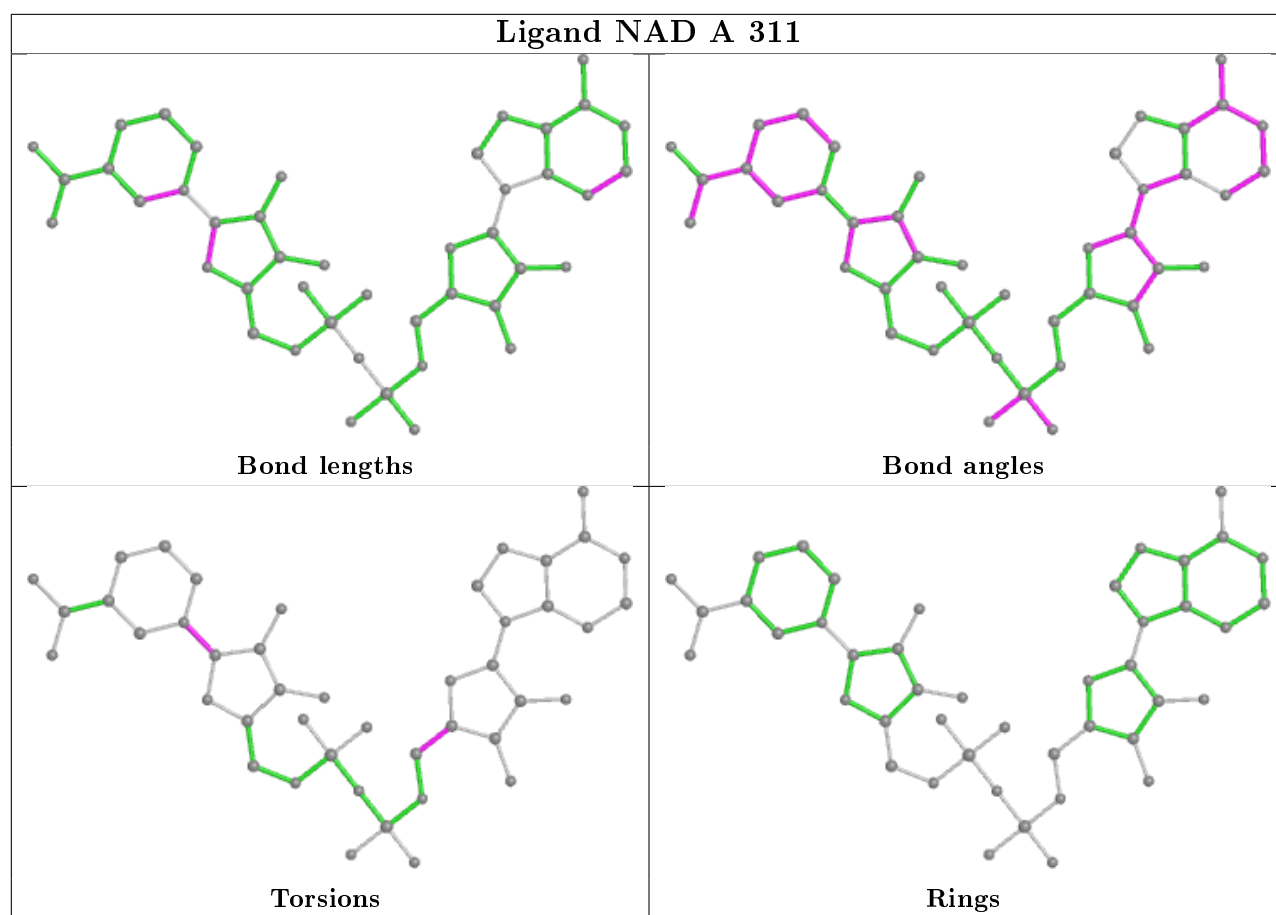
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	311	NAD	9	0
3	D	312	AKG	5	0
3	C	312	AKG	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	310/312 (99%)	0.05	6 (1%) 66 67	11, 18, 32, 43	0
1	B	310/312 (99%)	-0.04	5 (1%) 72 72	11, 17, 44, 126	0
1	C	310/312 (99%)	-0.00	7 (2%) 60 61	12, 19, 42, 173	0
1	D	309/312 (99%)	0.30	29 (9%) 8 8	13, 24, 73, 176	0
All	All	1239/1248 (99%)	0.08	47 (3%) 40 42	11, 19, 48, 176	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	GLY	10.0
1	D	256	PHE	9.7
1	C	310	GLY	9.3
1	A	310	GLY	8.3
1	D	259	GLY	6.9
1	D	260	PHE	6.3
1	D	261	THR	5.6
1	D	136	LEU	4.5
1	D	143	LEU	4.5
1	D	145	GLN	4.0
1	C	147	LYS	3.9
1	C	146	GLU	3.8
1	A	250	ASP	3.7
1	D	132	VAL	3.4
1	D	146	GLU	3.4
1	D	141	GLU	3.2
1	D	272	LEU	3.0
1	D	254	VAL	2.9
1	D	134	PRO	2.9
1	D	139	LEU	2.9
1	A	252	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	135	SER	2.7
1	C	145	GLN	2.6
1	C	148	GLY	2.6
1	A	145	GLN	2.6
1	D	156	TYR	2.6
1	C	149	ALA	2.5
1	D	255	GLU	2.5
1	D	144	GLY	2.5
1	A	119	ARG	2.4
1	D	138	ALA	2.4
1	D	258	GLU	2.4
1	D	128	LEU	2.4
1	D	263	LEU	2.4
1	D	147	LYS	2.4
1	D	182	ILE	2.4
1	D	273	ALA	2.3
1	D	257	SER	2.3
1	D	244	TYR	2.2
1	B	89[A]	MET	2.2
1	B	299	GLN	2.1
1	B	146	GLU	2.1
1	B	34	PRO	2.1
1	D	269	ARG	2.1
1	D	1	MET	2.0
1	A	258	GLU	2.0
1	C	168	TRP	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](#)

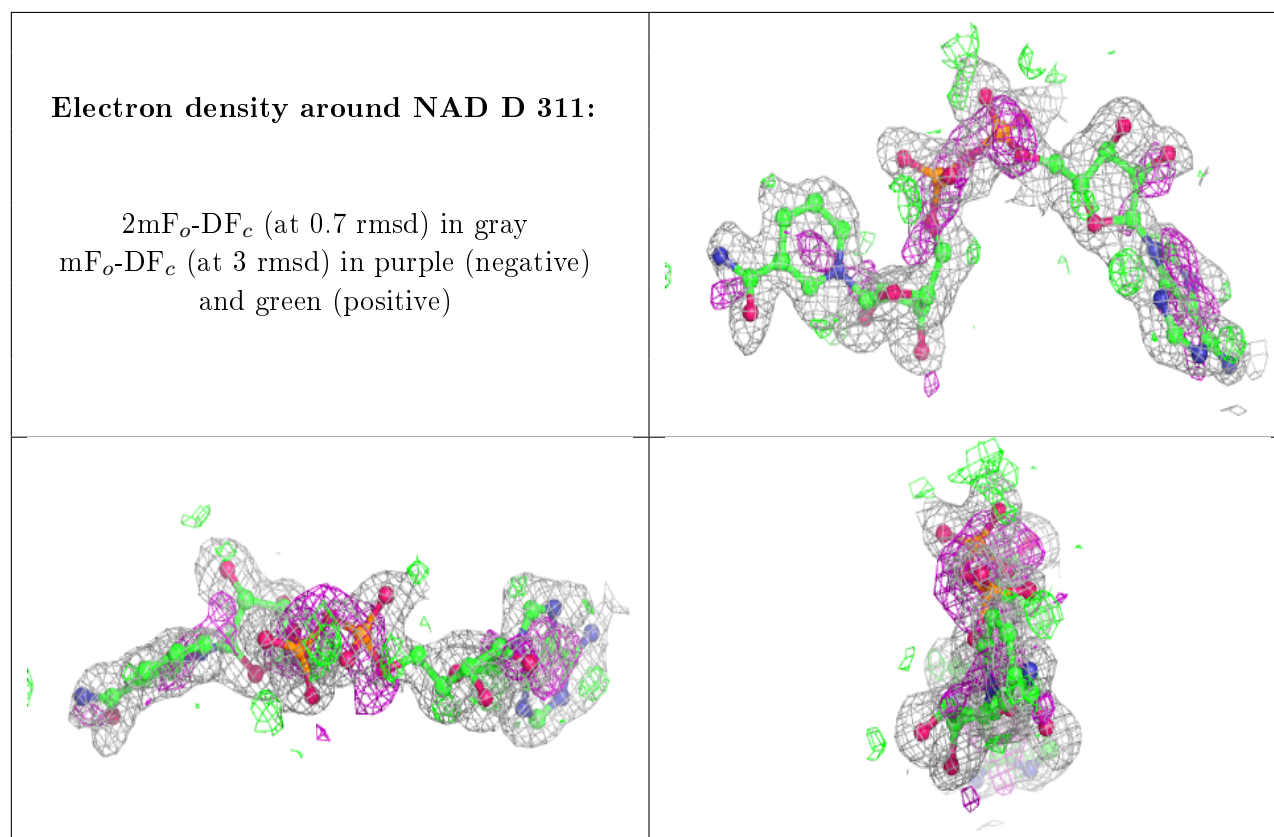
There are no carbohydrates in this entry.

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.

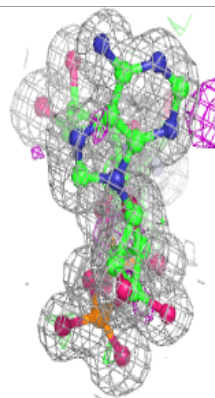
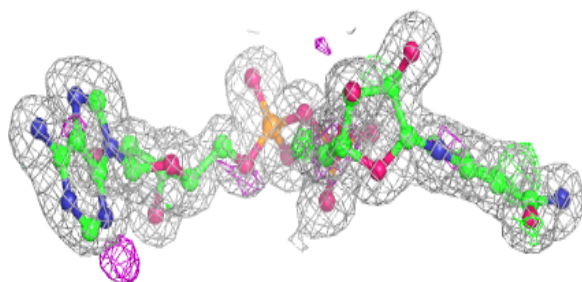
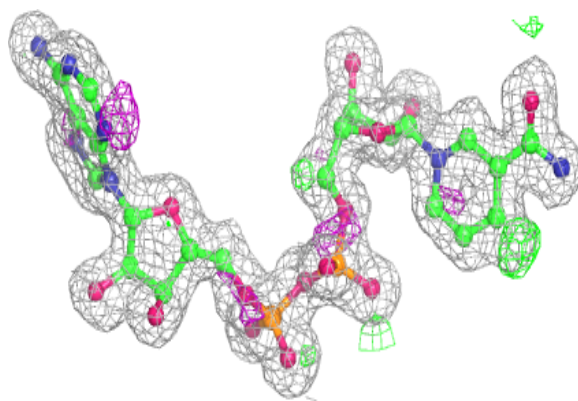
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	AKG	D	312	10/10	0.77	0.33	21,23,26,33	0
2	NAD	D	311	44/44	0.85	0.15	19,30,46,54	0
3	AKG	C	312	10/10	0.89	0.10	19,21,47,68	0
5	EDO	B	313	4/4	0.89	0.08	26,28,30,35	0
5	EDO	C	313	4/4	0.92	0.14	25,25,32,34	0
5	EDO	B	314	4/4	0.93	0.09	18,19,23,30	0
3	AKG	B	312	10/10	0.94	0.08	14,14,15,16	0
2	NAD	C	311	44/44	0.96	0.08	12,16,20,27	0
3	AKG	A	312	10/10	0.97	0.06	16,17,18,21	0
2	NAD	B	311	44/44	0.98	0.10	9,11,14,20	0
2	NAD	A	311	44/44	0.98	0.09	10,12,18,19	0
4	CL	D	313	1/1	0.98	0.11	19,19,19,19	0
4	CL	A	313	1/1	0.99	0.13	17,17,17,17	0
4	CL	B	315	1/1	1.00	0.15	14,14,14,14	0
4	CL	C	314	1/1	1.00	0.09	16,16,16,16	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.

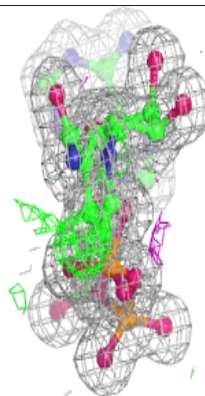
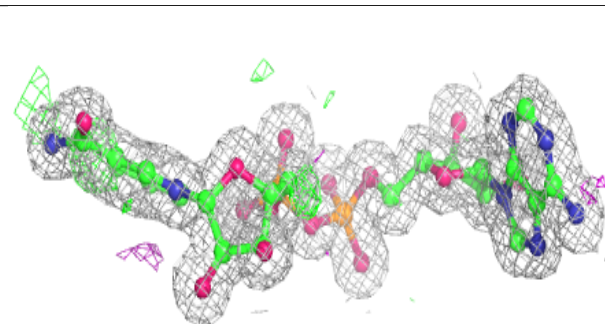
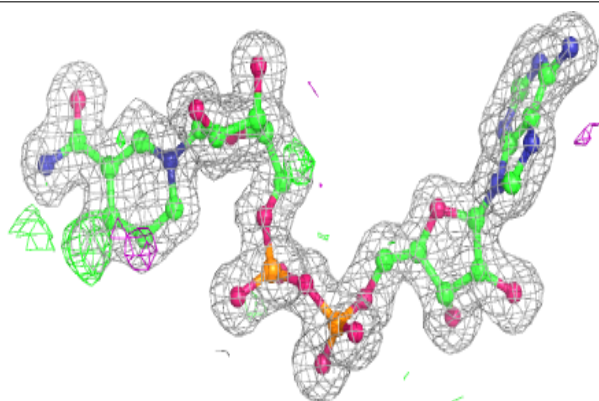


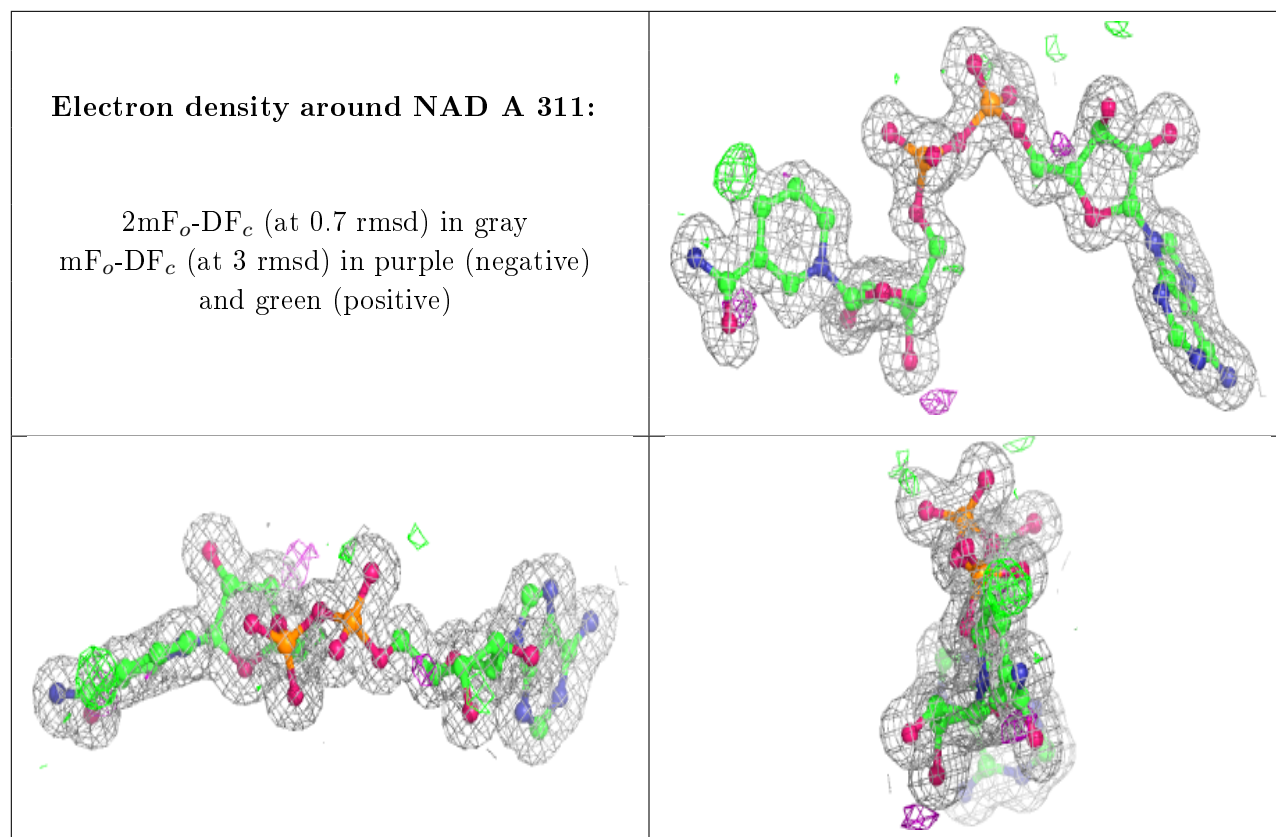
Electron density around NAD C 311:

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

**Electron density around NAD B 311:**

$2mF_o-DF_c$ (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.