



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:06 PM UTC

PDB ID : 3OA2 / pdb_00003oa2
Title : Crystal structure of the WlbA (WbpB) dehydrogenase from *Pseudomonas aeruginosa* in complex with NAD at 1.5 angstrom resolution
Authors : Holden, H.M.; Thoden, J.B.
Deposited on : 2010-08-04
Resolution : 1.50 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

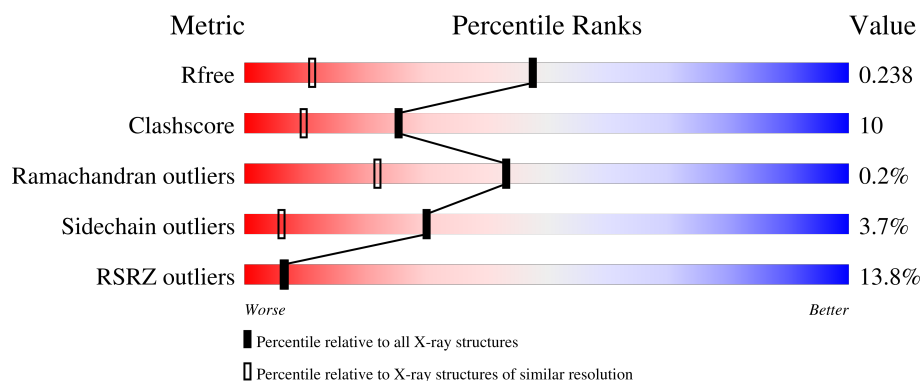
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	318	
1	B	318	
1	C	318	
1	D	318	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10958 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.

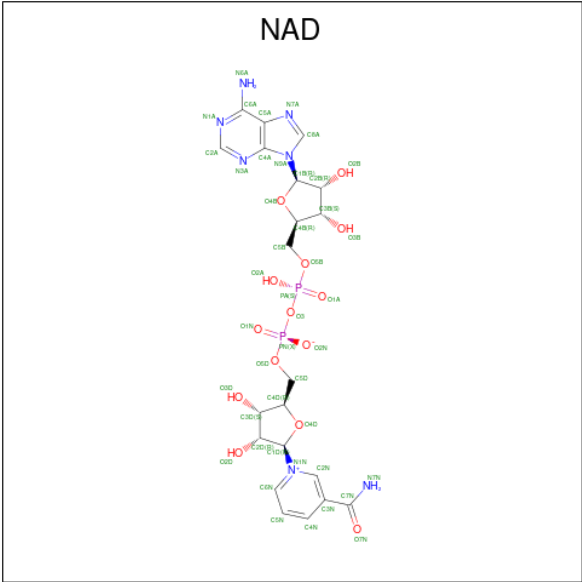
- Molecule 1 is a protein called WbpB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	2	0
			2453	1563	421	457	12			
1	B	311	Total	C	N	O	S	0	2	0
			2484	1582	429	461	12			
1	C	299	Total	C	N	O	S	0	5	0
			2427	1548	420	447	12			
1	D	298	Total	C	N	O	S	0	5	0
			2401	1531	412	446	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P72133
A	0	HIS	-	expression tag	UNP P72133
B	-1	GLY	-	expression tag	UNP P72133
B	0	HIS	-	expression tag	UNP P72133
C	-1	GLY	-	expression tag	UNP P72133
C	0	HIS	-	expression tag	UNP P72133
D	-1	GLY	-	expression tag	UNP P72133
D	0	HIS	-	expression tag	UNP P72133

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



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		

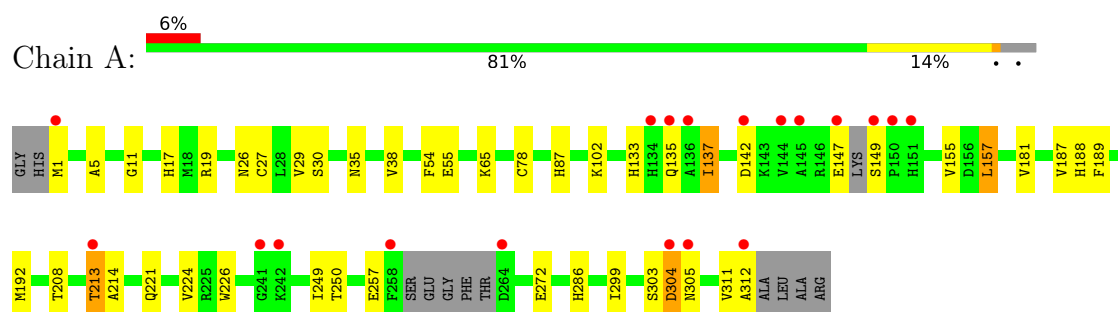
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	293	Total	O	0	0
			293	293		
3	B	267	Total	O	0	0
			267	267		
3	C	278	Total	O	0	0
			278	278		
3	D	179	Total	O	0	0
			179	179		

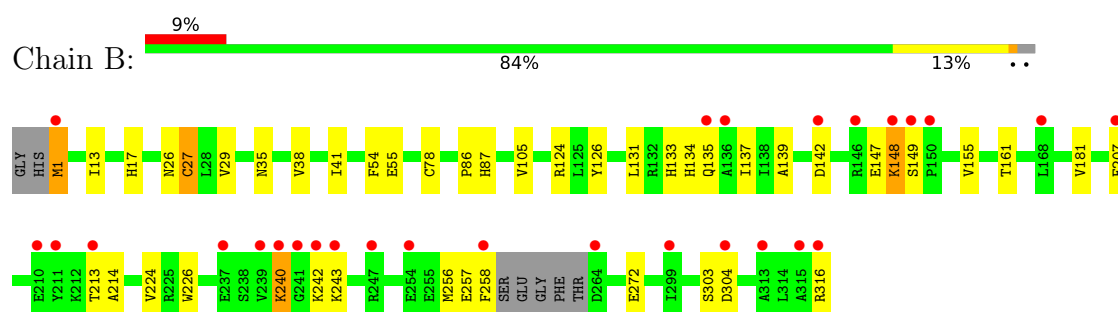
3 Residue-property plots [i](#)

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.

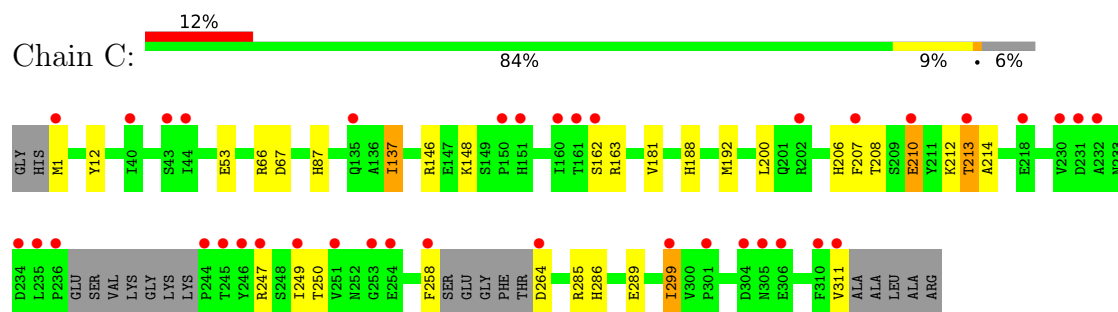
• Molecule 1: WbpB



• Molecule 1: WbpB

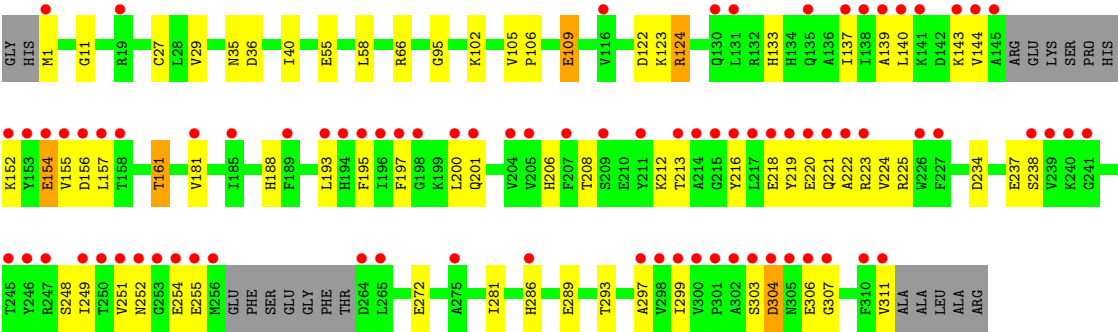


• Molecule 1: WbpB



• Molecule 1: WbpB





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.22Å 129.56Å 145.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 30.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.00-1.50) 93.5 (30.00-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.201 , 0.244 0.197 , 0.238	Depositor DCC
R_{free} test set	10383 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10958	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 11.81% 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

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	0.82	1/2518 (0.0%)	0.97	1/3412 (0.0%)
1	B	0.83	1/2550 (0.0%)	1.01	1/3456 (0.0%)
1	C	0.80	0/2502	0.92	2/3390 (0.1%)
1	D	0.71	1/2472 (0.0%)	0.88	2/3349 (0.1%)
All	All	0.79	3/10042 (0.0%)	0.95	6/13607 (0.0%)

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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	GLY	C-O	6.52	1.29	1.23
1	D	11	GLY	N-CA	5.16	1.49	1.44
1	B	105	VAL	CA-CB	5.16	1.60	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	181	VAL	N-CA-C	7.12	117.64	110.23
1	B	181	VAL	N-CA-C	6.86	117.36	110.23
1	A	181	VAL	N-CA-C	6.50	117.18	110.36
1	C	12	TYR	N-CA-C	5.23	116.66	111.07
1	D	281	ILE	N-CA-C	5.05	115.27	110.42
1	C	181	VAL	N-CA-C	5.04	115.27	110.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	303	SER	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	2453	0	2398	43	0
1	B	2484	0	2431	37	0
1	C	2427	0	2377	37	0
1	D	2401	0	2364	78	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	293	0	0	8	0
3	B	267	0	0	0	0
3	C	278	0	0	7	0
3	D	179	0	0	7	0
All	All	10958	0	9674	189	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 10.

All (189) 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:35:ASN:HB3	3:A:402:HOH:O	1.29	1.22
1:C:137:ILE:CD1	1:C:258:PHE:HE1	1.55	1.20
1:C:137:ILE:HD11	1:C:258:PHE:CE1	1.82	1.14
1:B:35:ASN:ND2	1:D:35[B]:ASN:OD1	1.81	1.13
1:D:124:ARG:HG3	1:D:124:ARG:HH21	1.10	1.11
1:C:137:ILE:HD11	1:C:258:PHE:HE1	1.01	1.10
1:D:216:TYR:CE2	1:D:218:GLU:CG	2.39	1.06
1:B:139:ALA:O	1:B:142:ASP:OD2	1.74	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:TYR:OH	1:D:223:ARG:HG3	1.59	1.02
1:C:53:GLU:OE2	3:C:752:HOH:O	1.77	0.99
1:D:216:TYR:CZ	1:D:218:GLU:HG2	1.98	0.97
1:A:213:THR:HG22	1:A:226:TRP:CH2	1.98	0.97
1:D:216:TYR:HE2	1:D:218:GLU:HG3	1.30	0.97
1:D:216:TYR:HH	1:D:223:ARG:HG3	1.32	0.94
1:D:216:TYR:CE2	1:D:218:GLU:HG3	2.03	0.93
1:D:216:TYR:CE2	1:D:218:GLU:HG2	2.01	0.93
1:D:208:THR:HG22	1:D:299:ILE:HD11	1.49	0.92
1:C:207:PHE:HA	1:C:299:ILE:CD1	1.99	0.92
1:A:213:THR:HG22	1:A:226:TRP:CZ3	2.05	0.91
1:A:213:THR:CG2	1:A:226:TRP:CH2	2.54	0.89
1:D:216:TYR:HE2	1:D:218:GLU:CG	1.81	0.89
1:C:163[B]:ARG:NH2	3:C:543:HOH:O	2.05	0.89
1:C:137:ILE:CD1	1:C:258:PHE:CE1	2.47	0.89
1:C:264:ASP:HB3	3:C:418:HOH:O	1.74	0.88
1:C:264:ASP:HB3	3:C:630:HOH:O	1.75	0.86
1:D:124:ARG:HH21	1:D:124:ARG:CG	1.88	0.86
1:B:213:THR:HG22	1:B:226:TRP:CH2	2.10	0.85
1:D:154:GLU:HB3	1:D:252:ASN:HA	1.56	0.85
1:D:154:GLU:HA	1:D:154:GLU:OE1	1.79	0.81
1:A:213:THR:HG21	1:A:226:TRP:HH2	1.45	0.80
1:D:216:TYR:OH	1:D:218:GLU:HG2	1.82	0.80
1:A:213:THR:CG2	1:A:226:TRP:HH2	1.92	0.79
1:D:124:ARG:HG3	1:D:124:ARG:NH2	1.92	0.77
1:C:207:PHE:HA	1:C:299:ILE:HD13	1.66	0.76
1:D:140:LEU:HD12	1:D:140:LEU:O	1.86	0.75
1:D:66:ARG:HD2	3:D:864:HOH:O	1.86	0.74
1:A:147:GLU:O	1:A:149:SER:N	2.21	0.74
1:A:65:LYS:HE2	3:A:977:HOH:O	1.87	0.74
1:C:208:THR:HA	1:C:213:THR:HG23	1.70	0.73
1:A:303:SER:O	1:A:305:ASN:N	2.23	0.72
1:B:124:ARG:HD3	1:B:126:TYR:OH	1.89	0.72
1:A:147:GLU:C	1:A:149:SER:N	2.48	0.72
1:D:140:LEU:HD12	1:D:144:VAL:HG23	1.70	0.72
1:B:242:LYS:HB3	1:B:242:LYS:HZ3	1.54	0.72
1:D:156:ASP:OD2	1:D:225:ARG:NH1	2.22	0.71
1:D:216:TYR:OH	1:D:223:ARG:CG	2.36	0.71
1:A:213:THR:CG2	1:A:214:ALA:N	2.54	0.70
1:C:137:ILE:HD12	1:C:258:PHE:HE1	1.52	0.69
1:D:155:VAL:HB	1:D:224:VAL:HG22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:GLY:O	1:D:123:LYS:HE3	1.96	0.66
1:D:154:GLU:HB2	1:D:252:ASN:OD1	1.95	0.66
1:A:1:MET:CE	3:A:573:HOH:O	2.42	0.66
1:B:27[B]:CYS:SG	1:B:29:VAL:HG12	2.37	0.65
1:B:213:THR:CG2	1:B:226:TRP:CH2	2.80	0.65
1:B:124:ARG:HD3	1:B:126:TYR:CZ	2.31	0.65
1:C:206:HIS:C	1:C:299:ILE:HD13	2.22	0.65
1:A:213:THR:HG22	1:A:214:ALA:N	2.12	0.65
1:B:213:THR:CG2	1:B:226:TRP:HH2	2.09	0.65
1:A:286:HIS:CD2	3:A:358:HOH:O	2.49	0.64
1:D:201:GLN:NE2	1:D:220:GLU:HA	2.12	0.64
1:D:139:ALA:O	1:D:143:LYS:HB2	1.97	0.64
1:A:1:MET:HE1	3:A:573:HOH:O	1.98	0.64
1:D:216:TYR:CZ	1:D:223:ARG:HG3	2.33	0.64
1:B:139:ALA:C	1:B:142:ASP:OD2	2.42	0.63
1:C:207:PHE:HA	1:C:299:ILE:HD11	1.80	0.63
1:D:286:HIS:NE2	3:D:340:HOH:O	2.31	0.63
1:D:140:LEU:CD1	1:D:144:VAL:HG23	2.31	0.61
1:D:40:ILE:HD12	3:D:855:HOH:O	2.01	0.61
1:C:207:PHE:CA	1:C:299:ILE:CD1	2.76	0.60
1:D:124:ARG:CG	1:D:124:ARG:NH2	2.56	0.60
1:B:1:MET:HE3	1:B:26:ASN:OD1	2.01	0.60
1:B:27[B]:CYS:SG	1:B:29:VAL:CG1	2.90	0.60
1:C:207:PHE:CA	1:C:299:ILE:HD13	2.31	0.60
1:A:192:MET:HE1	1:A:249:ILE:HD13	1.86	0.58
1:A:55:GLU:HG2	1:B:87:HIS:CD2	2.38	0.57
1:C:206:HIS:O	1:C:299:ILE:HD13	2.05	0.57
1:D:216:TYR:HH	1:D:218:GLU:HG2	1.69	0.57
1:D:133:HIS:CE1	1:D:272:GLU:HG3	2.40	0.57
1:D:311:VAL:HG12	1:D:311:VAL:O	2.05	0.56
1:C:67:ASP:HB2	3:C:491:HOH:O	2.04	0.56
1:A:221:GLN:NE2	3:A:492:HOH:O	2.34	0.56
1:B:147:GLU:O	1:B:148:LYS:C	2.50	0.54
1:C:208:THR:CA	1:C:213:THR:HG23	2.38	0.54
1:D:286:HIS:CD2	3:D:340:HOH:O	2.60	0.54
1:C:210:GLU:N	1:C:210:GLU:OE2	2.40	0.54
1:C:188:HIS:H	1:C:188:HIS:CD2	2.26	0.53
1:D:212:LYS:HE2	1:D:234:ASP:OD2	2.07	0.53
1:C:192:MET:HE1	1:C:249:ILE:HD13	1.89	0.53
1:D:154:GLU:HB3	1:D:252:ASN:CA	2.33	0.53
1:C:208:THR:CB	1:C:213:THR:HG23	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:TYR:OH	1:D:218:GLU:CG	2.54	0.53
1:C:137:ILE:HD12	1:C:258:PHE:CE1	2.34	0.52
1:A:1:MET:HE2	3:A:573:HOH:O	2.07	0.52
1:B:207:PHE:O	1:B:213:THR:HG23	2.10	0.52
1:D:195:PHE:HE2	3:D:648:HOH:O	1.91	0.52
1:A:55:GLU:HB3	1:B:86:PRO:HB2	1.92	0.51
1:B:213:THR:HG22	1:B:214:ALA:N	2.25	0.51
1:B:131:LEU:HB3	1:B:137:ILE:CD1	2.41	0.51
1:D:201:GLN:HE21	1:D:220:GLU:HA	1.76	0.50
1:D:303:SER:O	1:D:304:ASP:HB2	2.11	0.50
1:D:35[B]:ASN:HD22	1:D:36:ASP:N	2.10	0.50
1:A:87:HIS:CD2	1:B:55:GLU:HG2	2.46	0.49
1:B:242:LYS:HB3	1:B:242:LYS:NZ	2.21	0.49
1:A:188:HIS:H	1:A:188:HIS:CD2	2.29	0.49
1:D:161:THR:O	1:D:161:THR:CG2	2.60	0.49
1:A:213:THR:CG2	1:A:226:TRP:CZ3	2.86	0.49
1:D:27[B]:CYS:SG	1:D:29:VAL:HG12	2.52	0.49
1:D:216:TYR:CZ	1:D:218:GLU:CG	2.75	0.49
1:A:102:LYS:HD3	1:A:187:VAL:CG1	2.43	0.49
1:D:140:LEU:O	1:D:144:VAL:HG23	2.14	0.48
1:D:154:GLU:CB	1:D:252:ASN:HA	2.35	0.48
1:D:216:TYR:CE1	1:D:223:ARG:HG3	2.47	0.48
1:D:237:GLU:HA	1:D:237:GLU:OE1	2.12	0.48
1:D:311:VAL:O	1:D:311:VAL:CG1	2.61	0.48
1:B:147:GLU:O	1:B:149:SER:N	2.47	0.48
1:A:311:VAL:O	1:A:312:ALA:C	2.55	0.48
1:D:154:GLU:OE1	1:D:154:GLU:CA	2.48	0.47
1:D:216:TYR:OH	1:D:223:ARG:CD	2.62	0.47
1:C:207:PHE:CA	1:C:299:ILE:HD11	2.42	0.47
1:B:139:ALA:HA	1:B:142:ASP:OD2	2.15	0.47
1:C:250:THR:HG21	3:C:530:HOH:O	2.15	0.47
1:A:54:PHE:HD1	1:B:54:PHE:HD1	1.62	0.47
1:B:124:ARG:HG3	1:B:126:TYR:CE2	2.50	0.47
1:D:201:GLN:NE2	1:D:219:TYR:O	2.48	0.47
1:A:1:MET:HG3	3:A:683:HOH:O	2.15	0.47
1:A:17:HIS:CD2	1:A:78[B]:CYS:SG	3.09	0.46
1:B:213:THR:CG2	1:B:214:ALA:N	2.78	0.46
1:C:207:PHE:O	1:C:213:THR:HG22	2.16	0.46
1:D:221:GLN:HE21	1:D:221:GLN:HA	1.80	0.46
1:A:303:SER:O	1:A:304:ASP:C	2.59	0.46
1:A:213:THR:HG21	1:A:226:TRP:CH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:SER:C	1:C:163[B]:ARG:HG3	2.40	0.46
1:A:157:LEU:HD21	1:A:189:PHE:HB3	1.98	0.46
1:C:87:HIS:CD2	1:D:55:GLU:HG2	2.51	0.46
1:D:206:HIS:CD2	1:D:307:GLY:HA2	2.51	0.46
1:D:293:THR:O	1:D:297:ALA:HB2	2.16	0.46
1:B:161:THR:O	1:B:161:THR:HG23	2.16	0.45
1:D:102:LYS:O	1:D:102:LYS:HD2	2.16	0.45
1:B:240:LYS:C	1:B:242:LYS:H	2.24	0.45
1:C:214:ALA:HB3	1:C:311:VAL:HG21	1.99	0.45
1:D:155:VAL:O	1:D:224:VAL:HA	2.17	0.45
1:C:208:THR:N	1:C:299:ILE:HD11	2.31	0.44
1:A:133:HIS:CE1	1:A:272:GLU:HG3	2.52	0.44
1:C:285:ARG:O	1:C:289:GLU:HG3	2.17	0.44
1:B:213:THR:HG22	1:B:226:TRP:CZ3	2.49	0.44
1:B:213:THR:HG21	1:B:226:TRP:HH2	1.79	0.44
1:D:197:PHE:CD1	1:D:222:ALA:HB2	2.53	0.44
1:B:13:ILE:HD12	1:B:13:ILE:HA	1.89	0.43
1:D:40:ILE:HD11	3:D:848:HOH:O	2.18	0.43
1:D:216:TYR:OH	1:D:218:GLU:CD	2.60	0.43
1:D:193:LEU:CD1	1:D:224:VAL:HG11	2.48	0.43
1:D:152:LYS:HE2	1:D:219:TYR:O	2.18	0.43
1:C:207:PHE:CE1	1:C:212:LYS:HG3	2.53	0.43
1:D:200:LEU:HB2	1:D:286:HIS:HE1	1.83	0.43
1:D:105:VAL:HB	1:D:106:PRO:HD2	2.01	0.43
1:D:303:SER:O	1:D:306:GLU:HG3	2.19	0.43
1:D:248:SER:HA	1:D:255:GLU:OE2	2.18	0.43
1:A:137:ILE:HG12	1:A:192:MET:HG3	2.00	0.43
1:A:155:VAL:HA	1:A:250:THR:O	2.19	0.43
1:B:133:HIS:CE1	1:B:272:GLU:HG3	2.54	0.43
1:A:157:LEU:C	1:A:157:LEU:CD1	2.92	0.42
1:C:200:LEU:HB2	1:C:286[A]:HIS:CE1	2.55	0.42
1:D:193:LEU:HD13	1:D:224:VAL:HG11	2.00	0.42
1:A:38:VAL:HG22	1:A:38:VAL:O	2.20	0.42
1:A:213:THR:HG23	1:A:214:ALA:N	2.34	0.42
1:A:155:VAL:HB	1:A:224:VAL:HG22	2.02	0.42
1:D:197:PHE:O	1:D:219:TYR:HB3	2.19	0.42
1:A:208:THR:HG22	1:A:299:ILE:HD11	2.01	0.42
1:A:1:MET:HE3	1:A:26:ASN:OD1	2.20	0.41
1:A:27[B]:CYS:SG	1:A:29:VAL:CG1	3.08	0.41
1:B:134:HIS:CE1	1:B:258:PHE:HB2	2.55	0.41
1:A:5:ALA:HA	1:A:30:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:HIS:H	1:A:188:HIS:HD2	1.67	0.41
1:B:1:MET:HE3	1:B:1:MET:HB3	1.73	0.41
1:B:38:VAL:O	1:B:41:ILE:HG22	2.20	0.41
1:D:109:GLU:OE1	1:D:109:GLU:CA	2.68	0.41
1:C:207:PHE:HE1	1:C:212:LYS:HG3	1.86	0.41
1:D:95:GLY:C	1:D:123:LYS:HE3	2.44	0.41
1:D:188:HIS:CE1	3:D:376:HOH:O	2.74	0.41
1:B:155:VAL:HB	1:B:224:VAL:HG22	2.03	0.41
1:D:156:ASP:CG	1:D:225:ARG:HH11	2.22	0.41
1:B:17:HIS:CD2	1:B:78[A]:CYS:SG	3.14	0.40
1:D:27[B]:CYS:SG	1:D:29:VAL:CG1	3.09	0.40
1:B:135:GLN:HE21	1:B:135:GLN:HB3	1.73	0.40
1:C:66:ARG:HD2	3:C:881:HOH:O	2.21	0.40
1:C:207:PHE:HE1	1:C:212:LYS:CG	2.34	0.40
1:D:201:GLN:HE21	1:D:220:GLU:CA	2.34	0.40
1:D:35[B]:ASN:HD22	1:D:36:ASP:H	1.68	0.40
1:D:102:LYS:HD2	1:D:102:LYS:C	2.46	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	302/318 (95%)	295 (98%)	6 (2%)	1 (0%)	36	17
1	B	309/318 (97%)	299 (97%)	9 (3%)	1 (0%)	36	17
1	C	298/318 (94%)	294 (99%)	4 (1%)	0	100	100
1	D	297/318 (93%)	286 (96%)	11 (4%)	0	100	100
All	All	1206/1272 (95%)	1174 (97%)	30 (2%)	2 (0%)	43	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	ASP
1	B	148	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	266/272 (98%)	259 (97%)	7 (3%)	40	13
1	B	267/272 (98%)	258 (97%)	9 (3%)	32	7
1	C	264/272 (97%)	256 (97%)	8 (3%)	36	9
1	D	262/272 (96%)	246 (94%)	16 (6%)	17	1
All	All	1059/1088 (97%)	1019 (96%)	40 (4%)	30	6

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	135	GLN
1	A	137	ILE
1	A	142	ASP
1	A	157	LEU
1	A	213	THR
1	A	257	GLU
1	B	1	MET
1	B	27[A]	CYS
1	B	27[B]	CYS
1	B	240	LYS
1	B	243	LYS
1	B	256	MET
1	B	257	GLU
1	B	304	ASP
1	B	316	ARG
1	C	1	MET
1	C	137	ILE
1	C	146	ARG
1	C	148	LYS

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Mol	Chain	Res	Type
1	C	210	GLU
1	C	213	THR
1	C	247	ARG
1	C	299	ILE
1	D	1	MET
1	D	58	LEU
1	D	109	GLU
1	D	122	ASP
1	D	124	ARG
1	D	137	ILE
1	D	154	GLU
1	D	157	LEU
1	D	161	THR
1	D	213	THR
1	D	238	SER
1	D	249	ILE
1	D	251	VAL
1	D	254	GLU
1	D	289	GLU
1	D	304	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	165	ASN
1	A	188	HIS
1	A	221	GLN
1	A	286	HIS
1	B	127	ASN
1	B	135	GLN
1	B	188	HIS
1	B	221	GLN
1	C	127	ASN
1	C	188	HIS
1	D	127	ASN
1	D	201	GLN
1	D	206	HIS
1	D	221	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 ⓘ

4 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	317	-	46,48,48	1.56	5 (10%)	64,73,73	1.86	21 (32%)
2	NAD	D	317	-	46,48,48	1.06	2 (4%)	64,73,73	1.52	12 (18%)
2	NAD	B	317	-	46,48,48	0.99	1 (2%)	64,73,73	1.79	15 (23%)
2	NAD	C	317	-	46,48,48	1.33	6 (13%)	64,73,73	1.76	18 (28%)

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	317	-	-	7/30/62/62	0/5/5/5
2	NAD	D	317	-	-	8/30/62/62	0/5/5/5
2	NAD	B	317	-	-	6/30/62/62	0/5/5/5
2	NAD	C	317	-	-	6/30/62/62	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317	NAD	PA-O3	-5.25	1.53	1.59
2	A	317	NAD	PN-O3	4.95	1.64	1.59
2	C	317	NAD	PN-O3	3.96	1.63	1.59
2	A	317	NAD	O4D-C1D	3.50	1.45	1.40
2	D	317	NAD	PN-O3	3.47	1.63	1.59
2	C	317	NAD	O4D-C1D	2.90	1.44	1.40
2	C	317	NAD	PA-O3	2.87	1.62	1.59
2	B	317	NAD	O4D-C1D	2.72	1.44	1.40
2	D	317	NAD	O4D-C1D	2.66	1.44	1.40
2	A	317	NAD	C7N-N7N	2.43	1.37	1.33
2	A	317	NAD	O4B-C1B	2.22	1.47	1.42
2	C	317	NAD	C3N-C7N	-2.21	1.47	1.50
2	C	317	NAD	O4B-C1B	2.10	1.46	1.42
2	C	317	NAD	C7N-N7N	2.09	1.36	1.33

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	NAD	N3A-C2A-N1A	-4.55	121.70	128.58
2	B	317	NAD	N9A-C8A-N7A	-4.47	107.59	113.94
2	B	317	NAD	C4A-N9A-C8A	4.38	110.34	105.74
2	B	317	NAD	C5A-N7A-C8A	4.25	110.14	103.45
2	D	317	NAD	N3A-C2A-N1A	-4.14	122.31	128.58
2	A	317	NAD	C5A-N7A-C8A	4.10	109.89	103.45
2	A	317	NAD	C4A-C5A-N7A	-4.06	105.94	110.58
2	A	317	NAD	C3N-C7N-N7N	3.93	122.58	117.74
2	A	317	NAD	N9A-C8A-N7A	-3.83	108.50	113.94
2	C	317	NAD	N9A-C8A-N7A	-3.76	108.60	113.94
2	A	317	NAD	C6N-N1N-C2N	3.73	125.05	121.88
2	D	317	NAD	C4D-O4D-C1D	3.66	113.28	109.92
2	B	317	NAD	C4A-N9A-C1B	-3.64	118.11	126.63
2	C	317	NAD	C4A-N9A-C8A	3.56	109.48	105.74
2	C	317	NAD	C5A-N7A-C8A	3.51	108.96	103.45
2	B	317	NAD	C4A-C5A-N7A	-3.34	106.76	110.58
2	A	317	NAD	O2N-PN-O3	3.31	116.22	107.27
2	C	317	NAD	C5N-C4N-C3N	-3.28	117.14	120.36
2	B	317	NAD	C5B-C4B-C3B	-3.18	103.76	115.21
2	C	317	NAD	C5A-C4A-N3A	-3.18	122.34	126.72
2	B	317	NAD	O4B-C1B-C2B	-3.17	99.84	106.62
2	C	317	NAD	C4A-N9A-C1B	-3.09	119.41	126.63
2	C	317	NAD	O3-PA-O1A	-3.08	101.44	110.70
2	D	317	NAD	O2N-PN-O3	3.05	115.51	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	317	NAD	C4A-C5A-N7A	-2.99	107.17	110.58
2	B	317	NAD	C6N-N1N-C2N	2.99	124.42	121.88
2	B	317	NAD	C2A-N1A-C6A	2.98	123.62	118.73
2	D	317	NAD	C2A-N1A-C6A	2.91	123.51	118.73
2	A	317	NAD	C5B-C4B-C3B	-2.88	104.84	115.21
2	B	317	NAD	N6A-C6A-N1A	2.85	124.72	118.38
2	B	317	NAD	N3A-C2A-N1A	-2.83	124.29	128.58
2	D	317	NAD	O4B-C1B-C2B	-2.79	100.65	106.62
2	C	317	NAD	N3A-C4A-N9A	2.76	131.86	127.17
2	C	317	NAD	N3A-C2A-N1A	-2.69	124.51	128.58
2	A	317	NAD	C5A-C4A-N3A	-2.69	123.02	126.72
2	C	317	NAD	O4D-C4D-C5D	-2.66	100.82	109.33
2	A	317	NAD	C2A-N1A-C6A	2.65	123.09	118.73
2	C	317	NAD	C2N-C3N-C4N	2.61	121.30	118.26
2	C	317	NAD	O4B-C1B-C2B	-2.61	101.04	106.62
2	B	317	NAD	O2A-PA-O3	2.50	114.02	107.27
2	D	317	NAD	O3-PN-O1N	-2.49	103.21	110.70
2	D	317	NAD	O5D-PN-O1N	-2.45	99.22	108.94
2	B	317	NAD	O2N-PN-O3	2.44	113.86	107.27
2	A	317	NAD	O4B-C1B-C2B	-2.42	101.44	106.62
2	A	317	NAD	O3-PN-O1N	-2.39	103.52	110.70
2	D	317	NAD	O4D-C4D-C5D	-2.37	101.73	109.33
2	A	317	NAD	C5A-C4A-N9A	2.37	108.39	105.81
2	A	317	NAD	O3-PA-O1A	-2.34	103.66	110.70
2	D	317	NAD	C5B-C4B-C3B	-2.34	106.79	115.21
2	C	317	NAD	O3B-C3B-C2B	2.34	119.31	111.82
2	A	317	NAD	C6A-C5A-N7A	2.28	136.49	132.09
2	C	317	NAD	O2N-PN-O3	2.28	113.44	107.27
2	D	317	NAD	N9A-C8A-N7A	-2.26	110.72	113.94
2	A	317	NAD	C4B-O4B-C1B	-2.26	104.47	109.47
2	A	317	NAD	O5D-PN-O1N	-2.26	99.98	108.94
2	A	317	NAD	O5D-C5D-C4D	2.21	116.53	108.99
2	A	317	NAD	C2A-N3A-C4A	2.20	117.20	111.83
2	A	317	NAD	O4D-C4D-C5D	-2.18	102.36	109.33
2	C	317	NAD	C4B-O4B-C1B	-2.18	104.66	109.47
2	C	317	NAD	C2A-N3A-C4A	2.16	117.11	111.83
2	A	317	NAD	O7N-C7N-N7N	-2.16	119.50	122.62
2	B	317	NAD	O5D-PN-O1N	-2.13	100.48	108.94
2	C	317	NAD	O7N-C7N-C3N	-2.12	117.00	119.60
2	D	317	NAD	C4A-N9A-C1B	-2.06	121.82	126.63
2	B	317	NAD	O7N-C7N-N7N	-2.02	119.70	122.62
2	D	317	NAD	C4A-N9A-C8A	2.01	107.85	105.74

There are no chirality outliers.

All (27) torsion outliers are listed below:

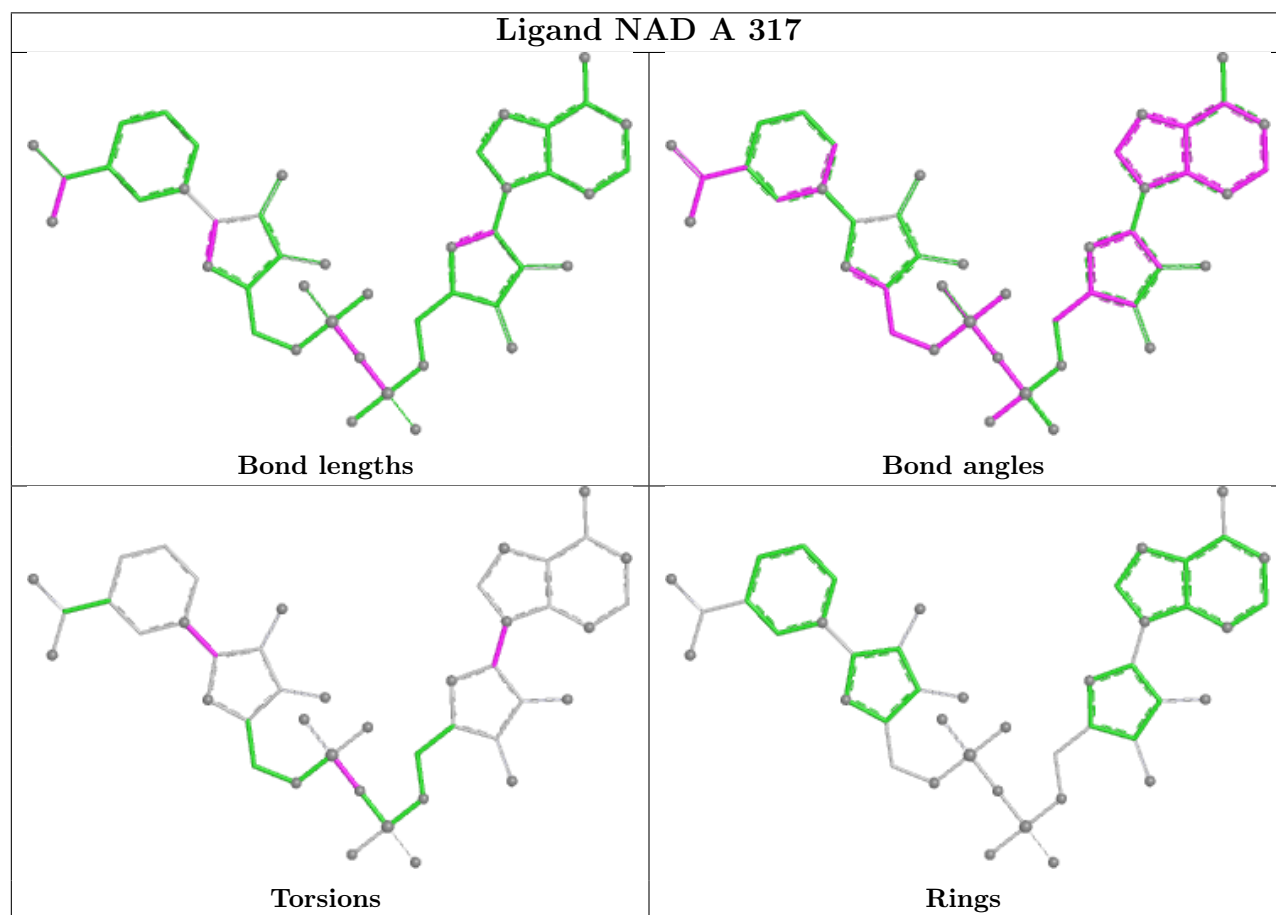
Mol	Chain	Res	Type	Atoms
2	A	317	NAD	O4D-C1D-N1N-C2N
2	A	317	NAD	O4D-C1D-N1N-C6N
2	A	317	NAD	C2D-C1D-N1N-C2N
2	B	317	NAD	O4D-C1D-N1N-C2N
2	B	317	NAD	O4D-C1D-N1N-C6N
2	B	317	NAD	C2D-C1D-N1N-C2N
2	C	317	NAD	O4D-C1D-N1N-C2N
2	C	317	NAD	O4D-C1D-N1N-C6N
2	C	317	NAD	C2D-C1D-N1N-C2N
2	D	317	NAD	O4D-C1D-N1N-C2N
2	D	317	NAD	O4D-C1D-N1N-C6N
2	D	317	NAD	C2D-C1D-N1N-C2N
2	D	317	NAD	C2D-C1D-N1N-C6N
2	A	317	NAD	C2B-C1B-N9A-C8A
2	C	317	NAD	C2B-C1B-N9A-C8A
2	D	317	NAD	C2B-C1B-N9A-C8A
2	B	317	NAD	C2B-C1B-N9A-C8A
2	A	317	NAD	PA-O3-PN-O2N
2	B	317	NAD	PA-O3-PN-O1N
2	B	317	NAD	PA-O3-PN-O2N
2	C	317	NAD	PA-O3-PN-O2N
2	D	317	NAD	PA-O3-PN-O2N
2	A	317	NAD	C2B-C1B-N9A-C4A
2	A	317	NAD	PA-O3-PN-O1N
2	C	317	NAD	PA-O3-PN-O1N
2	D	317	NAD	PA-O3-PN-O1N
2	D	317	NAD	O4B-C4B-C5B-O5B

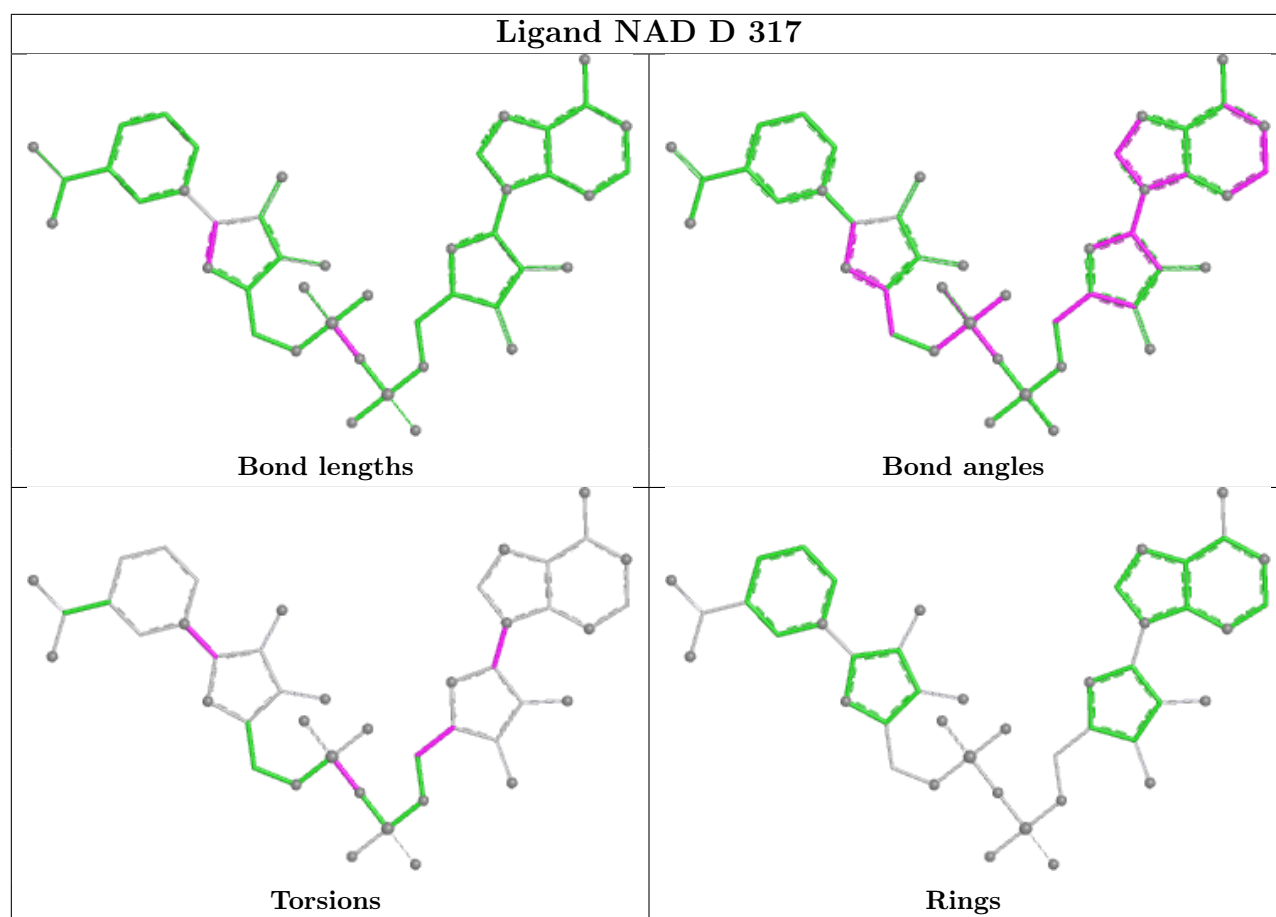
There are no ring outliers.

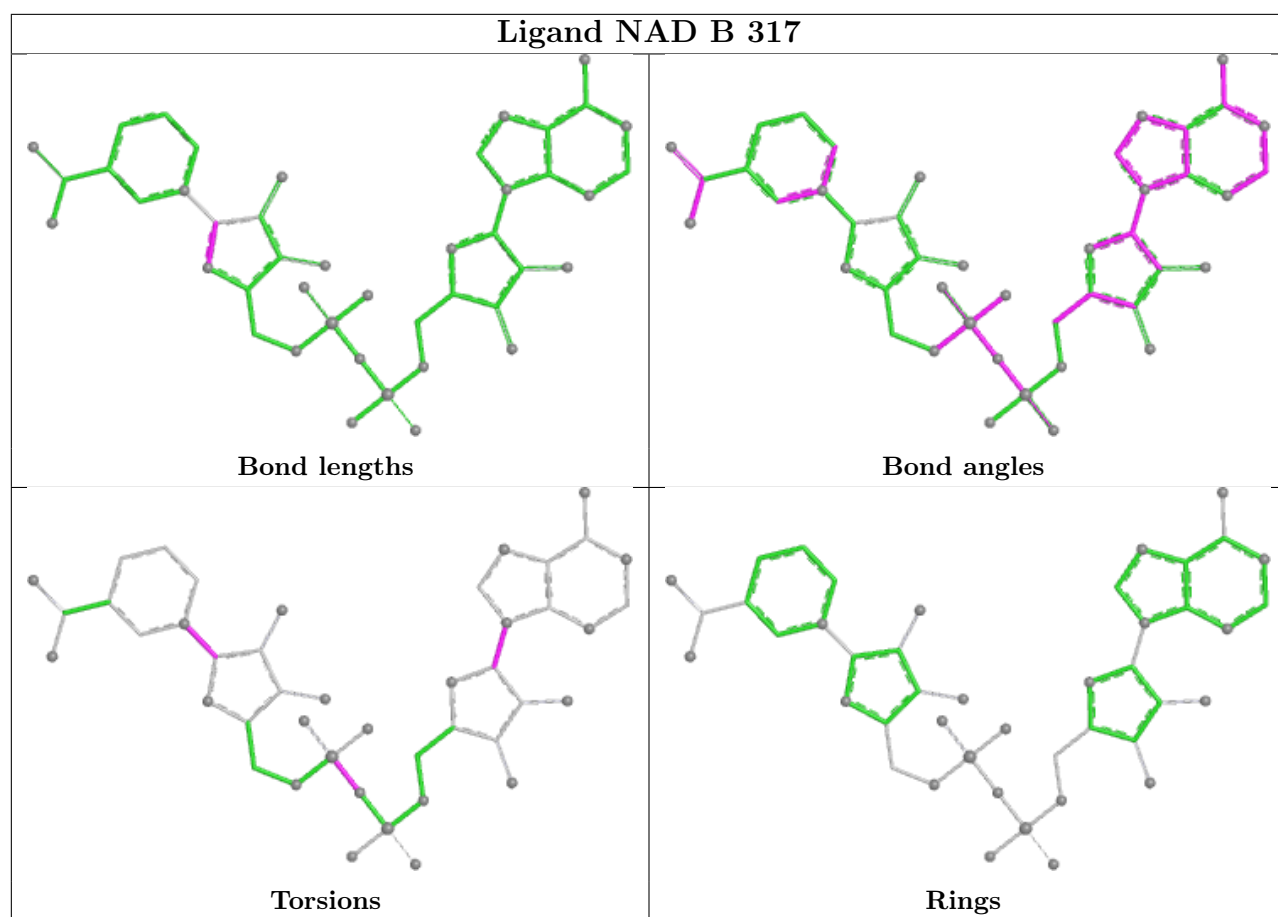
No monomer is involved in short contacts.

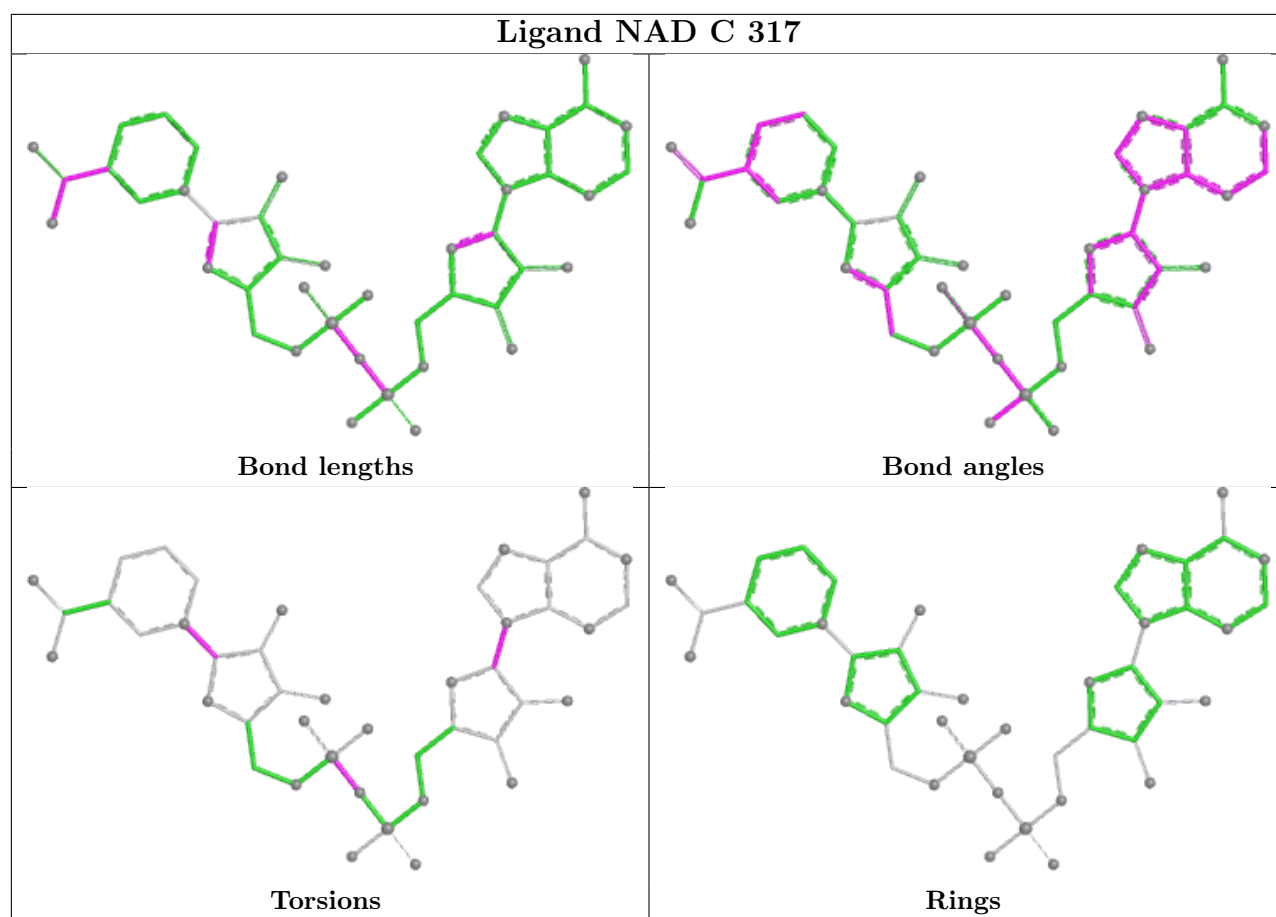
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	306/318 (96%)	0.22	19 (6%) 26 29	8, 19, 38, 53	2 (0%)
1	B	311/318 (97%)	0.42	28 (9%) 15 16	9, 20, 63, 156	2 (0%)
1	C	299/318 (94%)	0.51	38 (12%) 8 8	8, 20, 70, 130	5 (1%)
1	D	298/318 (93%)	1.27	82 (27%) 1 1	9, 28, 105, 160	5 (1%)
All	All	1214/1272 (95%)	0.60	167 (13%) 6 7	8, 21, 74, 160	14 (1%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	196	ILE	8.5
1	D	137	ILE	8.2
1	C	311	VAL	8.2
1	D	302	ALA	7.8
1	D	138	ILE	7.4
1	D	213	THR	7.4
1	D	145	ALA	7.1
1	B	213	THR	7.1
1	B	239	VAL	6.5
1	D	222	ALA	6.3
1	C	162	SER	6.3
1	D	139	ALA	6.2
1	D	157	LEU	6.0
1	D	311	VAL	5.8
1	D	153	TYR	5.7
1	C	161	THR	5.7
1	A	258	PHE	5.6
1	D	216	TYR	5.6
1	D	253	GLY	5.5
1	C	258	PHE	5.3
1	D	144	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	241	GLY	5.2
1	D	155	VAL	4.9
1	D	249	ILE	4.9
1	D	298	VAL	4.9
1	B	299	ILE	4.8
1	D	300	VAL	4.7
1	D	131	LEU	4.6
1	D	1	MET	4.6
1	D	197	PHE	4.5
1	B	150	PRO	4.5
1	C	244	PRO	4.5
1	A	312	ALA	4.2
1	D	219	TYR	4.1
1	D	135	GLN	4.1
1	D	305	ASN	4.1
1	D	254	GLU	4.0
1	B	142	ASP	4.0
1	D	223	ARG	4.0
1	A	150	PRO	4.0
1	D	306	GLU	3.9
1	D	198	GLY	3.9
1	B	315	ALA	3.8
1	D	141	LYS	3.7
1	D	189	PHE	3.7
1	D	264	ASP	3.7
1	D	251	VAL	3.7
1	D	143	LYS	3.7
1	C	305	ASN	3.6
1	B	211	TYR	3.6
1	D	301	PRO	3.6
1	B	258	PHE	3.6
1	D	239	VAL	3.5
1	D	250	THR	3.5
1	D	19[A]	ARG	3.5
1	B	1	MET	3.5
1	B	316	ARG	3.4
1	A	135	GLN	3.4
1	D	217	LEU	3.4
1	D	154	GLU	3.4
1	D	140	LEU	3.4
1	C	264	ASP	3.4
1	B	210	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	264	ASP	3.3
1	D	286	HIS	3.3
1	C	1	MET	3.2
1	B	240	LYS	3.2
1	B	148	LYS	3.1
1	C	232	ALA	3.1
1	C	207	PHE	3.1
1	D	195	PHE	3.1
1	C	310	PHE	3.1
1	C	299	ILE	3.1
1	C	210	GLU	3.0
1	B	242	LYS	3.0
1	D	193	LEU	3.0
1	B	304	ASP	3.0
1	A	147	GLU	3.0
1	D	303	SER	3.0
1	A	213	THR	3.0
1	D	205	VAL	3.0
1	C	151	HIS	3.0
1	D	304	ASP	3.0
1	D	310	PHE	3.0
1	D	297	ALA	2.9
1	D	185	ILE	2.9
1	D	221	GLN	2.9
1	A	304	ASP	2.9
1	C	218	GLU	2.9
1	A	305	ASN	2.9
1	C	150	PRO	2.9
1	D	201	GLN	2.9
1	D	247	ARG	2.9
1	C	213	THR	2.9
1	D	256	MET	2.9
1	D	215	GLY	2.9
1	D	209	SER	2.9
1	A	145	ALA	2.8
1	A	1	MET	2.8
1	D	252	ASN	2.8
1	B	247	ARG	2.8
1	D	218	GLU	2.8
1	D	181	VAL	2.7
1	A	149	SER	2.7
1	D	238	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	144	VAL	2.7
1	A	134	HIS	2.7
1	A	142	ASP	2.7
1	B	264	ASP	2.7
1	D	204	VAL	2.7
1	D	130	GLN	2.7
1	D	200	LEU	2.6
1	D	116	VAL	2.6
1	B	313	ALA	2.6
1	B	135	GLN	2.6
1	C	304	ASP	2.6
1	C	202	ARG	2.5
1	C	254	GLU	2.5
1	A	242	LYS	2.5
1	B	146	ARG	2.5
1	D	255	GLU	2.4
1	C	40	ILE	2.4
1	D	299	ILE	2.4
1	D	211	TYR	2.4
1	D	265	LEU	2.4
1	D	275	ALA	2.4
1	D	241	GLY	2.4
1	C	301	PRO	2.4
1	B	149	SER	2.4
1	C	135	GLN	2.4
1	A	241	GLY	2.4
1	D	307	GLY	2.4
1	C	306	GLU	2.4
1	C	249	ILE	2.4
1	C	245	THR	2.4
1	D	158	THR	2.4
1	B	207	PHE	2.4
1	C	231	ASP	2.3
1	D	156	ASP	2.3
1	C	236	PRO	2.3
1	D	152	LYS	2.3
1	B	243	LYS	2.3
1	D	194	HIS	2.3
1	C	247	ARG	2.2
1	D	220	GLU	2.2
1	B	136	ALA	2.2
1	D	227	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	246	TYR	2.2
1	A	151	HIS	2.2
1	A	136	ALA	2.1
1	C	160	ILE	2.1
1	B	237	GLU	2.1
1	C	230	VAL	2.1
1	C	43	SER	2.1
1	B	168	LEU	2.1
1	C	235	LEU	2.1
1	D	240	LYS	2.1
1	D	207	PHE	2.1
1	C	44	ILE	2.1
1	D	226	TRP	2.1
1	D	245	THR	2.0
1	D	214	ALA	2.0
1	C	234	ASP	2.0
1	C	253	GLY	2.0
1	B	254	GLU	2.0
1	C	251	VAL	2.0
1	C	246	TYR	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.

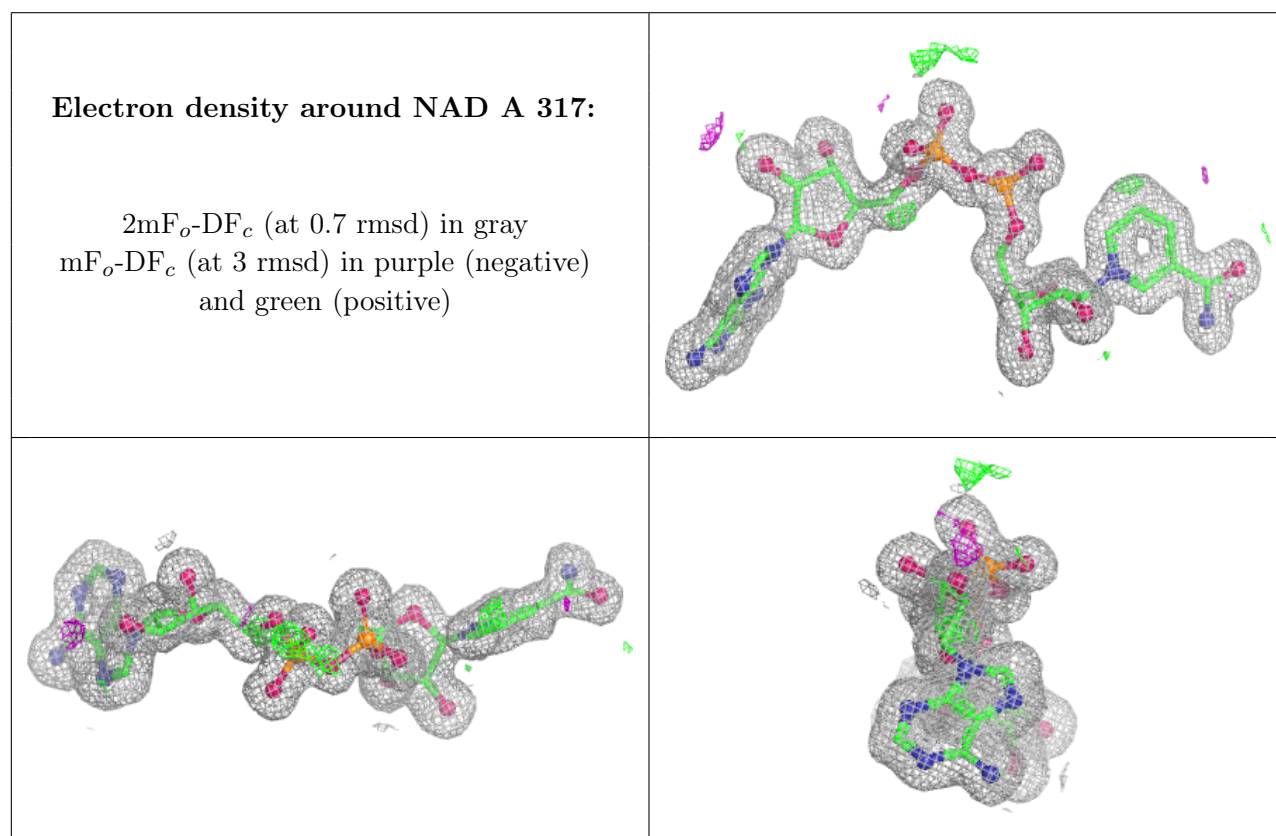
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	A	317	44/44	0.98	0.05	7,12,22,27	0
2	NAD	B	317	44/44	0.98	0.05	7,11,16,22	0
2	NAD	C	317	44/44	0.98	0.04	9,12,18,20	0

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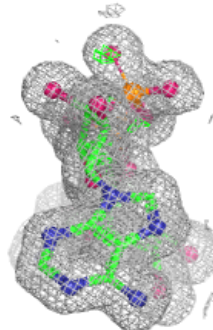
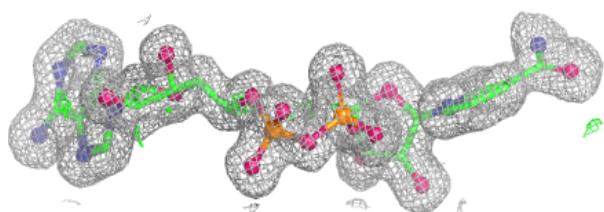
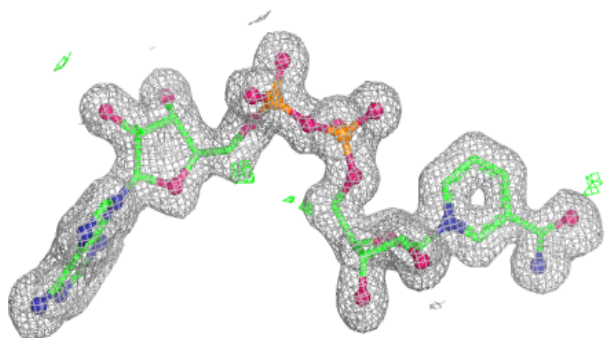
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	D	317	44/44	0.99	0.04	9,13,26,39	0

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.

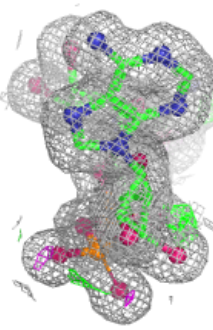
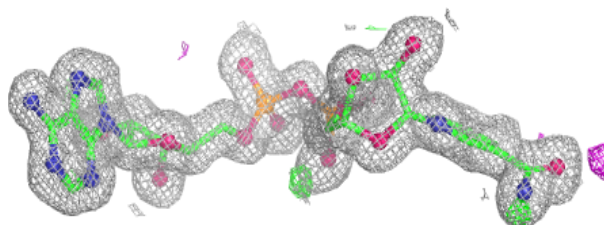
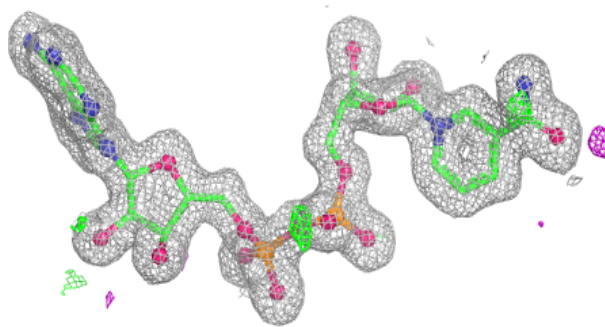


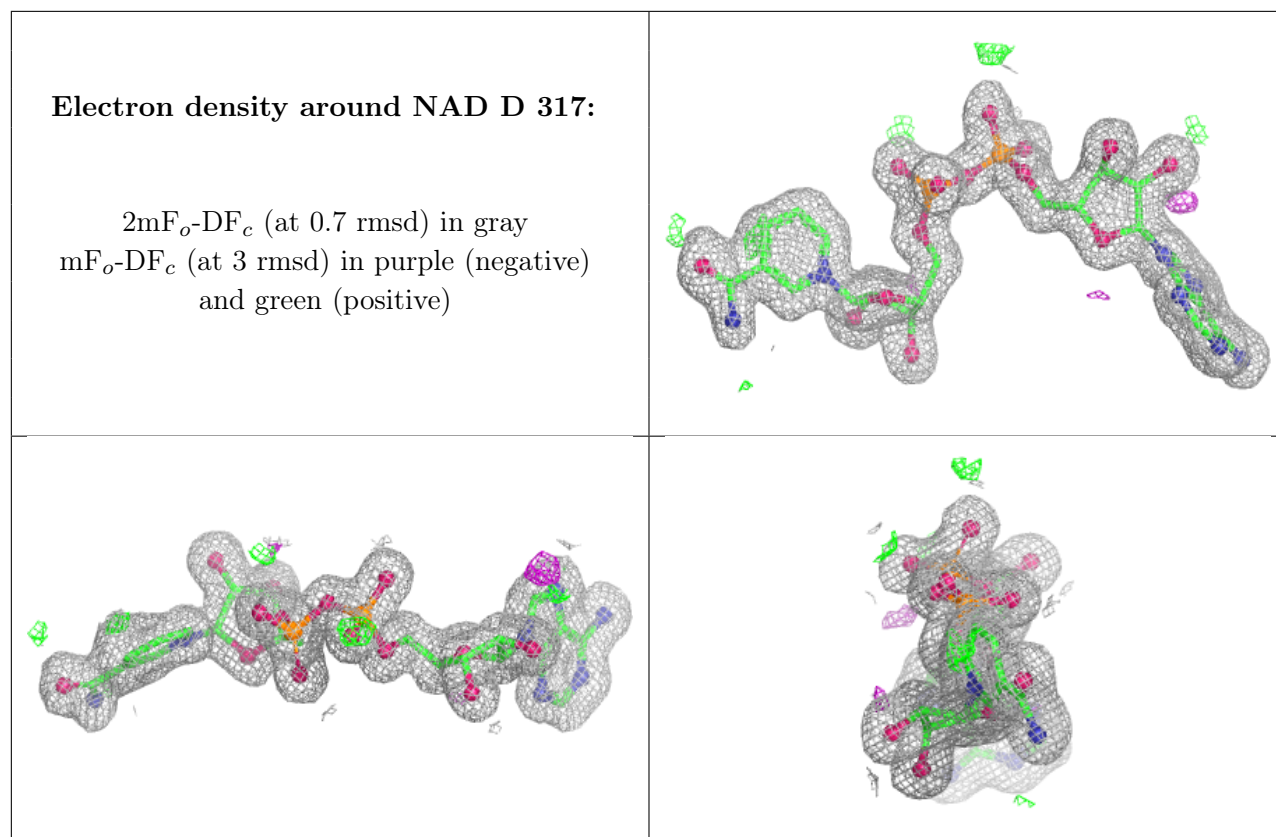
Electron density around NAD B 317:

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

**Electron density around NAD C 317:**

$2mF_o-DF_c$ (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.