



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 02:34 AM UTC

PDB ID : 2NSD / pdb_00002nsd
Title : Enoyl acyl carrier protein reductase InhA in complex with N-(4-methylbenzoyl)-4-benzylpiperidine
Authors : He, X.; Alian, A.; Ortiz de Montellano, P.R.
Deposited on : 2006-11-03
Resolution : 1.90 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

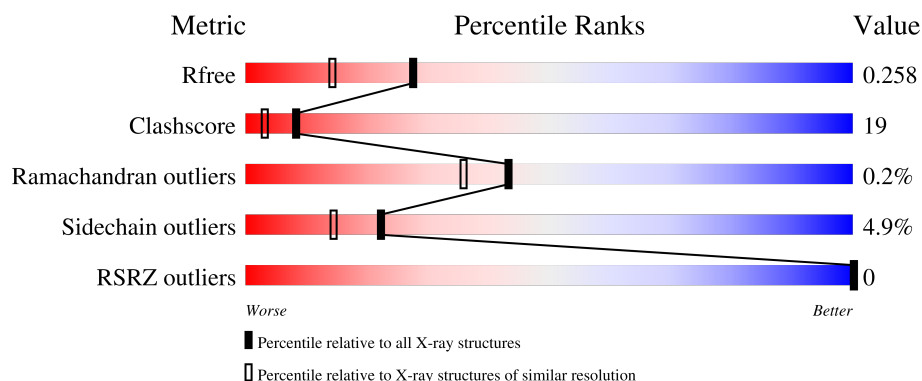
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	269	 73% 25% .
1	B	269	 65% 29% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4434 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 Enoyl-[acyl-carrier-protein] reductase.

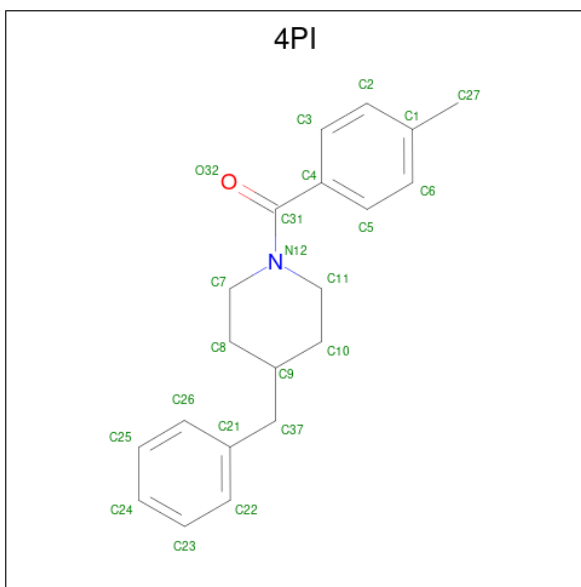
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			1996	1264	348	374	10			
1	B	268	Total	C	N	O	S	0	0	0
			1996	1264	348	374	10			

- 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		

- Molecule 3 is N-(4-METHYLBENZOYL)-4-BENZYLPIPERIDINE (CCD ID: 4PI) (formula: $C_{20}H_{23}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	20	1	1		
3	B	1	Total	C	N	O	0	0
			22	20	1	1		

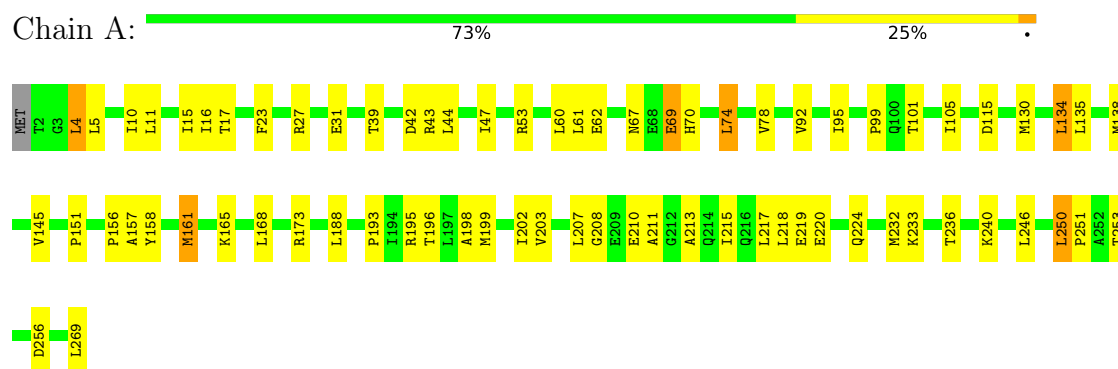
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	155	Total	O	0	0
			155	155		
4	B	155	Total	O	0	0
			155	155		

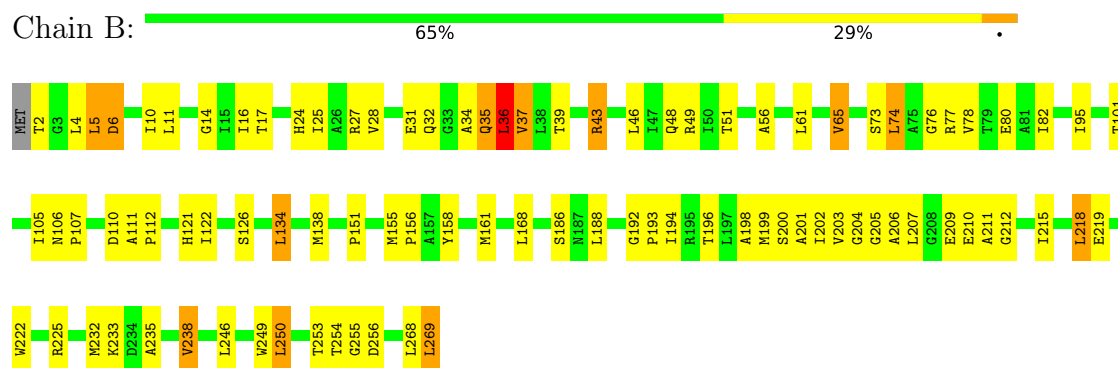
3 Residue-property plots

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: Enoyl-[acyl-carrier-protein] reductase



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.26Å 91.33Å 184.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.00 – 1.90 41.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.9 (41.00-1.90) 90.8 (41.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.259 0.235 , 0.258	Depositor DCC
R_{free} test set	4656 reflections (7.64%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.487 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4434	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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, 4PI

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	0.36	0/2034	0.91	6/2761 (0.2%)
1	B	0.37	0/2034	0.97	12/2761 (0.4%)
All	All	0.37	0/4068	0.94	18/5522 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	LEU	CA-C-N	6.78	126.41	119.56
1	A	250	LEU	C-N-CA	6.78	126.41	119.56
1	B	37	VAL	N-CA-C	-6.63	98.58	108.12
1	B	196	THR	N-CA-C	-6.60	101.64	110.55
1	B	192	GLY	N-CA-C	-6.55	104.04	112.10
1	B	250	LEU	CA-C-N	6.31	125.93	119.56
1	B	250	LEU	C-N-CA	6.31	125.93	119.56
1	B	36	LEU	N-CA-C	6.25	119.61	110.17
1	B	122	ILE	N-CA-C	6.04	116.83	110.72
1	A	161	MET	N-CA-C	-5.80	105.10	111.82
1	A	196	THR	N-CA-C	-5.68	102.88	110.55
1	B	256	ASP	N-CA-C	5.64	118.07	109.95
1	B	14	GLY	N-CA-C	5.36	122.72	115.32
1	B	161	MET	N-CA-C	-5.22	105.76	111.82
1	A	134	LEU	N-CA-C	5.16	119.84	113.50
1	B	25	ILE	N-CA-C	-5.12	105.72	110.53
1	B	134	LEU	N-CA-C	5.11	119.78	113.50
1	A	256	ASP	N-CA-C	5.11	117.30	109.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1996	0	2013	65	0
1	B	1996	0	2013	90	1
2	A	44	0	26	2	0
2	B	44	0	26	3	0
3	A	22	0	23	6	0
3	B	22	0	23	6	0
4	A	155	0	0	3	0
4	B	155	0	0	9	1
All	All	4434	0	4124	158	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (158) 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:101:THR:HG21	1:B:112:PRO:HD2	1.39	1.00
1:B:186:SER:H	1:B:254:THR:HG23	1.26	0.98
1:B:4:LEU:H	1:B:32:GLN:HE21	1.12	0.98
1:B:43:ARG:HD2	4:B:531:HOH:O	1.67	0.95
1:A:195:ARG:HD2	1:A:199:MET:HE1	1.49	0.94
1:B:65:VAL:HG21	1:B:126:SER:HB2	1.50	0.93
1:A:158:TYR:CE1	3:A:400:4PI:H111	2.03	0.92
1:B:105:ILE:HD11	1:B:206:ALA:HA	1.51	0.91
1:A:193:PRO:HB2	1:A:232:MET:HE3	1.52	0.90
1:A:67:ASN:HD22	1:A:70:HIS:H	1.19	0.89
1:B:5:LEU:HB3	1:B:34:ALA:HB2	1.56	0.86
1:A:173:ARG:NH2	4:A:503:HOH:O	2.12	0.82
1:B:254:THR:HG21	4:B:449:HOH:O	1.81	0.81
1:B:65:VAL:CG2	1:B:126:SER:HB2	2.11	0.81
1:B:158:TYR:CE1	3:B:400:4PI:H111	2.16	0.80
1:A:156:PRO:HD2	1:A:218:LEU:HD22	1.62	0.80
1:A:16:ILE:HG23	1:A:17:THR:HG23	1.63	0.79
1:B:253:THR:HG23	4:B:452:HOH:O	1.85	0.77
1:B:27:ARG:O	1:B:31:GLU:HG3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LYS:HG2	4:A:549:HOH:O	1.88	0.73
1:A:44:LEU:HD12	1:A:60:LEU:HD11	1.72	0.72
1:B:101:THR:HG22	1:B:111:ALA:HA	1.72	0.72
1:A:195:ARG:HD2	1:A:199:MET:CE	2.20	0.71
1:A:158:TYR:CE1	3:A:400:4PI:C11	2.73	0.70
1:A:207:LEU:HD12	1:A:208:GLY:N	2.05	0.70
1:A:27:ARG:O	1:A:31:GLU:HG3	1.92	0.69
1:A:101:THR:HG21	1:A:115:ASP:OD2	1.92	0.69
1:B:4:LEU:H	1:B:32:GLN:NE2	1.89	0.68
1:A:43:ARG:O	1:A:47:ILE:HG12	1.93	0.67
1:B:11:LEU:HD22	1:B:37:VAL:O	1.95	0.67
1:B:4:LEU:O	4:B:504:HOH:O	2.12	0.66
1:B:193:PRO:HB2	1:B:232:MET:HE3	1.77	0.66
1:A:74:LEU:O	1:A:78:VAL:HG23	1.96	0.66
1:B:105:ILE:HG21	1:B:210:GLU:HG3	1.76	0.66
1:B:101:THR:CG2	1:B:111:ALA:HA	2.25	0.66
1:A:16:ILE:HD12	1:A:47:ILE:HD11	1.78	0.66
1:B:207:LEU:HD11	4:B:517:HOH:O	1.97	0.65
1:B:16:ILE:HG23	1:B:17:THR:HG23	1.77	0.65
1:A:10:ILE:HD13	1:A:246:LEU:HD13	1.78	0.65
1:B:35:GLN:HE22	1:B:56:ALA:HB3	1.62	0.64
1:B:186:SER:N	1:B:254:THR:HG23	2.07	0.63
1:A:99:PRO:HB2	1:A:101:THR:HG22	1.80	0.63
1:B:101:THR:CG2	1:B:112:PRO:HD2	2.23	0.62
1:B:186:SER:H	1:B:254:THR:CG2	2.06	0.62
1:B:10:ILE:HD13	1:B:246:LEU:HD13	1.82	0.62
1:A:44:LEU:HD21	1:A:62:GLU:HG3	1.82	0.61
2:A:300:NAD:H2D	3:A:400:4PI:C3	2.30	0.61
1:A:67:ASN:ND2	1:A:70:HIS:ND1	2.49	0.61
1:A:158:TYR:CZ	3:A:400:4PI:H111	2.36	0.60
1:B:199:MET:HG2	3:B:400:4PI:H82	1.82	0.60
1:B:35:GLN:HA	1:B:35:GLN:OE1	2.01	0.60
1:B:158:TYR:CE1	3:B:400:4PI:C11	2.83	0.60
1:A:219:GLU:OE2	1:A:232:MET:HE1	2.01	0.60
1:B:10:ILE:O	1:B:36:LEU:HB3	2.02	0.59
1:B:212:GLY:HA2	1:B:215:ILE:HD12	1.84	0.59
1:B:268:LEU:O	1:B:269:LEU:HB3	2.04	0.58
1:A:11:LEU:C	1:A:11:LEU:HD23	2.29	0.58
1:B:158:TYR:CZ	3:B:400:4PI:H111	2.39	0.58
1:B:43:ARG:HD3	1:B:46:LEU:HD22	1.85	0.57
1:B:101:THR:HG21	1:B:112:PRO:CD	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASN:ND2	1:A:70:HIS:H	1.96	0.57
1:B:76:GLY:O	1:B:80:GLU:HG3	2.05	0.57
1:A:193:PRO:CB	1:A:232:MET:HE3	2.32	0.56
1:B:134:LEU:O	1:B:138:MET:HG3	2.06	0.56
1:B:235:ALA:O	1:B:238:VAL:HG13	2.05	0.56
1:A:99:PRO:HG2	1:A:115:ASP:HB3	1.87	0.56
1:A:199:MET:HG2	3:A:400:4PI:H82	1.86	0.56
1:A:269:LEU:OXT	1:A:269:LEU:HD13	2.06	0.56
1:B:199:MET:HE1	1:B:232:MET:HE2	1.87	0.56
1:B:73:SER:OG	1:B:77:ARG:NH1	2.39	0.55
1:B:203:VAL:HG13	1:B:204:GLY:N	2.22	0.55
1:B:105:ILE:N	1:B:105:ILE:HD12	2.22	0.54
1:A:105:ILE:HD13	1:A:211:ALA:HB2	1.89	0.54
1:B:105:ILE:HD12	1:B:105:ILE:H	1.73	0.54
1:B:200:SER:HA	1:B:203:VAL:HG12	1.90	0.54
1:B:35:GLN:NE2	1:B:56:ALA:HB3	2.24	0.53
1:A:134:LEU:O	1:A:138:MET:HG3	2.08	0.53
1:B:95:ILE:HD12	2:B:300:NAD:N3A	2.23	0.53
1:B:105:ILE:HD11	1:B:206:ALA:CA	2.30	0.53
1:A:44:LEU:HD12	1:A:60:LEU:CD1	2.36	0.53
1:A:198:ALA:O	1:A:202:ILE:HG13	2.08	0.53
1:B:11:LEU:C	1:B:11:LEU:HD13	2.34	0.53
1:B:203:VAL:HG13	1:B:204:GLY:H	1.73	0.52
1:A:215:ILE:HD12	1:A:215:ILE:N	2.26	0.51
1:B:78:VAL:O	1:B:82:ILE:HG12	2.11	0.51
1:A:101:THR:HG21	1:A:115:ASP:CG	2.35	0.51
1:B:11:LEU:HD21	1:B:39:THR:HG23	1.91	0.51
1:B:201:ALA:O	1:B:205:GLY:HA3	2.11	0.51
1:B:194:ILE:C	1:B:199:MET:HE3	2.37	0.50
1:A:213:ALA:O	1:A:217:LEU:HD13	2.12	0.50
1:B:106:ASN:ND2	1:B:107:PRO:HD2	2.25	0.50
1:A:39:THR:HA	1:A:61:LEU:O	2.13	0.49
1:B:207:LEU:CD1	4:B:517:HOH:O	2.59	0.49
1:B:39:THR:HA	1:B:61:LEU:O	2.13	0.49
1:A:16:ILE:HD12	1:A:47:ILE:CD1	2.43	0.49
1:B:207:LEU:C	1:B:209:GLU:H	2.21	0.49
1:A:5:LEU:HD23	1:A:10:ILE:HD12	1.96	0.48
1:A:203:VAL:HG13	1:A:215:ILE:HG21	1.95	0.47
1:A:211:ALA:O	1:A:215:ILE:HD13	2.14	0.47
1:B:155:MET:HB2	1:B:218:LEU:HD11	1.96	0.47
1:A:99:PRO:CG	1:A:115:ASP:HB3	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ALA:O	1:B:215:ILE:HG13	2.14	0.47
2:B:300:NAD:H51A	4:B:472:HOH:O	2.15	0.47
1:B:43:ARG:HB2	1:B:46:LEU:HB2	1.95	0.47
1:B:200:SER:HA	1:B:203:VAL:CG1	2.44	0.47
1:B:198:ALA:O	1:B:202:ILE:HG13	2.14	0.47
1:B:48:GLN:HA	1:B:51:THR:OG1	2.14	0.47
1:A:250:LEU:HB3	1:A:253:THR:CG2	2.45	0.46
1:B:107:PRO:HG2	1:B:110:ASP:OD2	2.14	0.46
1:A:4:LEU:HD13	1:A:5:LEU:CD1	2.45	0.46
1:B:121:HIS:HD2	4:B:426:HOH:O	1.98	0.46
1:B:199:MET:CE	1:B:232:MET:HE2	2.45	0.46
1:A:101:THR:HG21	1:A:115:ASP:CB	2.46	0.46
1:B:205:GLY:O	1:B:207:LEU:HD12	2.15	0.46
1:B:46:LEU:O	1:B:49:ARG:HB2	2.16	0.46
1:B:209:GLU:HA	1:B:209:GLU:OE1	2.16	0.46
1:A:236:THR:CG2	1:A:240:LYS:HE3	2.47	0.45
1:B:225:ARG:HH11	1:B:225:ARG:HG3	1.82	0.45
1:A:60:LEU:C	1:A:60:LEU:HD13	2.40	0.45
1:B:43:ARG:CD	1:B:46:LEU:HD22	2.45	0.45
1:A:220:GLU:O	1:A:224:GLN:HG3	2.17	0.45
1:B:218:LEU:HD22	1:B:222:TRP:HZ3	1.81	0.45
1:B:24:HIS:O	1:B:28:VAL:HG23	2.16	0.44
1:A:69:GLU:HG3	1:A:70:HIS:N	2.32	0.44
1:A:105:ILE:HD11	1:A:210:GLU:CG	2.48	0.44
1:B:249:TRP:C	1:B:250:LEU:HD22	2.42	0.44
1:B:268:LEU:HD12	1:B:268:LEU:HA	1.84	0.44
1:B:205:GLY:C	1:B:207:LEU:H	2.26	0.44
1:B:219:GLU:OE1	1:B:232:MET:HE1	2.18	0.44
1:B:11:LEU:HD23	1:B:37:VAL:HB	2.00	0.43
1:A:105:ILE:HB	1:A:207:LEU:HA	2.00	0.43
1:B:5:LEU:HB3	1:B:34:ALA:CB	2.39	0.43
1:A:250:LEU:HB3	1:A:253:THR:HG21	2.01	0.43
1:A:250:LEU:N	1:A:251:PRO:CD	2.82	0.43
1:B:46:LEU:HD12	1:B:46:LEU:N	2.34	0.43
1:A:16:ILE:HG22	2:A:300:NAD:O2A	2.19	0.43
1:B:11:LEU:HD21	1:B:39:THR:CG2	2.49	0.43
2:B:300:NAD:H2D	3:B:400:4PI:C5	2.49	0.42
1:A:218:LEU:HG	3:A:400:4PI:H24	2.00	0.42
1:B:254:THR:HG22	1:B:255:GLY:N	2.35	0.42
1:A:92:VAL:HG22	1:A:145:VAL:CG1	2.48	0.42
1:A:53:ARG:NH2	4:A:544:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LYS:NZ	4:B:479:HOH:O	2.52	0.42
1:A:5:LEU:HD23	1:A:10:ILE:CD1	2.50	0.42
1:A:219:GLU:CG	1:A:232:MET:SD	3.08	0.42
1:B:5:LEU:O	1:B:34:ALA:HB2	2.19	0.42
1:A:95:ILE:HD12	1:A:130:MET:HE1	2.01	0.41
1:B:74:LEU:O	1:B:78:VAL:HG23	2.20	0.41
1:B:156:PRO:HG2	1:B:218:LEU:HD12	2.02	0.41
1:B:2:THR:N	1:B:6:ASP:OD1	2.54	0.41
1:A:44:LEU:HD22	1:A:44:LEU:N	2.36	0.41
1:A:161:MET:HE3	1:A:165:LYS:HE2	2.03	0.41
1:B:43:ARG:HE	1:B:46:LEU:HD22	1.85	0.41
1:A:157:ALA:HB2	1:A:215:ILE:HD11	2.02	0.40
1:A:15:ILE:O	1:A:47:ILE:HD12	2.21	0.40
1:B:193:PRO:CB	1:B:232:MET:HE3	2.47	0.40
1:B:219:GLU:HB3	3:B:400:PI:H23	2.03	0.40
1:A:23:PHE:CD1	1:A:23:PHE:C	2.99	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:GLU:O	4:B:535:HOH:O[6_765]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	266/269 (99%)	244 (92%)	21 (8%)	1 (0%)	30	22
1	B	266/269 (99%)	248 (93%)	18 (7%)	0	100	100
All	All	532/538 (99%)	492 (92%)	39 (7%)	1 (0%)	43	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP

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	204/205 (100%)	197 (97%)	7 (3%)	32	25
1	B	204/205 (100%)	191 (94%)	13 (6%)	16	8
All	All	408/410 (100%)	388 (95%)	20 (5%)	22	14

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	69	GLU
1	A	74	LEU
1	A	135	LEU
1	A	151	PRO
1	A	168	LEU
1	A	188	LEU
1	B	5	LEU
1	B	6	ASP
1	B	35	GLN
1	B	36	LEU
1	B	43	ARG
1	B	65	VAL
1	B	74	LEU
1	B	151	PRO
1	B	168	LEU
1	B	188	LEU
1	B	218	LEU
1	B	238	VAL
1	B	269	LEU

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	66	GLN
1	A	67	ASN
1	A	100	GLN
1	A	106	ASN
1	A	121	HIS
1	A	214	GLN
1	A	265	HIS
1	B	32	GLN
1	B	48	GLN
1	B	86	ASN
1	B	106	ASN
1	B	187	ASN
1	B	214	GLN
1	B	224	GLN
1	B	265	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	4PI	B	400	-	24,24,24	4.57	16 (66%)	32,32,32	2.21	6 (18%)
2	NAD	A	300	-	46,48,48	1.88	7 (15%)	64,73,73	2.53	15 (23%)
2	NAD	B	300	-	46,48,48	1.88	9 (19%)	64,73,73	2.25	14 (21%)
3	4PI	A	400	-	24,24,24	4.56	17 (70%)	32,32,32	3.92	12 (37%)

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
3	4PI	B	400	-	-	2/12/22/22	0/3/3/3
2	NAD	A	300	-	-	7/30/62/62	0/5/5/5
2	NAD	B	300	-	-	6/30/62/62	0/5/5/5
3	4PI	A	400	-	-	2/12/22/22	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	4PI	O32-C31	-17.30	0.87	1.22
3	A	400	4PI	C22-C21	-12.27	1.14	1.38
3	A	400	4PI	C37-C21	9.08	1.72	1.51
3	A	400	4PI	C26-C21	8.70	1.56	1.38
2	B	300	NAD	O7N-C7N	7.12	1.37	1.24
2	A	300	NAD	O7N-C7N	6.97	1.37	1.24
3	B	400	4PI	C11-N12	6.07	1.57	1.47
3	A	400	4PI	C11-N12	5.92	1.57	1.47
3	B	400	4PI	C7-N12	4.89	1.55	1.47
3	A	400	4PI	C7-N12	4.60	1.55	1.47
2	A	300	NAD	PA-O3	4.53	1.64	1.59
2	B	300	NAD	C2N-N1N	4.52	1.39	1.35
2	A	300	NAD	C2N-N1N	4.40	1.39	1.35
3	B	400	4PI	C31-N12	4.32	1.43	1.34
3	B	400	4PI	C3-C4	4.21	1.45	1.39
2	B	300	NAD	PA-O3	4.07	1.63	1.59
3	A	400	4PI	C31-N12	4.02	1.43	1.34
3	A	400	4PI	C5-C4	4.01	1.45	1.39
3	A	400	4PI	C27-C1	-3.99	1.39	1.51
3	B	400	4PI	C27-C1	-3.97	1.39	1.51
3	A	400	4PI	C3-C4	3.87	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	4PI	C5-C4	3.63	1.44	1.39
3	B	400	4PI	C23-C22	3.49	1.44	1.38
2	A	300	NAD	C2A-N1A	3.49	1.40	1.33
3	A	400	4PI	C23-C22	3.45	1.44	1.38
2	B	300	NAD	C2A-N1A	3.43	1.40	1.33
2	A	300	NAD	PN-O3	3.33	1.63	1.59
3	B	400	4PI	C3-C2	3.17	1.43	1.38
3	A	400	4PI	C25-C24	3.15	1.45	1.38
3	A	400	4PI	O32-C31	-3.12	1.16	1.22
3	B	400	4PI	C25-C26	3.05	1.44	1.38
2	B	300	NAD	PN-O3	2.97	1.62	1.59
3	B	400	4PI	C25-C24	2.97	1.44	1.38
3	A	400	4PI	C25-C26	2.94	1.43	1.38
3	B	400	4PI	C22-C21	2.92	1.44	1.38
2	B	300	NAD	C2A-N3A	2.84	1.39	1.33
3	A	400	4PI	C6-C5	2.81	1.43	1.38
3	B	400	4PI	C23-C24	2.79	1.44	1.38
3	A	400	4PI	C23-C24	2.75	1.44	1.38
2	A	300	NAD	C2A-N3A	2.65	1.38	1.33
3	A	400	4PI	C3-C2	2.42	1.42	1.38
3	A	400	4PI	C6-C1	2.35	1.44	1.38
2	B	300	NAD	C4N-C3N	2.30	1.42	1.39
3	B	400	4PI	C6-C5	2.21	1.42	1.38
3	B	400	4PI	C2-C1	2.18	1.44	1.38
2	A	300	NAD	C4N-C3N	2.13	1.42	1.39
3	B	400	4PI	C26-C21	2.08	1.43	1.38
2	B	300	NAD	C6N-N1N	2.02	1.39	1.35
2	B	300	NAD	C5A-N7A	-2.02	1.35	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	4PI	C37-C21-C26	-11.69	99.16	120.90
3	A	400	4PI	C26-C21-C22	10.75	134.21	118.23
2	B	300	NAD	O2A-PA-O3	-9.31	82.10	107.27
2	A	300	NAD	O2A-PA-O3	8.54	130.37	107.27
3	B	400	4PI	C4-C31-N12	-8.29	108.31	118.66
3	A	400	4PI	C4-C31-N12	-8.23	108.39	118.66
2	B	300	NAD	O3-PA-O1A	-8.16	86.16	110.70
3	A	400	4PI	C25-C26-C21	-7.74	109.73	120.61
2	A	300	NAD	O3-PA-O1A	-7.71	87.51	110.70
2	A	300	NAD	O2A-PA-O5B	-7.07	75.51	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	NAD	O2A-PA-O1A	-6.37	82.79	112.44
2	A	300	NAD	O5B-PA-O1A	5.49	130.70	108.94
2	A	300	NAD	N3A-C2A-N1A	-5.28	120.58	128.58
2	A	300	NAD	C3N-C7N-N7N	5.14	124.08	117.74
2	B	300	NAD	N3A-C2A-N1A	-5.12	120.83	128.58
2	B	300	NAD	C3N-C7N-N7N	5.05	123.96	117.74
3	A	400	4PI	O32-C31-C4	4.86	129.91	120.29
3	B	400	4PI	C11-N12-C31	-4.64	108.45	122.79
3	A	400	4PI	C11-N12-C31	-4.60	108.56	122.79
2	A	300	NAD	N9A-C8A-N7A	-3.71	108.67	113.94
2	B	300	NAD	O2A-PA-O1A	3.58	129.11	112.44
2	B	300	NAD	N9A-C8A-N7A	-3.52	108.94	113.94
3	B	400	4PI	C21-C37-C9	3.36	120.62	114.45
2	B	300	NAD	C5A-N7A-C8A	3.33	108.68	103.45
3	A	400	4PI	C23-C22-C21	-3.27	116.02	120.61
2	A	300	NAD	C5A-N7A-C8A	3.22	108.52	103.45
3	A	400	4PI	C7-N12-C31	-3.17	113.00	122.79
3	B	400	4PI	C7-N12-C31	-3.09	113.22	122.79
2	B	300	NAD	C5A-C4A-N3A	-3.05	122.51	126.72
2	A	300	NAD	C2A-N3A-C4A	3.04	119.26	111.83
2	B	300	NAD	C2A-N3A-C4A	2.97	119.09	111.83
3	B	400	4PI	O32-C31-C4	2.95	126.14	120.29
2	A	300	NAD	C5A-C4A-N3A	-2.93	122.68	126.72
3	A	400	4PI	C37-C21-C22	2.87	126.25	120.90
2	A	300	NAD	O7N-C7N-N7N	-2.70	118.71	122.62
2	A	300	NAD	C4A-C5A-N7A	-2.64	107.57	110.58
2	B	300	NAD	O7N-C7N-N7N	-2.63	118.81	122.62
2	B	300	NAD	C4A-C5A-N7A	-2.56	107.66	110.58
3	A	400	4PI	C21-C37-C9	2.33	118.72	114.45
3	B	400	4PI	C8-C7-N12	2.26	115.09	110.66
3	A	400	4PI	C3-C4-C31	-2.25	114.51	120.28
2	B	300	NAD	C4B-O4B-C1B	-2.23	104.53	109.47
2	A	300	NAD	C4B-O4B-C1B	-2.20	104.61	109.47
3	A	400	4PI	C8-C7-N12	2.17	114.92	110.66
2	B	300	NAD	O5B-C5B-C4B	2.13	116.23	108.99
2	B	300	NAD	O4B-C4B-C5B	-2.08	102.68	109.33
2	A	300	NAD	C4A-N9A-C8A	2.05	107.89	105.74

There are no chirality outliers.

All (17) torsion outliers are listed below:

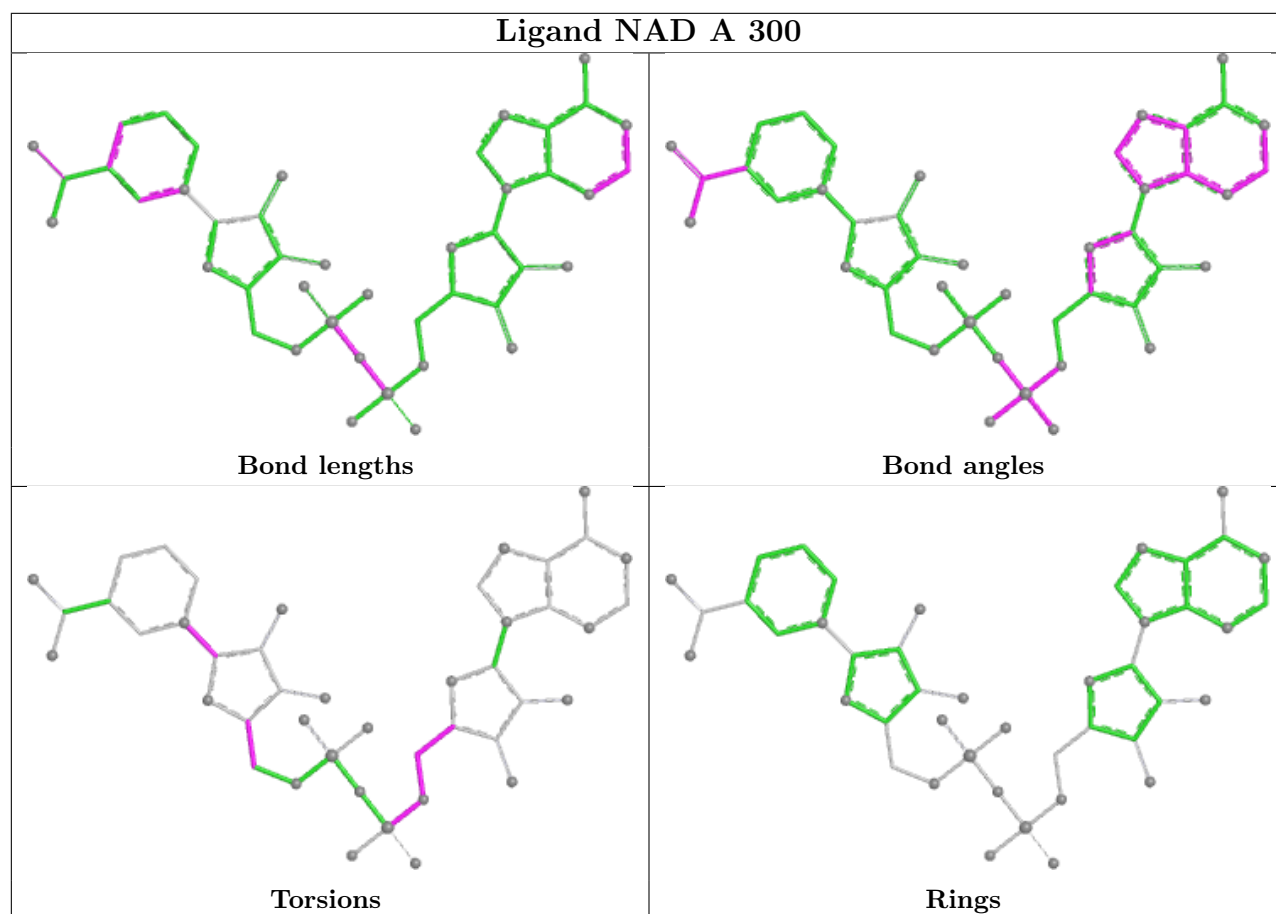
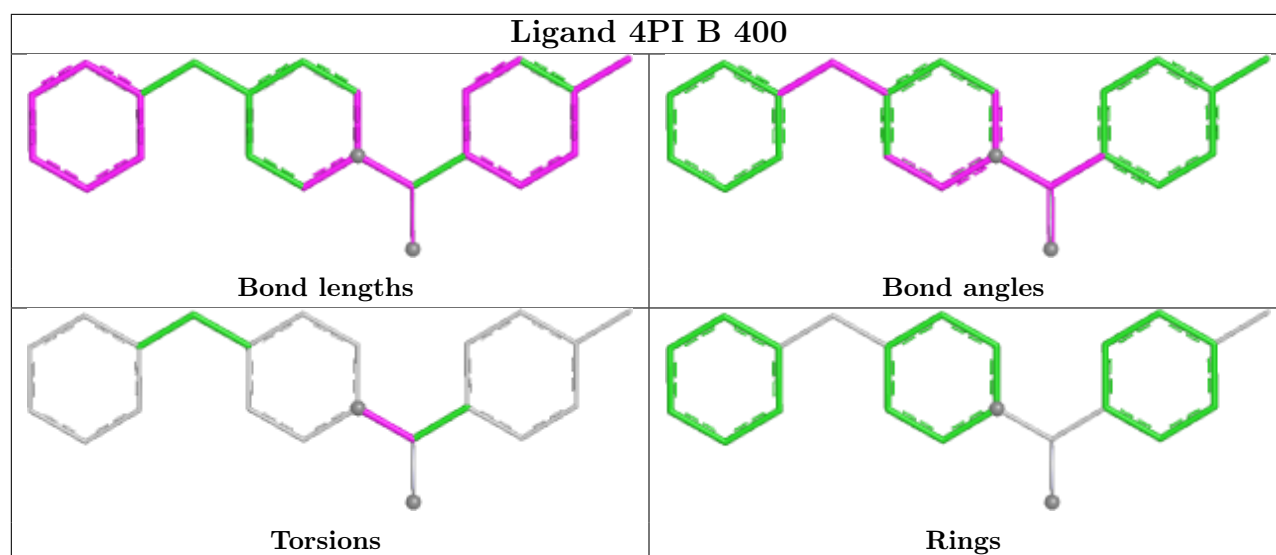
Mol	Chain	Res	Type	Atoms
2	A	300	NAD	C5B-O5B-PA-O2A
2	A	300	NAD	C5B-O5B-PA-O3
2	A	300	NAD	O4D-C1D-N1N-C2N
2	B	300	NAD	C5B-O5B-PA-O2A
2	B	300	NAD	C4B-C5B-O5B-PA
2	B	300	NAD	O4D-C1D-N1N-C2N
3	A	400	4PI	O32-C31-N12-C7
3	A	400	4PI	C4-C31-N12-C7
3	B	400	4PI	C4-C31-N12-C7
3	B	400	4PI	O32-C31-N12-C7
2	B	300	NAD	PA-O3-PN-O1N
2	B	300	NAD	C5B-O5B-PA-O3
2	A	300	NAD	O4D-C1D-N1N-C6N
2	B	300	NAD	O4D-C1D-N1N-C6N
2	A	300	NAD	C4B-C5B-O5B-PA
2	A	300	NAD	O4D-C4D-C5D-O5D
2	A	300	NAD	O4B-C4B-C5B-O5B

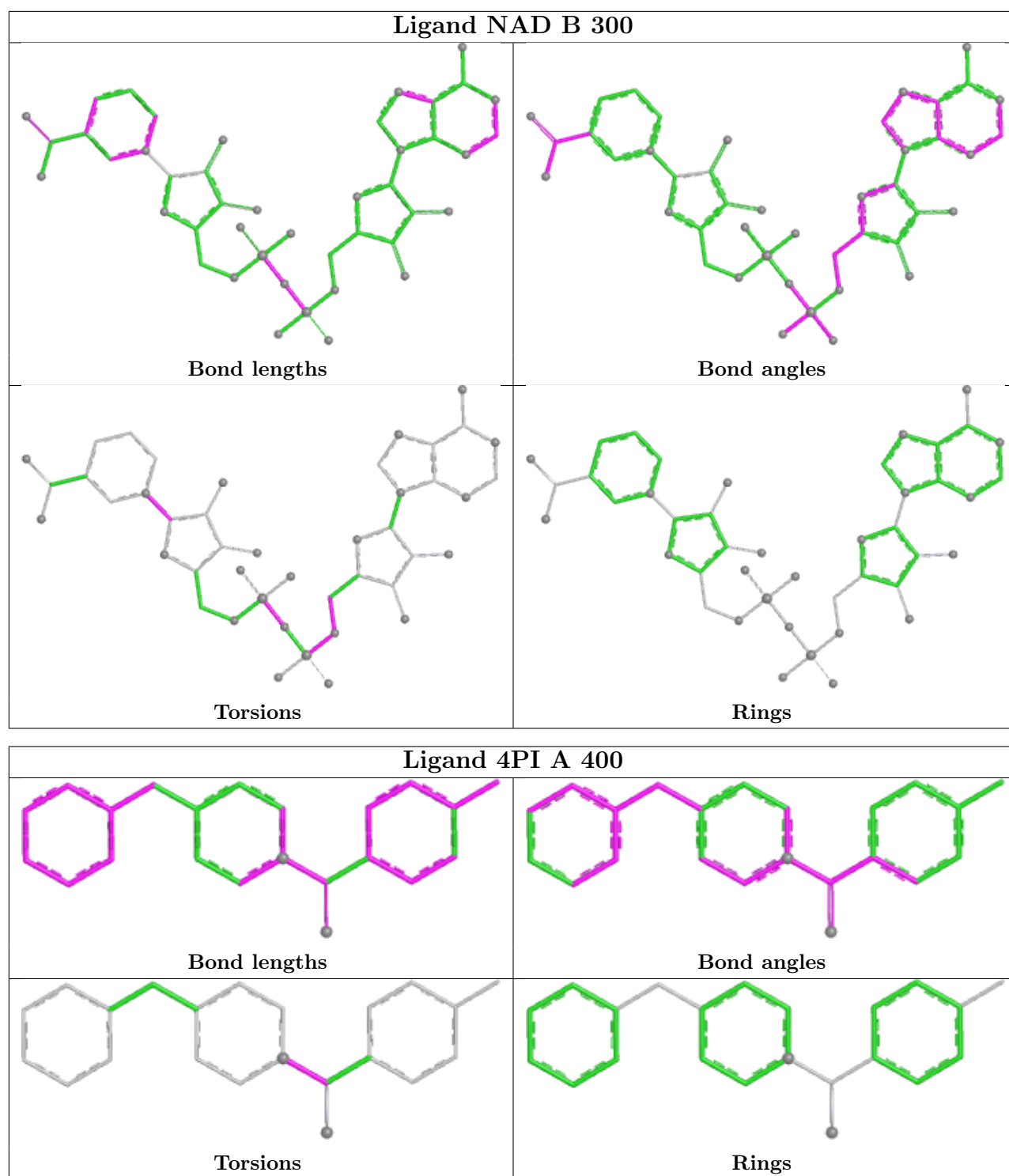
There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	400	4PI	6	0
2	A	300	NAD	2	0
2	B	300	NAD	3	0
3	A	400	4PI	6	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 ⓘ

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	268/269 (99%)	-1.02	0 100 100	19, 37, 65, 102	0
1	B	268/269 (99%)	-0.96	0 100 100	19, 36, 65, 111	0
All	All	536/538 (99%)	-0.99	0 100 100	19, 36, 67, 111	0

There are no RSRZ outliers to report.

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.

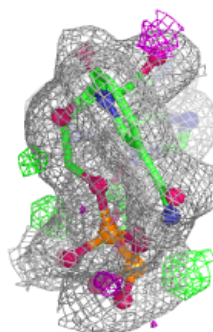
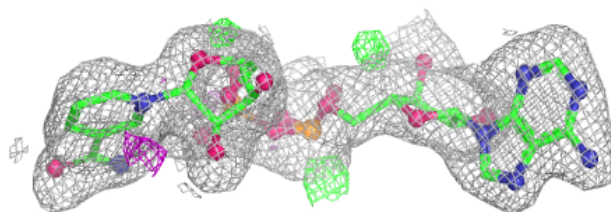
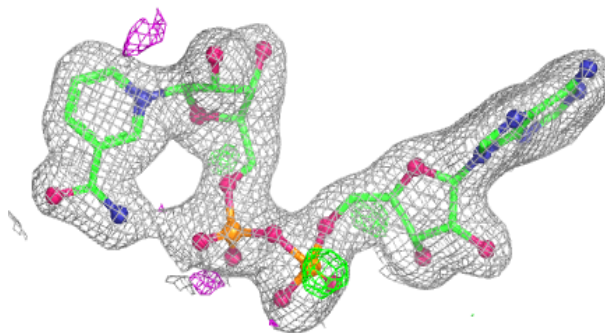
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	A	300	44/44	0.99	0.03	24,31,37,45	0
2	NAD	B	300	44/44	0.99	0.03	25,34,44,45	0
3	4PI	A	400	22/22	0.99	0.06	38,45,50,51	0
3	4PI	B	400	22/22	0.99	0.06	36,45,52,53	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

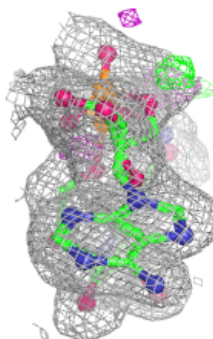
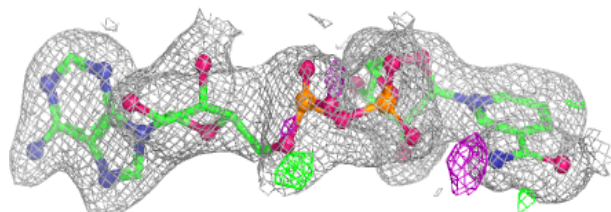
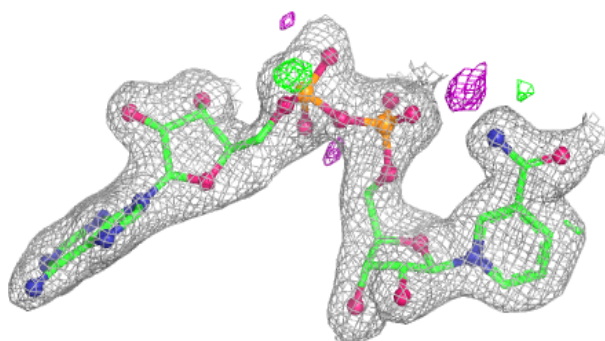
Electron density around NAD A 300:

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



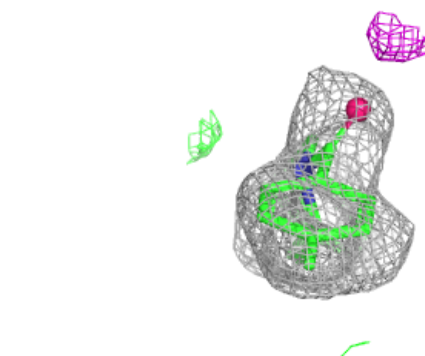
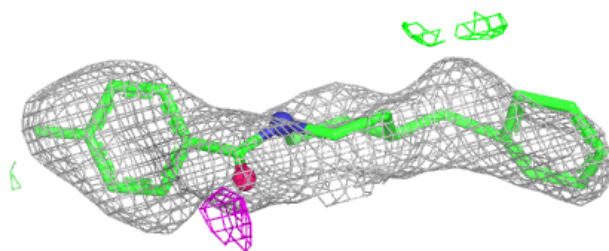
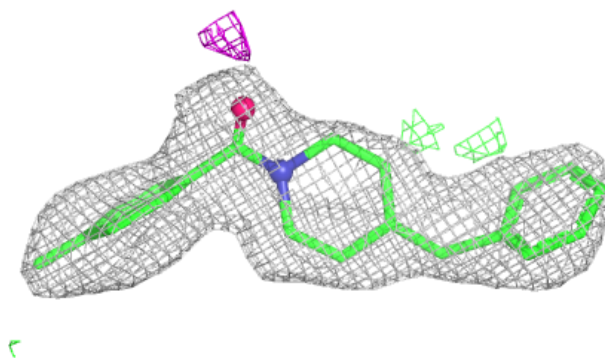
Electron density around NAD B 300:

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

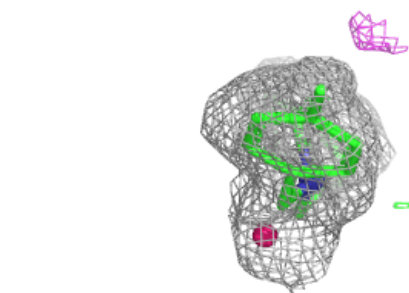
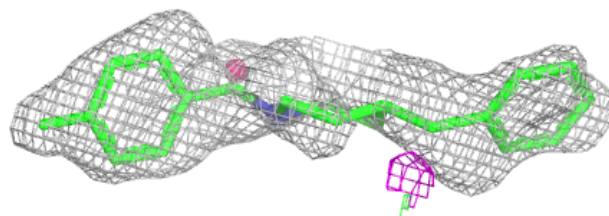
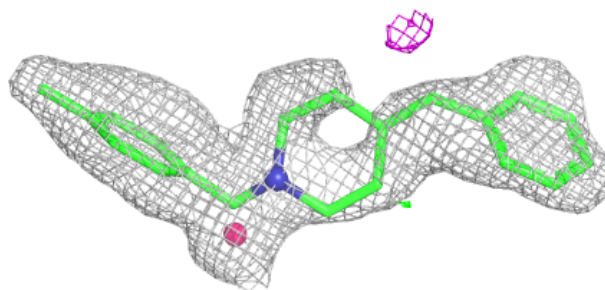


Electron density around 4PI A 400:

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

**Electron density around 4PI B 400:**

$2mF_o-DF_c$ (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.