



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:31 AM UTC

PDB ID : 1ZW1 / pdb_00001zw1
Title : Synthesis, Biological Activity, and X-Ray Crystal Structural Analysis of Diaryl Ether Inhibitors of Malarial Enoyl ACP Reductase. Part 1:4'-Substituted Triclosan Derivatives
Authors : Freundlich, J.S.; Anderson, J.W.; Sarantakis, D.; Shieh, H.M.; Yu, M.; Lucumi, E.; Kuo, M.; Schiehser, G.A.; Jacobus, D.P.; Jacobs Jr., W.R.; Fidock, D.A.; Sacchettini, J.C.
Deposited on : 2005-06-03
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

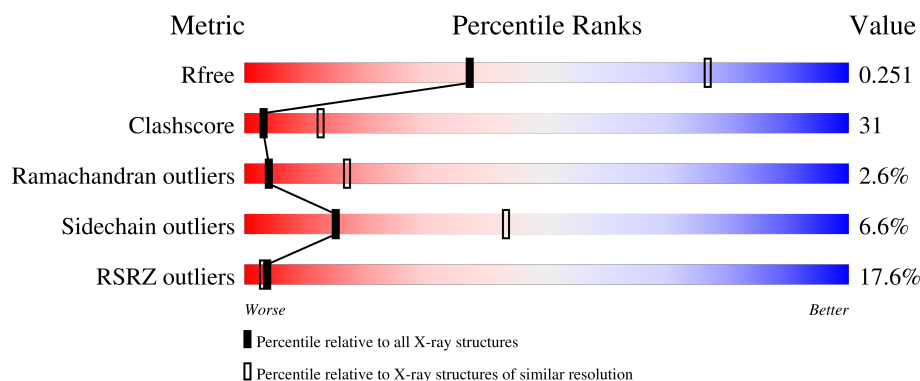
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	336	
1	B	336	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TN5	A	500	-	X	-	-
3	TN5	B	501	-	X	-	-

2 Entry composition [i](#)

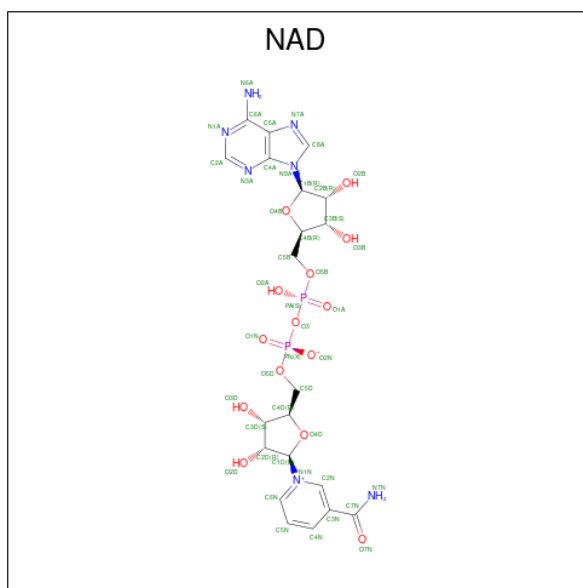
There are 3 unique types of molecules in this entry. The entry contains 4696 atoms, of which 0 are hydrogens and 0 are deuteriums.

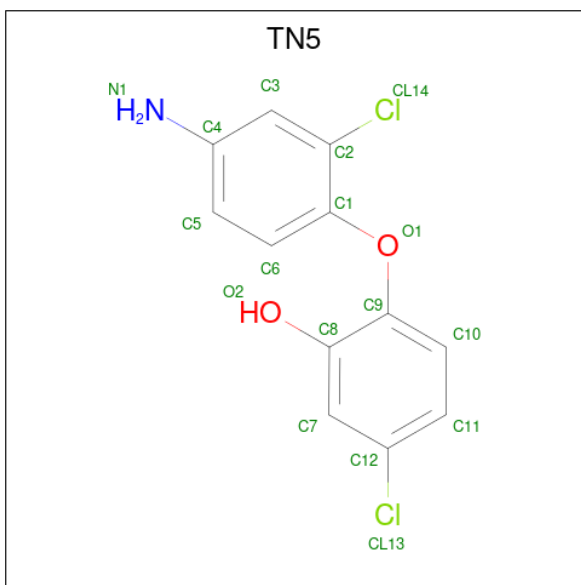
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called enoyl-acyl carrier reductase.

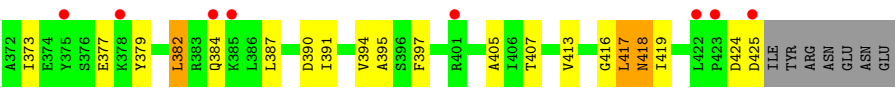
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2287	1458	384	434	11			
1	B	289	Total	C	N	O	S	0	0	0
			2287	1458	384	434	11			

- 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
3	A	1	Total	C	Cl	N	O	0	0
			17	12	2	1	2		
3	B	1	Total	C	Cl	N	O	0	0
			17	12	2	1	2		



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	131.27Å 131.27Å 82.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 – 2.90 29.72 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.72-2.90) 98.0 (29.72-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.38 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.297 0.252 , 0.251	Depositor DCC
R_{free} test set	822 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	4696	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: TN5, 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	0.48	0/2329	0.99	8/3141 (0.3%)
1	B	0.50	1/2329 (0.0%)	0.97	5/3141 (0.2%)
All	All	0.49	1/4658 (0.0%)	0.98	13/6282 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	274	VAL	CA-CB	5.71	1.59	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	SER	N-CA-C	-7.11	103.46	111.14
1	B	109	ASN	N-CA-C	6.61	121.20	113.20
1	A	383	ARG	N-CA-C	6.55	120.38	112.38
1	A	186	ARG	N-CA-C	6.54	118.20	111.14
1	A	278	GLY	N-CA-C	6.23	121.52	112.55
1	A	274	VAL	CA-C-N	6.21	127.61	119.84
1	A	274	VAL	C-N-CA	6.21	127.61	119.84
1	A	158	LYS	N-CA-C	-6.09	101.51	110.52
1	B	273	VAL	N-CA-C	5.85	116.56	108.84
1	B	302	ASN	N-CA-C	5.40	118.21	111.24
1	B	108	THR	N-CA-C	5.20	121.87	110.80
1	A	282	SER	N-CA-C	-5.08	105.20	111.40
1	A	178	ASP	N-CA-C	5.00	116.39	110.19

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	2287	0	2297	153	0
1	B	2287	0	2297	154	0
2	A	44	0	26	2	0
2	B	44	0	26	2	0
3	A	17	0	8	4	0
3	B	17	0	8	3	0
All	All	4696	0	4662	292	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 31.

All (292) 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)
3:A:500:TN5:N1	3:A:500:TN5:C4	1.69	1.52
3:B:501:TN5:N1	3:B:501:TN5:C4	1.69	1.52
1:A:212:LEU:HD21	1:A:248:LEU:HD22	1.46	0.98
1:B:217:ALA:HB1	1:B:281:MET:HE1	1.44	0.98
1:B:366:TYR:O	1:B:370:ASP:HB2	1.71	0.90
1:B:155:LYS:HE3	1:B:157:LYS:HE3	1.55	0.88
1:B:155:LYS:HD3	1:B:157:LYS:HZ1	1.42	0.83
1:A:259:GLN:HG2	1:A:304:ASN:ND2	1.93	0.83
1:A:281:MET:HE1	1:A:285:LYS:HE2	1.61	0.82
1:B:212:LEU:HB3	1:B:262:ILE:HG12	1.61	0.81
1:A:170:SER:HB3	1:A:240:LYS:HD2	1.61	0.81
1:A:301:ARG:NH2	1:B:379:TYR:HA	1.96	0.81
1:B:248:LEU:O	1:B:252:PHE:HB2	1.84	0.77
1:A:325:LYS:HB3	1:A:368:PHE:HB2	1.65	0.77
1:B:201:LEU:HD21	1:B:205:LYS:HE3	1.67	0.75
1:A:111:TYR:O	1:A:115:ILE:HG13	1.87	0.73
1:B:138:PHE:HE2	1:B:164:MET:HE3	1.54	0.72
1:B:170:SER:OG	1:B:240:LYS:HE2	1.90	0.72
1:B:151:MET:HE3	1:B:158:LYS:HE3	1.72	0.72
1:B:155:LYS:CD	1:B:157:LYS:HZ1	2.04	0.71
1:A:174:ALA:O	1:A:177:ILE:HG22	1.90	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:PHE:HD1	1:A:198:VAL:HG11	1.56	0.70
1:A:128:PHE:HB3	1:A:130:ILE:HD11	1.74	0.70
1:A:132:PRO:HB2	1:A:133:PRO:HD3	1.73	0.70
1:A:138:PHE:CE2	1:A:164:MET:HE2	2.27	0.70
1:A:281:MET:CE	1:A:285:LYS:HE2	2.22	0.69
1:B:99:ILE:HD13	1:B:125:LYS:HB2	1.74	0.69
1:A:159:MET:HE2	1:A:161:ILE:HG12	1.74	0.69
1:B:106:GLY:O	1:B:107:ASP:HB3	1.92	0.69
1:A:155:LYS:O	1:A:157:LYS:HG3	1.93	0.69
1:A:301:ARG:HH21	1:B:379:TYR:HA	1.55	0.69
1:B:108:THR:HG22	1:B:113:TRP:CE3	2.28	0.68
1:B:138:PHE:CE2	1:B:164:MET:HE3	2.28	0.68
1:A:178:ASP:OD2	1:A:180:GLU:HB3	1.93	0.68
1:A:154:ASP:O	1:A:156:ASP:N	2.27	0.68
1:A:177:ILE:HG23	1:A:177:ILE:O	1.94	0.68
1:B:177:ILE:HG13	1:B:177:ILE:O	1.93	0.67
1:A:379:TYR:OH	1:A:425:ASP:HB3	1.93	0.67
1:A:151:MET:HE3	1:A:158:LYS:NZ	2.09	0.67
1:B:210:ASN:HD22	1:B:257:LYS:NZ	1.93	0.67
1:B:194:THR:O	1:B:198:VAL:HG13	1.95	0.67
1:B:259:GLN:HG2	1:B:304:ASN:HD21	1.60	0.67
1:A:314:PRO:HB2	1:A:373:ILE:HG12	1.77	0.65
1:B:418:ASN:H	1:B:418:ASN:HD22	1.43	0.65
1:A:175:ASN:ND2	1:A:175:ASN:H	1.95	0.65
1:A:212:LEU:HB2	1:A:256:MET:HE1	1.78	0.65
1:A:125:LYS:N	1:A:125:LYS:HD2	2.12	0.64
1:A:252:PHE:O	1:A:256:MET:HG3	1.96	0.64
1:A:301:ARG:HH21	1:B:379:TYR:C	2.06	0.64
1:A:118:GLU:HG3	1:A:393:SER:N	2.13	0.64
1:B:195:ILE:HG23	1:B:248:LEU:HD23	1.80	0.64
1:A:414:ASP:CG	1:A:418:ASN:HD22	2.06	0.63
1:A:99:ILE:HB	1:A:209:ILE:HG22	1.81	0.63
1:A:387:LEU:O	1:A:390:ASP:HB2	1.99	0.63
1:B:259:GLN:HG2	1:B:304:ASN:ND2	2.14	0.62
1:B:183:ASN:HA	1:B:188:ASN:HD21	1.63	0.62
1:A:179:GLU:O	1:A:182:LYS:HB3	2.01	0.61
1:A:366:TYR:O	1:A:370:ASP:HB2	2.00	0.61
1:B:301:ARG:HG3	1:B:301:ARG:HH11	1.65	0.61
1:B:210:ASN:O	1:B:211:MET:HG3	1.99	0.61
1:B:274:VAL:O	1:B:274:VAL:CG2	2.49	0.61
1:B:148:ASP:HA	1:B:151:MET:HE2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PHE:O	1:A:151:MET:HG3	2.00	0.60
1:A:138:PHE:HE2	1:A:164:MET:HE2	1.67	0.60
1:B:174:ALA:HA	1:B:194:THR:HG21	1.84	0.60
1:B:154:ASP:O	1:B:156:ASP:N	2.26	0.60
1:A:120:SER:HB2	1:A:153:ILE:HG12	1.83	0.60
1:A:212:LEU:HB2	1:A:256:MET:CE	2.32	0.60
1:B:105:ILE:HD12	1:B:128:PHE:CD1	2.37	0.60
1:A:404:ARG:HH21	1:B:384:GLN:CD	2.10	0.59
1:B:105:ILE:HD12	1:B:128:PHE:CE1	2.37	0.59
1:B:301:ARG:HG3	1:B:301:ARG:NH1	2.16	0.59
1:A:277:TYR:CE2	1:A:281:MET:HB3	2.37	0.59
1:A:149:ASN:O	1:A:152:ILE:HG12	2.01	0.59
1:A:212:LEU:HD21	1:A:248:LEU:CD2	2.28	0.59
1:A:136:ASN:ND2	1:A:189:MET:HE2	2.17	0.59
1:A:215:SER:HA	1:A:265:LEU:HD23	1.84	0.59
1:B:200:ASN:HD22	1:B:200:ASN:N	2.00	0.59
1:A:125:LYS:HE3	1:A:160:ASN:HD22	1.68	0.59
1:B:155:LYS:HB2	1:B:157:LYS:NZ	2.18	0.59
1:A:379:TYR:HA	1:B:301:ARG:NH2	2.18	0.58
1:B:274:VAL:O	1:B:274:VAL:HG23	2.01	0.58
1:A:223:GLN:NE2	1:A:324:ASN:HB3	2.18	0.58
1:A:125:LYS:HE3	1:A:160:ASN:ND2	2.19	0.58
1:B:252:PHE:O	1:B:256:MET:HG3	2.03	0.58
1:A:306:ARG:HG2	1:B:382:LEU:HD21	1.85	0.57
1:A:301:ARG:HH21	1:B:379:TYR:CA	2.18	0.56
1:B:130:ILE:O	1:B:167:PHE:N	2.36	0.56
1:A:265:LEU:N	1:A:265:LEU:HD22	2.21	0.56
1:B:113:TRP:CH2	1:B:151:MET:HG2	2.41	0.56
1:A:179:GLU:OE1	1:A:182:LYS:HD3	2.06	0.56
1:B:126:ILE:HG22	1:B:127:ILE:H	1.71	0.56
1:A:263:ILE:HG23	1:A:399:LEU:HD21	1.87	0.56
1:A:276:GLY:HA2	1:A:325:LYS:HE3	1.88	0.56
1:B:139:MET:SD	1:B:164:MET:HE2	2.45	0.56
1:A:391:ILE:HD12	1:A:391:ILE:N	2.22	0.55
1:B:126:ILE:HG21	1:B:128:PHE:HE1	1.72	0.55
1:B:165:LEU:HD13	1:B:201:LEU:HD12	1.88	0.55
1:A:128:PHE:HB3	1:A:130:ILE:CD1	2.36	0.54
1:B:147:PHE:O	1:B:151:MET:HG3	2.07	0.54
1:A:379:TYR:HA	1:B:301:ARG:HH21	1.73	0.54
1:B:137:ILE:HD12	1:B:140:LYS:HD3	1.88	0.54
1:B:295:LEU:O	1:B:299:LEU:HG	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLN:HE21	1:A:304:ASN:HD21	1.55	0.54
1:B:132:PRO:HG2	1:B:187:TYR:CE2	2.43	0.54
1:A:379:TYR:C	1:B:301:ARG:HH21	2.16	0.53
1:B:108:THR:HG22	1:B:113:TRP:CD2	2.43	0.53
1:B:249:CYS:O	1:B:253:VAL:HB	2.09	0.53
1:A:232:LYS:O	1:A:236:ASP:HB2	2.08	0.53
1:A:125:LYS:HB3	1:A:162:LEU:HG	1.91	0.53
1:B:155:LYS:HD3	1:B:157:LYS:NZ	2.18	0.53
1:B:126:ILE:HG22	1:B:127:ILE:N	2.23	0.53
1:A:267:TYR:CD2	1:A:269:ALA:HB2	2.44	0.53
1:B:119:LEU:O	1:B:124:VAL:HG13	2.09	0.53
1:B:145:GLY:HA2	1:B:148:ASP:OD1	2.08	0.53
1:B:131:TRP:CG	1:B:133:PRO:HD2	2.44	0.53
1:B:148:ASP:O	1:B:158:LYS:NZ	2.42	0.53
1:A:99:ILE:HG23	1:A:162:LEU:HD12	1.91	0.52
1:A:178:ASP:O	1:A:182:LYS:HB2	2.08	0.52
1:A:187:TYR:HD2	1:A:193:TYR:OH	1.92	0.52
1:B:263:ILE:CD1	1:B:395:ALA:HB1	2.39	0.52
1:A:177:ILE:HD11	1:A:193:TYR:OH	2.09	0.52
1:A:245:LEU:HD22	1:A:288:LEU:CD1	2.39	0.52
1:A:264:SER:C	1:A:265:LEU:HD22	2.33	0.52
1:A:234:TYR:O	1:A:237:ALA:HB3	2.09	0.52
1:B:416:GLY:O	1:B:419:ILE:HG12	2.10	0.52
1:B:183:ASN:C	1:B:188:ASN:HD21	2.17	0.52
1:A:175:ASN:H	1:A:175:ASN:HD22	1.56	0.52
1:A:212:LEU:HD11	1:A:248:LEU:HD21	1.92	0.51
1:A:245:LEU:HD22	1:A:288:LEU:HD12	1.93	0.51
1:A:404:ARG:HH12	1:B:387:LEU:HD12	1.74	0.51
1:A:175:ASN:HD22	1:A:175:ASN:N	2.06	0.51
1:A:105:ILE:CG2	1:A:130:ILE:HD12	2.41	0.51
1:A:153:ILE:CD1	1:A:159:MET:HB2	2.41	0.51
1:A:391:ILE:N	1:A:391:ILE:CD1	2.74	0.51
1:B:178:ASP:O	1:B:182:LYS:HB2	2.10	0.50
1:B:209:ILE:O	1:B:256:MET:HA	2.11	0.50
1:B:269:ALA:HA	1:B:272:LYS:O	2.12	0.50
1:B:150:ASP:C	1:B:152:ILE:H	2.20	0.50
1:A:263:ILE:HA	1:A:308:ASN:O	2.10	0.50
1:B:153:ILE:HB	1:B:157:LYS:HB2	1.92	0.50
1:A:271:GLN:NE2	1:A:289:GLU:OE1	2.45	0.50
1:A:120:SER:CB	1:A:153:ILE:HG12	2.42	0.50
1:A:308:ASN:OD1	1:A:407:THR:HA	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LYS:HB2	1:B:157:LYS:HZ1	1.76	0.50
1:B:153:ILE:O	1:B:154:ASP:C	2.55	0.50
1:A:383:ARG:HE	1:B:301:ARG:HD2	1.76	0.50
1:B:104:GLY:O	2:B:451:NAD:H4B	2.12	0.50
1:B:171:PHE:O	1:B:195:ILE:HG13	2.12	0.50
1:B:184:ASN:ND2	1:B:186:ARG:H	2.09	0.50
1:B:202:ILE:HD12	1:B:252:PHE:HZ	1.77	0.50
1:A:304:ASN:CG	1:A:304:ASN:O	2.54	0.49
1:A:131:TRP:CG	1:A:133:PRO:HD2	2.47	0.49
1:A:153:ILE:O	1:A:154:ASP:C	2.55	0.49
1:A:259:GLN:HG2	1:A:304:ASN:HD21	1.74	0.49
1:A:183:ASN:O	1:A:184:ASN:C	2.55	0.49
1:A:366:TYR:N	1:A:366:TYR:CD2	2.79	0.49
1:B:117:LYS:HE3	1:B:150:ASP:O	2.12	0.49
1:B:113:TRP:HH2	1:B:151:MET:HG2	1.78	0.49
1:B:154:ASP:C	1:B:156:ASP:H	2.17	0.48
1:B:277:TYR:CE2	1:B:281:MET:HB3	2.48	0.48
1:B:155:LYS:HE3	1:B:157:LYS:CE	2.38	0.48
1:B:132:PRO:HB2	1:B:133:PRO:HD3	1.96	0.48
1:A:102:ILE:HA	1:A:213:VAL:HB	1.96	0.48
1:A:134:VAL:O	1:A:137:ILE:HG22	2.13	0.48
1:A:99:ILE:HD12	1:A:162:LEU:HD11	1.96	0.47
1:A:201:LEU:HD21	1:A:205:LYS:HE3	1.95	0.47
1:A:151:MET:O	1:A:153:ILE:HD12	2.14	0.47
1:A:128:PHE:CZ	1:A:159:MET:HE1	2.49	0.47
1:B:120:SER:O	1:B:123:ASN:N	2.31	0.47
1:B:217:ALA:CB	1:B:281:MET:HE1	2.32	0.47
1:A:136:ASN:HD21	1:A:189:MET:HE2	1.79	0.47
1:A:151:MET:HE3	1:A:158:LYS:HZ1	1.78	0.47
1:B:106:GLY:O	1:B:107:ASP:CB	2.62	0.47
1:B:183:ASN:CA	1:B:188:ASN:HD21	2.26	0.47
1:B:223:GLN:HE21	1:B:324:ASN:HB3	1.77	0.47
1:B:294:VAL:O	1:B:297:TYR:HB3	2.14	0.47
1:A:277:TYR:CZ	1:A:281:MET:HB3	2.50	0.47
1:A:401:ARG:C	1:A:403:SER:H	2.22	0.47
1:A:404:ARG:HH21	1:B:384:GLN:NE2	2.12	0.47
1:B:165:LEU:CD1	1:B:201:LEU:HD12	2.43	0.47
1:B:291:ASP:O	1:B:295:LEU:HG	2.15	0.47
1:B:390:ASP:O	1:B:394:VAL:HG23	2.15	0.47
1:A:269:ALA:HA	1:A:274:VAL:HG12	1.97	0.47
1:A:382:LEU:HD22	1:B:407:THR:HG21	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:THR:HA	1:B:285:LYS:HD2	1.96	0.47
1:A:203:HIS:HB2	1:A:255:ILE:HG21	1.97	0.47
1:B:108:THR:HA	1:B:113:TRP:HB2	1.97	0.47
1:A:208:LYS:HA	1:A:255:ILE:O	2.15	0.46
1:B:210:ASN:HB3	1:B:257:LYS:HE3	1.96	0.46
1:B:245:LEU:HD22	1:B:288:LEU:HD11	1.96	0.46
1:A:413:VAL:HG13	1:B:405:ALA:HB3	1.97	0.46
1:B:179:GLU:O	1:B:182:LYS:HB3	2.16	0.46
1:B:276:GLY:HA2	1:B:325:LYS:NZ	2.31	0.46
1:B:373:ILE:O	1:B:377:GLU:HG3	2.15	0.46
1:B:158:LYS:O	1:B:159:MET:C	2.59	0.46
1:B:252:PHE:CD1	1:B:255:ILE:HD11	2.50	0.46
1:A:218:ASN:HA	3:A:500:TN5:HN12	1.81	0.46
1:B:418:ASN:H	1:B:418:ASN:ND2	2.10	0.46
1:A:274:VAL:HG13	1:A:274:VAL:O	2.16	0.45
1:A:384:GLN:H	1:A:384:GLN:NE2	2.14	0.45
1:A:384:GLN:H	1:A:384:GLN:HE21	1.64	0.45
1:B:117:LYS:HE2	1:B:152:ILE:O	2.17	0.45
1:B:128:PHE:HB3	1:B:130:ILE:CD1	2.47	0.45
1:B:178:ASP:OD2	1:B:178:ASP:C	2.59	0.45
1:A:267:TYR:C	1:A:269:ALA:H	2.25	0.45
1:A:216:LEU:HD12	1:A:216:LEU:O	2.16	0.45
1:B:208:LYS:HA	1:B:255:ILE:O	2.16	0.45
1:B:391:ILE:HA	1:B:413:VAL:HG11	1.99	0.45
1:A:163:ASP:C	1:A:164:MET:HG3	2.42	0.45
1:A:216:LEU:HD12	1:A:216:LEU:C	2.42	0.45
1:B:108:THR:HG22	1:B:113:TRP:CZ3	2.51	0.45
1:B:231:ARG:O	1:B:235:LEU:HG	2.17	0.45
1:B:296:ALA:HA	1:B:307:ILE:HG22	1.99	0.44
1:A:173:THR:OG1	1:A:175:ASN:ND2	2.51	0.44
1:A:137:ILE:HD12	1:A:137:ILE:HA	1.81	0.44
1:A:155:LYS:O	1:A:156:ASP:C	2.61	0.44
1:A:223:GLN:HE21	1:A:324:ASN:HB3	1.82	0.44
1:A:320:ALA:HB1	1:A:369:ILE:HD13	1.99	0.44
1:B:245:LEU:HD22	1:B:288:LEU:CD1	2.47	0.44
1:B:314:PRO:HA	2:B:451:NAD:O7N	2.17	0.44
1:A:135:TYR:O	1:A:138:PHE:HB3	2.17	0.44
1:A:253:VAL:HG13	1:A:254:ASN:N	2.33	0.44
1:A:301:ARG:NH2	1:B:424:ASP:OD2	2.49	0.44
1:B:177:ILE:HD11	1:B:182:LYS:HE3	2.00	0.44
1:B:252:PHE:CE1	1:B:255:ILE:HD11	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ARG:O	1:B:123:ASN:HB2	2.18	0.44
1:B:366:TYR:N	1:B:366:TYR:CD2	2.86	0.44
1:A:263:ILE:HG23	1:A:399:LEU:CD2	2.48	0.44
1:B:217:ALA:HB3	3:B:501:TN5:CL14	2.54	0.44
1:A:181:THR:HB	1:A:187:TYR:CD2	2.52	0.43
1:A:201:LEU:C	1:A:201:LEU:HD13	2.43	0.43
1:A:253:VAL:CG1	1:A:254:ASN:N	2.80	0.43
1:B:222:VAL:HG21	3:B:501:TN5:H5	1.99	0.43
1:A:293:ARG:O	1:A:296:ALA:HB3	2.17	0.43
1:B:131:TRP:CD1	1:B:132:PRO:HD2	2.53	0.43
1:B:151:MET:HB3	1:B:159:MET:HB2	2.00	0.43
1:A:269:ALA:CB	1:A:277:TYR:CD2	3.01	0.43
1:A:253:VAL:HG23	1:A:305:ILE:HD12	2.01	0.43
1:A:234:TYR:HD1	1:A:235:LEU:HD23	1.84	0.43
1:A:404:ARG:NH1	1:B:387:LEU:HD12	2.34	0.43
1:A:416:GLY:O	1:A:419:ILE:HG12	2.18	0.43
1:B:148:ASP:HA	1:B:151:MET:CE	2.48	0.43
1:A:186:ARG:NH2	1:A:189:MET:SD	2.91	0.43
1:A:306:ARG:NH1	1:A:403:SER:O	2.52	0.43
1:A:414:ASP:OD1	1:A:418:ASN:ND2	2.51	0.43
1:B:101:PHE:CD1	1:B:252:PHE:CZ	3.07	0.43
1:B:162:LEU:HD21	1:B:206:TYR:CE1	2.53	0.43
1:B:189:MET:HG3	1:B:190:LEU:HD23	2.00	0.43
1:A:319:ALA:HB1	3:A:500:TN5:C2	2.49	0.43
1:B:418:ASN:ND2	1:B:418:ASN:N	2.66	0.43
1:A:132:PRO:CB	1:A:133:PRO:HD3	2.46	0.42
1:A:177:ILE:O	1:A:177:ILE:CG2	2.65	0.42
1:A:218:ASN:HA	3:A:500:TN5:N1	2.34	0.42
1:A:315:LEU:N	2:A:450:NAD:O7N	2.52	0.42
1:B:120:SER:O	1:B:121:LYS:C	2.62	0.42
1:B:263:ILE:HD11	1:B:395:ALA:HB1	2.00	0.42
1:A:171:PHE:HZ	1:A:181:THR:HG21	1.84	0.42
1:B:111:TYR:O	1:B:115:ILE:HG13	2.19	0.42
1:A:153:ILE:HD11	1:A:159:MET:HB2	2.02	0.42
1:A:201:LEU:CD1	1:A:205:LYS:HD2	2.49	0.42
1:A:267:TYR:C	1:A:269:ALA:N	2.77	0.42
1:A:105:ILE:HD11	1:A:113:TRP:HE3	1.85	0.42
1:B:162:LEU:CD2	1:B:162:LEU:C	2.93	0.42
1:A:113:TRP:CZ2	1:A:151:MET:HG2	2.55	0.42
1:B:183:ASN:HA	1:B:188:ASN:ND2	2.32	0.42
1:A:119:LEU:O	1:A:124:VAL:HG13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:O	1:B:120:SER:HB2	2.20	0.42
1:B:155:LYS:O	1:B:156:ASP:C	2.63	0.41
1:B:391:ILE:N	1:B:391:ILE:HD12	2.35	0.41
1:A:105:ILE:HD12	1:A:128:PHE:CE1	2.56	0.41
1:A:271:GLN:O	1:A:272:LYS:HD3	2.20	0.41
1:A:174:ALA:HA	1:A:194:THR:HG21	2.00	0.41
1:B:301:ARG:HH11	1:B:301:ARG:CG	2.32	0.41
1:A:169:ALA:H	2:A:450:NAD:C2A	2.30	0.41
1:B:317:SER:O	1:B:318:ARG:C	2.62	0.41
1:A:375:TYR:CD1	1:A:375:TYR:C	2.98	0.41
1:B:216:LEU:C	1:B:216:LEU:HD12	2.45	0.41
1:B:253:VAL:CG2	1:B:305:ILE:HD12	2.51	0.41
1:B:417:LEU:HD23	1:B:417:LEU:HA	1.90	0.41
1:A:118:GLU:HG3	1:A:392:GLY:C	2.46	0.41
1:B:136:ASN:OD1	1:B:189:MET:SD	2.79	0.41
1:A:323:ILE:O	1:A:324:ASN:HB3	2.21	0.41
1:A:394:VAL:HG22	1:B:397:PHE:HZ	1.85	0.41
1:A:203:HIS:O	1:A:207:GLY:HA2	2.22	0.40
1:B:225:ASP:O	1:B:226:LEU:C	2.64	0.40
1:B:325:LYS:HA	1:B:325:LYS:HD3	1.92	0.40
1:B:126:ILE:O	1:B:162:LEU:HB3	2.21	0.40
1:B:268:HIS:C	1:B:270:SER:H	2.30	0.40
1:B:120:SER:HB2	1:B:153:ILE:HD11	2.02	0.40
1:B:137:ILE:CD1	1:B:140:LYS:HD3	2.51	0.40
1:B:143:LYS:C	1:B:145:GLY:H	2.29	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	285/336 (85%)	247 (87%)	30 (10%)	8 (3%)	4 15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	285/336 (85%)	250 (88%)	28 (10%)	7 (2%)	4	17
All	All	570/672 (85%)	497 (87%)	58 (10%)	15 (3%)	4	17

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	ASP
1	A	155	LYS
1	B	107	ASP
1	B	155	LYS
1	A	156	ASP
1	A	404	ARG
1	B	154	ASP
1	B	159	MET
1	B	226	LEU
1	B	367	THR
1	A	324	ASN
1	A	367	THR
1	A	268	HIS
1	A	106	GLY
1	B	127	ILE

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	250/295 (85%)	235 (94%)	15 (6%)	17	47
1	B	250/295 (85%)	232 (93%)	18 (7%)	13	39
All	All	500/590 (85%)	467 (93%)	33 (7%)	15	43

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	130	ILE
1	A	137	ILE
1	A	165	LEU
1	A	175	ASN
1	A	227	LEU
1	A	238	LEU
1	A	240	LYS
1	A	265	LEU
1	A	273	VAL
1	A	282	SER
1	A	366	TYR
1	A	382	LEU
1	A	384	GLN
1	A	417	LEU
1	B	124	VAL
1	B	130	ILE
1	B	162	LEU
1	B	165	LEU
1	B	181	THR
1	B	182	LYS
1	B	200	ASN
1	B	204	GLN
1	B	226	LEU
1	B	227	LEU
1	B	273	VAL
1	B	274	VAL
1	B	366	TYR
1	B	367	THR
1	B	382	LEU
1	B	417	LEU
1	B	418	ASN
1	B	425	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	136	ASN
1	A	144	ASN
1	A	160	ASN
1	A	175	ASN
1	A	183	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	188	ASN
1	A	200	ASN
1	A	203	HIS
1	A	218	ASN
1	A	223	GLN
1	A	228	ASN
1	A	254	ASN
1	A	259	GLN
1	A	302	ASN
1	A	304	ASN
1	A	384	GLN
1	A	409	GLN
1	B	109	ASN
1	B	184	ASN
1	B	188	ASN
1	B	192	ASN
1	B	200	ASN
1	B	210	ASN
1	B	223	GLN
1	B	228	ASN
1	B	254	ASN
1	B	259	GLN
1	B	302	ASN
1	B	304	ASN
1	B	384	GLN
1	B	415	ASN
1	B	418	ASN

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
3	TN5	B	501	-	18,18,18	6.59	15 (83%)	25,25,25	1.81	7 (28%)
2	NAD	A	450	-	46,48,48	2.43	11 (23%)	64,73,73	2.69	15 (23%)
2	NAD	B	451	-	46,48,48	2.70	9 (19%)	64,73,73	2.61	15 (23%)
3	TN5	A	500	-	18,18,18	6.85	15 (83%)	25,25,25	1.63	8 (32%)

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	TN5	B	501	-	-	0/4/4/4	0/2/2/2
2	NAD	A	450	-	-	7/30/62/62	0/5/5/5
2	NAD	B	451	-	-	8/30/62/62	0/5/5/5
3	TN5	A	500	-	-	0/4/4/4	0/2/2/2

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	TN5	C3-C4	12.01	1.58	1.39
3	B	501	TN5	C3-C4	10.82	1.56	1.39
3	A	500	TN5	C1-C2	10.81	1.58	1.39
3	B	501	TN5	C7-C8	10.41	1.53	1.38
3	B	501	TN5	C1-C2	10.38	1.57	1.39
3	A	500	TN5	C7-C8	10.25	1.53	1.38
2	B	451	NAD	PN-O3	-9.69	1.49	1.59
3	A	500	TN5	C10-C11	8.83	1.53	1.38
3	A	500	TN5	C6-C1	8.75	1.57	1.39
3	B	501	TN5	C4-N1	8.65	1.69	1.38
3	A	500	TN5	C4-N1	8.62	1.69	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	451	NAD	C2N-N1N	8.49	1.44	1.35
3	B	501	TN5	C10-C11	8.18	1.52	1.38
2	A	450	NAD	C2N-N1N	8.18	1.44	1.35
3	B	501	TN5	C6-C1	7.95	1.56	1.39
3	A	500	TN5	C3-C2	7.80	1.51	1.38
2	B	451	NAD	PA-O3	-7.58	1.51	1.59
2	A	450	NAD	PN-O3	-7.39	1.51	1.59
3	B	501	TN5	C3-C2	7.37	1.50	1.38
3	B	501	TN5	C7-C12	6.99	1.49	1.38
3	A	500	TN5	C7-C12	6.50	1.48	1.38
3	A	500	TN5	C11-C12	5.78	1.48	1.38
3	A	500	TN5	C10-C9	5.57	1.51	1.39
3	B	501	TN5	C10-C9	5.54	1.51	1.39
3	B	501	TN5	C11-C12	5.43	1.48	1.38
2	A	450	NAD	O7N-C7N	5.28	1.34	1.24
3	A	500	TN5	C12-CL13	-5.15	1.62	1.74
3	B	501	TN5	C8-C9	5.09	1.49	1.40
2	B	451	NAD	O7N-C7N	5.07	1.33	1.24
3	A	500	TN5	C8-C9	5.04	1.49	1.40
2	A	450	NAD	PA-O3	-4.86	1.54	1.59
3	B	501	TN5	C12-CL13	-4.68	1.63	1.74
2	A	450	NAD	C5N-C4N	4.37	1.46	1.38
2	B	451	NAD	C5N-C4N	3.88	1.45	1.38
3	A	500	TN5	O1-C1	3.87	1.47	1.39
3	B	501	TN5	O1-C1	3.76	1.47	1.39
2	A	450	NAD	C4A-N3A	3.70	1.41	1.34
2	B	451	NAD	C4A-N3A	3.66	1.41	1.34
2	B	451	NAD	C6N-C5N	3.47	1.45	1.38
2	A	450	NAD	C6N-C5N	3.36	1.45	1.38
3	B	501	TN5	C2-CL14	-2.71	1.67	1.73
3	B	501	TN5	C5-C4	2.61	1.45	1.40
2	B	451	NAD	O4D-C1D	2.47	1.44	1.40
3	A	500	TN5	C5-C4	2.43	1.45	1.40
2	A	450	NAD	C5A-C4A	2.27	1.43	1.39
2	A	450	NAD	O4D-C1D	2.27	1.43	1.40
3	A	500	TN5	C2-CL14	-2.11	1.68	1.73
2	B	451	NAD	C6N-N1N	2.06	1.40	1.35
2	A	450	NAD	C4A-N9A	2.05	1.41	1.37
2	A	450	NAD	C2A-N1A	2.03	1.37	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	450	NAD	C5N-C4N-C3N	9.04	129.26	120.36
2	B	451	NAD	C5N-C4N-C3N	8.87	129.09	120.36
2	A	450	NAD	C2N-C3N-C4N	-8.15	108.77	118.26
2	B	451	NAD	C2N-C3N-C4N	-7.85	109.13	118.26
2	B	451	NAD	O7N-C7N-N7N	-7.55	111.71	122.62
2	A	450	NAD	O7N-C7N-N7N	-7.43	111.88	122.62
2	A	450	NAD	C1B-N9A-C8A	7.05	142.73	127.09
2	B	451	NAD	C1B-N9A-C8A	7.02	142.68	127.09
2	A	450	NAD	C4D-O4D-C1D	-6.53	103.95	109.92
2	B	451	NAD	C3N-C7N-N7N	6.29	125.48	117.74
2	A	450	NAD	C3N-C7N-N7N	6.17	125.33	117.74
2	B	451	NAD	C4A-N9A-C1B	-5.57	113.60	126.63
2	A	450	NAD	C4A-N9A-C1B	-5.36	114.09	126.63
2	B	451	NAD	C4D-O4D-C1D	-5.23	105.13	109.92
3	B	501	TN5	O1-C9-C8	4.81	124.72	116.59
3	A	500	TN5	O1-C9-C8	3.82	123.05	116.59
2	A	450	NAD	O2A-PA-O3	-3.57	97.64	107.27
2	B	451	NAD	C2N-C3N-C7N	3.13	128.49	119.46
2	B	451	NAD	O2A-PA-O3	-3.13	98.82	107.27
2	A	450	NAD	C2N-C3N-C7N	3.00	128.11	119.46
2	A	450	NAD	O3-PA-O1A	2.86	119.31	110.70
3	B	501	TN5	O1-C1-C6	2.70	127.83	120.74
3	B	501	TN5	C1-O1-C9	2.70	124.52	118.09
3	B	501	TN5	C6-C5-C4	2.68	123.94	120.66
3	A	500	TN5	C3-C2-C1	-2.64	117.66	121.01
2	A	450	NAD	C5N-C6N-N1N	-2.64	116.78	120.38
2	B	451	NAD	O7N-C7N-C3N	2.62	122.81	119.60
2	A	450	NAD	O7N-C7N-C3N	2.61	122.78	119.60
2	B	451	NAD	O3-PA-O1A	2.59	118.48	110.70
3	A	500	TN5	O1-C1-C6	2.53	127.38	120.74
2	A	450	NAD	C4A-N9A-C8A	-2.44	103.18	105.74
3	A	500	TN5	C6-C5-C4	2.39	123.58	120.66
3	A	500	TN5	C1-O1-C9	2.36	123.72	118.09
3	B	501	TN5	C7-C12-CL13	2.34	122.10	119.17
2	B	451	NAD	C5N-C6N-N1N	-2.27	117.28	120.38
3	B	501	TN5	O1-C1-C2	-2.19	114.61	119.51
3	B	501	TN5	C3-C4-N1	-2.18	116.89	120.56
3	A	500	TN5	O1-C1-C2	-2.11	114.80	119.51
2	B	451	NAD	O3B-C3B-C4B	-2.10	105.05	111.08
2	A	450	NAD	C6N-C5N-C4N	-2.07	116.46	119.45
2	B	451	NAD	C2B-C3B-C4B	2.06	106.59	102.61
3	A	500	TN5	C3-C4-N1	-2.04	117.12	120.56
3	A	500	TN5	C1-C2-CL14	2.03	121.77	119.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	451	NAD	O5D-PN-O1N	2.01	116.90	108.94
2	A	450	NAD	O2N-PN-O5D	-2.01	98.47	107.57

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	450	NAD	C5D-O5D-PN-O3
2	A	450	NAD	C5D-O5D-PN-O1N
2	A	450	NAD	C5D-O5D-PN-O2N
2	A	450	NAD	O4D-C1D-N1N-C2N
2	B	451	NAD	C5B-O5B-PA-O2A
2	B	451	NAD	C5D-O5D-PN-O3
2	B	451	NAD	C5D-O5D-PN-O1N
2	B	451	NAD	O4B-C4B-C5B-O5B
2	B	451	NAD	C3B-C4B-C5B-O5B
2	B	451	NAD	C5B-O5B-PA-O1A
2	B	451	NAD	C5D-O5D-PN-O2N
2	A	450	NAD	O4B-C4B-C5B-O5B
2	A	450	NAD	O4D-C1D-N1N-C6N
2	A	450	NAD	C3B-C4B-C5B-O5B
2	B	451	NAD	C4B-C5B-O5B-PA

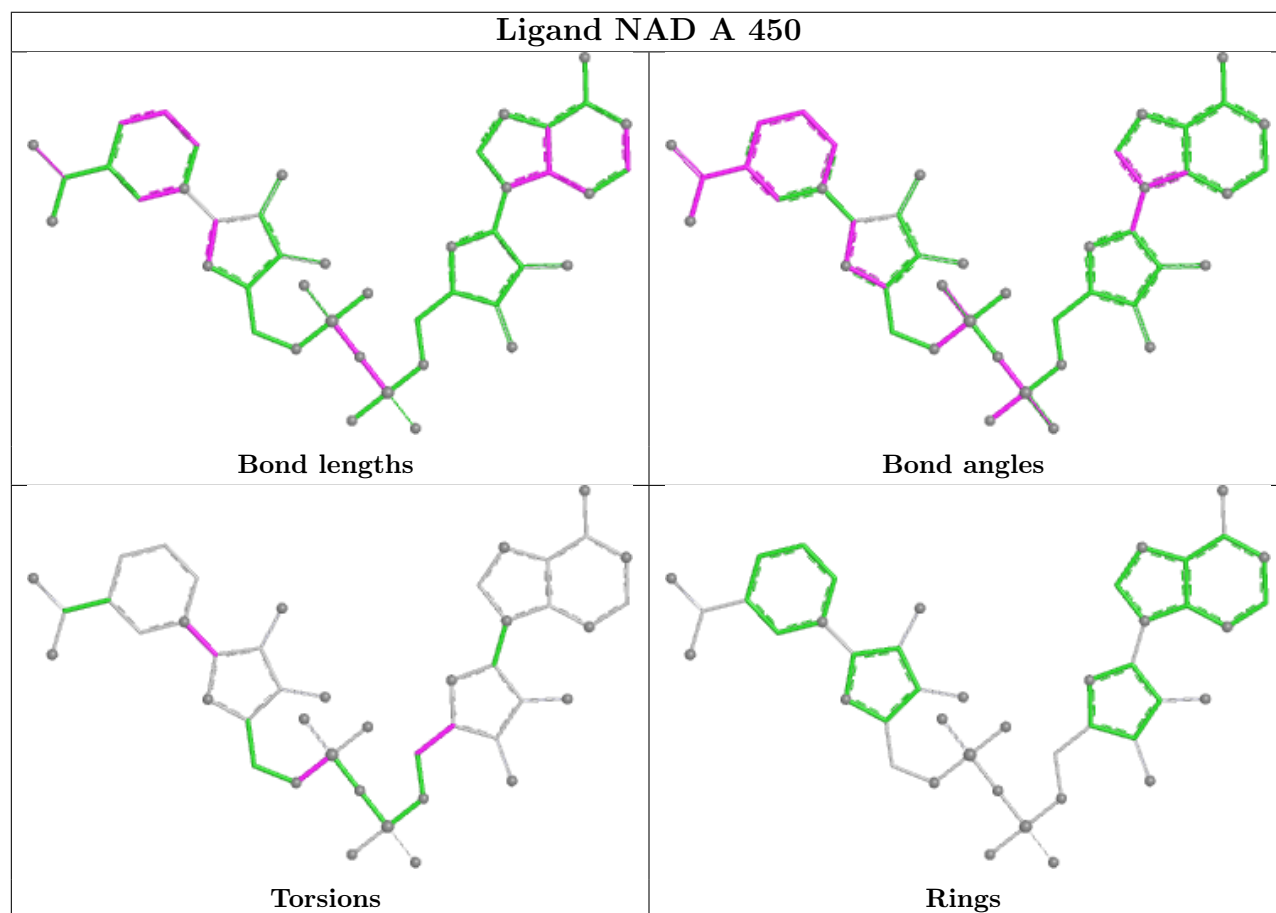
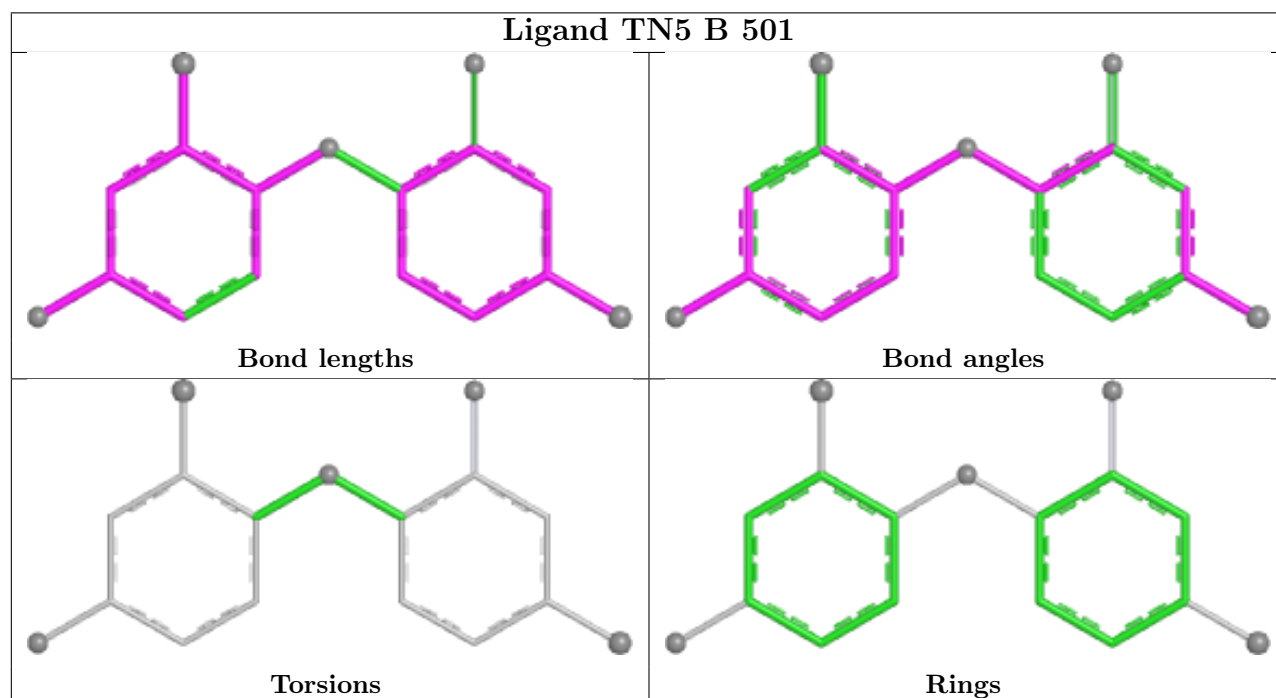
There are no ring outliers.

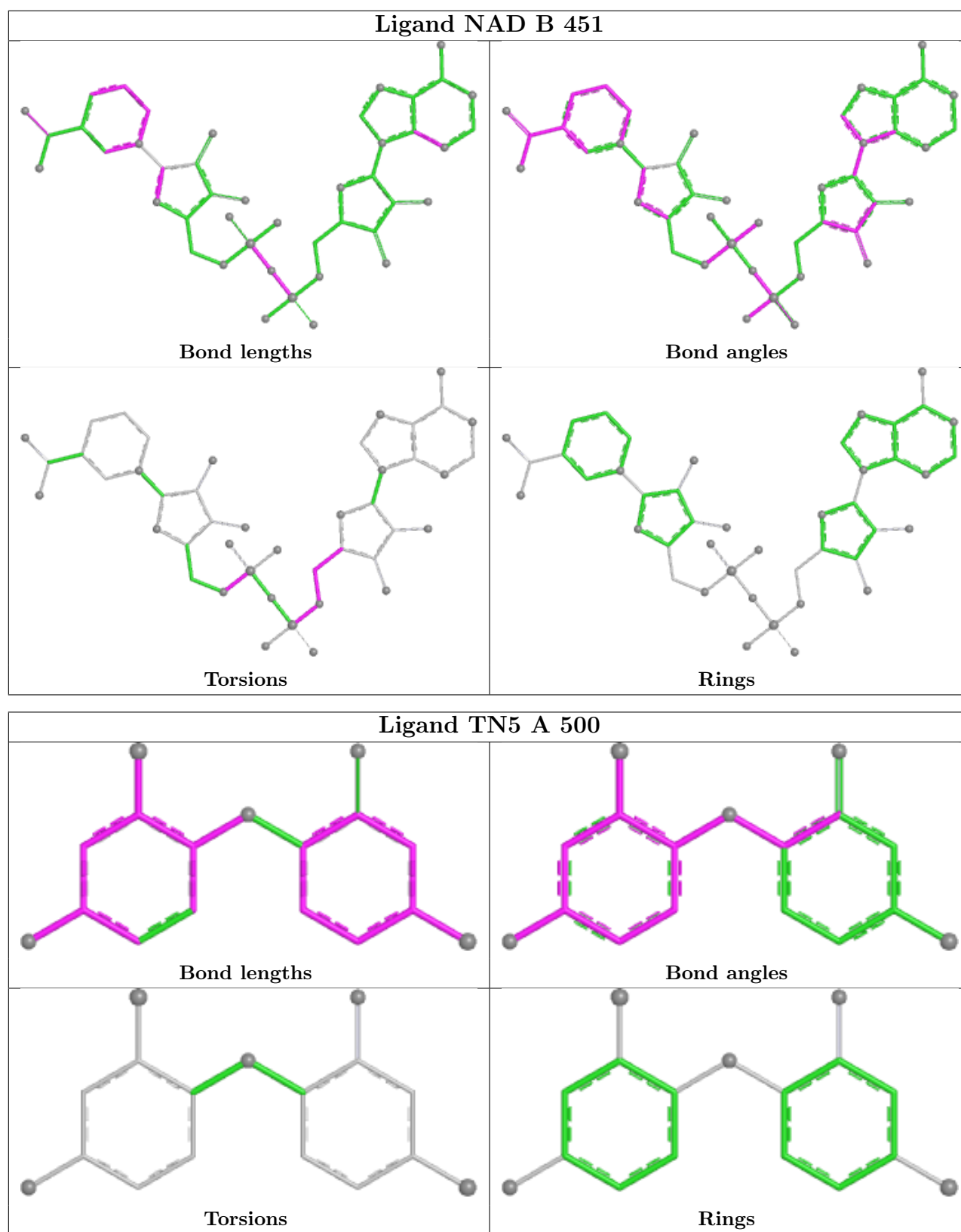
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	TN5	3	0
2	A	450	NAD	2	0
2	B	451	NAD	2	0
3	A	500	TN5	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

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

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	289/336 (86%)	1.14	50 (17%) 4 3	7, 25, 62, 76	0
1	B	289/336 (86%)	1.14	52 (17%) 3 3	7, 26, 67, 85	0
All	All	578/672 (86%)	1.14	102 (17%) 4 3	7, 26, 66, 85	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	ASP	6.7
1	A	366	TYR	6.1
1	A	179	GLU	5.1
1	B	155	LYS	5.0
1	B	324	ASN	4.9
1	B	149	ASN	4.5
1	A	324	ASN	4.5
1	A	183	ASN	4.4
1	B	425	ASP	4.2
1	A	175	ASN	4.2
1	B	152	ILE	4.1
1	B	160	ASN	3.9
1	B	366	TYR	3.9
1	A	423	PRO	3.6
1	B	159	MET	3.6
1	B	177	ILE	3.5
1	B	325	LYS	3.5
1	A	177	ILE	3.4
1	B	135	TYR	3.4
1	A	156	ASP	3.2
1	B	179	GLU	3.2
1	A	422	LEU	3.2
1	A	258	PRO	3.2
1	A	325	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	157	LYS	3.1
1	B	136	ASN	3.0
1	B	103	ALA	3.0
1	B	378	LYS	2.9
1	A	425	ASP	2.9
1	B	154	ASP	2.9
1	A	240	LYS	2.9
1	B	109	ASN	2.9
1	A	155	LYS	2.9
1	A	191	GLN	2.9
1	B	223	GLN	2.8
1	A	260	SER	2.8
1	A	158	LYS	2.8
1	B	147	PHE	2.8
1	A	300	GLY	2.8
1	A	186	ARG	2.7
1	A	383	ARG	2.7
1	B	375	TYR	2.7
1	B	142	TYR	2.7
1	B	371	TYR	2.7
1	B	207	GLY	2.7
1	A	144	ASN	2.7
1	A	184	ASN	2.7
1	B	254	ASN	2.7
1	B	368	PHE	2.6
1	A	185	LYS	2.6
1	A	189	MET	2.6
1	B	367	THR	2.6
1	B	422	LEU	2.6
1	A	323	ILE	2.6
1	A	180	GLU	2.6
1	B	303	TYR	2.6
1	B	321	THR	2.6
1	A	107	ASP	2.6
1	A	122	ARG	2.5
1	B	153	ILE	2.5
1	A	164	MET	2.5
1	B	318	ARG	2.5
1	A	146	LYS	2.5
1	B	122	ARG	2.4
1	B	141	ASN	2.4
1	B	144	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	182	LYS	2.4
1	B	116	ALA	2.4
1	A	137	ILE	2.4
1	B	110	GLY	2.3
1	A	393	SER	2.3
1	B	282	SER	2.3
1	A	297	TYR	2.3
1	B	129	GLY	2.3
1	A	259	GLN	2.2
1	A	178	ASP	2.2
1	B	167	PHE	2.2
1	B	97	GLU	2.2
1	B	322	ALA	2.2
1	B	385	LYS	2.2
1	B	323	ILE	2.2
1	B	384	GLN	2.2
1	B	401	ARG	2.2
1	A	181	THR	2.2
1	B	423	PRO	2.2
1	A	208	LYS	2.2
1	A	160	ASN	2.2
1	B	158	LYS	2.2
1	A	124	VAL	2.2
1	A	371	TYR	2.2
1	A	264	SER	2.1
1	A	369	ILE	2.1
1	A	424	ASP	2.1
1	B	150	ASP	2.1
1	A	384	GLN	2.1
1	B	189	MET	2.1
1	A	367	THR	2.1
1	B	156	ASP	2.1
1	B	238	LEU	2.1
1	A	149	ASN	2.0
1	A	299	LEU	2.0
1	B	121	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

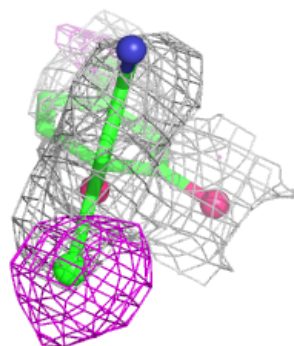
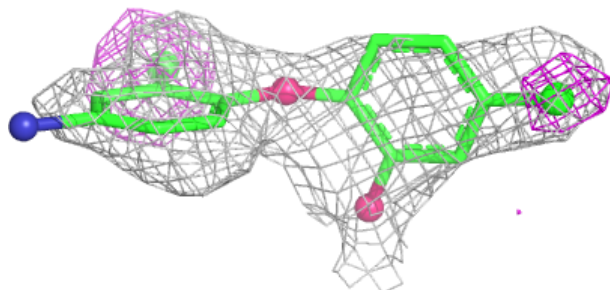
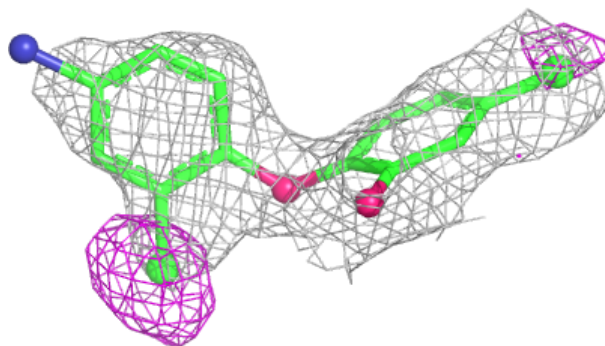
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TN5	B	501	17/17	0.70	0.24	25,30,33,34	0
3	TN5	A	500	17/17	0.81	0.18	9,19,20,21	0
2	NAD	A	450	44/44	0.87	0.17	29,38,58,58	0
2	NAD	B	451	44/44	0.92	0.11	20,27,31,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

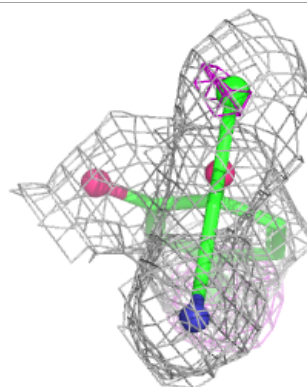
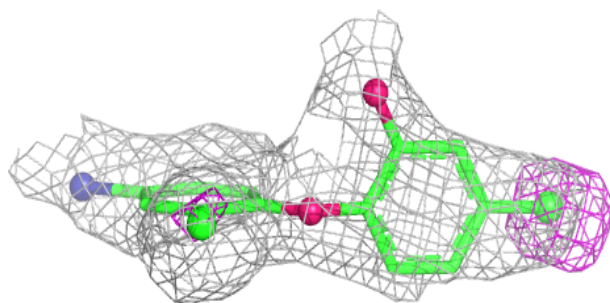
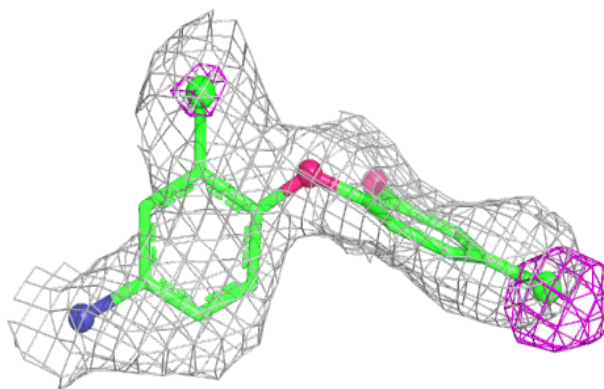
Electron density around TN5 B 501:

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

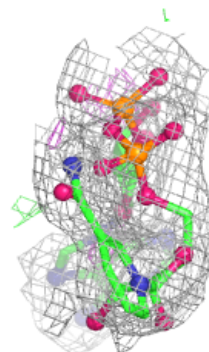
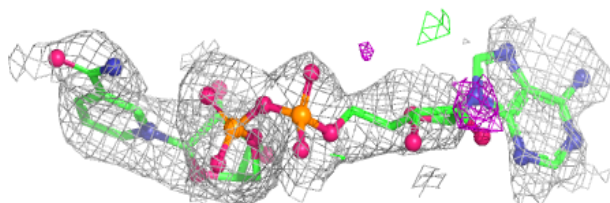
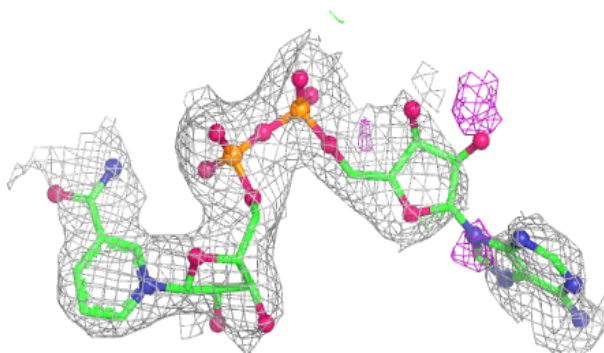


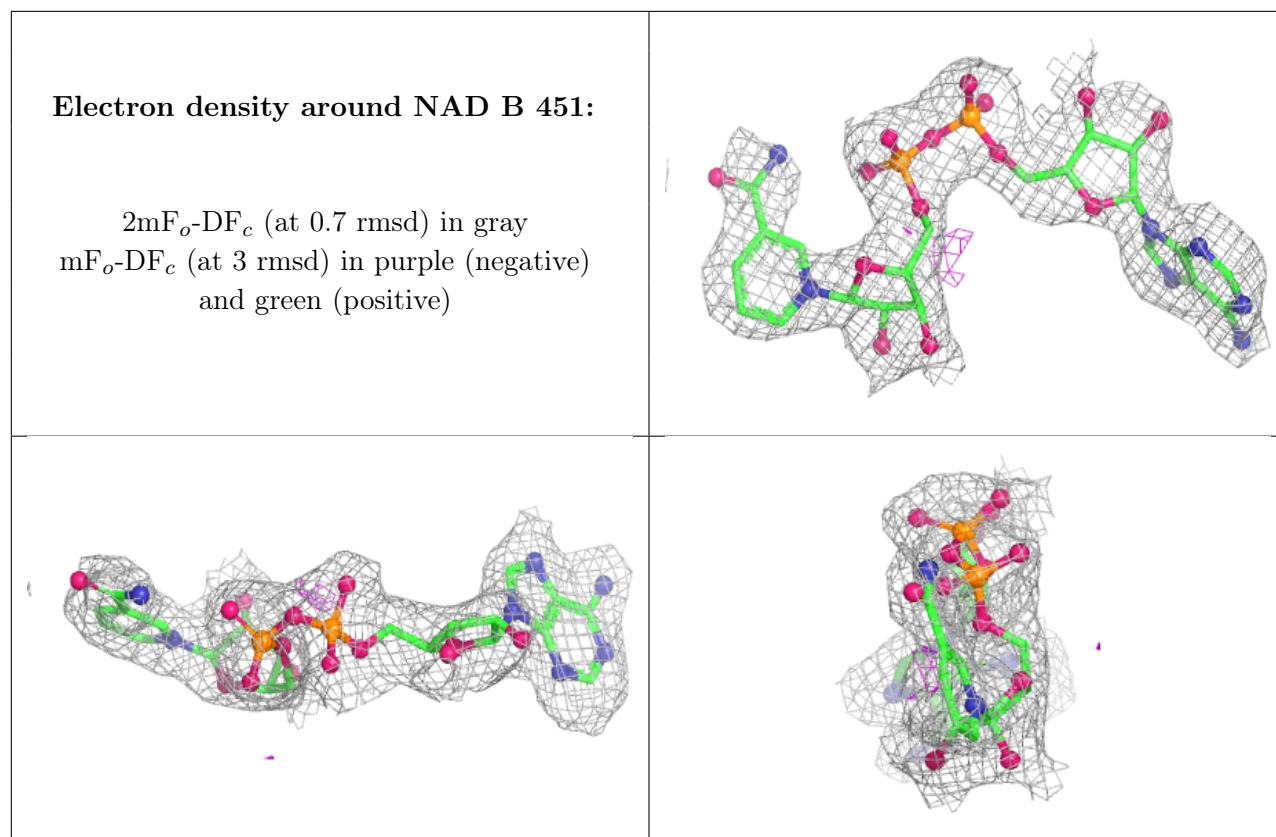
Electron density around TN5 A 500:

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

**Electron density around NAD A 450:**

$2mF_o-DF_c$ (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.