Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 01:22 AM EDT

PDB ID	:	3FNE
Title	:	Crystal structure of InhA bound to triclosan derivative 17
Authors	:	Wang, F.
Deposited on	:	2008-12-24
Resolution	:	1.98 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 (i) 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 (i)) were used in the production of this report:

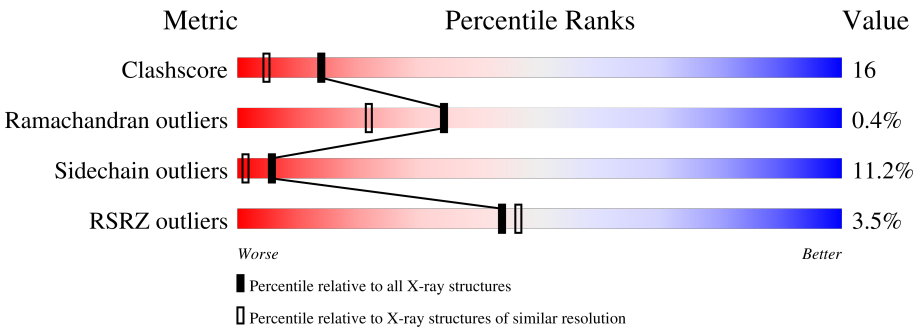
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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))
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 <=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	.% 71% 23% • •
1	B	269	6% 70% 19% 6% 6%
1	C	269	2% 71% 23% • •
1	D	269	4% 70% 23% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8797 atoms, of which 0 are hydrogens and 0 are deuteriums.

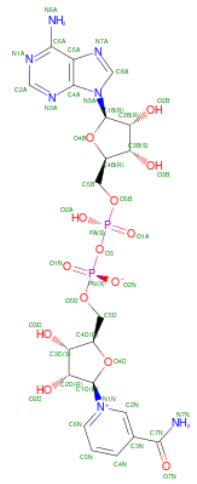
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	268	1994	1263	348	373	10	0	0	0
1	B	254	1908	1211	334	354	9	0	0	0
1	C	265	1977	1252	345	370	10	0	0	0
1	D	260	1947	1233	340	364	10	0	0	0

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

NAD



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

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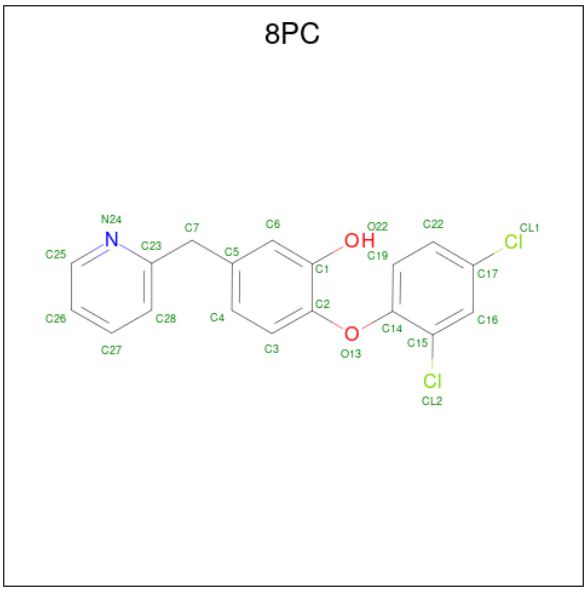
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	44	21	7	14	2	0	0
			Total	C	N	O	P		
2	D	1	44	21	7	14	2	0	0

- Molecule 3 is 2-(2,4-DICHLOROPHENOXY)-5-(PYRIDIN-2-YLMETHYL)PHENOL (three-letter code: 8PC) (formula: $C_{18}H_{13}Cl_2NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	A	1	23	18	2	1	2	0	0
			Total	C	Cl	N	O		
3	B	1	23	18	2	1	2	0	0
			Total	C	Cl	N	O		
3	C	1	23	18	2	1	2	0	0
			Total	C	Cl	N	O		
3	D	1	23	18	2	1	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	201	201	201	0	0
			Total	O		
4	B	180	180	180	0	0
			Total	O		
4	C	178	178	178	0	0

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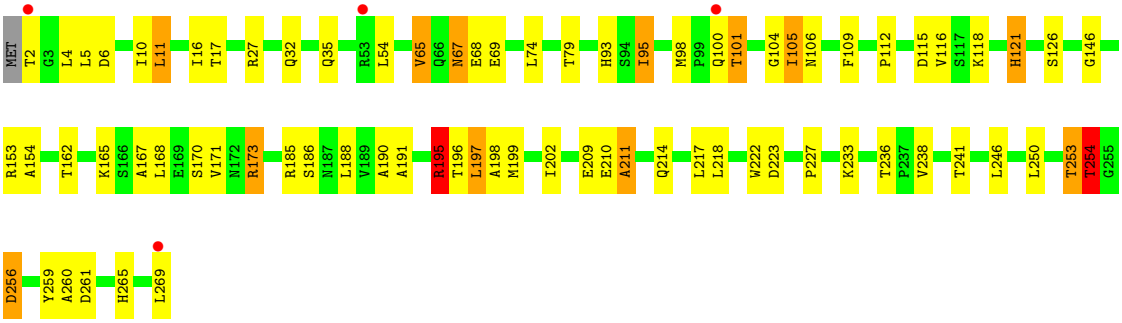
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	144	144	144	0	0

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.

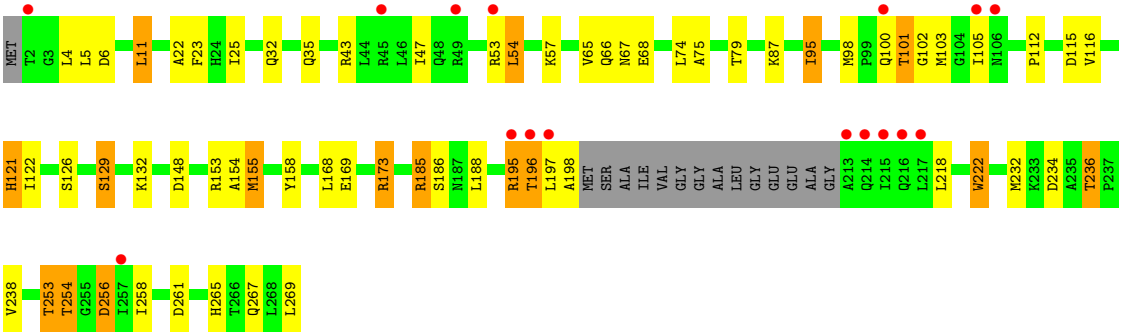
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain A:



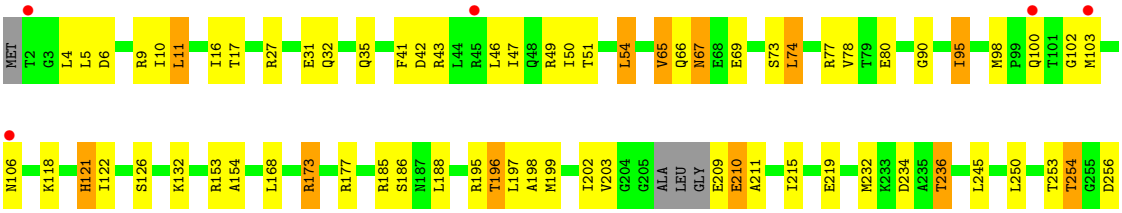
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain B:



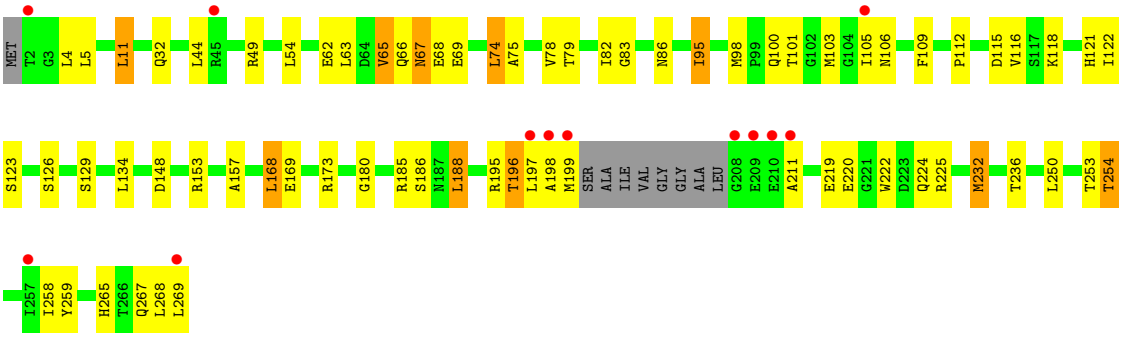
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	125.59Å 92.34Å 103.02Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	19.96 – 1.98 44.93 – 1.85	Depositor EDS
% Data completeness (in resolution range)	92.4 (19.96-1.98) 73.5 (44.93-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	0.71 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.253 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8797	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, 8PC

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	0.60	0/2032	0.83	4/2758 (0.1%)
1	B	0.61	0/1945	0.83	5/2640 (0.2%)
1	C	0.56	0/2014	0.77	2/2732 (0.1%)
1	D	0.55	0/1984	0.72	1/2691 (0.0%)
All	All	0.58	0/7975	0.79	12/10821 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	173	ARG	NE-CZ-NH2	-13.28	113.66	120.30
1	B	173	ARG	NE-CZ-NH2	-12.13	114.24	120.30
1	B	173	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	A	173	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	D	11	LEU	CA-CB-CG	7.44	132.41	115.30
1	C	173	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	11	LEU	CA-CB-CG	6.85	131.04	115.30
1	C	11	LEU	CA-CB-CG	6.79	130.93	115.30
1	B	185	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	185	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	254	THR	CB-CA-C	-5.51	96.73	111.60
1	A	11	LEU	CA-CB-CG	5.13	127.09	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1994	0	2008	77	0
1	B	1908	0	1923	67	0
1	C	1977	0	1988	67	0
1	D	1947	0	1955	70	0
2	A	44	0	26	2	0
2	B	44	0	26	1	0
2	C	44	0	26	1	0
2	D	44	0	26	1	0
3	A	23	0	12	1	0
3	B	23	0	12	3	0
3	C	23	0	12	1	0
3	D	23	0	12	2	0
4	A	201	0	0	21	0
4	B	180	0	0	16	0
4	C	178	0	0	13	0
4	D	144	0	0	8	0
All	All	8797	0	8026	255	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 16.

All (255) 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:65:VAL:HG21	1:B:126:SER:HB2	1.29	1.11
1:A:27:ARG:HH22	1:A:236:THR:HG22	1.16	1.05
1:B:87:LYS:HD3	4:B:306:HOH:O	1.61	0.98
1:D:106:ASN:HB2	4:D:279:HOH:O	1.64	0.97
1:C:254:THR:HG21	4:C:271:HOH:O	1.64	0.95
1:C:219:GLU:HG3	4:C:661:HOH:O	1.69	0.92
1:A:211:ALA:HA	1:A:214:GLN:HB2	1.51	0.92
1:A:196:THR:HB	4:A:668:HOH:O	1.73	0.89
1:A:101:THR:HG21	1:A:115:ASP:OD2	1.73	0.88
1:A:186:SER:H	1:A:254:THR:HG22	1.39	0.88
1:D:186:SER:H	1:D:254:THR:HG22	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:THR:HG21	2:A:300:NAD:O1N	1.72	0.88
1:A:79:THR:HG22	4:A:669:HOH:O	1.74	0.88
1:A:106:ASN:HB2	4:A:340:HOH:O	1.70	0.88
1:B:53:ARG:HG3	4:B:667:HOH:O	1.75	0.86
1:D:199:MET:HG3	3:D:430:8PC:H4	1.56	0.86
1:B:254:THR:HG21	4:B:273:HOH:O	1.76	0.86
1:A:265:HIS:O	1:C:153:ARG:NH1	2.08	0.86
1:C:4:LEU:H	1:C:32:GLN:HE21	1.21	0.85
1:C:186:SER:H	1:C:254:THR:HG22	1.41	0.85
4:A:270:HOH:O	1:D:253:THR:HG23	1.77	0.84
1:B:65:VAL:CG2	1:B:126:SER:HB2	2.08	0.83
1:A:4:LEU:H	1:A:32:GLN:HE21	1.25	0.81
1:C:196:THR:HG21	2:C:320:NAD:O1N	1.80	0.81
1:B:57:LYS:HD2	4:B:286:HOH:O	1.78	0.81
1:B:234:ASP:OD1	1:B:236:THR:HG23	1.80	0.81
1:A:27:ARG:NH2	1:A:236:THR:HG22	1.95	0.80
1:A:195:ARG:HH11	1:A:195:ARG:CG	1.93	0.80
1:A:196:THR:HG23	1:A:198:ALA:H	1.46	0.80
1:A:27:ARG:HH22	1:A:236:THR:CG2	1.93	0.80
1:B:4:LEU:H	1:B:32:GLN:HE21	1.31	0.79
1:D:49:ARG:HD3	4:D:288:HOH:O	1.83	0.79
1:A:254:THR:HG21	4:A:302:HOH:O	1.83	0.77
1:C:209:GLU:O	1:C:210:GLU:HB2	1.85	0.76
1:D:103:MET:O	1:D:157:ALA:O	2.04	0.75
1:C:186:SER:H	1:C:254:THR:CG2	1.98	0.75
1:D:185:ARG:HD2	4:D:322:HOH:O	1.86	0.74
1:A:256:ASP:OD2	1:D:265:HIS:HE1	1.71	0.74
1:A:185:ARG:HG2	1:A:254:THR:HG23	1.70	0.74
1:B:68:GLU:HG3	4:B:281:HOH:O	1.87	0.74
1:A:259:TYR:O	1:D:253:THR:HG22	1.89	0.73
1:C:195:ARG:HA	1:C:199:MET:HE2	1.71	0.72
1:A:196:THR:HG22	4:A:283:HOH:O	1.90	0.71
1:A:173:ARG:HB3	1:B:154:ALA:HB2	1.73	0.71
1:C:106:ASN:HB2	4:C:297:HOH:O	1.90	0.71
1:C:103:MET:HE2	1:C:202:ILE:HG12	1.71	0.71
1:B:79:THR:HG22	4:B:312:HOH:O	1.90	0.70
1:C:215:ILE:HG23	1:C:232:MET:HE1	1.72	0.70
1:B:195:ARG:HE	1:B:232:MET:HE2	1.56	0.70
1:C:195:ARG:HA	1:C:199:MET:CE	2.23	0.69
1:C:234:ASP:OD1	1:C:236:THR:HG23	1.91	0.69
1:D:254:THR:HG21	4:D:271:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:LEU:H	1:C:32:GLN:NE2	1.92	0.68
1:B:265:HIS:O	1:D:153:ARG:NH1	2.27	0.68
1:C:65:VAL:HG11	1:C:126:SER:CB	2.24	0.68
1:C:195:ARG:NH2	4:C:490:HOH:O	2.27	0.68
1:A:65:VAL:HG11	1:A:95:ILE:HD11	1.76	0.67
1:B:153:ARG:HD2	4:B:487:HOH:O	1.94	0.67
1:D:195:ARG:HG2	1:D:232:MET:HG2	1.75	0.66
1:B:155:MET:CE	1:D:268:LEU:HD22	2.26	0.66
1:C:103:MET:CE	1:C:202:ILE:HG12	2.26	0.65
1:C:245:LEU:HD11	1:C:258:ILE:HD13	1.77	0.65
1:A:185:ARG:CG	1:A:254:THR:HG23	2.26	0.65
1:D:74:LEU:HD13	1:D:134:LEU:HD21	1.78	0.65
1:C:198:ALA:HB1	3:C:420:8PC:C15	2.27	0.65
1:A:210:GLU:O	1:A:211:ALA:HB3	1.97	0.64
1:B:218:LEU:HA	1:D:269:LEU:HD21	1.78	0.64
1:D:4:LEU:H	1:D:32:GLN:HG3	1.62	0.64
1:B:57:LYS:CD	4:B:286:HOH:O	2.40	0.64
1:A:118:LYS:HE3	4:A:364:HOH:O	1.98	0.64
1:D:121:HIS:HD2	4:D:440:HOH:O	1.78	0.63
1:A:253:THR:HG22	4:D:275:HOH:O	1.98	0.63
1:B:101:THR:HG21	1:B:115:ASP:OD2	1.99	0.63
1:A:195:ARG:HH11	1:A:195:ARG:HG3	1.63	0.63
1:C:195:ARG:HG2	1:C:199:MET:HE1	1.80	0.63
1:A:153:ARG:NH2	1:C:153:ARG:HE	1.96	0.63
1:C:69:GLU:HG3	4:C:583:HOH:O	1.98	0.63
1:D:4:LEU:N	1:D:32:GLN:HG3	2.14	0.62
1:D:79:THR:HG22	4:D:324:HOH:O	1.99	0.62
1:D:196:THR:HG21	2:D:330:NAD:O1N	1.99	0.62
1:A:195:ARG:HH11	1:A:195:ARG:HG2	1.64	0.62
1:C:80:GLU:HB3	4:C:630:HOH:O	1.98	0.62
1:B:196:THR:HG23	1:B:198:ALA:H	1.65	0.61
1:D:101:THR:HG21	1:D:115:ASP:OD2	2.01	0.60
1:D:168:LEU:HD13	1:D:188:LEU:HD21	1.83	0.60
1:A:35:GLN:HB2	4:A:672:HOH:O	2.00	0.60
1:A:79:THR:CG2	4:A:669:HOH:O	2.42	0.60
1:C:65:VAL:CG1	1:C:126:SER:HB2	2.32	0.60
1:B:256:ASP:OD2	1:C:265:HIS:HE1	1.85	0.60
1:C:65:VAL:CG1	1:C:126:SER:CB	2.79	0.60
1:B:173:ARG:NH2	4:B:455:HOH:O	2.07	0.60
1:B:186:SER:H	1:B:254:THR:CG2	2.15	0.59
1:B:153:ARG:CZ	1:D:153:ARG:HE	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ARG:HE	1:B:232:MET:CE	2.15	0.59
1:B:155:MET:HE2	1:D:268:LEU:HD22	1.85	0.59
1:C:209:GLU:N	4:C:660:HOH:O	2.34	0.59
1:B:265:HIS:HE1	1:C:256:ASP:OD2	1.85	0.58
1:A:154:ALA:HB2	1:B:173:ARG:HB3	1.84	0.58
1:A:79:THR:HB	4:A:688:HOH:O	2.02	0.58
1:A:105:ILE:CD1	1:A:211:ALA:HB3	2.34	0.58
1:D:95:ILE:HD12	1:D:122:ILE:HG23	1.86	0.58
1:D:196:THR:HG23	1:D:198:ALA:H	1.67	0.57
1:A:109:PHE:HB3	1:B:132:LYS:HG3	1.87	0.57
1:A:223:ASP:HB3	4:A:408:HOH:O	2.03	0.57
1:B:185:ARG:HD2	4:B:352:HOH:O	2.05	0.57
1:B:121:HIS:HD2	4:B:337:HOH:O	1.88	0.57
1:D:83:GLY:O	1:D:86:ASN:HB2	2.04	0.57
1:B:158:TYR:HB2	3:B:410:8PC:H27	1.87	0.57
1:A:199:MET:HA	1:A:199:MET:CE	2.35	0.56
1:B:196:THR:HG21	2:B:310:NAD:O1N	2.04	0.56
1:A:210:GLU:O	1:A:211:ALA:CB	2.53	0.56
1:C:43:ARG:HB3	1:C:46:LEU:HG	1.86	0.56
1:C:196:THR:HG22	1:C:199:MET:H	1.69	0.56
1:B:79:THR:CG2	4:B:312:HOH:O	2.52	0.55
1:B:153:ARG:CZ	1:D:153:ARG:HH21	2.19	0.55
1:A:185:ARG:HA	1:A:254:THR:CG2	2.37	0.55
1:C:173:ARG:NH2	4:C:310:HOH:O	2.15	0.55
1:C:16:ILE:HG23	1:C:17:THR:HG23	1.88	0.54
1:B:66:GLN:HE21	1:B:121:HIS:CD2	2.25	0.54
1:B:98:MET:HE2	1:B:102:GLY:HA3	1.88	0.54
1:D:185:ARG:HA	1:D:254:THR:CG2	2.38	0.54
1:A:4:LEU:H	1:A:32:GLN:NE2	2.02	0.54
1:A:98:MET:CE	1:A:116:VAL:HA	2.38	0.54
1:B:222:TRP:HE1	1:B:261:ASP:HB2	1.72	0.54
1:C:65:VAL:HG11	1:C:126:SER:HB2	1.90	0.54
1:D:66:GLN:HE21	1:D:121:HIS:CD2	2.26	0.53
1:B:186:SER:H	1:B:254:THR:HG23	1.73	0.53
1:B:22:ALA:HA	1:B:25:ILE:HD12	1.89	0.53
1:C:27:ARG:O	1:C:31:GLU:HG3	2.09	0.53
1:C:185:ARG:HA	1:C:254:THR:HG23	1.90	0.53
1:B:155:MET:HE2	1:D:268:LEU:CD2	2.40	0.52
1:B:258:ILE:HD12	1:B:258:ILE:N	2.24	0.52
1:A:67:ASN:HD21	1:A:69:GLU:HB3	1.74	0.52
1:C:46:LEU:O	1:C:50:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ILE:CD1	1:D:122:ILE:HG23	2.40	0.52
1:B:148:ASP:OD2	1:B:169:GLU:OE2	2.28	0.51
1:C:65:VAL:CG1	1:C:126:SER:HB3	2.40	0.51
1:C:66:GLN:HE21	1:C:121:HIS:CD2	2.27	0.51
1:C:185:ARG:CD	4:C:311:HOH:O	2.58	0.51
1:A:105:ILE:HD11	1:A:210:GLU:O	2.11	0.51
1:A:167:ALA:O	1:A:171:VAL:HG23	2.11	0.51
1:A:227:PRO:O	1:D:180:GLY:HA3	2.11	0.50
1:B:4:LEU:H	1:B:32:GLN:NE2	2.06	0.50
1:B:153:ARG:NH2	1:D:153:ARG:HE	2.09	0.50
1:D:225:ARG:HD2	1:D:267:GLN:O	2.12	0.50
1:A:118:LYS:CE	4:A:364:HOH:O	2.56	0.50
1:A:121:HIS:HD2	4:A:339:HOH:O	1.94	0.50
1:A:185:ARG:HD3	4:A:350:HOH:O	2.12	0.50
1:C:10:ILE:HG12	1:C:90:GLY:HA3	1.92	0.50
1:D:63:LEU:HD13	1:D:74:LEU:HG	1.92	0.50
1:D:98:MET:HE3	1:D:116:VAL:HA	1.94	0.49
1:B:95:ILE:HD12	1:B:122:ILE:HG23	1.94	0.49
1:B:185:ARG:HA	1:B:254:THR:HG23	1.95	0.49
1:B:198:ALA:HB1	3:B:410:8PC:C15	2.43	0.49
1:D:4:LEU:H	1:D:32:GLN:HE21	1.60	0.48
1:D:148:ASP:OD2	1:D:169:GLU:OE2	2.31	0.48
1:A:253:THR:HB	1:D:259:TYR:O	2.14	0.48
1:A:265:HIS:HD2	4:A:285:HOH:O	1.96	0.48
1:B:267:GLN:OE1	1:C:177:ARG:HD2	2.14	0.48
1:C:65:VAL:HG11	1:C:126:SER:HB3	1.95	0.48
1:D:105:ILE:HB	1:D:211:ALA:HB2	1.96	0.48
1:A:222:TRP:HE1	1:A:261:ASP:HB2	1.79	0.48
1:B:75:ALA:O	1:B:79:THR:HG23	2.13	0.48
1:A:104:GLY:HA3	1:A:202:ILE:HD12	1.96	0.48
1:B:53:ARG:NH1	4:B:340:HOH:O	2.46	0.47
1:B:23:PHE:CE2	1:B:54:LEU:HD13	2.50	0.47
1:D:65:VAL:CG1	1:D:126:SER:HB2	2.44	0.47
1:A:153:ARG:HD2	4:A:369:HOH:O	2.14	0.47
1:C:154:ALA:HB2	1:D:173:ARG:HB3	1.96	0.47
1:B:129:SER:HB3	4:B:577:HOH:O	2.13	0.47
1:C:100:GLN:HB2	4:C:315:HOH:O	2.15	0.47
1:C:185:ARG:HA	1:C:254:THR:CG2	2.44	0.47
1:A:65:VAL:HG21	1:A:126:SER:HB2	1.96	0.47
1:A:233:LYS:HD2	4:A:388:HOH:O	2.14	0.46
1:B:101:THR:HG21	1:B:112:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ARG:HG3	1:C:232:MET:HE3	1.96	0.46
1:B:103:MET:SD	3:B:410:8PC:H22	2.55	0.46
1:B:195:ARG:HA	1:B:195:ARG:HD3	1.73	0.46
1:D:68:GLU:CG	1:D:69:GLU:N	2.78	0.46
1:A:10:ILE:HD13	1:A:246:LEU:HD13	1.97	0.46
1:B:153:ARG:NE	1:D:153:ARG:HH21	2.13	0.46
1:D:65:VAL:HG11	1:D:126:SER:CB	2.46	0.46
1:C:67:ASN:C	1:C:67:ASN:HD22	2.19	0.45
1:A:105:ILE:HD12	1:A:211:ALA:HB3	1.98	0.45
1:D:258:ILE:N	1:D:258:ILE:HD12	2.31	0.45
1:D:185:ARG:HB3	1:D:254:THR:HG23	1.99	0.45
1:C:9:ARG:NH1	1:C:35:GLN:OE1	2.50	0.45
1:A:196:THR:CB	4:A:668:HOH:O	2.47	0.45
1:A:199:MET:HA	1:A:199:MET:HE3	1.99	0.45
1:D:4:LEU:HB3	1:D:32:GLN:CG	2.47	0.45
1:A:223:ASP:CB	4:A:408:HOH:O	2.64	0.45
1:C:66:GLN:OE1	1:C:118:LYS:NZ	2.50	0.45
1:D:196:THR:HG22	1:D:199:MET:HB2	1.99	0.45
1:D:65:VAL:CG1	1:D:126:SER:CB	2.94	0.45
1:A:105:ILE:HD11	1:A:211:ALA:HB3	1.98	0.44
1:D:4:LEU:HB3	1:D:32:GLN:HG2	1.98	0.44
1:A:98:MET:HE1	1:A:116:VAL:HA	1.98	0.44
1:A:101:THR:HG21	1:A:112:PRO:HD2	1.99	0.44
1:D:126:SER:HA	1:D:129:SER:OG	2.18	0.44
1:A:165:LYS:HE2	4:A:683:HOH:O	2.17	0.44
1:C:47:ILE:O	1:C:51:THR:HG23	2.17	0.44
1:C:51:THR:O	1:C:54:LEU:HB2	2.17	0.44
1:A:191:ALA:HB3	2:A:300:NAD:C5N	2.48	0.44
1:C:132:LYS:HG3	1:D:109:PHE:HB3	2.00	0.44
1:D:67:ASN:C	1:D:67:ASN:HD22	2.21	0.43
1:A:202:ILE:HD13	1:A:202:ILE:HA	1.94	0.43
1:C:41:PHE:C	1:C:41:PHE:CD1	2.90	0.43
1:C:185:ARG:HD3	4:C:311:HOH:O	2.17	0.43
1:B:98:MET:CE	1:B:116:VAL:HA	2.49	0.43
1:A:65:VAL:HG11	1:A:95:ILE:CD1	2.46	0.43
1:C:203:VAL:HG12	1:C:211:ALA:HA	2.00	0.43
1:D:220:GLU:O	1:D:224:GLN:HG3	2.18	0.43
3:D:430:8PC:H25	4:D:673:HOH:O	2.18	0.43
1:C:95:ILE:HD12	1:C:122:ILE:HG23	2.01	0.43
1:C:185:ARG:CA	1:C:254:THR:HG23	2.48	0.43
1:D:75:ALA:O	1:D:79:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ARG:CB	1:D:254:THR:HG23	2.49	0.43
1:A:190:ALA:HB3	1:A:259:TYR:CD2	2.54	0.42
1:B:155:MET:HG3	1:B:218:LEU:HD11	2.00	0.42
1:C:74:LEU:O	1:C:78:VAL:HG23	2.19	0.42
1:D:78:VAL:O	1:D:82:ILE:HG12	2.19	0.42
1:D:196:THR:HG22	1:D:199:MET:H	1.83	0.42
1:B:265:HIS:O	1:D:153:ARG:HD3	2.19	0.42
1:D:68:GLU:HG2	1:D:69:GLU:N	2.34	0.42
1:C:98:MET:HE2	1:C:102:GLY:HA3	2.00	0.42
1:D:74:LEU:O	1:D:78:VAL:HG23	2.19	0.42
1:A:16:ILE:HG23	1:A:17:THR:HG23	2.01	0.42
1:A:17:THR:HG21	1:A:197:LEU:HD23	2.01	0.42
1:D:232:MET:HE2	1:D:232:MET:HB2	1.96	0.42
1:B:153:ARG:NH1	4:B:329:HOH:O	2.52	0.42
1:A:101:THR:CG2	1:A:115:ASP:OD2	2.58	0.41
1:A:27:ARG:NH2	1:A:236:THR:CG2	2.71	0.41
1:A:93:HIS:O	1:A:146:GLY:HA2	2.20	0.41
1:A:68:GLU:HB3	4:A:355:HOH:O	2.19	0.41
1:A:199:MET:HE1	3:A:400:8PC:H22	2.02	0.41
1:B:65:VAL:HG11	1:B:95:ILE:HD11	2.03	0.41
1:C:65:VAL:HG13	1:C:126:SER:CB	2.50	0.41
1:C:121:HIS:HD2	4:C:410:HOH:O	2.03	0.41
1:B:43:ARG:O	1:B:47:ILE:HG13	2.20	0.41
1:B:153:ARG:NH2	1:D:153:ARG:NE	2.68	0.41
1:D:219:GLU:OE2	1:D:232:MET:SD	2.78	0.41
1:B:186:SER:H	1:B:254:THR:HG22	1.86	0.41
1:B:253:THR:HB	1:C:259:TYR:O	2.21	0.41
1:C:210:GLU:N	4:C:670:HOH:O	2.54	0.41
1:D:196:THR:HG23	1:D:198:ALA:N	2.36	0.41
1:A:2:THR:O	1:A:6:ASP:OD2	2.40	0.40
1:A:186:SER:N	1:A:254:THR:HG22	2.20	0.40
1:A:241:THR:HG21	1:A:260:ALA:HB2	2.03	0.40
1:C:73:SER:O	1:C:77:ARG:HG3	2.21	0.40
1:D:101:THR:HG21	1:D:112:PRO:HD2	2.03	0.40
1:B:236:THR:HG21	4:B:563:HOH:O	2.21	0.40
1:C:16:ILE:HD11	1:C:43:ARG:HD3	2.02	0.40
1:D:44:LEU:HD21	1:D:62:GLU:HB2	2.02	0.40
1:B:218:LEU:HA	1:D:269:LEU:CD2	2.50	0.40
1:C:65:VAL:HG13	1:C:126:SER:HB2	2.03	0.40

There are no symmetry-related clashes.

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%)	252 (95%)	12 (4%)	2 (1%)	19 9
1	B	250/269 (93%)	237 (95%)	12 (5%)	1 (0%)	34 22
1	C	261/269 (97%)	246 (94%)	14 (5%)	1 (0%)	34 22
1	D	256/269 (95%)	238 (93%)	18 (7%)	0	100 100
All	All	1033/1076 (96%)	973 (94%)	56 (5%)	4 (0%)	34 22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	210	GLU
1	B	195	ARG
1	A	211	ALA
1	A	195	ARG

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	203/205 (99%)	177 (87%)	26 (13%)	4 1
1	B	196/205 (96%)	171 (87%)	25 (13%)	4 1
1	C	202/205 (98%)	182 (90%)	20 (10%)	8 1
1	D	199/205 (97%)	180 (90%)	19 (10%)	8 1
All	All	800/820 (98%)	710 (89%)	90 (11%)	6 1

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	11	LEU
1	A	54	LEU
1	A	65	VAL
1	A	67	ASN
1	A	74	LEU
1	A	95	ILE
1	A	100	GLN
1	A	101	THR
1	A	105	ILE
1	A	121	HIS
1	A	162	THR
1	A	168	LEU
1	A	170	SER
1	A	188	LEU
1	A	195	ARG
1	A	197	LEU
1	A	209	GLU
1	A	217	LEU
1	A	218	LEU
1	A	238	VAL
1	A	250	LEU
1	A	253	THR
1	A	254	THR
1	A	256	ASP
1	A	269	LEU
1	B	5	LEU
1	B	6	ASP
1	B	11	LEU
1	B	35	GLN
1	B	54	LEU
1	B	67	ASN
1	B	74	LEU
1	B	95	ILE
1	B	100	GLN
1	B	101	THR
1	B	105	ILE
1	B	121	HIS
1	B	129	SER
1	B	155	MET
1	B	168	LEU
1	B	188	LEU

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Mol	Chain	Res	Type
1	B	196	THR
1	B	197	LEU
1	B	222	TRP
1	B	236	THR
1	B	238	VAL
1	B	253	THR
1	B	254	THR
1	B	256	ASP
1	B	269	LEU
1	C	5	LEU
1	C	6	ASP
1	C	11	LEU
1	C	42	ASP
1	C	49	ARG
1	C	54	LEU
1	C	65	VAL
1	C	67	ASN
1	C	74	LEU
1	C	95	ILE
1	C	121	HIS
1	C	168	LEU
1	C	188	LEU
1	C	196	THR
1	C	197	LEU
1	C	236	THR
1	C	250	LEU
1	C	253	THR
1	C	254	THR
1	C	269	LEU
1	D	5	LEU
1	D	11	LEU
1	D	54	LEU
1	D	65	VAL
1	D	67	ASN
1	D	74	LEU
1	D	95	ILE
1	D	100	GLN
1	D	118	LYS
1	D	123	SER
1	D	168	LEU
1	D	188	LEU
1	D	196	THR

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Mol	Chain	Res	Type
1	D	197	LEU
1	D	222	TRP
1	D	232	MET
1	D	236	THR
1	D	250	LEU
1	D	254	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	67	ASN
1	A	86	ASN
1	A	100	GLN
1	A	121	HIS
1	A	187	ASN
1	A	216	GLN
1	A	265	HIS
1	B	32	GLN
1	B	35	GLN
1	B	67	ASN
1	B	86	ASN
1	B	121	HIS
1	B	187	ASN
1	B	224	GLN
1	B	265	HIS
1	C	32	GLN
1	C	67	ASN
1	C	86	ASN
1	C	121	HIS
1	C	187	ASN
1	C	265	HIS
1	D	32	GLN
1	D	66	GLN
1	D	67	ASN
1	D	86	ASN
1	D	187	ASN
1	D	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	B	310	-	42,48,48	1.72	4 (9%)	50,73,73	1.37	5 (10%)
2	NAD	A	300	-	42,48,48	1.56	3 (7%)	50,73,73	1.32	4 (8%)
3	8PC	C	420	-	25,25,25	0.89	2 (8%)	33,34,34	1.03	2 (6%)
3	8PC	D	430	-	25,25,25	0.68	0	33,34,34	1.31	5 (15%)
2	NAD	D	330	-	42,48,48	1.72	4 (9%)	50,73,73	1.46	7 (14%)
2	NAD	C	320	-	42,48,48	1.68	4 (9%)	50,73,73	1.45	4 (8%)
3	8PC	A	400	-	25,25,25	0.70	0	33,34,34	1.10	3 (9%)
3	8PC	B	410	-	25,25,25	0.80	2 (8%)	33,34,34	0.99	2 (6%)

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	B	310	-	-	9/26/62/62	0/5/5/5
2	NAD	A	300	-	-	7/26/62/62	0/5/5/5
3	8PC	C	420	-	-	2/8/8/8	0/3/3/3
3	8PC	D	430	-	-	2/8/8/8	0/3/3/3
2	NAD	D	330	-	-	8/26/62/62	0/5/5/5
2	NAD	C	320	-	-	5/26/62/62	0/5/5/5
3	8PC	A	400	-	-	2/8/8/8	0/3/3/3
3	8PC	B	410	-	-	2/8/8/8	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	310	NAD	O7N-C7N	8.67	1.40	1.24
2	D	330	NAD	O7N-C7N	8.26	1.40	1.24
2	C	320	NAD	O7N-C7N	7.93	1.39	1.24
2	A	300	NAD	O7N-C7N	7.69	1.38	1.24
2	D	330	NAD	C2A-N3A	4.23	1.38	1.32
2	C	320	NAD	C2A-N3A	3.98	1.38	1.32
2	A	300	NAD	C2A-N3A	3.93	1.38	1.32
2	B	310	NAD	C2A-N3A	3.92	1.38	1.32
2	C	320	NAD	C2N-N1N	3.32	1.39	1.35
2	B	310	NAD	C2N-N1N	2.93	1.38	1.35
2	A	300	NAD	C2A-N1A	2.80	1.39	1.33
2	C	320	NAD	C2A-N1A	2.64	1.38	1.33
2	D	330	NAD	C2A-N1A	2.60	1.38	1.33
3	C	420	8PC	C15-CL2	2.42	1.79	1.73
3	B	410	8PC	C15-CL2	2.36	1.79	1.73
2	D	330	NAD	C2N-N1N	2.32	1.37	1.35
2	B	310	NAD	C2A-N1A	2.24	1.38	1.33
3	B	410	8PC	C17-CL1	2.11	1.79	1.74
3	C	420	8PC	C17-CL1	2.11	1.79	1.74

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	310	NAD	N3A-C2A-N1A	-6.14	119.08	128.68
2	D	330	NAD	N3A-C2A-N1A	-5.69	119.79	128.68
2	A	300	NAD	N3A-C2A-N1A	-5.49	120.09	128.68
2	C	320	NAD	N3A-C2A-N1A	-5.23	120.50	128.68
2	C	320	NAD	C3N-C7N-N7N	4.70	123.39	117.75
2	D	330	NAD	C3N-C7N-N7N	4.08	122.65	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	430	8PC	C16-C17-CL1	-3.36	114.96	119.15
2	D	330	NAD	O7N-C7N-C3N	-3.12	115.90	119.63
2	A	300	NAD	PN-O3-PA	-3.04	122.40	132.83
3	B	410	8PC	C25-N24-C23	3.00	121.53	117.42
3	D	430	8PC	C22-C17-CL1	2.96	123.98	119.35
3	D	430	8PC	C14-C15-CL2	2.90	122.83	119.43
2	A	300	NAD	C3N-C7N-N7N	2.88	121.21	117.75
3	A	400	8PC	C2-O13-C14	2.71	124.48	118.04
2	C	320	NAD	O7N-C7N-N7N	-2.70	118.74	122.58
2	D	330	NAD	O4D-C1D-C2D	-2.68	103.01	106.93
2	B	310	NAD	O4B-C1B-C2B	-2.64	103.07	106.93
3	A	400	8PC	C14-C15-CL2	2.60	122.47	119.43
2	B	310	NAD	PN-O3-PA	-2.51	124.22	132.83
3	C	420	8PC	C25-N24-C23	2.50	120.85	117.42
2	D	330	NAD	O4B-C1B-C2B	-2.44	103.36	106.93
3	A	400	8PC	C25-N24-C23	2.44	120.76	117.42
2	D	330	NAD	C6N-N1N-C2N	-2.41	119.77	121.97
3	C	420	8PC	C7-C23-N24	2.35	120.27	117.32
2	B	310	NAD	C3N-C7N-N7N	2.33	120.55	117.75
2	A	300	NAD	O4B-C1B-C2B	-2.32	103.54	106.93
2	C	320	NAD	C4A-C5A-N7A	-2.28	107.02	109.40
2	B	310	NAD	C6N-N1N-C2N	-2.20	119.97	121.97
2	D	330	NAD	C1B-N9A-C4A	-2.13	122.89	126.64
3	B	410	8PC	C2-O13-C14	2.10	123.03	118.04
3	D	430	8PC	C16-C15-CL2	-2.09	115.12	118.49
3	D	430	8PC	C25-N24-C23	2.06	120.24	117.42

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	NAD	C5D-O5D-PN-O1N
2	A	300	NAD	C5D-O5D-PN-O2N
2	A	300	NAD	O4D-C1D-N1N-C2N
2	B	310	NAD	C5B-O5B-PA-O1A
2	B	310	NAD	PN-O3-PA-O5B
2	B	310	NAD	C5D-O5D-PN-O3
2	B	310	NAD	O4D-C1D-N1N-C2N
2	C	320	NAD	C5D-O5D-PN-O1N
2	C	320	NAD	C5D-O5D-PN-O2N
2	C	320	NAD	O4D-C1D-N1N-C2N
2	D	330	NAD	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	D	330	NAD	C5D-O5D-PN-O2N
2	D	330	NAD	O4D-C1D-N1N-C2N
2	D	330	NAD	O4D-C1D-N1N-C6N
3	A	400	8PC	N24-C23-C7-C5
3	A	400	8PC	C28-C23-C7-C5
3	D	430	8PC	N24-C23-C7-C5
2	A	300	NAD	PA-O3-PN-O1N
2	B	310	NAD	O4B-C4B-C5B-O5B
3	D	430	8PC	C28-C23-C7-C5
2	B	310	NAD	C5B-O5B-PA-O3
2	B	310	NAD	C5B-O5B-PA-O2A
2	B	310	NAD	C5D-O5D-PN-O1N
2	A	300	NAD	PA-O3-PN-O2N
3	B	410	8PC	N24-C23-C7-C5
3	C	420	8PC	N24-C23-C7-C5
2	B	310	NAD	C3B-C4B-C5B-O5B
2	C	320	NAD	O4B-C4B-C5B-O5B
3	B	410	8PC	C28-C23-C7-C5
3	C	420	8PC	C28-C23-C7-C5
2	A	300	NAD	O4B-C4B-C5B-O5B
2	A	300	NAD	C5D-O5D-PN-O3
2	C	320	NAD	C5D-O5D-PN-O3
2	D	330	NAD	C5D-O5D-PN-O3
2	D	330	NAD	C2D-C1D-N1N-C6N
2	D	330	NAD	PA-O3-PN-O2N
2	D	330	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

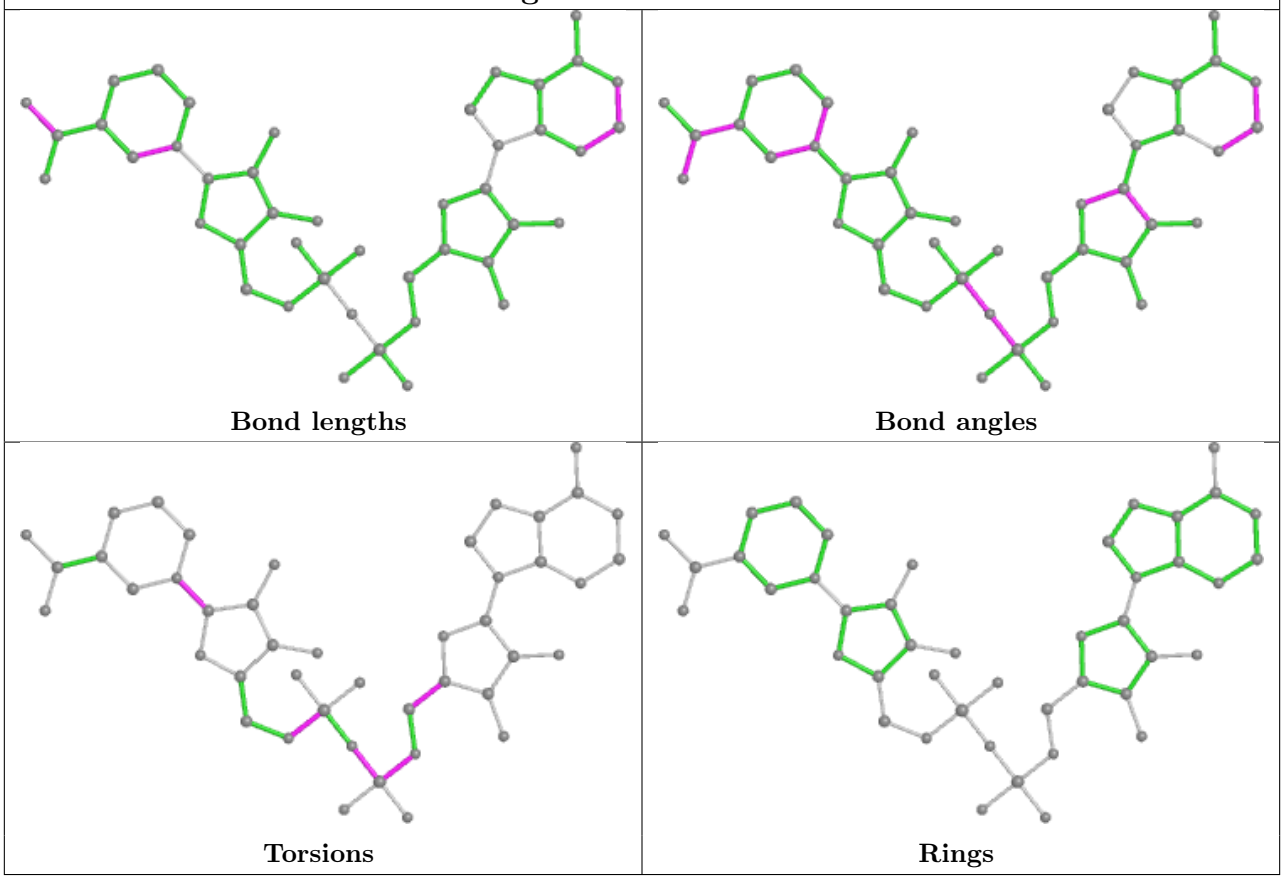
8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	310	NAD	1	0
2	A	300	NAD	2	0
3	C	420	8PC	1	0
3	D	430	8PC	2	0
2	D	330	NAD	1	0
2	C	320	NAD	1	0
3	A	400	8PC	1	0
3	B	410	8PC	3	0

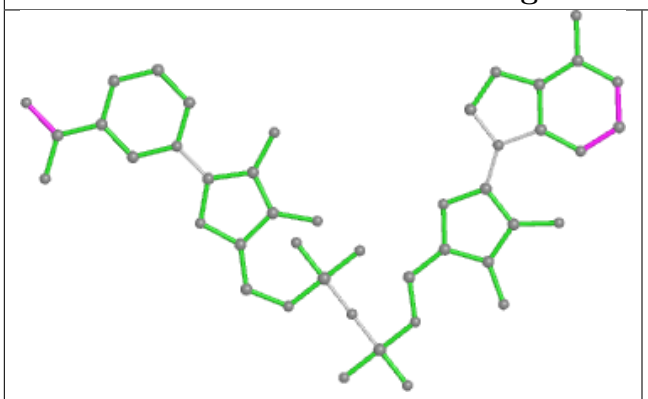
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

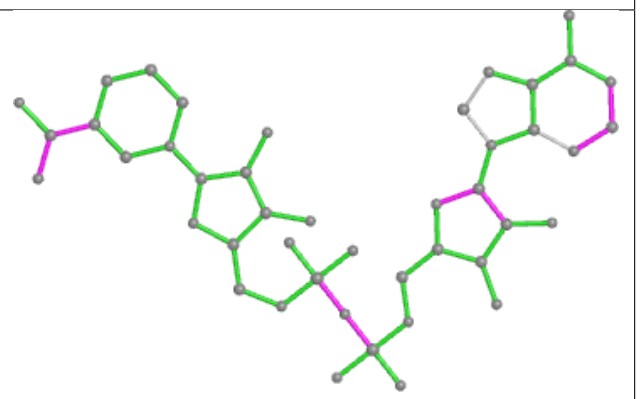
Ligand NAD B 310



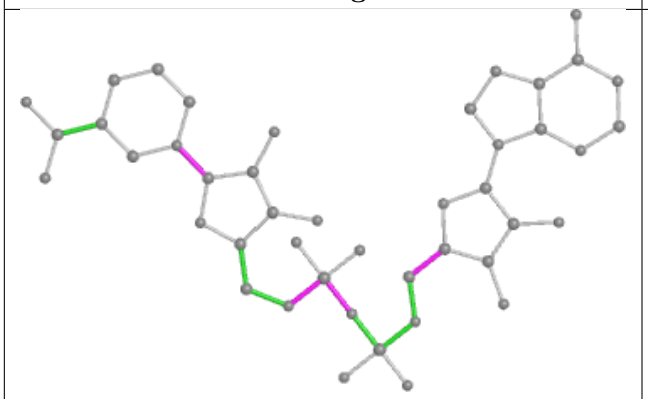
Ligand NAD A 300



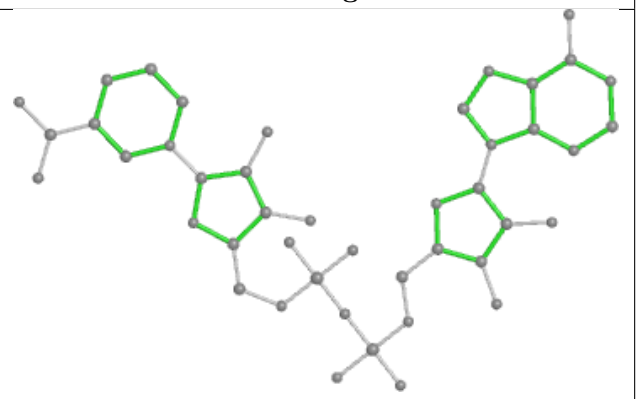
Bond lengths



Bond angles

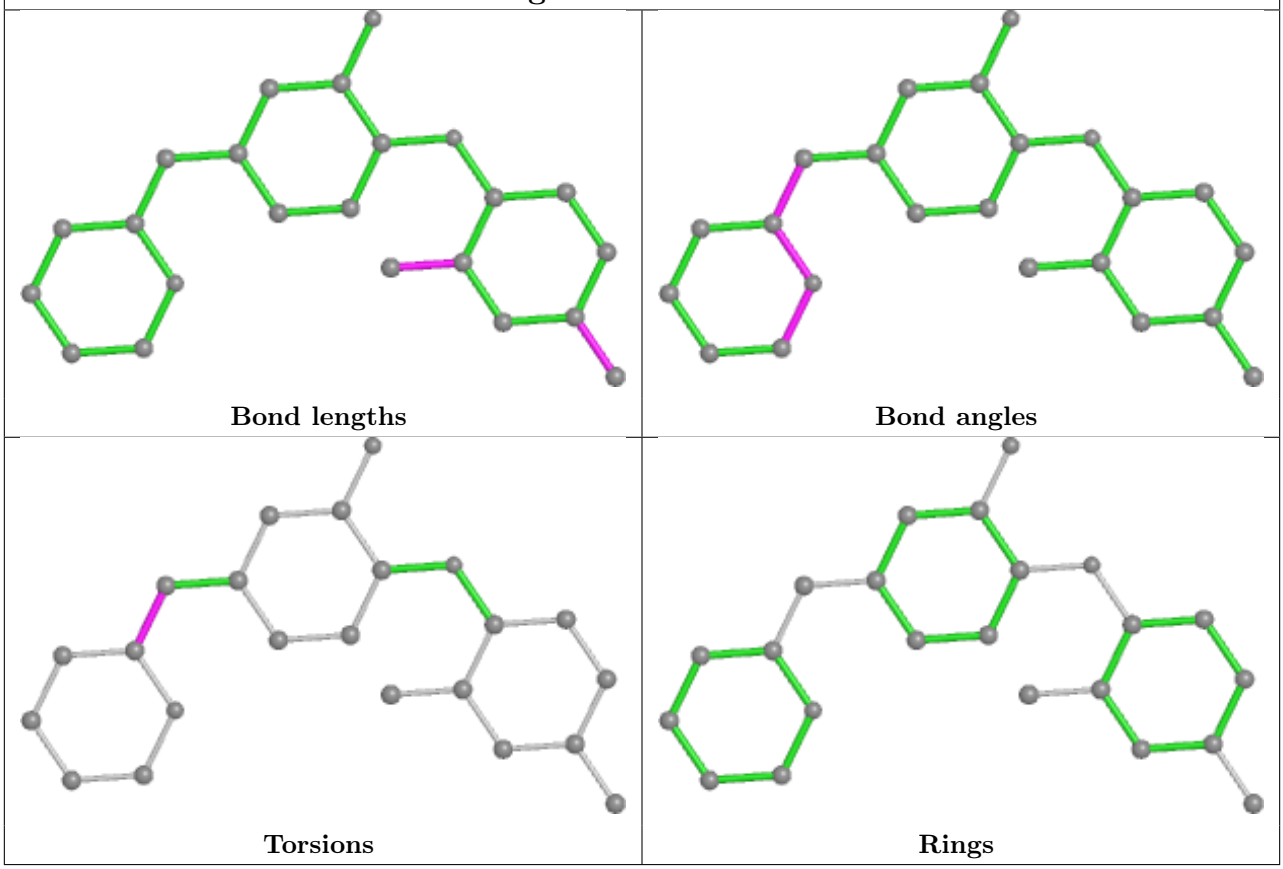


Torsions

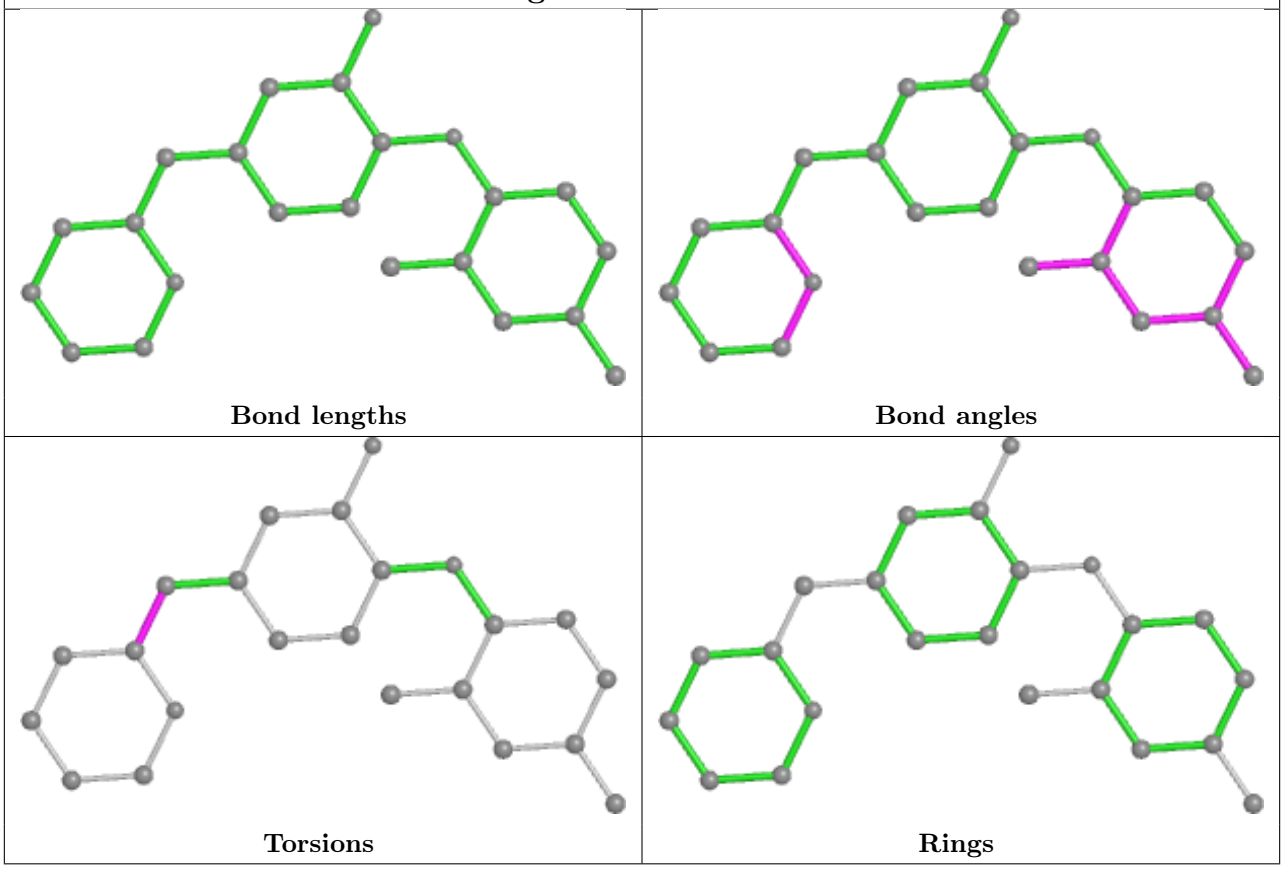


Rings

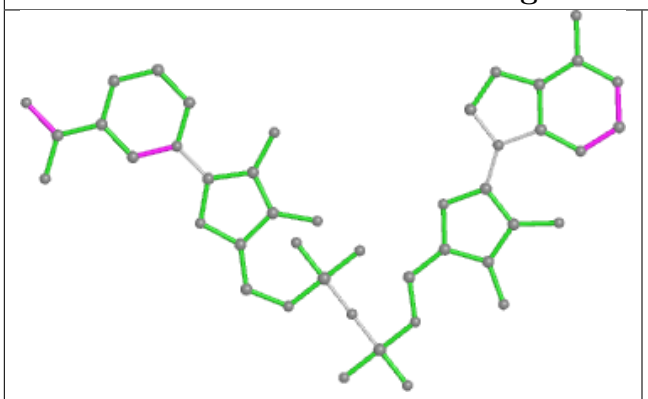
Ligand 8PC C 420



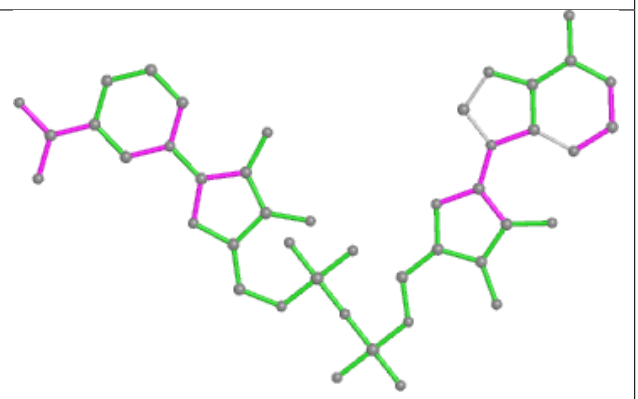
Ligand 8PC D 430



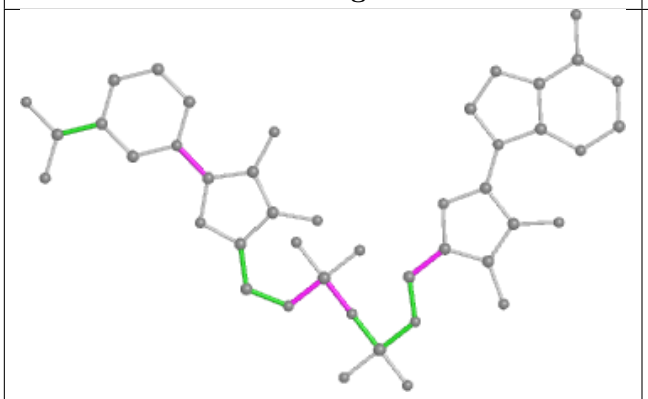
Ligand NAD D 330



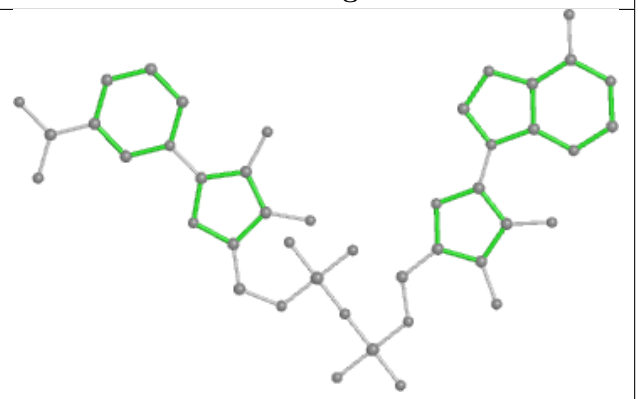
Bond lengths



Bond angles

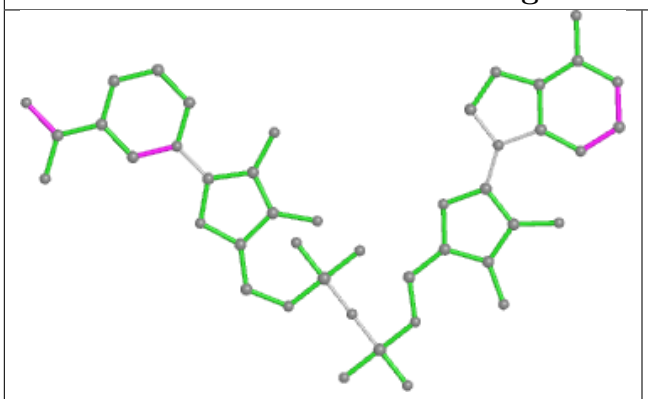


Torsions

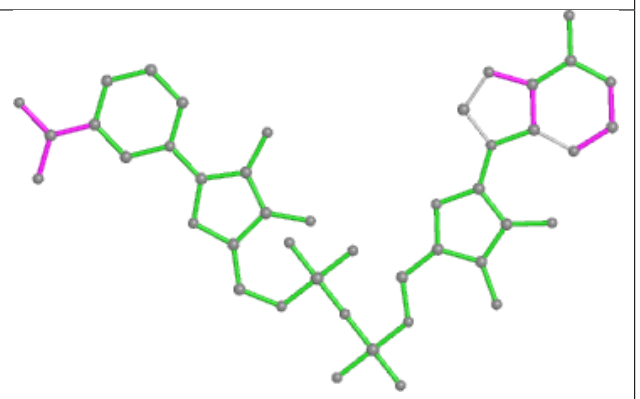


Rings

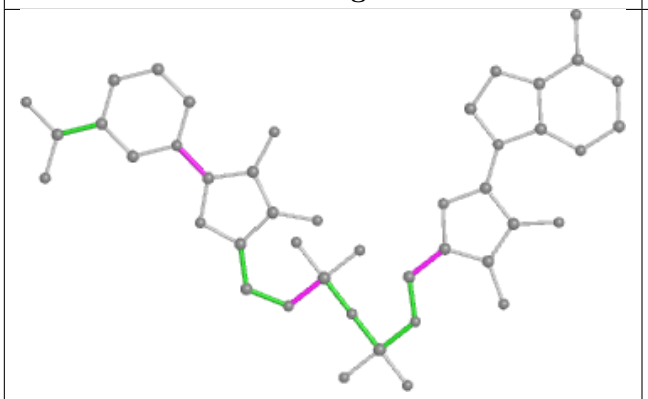
Ligand NAD C 320



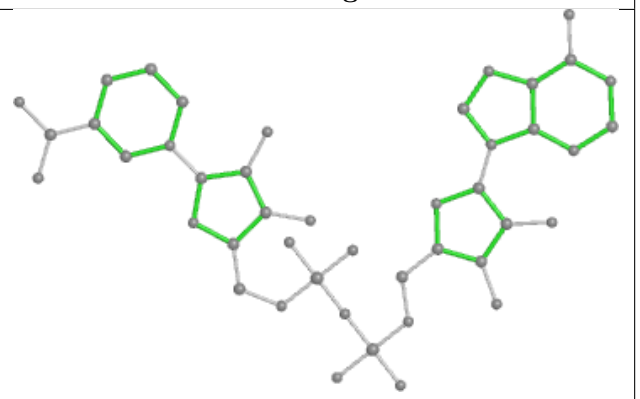
Bond lengths



Bond angles

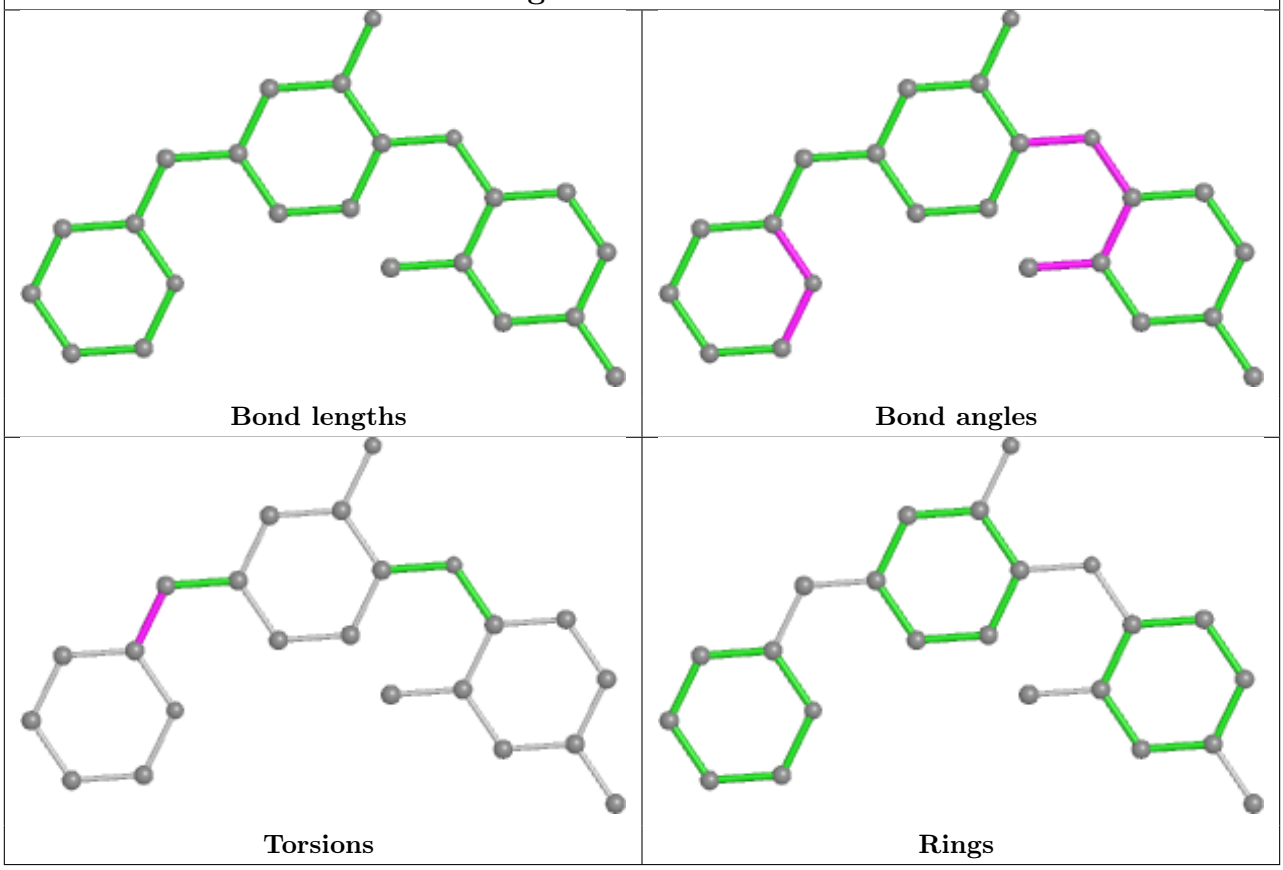


Torsions

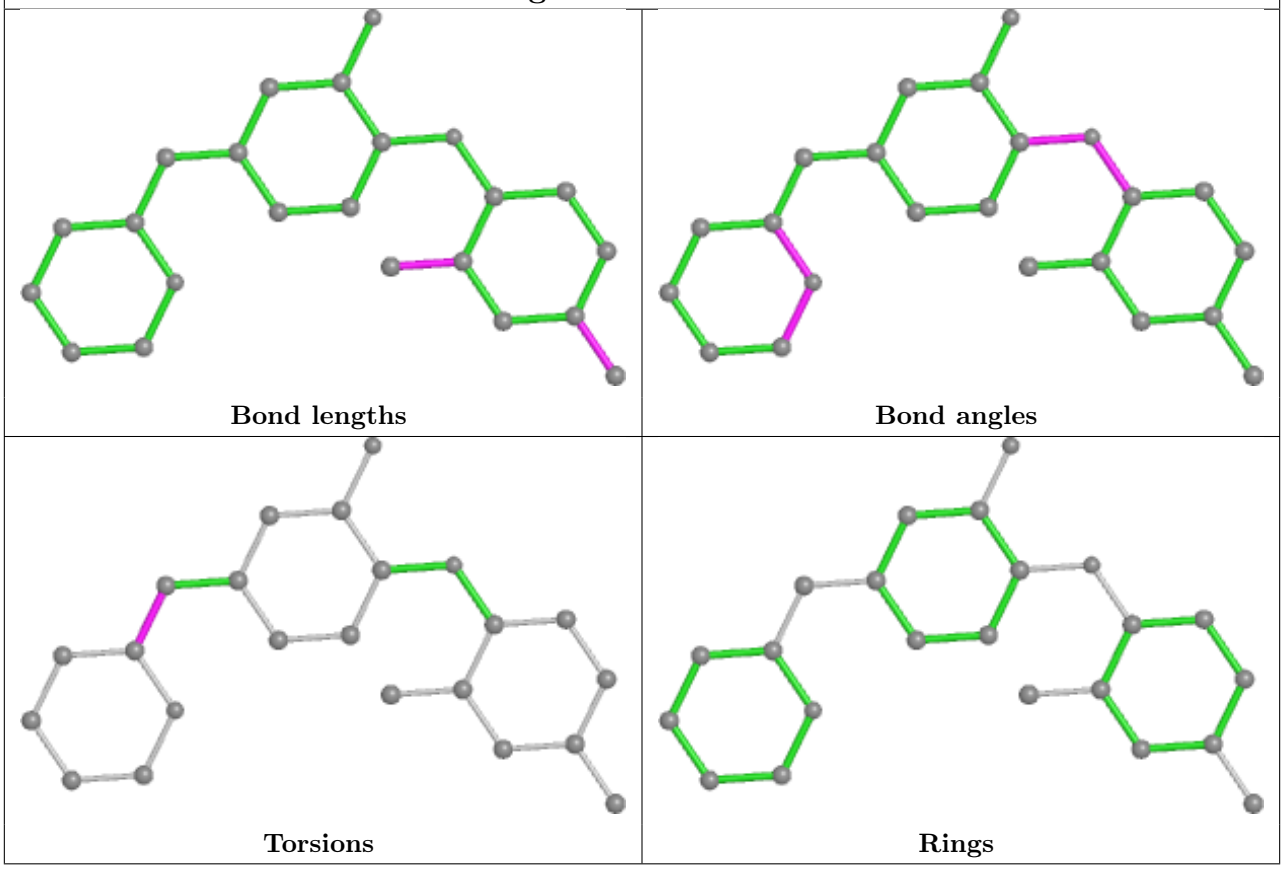


Rings

Ligand 8PC A 400



Ligand 8PC B 410



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	268/269 (99%)	-0.15	4 (1%)	73	75	22, 31, 41, 52	0
1	B	254/269 (94%)	0.06	16 (6%)	20	22	20, 30, 51, 72	0
1	C	265/269 (98%)	-0.07	5 (1%)	66	68	23, 33, 46, 54	0
1	D	260/269 (96%)	0.08	12 (4%)	32	34	24, 35, 54, 77	0
All	All	1047/1076 (97%)	-0.02	37 (3%)	44	46	20, 32, 48, 77	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	THR	6.3
1	D	208	GLY	5.5
1	B	197	LEU	5.5
1	B	2	THR	5.1
1	B	105	ILE	4.7
1	D	105	ILE	4.6
1	D	211	ALA	4.6
1	B	213	ALA	4.3
1	B	214	GLN	4.3
1	D	210	GLU	3.7
1	B	215	ILE	3.6
1	D	199	MET	3.6
1	B	45	ARG	3.1
1	B	217	LEU	3.0
1	B	257	ILE	3.0
1	C	106	ASN	2.9
1	D	2	THR	2.8
1	A	2	THR	2.8
1	D	209	GLU	2.8
1	D	197	LEU	2.7
1	A	269	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	100	GLN	2.7
1	B	196	THR	2.6
1	B	49	ARG	2.4
1	B	195	ARG	2.3
1	C	103	MET	2.3
1	B	216	GLN	2.2
1	D	45	ARG	2.2
1	D	269	LEU	2.2
1	C	45	ARG	2.1
1	C	100	GLN	2.1
1	B	106	ASN	2.1
1	D	198	ALA	2.1
1	D	257	ILE	2.1
1	B	53	ARG	2.1
1	B	100	GLN	2.0
1	A	53	ARG	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 monosaccharides 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
3	8PC	B	410	23/23	0.85	0.18	59,60,61,62	0
3	8PC	D	430	23/23	0.91	0.12	44,47,48,48	0
2	NAD	B	310	44/44	0.93	0.10	34,45,49,49	0
3	8PC	C	420	23/23	0.94	0.08	36,37,38,38	0
3	8PC	A	400	23/23	0.95	0.09	28,34,36,37	0
2	NAD	D	330	44/44	0.95	0.08	33,36,40,41	0
2	NAD	C	320	44/44	0.97	0.07	22,30,34,35	0

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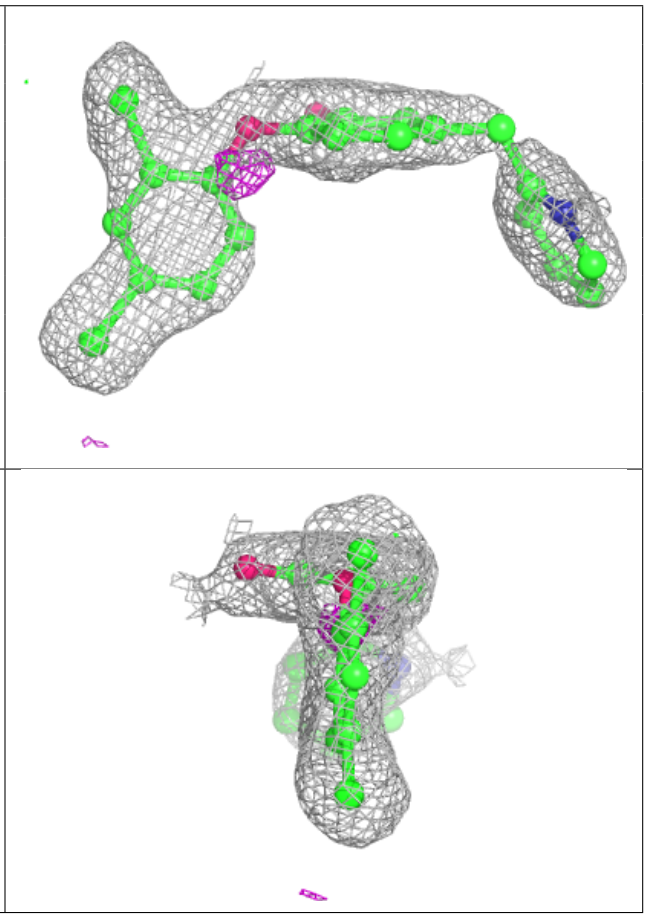
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	A	300	44/44	0.97	0.07	22,29,32,33	0

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.

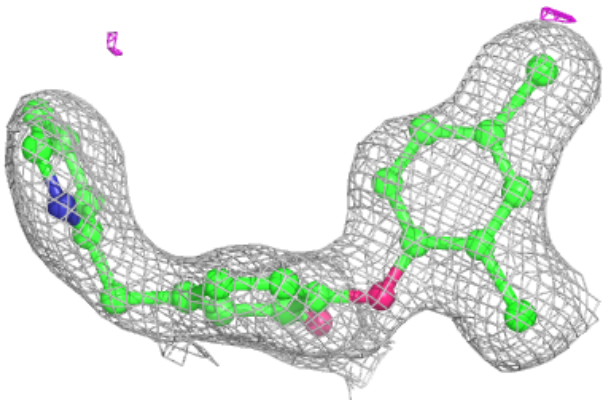
Electron density around 8PC B 410:

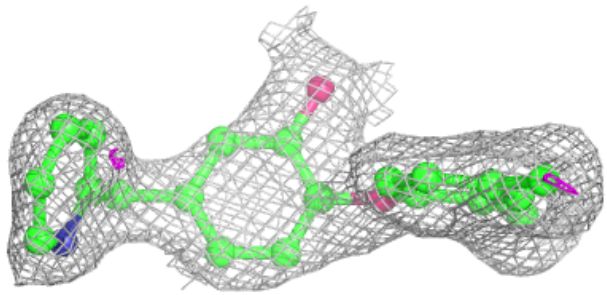
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

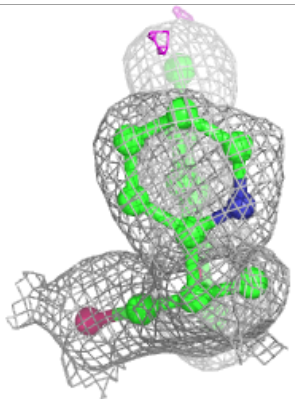


Electron density around 8PC D 430:

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

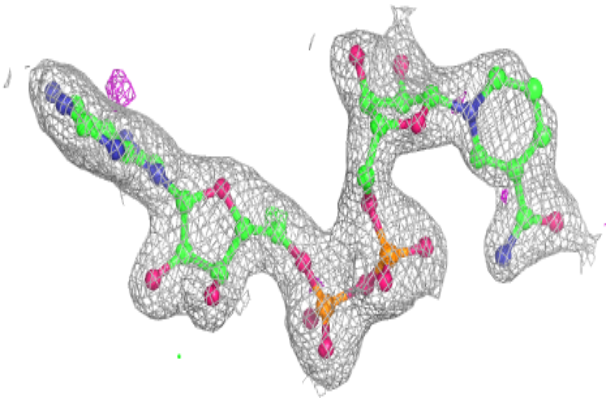


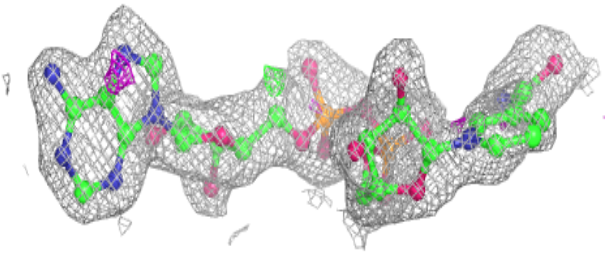


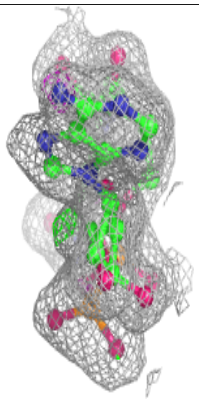


Electron density around NAD B 310:

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

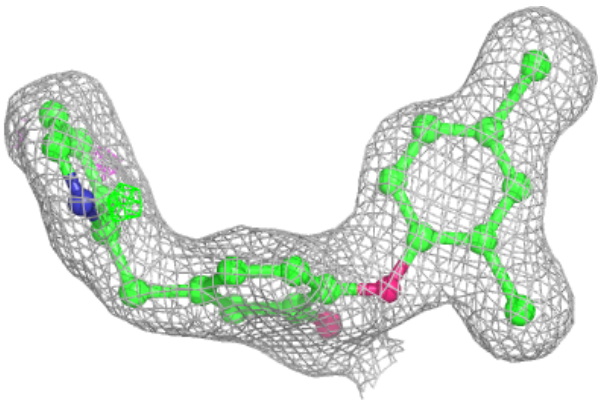


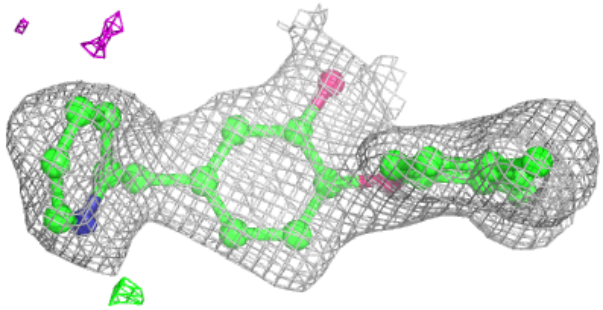


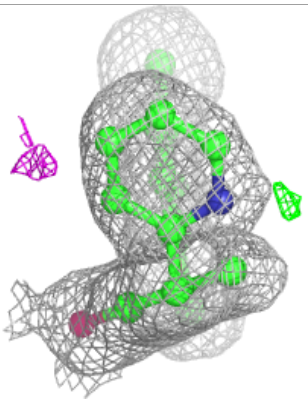


Electron density around 8PC C 420:

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

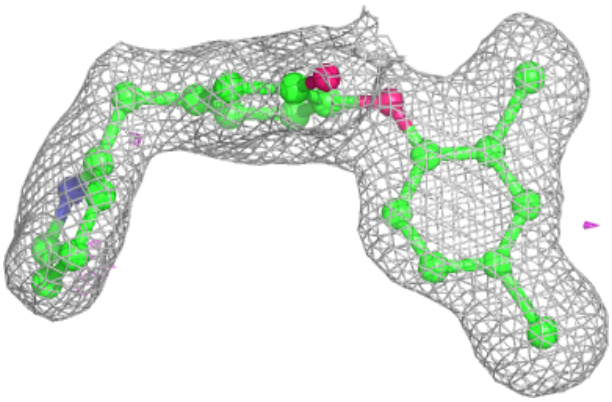


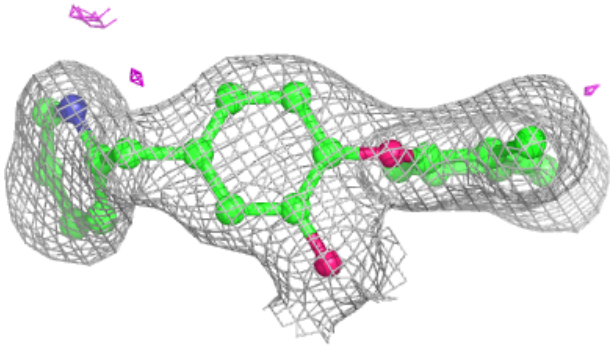


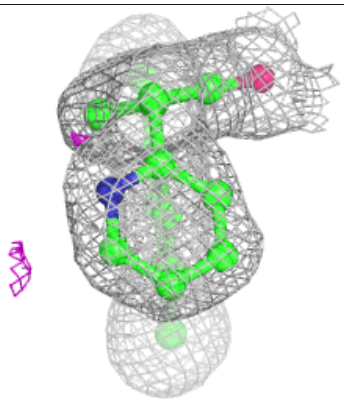


Electron density around 8PC A 400:

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

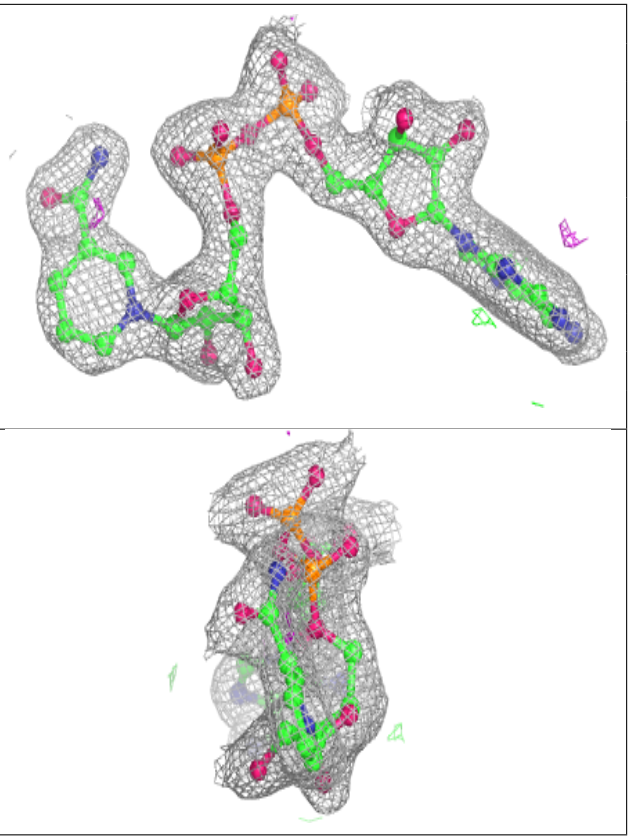


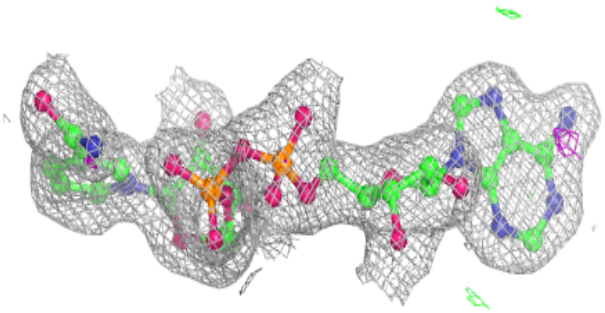




Electron density around NAD D 330:

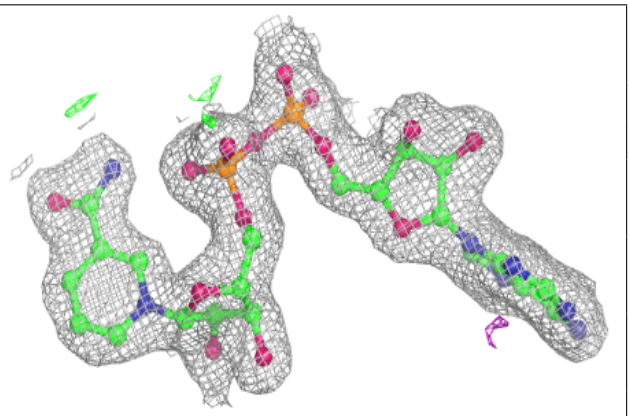
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

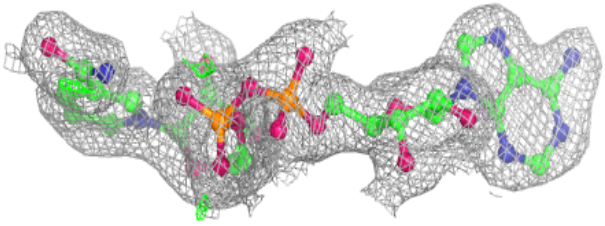


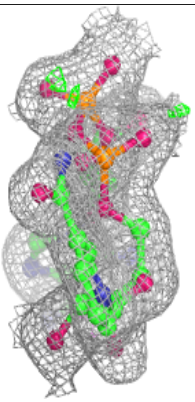


Electron density around NAD C 320:

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

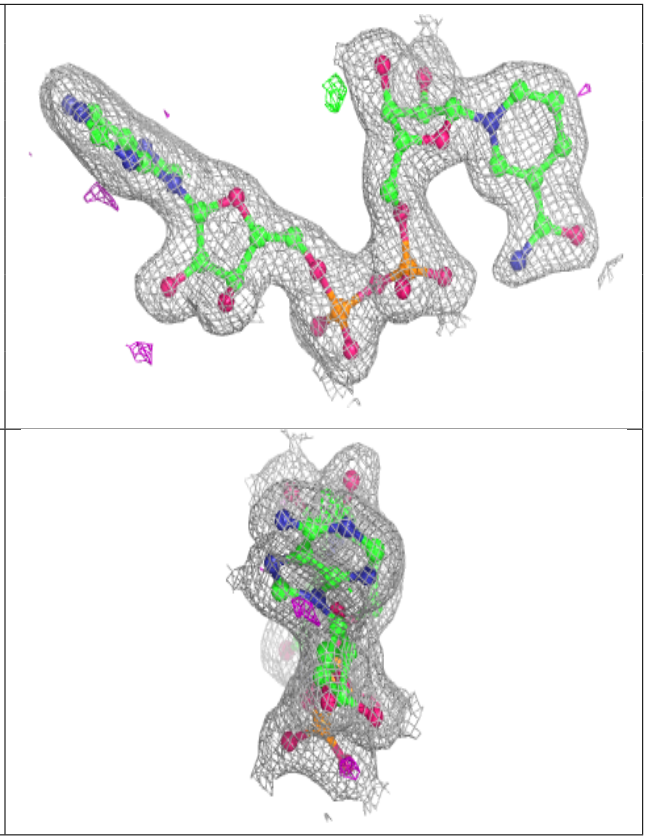






Electron density around NAD A 300:

$2mF_o$-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.