Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:45 am BST

PDB ID	:	2B36
Title	:	Crystal structure of Mycobacterium tuberculosis enoyl reductase (InhA) inhibited by 5-pentyl-2-phenoxyphenol
Authors	:	Sullivan, T.J.; Truglio, J.J.; Novichenok, P.; Stratton, C.; Zhang, X.; Kaur, T.; Johnson, F.; Boyne, M.S.; Amin, A.
Deposited on	:	2005-09-19
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

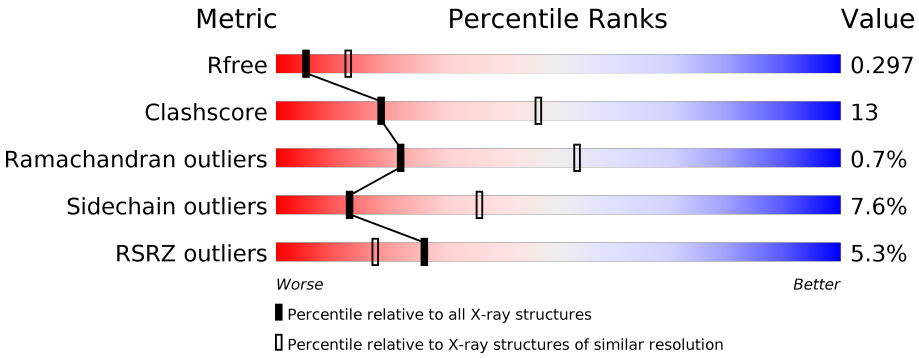
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	4% 70% 27%
1	B	269	% 73% 19%
1	C	269	6% 68% 20% 8%
1	D	269	4% 63% 26% 8%
1	E	269	4% 63% 28% 6%
1	F	269	10% 65% 25% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	5PP	C	292	-	-	-	X
2	5PP	E	294	-	-	-	X
2	5PP	F	295	-	-	-	X

2 Entry composition

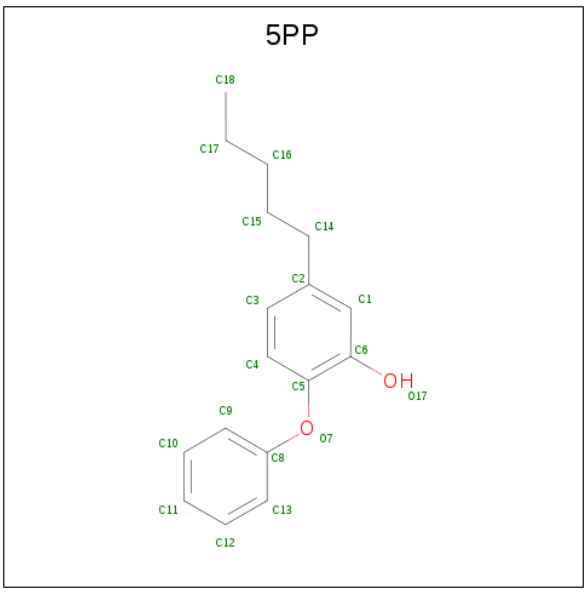
There are 3 unique types of molecules in this entry. The entry contains 11841 atoms, of which 0 are hydrogens and 0 are deuteriums.

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].

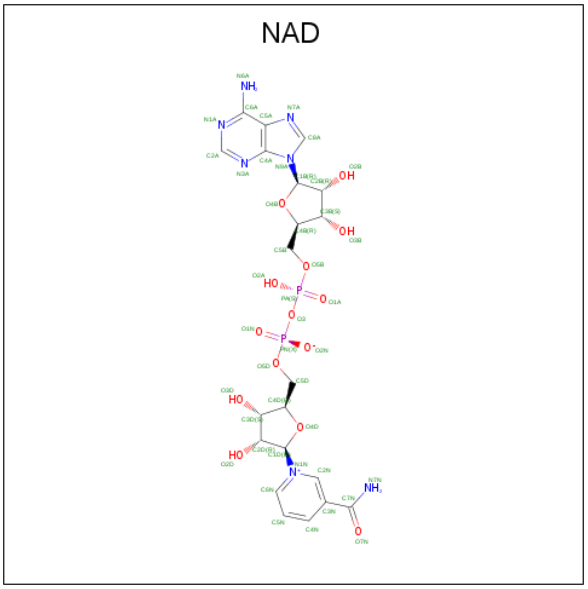
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			1996	1264	348	374	10			
1	B	259	Total	C	N	O	S	0	0	0
			1941	1229	339	364	9			
1	C	248	Total	C	N	O	S	0	0	0
			1866	1184	326	347	9			
1	D	248	Total	C	N	O	S	0	0	0
			1862	1181	326	345	10			
1	E	254	Total	C	N	O	S	0	0	0
			1906	1208	334	355	9			
1	F	251	Total	C	N	O	S	0	0	0
			1892	1200	331	352	9			

- Molecule 2 is 5-PENTYL-2-PHENOXYPHENOL (three-letter code: 5PP) (formula: $C_{17}H_{20}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 19 17 2	0	0
2	B	1	Total C O 19 17 2	0	0
2	C	1	Total C O 19 17 2	0	0
2	D	1	Total C O 19 17 2	0	0
2	E	1	Total C O 19 17 2	0	0
2	F	1	Total C O 19 17 2	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

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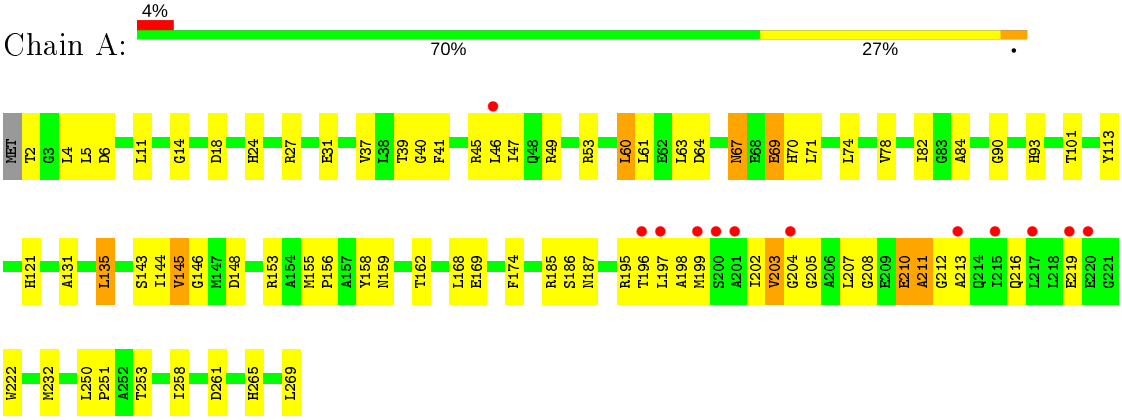
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

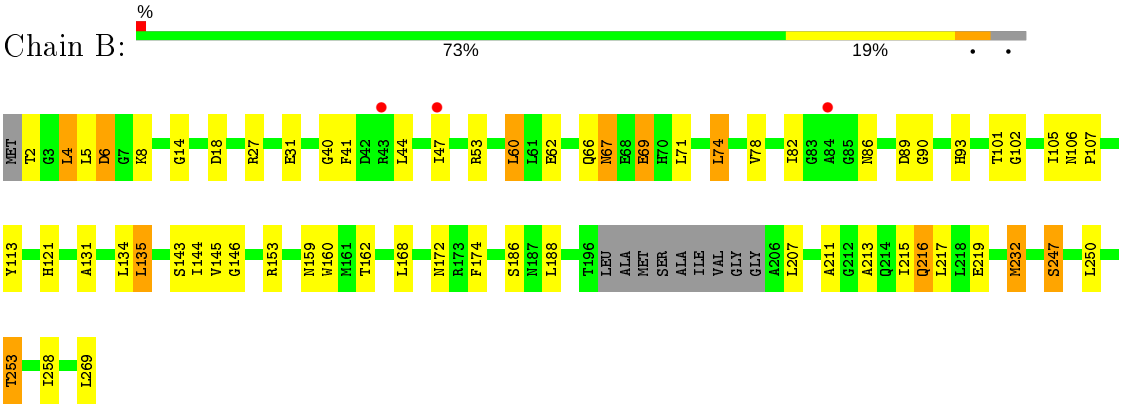
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain A:



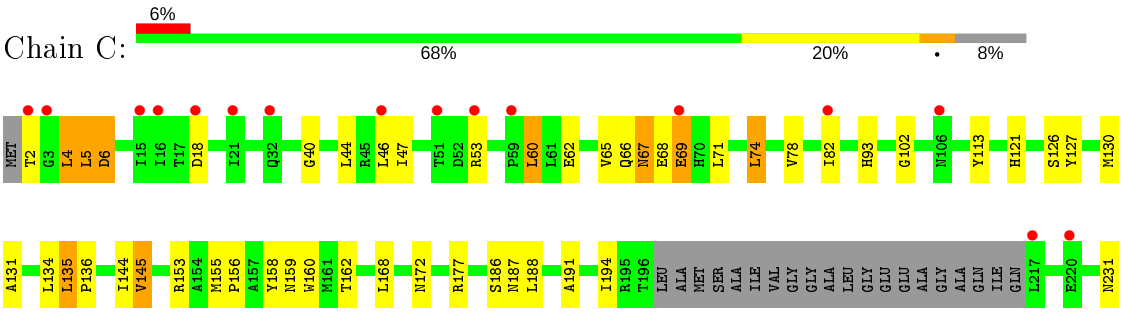
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain B:

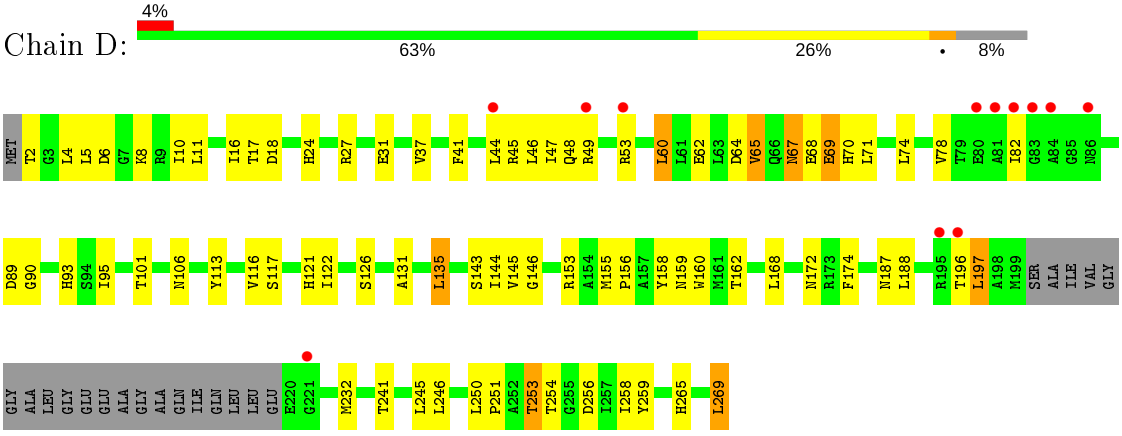


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

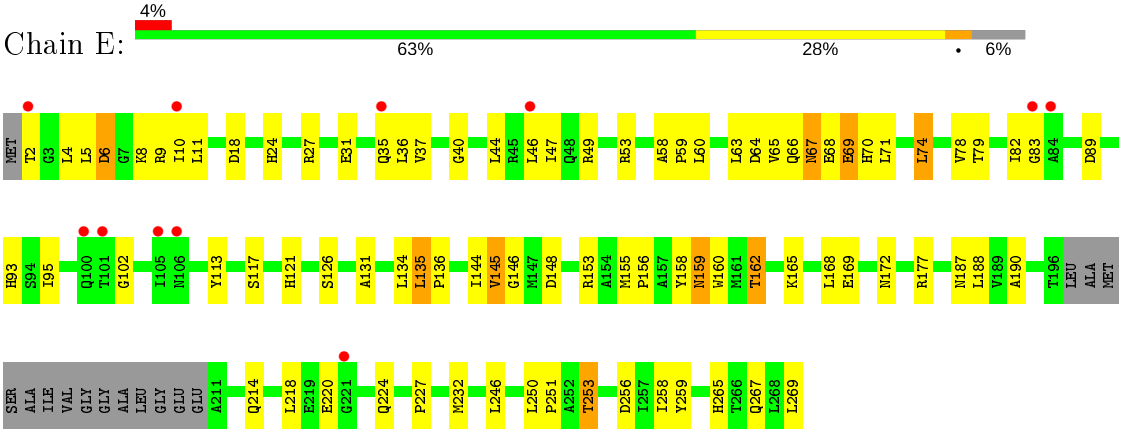
Chain C:



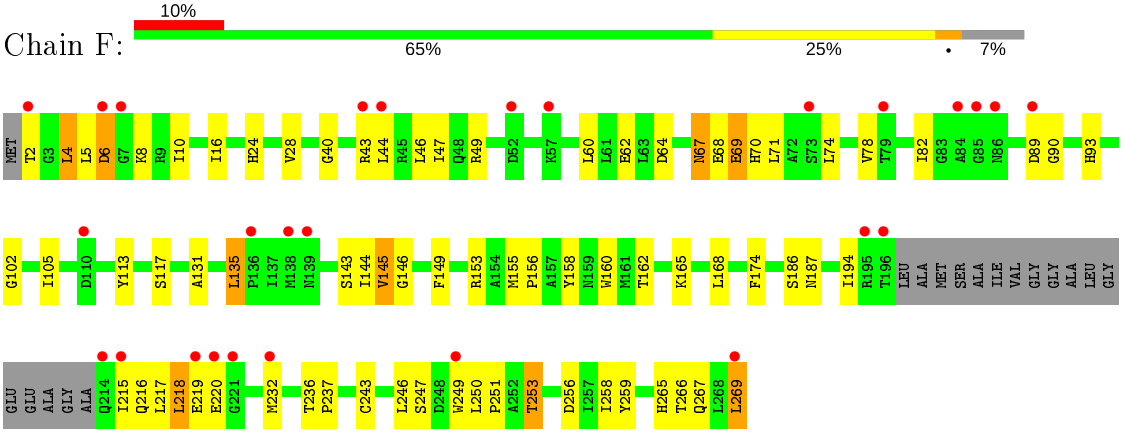
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



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



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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	99.95Å 81.83Å 188.66Å 90.00° 95.69° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 38.87 – 2.78	Depositor EDS
% Data completeness (in resolution range)	98.5 (10.00-2.80) 97.7 (38.87-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.03 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.242 , 0.295 0.250 , 0.297	Depositor DCC
R_{free} test set	1929 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	11841	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.72% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, 5PP

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	0.80	0/2034	0.71	0/2761
1	B	0.83	0/1978	0.73	0/2684
1	C	0.70	0/1903	0.67	0/2583
1	D	0.69	0/1899	0.68	0/2577
1	E	0.67	0/1943	0.66	0/2637
1	F	0.74	1/1929 (0.1%)	0.69	0/2618
All	All	0.74	1/11686 (0.0%)	0.69	0/15860

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	243	CYS	CB-SG	-5.61	1.72	1.81

There are no bond angle outliers.

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	56	1
1	B	1941	0	1951	45	0
1	C	1866	0	1880	59	0
1	D	1862	0	1877	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1906	0	1920	66	0
1	F	1892	0	1907	67	0
2	A	19	0	19	0	0
2	B	19	0	19	0	0
2	C	19	0	19	0	0
2	D	19	0	19	0	0
2	E	19	0	19	0	0
2	F	19	0	19	0	0
3	A	44	0	26	4	0
3	B	44	0	26	1	0
3	C	44	0	26	1	0
3	D	44	0	26	1	0
3	E	44	0	26	0	0
3	F	44	0	26	3	0
All	All	11841	0	11818	312	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 13.

All (312) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HG2	1:C:136:PRO:HB3	1.59	0.84
1:D:2:THR:HB	1:D:6:ASP:OD2	1.82	0.80
1:D:101:THR:O	1:D:106:ASN:ND2	2.16	0.79
1:A:2:THR:HB	1:A:6:ASP:OD2	1.81	0.78
1:C:265:HIS:O	1:E:153:ARG:NH1	2.20	0.75
1:B:27:ARG:HG2	1:B:31:GLU:OE2	1.87	0.73
1:E:47:ILE:HD11	1:E:60:LEU:HD21	1.73	0.71
1:E:2:THR:HB	1:E:6:ASP:OD2	1.90	0.71
1:E:156:PRO:HG3	1:E:214:GLN:HE21	1.56	0.71
1:D:153:ARG:NE	1:F:153:ARG:HH21	1.89	0.70
1:C:2:THR:HB	1:C:6:ASP:OD2	1.91	0.70
1:E:78:VAL:O	1:E:82:ILE:HG12	1.92	0.69
1:B:131:ALA:O	1:B:135:LEU:HB2	1.93	0.66
1:D:253:THR:HB	1:E:259:TYR:O	1.95	0.66
1:C:153:ARG:HH21	1:E:153:ARG:NE	1.93	0.65
1:A:202:ILE:HG22	1:A:207:LEU:HD13	1.78	0.65
1:C:153:ARG:NH1	1:E:265:HIS:O	2.31	0.64
1:B:215:ILE:HG22	1:B:216:GLN:OE1	1.97	0.63
1:B:213:ALA:O	1:B:217:LEU:HB2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:THR:HB	1:B:6:ASP:OD2	1.98	0.63
1:C:153:ARG:NE	1:E:153:ARG:HH21	1.96	0.63
1:D:47:ILE:HG13	1:D:60:LEU:HD11	1.80	0.63
1:C:259:TYR:O	1:F:253:THR:HB	1.98	0.63
1:F:194:ILE:HB	3:F:306:NAD:N7N	2.13	0.63
1:C:145:VAL:HA	1:C:187:ASN:O	1.99	0.63
1:D:153:ARG:HH21	1:F:153:ARG:CZ	2.12	0.62
1:A:27:ARG:HG2	1:A:31:GLU:OE2	1.99	0.62
1:E:47:ILE:HG13	1:E:60:LEU:HD11	1.81	0.62
1:A:196:THR:O	1:A:197:LEU:HD22	1.99	0.62
1:A:113:TYR:CE2	1:B:121:HIS:HB2	2.35	0.62
1:D:47:ILE:HD11	1:D:60:LEU:HD21	1.82	0.61
1:F:44:LEU:HD23	1:F:47:ILE:HD11	1.83	0.61
1:A:64:ASP:H	1:A:70:HIS:CD2	2.19	0.60
1:C:47:ILE:HG13	1:C:60:LEU:HD11	1.83	0.60
1:A:131:ALA:O	1:A:135:LEU:HB2	2.01	0.60
1:C:158:TYR:HD2	1:C:162:THR:HG1	1.50	0.60
1:D:78:VAL:O	1:D:82:ILE:HG12	2.01	0.60
1:B:67:ASN:HD22	1:B:67:ASN:C	2.05	0.60
1:E:65:VAL:HB	1:E:126:SER:HB2	1.83	0.60
1:A:203:VAL:HG23	1:A:204:GLY:H	1.65	0.59
1:A:78:VAL:O	1:A:82:ILE:HG12	2.02	0.59
1:B:47:ILE:HD11	1:B:60:LEU:HD21	1.85	0.59
1:A:11:LEU:HA	1:A:37:VAL:O	2.03	0.59
1:C:131:ALA:O	1:C:135:LEU:HB2	2.02	0.59
1:C:67:ASN:C	1:C:67:ASN:HD22	2.05	0.59
1:C:78:VAL:O	1:C:82:ILE:HG12	2.01	0.58
1:A:47:ILE:HD11	1:A:60:LEU:HD21	1.86	0.58
1:E:131:ALA:O	1:E:135:LEU:HB2	2.04	0.58
1:C:153:ARG:CZ	1:E:153:ARG:HH21	2.16	0.58
1:D:258:ILE:N	1:D:258:ILE:HD12	2.18	0.58
1:F:67:ASN:HD22	1:F:67:ASN:C	2.07	0.58
1:D:158:TYR:HD2	1:D:162:THR:HG1	1.51	0.57
1:F:135:LEU:HD13	1:F:144:ILE:HD11	1.86	0.57
1:D:10:ILE:HD13	1:D:246:LEU:HD13	1.85	0.57
1:D:67:ASN:ND2	1:D:69:GLU:H	2.02	0.57
1:B:153:ARG:HH11	1:B:153:ARG:HG2	1.70	0.57
1:D:153:ARG:NH1	1:F:265:HIS:O	2.37	0.57
1:C:253:THR:HB	1:F:259:TYR:O	2.05	0.56
1:C:153:ARG:HH21	1:E:153:ARG:CZ	2.18	0.56
1:A:195:ARG:HD3	1:A:199:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:VAL:O	1:B:82:ILE:HG12	2.05	0.55
1:F:215:ILE:HA	1:F:218:LEU:HD21	1.88	0.55
1:D:113:TYR:CE2	1:D:117:SER:HB2	2.41	0.55
1:D:153:ARG:HH21	1:F:153:ARG:NE	2.04	0.55
1:A:47:ILE:HG13	1:A:60:LEU:HD11	1.88	0.55
1:B:40:GLY:HA3	1:B:47:ILE:CD1	2.36	0.55
1:C:256:ASP:OD2	1:F:259:TYR:HB2	2.07	0.55
1:C:47:ILE:HD11	1:C:60:LEU:HD21	1.90	0.54
1:D:196:THR:HG22	1:D:197:LEU:HG	1.90	0.54
1:D:241:THR:O	1:D:245:LEU:HD23	2.08	0.54
1:F:131:ALA:O	1:F:135:LEU:HB2	2.08	0.53
1:F:258:ILE:HD12	1:F:258:ILE:N	2.22	0.53
1:B:207:LEU:HD22	1:B:211:ALA:HB2	1.89	0.53
1:B:105:ILE:HB	1:B:207:LEU:CD2	2.39	0.53
1:C:44:LEU:HD11	1:C:62:GLU:HB2	1.91	0.53
1:F:44:LEU:HA	1:F:47:ILE:HG12	1.91	0.53
1:D:67:ASN:HD22	1:D:67:ASN:C	2.12	0.53
1:E:135:LEU:HD13	1:E:144:ILE:HD11	1.90	0.53
1:D:259:TYR:O	1:E:253:THR:HB	2.09	0.53
1:D:64:ASP:H	1:D:70:HIS:CD2	2.27	0.53
1:A:46:LEU:HA	1:A:49:ARG:HH12	1.74	0.52
1:D:67:ASN:HD21	1:D:69:GLU:HB2	1.74	0.52
1:D:27:ARG:HG2	1:D:31:GLU:OE2	2.10	0.52
1:B:67:ASN:HD21	1:B:69:GLU:HB2	1.74	0.52
1:F:144:ILE:O	1:F:186:SER:HA	2.10	0.52
1:A:174:PHE:CE2	1:B:159:ASN:HA	2.45	0.52
1:B:47:ILE:HG13	1:B:60:LEU:HD11	1.91	0.52
1:D:131:ALA:O	1:D:135:LEU:HB2	2.09	0.52
1:A:67:ASN:HD22	1:A:67:ASN:C	2.13	0.52
1:D:18:ASP:HB3	1:D:53:ARG:HH21	1.76	0.51
1:D:172:ASN:CG	1:D:188:LEU:HD13	2.30	0.51
1:A:158:TYR:HD2	1:A:162:THR:HG1	1.57	0.51
1:A:211:ALA:O	1:A:213:ALA:N	2.44	0.51
1:F:153:ARG:HH11	1:F:153:ARG:HG2	1.76	0.51
1:C:191:ALA:HA	1:C:260:ALA:O	2.11	0.51
1:C:67:ASN:ND2	1:C:69:GLU:H	2.09	0.51
1:E:64:ASP:H	1:E:70:HIS:CD2	2.29	0.51
1:B:67:ASN:ND2	1:B:69:GLU:H	2.08	0.51
1:A:93:HIS:O	1:A:146:GLY:HA2	2.11	0.51
1:A:45:ARG:CG	1:C:136:PRO:HB3	2.36	0.51
1:D:259:TYR:HB2	1:E:256:ASP:OD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LEU:HA	1:D:49:ARG:HH12	1.75	0.50
1:D:67:ASN:ND2	1:D:69:GLU:N	2.59	0.50
1:F:218:LEU:C	1:F:220:GLU:N	2.65	0.50
1:A:198:ALA:O	1:A:202:ILE:HG23	2.10	0.50
1:F:47:ILE:HG13	1:F:60:LEU:HD11	1.93	0.50
1:B:40:GLY:HA3	1:B:47:ILE:HD13	1.93	0.50
1:C:153:ARG:NH2	1:E:153:ARG:NH2	2.60	0.50
1:C:46:LEU:HD23	1:C:46:LEU:O	2.12	0.50
1:D:122:ILE:HD13	3:D:304:NAD:H61A	1.75	0.50
1:F:40:GLY:HA3	1:F:47:ILE:CD1	2.41	0.50
1:F:47:ILE:HD11	1:F:60:LEU:HD21	1.94	0.50
1:C:236:THR:HB	1:C:237:PRO:HD3	1.94	0.49
1:F:93:HIS:O	1:F:146:GLY:HA2	2.11	0.49
1:A:202:ILE:C	1:A:202:ILE:HD12	2.33	0.49
1:F:165:LYS:NZ	3:F:306:NAD:O2D	2.38	0.49
1:B:219:GLU:OE2	1:B:232:MET:CB	2.60	0.49
1:A:148:ASP:OD2	1:A:169:GLU:OE2	2.30	0.49
1:A:121:HIS:HB2	1:B:113:TYR:CE2	2.48	0.49
1:C:258:ILE:N	1:C:258:ILE:HD12	2.27	0.49
1:E:24:HIS:CD2	1:E:27:ARG:HH21	2.31	0.49
1:C:241:THR:HG23	1:F:250:LEU:HD23	1.95	0.49
1:F:67:ASN:HD22	1:F:68:GLU:N	2.10	0.49
1:E:102:GLY:O	1:E:160:TRP:HB2	2.13	0.49
1:B:258:ILE:HD12	1:B:258:ILE:N	2.28	0.48
1:D:135:LEU:HD13	1:D:144:ILE:HD11	1.94	0.48
1:E:250:LEU:N	1:E:251:PRO:CD	2.76	0.48
1:E:40:GLY:HA3	1:E:47:ILE:CD1	2.43	0.48
1:F:155:MET:HB2	1:F:156:PRO:HD2	1.93	0.48
1:E:11:LEU:HA	1:E:37:VAL:O	2.13	0.48
1:F:145:VAL:HA	1:F:187:ASN:O	2.12	0.48
1:F:236:THR:HB	1:F:237:PRO:HD3	1.94	0.48
1:D:67:ASN:HD22	1:D:69:GLU:N	2.10	0.48
1:A:258:ILE:HD12	1:A:258:ILE:N	2.29	0.48
1:B:67:ASN:HD22	1:B:69:GLU:N	2.12	0.48
1:C:67:ASN:HD21	1:C:69:GLU:HB2	1.77	0.48
1:E:159:ASN:HA	1:F:174:PHE:CE2	2.49	0.48
1:B:14:GLY:O	3:B:302:NAD:O3B	2.27	0.48
1:C:241:THR:HG23	1:F:250:LEU:CD2	2.44	0.48
1:F:218:LEU:C	1:F:220:GLU:H	2.17	0.48
1:F:43:ARG:CZ	1:F:46:LEU:HD13	2.44	0.48
1:F:2:THR:HB	1:F:6:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:LEU:HD23	1:F:46:LEU:O	2.13	0.48
1:D:46:LEU:HD23	1:D:46:LEU:O	2.14	0.48
1:E:67:ASN:C	1:E:67:ASN:HD22	2.18	0.48
1:C:66:GLN:HG2	1:C:121:HIS:CE1	2.50	0.47
1:C:158:TYR:HD2	1:C:162:THR:OG1	1.97	0.47
1:E:74:LEU:HD13	1:E:134:LEU:HD21	1.97	0.47
1:E:165:LYS:O	1:E:169:GLU:HG3	2.14	0.47
1:E:67:ASN:HD21	1:E:69:GLU:HB2	1.78	0.47
1:C:155:MET:HB2	1:C:156:PRO:HD2	1.95	0.47
1:C:269:LEU:HD23	1:E:218:LEU:HD12	1.95	0.47
1:C:65:VAL:HB	1:C:126:SER:HB2	1.97	0.47
1:D:67:ASN:HD22	1:D:68:GLU:N	2.13	0.47
1:F:10:ILE:HD13	1:F:246:LEU:HD13	1.95	0.47
1:B:67:ASN:ND2	1:B:69:GLU:N	2.63	0.47
1:E:155:MET:HB2	1:E:156:PRO:HD2	1.97	0.47
1:E:27:ARG:HG2	1:E:31:GLU:OE2	2.15	0.47
1:A:222:TRP:HE1	1:A:261:ASP:HB2	1.80	0.47
1:D:153:ARG:NH2	1:F:153:ARG:NH2	2.63	0.47
1:D:265:HIS:O	1:F:153:ARG:NH1	2.47	0.47
1:C:259:TYR:HB2	1:F:256:ASP:OD2	2.15	0.47
1:F:113:TYR:CE2	1:F:117:SER:HB2	2.49	0.47
1:B:93:HIS:O	1:B:146:GLY:HA2	2.15	0.46
1:B:4:LEU:HD22	1:B:247:SER:HB2	1.97	0.46
1:D:153:ARG:HE	1:F:153:ARG:HH21	1.60	0.46
1:F:90:GLY:HA2	1:F:143:SER:O	2.16	0.46
1:F:64:ASP:H	1:F:70:HIS:CD2	2.33	0.46
1:A:135:LEU:HD13	1:A:144:ILE:HD11	1.97	0.46
1:A:250:LEU:N	1:A:251:PRO:CD	2.79	0.46
1:B:66:GLN:HG2	1:B:121:HIS:CE1	2.50	0.46
1:F:67:ASN:OD1	1:F:70:HIS:CE1	2.68	0.46
1:B:216:GLN:OE1	1:B:216:GLN:N	2.49	0.46
1:D:153:ARG:CZ	1:F:153:ARG:HH21	2.28	0.46
1:A:153:ARG:HH11	1:A:153:ARG:HG2	1.80	0.46
1:C:74:LEU:HD13	1:C:134:LEU:HD21	1.96	0.46
1:C:40:GLY:HA3	1:C:47:ILE:CD1	2.46	0.46
1:A:202:ILE:HD12	1:A:202:ILE:O	2.14	0.46
1:B:74:LEU:HD13	1:B:134:LEU:HD21	1.97	0.46
1:E:44:LEU:HA	1:E:47:ILE:HG12	1.97	0.46
1:A:144:ILE:O	1:A:186:SER:HA	2.15	0.46
1:F:158:TYR:HD2	1:F:162:THR:OG1	1.99	0.46
1:A:40:GLY:HA3	1:A:47:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ILE:HG23	1:D:17:THR:HG23	1.98	0.46
1:D:256:ASP:OD2	1:E:259:TYR:HB2	2.16	0.45
1:E:135:LEU:N	1:E:136:PRO:CD	2.79	0.45
1:E:18:ASP:HB3	1:E:53:ARG:HH21	1.81	0.45
1:B:41:PHE:C	1:B:41:PHE:CD1	2.90	0.45
1:C:159:ASN:HA	1:D:174:PHE:CE2	2.51	0.45
1:A:63:LEU:O	3:A:301:NAD:H2A	2.17	0.45
1:D:67:ASN:HD22	1:D:69:GLU:H	1.63	0.45
1:E:79:THR:O	1:E:83:GLY:N	2.47	0.45
1:E:46:LEU:HG	1:E:49:ARG:HH12	1.80	0.45
1:C:102:GLY:O	1:C:160:TRP:HB2	2.16	0.45
1:D:250:LEU:N	1:D:251:PRO:CD	2.80	0.45
1:F:46:LEU:HA	1:F:49:ARG:HH12	1.82	0.45
1:B:172:ASN:CG	1:B:188:LEU:HD13	2.37	0.45
1:A:67:ASN:ND2	1:A:69:GLU:H	2.15	0.45
1:A:14:GLY:O	3:A:301:NAD:O3B	2.30	0.45
1:B:8:LYS:HA	1:B:89:ASP:OD2	2.17	0.45
1:E:158:TYR:HD2	1:E:162:THR:OG1	2.00	0.45
1:C:156:PRO:O	1:C:158:TYR:N	2.41	0.45
1:E:148:ASP:O	1:E:190:ALA:HA	2.17	0.45
1:C:93:HIS:HA	1:C:130:MET:HE1	1.99	0.45
1:D:45:ARG:O	1:D:48:GLN:HB2	2.17	0.45
1:E:9:ARG:HA	1:E:35:GLN:O	2.17	0.45
1:F:249:TRP:O	1:F:250:LEU:HG	2.17	0.45
1:F:44:LEU:HD11	1:F:62:GLU:HB2	1.98	0.45
1:E:93:HIS:CE1	1:E:95:ILE:HB	2.52	0.44
1:E:93:HIS:O	1:E:146:GLY:HA2	2.17	0.44
1:D:11:LEU:HA	1:D:37:VAL:O	2.17	0.44
1:A:145:VAL:HA	1:A:187:ASN:O	2.17	0.44
1:D:8:LYS:HA	1:D:89:ASP:OD2	2.17	0.44
1:E:66:GLN:HG2	1:E:121:HIS:CE1	2.52	0.44
1:F:67:ASN:HD21	1:F:69:GLU:HB2	1.81	0.44
1:A:39:THR:HA	1:A:61:LEU:O	2.17	0.44
1:C:194:ILE:N	3:C:303:NAD:O7N	2.36	0.44
1:F:250:LEU:N	1:F:251:PRO:CD	2.81	0.44
1:F:4:LEU:HD22	1:F:247:SER:HB2	1.99	0.44
1:A:113:TYR:CZ	1:B:121:HIS:HB2	2.52	0.44
1:B:90:GLY:HA2	1:B:143:SER:O	2.17	0.44
1:B:207:LEU:HD13	1:B:211:ALA:HB1	2.00	0.44
1:C:250:LEU:N	1:C:251:PRO:HD3	2.32	0.44
1:D:65:VAL:HB	1:D:126:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:HIS:HB2	1:F:113:TYR:CE2	2.53	0.44
1:F:78:VAL:O	1:F:82:ILE:HG12	2.18	0.44
1:B:67:ASN:ND2	1:B:67:ASN:C	2.71	0.44
1:A:41:PHE:C	1:A:41:PHE:CD1	2.90	0.44
1:B:219:GLU:OE2	1:B:232:MET:HB2	2.18	0.43
1:E:10:ILE:HB	1:E:36:LEU:CD2	2.47	0.43
1:E:220:GLU:HG2	1:E:224:GLN:HE21	1.83	0.43
1:E:40:GLY:HA3	1:E:47:ILE:HD13	2.00	0.43
1:B:144:ILE:O	1:B:186:SER:HA	2.17	0.43
1:E:172:ASN:CG	1:E:188:LEU:HD13	2.38	0.43
1:A:159:ASN:HA	1:B:174:PHE:CE2	2.53	0.43
1:A:196:THR:HG21	3:A:301:NAD:O2A	2.19	0.43
1:E:145:VAL:HA	1:E:187:ASN:O	2.18	0.43
1:C:60:LEU:C	1:C:60:LEU:CD2	2.87	0.43
1:A:18:ASP:CB	1:A:53:ARG:HH21	2.31	0.43
1:C:250:LEU:N	1:C:251:PRO:CD	2.82	0.43
1:C:4:LEU:O	1:C:5:LEU:HD13	2.19	0.43
1:D:269:LEU:O	1:E:177:ARG:NH2	2.51	0.43
1:A:64:ASP:H	1:A:70:HIS:HD2	1.65	0.43
1:E:63:LEU:HD22	1:E:74:LEU:HD11	1.99	0.43
1:A:67:ASN:HD22	1:A:69:GLU:H	1.67	0.43
1:F:105:ILE:O	1:F:105:ILE:HG13	2.19	0.43
1:F:266:THR:OG1	1:F:267:GLN:NE2	2.45	0.43
1:F:24:HIS:O	1:F:28:VAL:HG23	2.19	0.43
1:C:113:TYR:CE2	1:D:121:HIS:HB2	2.54	0.43
1:C:74:LEU:O	1:C:78:VAL:HG23	2.19	0.42
1:D:90:GLY:HA2	1:D:143:SER:O	2.18	0.42
1:A:18:ASP:HB3	1:A:53:ARG:HH21	1.84	0.42
1:A:24:HIS:CD2	1:A:27:ARG:HH21	2.37	0.42
1:A:24:HIS:HD2	1:A:27:ARG:HH21	1.66	0.42
1:D:41:PHE:C	1:D:41:PHE:CD1	2.92	0.42
1:D:44:LEU:HA	1:D:47:ILE:HG12	2.01	0.42
1:E:8:LYS:HA	1:E:89:ASP:OD2	2.20	0.42
1:F:67:ASN:ND2	1:F:69:GLU:H	2.17	0.42
1:B:102:GLY:O	1:B:160:TRP:HB2	2.19	0.42
1:C:177:ARG:NH2	1:F:269:LEU:O	2.52	0.42
1:F:8:LYS:HA	1:F:89:ASP:OD2	2.18	0.42
1:A:155:MET:HB2	1:A:156:PRO:HD2	2.01	0.42
1:A:185:ARG:HH11	1:A:185:ARG:HG3	1.84	0.42
1:C:93:HIS:CD2	1:C:127:TYR:HA	2.54	0.42
1:A:208:GLY:HA3	1:A:210:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ASN:OD1	1:B:107:PRO:HD2	2.19	0.42
1:C:135:LEU:HD13	1:C:144:ILE:HD11	2.02	0.42
1:D:18:ASP:CB	1:D:53:ARG:HH21	2.31	0.42
1:E:10:ILE:HD13	1:E:246:LEU:HD13	2.01	0.42
1:E:258:ILE:HD12	1:E:258:ILE:N	2.35	0.42
1:E:67:ASN:ND2	1:E:69:GLU:H	2.18	0.42
1:C:172:ASN:CG	1:C:188:LEU:HD13	2.40	0.42
1:D:155:MET:HB2	1:D:156:PRO:HD2	2.02	0.42
1:E:250:LEU:N	1:E:251:PRO:HD3	2.35	0.42
1:E:46:LEU:O	1:E:46:LEU:HD23	2.19	0.42
1:A:41:PHE:HB2	3:A:301:NAD:N3A	2.35	0.42
1:B:44:LEU:HD11	1:B:62:GLU:HB2	2.01	0.42
1:F:46:LEU:HG	1:F:49:ARG:HH12	1.84	0.42
1:B:82:ILE:O	1:B:86:ASN:ND2	2.38	0.41
1:D:44:LEU:HD11	1:D:62:GLU:HB2	2.02	0.41
1:B:250:LEU:HB3	1:B:253:THR:CG2	2.49	0.41
1:D:93:HIS:O	1:D:146:GLY:HA2	2.20	0.41
1:D:93:HIS:CE1	1:D:95:ILE:HB	2.55	0.41
1:F:215:ILE:HD12	1:F:215:ILE:O	2.21	0.41
1:A:27:ARG:O	1:A:31:GLU:HG3	2.21	0.41
1:C:67:ASN:HD22	1:C:69:GLU:N	2.18	0.41
1:E:113:TYR:CE2	1:E:117:SER:HB2	2.55	0.41
1:E:156:PRO:CG	1:E:214:GLN:HB3	2.50	0.41
1:E:58:ALA:HA	1:E:59:PRO:HD3	1.94	0.41
1:A:90:GLY:HA2	1:A:143:SER:O	2.21	0.41
1:C:44:LEU:HA	1:C:47:ILE:HG12	2.02	0.41
1:C:231:ASN:ND2	1:C:234:ASP:HB2	2.36	0.41
1:D:116:VAL:HG11	1:D:160:TRP:CE3	2.55	0.41
1:C:153:ARG:NH2	1:E:153:ARG:CZ	2.83	0.41
1:D:153:ARG:CZ	1:F:153:ARG:NH2	2.84	0.41
1:C:144:ILE:O	1:C:186:SER:HA	2.19	0.41
1:C:18:ASP:HB3	1:C:53:ARG:HH21	1.85	0.41
1:D:187:ASN:OD1	1:D:254:THR:HA	2.21	0.41
1:E:227:PRO:HD3	1:E:267:GLN:HG3	2.03	0.41
1:E:250:LEU:HB3	1:E:253:THR:CG2	2.51	0.40
1:A:210:GLU:CD	1:A:210:GLU:H	2.23	0.40
1:F:218:LEU:O	1:F:220:GLU:N	2.55	0.40
1:A:216:GLN:HA	1:A:219:GLU:OE1	2.22	0.40
1:D:24:HIS:HD2	1:D:27:ARG:HH21	1.68	0.40
1:F:102:GLY:O	1:F:160:TRP:HB2	2.22	0.40
1:F:215:ILE:HB	1:F:218:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:ILE:HD11	1:F:43:ARG:HH21	1.87	0.40
1:E:27:ARG:O	1:E:31:GLU:HG3	2.22	0.40
1:E:67:ASN:HD22	1:E:68:GLU:N	2.20	0.40
1:B:18:ASP:HB3	1:B:53:ARG:HH21	1.86	0.40
1:C:67:ASN:HD22	1:C:68:GLU:N	2.19	0.40
1:F:149:PHE:CD2	3:F:306:NAD:H5N	2.57	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:A:153:ARG:NH1	1:A:265:HIS:O[2_555]	2.18	0.02

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%)	240 (90%)	21 (8%)	5 (2%)	8 26
1	B	255/269 (95%)	239 (94%)	15 (6%)	1 (0%)	34 66
1	C	244/269 (91%)	227 (93%)	17 (7%)	0	100 100
1	D	244/269 (91%)	223 (91%)	19 (8%)	2 (1%)	19 49
1	E	250/269 (93%)	234 (94%)	15 (6%)	1 (0%)	34 66
1	F	247/269 (92%)	220 (89%)	26 (10%)	1 (0%)	34 66
All	All	1506/1614 (93%)	1383 (92%)	113 (8%)	10 (1%)	22 53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	ALA
1	A	212	GLY

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Mol	Chain	Res	Type
1	A	203	VAL
1	D	159	ASN
1	E	159	ASN
1	A	205	GLY
1	B	247	SER
1	F	219	GLU
1	A	84	ALA
1	D	65	VAL

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%)	189 (93%)	15 (7%)	13	37
1	B	199/205 (97%)	182 (92%)	17 (8%)	10	31
1	C	193/205 (94%)	179 (93%)	14 (7%)	14	38
1	D	192/205 (94%)	178 (93%)	14 (7%)	14	38
1	E	196/205 (96%)	182 (93%)	14 (7%)	14	39
1	F	196/205 (96%)	180 (92%)	16 (8%)	11	33
All	All	1180/1230 (96%)	1090 (92%)	90 (8%)	13	36

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

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	LEU
1	A	60	LEU
1	A	67	ASN
1	A	69	GLU
1	A	71	LEU
1	A	74	LEU
1	A	101	THR
1	A	135	LEU
1	A	145	VAL

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Mol	Chain	Res	Type
1	A	168	LEU
1	A	210	GLU
1	A	232	MET
1	A	253	THR
1	A	269	LEU
1	B	4	LEU
1	B	5	LEU
1	B	6	ASP
1	B	60	LEU
1	B	67	ASN
1	B	69	GLU
1	B	71	LEU
1	B	74	LEU
1	B	101	THR
1	B	135	LEU
1	B	145	VAL
1	B	162	THR
1	B	168	LEU
1	B	216	GLN
1	B	232	MET
1	B	253	THR
1	B	269	LEU
1	C	4	LEU
1	C	5	LEU
1	C	6	ASP
1	C	60	LEU
1	C	67	ASN
1	C	69	GLU
1	C	71	LEU
1	C	74	LEU
1	C	135	LEU
1	C	145	VAL
1	C	168	LEU
1	C	232	MET
1	C	253	THR
1	C	269	LEU
1	D	4	LEU
1	D	5	LEU
1	D	60	LEU
1	D	67	ASN
1	D	69	GLU
1	D	71	LEU

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Mol	Chain	Res	Type
1	D	74	LEU
1	D	135	LEU
1	D	145	VAL
1	D	168	LEU
1	D	197	LEU
1	D	232	MET
1	D	253	THR
1	D	269	LEU
1	E	4	LEU
1	E	5	LEU
1	E	6	ASP
1	E	67	ASN
1	E	69	GLU
1	E	71	LEU
1	E	74	LEU
1	E	135	LEU
1	E	145	VAL
1	E	162	THR
1	E	168	LEU
1	E	232	MET
1	E	253	THR
1	E	269	LEU
1	F	4	LEU
1	F	5	LEU
1	F	6	ASP
1	F	67	ASN
1	F	69	GLU
1	F	71	LEU
1	F	74	LEU
1	F	135	LEU
1	F	145	VAL
1	F	168	LEU
1	F	216	GLN
1	F	217	LEU
1	F	218	LEU
1	F	232	MET
1	F	253	THR
1	F	269	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	67	ASN
1	A	70	HIS
1	A	139	ASN
1	A	214	GLN
1	A	224	GLN
1	B	67	ASN
1	B	139	ASN
1	B	214	GLN
1	C	67	ASN
1	C	139	ASN
1	C	224	GLN
1	D	67	ASN
1	D	139	ASN
1	E	24	HIS
1	E	67	ASN
1	E	139	ASN
1	E	214	GLN
1	E	224	GLN
1	F	67	ASN
1	F	139	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 carbohydrates in this entry.

5.6 Ligand geometry

12 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	NAD	A	301	-	42,48,48	1.71	4 (9%)	50,73,73	1.60	8 (16%)
2	5PP	A	290	-	20,20,20	0.97	2 (10%)	25,25,25	1.03	2 (8%)
2	5PP	E	294	-	20,20,20	1.17	1 (5%)	25,25,25	1.10	1 (4%)
3	NAD	D	304	-	42,48,48	1.67	2 (4%)	50,73,73	1.45	4 (8%)
2	5PP	D	293	-	20,20,20	1.04	3 (15%)	25,25,25	1.27	3 (12%)
3	NAD	C	303	-	42,48,48	1.73	5 (11%)	50,73,73	1.39	4 (8%)
3	NAD	E	305	-	42,48,48	1.90	4 (9%)	50,73,73	1.50	3 (6%)
2	5PP	F	295	-	20,20,20	1.23	1 (5%)	25,25,25	1.51	3 (12%)
3	NAD	F	306	-	42,48,48	1.69	4 (9%)	50,73,73	1.62	9 (18%)
3	NAD	B	302	-	42,48,48	1.60	2 (4%)	50,73,73	1.36	4 (8%)
2	5PP	C	292	-	20,20,20	1.18	1 (5%)	25,25,25	1.49	4 (16%)
2	5PP	B	291	-	20,20,20	1.07	2 (10%)	25,25,25	1.05	1 (4%)

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	NAD	A	301	-	-	4/26/62/62	0/5/5/5
2	5PP	A	290	-	-	4/9/9/9	0/2/2/2
2	5PP	E	294	-	-	4/9/9/9	0/2/2/2
3	NAD	D	304	-	-	2/26/62/62	0/5/5/5
2	5PP	D	293	-	-	4/9/9/9	0/2/2/2
3	NAD	C	303	-	-	2/26/62/62	0/5/5/5
3	NAD	E	305	-	-	4/26/62/62	0/5/5/5
2	5PP	F	295	-	-	2/9/9/9	0/2/2/2
3	NAD	F	306	-	-	7/26/62/62	0/5/5/5
3	NAD	B	302	-	-	4/26/62/62	0/5/5/5
2	5PP	C	292	-	-	2/9/9/9	0/2/2/2
2	5PP	B	291	-	-	4/9/9/9	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	305	NAD	O7N-C7N	9.60	1.42	1.24
3	C	303	NAD	O7N-C7N	8.32	1.40	1.24
3	F	306	NAD	O7N-C7N	8.22	1.39	1.24
3	D	304	NAD	O7N-C7N	7.94	1.39	1.24
3	B	302	NAD	O7N-C7N	7.87	1.39	1.24
3	A	301	NAD	O7N-C7N	7.50	1.38	1.24
3	A	301	NAD	C2A-N3A	5.15	1.40	1.32
2	F	295	5PP	C6-C5	4.07	1.47	1.40
2	C	292	5PP	C6-C5	4.00	1.47	1.40
3	D	304	NAD	C2A-N3A	3.95	1.38	1.32
3	F	306	NAD	C2A-N3A	3.94	1.38	1.32
3	E	305	NAD	C2A-N3A	3.89	1.38	1.32
2	E	294	5PP	C6-C5	3.75	1.47	1.40
3	C	303	NAD	C2A-N3A	3.70	1.38	1.32
2	B	291	5PP	C6-C5	3.62	1.46	1.40
3	F	306	NAD	C2A-N1A	3.17	1.39	1.33
3	B	302	NAD	C2A-N3A	3.04	1.37	1.32
3	A	301	NAD	C2A-N1A	2.77	1.39	1.33
3	E	305	NAD	C2A-N1A	2.67	1.38	1.33
2	A	290	5PP	C6-C5	2.67	1.45	1.40
2	D	293	5PP	C6-C5	2.63	1.45	1.40
3	C	303	NAD	C2A-N1A	2.51	1.38	1.33
2	D	293	5PP	O17-C6	-2.42	1.31	1.36
2	B	291	5PP	O17-C6	-2.38	1.31	1.36
3	A	301	NAD	C2B-C1B	-2.37	1.50	1.53
3	C	303	NAD	O4B-C1B	-2.32	1.37	1.41
2	A	290	5PP	O17-C6	-2.23	1.31	1.36
3	F	306	NAD	C2N-N1N	2.18	1.37	1.35
3	C	303	NAD	O4D-C1D	2.07	1.44	1.41
2	D	293	5PP	C13-C8	2.03	1.42	1.38
3	E	305	NAD	C4A-N3A	2.02	1.38	1.35

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	305	NAD	N3A-C2A-N1A	-6.57	118.42	128.68
3	F	306	NAD	N3A-C2A-N1A	-6.42	118.65	128.68
3	C	303	NAD	N3A-C2A-N1A	-6.27	118.87	128.68
3	B	302	NAD	N3A-C2A-N1A	-5.68	119.80	128.68
3	D	304	NAD	N3A-C2A-N1A	-5.68	119.81	128.68
3	A	301	NAD	N3A-C2A-N1A	-5.24	120.49	128.68
2	F	295	5PP	C5-O7-C8	5.13	130.78	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	292	5PP	C5-O7-C8	4.45	129.11	118.00
3	A	301	NAD	O4B-C1B-C2B	-3.84	101.31	106.93
3	E	305	NAD	C1B-N9A-C4A	-3.59	120.33	126.64
3	D	304	NAD	C6N-N1N-C2N	-3.36	118.91	121.97
3	C	303	NAD	C1B-N9A-C4A	-3.31	120.82	126.64
2	E	294	5PP	C5-O7-C8	3.27	126.15	118.00
2	C	292	5PP	C3-C2-C1	3.19	123.00	118.54
3	F	306	NAD	C6N-N1N-C2N	-3.19	119.07	121.97
3	A	301	NAD	O2N-PN-O1N	3.04	127.26	112.24
3	A	301	NAD	C2N-C3N-C4N	2.86	121.50	118.26
3	C	303	NAD	PN-O3-PA	-2.77	123.32	132.83
3	F	306	NAD	C3D-C2D-C1D	2.76	105.14	100.98
3	F	306	NAD	C2N-C3N-C4N	2.76	121.39	118.26
3	F	306	NAD	PN-O3-PA	-2.74	123.41	132.83
3	A	301	NAD	C5A-C6A-N6A	-2.69	116.26	120.35
2	A	290	5PP	O17-C6-C5	-2.65	113.91	120.09
2	B	291	5PP	C3-C2-C1	2.62	122.22	118.54
3	A	301	NAD	C6N-N1N-C2N	-2.51	119.68	121.97
3	B	302	NAD	O4B-C1B-C2B	-2.43	103.38	106.93
2	C	292	5PP	C15-C14-C2	-2.42	104.57	113.68
2	D	293	5PP	C3-C2-C1	2.42	121.92	118.54
3	D	304	NAD	PN-O3-PA	-2.34	124.81	132.83
3	B	302	NAD	C1B-N9A-C4A	-2.33	122.55	126.64
3	E	305	NAD	O7N-C7N-C3N	-2.24	116.96	119.63
3	A	301	NAD	O3B-C3B-C4B	-2.23	104.59	111.05
3	B	302	NAD	O7N-C7N-N7N	-2.22	119.42	122.58
3	A	301	NAD	O4B-C4B-C5B	2.22	116.67	109.37
2	F	295	5PP	C14-C2-C3	-2.20	115.67	121.23
3	D	304	NAD	O4B-C1B-C2B	-2.20	103.71	106.93
3	F	306	NAD	C2N-N1N-C1D	2.19	124.01	119.14
3	F	306	NAD	C3N-C7N-N7N	2.18	120.37	117.75
3	C	303	NAD	C2N-C3N-C4N	2.16	120.71	118.26
2	C	292	5PP	C6-C1-C2	-2.14	118.55	120.83
2	F	295	5PP	C9-C8-C13	-2.14	116.87	120.18
3	F	306	NAD	C4N-C3N-C7N	-2.13	115.35	121.04
2	D	293	5PP	C6-C1-C2	-2.10	118.60	120.83
2	D	293	5PP	C9-C8-C13	-2.07	116.98	120.18
3	F	306	NAD	C1B-N9A-C4A	-2.07	123.00	126.64
2	A	290	5PP	C3-C2-C1	2.04	121.40	118.54

There are no chirality outliers.

All (43) torsion outliers are listed below:

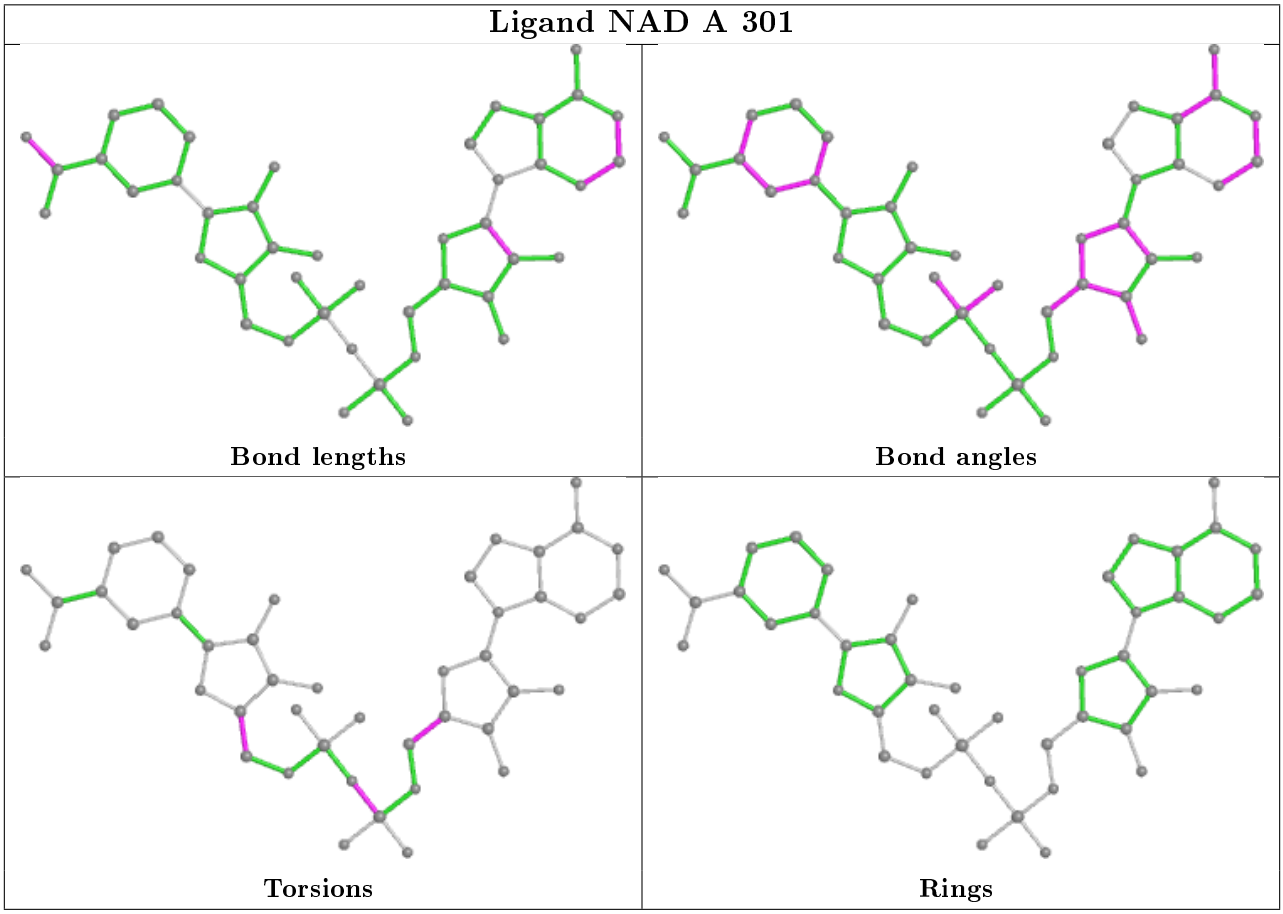
Mol	Chain	Res	Type	Atoms
3	D	304	NAD	O4D-C1D-N1N-C2N
3	C	303	NAD	O4D-C1D-N1N-C2N
3	B	302	NAD	O4D-C1D-N1N-C2N
3	E	305	NAD	C5B-O5B-PA-O1A
3	F	306	NAD	C2N-C3N-C7N-O7N
2	E	294	5PP	C2-C14-C15-C16
2	A	290	5PP	C2-C14-C15-C16
2	F	295	5PP	C2-C14-C15-C16
2	B	291	5PP	C2-C14-C15-C16
3	F	306	NAD	C2N-C3N-C7N-N7N
2	D	293	5PP	C2-C14-C15-C16
2	E	294	5PP	C14-C15-C16-C17
2	B	291	5PP	C14-C15-C16-C17
2	C	292	5PP	C14-C15-C16-C17
2	F	295	5PP	C14-C15-C16-C17
2	A	290	5PP	C15-C16-C17-C18
2	D	293	5PP	C15-C16-C17-C18
2	A	290	5PP	C14-C15-C16-C17
2	C	292	5PP	C15-C16-C17-C18
2	E	294	5PP	C15-C16-C17-C18
3	E	305	NAD	C5B-O5B-PA-O3
3	F	306	NAD	PN-O3-PA-O1A
2	D	293	5PP	C14-C15-C16-C17
3	A	301	NAD	O4D-C4D-C5D-O5D
2	B	291	5PP	C15-C16-C17-C18
3	F	306	NAD	PN-O3-PA-O2A
3	B	302	NAD	PA-O3-PN-O2N
2	B	291	5PP	C6-C5-O7-C8
2	A	290	5PP	C6-C5-O7-C8
3	F	306	NAD	C4N-C3N-C7N-N7N
3	E	305	NAD	O4B-C4B-C5B-O5B
3	A	301	NAD	PN-O3-PA-O1A
3	F	306	NAD	C4N-C3N-C7N-O7N
3	B	302	NAD	O4B-C4B-C5B-O5B
2	E	294	5PP	C6-C5-O7-C8
3	A	301	NAD	O4B-C4B-C5B-O5B
3	A	301	NAD	C3D-C4D-C5D-O5D
3	F	306	NAD	O4B-C4B-C5B-O5B
3	D	304	NAD	O4B-C4B-C5B-O5B
3	B	302	NAD	PA-O3-PN-O1N
3	E	305	NAD	C5B-O5B-PA-O2A
3	C	303	NAD	O4B-C4B-C5B-O5B
2	D	293	5PP	C6-C5-O7-C8

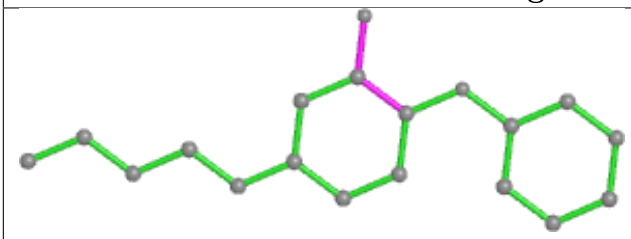
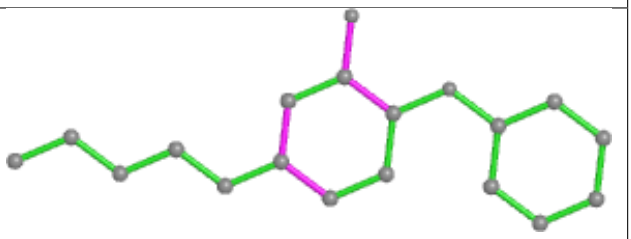
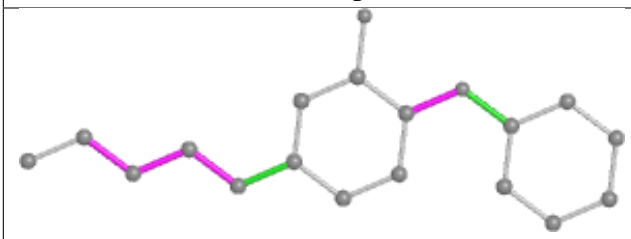
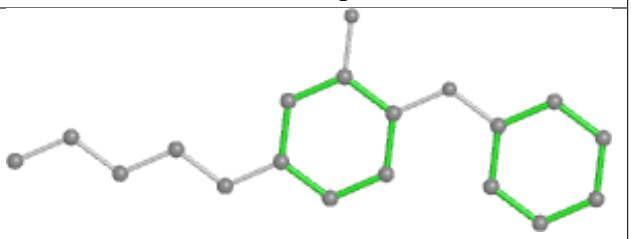
There are no ring outliers.

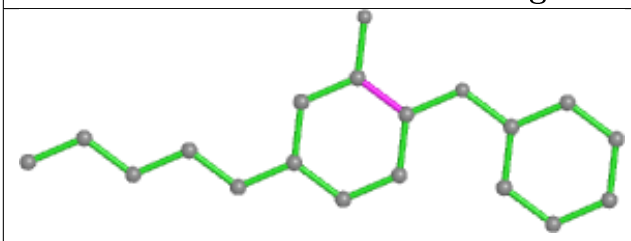
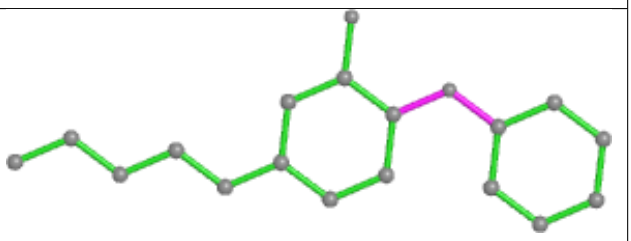
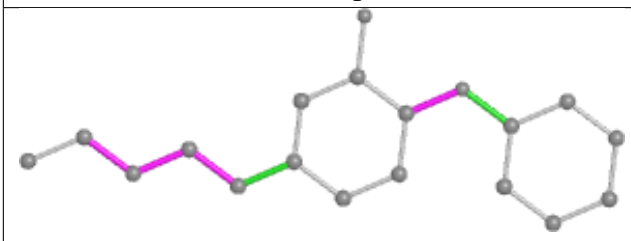
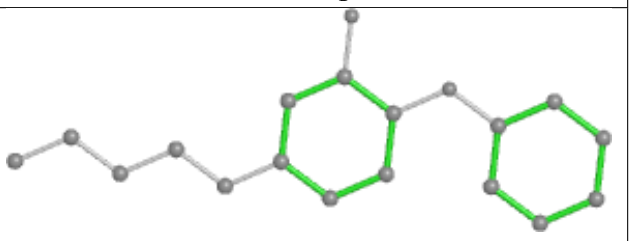
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	NAD	4	0
3	D	304	NAD	1	0
3	C	303	NAD	1	0
3	F	306	NAD	3	0
3	B	302	NAD	1	0

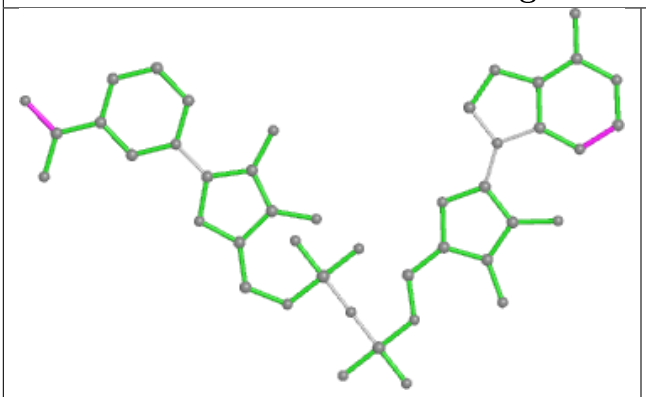
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



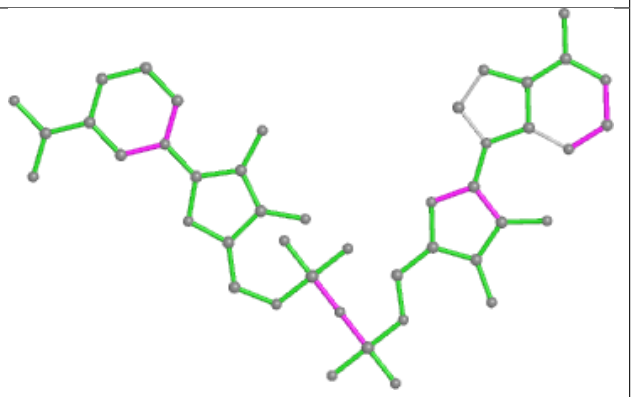
Ligand 5PP A 290	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 5PP E 294	
 Bond lengths	 Bond angles
 Torsions	 Rings

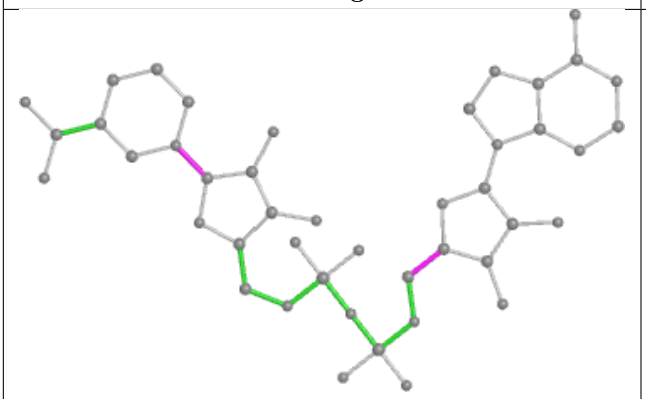
Ligand NAD D 304



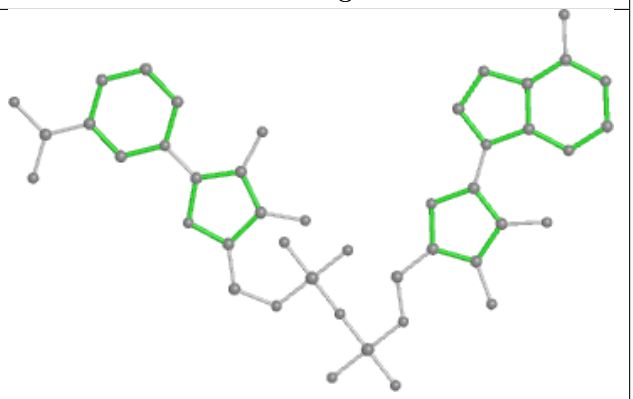
Bond lengths



Bond angles

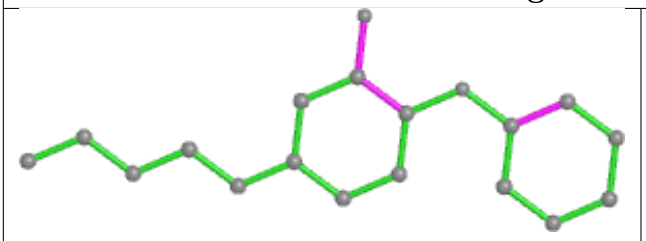


Torsions

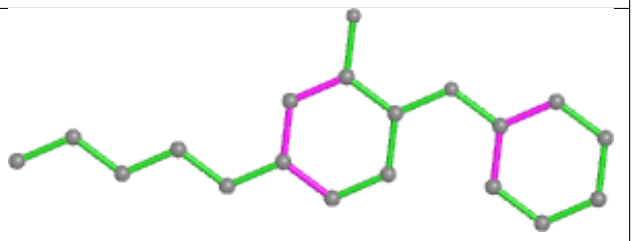


Rings

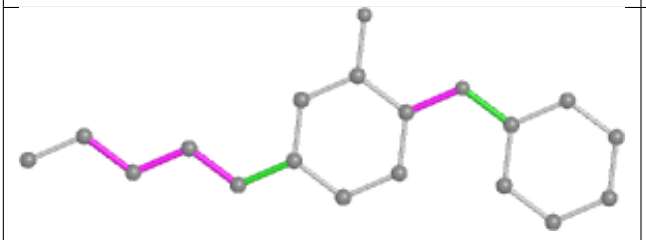
Ligand 5PP D 293



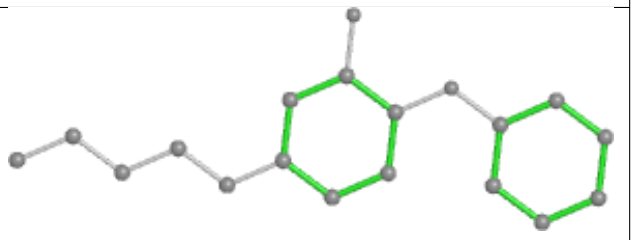
Bond lengths



Bond angles

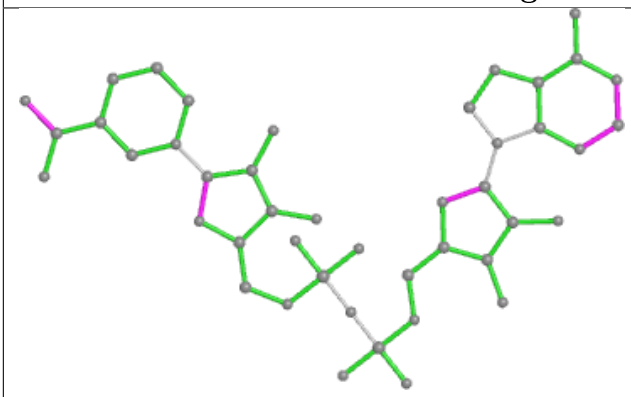


Torsions

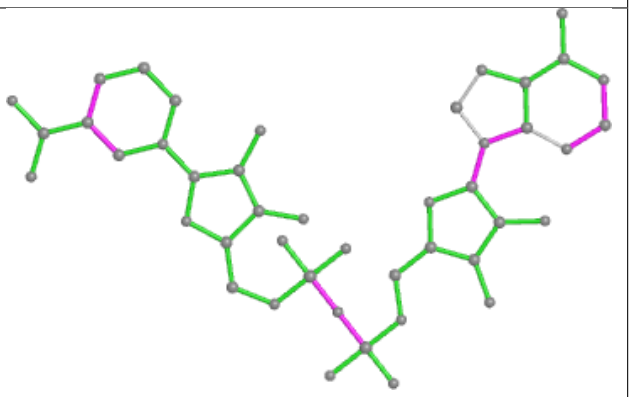


Rings

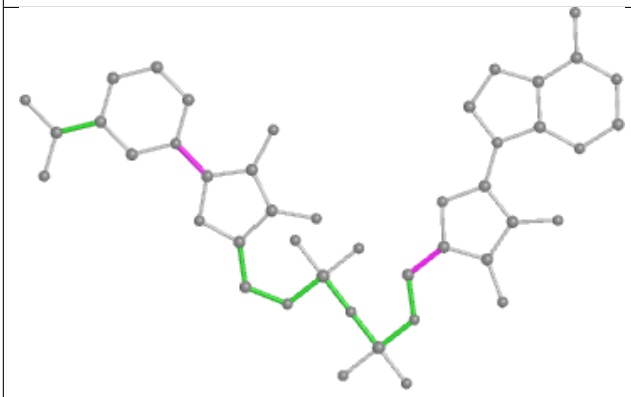
Ligand NAD C 303



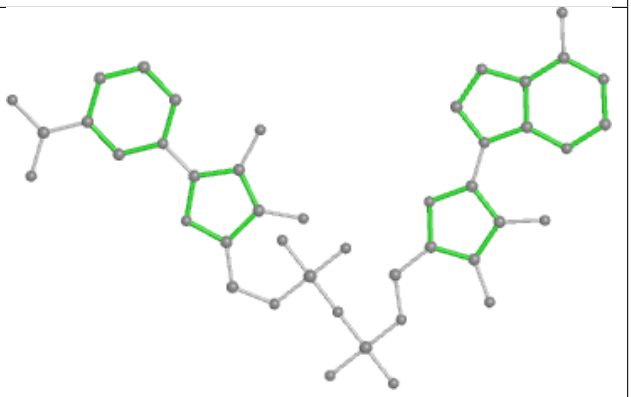
Bond lengths



Bond angles

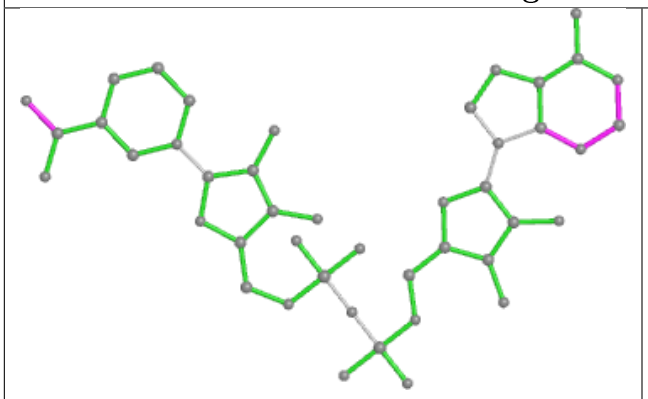


Torsions

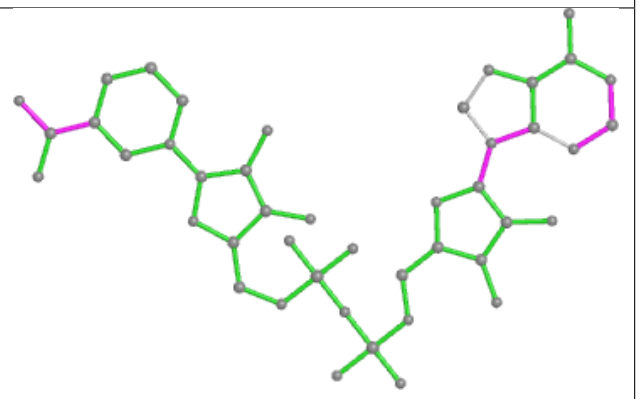


Rings

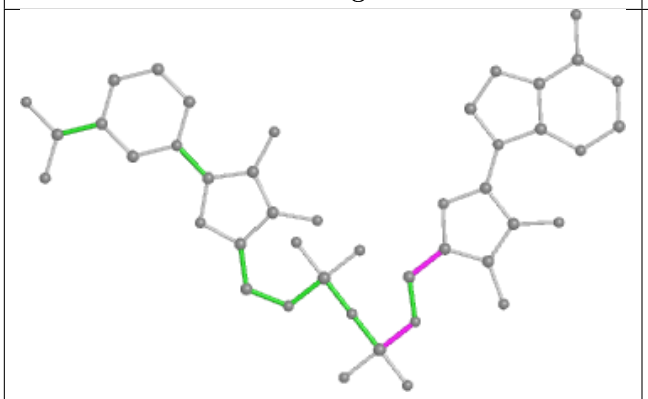
Ligand NAD E 305



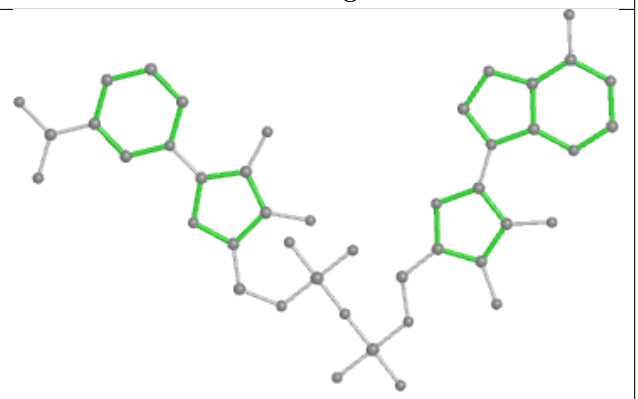
Bond lengths



Bond angles

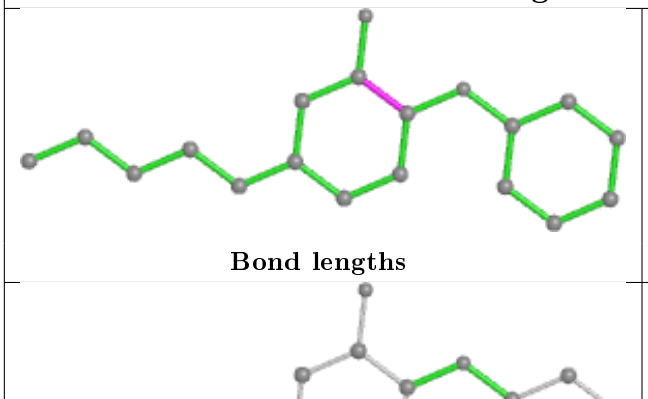


Torsions

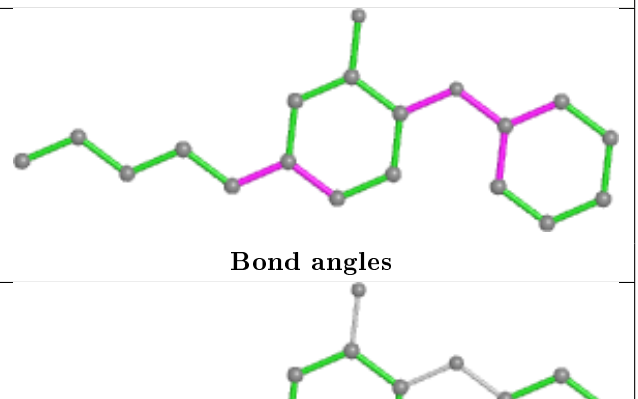


Rings

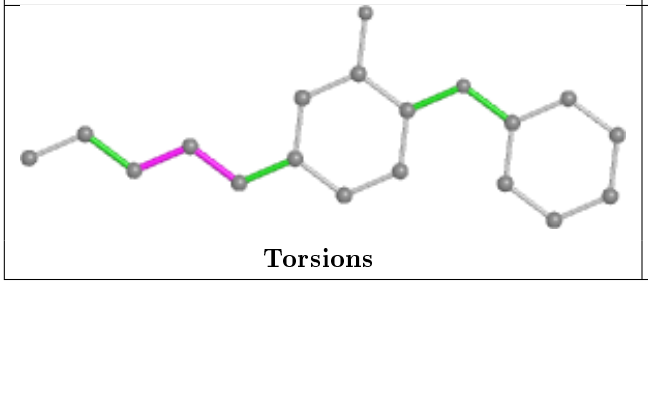
Ligand 5PP F 295



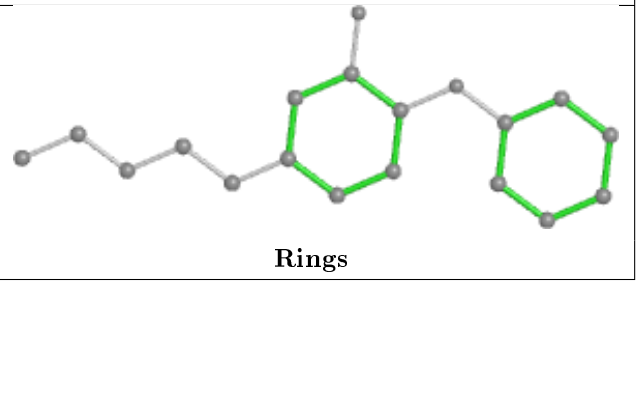
Bond lengths



Bond angles

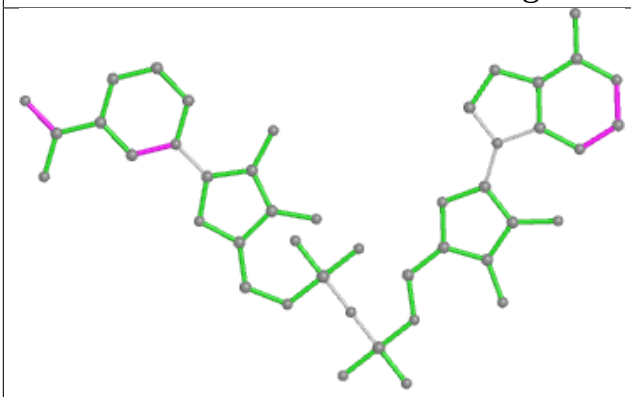


Torsions

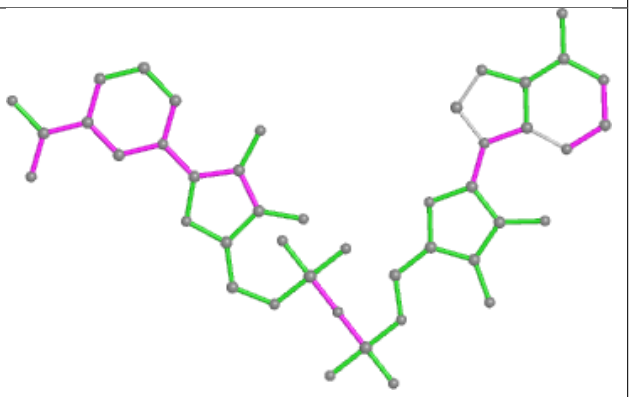


Rings

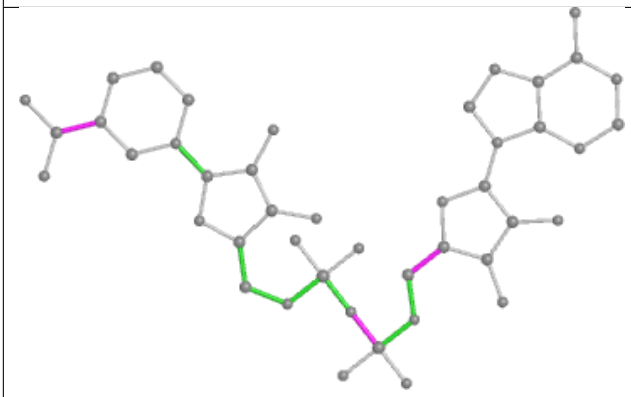
Ligand NAD F 306



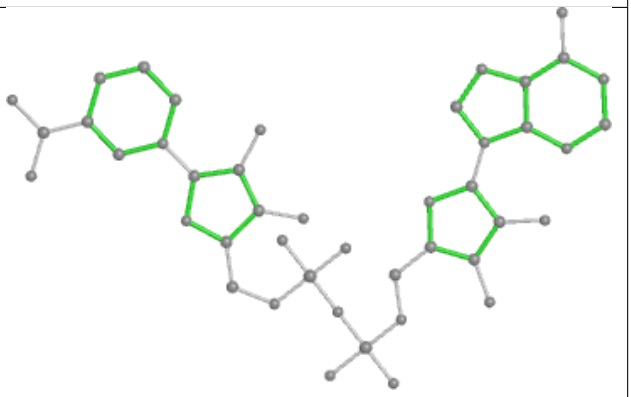
Bond lengths



Bond angles

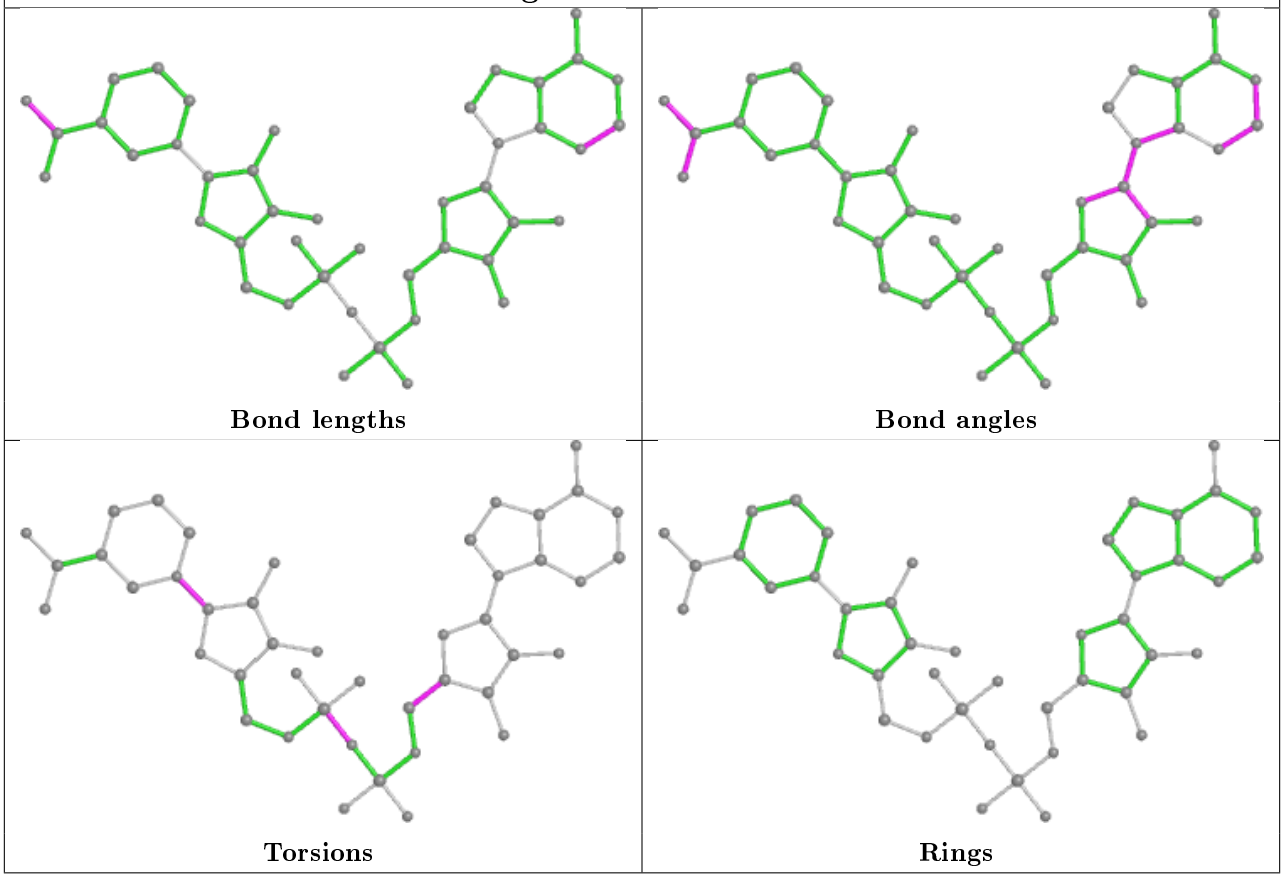


Torsions

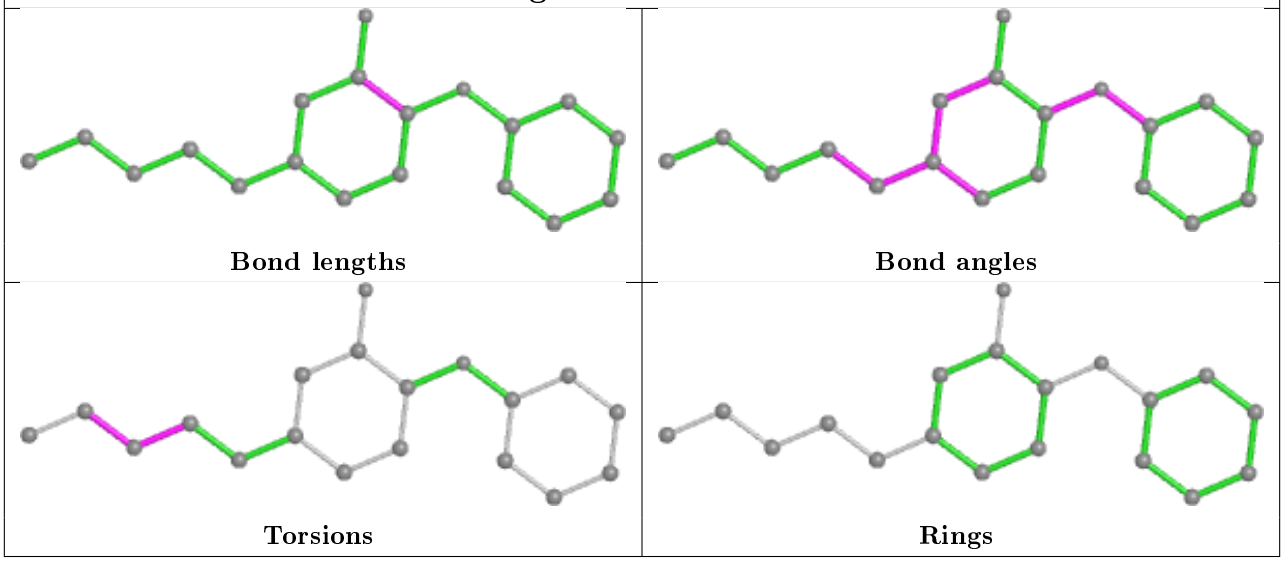


Rings

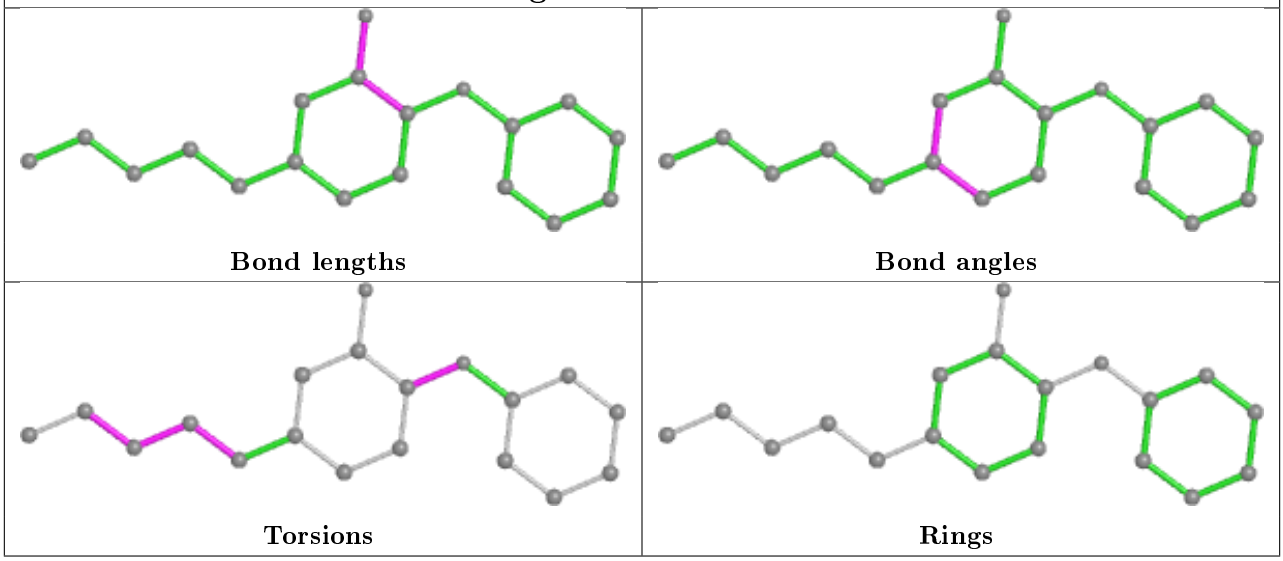
Ligand NAD B 302



Ligand 5PP C 292



Ligand 5PP B 291



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.01	12 (4%) 33 23	6, 22, 55, 80	0
1	B	259/269 (96%)	-0.11	3 (1%) 79 73	4, 21, 48, 63	0
1	C	248/269 (92%)	0.34	16 (6%) 18 11	18, 35, 59, 64	0
1	D	248/269 (92%)	0.45	12 (4%) 30 21	19, 35, 58, 66	0
1	E	254/269 (94%)	0.32	11 (4%) 35 25	16, 33, 52, 63	0
1	F	251/269 (93%)	0.48	27 (10%) 5 3	14, 33, 57, 68	0
All	All	1528/1614 (94%)	0.24	81 (5%) 26 17	4, 31, 56, 80	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	LEU	6.1
1	A	200	SER	5.8
1	D	196	THR	5.7
1	F	221	GLY	4.8
1	D	86	ASN	4.7
1	C	2	THR	4.5
1	D	195	ARG	4.4
1	F	220	GLU	4.2
1	D	84	ALA	4.1
1	F	2	THR	3.9
1	A	213	ALA	3.8
1	C	3	GLY	3.8
1	D	44	LEU	3.6
1	C	16	ILE	3.6
1	F	57	LYS	3.5
1	A	199	MET	3.5
1	F	196	THR	3.4
1	F	110	ASP	3.3
1	F	139	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	32	GLN	3.2
1	A	204	GLY	3.2
1	E	84	ALA	3.2
1	F	85	GLY	3.1
1	D	221	GLY	3.1
1	E	83	GLY	3.1
1	F	73	SER	3.0
1	F	44	LEU	3.0
1	F	219	GLU	3.0
1	F	79	THR	3.0
1	E	106	ASN	2.9
1	F	86	ASN	2.9
1	C	46	LEU	2.9
1	D	49	ARG	2.8
1	F	269	LEU	2.7
1	D	82	ILE	2.7
1	D	80	GLU	2.7
1	C	82	ILE	2.6
1	D	53	ARG	2.5
1	E	100	GLN	2.5
1	A	196	THR	2.5
1	E	221	GLY	2.5
1	D	83	GLY	2.4
1	C	21	ILE	2.4
1	F	84	ALA	2.4
1	E	2	THR	2.4
1	B	84	ALA	2.4
1	F	215	ILE	2.4
1	A	217	LEU	2.4
1	B	43	ARG	2.4
1	E	35	GLN	2.4
1	B	47	ILE	2.4
1	A	215	ILE	2.3
1	F	214	GLN	2.3
1	A	219	GLU	2.3
1	F	232	MET	2.3
1	C	51	THR	2.2
1	C	15	ILE	2.2
1	E	101	THR	2.2
1	D	81	ALA	2.2
1	C	18	ASP	2.2
1	A	220	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	195	ARG	2.2
1	F	6	ASP	2.2
1	E	10	ILE	2.1
1	C	53	ARG	2.1
1	C	220	GLU	2.1
1	E	46	LEU	2.1
1	C	69	GLU	2.1
1	C	106	ASN	2.1
1	F	249	TRP	2.1
1	E	105	ILE	2.1
1	F	136	PRO	2.1
1	A	46	LEU	2.1
1	C	217	LEU	2.1
1	C	59	PRO	2.1
1	F	52	ASP	2.0
1	F	89	ASP	2.0
1	F	43	ARG	2.0
1	F	7	GLY	2.0
1	F	138	MET	2.0
1	A	201	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	5PP	E	294	19/19	0.41	0.69	59,60,61,61	19
2	5PP	F	295	19/19	0.51	0.62	46,50,51,51	19
2	5PP	C	292	19/19	0.74	0.44	20,23,27,27	19

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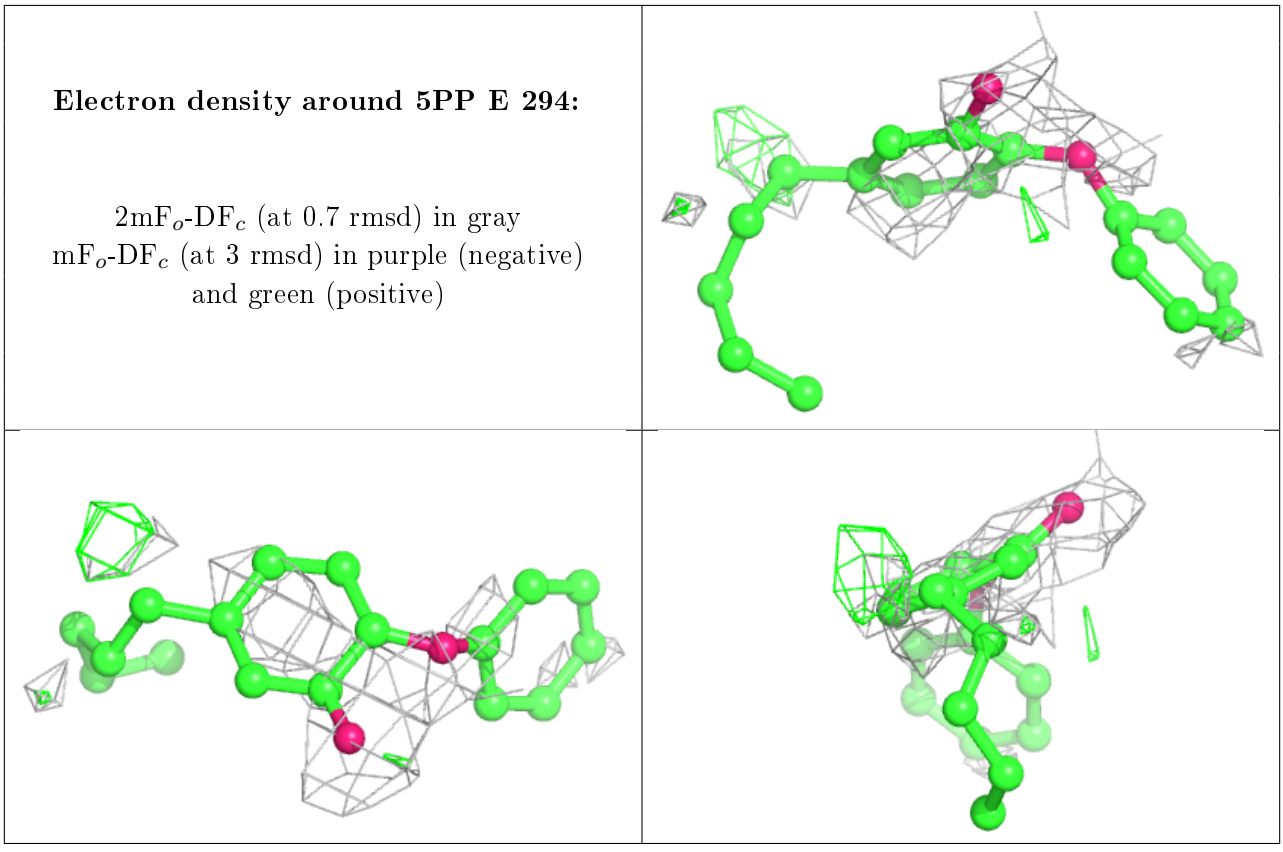
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	5PP	B	291	19/19	0.80	0.54	26,29,30,31	19
2	5PP	D	293	19/19	0.82	0.39	18,20,21,21	19
2	5PP	A	290	19/19	0.83	0.48	22,25,27,27	19
3	NAD	C	303	44/44	0.91	0.21	24,39,46,49	0
3	NAD	D	304	44/44	0.92	0.19	22,36,45,46	0
3	NAD	F	306	44/44	0.92	0.19	22,34,49,50	0
3	NAD	E	305	44/44	0.94	0.16	19,23,27,29	0
3	NAD	B	302	44/44	0.96	0.12	4,11,18,21	0
3	NAD	A	301	44/44	0.97	0.12	2,11,19,20	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.

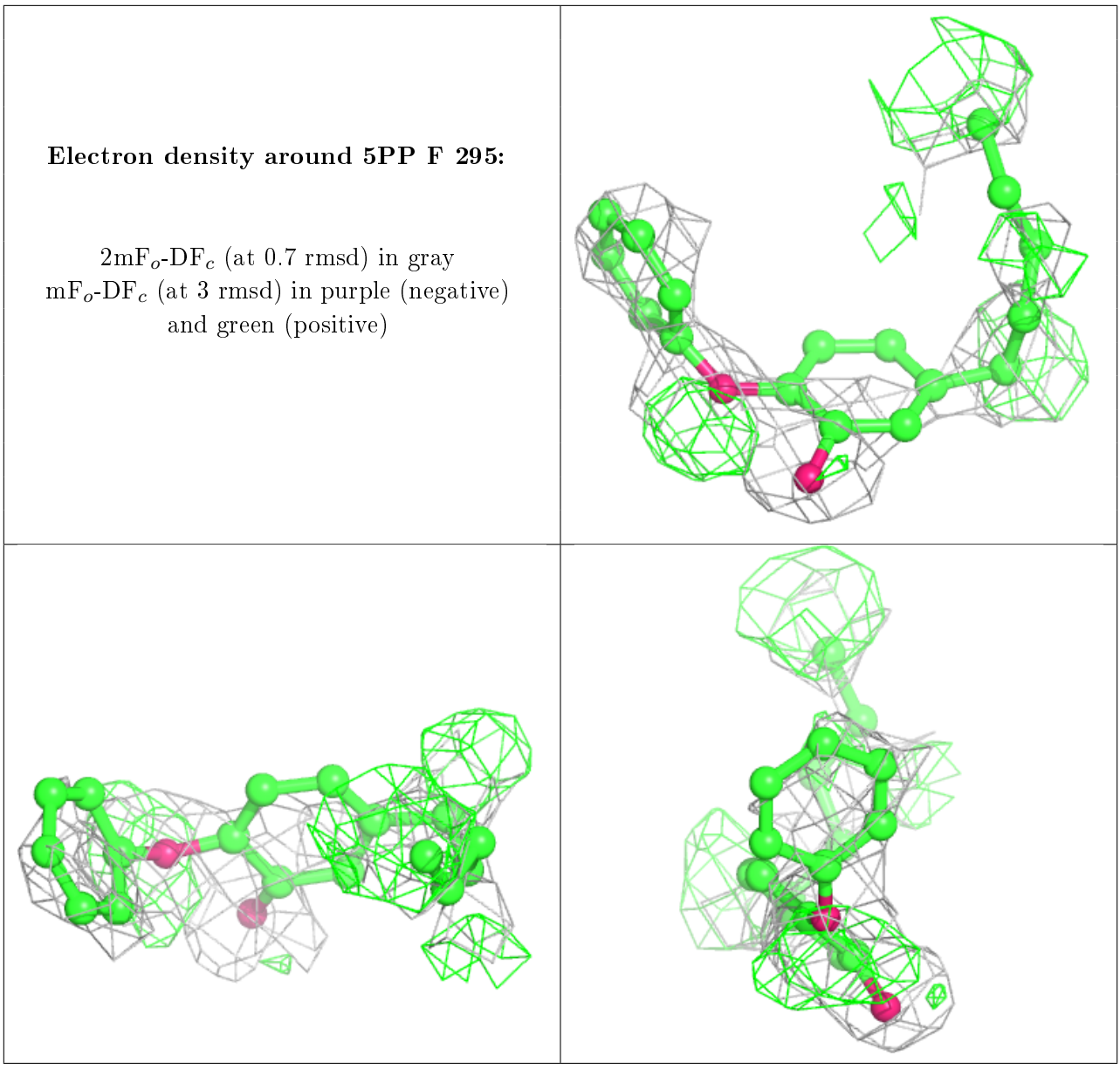
Electron density around 5PP E 294:

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



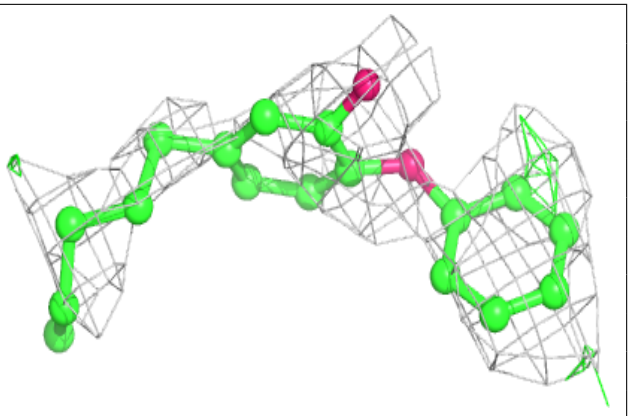
Electron density around 5PP F 295:

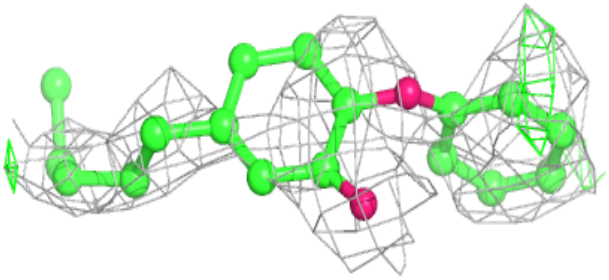
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

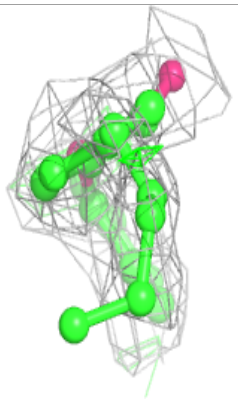


Electron density around 5PP C 292:

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

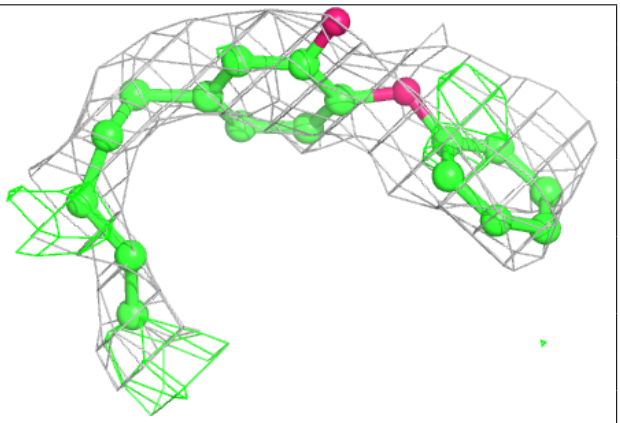


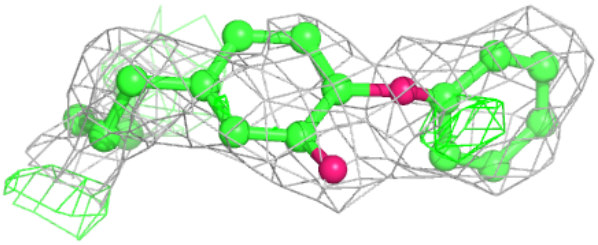


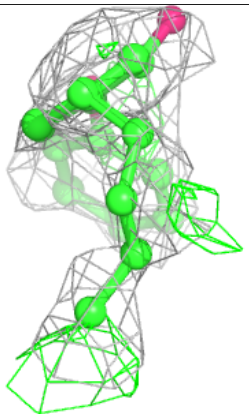


Electron density around 5PP B 291:

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

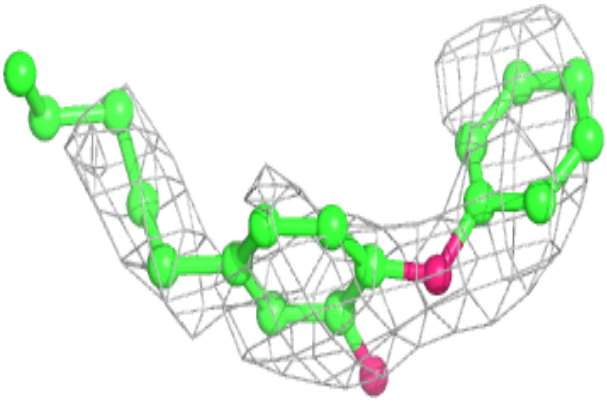


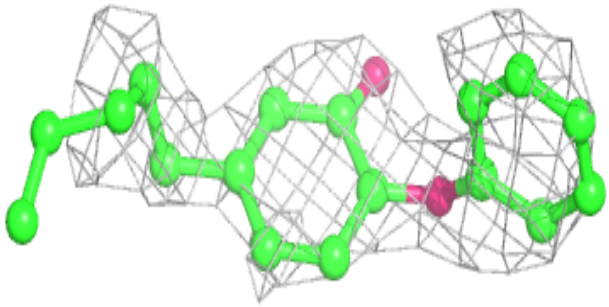


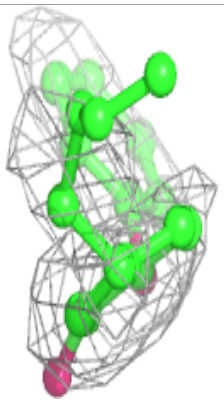


Electron density around 5PP D 293:

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

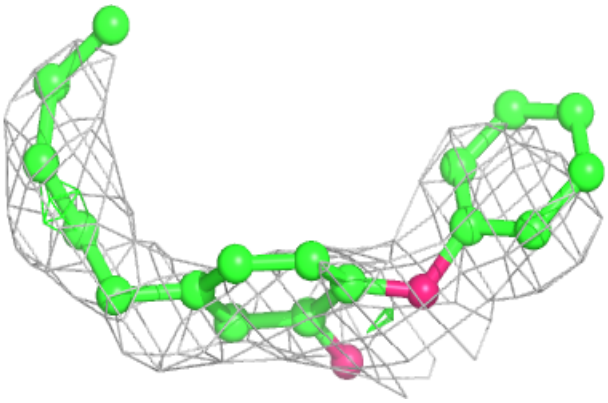


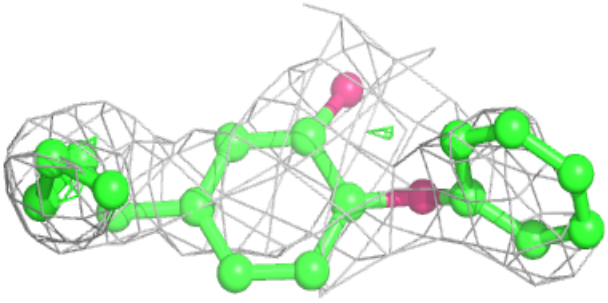


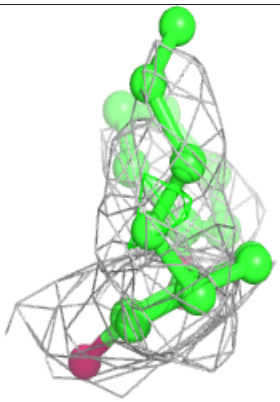


Electron density around 5PP A 290:

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

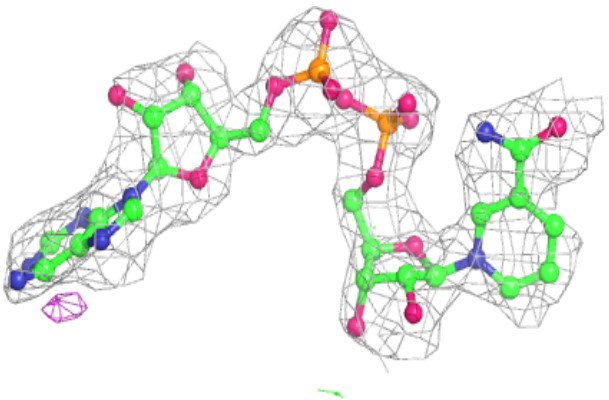


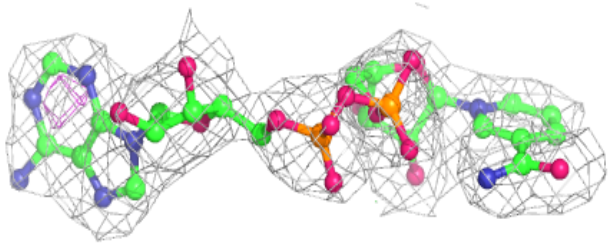


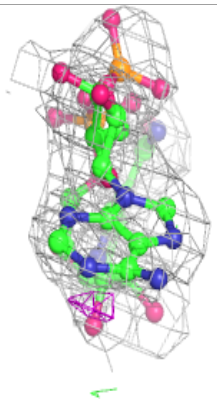


Electron density around NAD C 303:

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

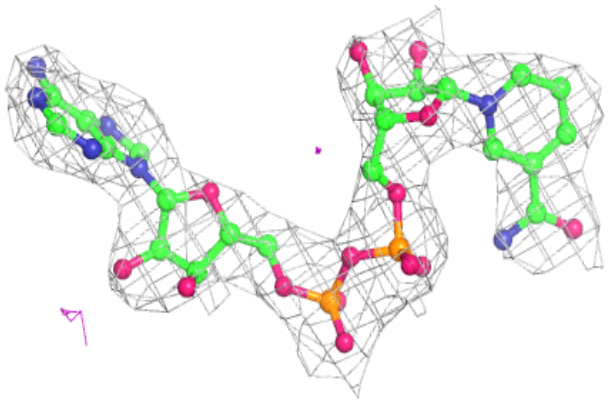


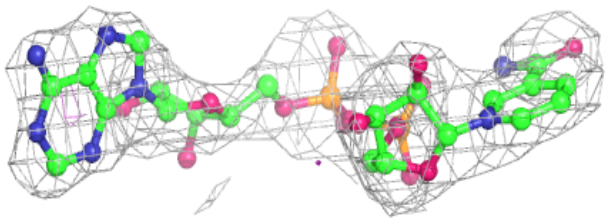


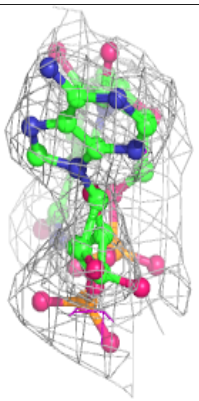


Electron density around NAD D 304:

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

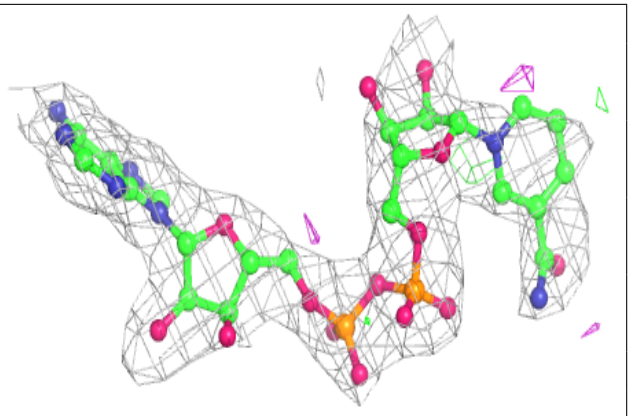


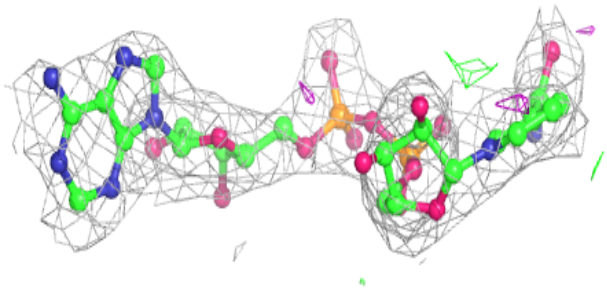


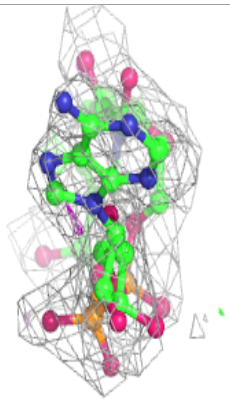


Electron density around NAD F 306:

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

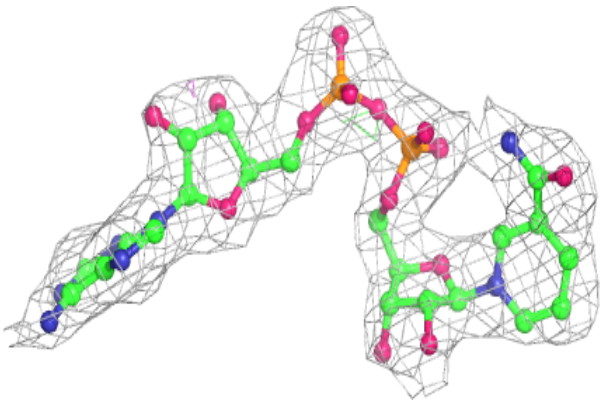


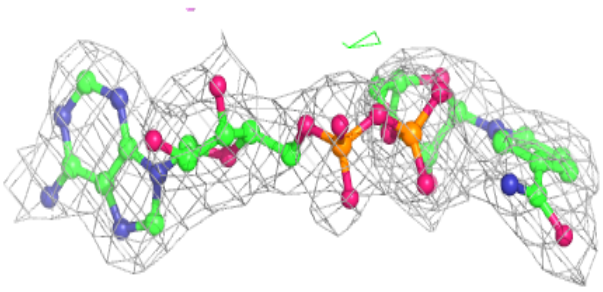


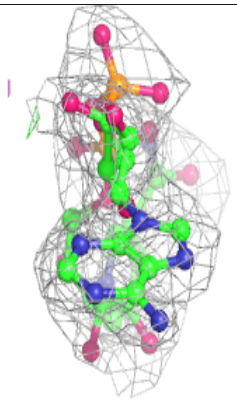


Electron density around NAD E 305:

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

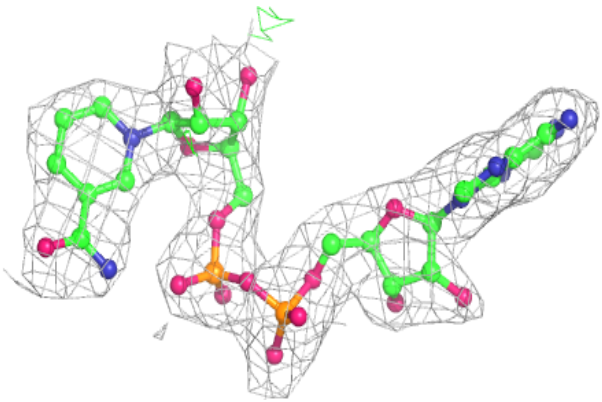


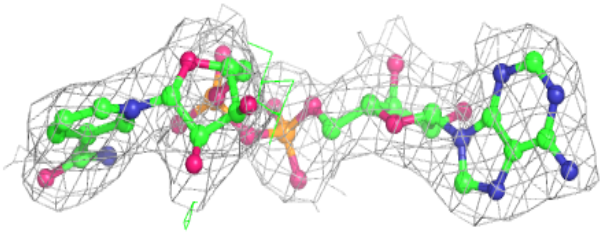


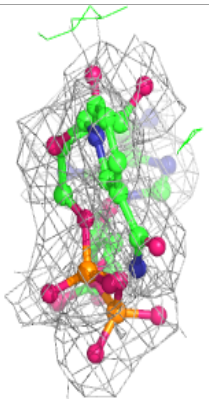


Electron density around NAD B 302:

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

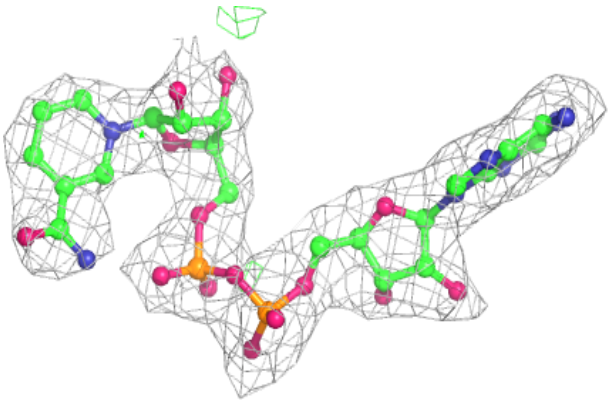


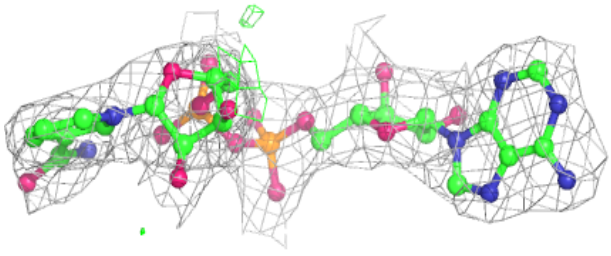


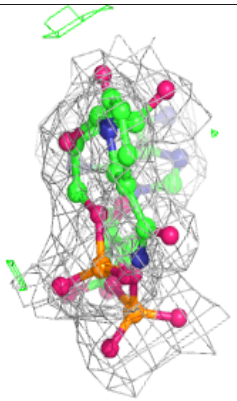


Electron density around NAD A 301:

$2mF_o$-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.