Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:00 am BST

PDB ID	:	2B35
Title	:	Crystal structure of Mycobacterium tuberculosis enoyl reductase (InhA) inhibited by triclosan
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	:	2.30 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:

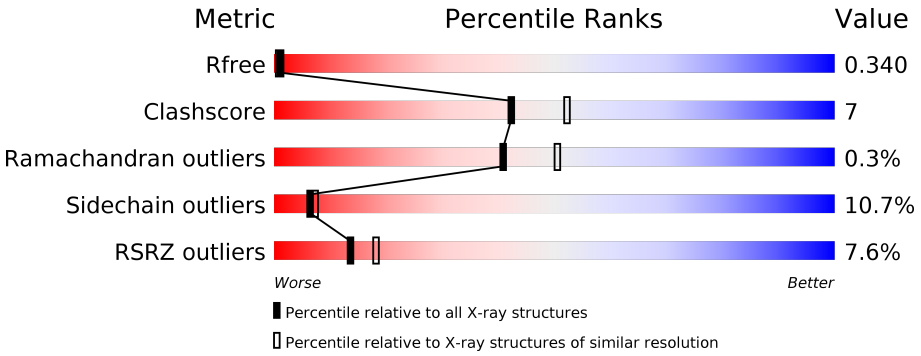
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	2% 74% 17% • 6%
1	B	269	2% 72% 17% • 9%
1	C	269	11% 66% 23% • 8%
1	D	269	8% 72% 18% • 8%
1	E	269	9% 74% 18% • 6%
1	F	269	10% 73% 18% • 7%

2 Entry composition

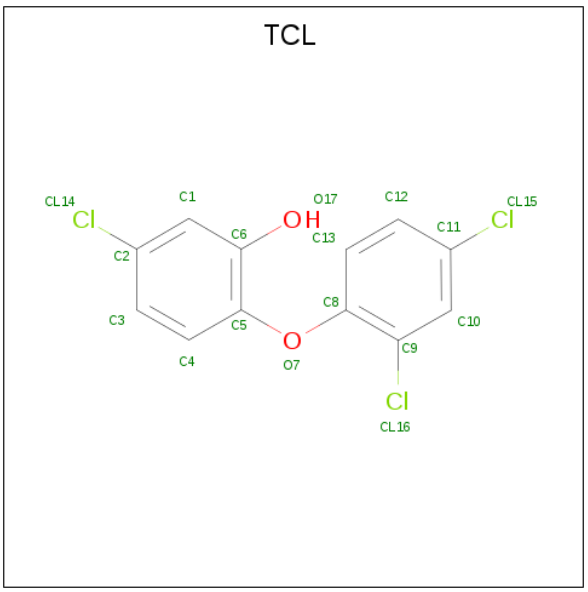
There are 3 unique types of molecules in this entry. The entry contains 11637 atoms, of which 0 are hydrogens and 0 are deuteriums.

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].

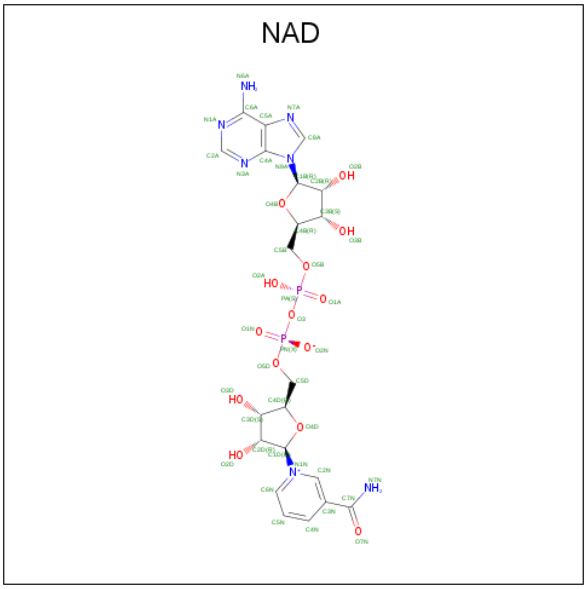
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1900	1205	333	353	9			
1	B	246	Total	C	N	O	S	0	0	0
			1849	1172	324	344	9			
1	C	248	Total	C	N	O	S	0	0	0
			1865	1184	326	346	9			
1	D	248	Total	C	N	O	S	0	0	0
			1861	1181	326	344	10			
1	E	254	Total	C	N	O	S	0	0	0
			1905	1208	334	354	9			
1	F	251	Total	C	N	O	S	0	0	0
			1891	1200	331	351	9			

- Molecule 2 is TRICLOSAN (three-letter code: TCL) (formula: $C_{12}H_7Cl_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	B	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	C	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	D	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	E	1	Total	C	Cl	O	0	0
			17	12	3	2		
2	F	1	Total	C	Cl	O	0	0
			17	12	3	2		

- 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	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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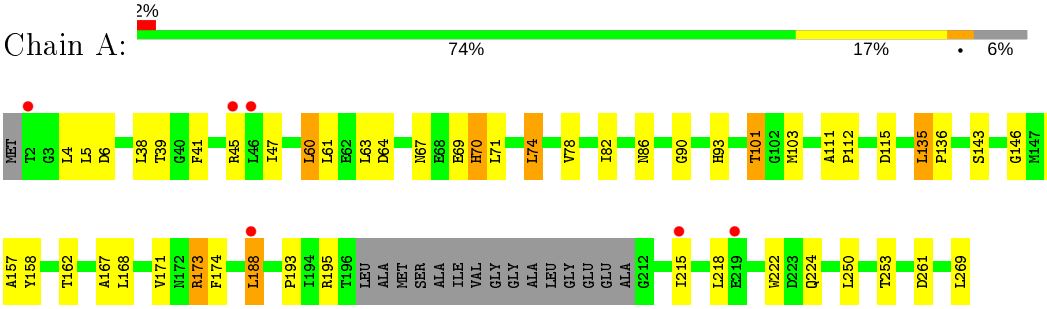
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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.

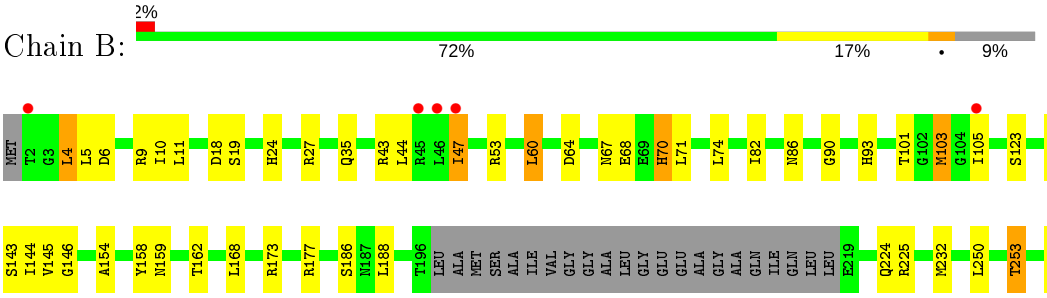
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain A:



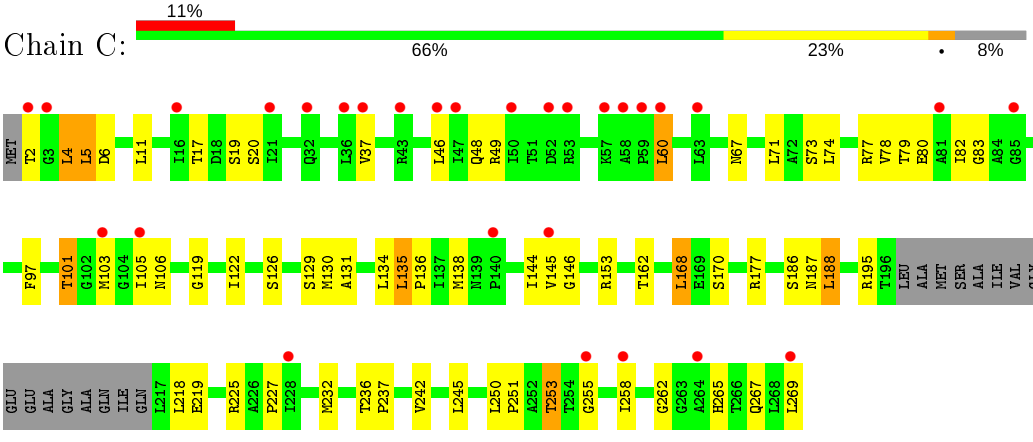
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain B:



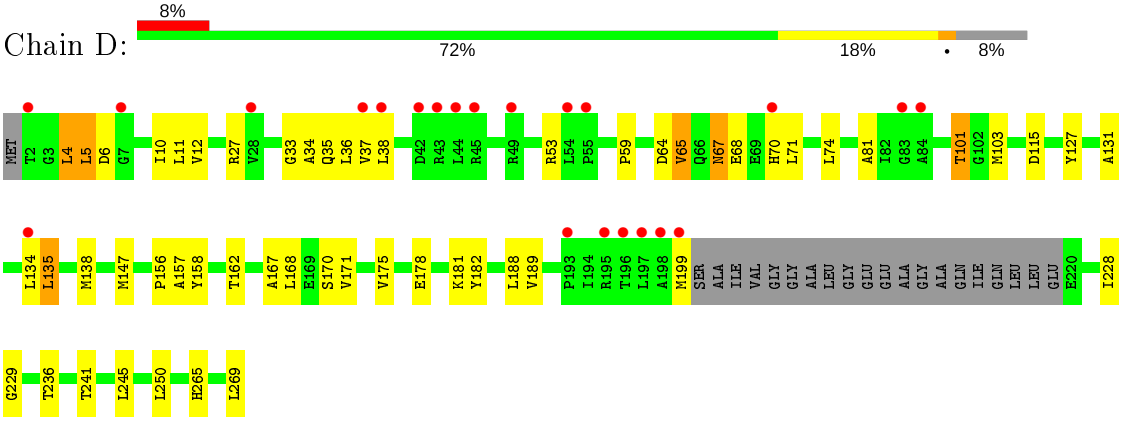
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain C:



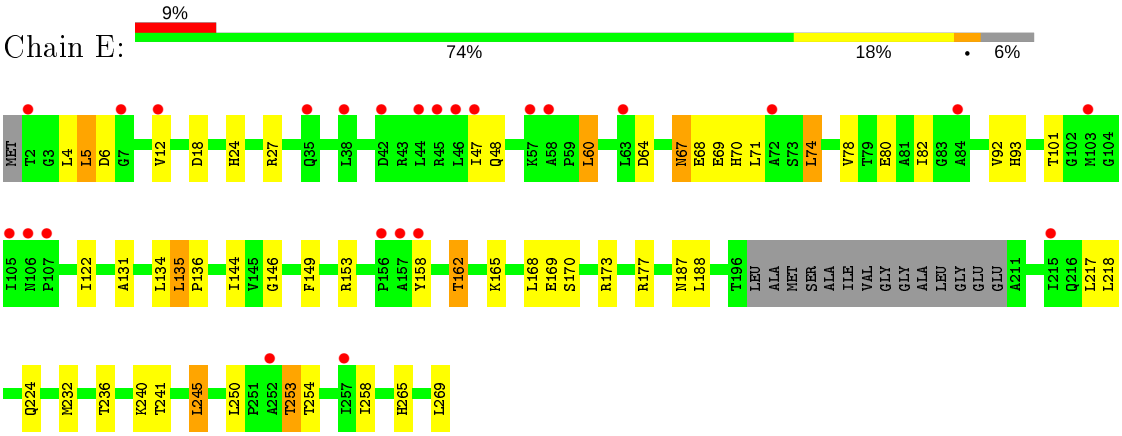
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain D:



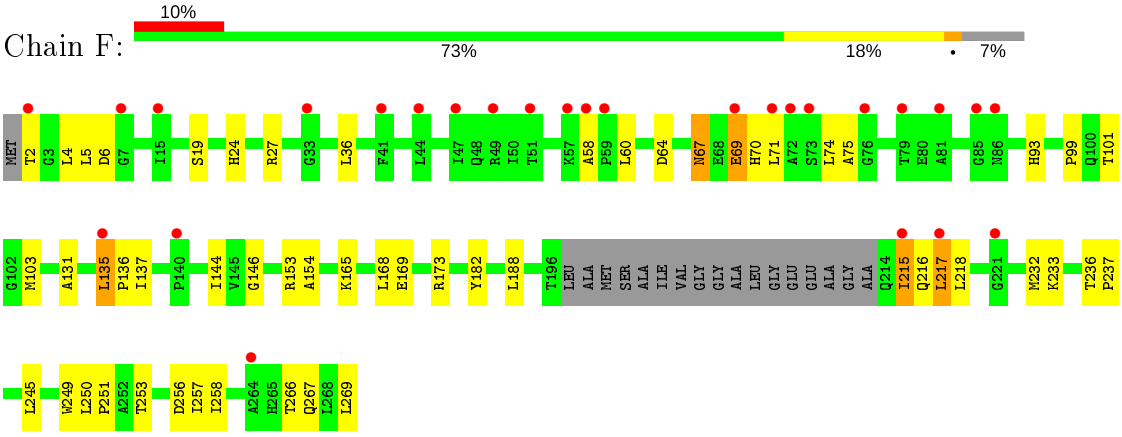
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain E:



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

Chain F:



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 – 2.30 46.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.1 (10.00-2.30) 82.2 (46.93-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005, CNS	Depositor
R, R_{free}	0.268 , 0.334 0.278 , 0.340	Depositor DCC
R_{free} test set	3633 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	11637	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 13.25% 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: TCL, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.68	0/1937	0.74	1/2630 (0.0%)
1	B	0.67	0/1886	0.77	3/2561 (0.1%)
1	C	0.62	0/1902	0.67	0/2583
1	D	0.63	0/1898	0.71	0/2577
1	E	0.60	0/1942	0.71	1/2637 (0.0%)
1	F	0.62	0/1928	0.71	0/2618
All	All	0.64	0/11493	0.72	5/15606 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	177	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	4	LEU	CA-CB-CG	6.00	129.09	115.30
1	E	177	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	173	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	173	ARG	NE-CZ-NH2	-5.65	117.48	120.30

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	1900	0	1915	27	0
1	B	1849	0	1858	18	0
1	C	1865	0	1880	38	0
1	D	1861	0	1877	28	0
1	E	1905	0	1920	34	0
1	F	1891	0	1907	29	0
2	A	17	0	6	2	0
2	B	17	0	6	1	0
2	C	17	0	6	1	0
2	D	17	0	6	2	0
2	E	17	0	6	1	0
2	F	17	0	6	2	0
3	A	44	0	26	1	0
3	B	44	0	26	0	0
3	C	44	0	26	0	0
3	D	44	0	26	2	0
3	E	44	0	26	2	0
3	F	44	0	26	2	0
All	All	11637	0	11549	160	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 7.

All (160) 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:C:103:MET:SD	2:C:304:TCL:H121	2.25	0.77
1:A:173:ARG:HB3	1:B:154:ALA:HB2	1.69	0.74
1:E:173:ARG:HB3	1:F:154:ALA:HB2	1.70	0.74
1:F:215:ILE:HG23	1:F:218:LEU:HD12	1.70	0.72
1:C:265:HIS:O	1:E:153:ARG:NH1	2.22	0.72
1:B:47:ILE:HD11	1:B:60:LEU:HD21	1.72	0.70
1:F:64:ASP:H	1:F:70:HIS:HD2	1.38	0.70
1:C:265:HIS:O	1:E:153:ARG:HD3	1.92	0.69
1:D:64:ASP:H	1:D:70:HIS:HD2	1.41	0.69
1:F:131:ALA:O	1:F:135:LEU:HB2	1.93	0.68
1:D:199:MET:HB3	2:D:306:TCL:H31	1.77	0.66
1:F:103:MET:SD	2:F:311:TCL:H121	2.35	0.66
1:C:101:THR:O	1:C:106:ASN:ND2	2.28	0.65
1:F:215:ILE:HG22	1:F:216:GLN:H	1.60	0.65
1:C:168:LEU:HD13	1:C:188:LEU:HD21	1.78	0.65
1:A:38:LEU:HB2	1:A:60:LEU:HD23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ASP:H	1:A:70:HIS:HD2	1.43	0.63
1:E:67:ASN:HD21	1:E:69:GLU:HB2	1.65	0.62
1:B:103:MET:SD	2:B:302:TCL:H121	2.41	0.60
1:F:67:ASN:HD21	1:F:69:GLU:HB2	1.66	0.60
1:C:265:HIS:O	1:E:153:ARG:CZ	2.51	0.58
1:E:131:ALA:O	1:E:135:LEU:HB2	2.04	0.58
1:D:67:ASN:OD1	1:D:70:HIS:CE1	2.57	0.57
1:E:4:LEU:HD13	1:E:5:LEU:HD13	1.87	0.57
1:B:24:HIS:HD2	1:B:27:ARG:HH21	1.53	0.57
1:F:249:TRP:O	1:F:250:LEU:HG	2.05	0.56
1:B:158:TYR:HD2	1:B:162:THR:HG1	1.53	0.56
1:E:24:HIS:HD2	1:E:27:ARG:HH21	1.53	0.56
1:A:45:ARG:HG2	1:C:136:PRO:HB3	1.88	0.56
1:A:86:ASN:OD1	1:F:233:LYS:HE3	2.05	0.56
1:D:250:LEU:HD23	1:E:241:THR:HG23	1.89	0.54
1:F:258:ILE:HD12	1:F:258:ILE:N	2.23	0.54
1:D:4:LEU:HD13	1:D:5:LEU:HD13	1.90	0.53
1:D:67:ASN:HD22	1:D:68:GLU:N	2.05	0.53
1:A:74:LEU:O	1:A:78:VAL:HG23	2.08	0.53
1:B:18:ASP:OD2	1:B:53:ARG:NH2	2.41	0.53
1:C:48:GLN:HG2	1:C:60:LEU:HD12	1.90	0.53
1:F:236:THR:HB	1:F:237:PRO:HD3	1.91	0.53
1:E:158:TYR:CE1	2:E:309:TCL:C1	2.92	0.53
1:E:158:TYR:HD2	1:E:162:THR:HG1	1.57	0.53
1:C:145:VAL:HG11	1:C:242:VAL:HG13	1.90	0.52
2:F:311:TCL:CL16	3:F:312:NAD:O3	2.66	0.51
1:E:67:ASN:HD22	1:E:70:HIS:H	1.58	0.51
1:B:93:HIS:O	1:B:146:GLY:HA2	2.11	0.51
1:C:122:ILE:O	1:C:126:SER:OG	2.29	0.51
1:A:93:HIS:O	1:A:146:GLY:HA2	2.10	0.51
1:D:135:LEU:HG	1:D:182:TYR:CD1	2.45	0.51
1:F:99:PRO:HB2	1:F:101:THR:HG22	1.93	0.50
1:E:74:LEU:HD13	1:E:134:LEU:HD21	1.92	0.50
1:E:149:PHE:HD2	3:E:310:NAD:H5N	1.76	0.50
1:E:122:ILE:HG12	3:E:310:NAD:H61A	1.76	0.50
1:E:135:LEU:HD13	1:E:144:ILE:HD11	1.93	0.50
1:F:169:GLU:HG2	1:F:257:ILE:HD11	1.93	0.50
1:D:64:ASP:OD1	3:D:307:NAD:N6A	2.44	0.50
1:F:215:ILE:O	1:F:217:LEU:N	2.44	0.49
1:D:158:TYR:OH	2:D:306:TCL:O17	2.30	0.49
1:F:36:LEU:O	1:F:58:ALA:HB1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:LEU:O	1:D:138:MET:HG3	2.13	0.49
1:C:131:ALA:O	1:C:135:LEU:HB2	2.13	0.49
1:A:103:MET:SD	2:A:300:TCL:H121	2.53	0.49
1:F:135:LEU:HD13	1:F:144:ILE:HD11	1.94	0.48
1:B:131:ALA:O	1:B:135:LEU:HB2	2.13	0.48
1:E:48:GLN:HE21	1:E:60:LEU:HB3	1.78	0.48
1:C:17:THR:H	1:C:20:SER:HG	1.62	0.48
1:D:147:MET:HE1	1:D:189:VAL:HB	1.96	0.48
1:A:63:LEU:O	3:A:301:NAD:H2A	2.14	0.48
1:A:101:THR:HG21	1:A:115:ASP:OD1	2.14	0.47
1:C:11:LEU:HA	1:C:37:VAL:O	2.14	0.47
1:C:225:ARG:HG2	1:C:267:GLN:HB2	1.96	0.47
1:C:93:HIS:O	1:C:146:GLY:HA2	2.14	0.47
1:D:156:PRO:O	1:D:157:ALA:HB3	2.15	0.47
1:E:187:ASN:ND2	1:E:253:THR:O	2.32	0.47
1:C:153:ARG:HH21	1:E:153:ARG:NE	2.13	0.47
1:D:67:ASN:HD22	1:D:67:ASN:C	2.18	0.47
1:F:250:LEU:N	1:F:251:PRO:HD3	2.30	0.47
1:E:135:LEU:N	1:E:136:PRO:CD	2.78	0.46
1:E:12:VAL:HA	1:E:92:VAL:HB	1.97	0.46
1:C:227:PRO:HD2	1:C:262:GLY:O	2.15	0.46
1:C:79:THR:O	1:C:83:GLY:N	2.46	0.46
1:D:127:TYR:CD2	1:D:175:VAL:HG21	2.51	0.46
1:E:236:THR:O	1:E:240:LYS:HG3	2.16	0.46
1:D:27:ARG:NH2	1:D:236:THR:OG1	2.49	0.46
1:A:148:ASP:HB2	1:A:188:LEU:HG	1.98	0.46
1:B:9:ARG:HA	1:B:35:GLN:O	2.15	0.46
1:C:153:ARG:NH1	1:E:265:HIS:O	2.47	0.46
1:D:131:ALA:O	1:D:135:LEU:HB2	2.17	0.45
1:D:12:VAL:O	1:D:38:LEU:HA	2.17	0.45
1:C:97:PHE:O	1:C:119:GLY:HA2	2.17	0.45
1:D:65:VAL:HG22	3:D:307:NAD:N1A	2.32	0.45
1:D:101:THR:HG21	1:D:115:ASP:OD1	2.15	0.45
1:D:265:HIS:O	1:F:153:ARG:NH1	2.50	0.45
1:C:265:HIS:O	1:E:153:ARG:CD	2.63	0.45
1:C:4:LEU:HD13	1:C:5:LEU:HD13	1.98	0.45
1:B:43:ARG:O	1:B:47:ILE:HG23	2.18	0.44
1:C:186:SER:O	1:C:255:GLY:N	2.48	0.44
1:E:67:ASN:ND2	1:E:69:GLU:HB2	2.31	0.44
1:B:82:ILE:O	1:B:86:ASN:ND2	2.50	0.44
1:E:78:VAL:O	1:E:82:ILE:HG12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:LEU:HB3	1:E:253:THR:CG2	2.47	0.44
1:F:67:ASN:ND2	1:F:69:GLU:HB2	2.31	0.44
1:A:253:THR:O	1:A:253:THR:HG23	2.17	0.44
1:E:187:ASN:OD1	1:E:254:THR:HA	2.17	0.44
1:A:193:PRO:HD3	1:A:222:TRP:CE2	2.53	0.44
1:B:64:ASP:H	1:B:70:HIS:HD2	1.66	0.44
1:C:46:LEU:HG	1:C:49:ARG:HH12	1.83	0.43
1:F:266:THR:OG1	1:F:267:GLN:NE2	2.47	0.43
1:A:135:LEU:N	1:A:136:PRO:CD	2.81	0.43
1:C:135:LEU:HD13	1:C:144:ILE:HD11	2.00	0.43
1:F:169:GLU:HB3	1:F:173:ARG:NH2	2.33	0.43
1:A:155:MET:HB2	1:A:156:PRO:HD2	2.01	0.43
1:D:178:GLU:OE1	1:D:181:LYS:NZ	2.49	0.43
1:A:222:TRP:HE1	1:A:261:ASP:HB2	1.84	0.43
1:B:10:ILE:HG12	1:B:90:GLY:HA3	2.01	0.43
1:B:90:GLY:HA2	1:B:143:SER:O	2.19	0.43
1:E:165:LYS:O	1:E:169:GLU:HG3	2.18	0.43
1:C:134:LEU:O	1:C:138:MET:HG3	2.18	0.43
1:D:6:ASP:OD1	1:D:33:GLY:HA3	2.18	0.43
1:E:47:ILE:HD11	1:E:60:LEU:HD21	2.00	0.43
1:A:167:ALA:O	1:A:171:VAL:HG23	2.19	0.43
1:A:39:THR:HA	1:A:61:LEU:O	2.18	0.43
1:C:78:VAL:O	1:C:82:ILE:HG12	2.18	0.43
1:F:67:ASN:HD22	1:F:67:ASN:C	2.22	0.43
1:C:187:ASN:ND2	1:C:253:THR:O	2.39	0.42
1:B:144:ILE:O	1:B:186:SER:HA	2.19	0.42
1:D:167:ALA:O	1:D:171:VAL:HG23	2.19	0.42
1:A:41:PHE:C	1:A:41:PHE:CD1	2.91	0.42
1:F:93:HIS:O	1:F:146:GLY:HA2	2.19	0.42
1:F:135:LEU:N	1:F:136:PRO:CD	2.83	0.42
1:A:82:ILE:O	1:A:86:ASN:ND2	2.53	0.42
1:D:59:PRO:HG2	1:D:81:ALA:HB1	2.01	0.42
1:A:90:GLY:HA2	1:A:143:SER:O	2.20	0.42
1:D:5:LEU:HB3	1:D:34:ALA:HB2	2.02	0.42
1:C:88:LEU:O	1:C:138:MET:HA	2.20	0.41
1:C:153:ARG:HH21	1:E:153:ARG:CZ	2.33	0.41
1:B:250:LEU:HB3	1:B:253:THR:CG2	2.50	0.41
1:F:135:LEU:HG	1:F:182:TYR:CD1	2.55	0.41
1:A:156:PRO:O	1:A:157:ALA:HB3	2.20	0.41
1:D:241:THR:O	1:D:245:LEU:HD23	2.18	0.41
1:F:24:HIS:HD2	1:F:27:ARG:HH21	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:ASP:H	1:E:70:HIS:HD2	1.69	0.41
1:C:245:LEU:HD22	1:C:250:LEU:CD1	2.50	0.41
1:D:11:LEU:HA	1:D:37:VAL:O	2.20	0.41
1:F:75:ALA:HA	1:F:137:ILE:HD11	2.02	0.41
1:C:236:THR:HB	1:C:237:PRO:HD3	2.02	0.41
1:A:111:ALA:HA	1:A:112:PRO:HD3	1.97	0.41
1:B:225:ARG:HG2	1:B:267:GLN:HB2	2.02	0.41
1:C:145:VAL:HA	1:C:187:ASN:O	2.21	0.41
1:E:245:LEU:HD11	1:E:258:ILE:HD13	2.02	0.41
1:C:258:ILE:N	1:C:258:ILE:HD12	2.36	0.41
1:D:10:ILE:O	1:D:36:LEU:HA	2.21	0.41
1:A:250:LEU:O	1:A:253:THR:HG22	2.20	0.41
1:C:2:THR:HG1	1:F:2:THR:N	2.19	0.41
1:E:93:HIS:O	1:E:146:GLY:HA2	2.21	0.41
1:A:47:ILE:HD11	1:A:60:LEU:HD11	2.03	0.41
1:C:126:SER:HA	1:C:129:SER:OG	2.21	0.41
1:A:174:PHE:CE2	1:B:159:ASN:HA	2.55	0.40
1:F:165:LYS:NZ	3:F:312:NAD:O2D	2.50	0.40
1:C:73:SER:OG	1:C:77:ARG:NE	2.54	0.40
1:A:158:TYR:OH	2:A:300:TCL:O17	2.34	0.40
1:C:135:LEU:N	1:C:136:PRO:CD	2.85	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	249/269 (93%)	235 (94%)	13 (5%)	1 (0%)	34 42
1	B	242/269 (90%)	233 (96%)	9 (4%)	0	100 100
1	C	244/269 (91%)	227 (93%)	16 (7%)	1 (0%)	34 42
1	D	244/269 (91%)	224 (92%)	18 (7%)	2 (1%)	19 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	250/269 (93%)	241 (96%)	9 (4%)	0	100 100
1	F	247/269 (92%)	229 (93%)	17 (7%)	1 (0%)	34 42
All	All	1476/1614 (91%)	1389 (94%)	82 (6%)	5 (0%)	41 50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	195	ARG
1	A	195	ARG
1	D	229	GLY
1	F	215	ILE
1	D	65	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	196/205 (96%)	178 (91%)	18 (9%)	9 11
1	B	191/205 (93%)	166 (87%)	25 (13%)	4 4
1	C	193/205 (94%)	168 (87%)	25 (13%)	4 4
1	D	192/205 (94%)	176 (92%)	16 (8%)	11 14
1	E	196/205 (96%)	174 (89%)	22 (11%)	6 6
1	F	196/205 (96%)	178 (91%)	18 (9%)	9 11
All	All	1164/1230 (95%)	1040 (89%)	124 (11%)	6 7

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	LEU
1	A	6	ASP
1	A	60	LEU
1	A	67	ASN

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Mol	Chain	Res	Type
1	A	69	GLU
1	A	70	HIS
1	A	71	LEU
1	A	74	LEU
1	A	101	THR
1	A	135	LEU
1	A	162	THR
1	A	168	LEU
1	A	188	LEU
1	A	215	ILE
1	A	218	LEU
1	A	224	GLN
1	A	269	LEU
1	B	4	LEU
1	B	5	LEU
1	B	6	ASP
1	B	11	LEU
1	B	19	SER
1	B	44	LEU
1	B	47	ILE
1	B	60	LEU
1	B	67	ASN
1	B	68	GLU
1	B	70	HIS
1	B	71	LEU
1	B	74	LEU
1	B	101	THR
1	B	103	MET
1	B	105	ILE
1	B	123	SER
1	B	135	LEU
1	B	145	VAL
1	B	168	LEU
1	B	188	LEU
1	B	224	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	19	SER

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Mol	Chain	Res	Type
1	C	60	LEU
1	C	67	ASN
1	C	71	LEU
1	C	74	LEU
1	C	80	GLU
1	C	89	ASP
1	C	101	THR
1	C	105	ILE
1	C	130	MET
1	C	135	LEU
1	C	162	THR
1	C	168	LEU
1	C	170	SER
1	C	177	ARG
1	C	188	LEU
1	C	218	LEU
1	C	219	GLU
1	C	232	MET
1	C	251	PRO
1	C	253	THR
1	C	269	LEU
1	D	4	LEU
1	D	5	LEU
1	D	35	GLN
1	D	53	ARG
1	D	67	ASN
1	D	71	LEU
1	D	74	LEU
1	D	101	THR
1	D	103	MET
1	D	135	LEU
1	D	162	THR
1	D	168	LEU
1	D	170	SER
1	D	188	LEU
1	D	228	ILE
1	D	269	LEU
1	E	5	LEU
1	E	6	ASP
1	E	18	ASP
1	E	60	LEU
1	E	67	ASN

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Mol	Chain	Res	Type
1	E	68	GLU
1	E	71	LEU
1	E	74	LEU
1	E	80	GLU
1	E	101	THR
1	E	135	LEU
1	E	162	THR
1	E	168	LEU
1	E	170	SER
1	E	188	LEU
1	E	217	LEU
1	E	218	LEU
1	E	224	GLN
1	E	232	MET
1	E	245	LEU
1	E	253	THR
1	E	269	LEU
1	F	4	LEU
1	F	5	LEU
1	F	6	ASP
1	F	19	SER
1	F	60	LEU
1	F	67	ASN
1	F	69	GLU
1	F	71	LEU
1	F	74	LEU
1	F	135	LEU
1	F	168	LEU
1	F	188	LEU
1	F	217	LEU
1	F	232	MET
1	F	245	LEU
1	F	253	THR
1	F	256	ASP
1	F	269	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	70	HIS
1	A	139	ASN

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Mol	Chain	Res	Type
1	B	24	HIS
1	B	67	ASN
1	B	70	HIS
1	B	139	ASN
1	C	67	ASN
1	C	70	HIS
1	D	67	ASN
1	D	70	HIS
1	D	106	ASN
1	D	139	ASN
1	E	24	HIS
1	E	48	GLN
1	E	67	ASN
1	E	70	HIS
1	E	139	ASN
1	F	24	HIS
1	F	67	ASN
1	F	70	HIS
1	F	139	ASN
1	F	216	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no 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	F	312	-	42,48,48	1.69	3 (7%)	50,73,73	1.47	4 (8%)
3	NAD	E	310	-	42,48,48	1.68	4 (9%)	50,73,73	1.48	5 (10%)
2	TCL	F	311	-	18,18,18	2.04	3 (16%)	25,25,25	1.02	2 (8%)
2	TCL	D	306	-	18,18,18	2.03	5 (27%)	25,25,25	1.30	3 (12%)
2	TCL	B	302	-	18,18,18	1.95	4 (22%)	25,25,25	1.39	2 (8%)
3	NAD	B	303	-	42,48,48	1.65	4 (9%)	50,73,73	1.56	5 (10%)
3	NAD	A	301	-	42,48,48	1.68	3 (7%)	50,73,73	1.51	6 (12%)
3	NAD	C	305	-	42,48,48	1.72	4 (9%)	50,73,73	1.31	4 (8%)
3	NAD	D	307	-	42,48,48	1.68	4 (9%)	50,73,73	1.38	5 (10%)
2	TCL	E	309	-	18,18,18	2.11	5 (27%)	25,25,25	1.12	1 (4%)
2	TCL	A	300	-	18,18,18	2.21	5 (27%)	25,25,25	1.44	3 (12%)
2	TCL	C	304	-	18,18,18	2.01	4 (22%)	25,25,25	1.40	5 (20%)

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	F	312	-	-	6/26/62/62	0/5/5/5
3	NAD	E	310	-	-	7/26/62/62	0/5/5/5
2	TCL	F	311	-	-	1/4/4/4	0/2/2/2
2	TCL	D	306	-	-	0/4/4/4	0/2/2/2
2	TCL	B	302	-	-	1/4/4/4	0/2/2/2
3	NAD	B	303	-	-	7/26/62/62	0/5/5/5
3	NAD	A	301	-	-	1/26/62/62	0/5/5/5
3	NAD	C	305	-	-	10/26/62/62	0/5/5/5
3	NAD	D	307	-	-	7/26/62/62	0/5/5/5
2	TCL	E	309	-	-	0/4/4/4	0/2/2/2
2	TCL	A	300	-	-	1/4/4/4	0/2/2/2
2	TCL	C	304	-	-	0/4/4/4	0/2/2/2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	312	NAD	O7N-C7N	8.66	1.40	1.24
3	A	301	NAD	O7N-C7N	8.30	1.40	1.24
3	E	310	NAD	O7N-C7N	8.29	1.40	1.24
3	D	307	NAD	O7N-C7N	8.14	1.39	1.24
3	C	305	NAD	O7N-C7N	8.14	1.39	1.24
3	B	303	NAD	O7N-C7N	7.56	1.38	1.24
2	F	311	TCL	C8-C9	5.70	1.49	1.39
2	A	300	TCL	C8-C9	5.69	1.49	1.39
2	A	300	TCL	C6-C5	5.31	1.49	1.40
2	E	309	TCL	C8-C9	5.11	1.48	1.39
2	B	302	TCL	C6-C5	4.97	1.49	1.40
2	D	306	TCL	C6-C5	4.91	1.49	1.40
2	C	304	TCL	C6-C5	4.87	1.49	1.40
2	E	309	TCL	C6-C5	4.86	1.49	1.40
2	D	306	TCL	C8-C9	4.76	1.47	1.39
2	C	304	TCL	C8-C9	4.52	1.47	1.39
2	B	302	TCL	C8-C9	4.50	1.47	1.39
3	B	303	NAD	C2A-N3A	4.48	1.39	1.32
2	F	311	TCL	C6-C5	4.25	1.48	1.40
3	D	307	NAD	C2A-N3A	4.06	1.38	1.32
3	C	305	NAD	C2A-N3A	4.04	1.38	1.32
3	A	301	NAD	C2A-N3A	4.04	1.38	1.32
3	E	310	NAD	C2A-N3A	3.79	1.38	1.32
3	F	312	NAD	C2A-N3A	3.68	1.38	1.32
3	B	303	NAD	C2A-N1A	3.14	1.39	1.33
2	E	309	TCL	C2-CL14	3.03	1.81	1.74
2	C	304	TCL	C2-CL14	2.93	1.80	1.74
2	B	302	TCL	C11-CL15	2.90	1.80	1.74
2	C	304	TCL	C11-CL15	2.90	1.80	1.74
2	D	306	TCL	C2-CL14	2.90	1.80	1.74
3	C	305	NAD	C2A-N1A	2.88	1.39	1.33
2	F	311	TCL	C2-CL14	2.80	1.80	1.74
2	D	306	TCL	C9-CL16	2.72	1.80	1.73
2	A	300	TCL	C2-CL14	2.66	1.80	1.74
3	D	307	NAD	C2A-N1A	2.65	1.38	1.33
3	C	305	NAD	C2N-N1N	2.63	1.38	1.35
3	B	303	NAD	C2N-N1N	2.54	1.38	1.35
2	B	302	TCL	C2-CL14	2.50	1.79	1.74
2	E	309	TCL	C11-CL15	2.48	1.79	1.74
3	F	312	NAD	O4B-C4B	-2.45	1.39	1.45
3	E	310	NAD	C2A-N1A	2.43	1.38	1.33
2	D	306	TCL	C11-CL15	2.42	1.79	1.74
2	A	300	TCL	C11-CL15	2.36	1.79	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	307	NAD	C2N-N1N	2.28	1.37	1.35
2	E	309	TCL	C9-CL16	2.27	1.79	1.73
3	A	301	NAD	C2A-N1A	2.26	1.38	1.33
3	E	310	NAD	C2N-N1N	2.25	1.37	1.35
2	A	300	TCL	C9-CL16	2.02	1.78	1.73

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	310	NAD	N3A-C2A-N1A	-6.97	117.79	128.68
3	A	301	NAD	N3A-C2A-N1A	-6.85	117.97	128.68
3	C	305	NAD	N3A-C2A-N1A	-6.44	118.62	128.68
3	B	303	NAD	N3A-C2A-N1A	-6.35	118.75	128.68
3	D	307	NAD	N3A-C2A-N1A	-6.22	118.96	128.68
3	F	312	NAD	N3A-C2A-N1A	-6.20	118.98	128.68
3	B	303	NAD	C3N-C7N-N7N	4.78	123.48	117.75
2	B	302	TCL	C8-O7-C5	3.72	126.89	118.04
2	A	300	TCL	C8-O7-C5	3.63	126.68	118.04
2	C	304	TCL	C13-C12-C11	3.46	122.89	119.24
2	B	302	TCL	C13-C12-C11	3.45	122.88	119.24
2	D	306	TCL	O7-C5-C6	3.35	122.49	116.22
2	A	300	TCL	C8-C9-CL16	3.33	123.34	119.43
3	F	312	NAD	C3N-C7N-N7N	3.04	121.40	117.75
3	F	312	NAD	PN-O3-PA	-3.01	122.49	132.83
3	A	301	NAD	O4B-C1B-C2B	-2.89	102.71	106.93
3	E	310	NAD	PN-O3-PA	-2.84	123.08	132.83
3	A	301	NAD	C6N-N1N-C2N	-2.73	119.49	121.97
2	D	306	TCL	C4-C3-C2	2.63	122.01	119.24
3	D	307	NAD	C1B-N9A-C4A	-2.62	122.03	126.64
3	E	310	NAD	C1B-N9A-C4A	-2.60	122.07	126.64
2	F	311	TCL	C13-C12-C11	2.60	121.99	119.24
3	A	301	NAD	O7N-C7N-N7N	-2.57	118.93	122.58
3	A	301	NAD	O4D-C1D-C2D	-2.47	103.32	106.93
3	D	307	NAD	O2N-PN-O1N	2.43	124.26	112.24
3	A	301	NAD	O2N-PN-O1N	2.43	124.26	112.24
2	E	309	TCL	C13-C12-C11	2.43	121.80	119.24
2	F	311	TCL	C8-O7-C5	2.41	123.77	118.04
3	C	305	NAD	PN-O3-PA	-2.38	124.67	132.83
2	A	300	TCL	C13-C12-C11	2.33	121.70	119.24
2	C	304	TCL	C4-C3-C2	2.31	121.68	119.24
3	C	305	NAD	C1B-N9A-C4A	-2.30	122.60	126.64
3	C	305	NAD	C3N-C7N-N7N	2.30	120.51	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	307	NAD	C3N-C7N-N7N	2.29	120.50	117.75
2	D	306	TCL	C10-C9-CL16	2.22	122.08	118.49
3	B	303	NAD	O7N-C7N-N7N	-2.22	119.42	122.58
3	E	310	NAD	C4A-C5A-N7A	-2.19	107.12	109.40
3	B	303	NAD	O4D-C1D-C2D	-2.16	103.77	106.93
3	B	303	NAD	O7N-C7N-C3N	-2.16	117.05	119.63
2	C	304	TCL	O7-C5-C6	2.14	120.23	116.22
2	C	304	TCL	C12-C11-CL15	2.07	122.60	119.35
3	D	307	NAD	C6N-N1N-C2N	-2.07	120.09	121.97
2	C	304	TCL	C8-O7-C5	2.03	122.87	118.04
3	E	310	NAD	O3B-C3B-C2B	-2.02	105.28	111.82
3	F	312	NAD	C2A-N1A-C6A	2.02	122.20	118.75

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	312	NAD	O4D-C1D-N1N-C2N
3	F	312	NAD	O4D-C1D-N1N-C6N
3	E	310	NAD	C5D-O5D-PN-O1N
3	E	310	NAD	C5D-O5D-PN-O2N
3	E	310	NAD	O4D-C1D-N1N-C2N
3	B	303	NAD	C5D-O5D-PN-O2N
3	B	303	NAD	O4D-C1D-N1N-C2N
3	C	305	NAD	C5B-O5B-PA-O1A
3	C	305	NAD	PN-O3-PA-O5B
3	C	305	NAD	C5D-O5D-PN-O1N
3	C	305	NAD	C5D-O5D-PN-O2N
3	C	305	NAD	O4D-C1D-N1N-C2N
3	C	305	NAD	O4D-C1D-N1N-C6N
3	D	307	NAD	O4D-C1D-N1N-C2N
3	D	307	NAD	O4D-C4D-C5D-O5D
3	D	307	NAD	C3D-C4D-C5D-O5D
3	F	312	NAD	PN-O3-PA-O1A
3	B	303	NAD	PA-O3-PN-O1N
3	D	307	NAD	O4B-C4B-C5B-O5B
3	B	303	NAD	C5D-O5D-PN-O3
3	C	305	NAD	C5B-O5B-PA-O3
3	E	310	NAD	PA-O3-PN-O1N
3	E	310	NAD	PA-O3-PN-O2N
3	B	303	NAD	C5D-O5D-PN-O1N
3	C	305	NAD	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	F	311	TCL	C6-C5-O7-C8
3	F	312	NAD	O4B-C4B-C5B-O5B
2	B	302	TCL	C6-C5-O7-C8
3	B	303	NAD	PA-O3-PN-O2N
3	D	307	NAD	PN-O3-PA-O1A
3	D	307	NAD	PN-O3-PA-O2A
3	C	305	NAD	O4B-C4B-C5B-O5B
3	D	307	NAD	PA-O3-PN-O2N
3	E	310	NAD	C5D-O5D-PN-O3
3	C	305	NAD	C5D-O5D-PN-O3
3	E	310	NAD	O4B-C4B-C5B-O5B
3	A	301	NAD	O4B-C4B-C5B-O5B
3	F	312	NAD	PN-O3-PA-O2A
3	F	312	NAD	PA-O3-PN-O2N
2	A	300	TCL	C6-C5-O7-C8
3	B	303	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

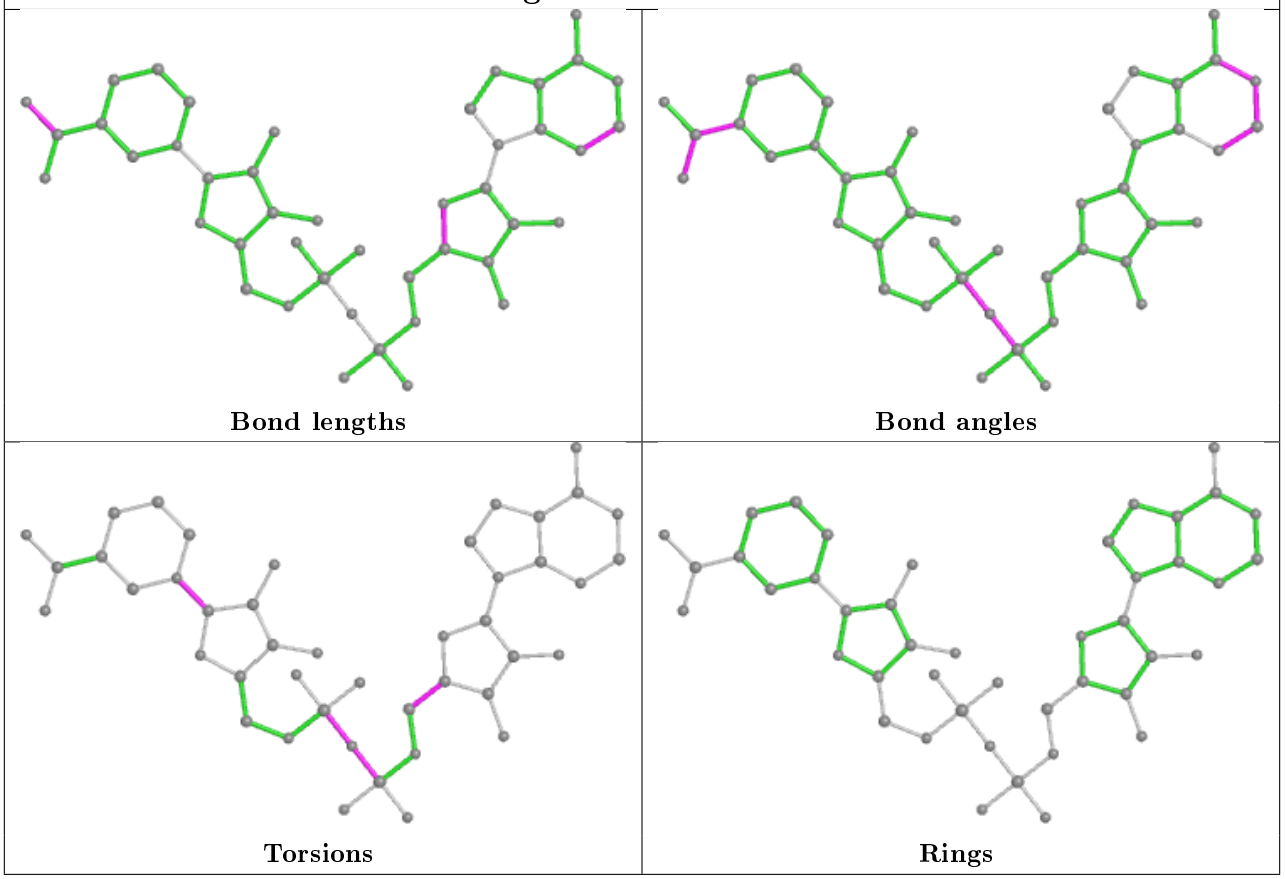
10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	312	NAD	2	0
3	E	310	NAD	2	0
2	F	311	TCL	2	0
2	D	306	TCL	2	0
2	B	302	TCL	1	0
3	A	301	NAD	1	0
3	D	307	NAD	2	0
2	E	309	TCL	1	0
2	A	300	TCL	2	0
2	C	304	TCL	1	0

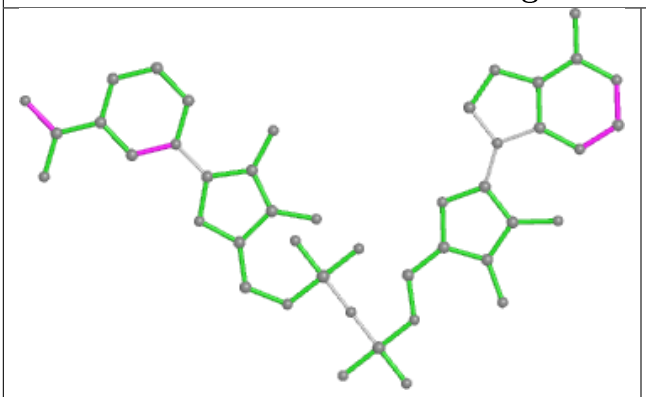
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

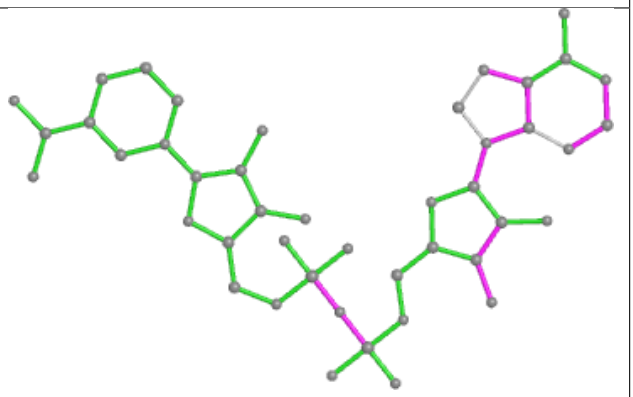
Ligand NAD F 312



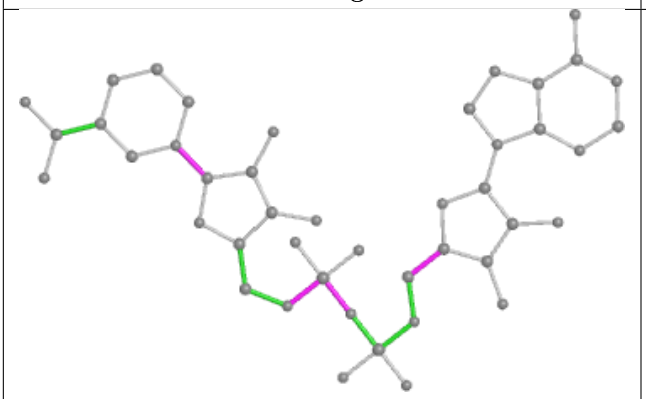
Ligand NAD E 310



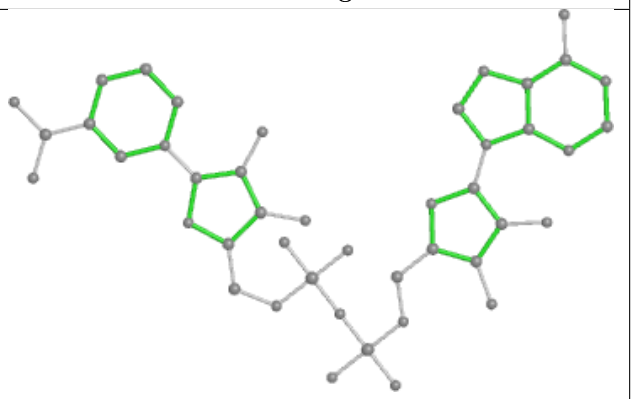
Bond lengths



Bond angles

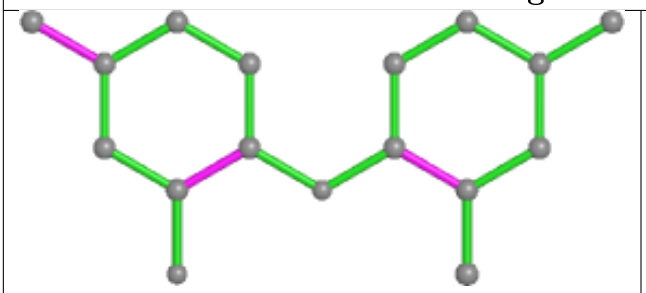


Torsions

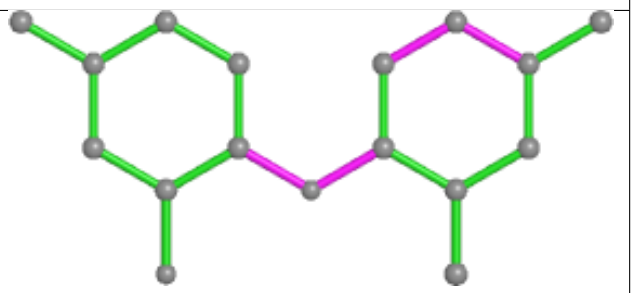


Rings

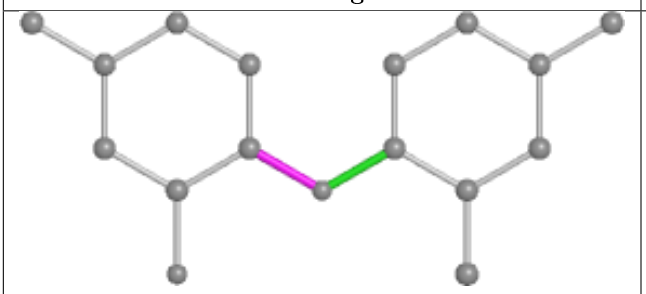
Ligand TCL F 311



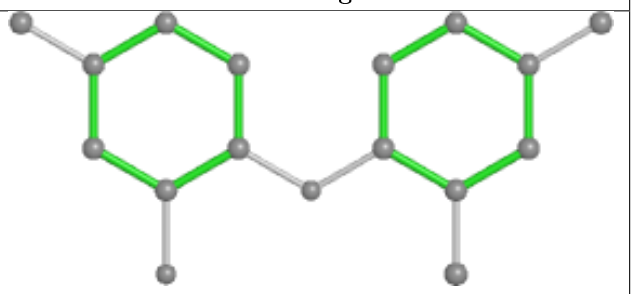
Bond lengths



Bond angles

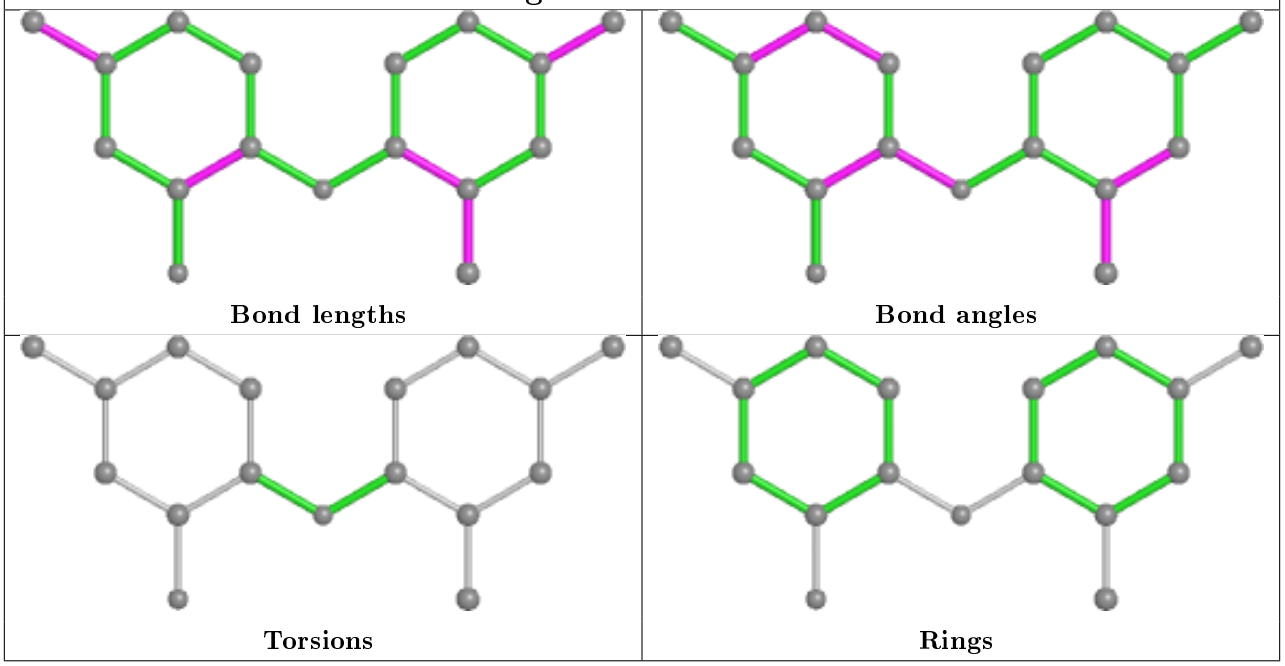


Torsions

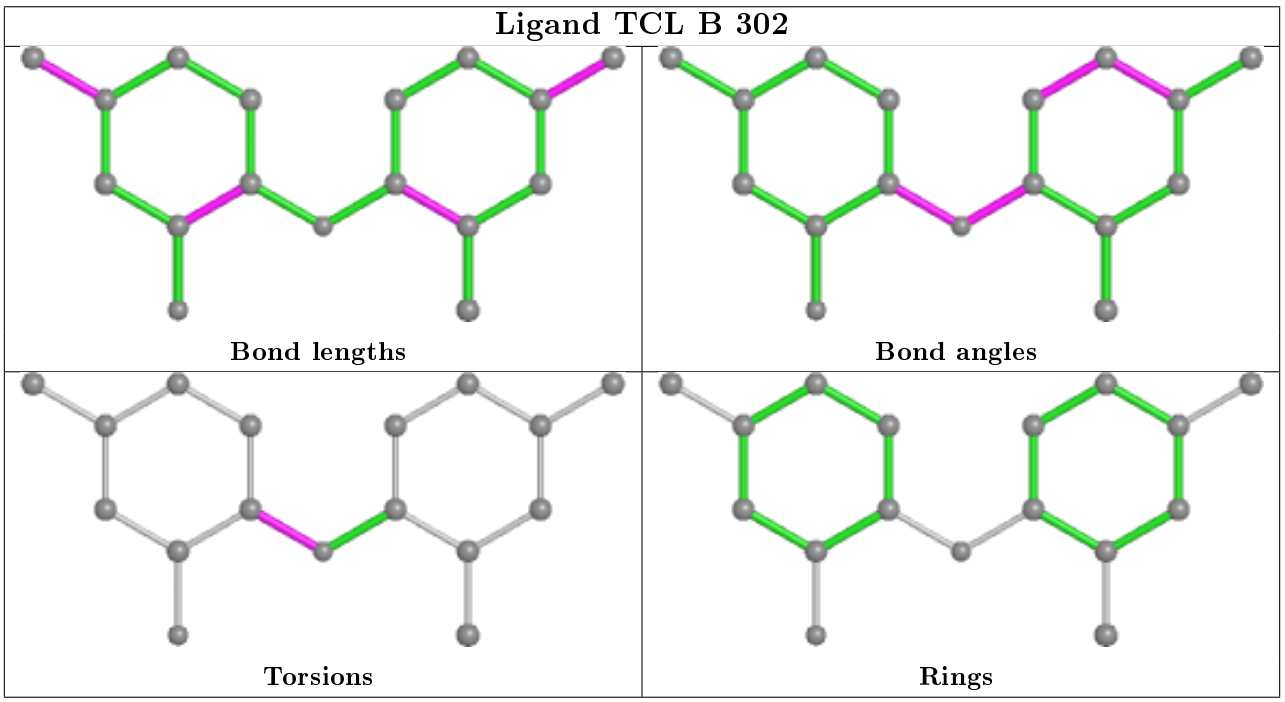


Rings

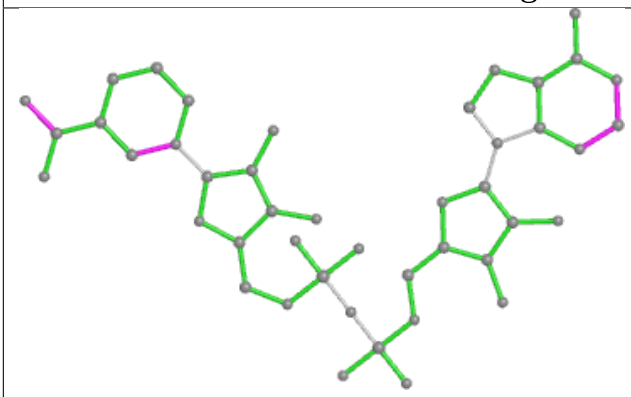
Ligand TCL D 306



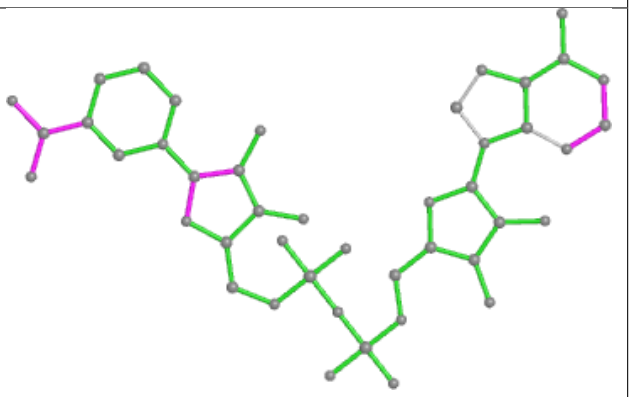
Ligand TCL B 302



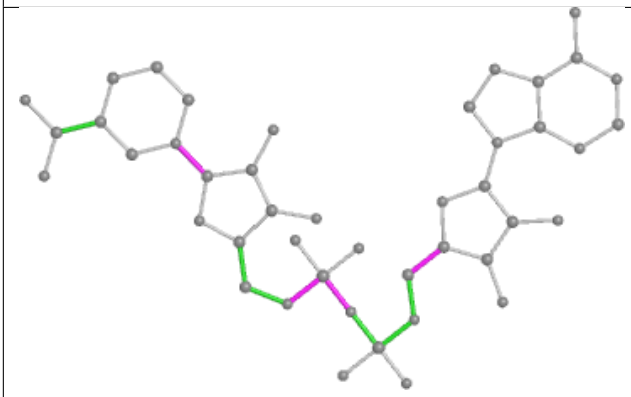
Ligand NAD B 303



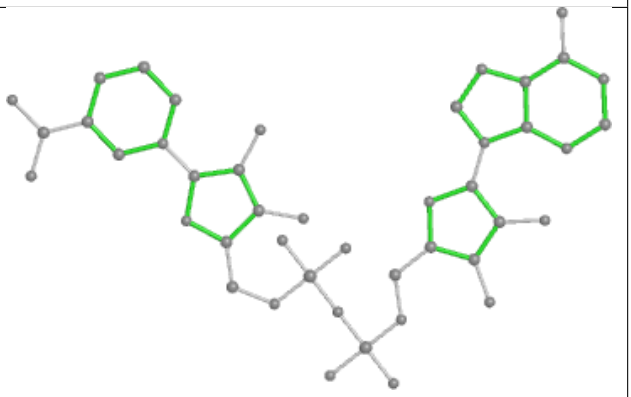
Bond lengths



Bond angles

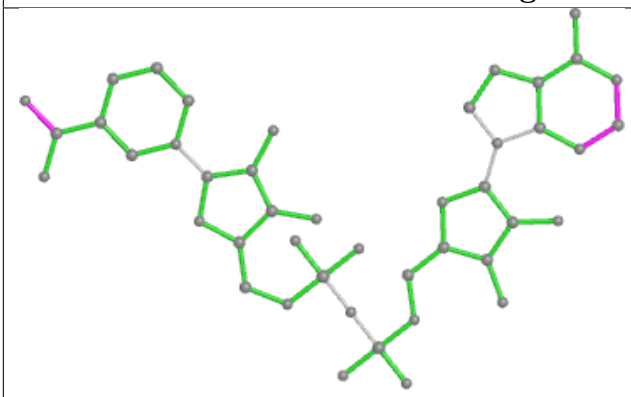


Torsions

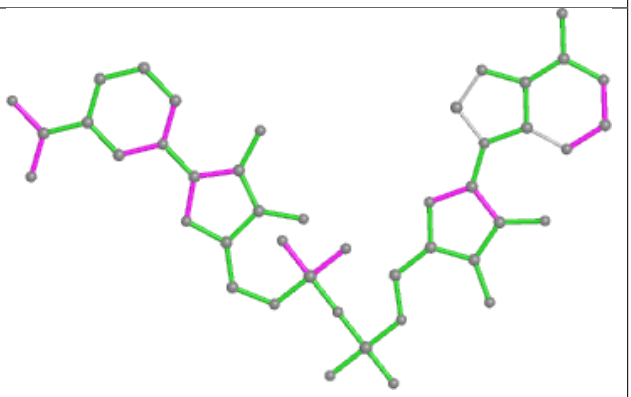


Rings

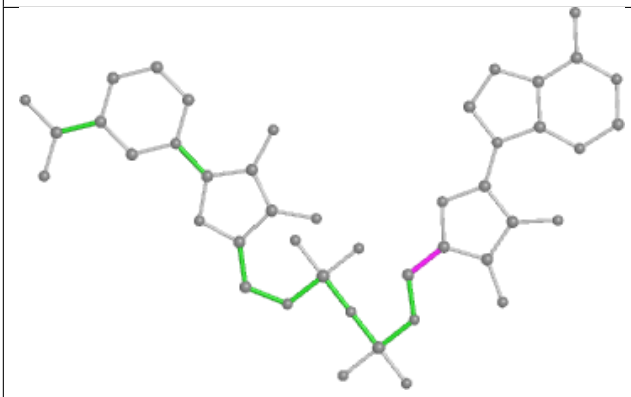
Ligand NAD A 301



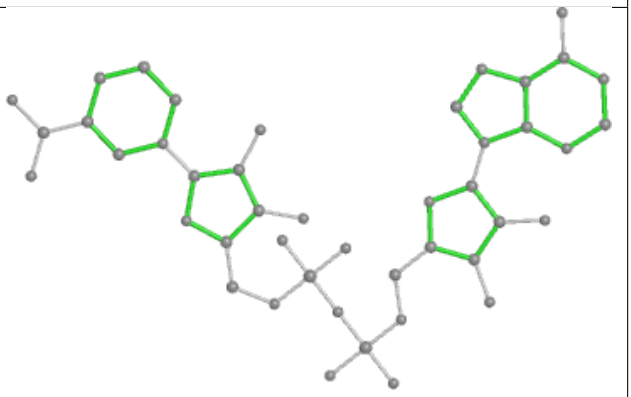
Bond lengths



Bond angles

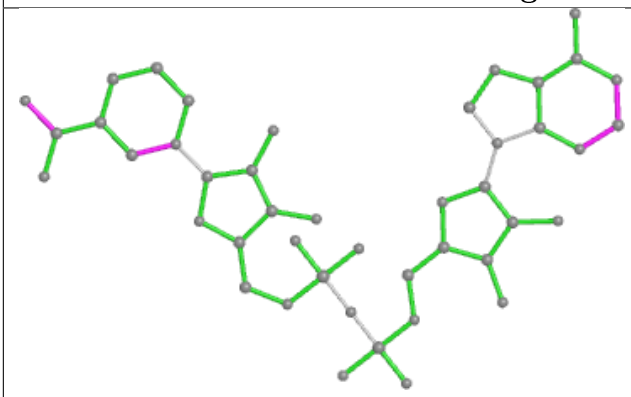


Torsions

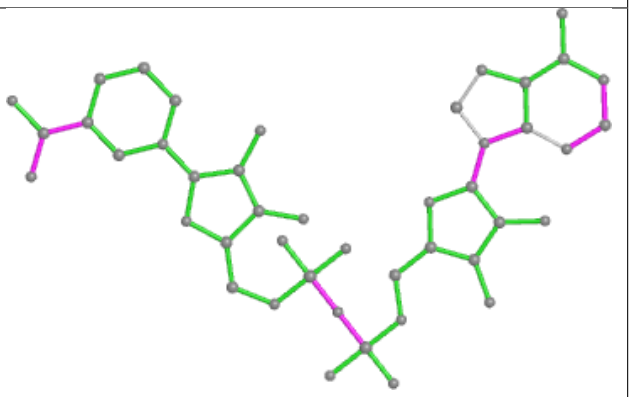


Rings

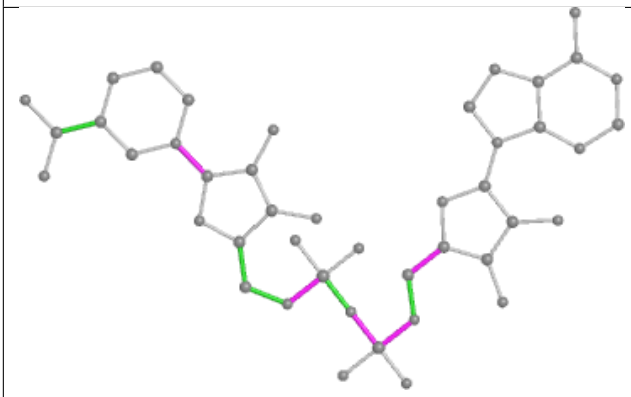
Ligand NAD C 305



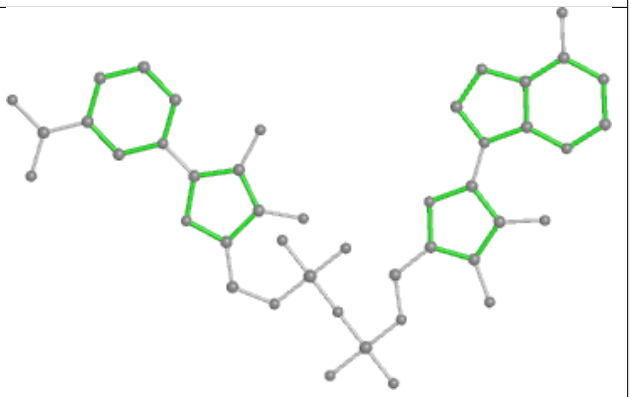
Bond lengths



Bond angles

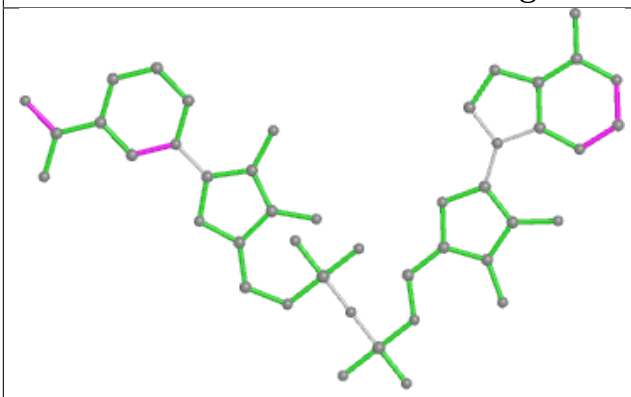


Torsions

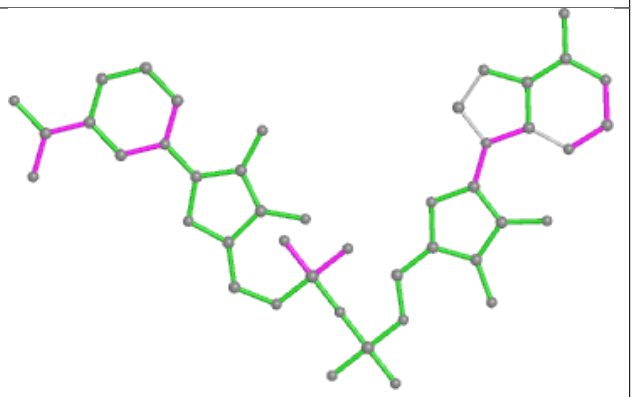


Rings

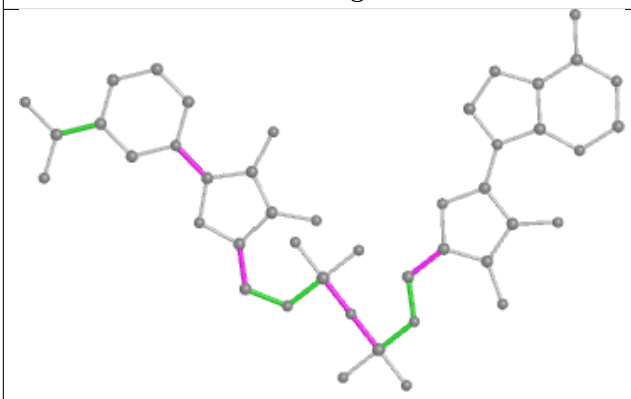
Ligand NAD D 307



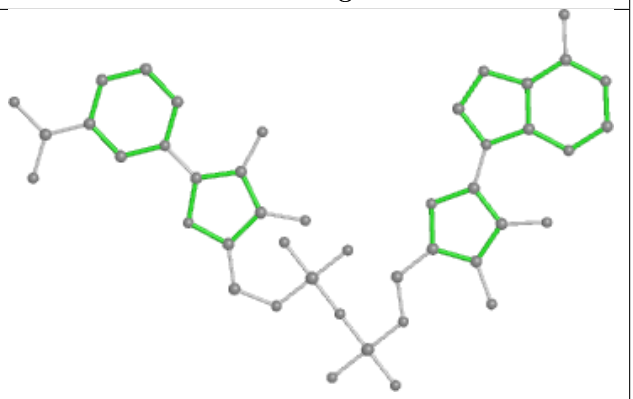
Bond lengths



Bond angles

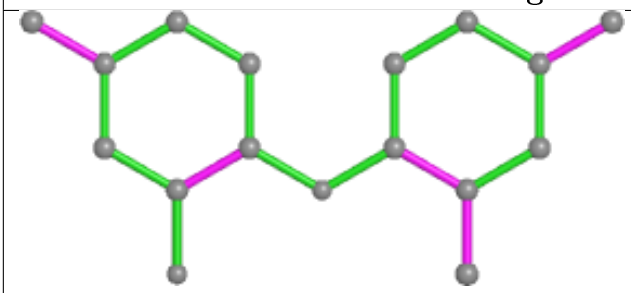


Torsions

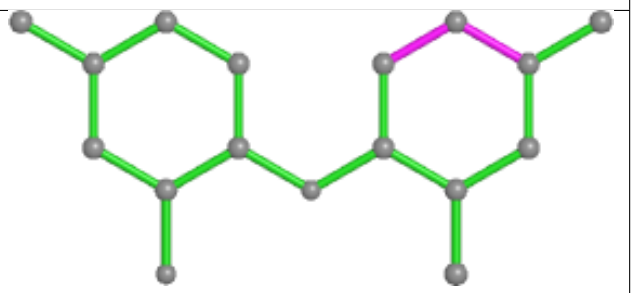


Rings

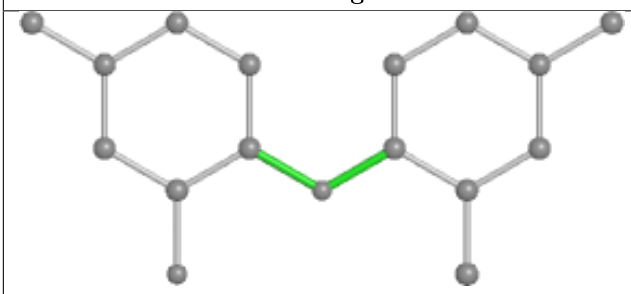
Ligand TCL E 309



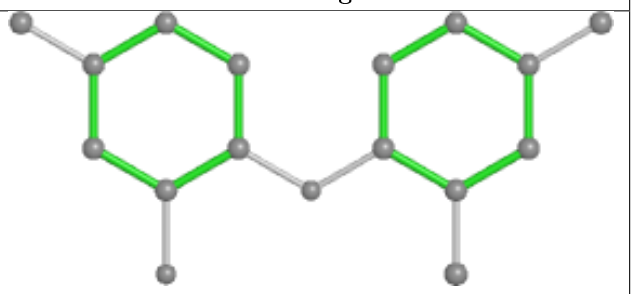
Bond lengths



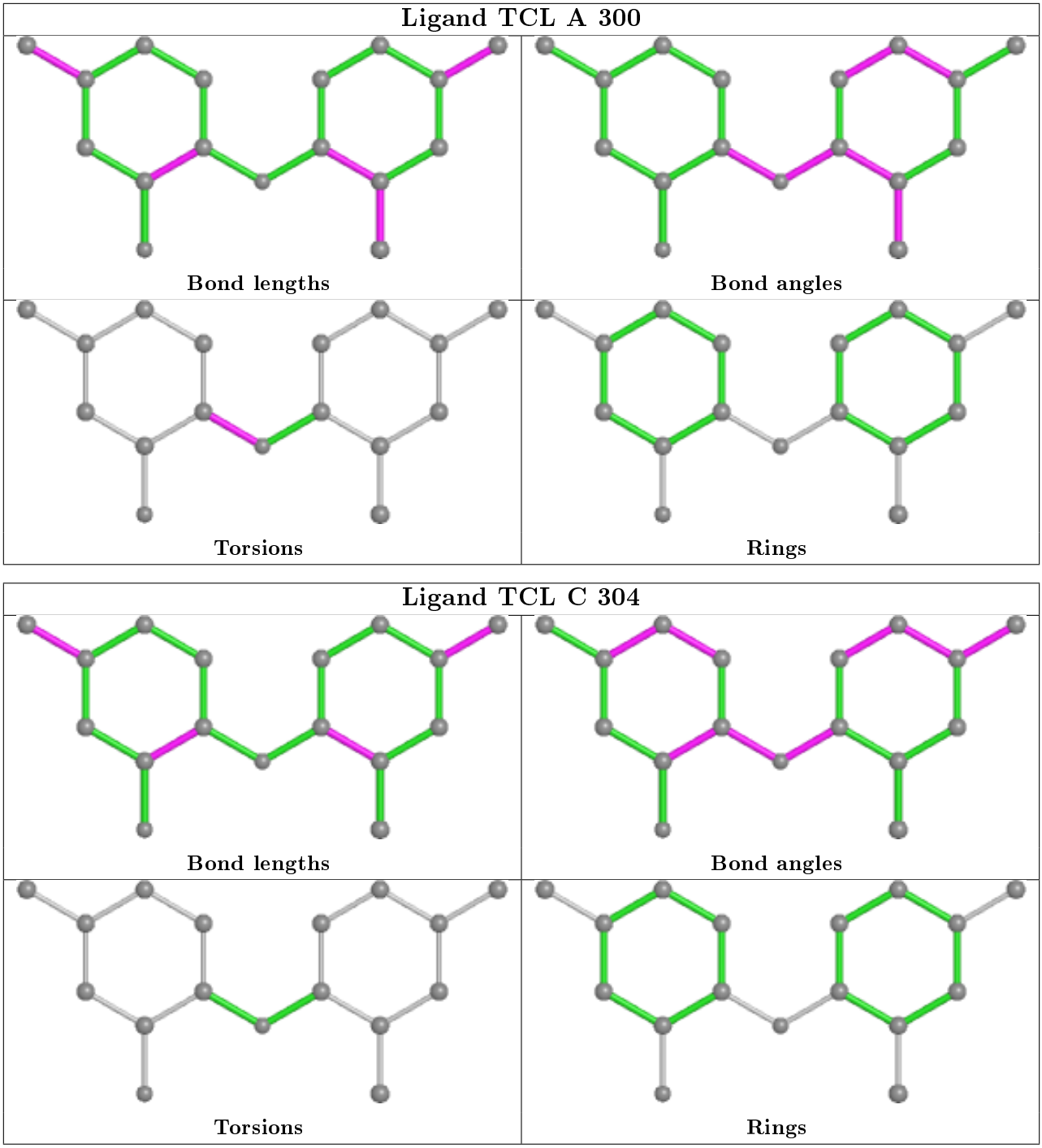
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	253/269 (94%)	0.40	6 (2%) 59 66	13, 25, 45, 53	0
1	B	246/269 (91%)	0.52	5 (2%) 65 71	14, 25, 43, 54	0
1	C	248/269 (92%)	0.98	29 (11%) 4 6	23, 34, 51, 58	0
1	D	248/269 (92%)	0.88	22 (8%) 9 13	22, 34, 50, 55	0
1	E	254/269 (94%)	0.74	25 (9%) 7 10	21, 33, 46, 50	0
1	F	251/269 (93%)	0.97	27 (10%) 5 8	20, 35, 51, 57	0
All	All	1500/1614 (92%)	0.75	114 (7%) 13 18	13, 32, 48, 58	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	79	THR	6.2
1	D	55	PRO	5.5
1	C	58	ALA	5.2
1	E	2	THR	5.2
1	C	21	ILE	4.9
1	F	81	ALA	4.9
1	C	2	THR	4.4
1	F	2	THR	4.4
1	C	50	ILE	4.3
1	D	44	LEU	4.3
1	C	46	LEU	4.2
1	C	85	GLY	4.0
1	D	54	LEU	3.7
1	A	46	LEU	3.7
1	D	38	LEU	3.6
1	F	44	LEU	3.6
1	E	84	ALA	3.5
1	E	105	ILE	3.4
1	F	47	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	37	VAL	3.4
1	D	70	HIS	3.4
1	F	76	GLY	3.4
1	F	86	ASN	3.3
1	B	45	ARG	3.1
1	E	35	GLN	3.1
1	C	36	LEU	3.1
1	E	103	MET	3.1
1	C	52	ASP	3.1
1	C	140	PRO	3.1
1	F	221	GLY	3.0
1	D	196	THR	3.0
1	E	46	LEU	3.0
1	D	45	ARG	3.0
1	C	63	LEU	2.9
1	B	2	THR	2.9
1	F	73	SER	2.8
1	F	58	ALA	2.8
1	C	59	PRO	2.8
1	E	7	GLY	2.8
1	F	51	THR	2.8
1	C	60	LEU	2.8
1	C	57	LYS	2.8
1	F	71	LEU	2.7
1	E	157	ALA	2.7
1	B	47	ILE	2.7
1	A	2	THR	2.7
1	C	81	ALA	2.6
1	D	198	ALA	2.6
1	C	3	GLY	2.6
1	E	58	ALA	2.6
1	D	42	ASP	2.6
1	D	134	LEU	2.6
1	D	84	ALA	2.6
1	F	69	GLU	2.6
1	F	57	LYS	2.6
1	C	269	LEU	2.5
1	E	72	ALA	2.5
1	C	16	ILE	2.5
1	F	215	ILE	2.5
1	C	37	VAL	2.5
1	E	257	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	33	GLY	2.5
1	E	42	ASP	2.4
1	D	49	ARG	2.4
1	D	28	VAL	2.4
1	E	12	VAL	2.4
1	F	59	PRO	2.4
1	E	158	TYR	2.4
1	E	57	LYS	2.4
1	D	199	MET	2.4
1	F	72	ALA	2.4
1	D	197	LEU	2.4
1	E	106	ASN	2.4
1	F	49	ARG	2.3
1	F	135	LEU	2.3
1	E	38	LEU	2.3
1	D	193	PRO	2.3
1	F	7	GLY	2.3
1	A	215	ILE	2.3
1	B	46	LEU	2.3
1	E	44	LEU	2.2
1	E	156	PRO	2.2
1	C	103	MET	2.2
1	C	47	ILE	2.2
1	A	219	GLU	2.2
1	C	105	ILE	2.2
1	E	47	ILE	2.2
1	E	215	ILE	2.2
1	D	7	GLY	2.2
1	F	41	PHE	2.2
1	F	264	ALA	2.2
1	C	255	GLY	2.2
1	F	85	GLY	2.2
1	E	63	LEU	2.1
1	F	217	LEU	2.1
1	C	258	ILE	2.1
1	C	43	ARG	2.1
1	E	45	ARG	2.1
1	D	2	THR	2.1
1	C	32	GLN	2.1
1	A	45	ARG	2.1
1	D	195	ARG	2.1
1	A	188	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	140	PRO	2.1
1	B	105	ILE	2.1
1	C	228	ILE	2.1
1	C	53	ARG	2.1
1	C	145	VAL	2.1
1	D	83	GLY	2.0
1	C	264	ALA	2.0
1	E	252	ALA	2.0
1	E	107	PRO	2.0
1	F	15	ILE	2.0
1	D	43	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 carbohydrates in this entry.

6.4 Ligands (i)

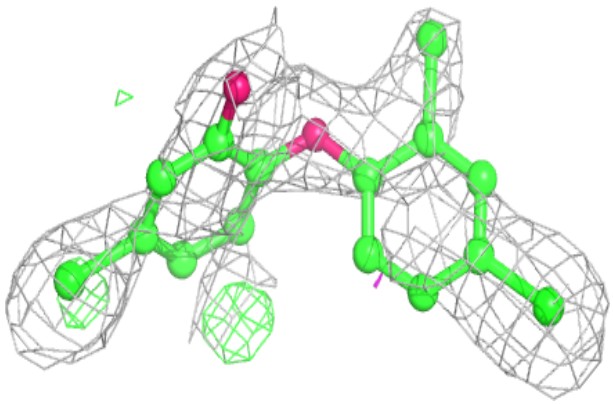
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

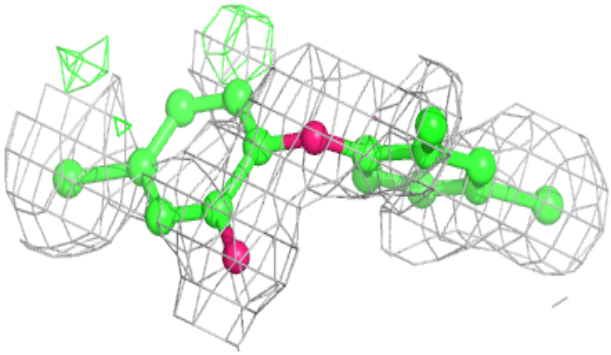
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TCL	E	309	17/17	0.60	0.29	61,62,62,63	0
2	TCL	F	311	17/17	0.75	0.30	53,55,58,58	0
2	TCL	C	304	17/17	0.76	0.23	48,50,51,52	0
2	TCL	B	302	17/17	0.80	0.25	54,55,59,60	0
2	TCL	A	300	17/17	0.82	0.22	43,44,49,51	0
3	NAD	C	305	44/44	0.86	0.16	28,37,40,43	0
2	TCL	D	306	17/17	0.86	0.19	46,46,48,49	0
3	NAD	D	307	44/44	0.88	0.16	28,34,37,40	0
3	NAD	F	312	44/44	0.88	0.20	28,36,42,44	0
3	NAD	B	303	44/44	0.90	0.15	22,27,30,32	0
3	NAD	E	310	44/44	0.90	0.15	25,29,33,34	0
3	NAD	A	301	44/44	0.91	0.15	25,30,34,37	0

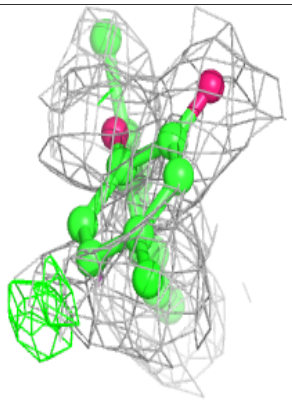
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TCL E 309:

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

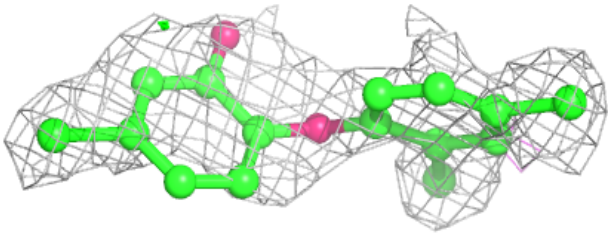


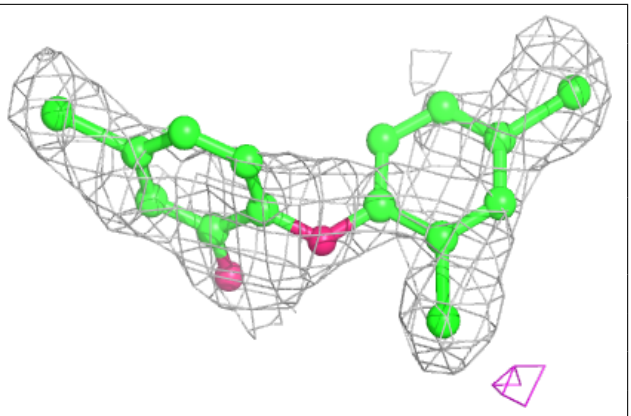


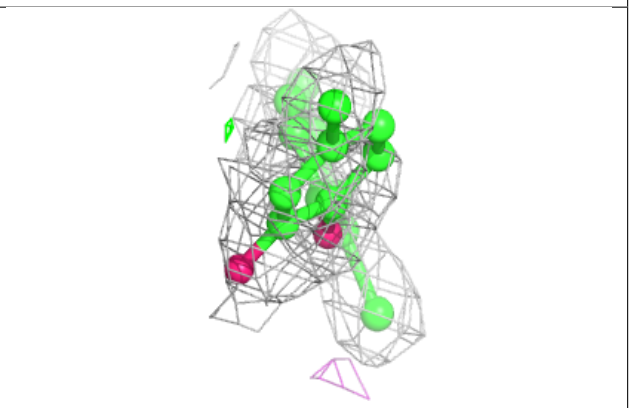


Electron density around TCL F 311:

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

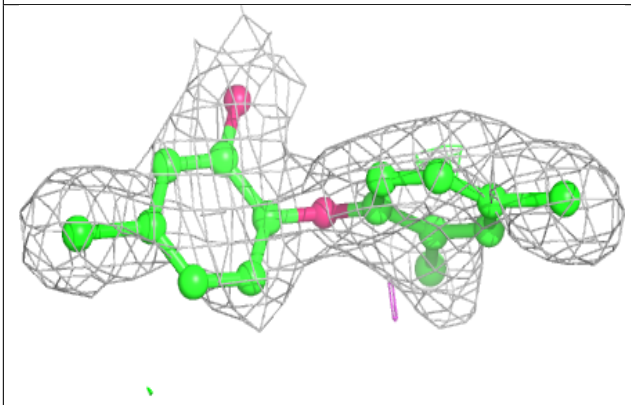


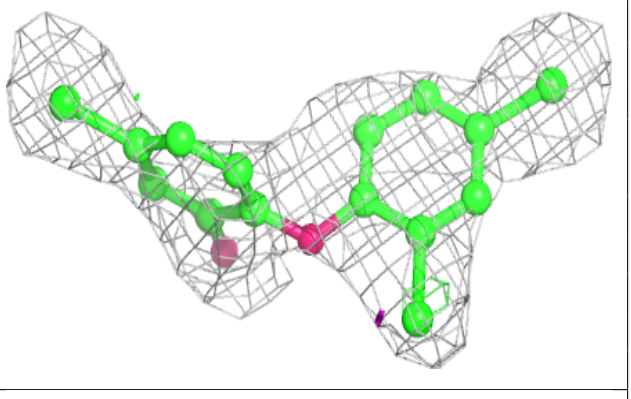


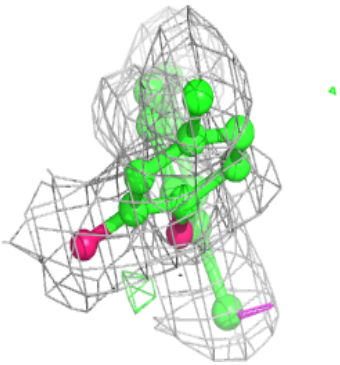


Electron density around TCL C 304:

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

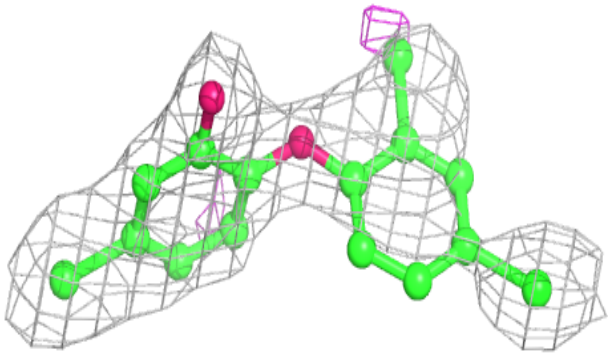


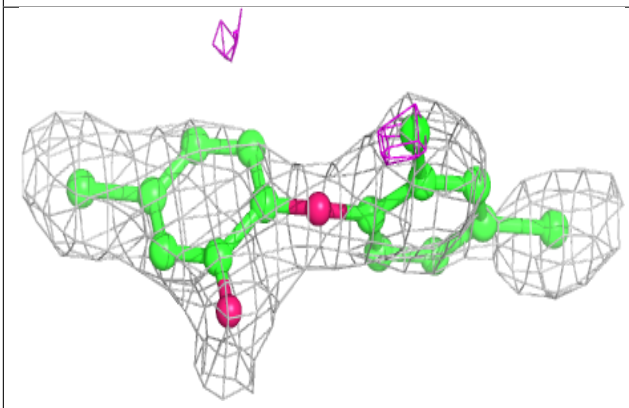


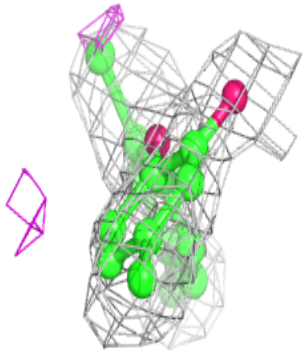


Electron density around TCL B 302:

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

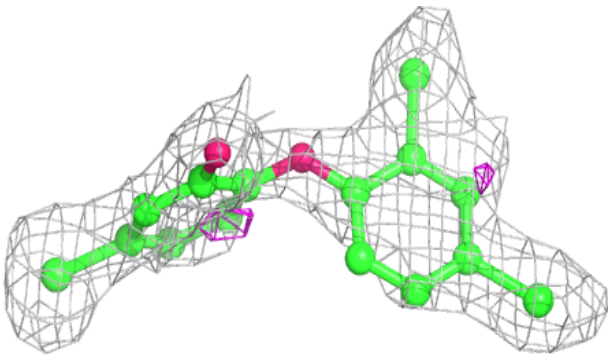


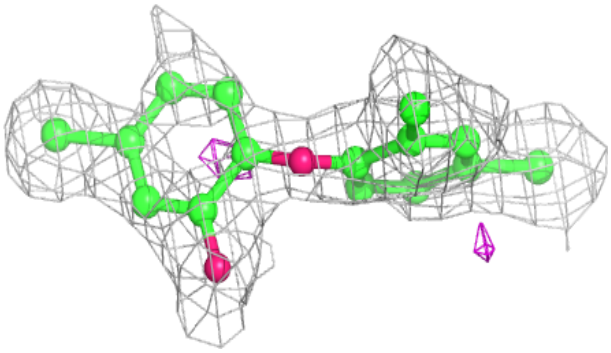


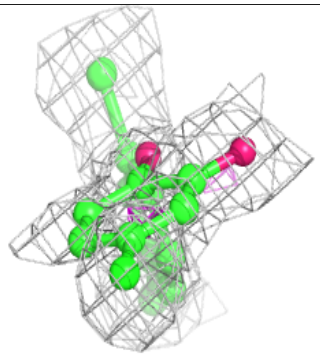


Electron density around TCL A 300:

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

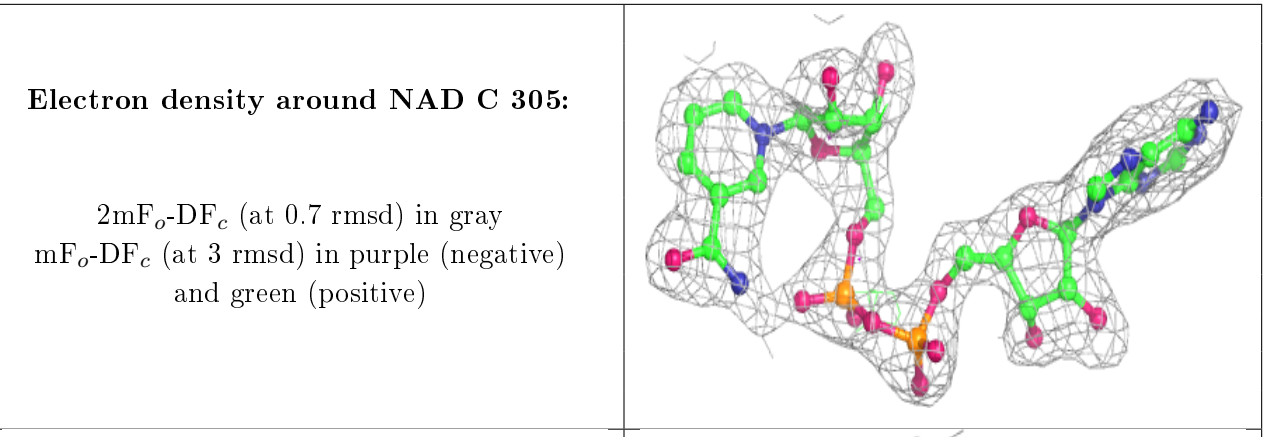






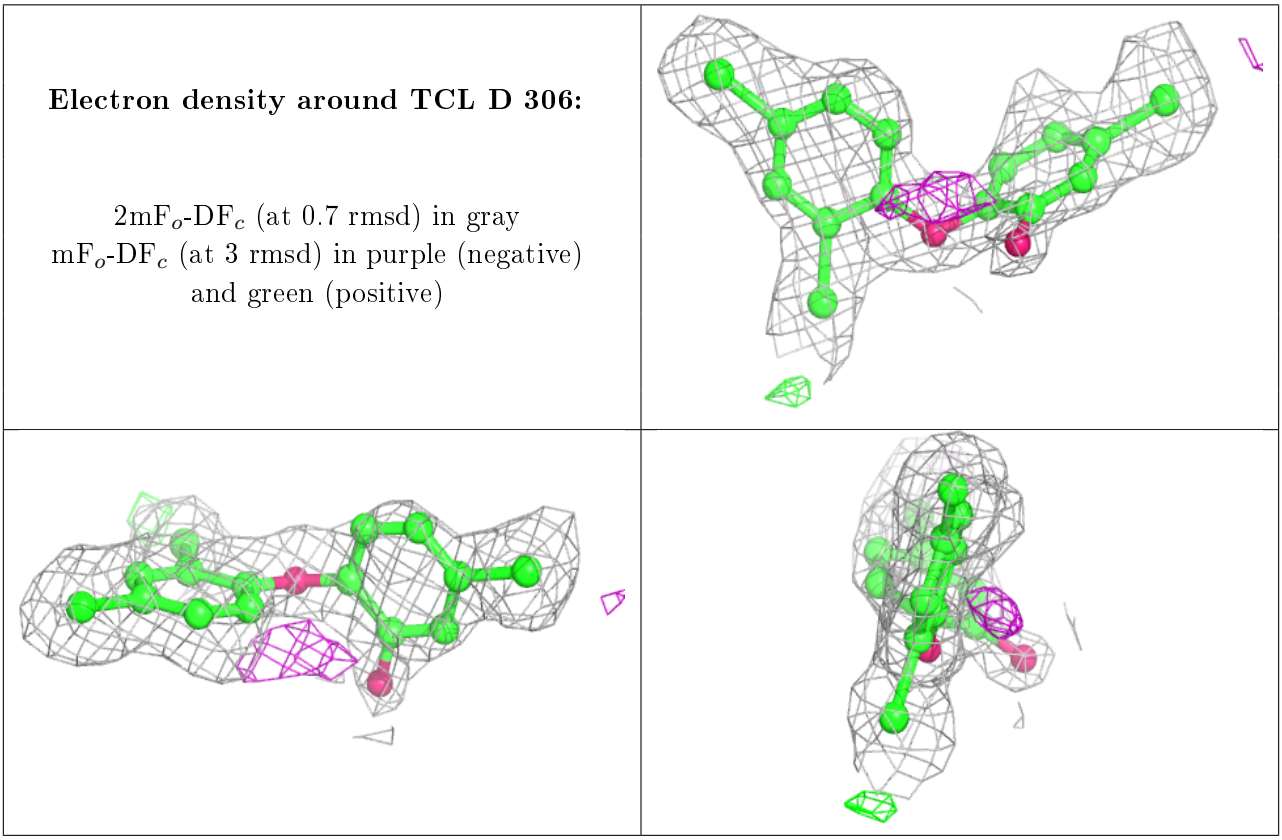
Electron density around NAD C 305:

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



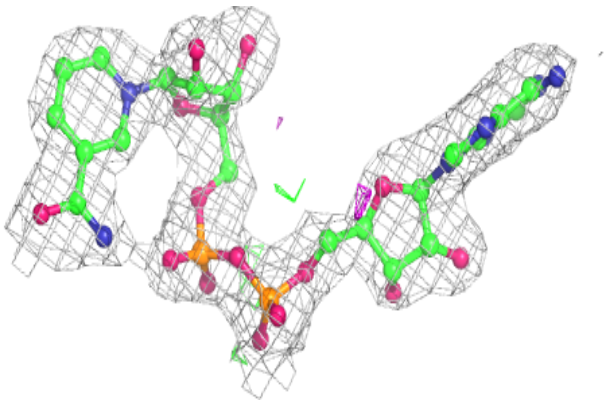
Electron density around TCL D 306:

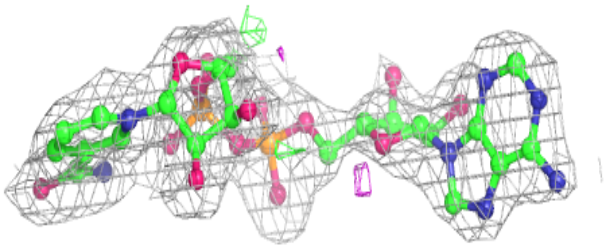
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

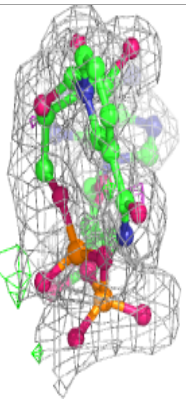


Electron density around NAD D 307:

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

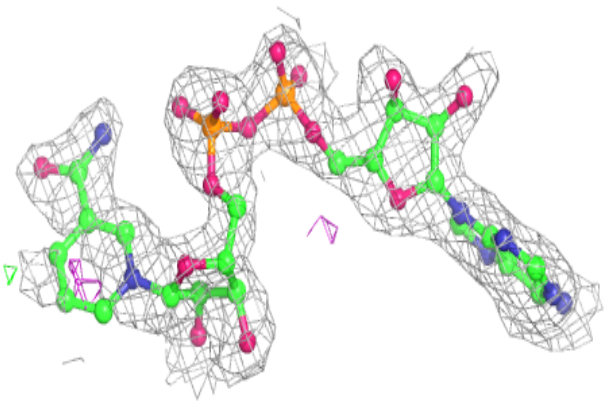


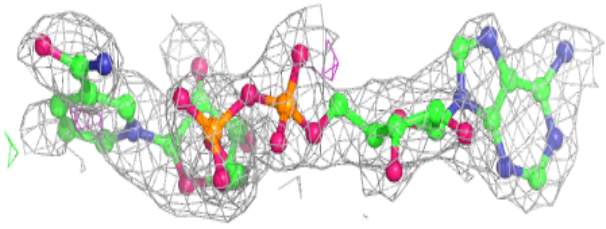


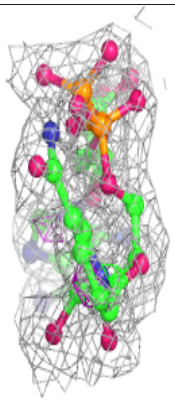


Electron density around NAD F 312:

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

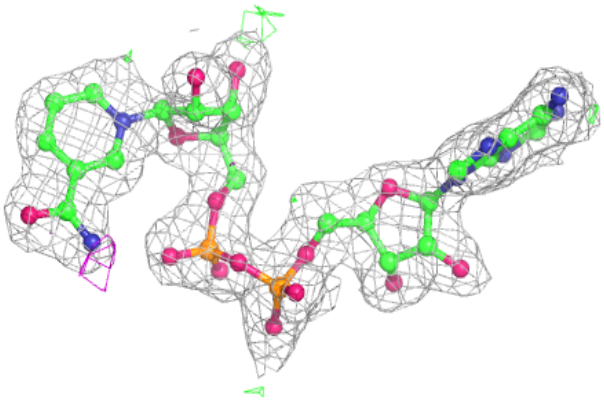


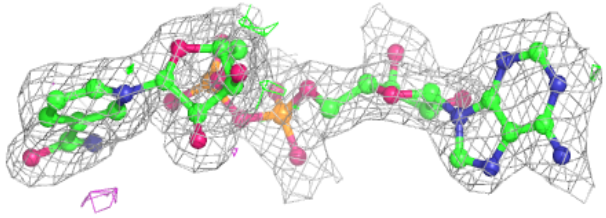


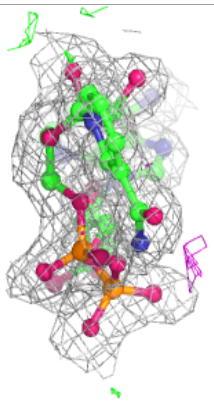


Electron density around NAD B 303:

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

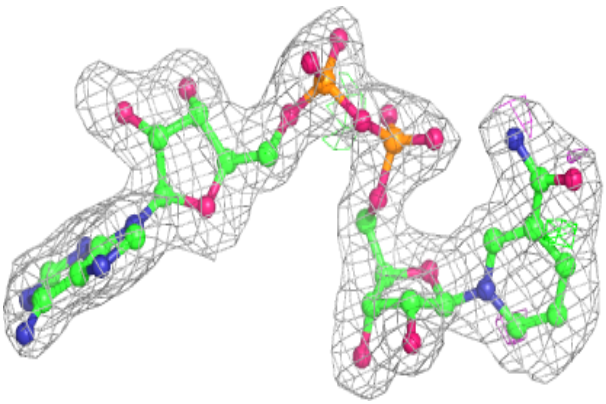


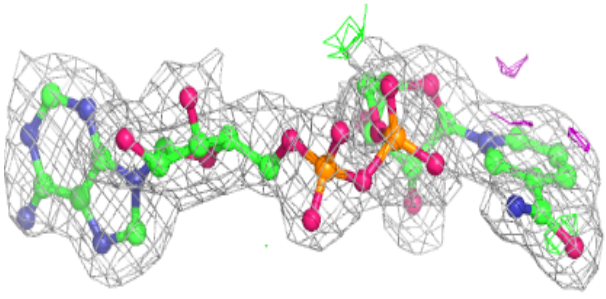


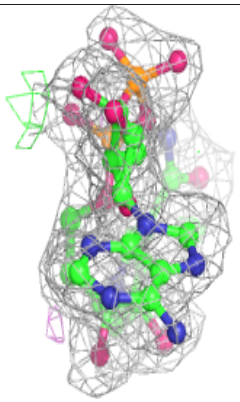


Electron density around NAD E 310:

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

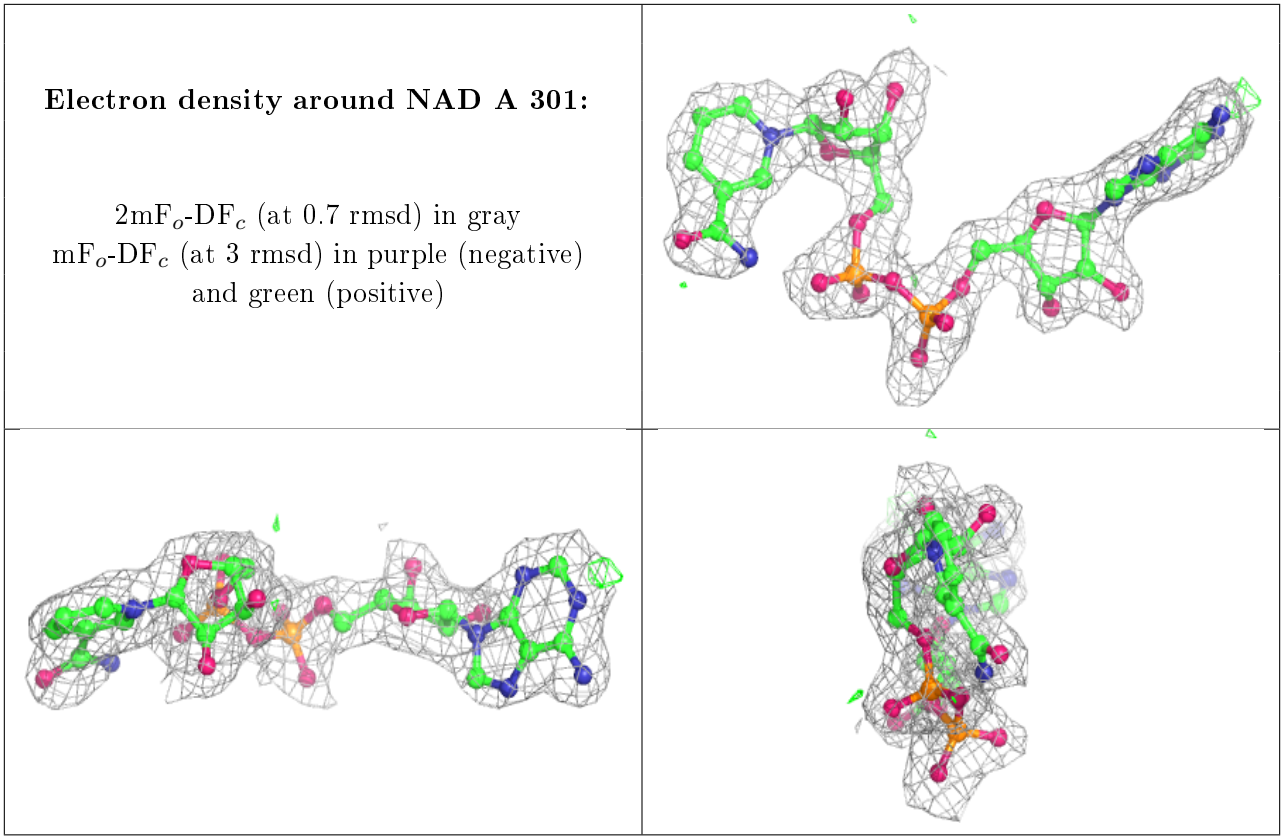






Electron density around NAD A 301:

$2mF_o$-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

There are no such residues in this entry.