



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 12:41 am BST

PDB ID : 2B37
Title : Crystal structure of Mycobacterium tuberculosis enoyl reductase (InhA) inhibited by 5-octyl-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 : 2.60 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

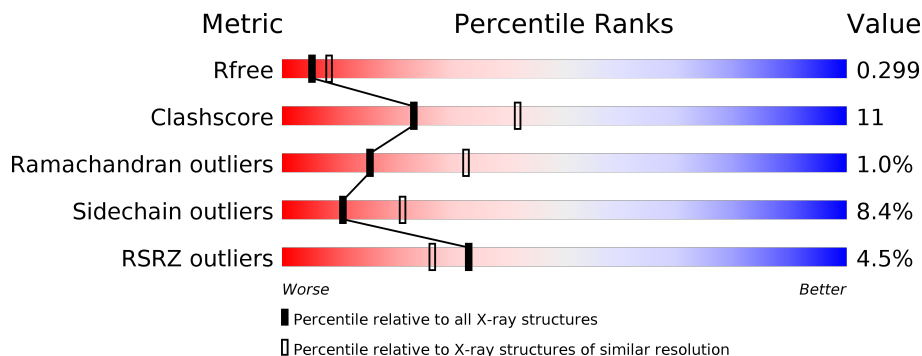
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	269	
1	B	269	
1	C	269	
1	D	269	
1	E	269	
1	F	269	

2 Entry composition [i](#)

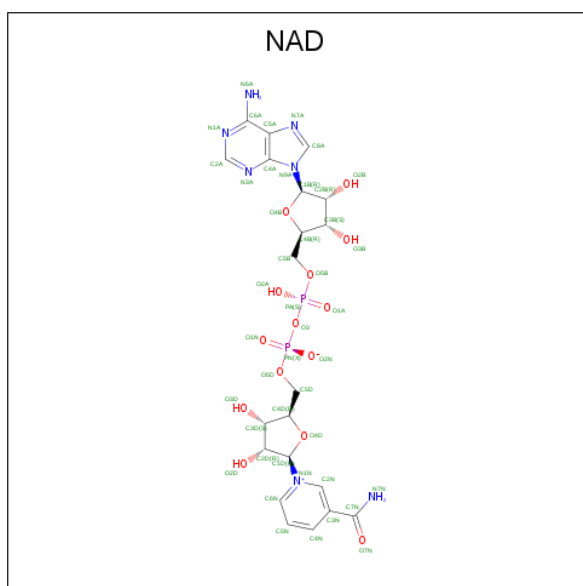
There are 4 unique types of molecules in this entry. The entry contains 11736 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

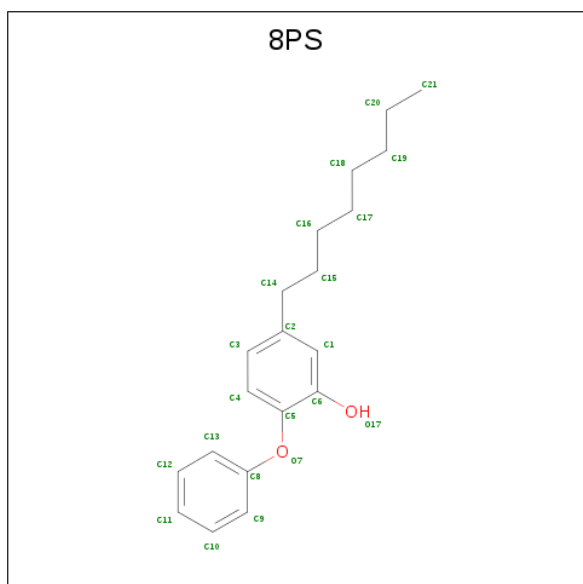
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	248	Total 1865	C 1184	N 326	O 346	S 9	0	0	0
1	B	245	Total 1840	C 1167	N 323	O 341	S 9	0	0	0
1	C	260	Total 1944	C 1231	N 340	O 364	S 9	0	0	0
1	D	260	Total 1944	C 1231	N 340	O 364	S 9	0	0	0
1	E	260	Total 1944	C 1231	N 340	O 364	S 9	0	0	0
1	F	248	Total 1861	C 1181	N 326	O 344	S 10	0	0	0

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



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

- Molecule 3 is 5-OCTYL-2-PHENOXYPHENOL (three-letter code: 8PS) (formula: $C_{20}H_{26}O_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	C O	0	0
			22	20 2		
3	D	1	Total	C O	0	0
			22	20 2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O	0	0
			7 7		

Continued on next page...

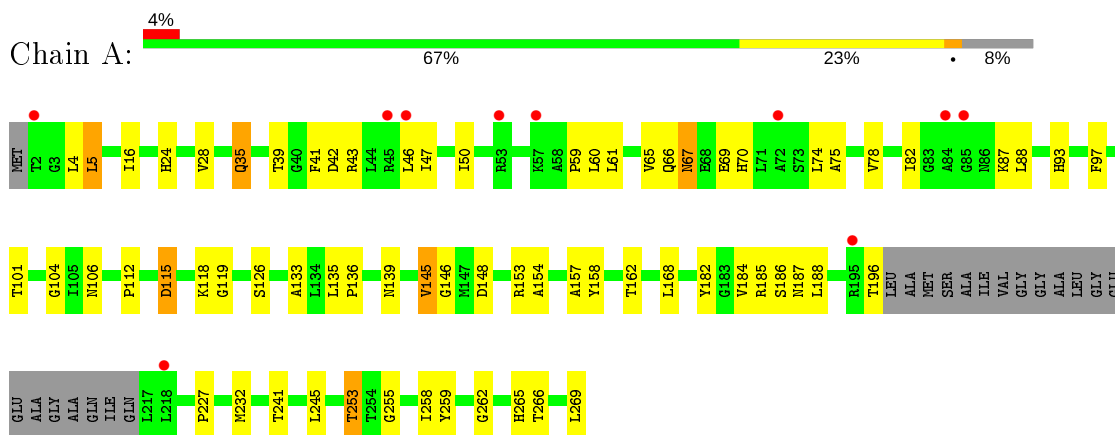
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total O 2 2	0	0
4	C	7	Total O 7 7	0	0
4	D	6	Total O 6 6	0	0
4	E	3	Total O 3 3	0	0
4	F	5	Total O 5 5	0	0

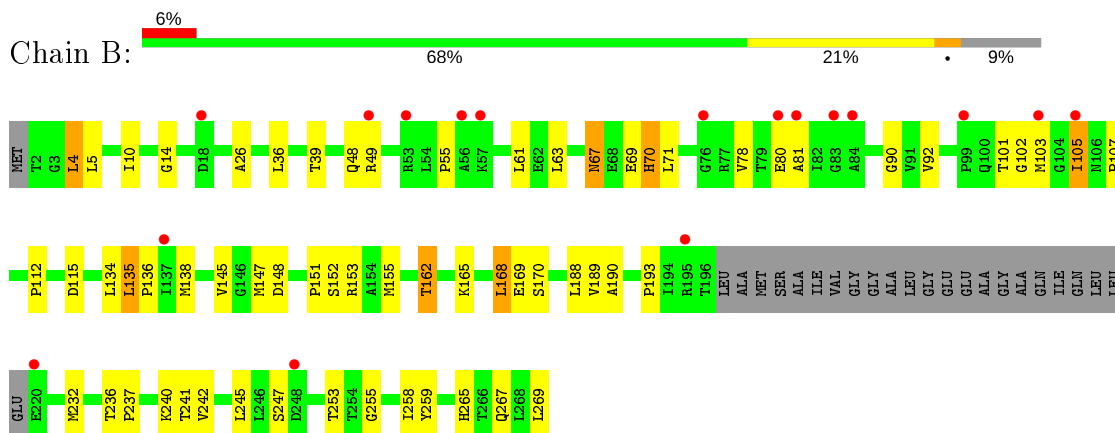
3 Residue-property plots [i](#)

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.

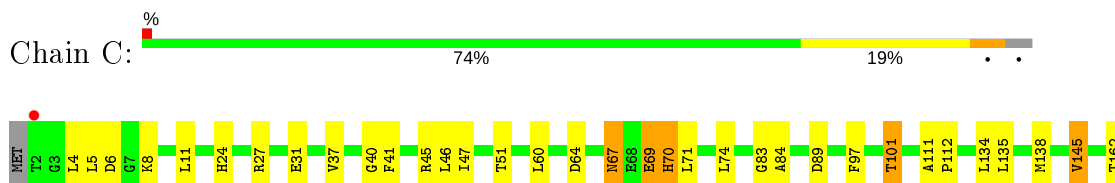
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

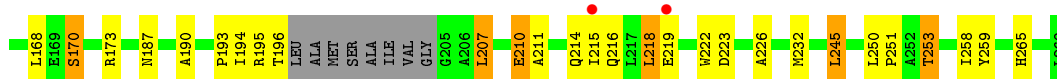


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

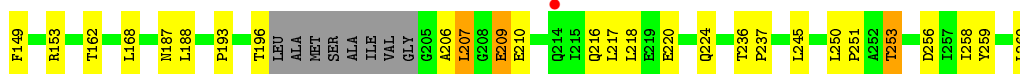
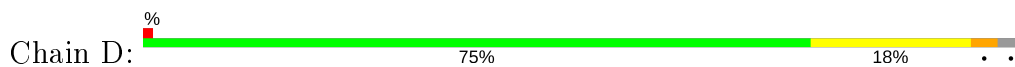


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

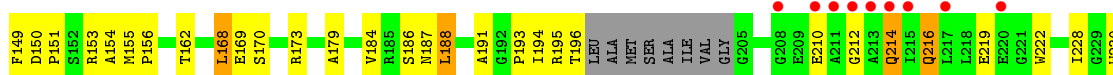
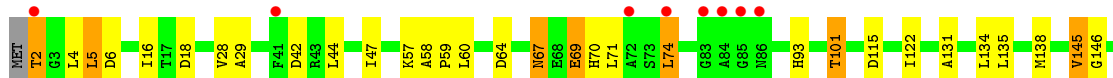




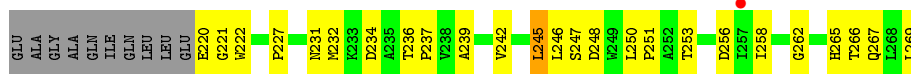
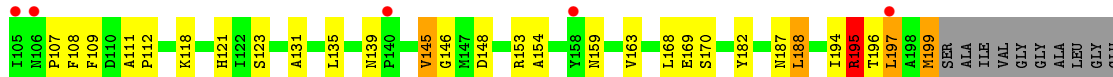
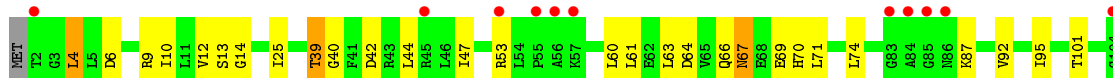
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	82.34Å 100.29Å 379.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 39.29 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (15.00-2.60) 96.3 (39.29-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.225 , 0.294 0.231 , 0.299	Depositor DCC
R_{free} test set	2384 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtrriage
Anisotropy	0.817	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11736	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2140e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 8PS, 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	0.67	0/1902	0.62	0/2583
1	B	0.70	0/1877	0.62	0/2549
1	C	0.84	1/1981 (0.1%)	0.70	0/2689
1	D	0.85	0/1981	0.70	0/2689
1	E	0.78	0/1981	0.66	0/2689
1	F	0.73	0/1898	0.64	1/2577 (0.0%)
All	All	0.77	1/11620 (0.0%)	0.65	1/15776 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	222	TRP	CB-CG	-5.46	1.40	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	195	ARG	NE-CZ-NH1	5.11	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1865	0	1880	48	0
1	B	1840	0	1852	44	0
1	C	1944	0	1954	40	0
1	D	1944	0	1954	43	0
1	E	1944	0	1954	55	0
1	F	1861	0	1877	59	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	2	0
2	D	44	0	26	5	0
2	E	44	0	26	4	0
2	F	44	0	26	2	0
3	C	22	0	25	3	0
3	D	22	0	25	7	0
4	A	7	0	0	0	0
4	B	2	0	0	0	0
4	C	7	0	0	3	0
4	D	6	0	0	0	0
4	E	3	0	0	1	0
4	F	5	0	0	0	0
All	All	11736	0	11677	265	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 11.

All (265) 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:F:101:THR:HG21	1:F:112:PRO:HD2	1.57	0.85
1:F:195:ARG:HG2	1:F:195:ARG:HH11	1.47	0.79
1:E:168:LEU:HD22	1:E:188:LEU:HD21	1.65	0.78
1:A:35:GLN:HE22	1:A:82:ILE:HG22	1.51	0.76
1:E:4:LEU:HD13	1:E:5:LEU:HD13	1.67	0.75
1:D:101:THR:HG21	1:D:115:ASP:OD1	1.85	0.74
1:A:241:THR:HG23	1:E:250:LEU:HD23	1.68	0.73
1:E:245:LEU:HD11	1:E:258:ILE:HD12	1.70	0.73
1:F:195:ARG:CG	1:F:195:ARG:HH11	2.02	0.71
1:C:218:LEU:HB2	3:C:300:8PS:H212	1.72	0.71
1:F:101:THR:CG2	1:F:111:ALA:HA	2.21	0.70
1:A:101:THR:CG2	1:A:112:PRO:HD2	2.23	0.68
1:A:101:THR:HG21	1:A:112:PRO:HD2	1.73	0.68
1:D:67:ASN:HD22	1:D:67:ASN:C	1.98	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:NH1	1:F:265:HIS:O	2.28	0.66
1:A:153:ARG:HH21	1:F:153:ARG:NE	1.94	0.65
1:D:218:LEU:HD11	3:D:301:8PS:H192	1.78	0.65
1:D:206:ALA:HA	1:D:209:GLU:HG2	1.80	0.64
1:F:168:LEU:HD23	1:F:188:LEU:HD21	1.80	0.63
1:F:168:LEU:CD2	1:F:188:LEU:HD21	2.29	0.63
1:B:101:THR:HG21	1:B:112:PRO:HD2	1.81	0.62
1:D:218:LEU:HD11	3:D:301:8PS:C19	2.30	0.62
1:E:212:GLY:O	1:E:216:GLN:HB2	1.99	0.62
1:F:196:THR:HG23	1:F:197:LEU:HD23	1.80	0.62
1:A:253:THR:HB	1:E:259:TYR:O	2.00	0.62
1:A:259:TYR:O	1:E:253:THR:HB	2.00	0.62
1:E:173:ARG:HB3	1:F:154:ALA:HB2	1.82	0.62
4:C:408:HOH:O	1:D:253:THR:HG22	2.01	0.61
1:D:67:ASN:ND2	1:D:70:HIS:H	1.98	0.61
1:E:67:ASN:HD21	1:E:69:GLU:HB2	1.64	0.61
1:A:153:ARG:HH21	1:F:153:ARG:HE	1.47	0.61
1:A:158:TYR:HD2	1:A:162:THR:HG1	1.44	0.61
1:D:99:PRO:HB2	1:D:101:THR:HG22	1.82	0.61
1:B:148:ASP:O	1:B:190:ALA:HA	2.01	0.60
1:F:123:SER:O	1:F:168:LEU:HD12	2.01	0.60
1:E:210:GLU:O	1:E:214:GLN:NE2	2.34	0.60
1:F:253:THR:HG21	1:F:258:ILE:HD11	1.83	0.60
1:B:255:GLY:O	1:F:266:THR:HG21	2.02	0.60
1:C:245:LEU:HD11	1:C:258:ILE:HD13	1.83	0.59
1:D:218:LEU:HG	3:D:301:8PS:H213	1.83	0.59
1:A:60:LEU:HD23	1:A:61:LEU:N	2.17	0.59
1:A:265:HIS:O	1:F:153:ARG:NH1	2.35	0.59
1:D:245:LEU:HD11	1:D:258:ILE:HD13	1.84	0.59
1:E:101:THR:HG21	1:E:115:ASP:OD1	2.02	0.59
1:D:218:LEU:HD21	3:D:301:8PS:H201	1.84	0.59
1:B:14:GLY:O	2:B:402:NAD:O3B	2.20	0.59
1:A:241:THR:HG23	1:E:250:LEU:CD2	2.33	0.58
1:F:131:ALA:O	1:F:135:LEU:HB2	2.03	0.58
1:B:101:THR:HG21	1:B:115:ASP:OD1	2.03	0.58
1:E:145:VAL:HA	1:E:187:ASN:O	2.04	0.58
1:F:40:GLY:HA3	1:F:47:ILE:CD1	2.33	0.58
1:B:67:ASN:HD22	1:B:67:ASN:C	2.07	0.57
1:F:145:VAL:HA	1:F:187:ASN:O	2.04	0.57
1:A:101:THR:O	1:A:106:ASN:ND2	2.38	0.57
1:A:66:GLN:HE22	1:A:118:LYS:HG3	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LEU:O	1:C:138:MET:HG3	2.05	0.57
1:F:195:ARG:N	1:F:232:MET:O	2.32	0.57
1:F:145:VAL:HG21	1:F:242:VAL:HG13	1.87	0.56
1:D:4:LEU:HB3	1:D:5:LEU:HD13	1.86	0.56
1:A:24:HIS:O	1:A:28:VAL:HG23	2.05	0.56
1:E:131:ALA:O	1:E:135:LEU:HB2	2.05	0.56
1:A:87:LYS:HB2	1:A:139:ASN:ND2	2.21	0.56
1:D:21:ILE:O	1:D:25:ILE:HG13	2.06	0.56
1:B:67:ASN:ND2	1:B:70:HIS:H	2.04	0.55
1:F:95:ILE:HD13	2:F:406:NAD:C2A	2.36	0.55
1:B:267:GLN:OE1	1:E:154:ALA:HB3	2.07	0.55
1:F:14:GLY:O	2:F:406:NAD:O3B	2.24	0.55
1:F:60:LEU:O	1:F:60:LEU:HD13	2.07	0.55
1:C:253:THR:HB	1:D:259:TYR:O	2.07	0.55
1:C:259:TYR:O	1:D:253:THR:HB	2.07	0.55
1:A:158:TYR:HD2	1:A:162:THR:OG1	1.90	0.54
1:B:193:PRO:O	1:B:232:MET:HB3	2.08	0.54
1:F:220:GLU:O	1:F:222:TRP:N	2.40	0.54
1:B:147:MET:HE1	1:B:189:VAL:HB	1.89	0.54
1:B:78:VAL:O	1:B:81:ALA:N	2.40	0.54
1:C:196:THR:HG21	2:C:403:NAD:PN	2.47	0.54
1:C:64:ASP:H	1:C:70:HIS:HD2	1.54	0.54
1:E:196:THR:O	4:E:407:HOH:O	2.18	0.54
1:D:60:LEU:HD13	1:D:60:LEU:O	2.08	0.53
1:A:154:ALA:HB3	1:F:267:GLN:OE1	2.08	0.53
1:F:4:LEU:HD22	1:F:247:SER:HB2	1.89	0.52
1:A:182:TYR:HB2	1:A:184:VAL:HG23	1.91	0.52
1:B:265:HIS:O	1:E:153:ARG:NH1	2.42	0.52
1:E:214:GLN:N	1:E:214:GLN:HE21	2.07	0.52
1:D:63:LEU:HD11	1:D:71:LEU:CD1	2.39	0.52
1:E:214:GLN:HE21	1:E:214:GLN:H	1.58	0.52
1:E:16:ILE:HD12	1:E:47:ILE:CG2	2.39	0.52
1:B:147:MET:HE3	1:B:242:VAL:HG22	1.92	0.52
1:C:8:LYS:HA	1:C:89:ASP:OD2	2.10	0.51
1:E:191:ALA:HB1	1:E:238:VAL:HG21	1.92	0.51
1:D:14:GLY:O	2:D:404:NAD:O3B	2.23	0.51
1:E:134:LEU:O	1:E:138:MET:HG3	2.11	0.51
1:F:195:ARG:NH1	1:F:195:ARG:HG2	2.16	0.51
1:F:135:LEU:HG	1:F:182:TYR:CD1	2.45	0.51
1:E:2:THR:HG22	1:E:6:ASP:OD2	2.11	0.50
1:C:210:GLU:CD	1:C:210:GLU:H	2.15	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ASP:O	4:C:407:HOH:O	2.19	0.50
1:C:216:GLN:HA	1:C:219:GLU:CD	2.32	0.50
1:C:64:ASP:H	1:C:70:HIS:CD2	2.30	0.50
1:C:67:ASN:HD22	1:C:69:GLU:H	1.58	0.50
1:B:241:THR:HG23	1:F:250:LEU:HD23	1.94	0.49
1:A:145:VAL:HA	1:A:187:ASN:O	2.12	0.49
1:C:101:THR:HG23	1:C:111:ALA:HA	1.93	0.49
1:B:190:ALA:HB3	1:B:259:TYR:CD2	2.48	0.49
1:C:101:THR:HG21	1:C:112:PRO:HD2	1.95	0.49
1:D:24:HIS:CD2	1:D:27:ARG:HH21	2.30	0.49
1:B:4:LEU:HD11	1:B:247:SER:HB3	1.95	0.49
1:D:269:LEU:C	1:D:269:LEU:HD13	2.33	0.49
1:F:231:ASN:HD22	1:F:234:ASP:HB2	1.78	0.49
1:F:107:PRO:O	1:F:109:PHE:N	2.46	0.49
1:F:25:ILE:HG12	1:F:239:ALA:HA	1.95	0.48
1:A:227:PRO:HD2	1:A:262:GLY:O	2.14	0.48
1:B:147:MET:O	1:B:165:LYS:NZ	2.46	0.48
1:B:26:ALA:HB1	1:B:36:LEU:CD1	2.44	0.48
1:A:67:ASN:HD22	1:A:70:HIS:H	1.62	0.48
1:C:27:ARG:HD2	1:C:31:GLU:OE2	2.13	0.48
1:E:155:MET:HB2	1:E:156:PRO:HD2	1.95	0.48
1:D:196:THR:HG21	2:D:404:NAD:O1N	2.13	0.48
1:D:65:VAL:HG22	2:D:404:NAD:C6A	2.44	0.48
1:D:65:VAL:HG22	2:D:404:NAD:N1A	2.28	0.48
1:E:210:GLU:CD	1:E:210:GLU:H	2.16	0.48
1:A:186:SER:O	1:A:255:GLY:N	2.46	0.48
1:E:236:THR:HB	1:E:237:PRO:HD3	1.96	0.48
1:B:4:LEU:HD13	1:B:5:LEU:CD1	2.44	0.47
1:D:145:VAL:HA	1:D:187:ASN:O	2.14	0.47
1:E:193:PRO:HA	2:E:405:NAD:O7N	2.13	0.47
1:B:105:ILE:O	1:B:105:ILE:HD13	2.14	0.47
1:B:148:ASP:OD2	1:B:169:GLU:OE2	2.33	0.47
1:C:218:LEU:CB	3:C:300:8PS:H212	2.43	0.47
1:E:250:LEU:N	1:E:251:PRO:HD3	2.30	0.47
1:A:241:THR:O	1:A:245:LEU:HD23	2.14	0.47
1:B:153:ARG:NH1	1:E:265:HIS:O	2.48	0.47
1:C:250:LEU:N	1:C:251:PRO:HD3	2.30	0.47
1:E:93:HIS:O	1:E:146:GLY:HA2	2.14	0.47
1:C:207:LEU:HB2	1:C:211:ALA:CB	2.44	0.47
1:C:245:LEU:CD1	1:C:250:LEU:HD13	2.44	0.47
1:B:236:THR:O	1:B:240:LYS:N	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:PHE:CE2	3:D:301:8PS:H142	2.50	0.47
1:C:265:HIS:NE2	1:D:256:ASP:OD2	2.28	0.47
1:A:245:LEU:HD11	1:A:258:ILE:HD13	1.97	0.46
1:F:101:THR:HG21	1:F:112:PRO:CD	2.35	0.46
1:D:24:HIS:HD2	1:D:27:ARG:HH21	1.62	0.46
1:E:67:ASN:ND2	1:E:69:GLU:HB2	2.31	0.46
1:C:207:LEU:HB2	1:C:211:ALA:HB3	1.98	0.46
1:F:66:GLN:HE22	1:F:118:LYS:HG3	1.80	0.46
1:A:16:ILE:HD12	1:A:47:ILE:CG2	2.44	0.46
1:D:93:HIS:O	1:D:146:GLY:HA2	2.15	0.46
1:E:67:ASN:C	1:E:67:ASN:HD22	2.18	0.46
1:E:58:ALA:HB1	1:E:59:PRO:HD2	1.97	0.46
1:A:185:ARG:HG2	1:E:228:ILE:HD13	1.97	0.45
1:B:151:PRO:CB	1:B:162:THR:HG22	2.46	0.45
1:E:28:VAL:O	1:E:29:ALA:C	2.55	0.45
1:A:93:HIS:O	1:A:146:GLY:HA2	2.16	0.45
1:F:197:LEU:HD23	1:F:197:LEU:H	1.82	0.45
1:B:39:THR:HB	1:B:63:LEU:HB3	1.99	0.45
1:C:24:HIS:HD2	1:C:27:ARG:HH21	1.65	0.45
1:B:153:ARG:HH21	1:E:153:ARG:NE	2.13	0.45
1:D:5:LEU:HB3	1:D:34:ALA:HB2	1.97	0.45
1:A:60:LEU:C	1:A:60:LEU:HD23	2.37	0.45
1:A:66:GLN:NE2	1:A:118:LYS:HG3	2.31	0.45
1:A:148:ASP:O	2:A:401:NAD:H6N	2.17	0.45
1:A:97:PHE:O	1:A:119:GLY:HA2	2.16	0.45
1:E:74:LEU:HD13	1:E:134:LEU:HD21	1.98	0.45
1:B:253:THR:HG21	1:B:258:ILE:HD11	1.99	0.45
1:C:40:GLY:HA3	1:C:47:ILE:HD11	1.98	0.45
1:F:227:PRO:HD2	1:F:262:GLY:O	2.16	0.44
1:F:12:VAL:HA	1:F:92:VAL:HB	1.98	0.44
1:B:236:THR:N	1:B:237:PRO:HD2	2.32	0.44
1:E:122:ILE:HD13	2:E:405:NAD:H61A	1.82	0.44
1:A:153:ARG:HD3	1:F:265:HIS:O	2.17	0.44
1:D:206:ALA:O	1:D:207:LEU:C	2.55	0.44
1:D:64:ASP:H	1:D:70:HIS:HD2	1.64	0.44
1:E:64:ASP:H	1:E:70:HIS:CD2	2.35	0.44
1:B:134:LEU:O	1:B:138:MET:HG3	2.16	0.44
1:F:168:LEU:HD23	1:F:168:LEU:C	2.38	0.44
1:F:39:THR:HA	1:F:61:LEU:O	2.17	0.44
1:C:218:LEU:HD23	1:C:219:GLU:N	2.33	0.44
1:F:66:GLN:HG2	1:F:121:HIS:CE1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:HIS:CD2	1:A:266:THR:HG23	2.52	0.44
1:E:245:LEU:HD11	1:E:258:ILE:CD1	2.42	0.44
1:A:16:ILE:O	1:A:50:ILE:HD12	2.17	0.44
1:B:102:GLY:O	1:B:103:MET:HG2	2.18	0.44
1:D:65:VAL:HB	1:D:126:SER:HB2	2.00	0.44
1:E:179:ALA:HB1	1:E:184:VAL:HB	2.00	0.44
1:A:75:ALA:HB2	1:A:133:ALA:O	2.18	0.43
1:B:10:ILE:HG13	1:B:90:GLY:HA3	2.00	0.43
1:C:194:ILE:O	1:C:196:THR:N	2.51	0.43
1:C:219:GLU:HG2	1:C:232:MET:SD	2.58	0.43
1:D:218:LEU:HD11	3:D:301:8PS:C20	2.48	0.43
1:B:92:VAL:HG22	1:B:145:VAL:CG1	2.47	0.43
1:C:97:PHE:HA	3:C:300:8PS:H11	2.00	0.43
1:C:83:GLY:O	1:C:84:ALA:C	2.56	0.43
1:D:236:THR:N	1:D:237:PRO:CD	2.80	0.43
1:A:43:ARG:HE	1:A:46:LEU:HD22	1.82	0.43
1:C:190:ALA:HB3	1:C:259:TYR:CD2	2.54	0.43
1:F:194:ILE:HA	1:F:232:MET:O	2.18	0.43
1:F:195:ARG:CG	1:F:195:ARG:NH1	2.71	0.43
1:F:64:ASP:H	1:F:70:HIS:HD2	1.65	0.43
1:D:135:LEU:N	1:D:136:PRO:CD	2.81	0.43
1:C:170:SER:HA	1:C:173:ARG:NH1	2.33	0.43
1:B:67:ASN:ND2	1:B:69:GLU:H	2.17	0.43
1:C:145:VAL:HA	1:C:187:ASN:O	2.18	0.43
1:C:41:PHE:HB2	2:C:403:NAD:C2A	2.48	0.43
1:D:250:LEU:N	1:D:251:PRO:HD3	2.34	0.43
1:A:41:PHE:CG	1:A:42:ASP:N	2.87	0.43
1:A:65:VAL:HB	1:A:126:SER:HB2	1.99	0.43
1:F:236:THR:N	1:F:237:PRO:CD	2.82	0.43
1:B:168:LEU:HD22	1:B:168:LEU:O	2.19	0.43
1:D:153:ARG:HG2	1:D:153:ARG:HH11	1.83	0.43
1:B:67:ASN:ND2	1:B:69:GLU:N	2.66	0.42
1:C:193:PRO:O	1:C:194:ILE:HD13	2.19	0.42
1:E:4:LEU:CD1	1:E:5:LEU:HD13	2.44	0.42
1:A:158:TYR:CD2	1:A:162:THR:OG1	2.61	0.42
1:C:47:ILE:O	1:C:51:THR:HG23	2.19	0.42
1:C:67:ASN:HD22	1:C:69:GLU:N	2.17	0.42
1:E:67:ASN:HD22	1:E:69:GLU:H	1.67	0.42
1:B:4:LEU:CD1	1:B:247:SER:HB3	2.50	0.42
1:F:146:GLY:O	1:F:188:LEU:HA	2.19	0.42
1:E:194:ILE:N	2:E:405:NAD:O7N	2.42	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASN:ND2	1:B:67:ASN:C	2.72	0.42
1:F:148:ASP:OD2	1:F:169:GLU:OE2	2.38	0.42
1:F:42:ASP:O	1:F:44:LEU:HD23	2.20	0.42
1:E:151:PRO:HD2	1:E:169:GLU:OE2	2.19	0.42
1:F:196:THR:HB	1:F:199:MET:HA	2.00	0.42
1:E:149:PHE:HB2	2:E:405:NAD:C5N	2.50	0.42
1:B:67:ASN:HD21	1:B:69:GLU:HB2	1.85	0.42
1:F:245:LEU:CD1	1:F:250:LEU:HD13	2.49	0.42
1:A:104:GLY:O	1:A:157:ALA:HA	2.19	0.42
1:E:42:ASP:OD1	1:E:42:ASP:C	2.58	0.42
1:B:135:LEU:N	1:B:136:PRO:CD	2.83	0.42
1:C:11:LEU:HA	1:C:37:VAL:O	2.20	0.42
1:E:186:SER:O	1:E:255:GLY:N	2.50	0.42
1:E:250:LEU:N	1:E:251:PRO:CD	2.83	0.42
1:A:101:THR:HB	1:A:115:ASP:OD1	2.19	0.41
1:B:155:MET:CE	1:E:268:LEU:HD22	2.49	0.41
1:B:39:THR:HA	1:B:61:LEU:O	2.20	0.41
1:C:214:GLN:O	1:C:215:ILE:C	2.54	0.41
1:F:250:LEU:N	1:F:251:PRO:HD3	2.35	0.41
1:A:78:VAL:HG11	1:A:88:LEU:HD11	2.03	0.41
1:D:220:GLU:O	1:D:224:GLN:HG3	2.20	0.41
1:D:193:PRO:HA	2:D:404:NAD:O7N	2.20	0.41
1:F:87:LYS:HB2	1:F:139:ASN:ND2	2.35	0.41
1:B:193:PRO:HB2	1:B:232:MET:SD	2.61	0.41
1:A:4:LEU:HB3	1:A:5:LEU:HD13	2.03	0.41
1:E:101:THR:HG21	1:E:115:ASP:CB	2.51	0.41
1:E:170:SER:HB3	1:F:163:VAL:HG22	2.03	0.41
1:E:4:LEU:HD11	1:E:247:SER:HB3	2.01	0.41
1:F:13:SER:HB2	1:F:95:ILE:HD11	2.03	0.41
1:F:220:GLU:C	1:F:222:TRP:N	2.74	0.41
1:E:230:TRP:CZ3	1:E:261:ASP:HA	2.55	0.41
1:F:10:ILE:HD13	1:F:246:LEU:HD13	2.03	0.41
1:A:67:ASN:HD21	1:A:69:GLU:HB2	1.85	0.41
1:F:39:THR:HB	1:F:63:LEU:HB3	2.02	0.41
1:C:226:ALA:O	4:C:407:HOH:O	2.22	0.41
1:B:165:LYS:HA	1:B:165:LYS:HD3	1.95	0.40
1:D:9:ARG:HA	1:D:35:GLN:O	2.21	0.40
1:B:147:MET:HE3	1:B:242:VAL:CG2	2.51	0.40
1:D:97:PHE:HA	3:D:301:8PS:H11	2.04	0.40
1:F:250:LEU:N	1:F:251:PRO:CD	2.85	0.40
1:F:67:ASN:ND2	1:F:69:GLU:H	2.19	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PRO:HG2	1:C:45:ARG:NH2	2.37	0.40
1:E:135:LEU:HD21	1:E:179:ALA:HA	2.03	0.40
1:D:134:LEU:O	1:D:138:MET:HG3	2.22	0.40
1:A:39:THR:HA	1:A:61:LEU:O	2.22	0.40
1:D:216:GLN:C	1:D:218:LEU:N	2.75	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	244/269 (91%)	224 (92%)	18 (7%)	2 (1%)	19	39
1	B	241/269 (90%)	220 (91%)	19 (8%)	2 (1%)	19	39
1	C	256/269 (95%)	237 (93%)	18 (7%)	1 (0%)	34	57
1	D	256/269 (95%)	234 (91%)	18 (7%)	4 (2%)	9	19
1	E	256/269 (95%)	237 (93%)	17 (7%)	2 (1%)	19	39
1	F	244/269 (91%)	217 (89%)	23 (9%)	4 (2%)	9	19
All	All	1497/1614 (93%)	1369 (91%)	113 (8%)	15 (1%)	15	32

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	195	ARG
1	D	207	LEU
1	D	209	GLU
1	E	195	ARG
1	F	108	PHE
1	A	74	LEU
1	D	217	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	221	GLY
1	A	59	PRO
1	F	53	ARG
1	B	55	PRO
1	E	150	ASP
1	F	159	ASN
1	D	210	GLU
1	B	107	PRO

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	193/205 (94%)	181 (94%)	12 (6%)	18	37
1	B	190/205 (93%)	174 (92%)	16 (8%)	11	21
1	C	199/205 (97%)	178 (89%)	21 (11%)	6	12
1	D	199/205 (97%)	187 (94%)	12 (6%)	19	39
1	E	199/205 (97%)	178 (89%)	21 (11%)	6	12
1	F	192/205 (94%)	175 (91%)	17 (9%)	9	19
All	All	1172/1230 (95%)	1073 (92%)	99 (8%)	11	21

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	35	GLN
1	A	67	ASN
1	A	115	ASP
1	A	135	LEU
1	A	145	VAL
1	A	168	LEU
1	A	188	LEU
1	A	196	THR
1	A	232	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	253	THR
1	A	269	LEU
1	B	4	LEU
1	B	48	GLN
1	B	49	ARG
1	B	67	ASN
1	B	70	HIS
1	B	71	LEU
1	B	80	GLU
1	B	105	ILE
1	B	135	LEU
1	B	152	SER
1	B	162	THR
1	B	168	LEU
1	B	170	SER
1	B	188	LEU
1	B	245	LEU
1	B	269	LEU
1	C	4	LEU
1	C	5	LEU
1	C	6	ASP
1	C	46	LEU
1	C	60	LEU
1	C	67	ASN
1	C	69	GLU
1	C	70	HIS
1	C	71	LEU
1	C	74	LEU
1	C	101	THR
1	C	135	LEU
1	C	145	VAL
1	C	162	THR
1	C	168	LEU
1	C	170	SER
1	C	207	LEU
1	C	210	GLU
1	C	218	LEU
1	C	245	LEU
1	C	253	THR
1	D	5	LEU
1	D	44	LEU
1	D	67	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	70	HIS
1	D	71	LEU
1	D	74	LEU
1	D	135	LEU
1	D	145	VAL
1	D	162	THR
1	D	168	LEU
1	D	188	LEU
1	D	253	THR
1	E	2	THR
1	E	5	LEU
1	E	18	ASP
1	E	44	LEU
1	E	57	LYS
1	E	60	LEU
1	E	67	ASN
1	E	69	GLU
1	E	71	LEU
1	E	74	LEU
1	E	101	THR
1	E	145	VAL
1	E	162	THR
1	E	168	LEU
1	E	188	LEU
1	E	214	GLN
1	E	216	GLN
1	E	219	GLU
1	E	222	TRP
1	E	233	LYS
1	E	253	THR
1	F	4	LEU
1	F	6	ASP
1	F	9	ARG
1	F	39	THR
1	F	67	ASN
1	F	71	LEU
1	F	74	LEU
1	F	145	VAL
1	F	170	SER
1	F	188	LEU
1	F	195	ARG
1	F	197	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	199	MET
1	F	245	LEU
1	F	248	ASP
1	F	256	ASP
1	F	269	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	35	GLN
1	A	67	ASN
1	A	139	ASN
1	B	35	GLN
1	B	66	GLN
1	B	67	ASN
1	B	224	GLN
1	C	24	HIS
1	C	67	ASN
1	C	70	HIS
1	D	35	GLN
1	D	67	ASN
1	D	70	HIS
1	D	139	ASN
1	E	67	ASN
1	E	139	ASN
1	E	214	GLN
1	E	216	GLN
1	F	24	HIS
1	F	67	ASN
1	F	70	HIS
1	F	106	ASN
1	F	139	ASN
1	F	231	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	402	-	42,48,48	1.71	4 (9%)	50,73,73	1.26	5 (10%)
3	8PS	D	301	-	23,23,23	1.25	1 (4%)	28,28,28	1.27	3 (10%)
2	NAD	E	405	-	42,48,48	1.84	6 (14%)	50,73,73	1.56	7 (14%)
3	8PS	C	300	-	23,23,23	1.21	1 (4%)	28,28,28	1.10	4 (14%)
2	NAD	F	406	-	42,48,48	1.70	3 (7%)	50,73,73	1.31	3 (6%)
2	NAD	D	404	-	42,48,48	1.82	3 (7%)	50,73,73	1.46	8 (16%)
2	NAD	C	403	-	42,48,48	1.97	5 (11%)	50,73,73	1.47	5 (10%)
2	NAD	A	401	-	42,48,48	1.67	5 (11%)	50,73,73	1.33	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	402	-	-	6/26/62/62	0/5/5/5
3	8PS	D	301	-	-	2/12/12/12	0/2/2/2
2	NAD	E	405	-	-	6/26/62/62	0/5/5/5
3	8PS	C	300	-	-	1/12/12/12	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	F	406	-	-	9/26/62/62	0/5/5/5
2	NAD	D	404	-	-	9/26/62/62	0/5/5/5
2	NAD	C	403	-	-	6/26/62/62	0/5/5/5
2	NAD	A	401	-	-	6/26/62/62	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	405	NAD	O7N-C7N	8.99	1.41	1.24
2	D	404	NAD	O7N-C7N	8.87	1.41	1.24
2	C	403	NAD	O7N-C7N	8.82	1.41	1.24
2	F	406	NAD	O7N-C7N	8.78	1.41	1.24
2	B	402	NAD	O7N-C7N	8.45	1.40	1.24
2	A	401	NAD	O7N-C7N	8.04	1.39	1.24
2	C	403	NAD	C2A-N3A	6.16	1.42	1.32
2	D	404	NAD	C2A-N3A	4.68	1.39	1.32
3	C	300	8PS	C6-C5	4.55	1.48	1.40
2	B	402	NAD	C2A-N3A	4.34	1.39	1.32
3	D	301	8PS	C6-C5	4.06	1.47	1.40
2	F	406	NAD	C2A-N3A	3.83	1.38	1.32
2	E	405	NAD	C2A-N3A	3.48	1.37	1.32
2	A	401	NAD	C2B-C1B	-3.27	1.48	1.53
2	D	404	NAD	C2N-N1N	3.23	1.38	1.35
2	C	403	NAD	O4D-C1D	2.99	1.45	1.41
2	A	401	NAD	C2A-N3A	2.96	1.36	1.32
2	B	402	NAD	C2A-N1A	2.62	1.38	1.33
2	A	401	NAD	C2A-N1A	2.60	1.38	1.33
2	E	405	NAD	C2N-N1N	2.56	1.38	1.35
2	F	406	NAD	C2A-N1A	2.44	1.38	1.33
2	E	405	NAD	C2A-N1A	2.40	1.38	1.33
2	E	405	NAD	C2B-C1B	-2.19	1.50	1.53
2	E	405	NAD	PN-O2N	-2.12	1.45	1.55
2	C	403	NAD	C2A-N1A	2.09	1.37	1.33
2	A	401	NAD	C2N-N1N	2.07	1.37	1.35
2	C	403	NAD	C2B-C1B	-2.02	1.50	1.53
2	B	402	NAD	C2N-N1N	2.01	1.37	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	406	NAD	N3A-C2A-N1A	-6.19	119.00	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAD	N3A-C2A-N1A	-5.93	119.42	128.68
2	C	403	NAD	N3A-C2A-N1A	-5.92	119.43	128.68
2	E	405	NAD	N3A-C2A-N1A	-5.90	119.45	128.68
2	D	404	NAD	N3A-C2A-N1A	-5.06	120.77	128.68
2	B	402	NAD	N3A-C2A-N1A	-5.05	120.79	128.68
3	D	301	8PS	C5-O7-C8	3.71	127.25	118.00
2	C	403	NAD	C3N-C7N-N7N	3.58	122.04	117.75
2	D	404	NAD	O4B-C1B-C2B	-3.50	101.81	106.93
2	C	403	NAD	PN-O3-PA	-3.38	121.22	132.83
2	E	405	NAD	O7N-C7N-C3N	-3.33	115.64	119.63
2	E	405	NAD	C3N-C2N-N1N	-3.30	117.20	120.43
2	E	405	NAD	C3N-C7N-N7N	3.12	121.49	117.75
2	D	404	NAD	PN-O3-PA	-3.10	122.18	132.83
2	A	401	NAD	C1B-N9A-C4A	-2.93	121.50	126.64
2	A	401	NAD	PN-O3-PA	-2.92	122.81	132.83
2	F	406	NAD	PN-O3-PA	-2.91	122.83	132.83
2	B	402	NAD	O4B-C1B-C2B	-2.90	102.68	106.93
2	C	403	NAD	C5A-C6A-N6A	-2.87	115.99	120.35
2	B	402	NAD	PN-O3-PA	-2.86	123.03	132.83
2	E	405	NAD	O4B-C1B-C2B	-2.74	102.92	106.93
2	D	404	NAD	C2N-C3N-C4N	2.59	121.20	118.26
2	D	404	NAD	C3N-C7N-N7N	2.57	120.83	117.75
2	D	404	NAD	C4A-C5A-N7A	-2.53	106.77	109.40
2	B	402	NAD	C3N-C7N-N7N	2.52	120.78	117.75
2	C	403	NAD	O4B-C1B-C2B	-2.47	103.31	106.93
2	E	405	NAD	C2N-C3N-C4N	2.44	121.03	118.26
3	C	300	8PS	C3-C2-C1	2.41	121.91	118.54
3	C	300	8PS	C1-C6-C5	-2.40	117.35	119.81
3	D	301	8PS	C3-C2-C1	2.39	121.89	118.54
3	D	301	8PS	C15-C14-C2	-2.24	105.23	113.68
2	D	404	NAD	O7N-C7N-C3N	-2.19	117.01	119.63
2	F	406	NAD	C1B-N9A-C4A	-2.15	122.86	126.64
3	C	300	8PS	C15-C14-C2	-2.13	105.66	113.68
2	B	402	NAD	O2N-PN-O1N	2.12	122.72	112.24
2	E	405	NAD	C5A-C6A-N6A	-2.08	117.20	120.35
2	D	404	NAD	C3N-C2N-N1N	-2.04	118.43	120.43
3	C	300	8PS	C5-O7-C8	2.02	123.05	118.00

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	406	NAD	C5B-O5B-PA-O1A
2	F	406	NAD	C5D-O5D-PN-O3
2	F	406	NAD	O4D-C1D-N1N-C2N
2	E	405	NAD	C5D-O5D-PN-O2N
2	B	402	NAD	C5D-O5D-PN-O1N
2	B	402	NAD	C5D-O5D-PN-O2N
2	B	402	NAD	O4D-C1D-N1N-C2N
2	D	404	NAD	C5B-O5B-PA-O1A
2	D	404	NAD	PN-O3-PA-O5B
2	D	404	NAD	C5D-O5D-PN-O3
2	D	404	NAD	O4D-C1D-N1N-C2N
2	C	403	NAD	C5D-O5D-PN-O1N
2	C	403	NAD	C5D-O5D-PN-O2N
2	C	403	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	C5D-O5D-PN-O3
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
3	D	301	8PS	C2-C14-C15-C16
2	D	404	NAD	O4B-C4B-C5B-O5B
3	D	301	8PS	C16-C17-C18-C19
3	C	300	8PS	C16-C17-C18-C19
2	F	406	NAD	PN-O3-PA-O5B
2	A	401	NAD	PN-O3-PA-O5B
2	F	406	NAD	O4B-C4B-C5B-O5B
2	F	406	NAD	C5B-O5B-PA-O3
2	E	405	NAD	C5D-O5D-PN-O3
2	D	404	NAD	C5B-O5B-PA-O3
2	F	406	NAD	C5B-O5B-PA-O2A
2	F	406	NAD	C5D-O5D-PN-O1N
2	E	405	NAD	C5D-O5D-PN-O1N
2	D	404	NAD	C5B-O5B-PA-O2A
2	D	404	NAD	C5D-O5D-PN-O1N
2	A	401	NAD	C5D-O5D-PN-O1N
2	D	404	NAD	C3B-C4B-C5B-O5B
2	C	403	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	O4B-C4B-C5B-O5B
2	E	405	NAD	PA-O3-PN-O1N
2	B	402	NAD	PA-O3-PN-O2N
2	B	402	NAD	C5D-O5D-PN-O3
2	C	403	NAD	C5D-O5D-PN-O3
2	F	406	NAD	C3B-C4B-C5B-O5B
2	E	405	NAD	O4B-C4B-C5B-O5B
2	E	405	NAD	PA-O3-PN-O2N

Continued on next page...

Continued from previous page...

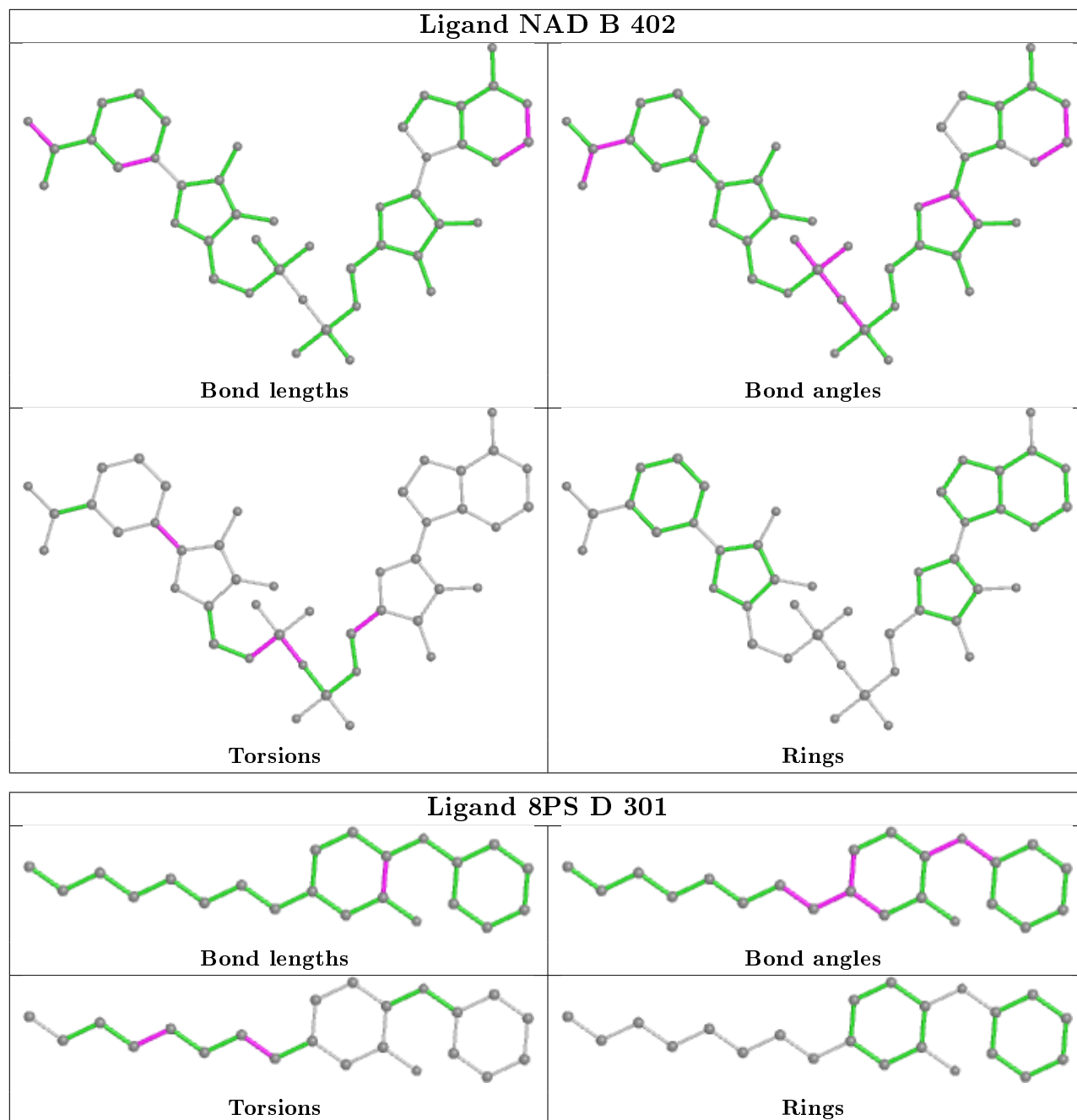
Mol	Chain	Res	Type	Atoms
2	C	403	NAD	PA-O3-PN-O2N
2	B	402	NAD	O4B-C4B-C5B-O5B

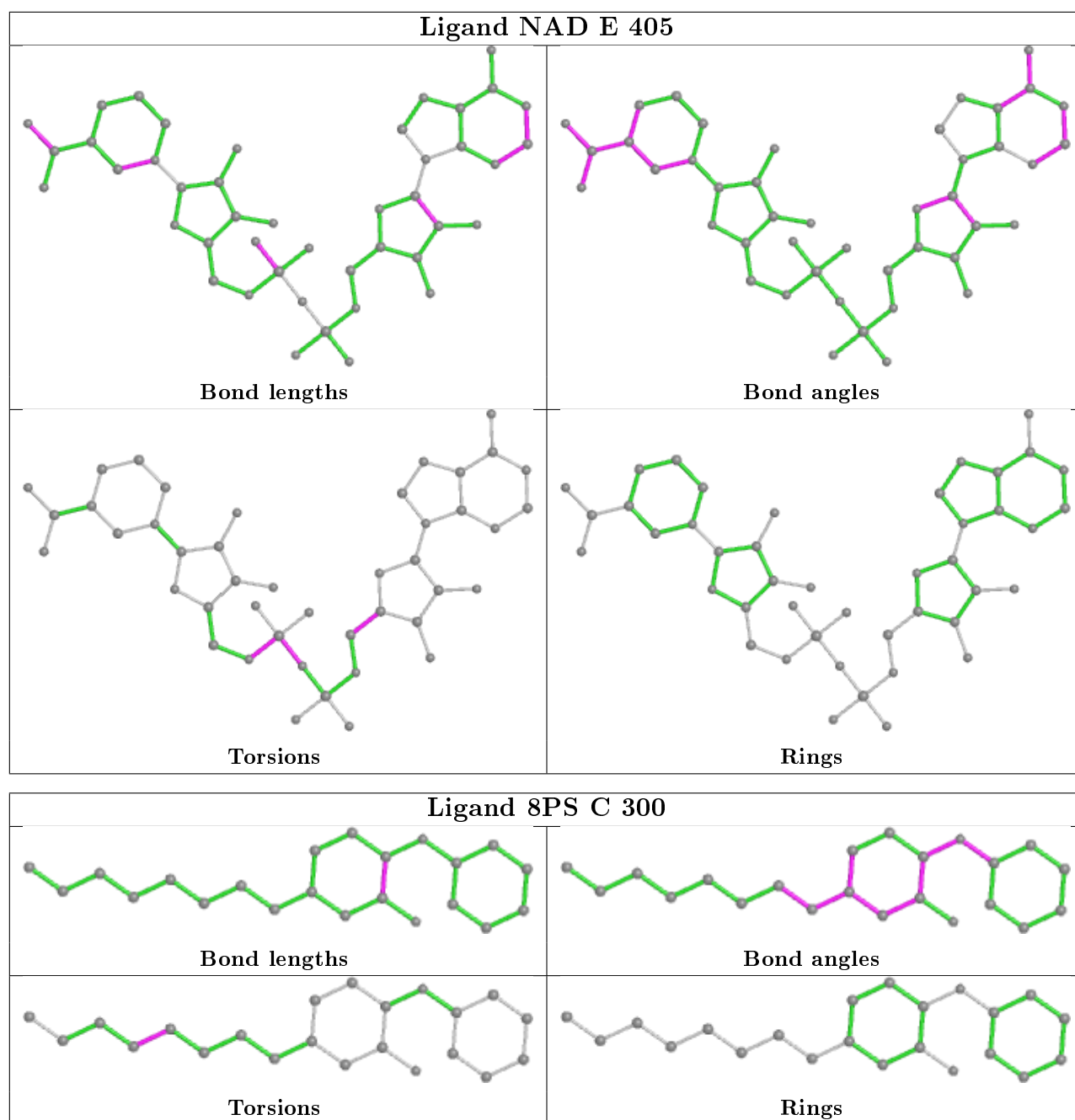
There are no ring outliers.

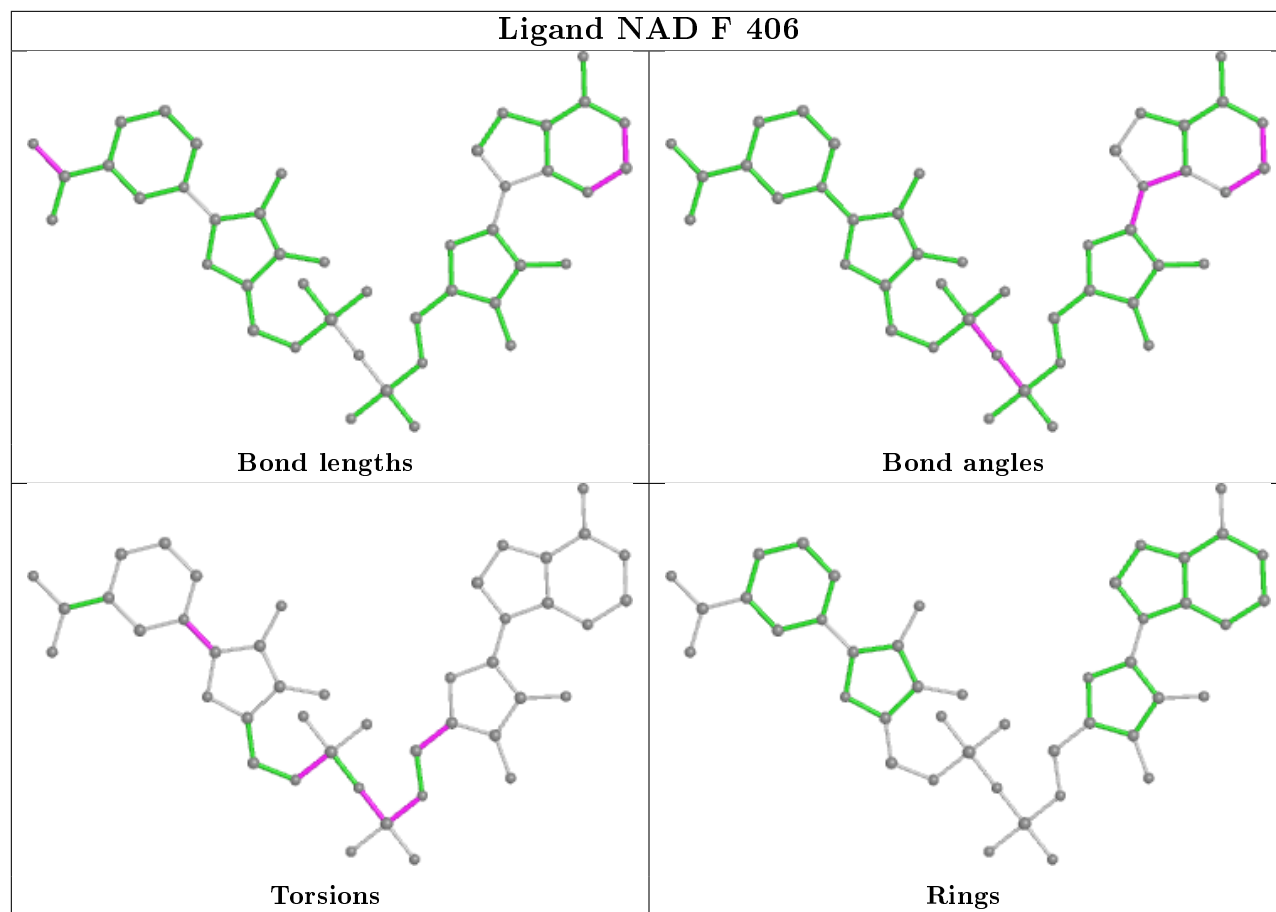
8 monomers are involved in 25 short contacts:

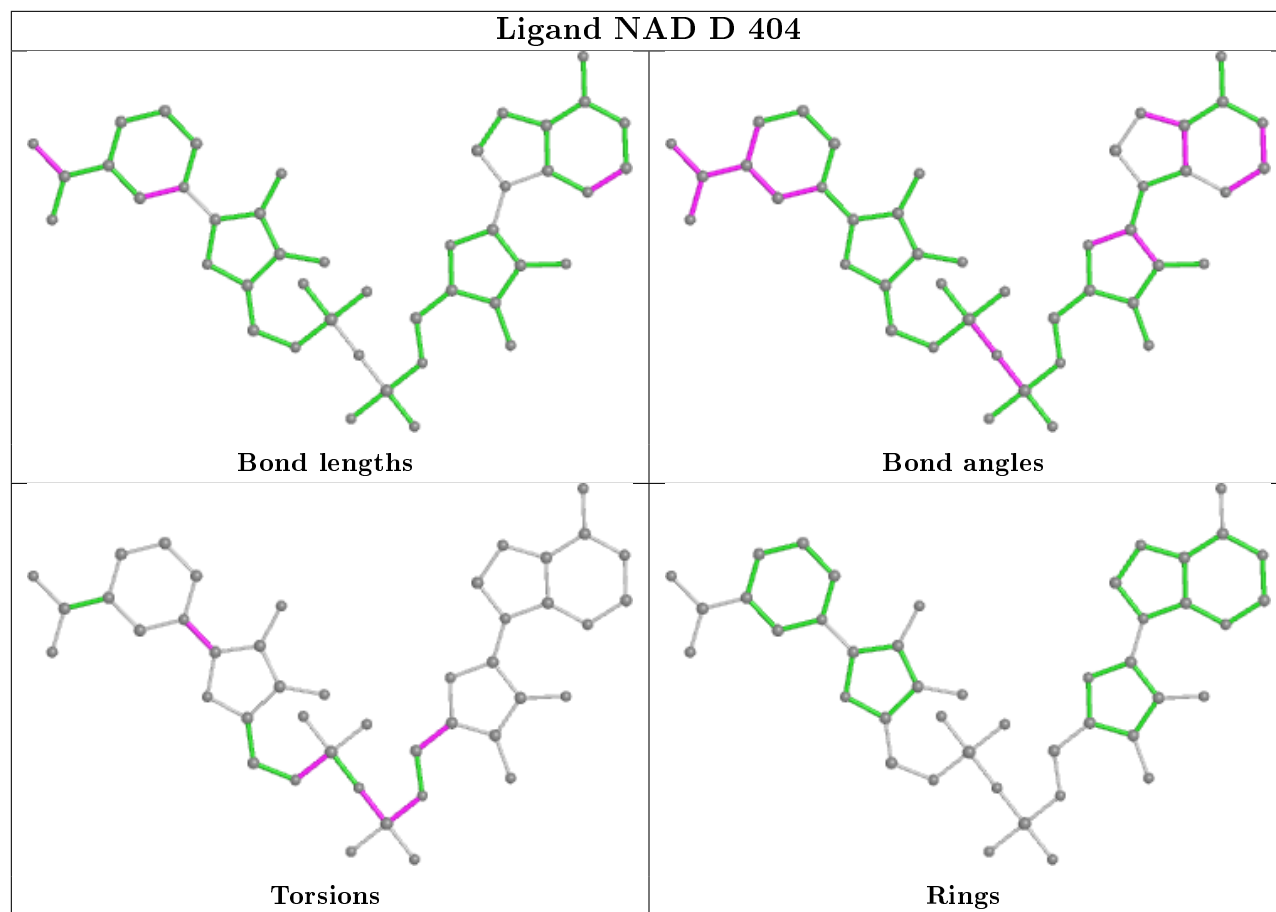
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	NAD	1	0
3	D	301	8PS	7	0
2	E	405	NAD	4	0
3	C	300	8PS	3	0
2	F	406	NAD	2	0
2	D	404	NAD	5	0
2	C	403	NAD	2	0
2	A	401	NAD	1	0

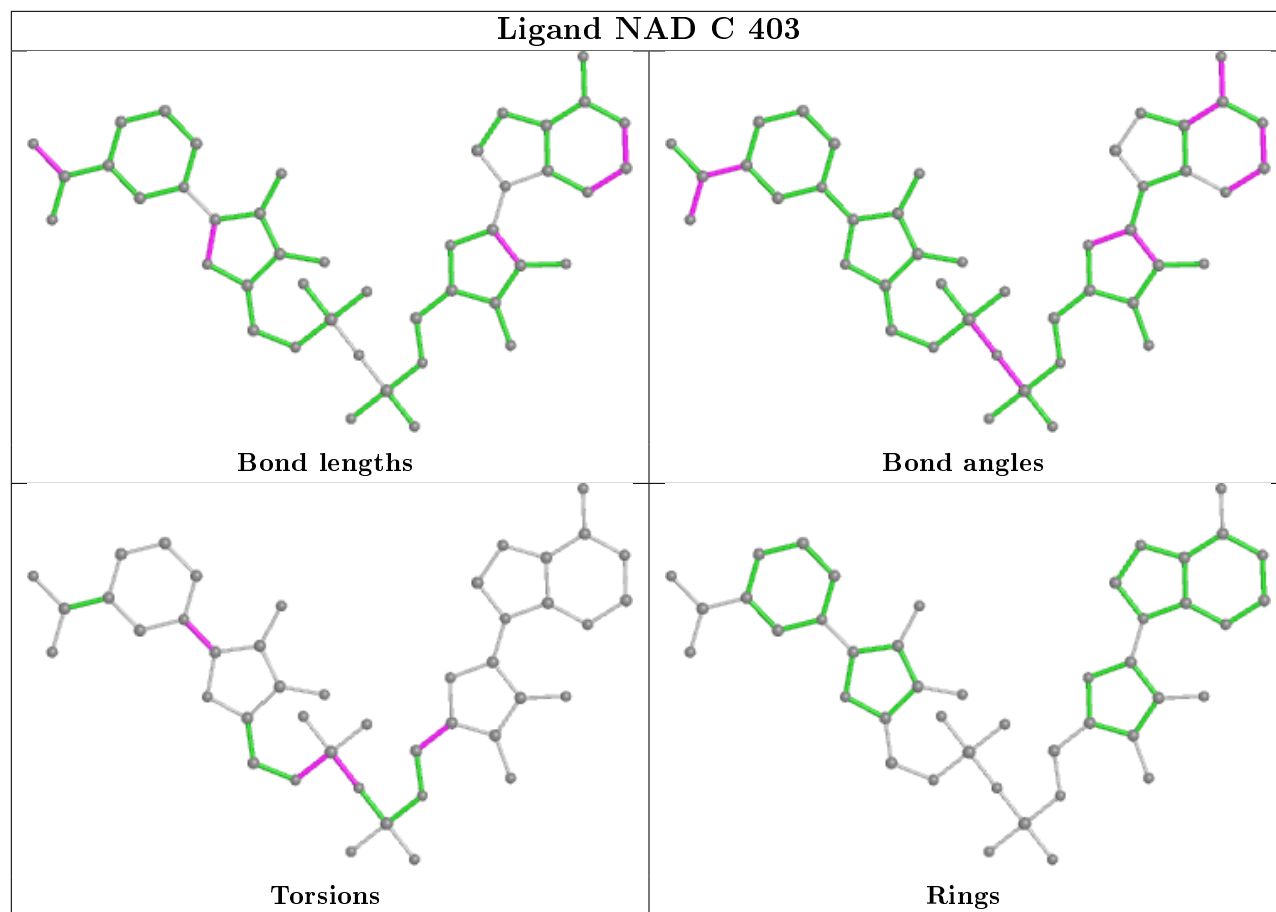
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

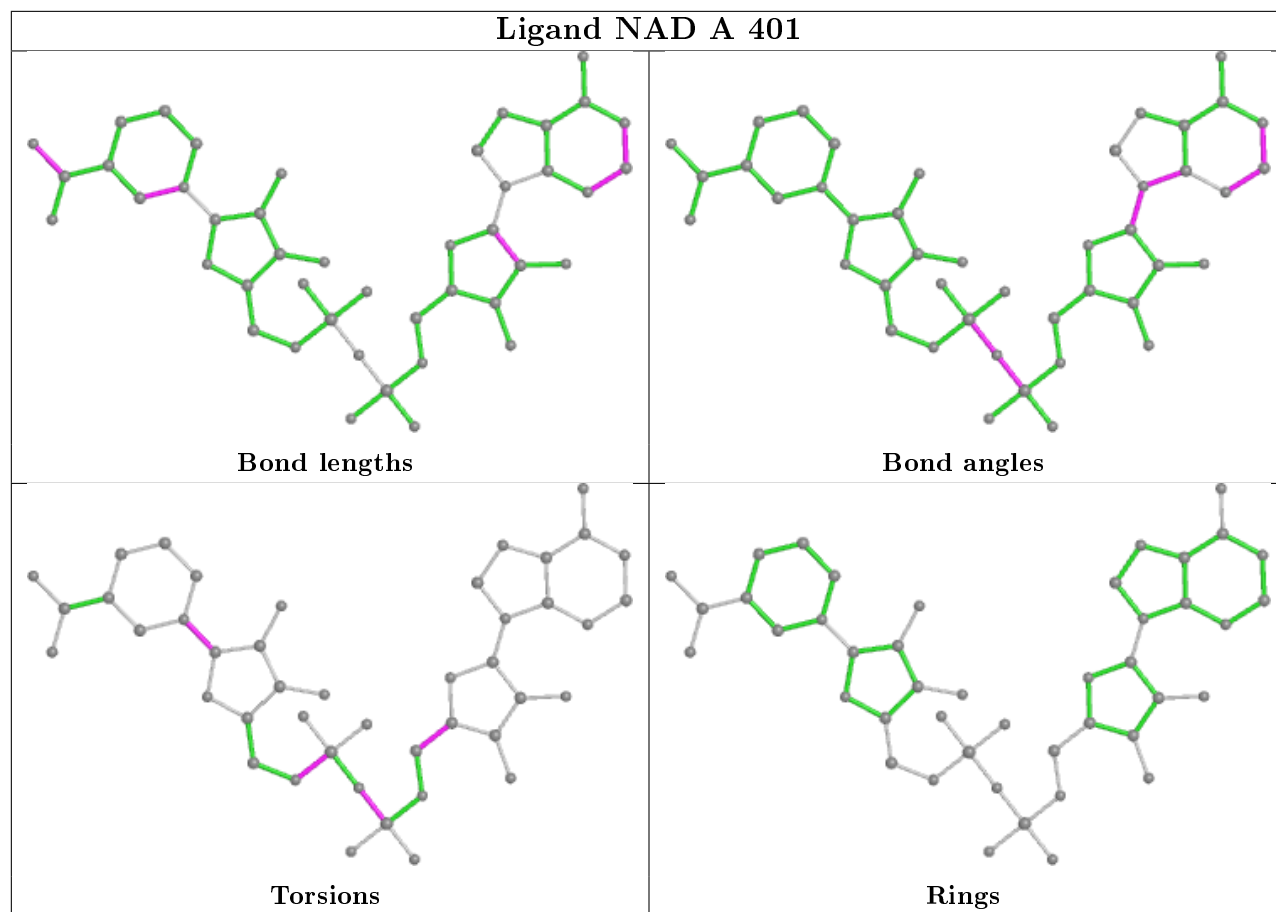












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	248/269 (92%)	0.17	10 (4%) 38 31	28, 44, 66, 77	0
1	B	245/269 (91%)	0.48	17 (6%) 16 12	32, 51, 78, 91	0
1	C	260/269 (96%)	-0.24	3 (1%) 79 76	9, 25, 54, 66	0
1	D	260/269 (96%)	-0.18	4 (1%) 73 70	9, 24, 58, 70	0
1	E	260/269 (96%)	0.19	18 (6%) 16 12	25, 39, 63, 73	0
1	F	248/269 (92%)	0.34	17 (6%) 16 12	25, 44, 64, 76	0
All	All	1521/1614 (94%)	0.12	69 (4%) 33 26	9, 39, 65, 91	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	ARG	4.9
1	A	218	LEU	4.2
1	B	80	GLU	4.2
1	A	46	LEU	4.1
1	B	56	ALA	3.8
1	E	83	GLY	3.7
1	F	85	GLY	3.7
1	E	208	GLY	3.6
1	E	2	THR	3.6
1	A	84	ALA	3.5
1	C	219	GLU	3.5
1	F	57	LYS	3.5
1	E	213	ALA	3.4
1	F	86	ASN	3.4
1	B	195	ARG	3.3
1	F	105	ILE	3.2
1	F	104	GLY	3.2
1	F	2	THR	3.2
1	E	217	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	84	ALA	3.1
1	B	57	LYS	3.0
1	C	215	ILE	2.9
1	B	137	ILE	2.9
1	C	2	THR	2.9
1	B	53	ARG	2.9
1	D	45	ARG	2.9
1	A	2	THR	2.8
1	B	105	ILE	2.8
1	B	76	GLY	2.8
1	B	99	PRO	2.8
1	E	212	GLY	2.8
1	A	195	ARG	2.7
1	F	140	PRO	2.7
1	D	49	ARG	2.6
1	E	84	ALA	2.6
1	E	220	GLU	2.6
1	E	269	LEU	2.6
1	E	41	PHE	2.5
1	F	56	ALA	2.5
1	F	83	GLY	2.5
1	E	74	LEU	2.5
1	B	81	ALA	2.4
1	F	197	LEU	2.4
1	B	220	GLU	2.4
1	B	103	MET	2.4
1	F	158	TYR	2.4
1	A	53	ARG	2.4
1	F	55	PRO	2.4
1	F	53	ARG	2.3
1	B	83	GLY	2.3
1	A	45	ARG	2.3
1	D	43	ARG	2.3
1	D	214	GLN	2.3
1	B	18	ASP	2.3
1	E	214	GLN	2.2
1	A	72	ALA	2.2
1	A	57	LYS	2.2
1	F	106	ASN	2.2
1	B	248	ASP	2.2
1	E	85	GLY	2.2
1	E	86	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	215	ILE	2.1
1	E	211	ALA	2.1
1	F	257	ILE	2.1
1	E	72	ALA	2.1
1	F	84	ALA	2.0
1	A	85	GLY	2.0
1	E	210	GLU	2.0
1	F	45	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](#)

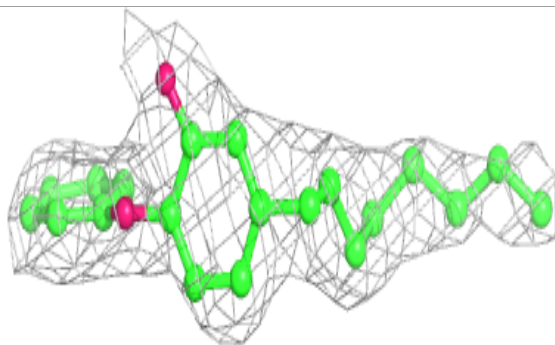
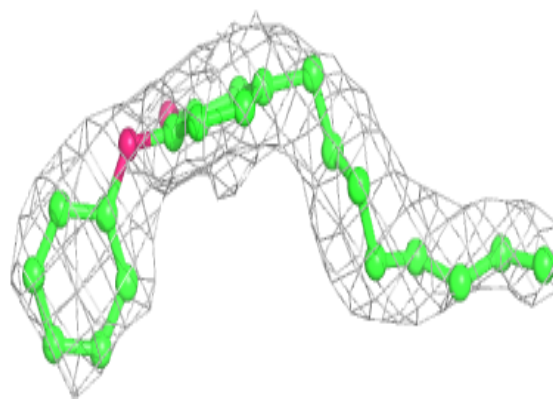
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	8PS	D	301	22/22	0.89	0.21	36,39,43,44	0
2	NAD	B	402	44/44	0.90	0.19	45,53,55,56	0
3	8PS	C	300	22/22	0.93	0.16	34,35,37,38	0
2	NAD	F	406	44/44	0.93	0.15	24,46,55,55	0
2	NAD	A	401	44/44	0.93	0.15	38,42,44,44	0
2	NAD	D	404	44/44	0.96	0.13	15,26,31,35	0
2	NAD	C	403	44/44	0.96	0.15	22,27,33,34	0
2	NAD	E	405	44/44	0.96	0.12	29,36,40,41	0

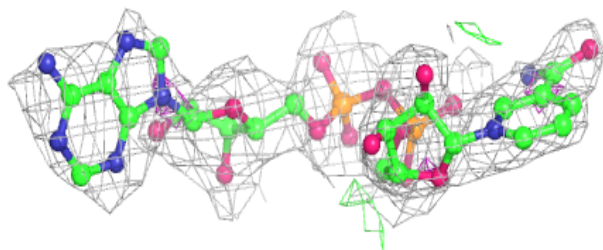
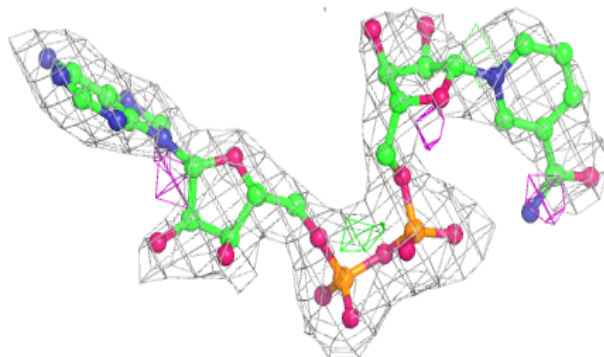
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8PS D 301:

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

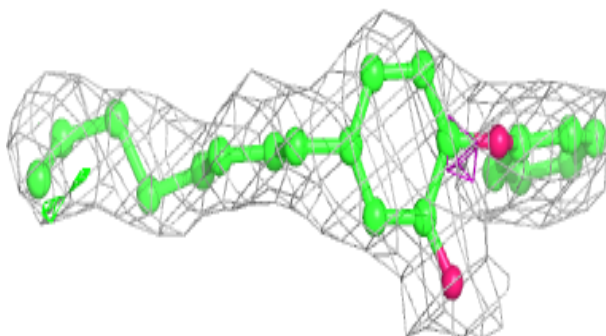
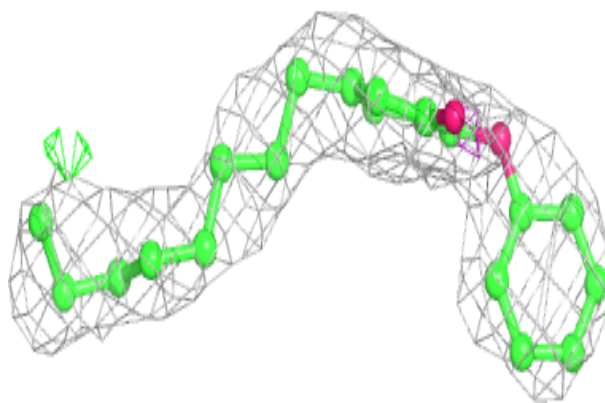
**Electron density around NAD B 402:**

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

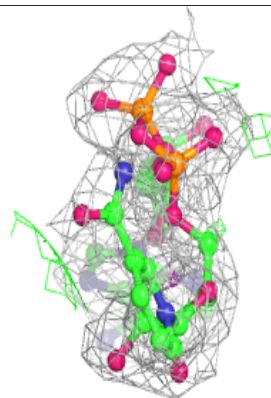
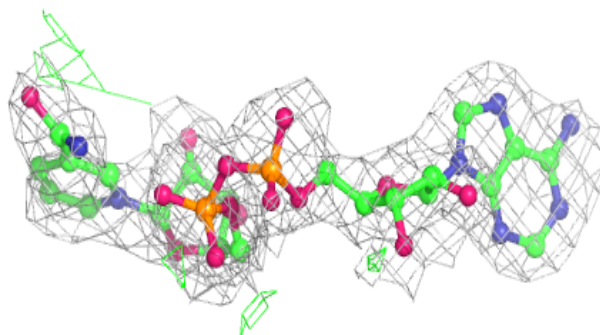
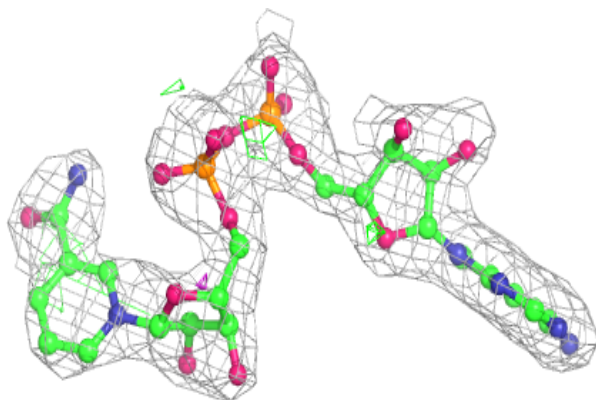


Electron density around 8PS C 300:

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

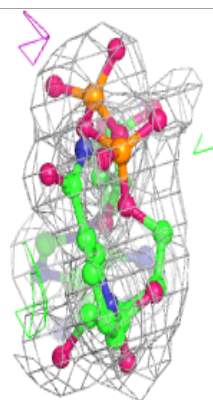
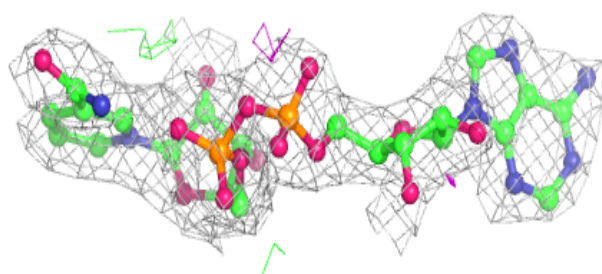
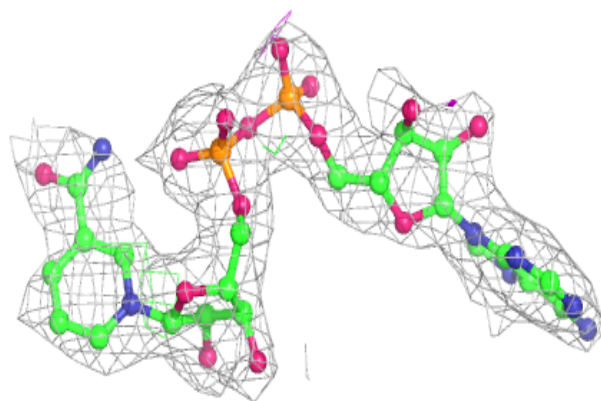
**Electron density around NAD F 406:**

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

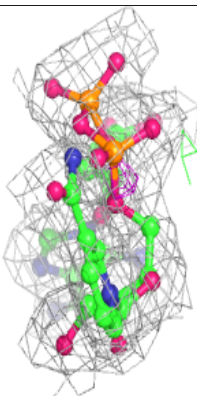
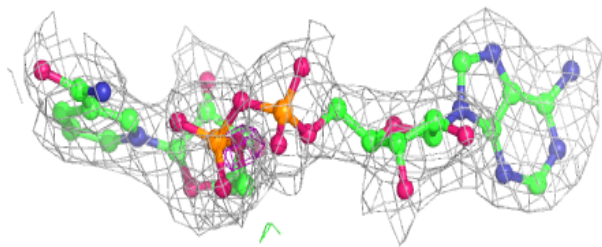
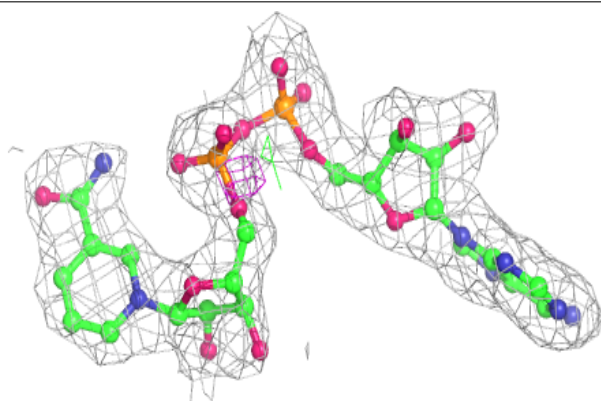


Electron density around NAD A 401:

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

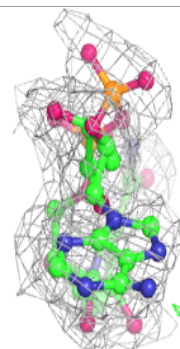
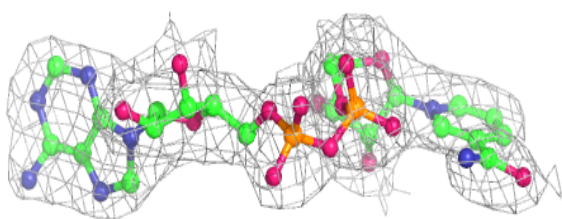
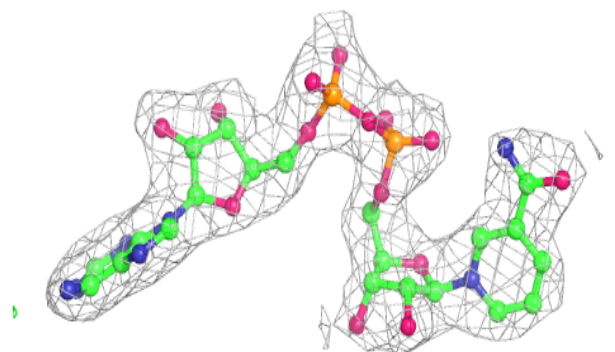
**Electron density around NAD D 404:**

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

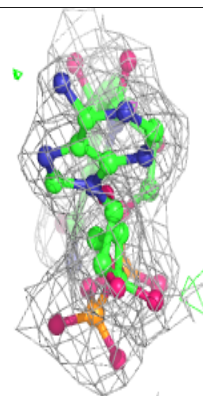
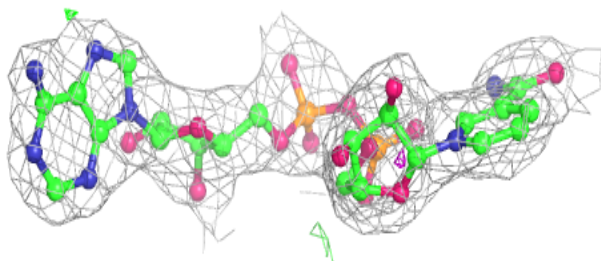
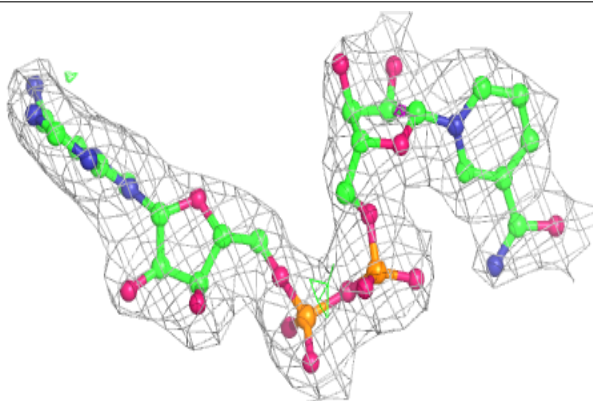


Electron density around NAD C 403:

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

**Electron density around NAD E 405:**

$2mF_o-DF_c$ (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.