



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:32 AM UTC

PDB ID : 2B36 / pdb_00002b36
Title : Crystal structure of Mycobacterium tuberculosis enoyl reductase (InhA) inhibited by 5-pentyl-2-phenoxyphenol
Authors : Sullivan, T.J.; Truglio, J.J.; Novichenok, P.; Stratton, C.; Zhang, X.; Kaur, T.; Johnson, F.; Boyne, M.S.; Amin, A.
Deposited on : 2005-09-19
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

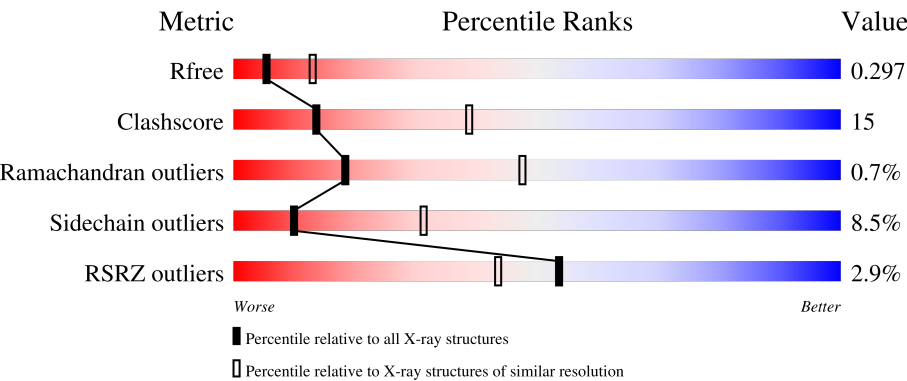
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	269	4% 67% 29% .
1	B	269	% 70% 22% . .
1	C	269	% 65% 23% . 8%
1	D	269	6% 62% 27% . 8%

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Mol	Chain	Length	Quality of chain
1	E	269	% 61% 29% • 6%
1	F	269	4% 62% 26% 5% 7%

2 Entry composition [i](#)

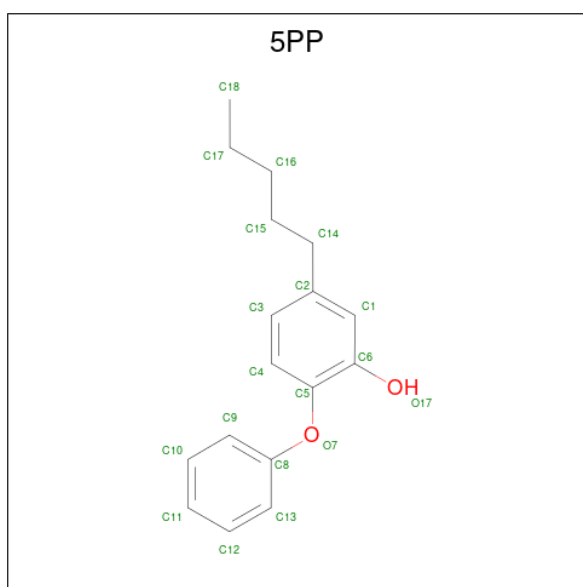
There are 3 unique types of molecules in this entry. The entry contains 11841 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

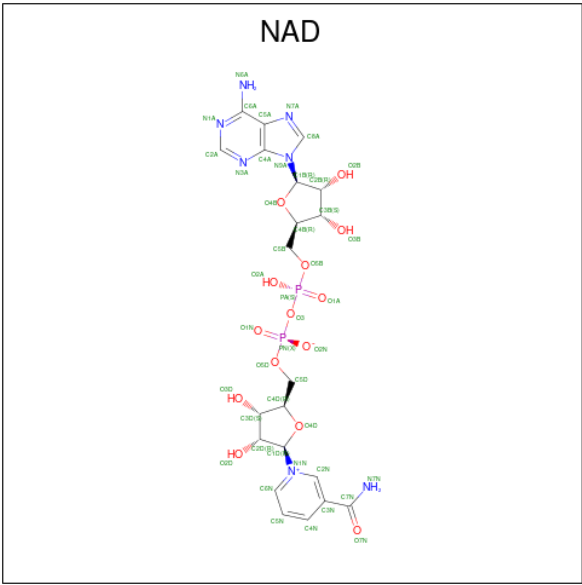
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			1996	1264	348	374	10			
1	B	259	Total	C	N	O	S	0	0	0
			1941	1229	339	364	9			
1	C	248	Total	C	N	O	S	0	0	0
			1866	1184	326	347	9			
1	D	248	Total	C	N	O	S	0	0	0
			1862	1181	326	345	10			
1	E	254	Total	C	N	O	S	0	0	0
			1906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

- Molecule 2 is 5-PENTYL-2-PHENOXYPHENOL (CCD ID: 5PP) (formula: C₁₇H₂₀O₂).



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

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



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

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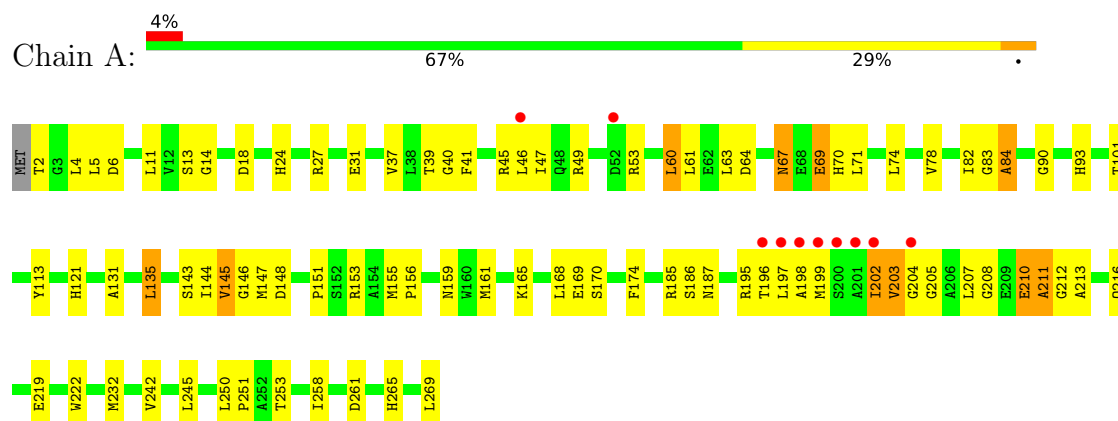
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

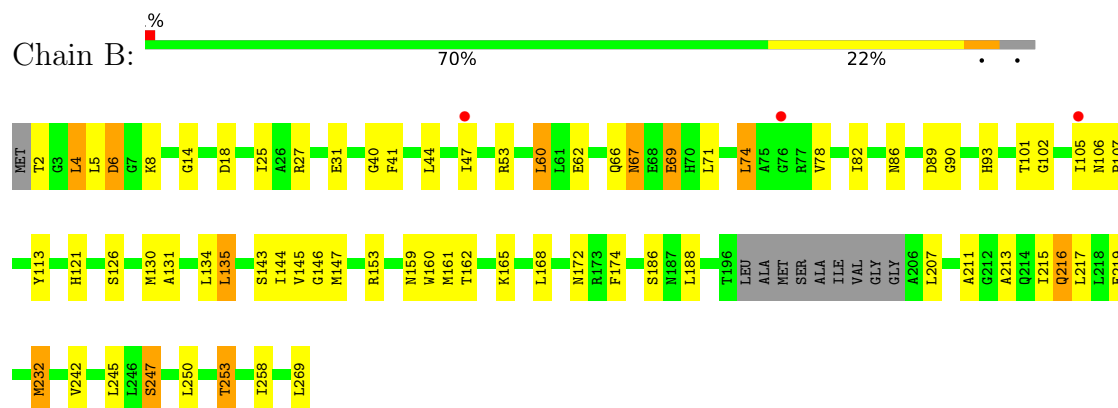
3 Residue-property plots

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

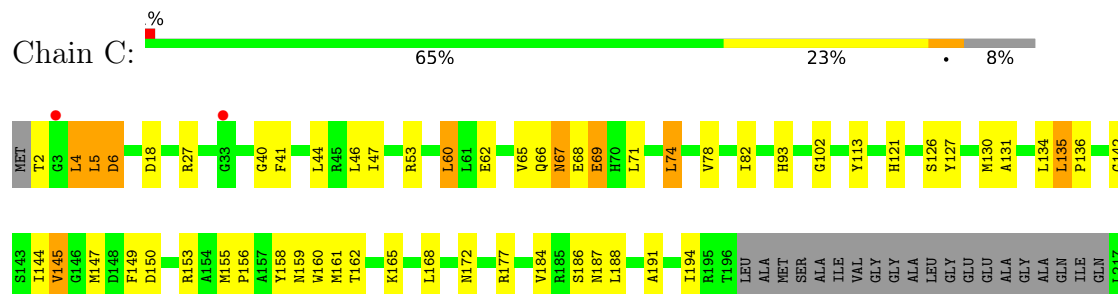
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

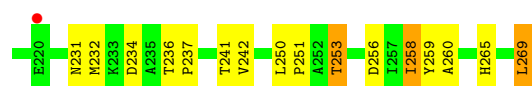


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

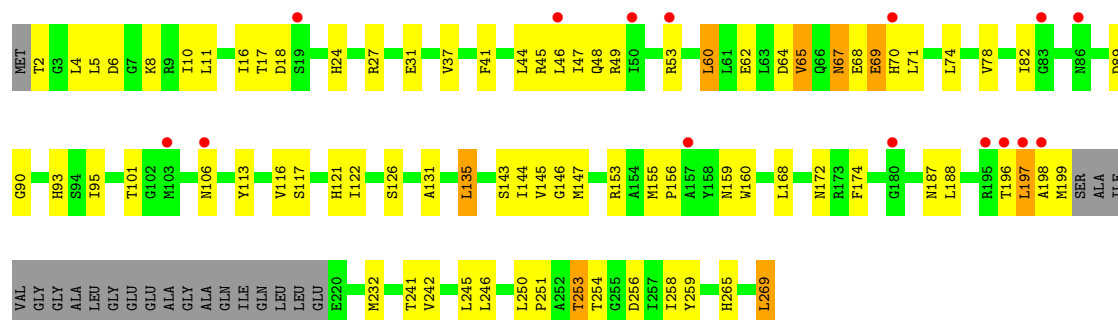


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

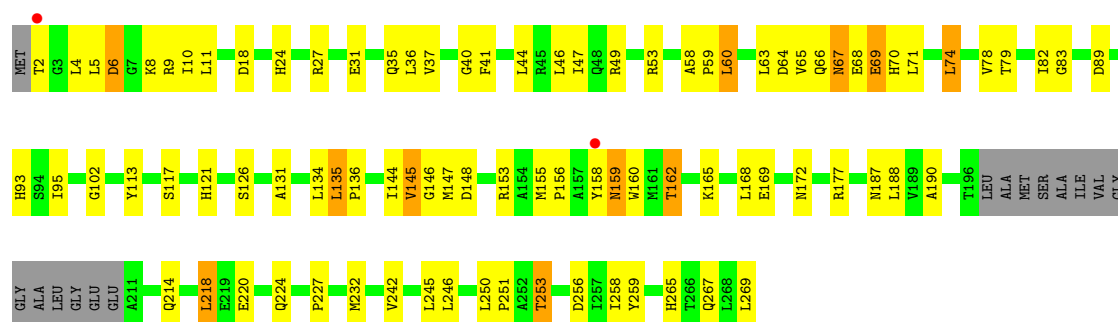




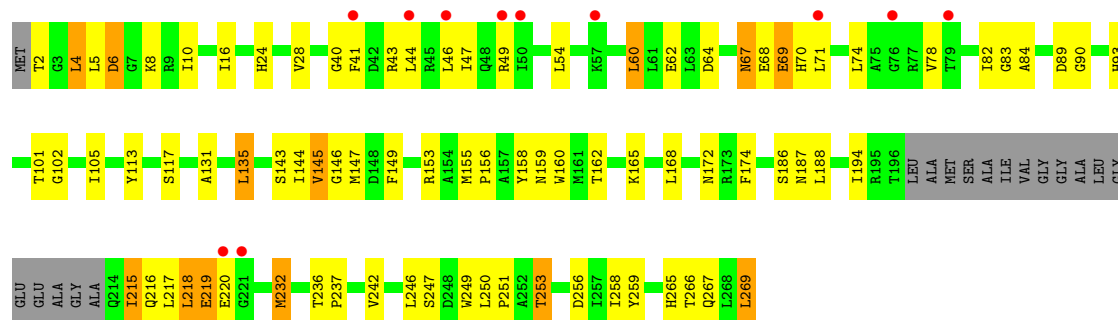
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



- 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 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.95Å 81.83Å 188.66Å 90.00° 95.69° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (10.00-2.80) 96.2 (10.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.03 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.242 , 0.295 0.250 , 0.297	Depositor DCC
R_{free} test set	1929 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	11841	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 5PP, 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	1.12	2/2034 (0.1%)	0.96	1/2761 (0.0%)
1	B	1.10	1/1978 (0.1%)	0.99	1/2684 (0.0%)
1	C	0.91	0/1903	0.93	1/2583 (0.0%)
1	D	0.92	0/1899	0.93	1/2577 (0.0%)
1	E	0.89	0/1943	0.90	0/2637
1	F	0.95	0/1929	0.91	2/2618 (0.1%)
All	All	0.99	3/11686 (0.0%)	0.94	6/15860 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	PRO	N-CA	-6.75	1.42	1.47
1	A	13	SER	CA-C	-5.73	1.45	1.53
1	B	126	SER	C-O	-5.64	1.16	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	ILE	N-CA-C	-7.05	103.90	110.53
1	D	198	ALA	N-CA-C	-6.40	105.77	112.93
1	A	170	SER	N-CA-C	-5.76	104.37	111.40
1	F	54	LEU	CA-C-N	5.34	126.52	119.84
1	F	54	LEU	C-N-CA	5.34	126.52	119.84
1	C	27	ARG	N-CA-C	-5.28	105.22	110.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1996	0	2013	60	1
1	B	1941	0	1951	49	0
1	C	1866	0	1880	66	0
1	D	1862	0	1877	65	0
1	E	1906	0	1920	69	0
1	F	1892	0	1907	78	0
2	A	19	0	19	0	0
2	B	19	0	19	0	0
2	C	19	0	19	0	0
2	D	19	0	19	0	0
2	E	19	0	19	0	0
2	F	19	0	19	0	0
3	A	44	0	26	4	0
3	B	44	0	26	1	0
3	C	44	0	26	1	0
3	D	44	0	26	1	0
3	E	44	0	26	0	0
3	F	44	0	26	3	0
All	All	11841	0	11818	346	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (346) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HG2	1:C:136:PRO:HB3	1.59	0.84
1:D:2:THR:HB	1:D:6:ASP:OD2	1.82	0.80
1:D:101:THR:O	1:D:106:ASN:ND2	2.16	0.79
1:A:2:THR:HB	1:A:6:ASP:OD2	1.81	0.78
1:C:265:HIS:O	1:E:153:ARG:NH1	2.20	0.75
1:B:27:ARG:HG2	1:B:31:GLU:OE2	1.87	0.73
1:E:47:ILE:HD11	1:E:60:LEU:HD21	1.73	0.71
1:E:2:THR:HB	1:E:6:ASP:OD2	1.90	0.71
1:E:156:PRO:HG3	1:E:214:GLN:HE21	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:ARG:NE	1:F:153:ARG:HH21	1.89	0.70
1:C:2:THR:HB	1:C:6:ASP:OD2	1.91	0.70
1:E:78:VAL:O	1:E:82:ILE:HG12	1.92	0.69
1:F:219:GLU:HB2	1:F:232:MET:HE3	1.77	0.67
1:B:131:ALA:O	1:B:135:LEU:HB2	1.93	0.66
1:D:253:THR:HB	1:E:259:TYR:O	1.95	0.66
1:C:153:ARG:HH21	1:E:153:ARG:NE	1.93	0.65
1:A:202:ILE:HG22	1:A:207:LEU:HD13	1.78	0.65
1:B:67:ASN:HD22	1:B:67:ASN:C	2.05	0.65
1:C:153:ARG:NH1	1:E:265:HIS:O	2.31	0.64
1:B:2:THR:HB	1:B:6:ASP:OD2	1.98	0.63
1:B:213:ALA:O	1:B:217:LEU:HB2	1.97	0.63
1:B:215:ILE:HG22	1:B:216:GLN:OE1	1.97	0.63
1:C:153:ARG:NE	1:E:153:ARG:HH21	1.96	0.63
1:C:67:ASN:C	1:C:67:ASN:HD22	2.05	0.63
1:D:47:ILE:HG13	1:D:60:LEU:HD11	1.80	0.63
1:C:259:TYR:O	1:F:253:THR:HB	1.98	0.63
1:F:194:ILE:HB	3:F:306:NAD:N7N	2.13	0.63
1:C:145:VAL:HA	1:C:187:ASN:O	1.99	0.63
1:F:67:ASN:C	1:F:67:ASN:HD22	2.07	0.62
1:D:153:ARG:HH21	1:F:153:ARG:CZ	2.12	0.62
1:A:27:ARG:HG2	1:A:31:GLU:OE2	1.99	0.62
1:E:47:ILE:HG13	1:E:60:LEU:HD11	1.81	0.62
1:A:113:TYR:CE2	1:B:121:HIS:HB2	2.35	0.62
1:A:147:MET:HE1	1:A:242:VAL:HG22	1.80	0.62
1:A:196:THR:O	1:A:197:LEU:HD22	1.99	0.62
1:D:47:ILE:HD11	1:D:60:LEU:HD21	1.82	0.61
1:F:44:LEU:HD23	1:F:47:ILE:HD11	1.83	0.61
1:A:64:ASP:H	1:A:70:HIS:CD2	2.19	0.60
1:C:47:ILE:HG13	1:C:60:LEU:HD11	1.83	0.60
1:A:131:ALA:O	1:A:135:LEU:HB2	2.01	0.60
1:D:78:VAL:O	1:D:82:ILE:HG12	2.01	0.60
1:B:219:GLU:HG2	1:B:232:MET:HE3	1.84	0.60
1:E:65:VAL:HB	1:E:126:SER:HB2	1.83	0.60
1:A:203:VAL:HG23	1:A:204:GLY:H	1.65	0.59
1:A:78:VAL:O	1:A:82:ILE:HG12	2.02	0.59
1:B:47:ILE:HD11	1:B:60:LEU:HD21	1.85	0.59
1:A:11:LEU:HA	1:A:37:VAL:O	2.03	0.59
1:C:131:ALA:O	1:C:135:LEU:HB2	2.02	0.59
1:C:78:VAL:O	1:C:82:ILE:HG12	2.01	0.58
1:A:147:MET:HE1	1:A:242:VAL:CG2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HD11	1:A:60:LEU:HD21	1.86	0.58
1:C:153:ARG:CZ	1:E:153:ARG:HH21	2.16	0.58
1:E:131:ALA:O	1:E:135:LEU:HB2	2.04	0.58
1:D:258:ILE:N	1:D:258:ILE:HD12	2.18	0.58
1:D:67:ASN:C	1:D:67:ASN:HD22	2.12	0.57
1:F:135:LEU:HD13	1:F:144:ILE:HD11	1.86	0.57
1:D:10:ILE:HD13	1:D:246:LEU:HD13	1.85	0.57
1:D:67:ASN:ND2	1:D:69:GLU:H	2.02	0.57
1:B:153:ARG:HH11	1:B:153:ARG:HG2	1.70	0.57
1:A:195:ARG:HD3	1:A:199:MET:HE2	1.86	0.57
1:D:153:ARG:NH1	1:F:265:HIS:O	2.37	0.57
1:A:67:ASN:C	1:A:67:ASN:HD22	2.13	0.56
1:C:253:THR:HB	1:F:259:TYR:O	2.05	0.56
1:D:147:MET:HE1	1:D:242:VAL:CG2	2.35	0.56
1:C:153:ARG:HH21	1:E:153:ARG:CZ	2.18	0.56
1:D:172:ASN:CG	1:D:188:LEU:HD13	2.30	0.56
1:E:147:MET:HE1	1:E:242:VAL:HG22	1.87	0.56
1:F:147:MET:HE1	1:F:242:VAL:CG2	2.36	0.56
1:B:78:VAL:O	1:B:82:ILE:HG12	2.05	0.55
1:F:215:ILE:HA	1:F:218:LEU:HD21	1.88	0.55
1:D:113:TYR:CE2	1:D:117:SER:HB2	2.41	0.55
1:D:153:ARG:HH21	1:F:153:ARG:NE	2.04	0.55
1:A:47:ILE:HG13	1:A:60:LEU:HD11	1.88	0.55
1:B:40:GLY:HA3	1:B:47:ILE:CD1	2.36	0.55
1:C:256:ASP:OD2	1:F:259:TYR:HB2	2.07	0.55
1:C:47:ILE:HD11	1:C:60:LEU:HD21	1.90	0.54
1:D:196:THR:HG22	1:D:197:LEU:HG	1.90	0.54
1:A:202:ILE:HD12	1:A:202:ILE:C	2.33	0.54
1:D:241:THR:O	1:D:245:LEU:HD23	2.08	0.54
1:F:131:ALA:O	1:F:135:LEU:HB2	2.08	0.53
1:F:258:ILE:N	1:F:258:ILE:HD12	2.22	0.53
1:B:207:LEU:HD22	1:B:211:ALA:HB2	1.89	0.53
1:B:105:ILE:HB	1:B:207:LEU:CD2	2.39	0.53
1:C:44:LEU:HD11	1:C:62:GLU:HB2	1.91	0.53
1:C:147:MET:HE1	1:C:242:VAL:HG22	1.91	0.53
1:F:44:LEU:HA	1:F:47:ILE:HG12	1.91	0.53
1:E:135:LEU:HD13	1:E:144:ILE:HD11	1.90	0.53
1:D:259:TYR:O	1:E:253:THR:HB	2.09	0.53
1:D:64:ASP:H	1:D:70:HIS:CD2	2.27	0.53
1:A:46:LEU:HA	1:A:49:ARG:HH12	1.74	0.52
1:D:67:ASN:HD21	1:D:69:GLU:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:LEU:C	1:F:220:GLU:H	2.17	0.52
1:D:27:ARG:HG2	1:D:31:GLU:OE2	2.10	0.52
1:E:67:ASN:C	1:E:67:ASN:HD22	2.18	0.52
1:B:67:ASN:HD21	1:B:69:GLU:HB2	1.74	0.52
1:F:144:ILE:O	1:F:186:SER:HA	2.10	0.52
1:A:174:PHE:CE2	1:B:159:ASN:HA	2.45	0.52
1:B:47:ILE:HG13	1:B:60:LEU:HD11	1.91	0.52
1:D:131:ALA:O	1:D:135:LEU:HB2	2.09	0.52
1:F:218:LEU:C	1:F:220:GLU:N	2.65	0.52
1:D:18:ASP:HB3	1:D:53:ARG:HH21	1.76	0.51
1:A:211:ALA:O	1:A:213:ALA:N	2.44	0.51
1:F:153:ARG:HG2	1:F:153:ARG:HH11	1.76	0.51
1:C:191:ALA:HA	1:C:260:ALA:O	2.11	0.51
1:C:67:ASN:ND2	1:C:69:GLU:H	2.09	0.51
1:E:64:ASP:H	1:E:70:HIS:CD2	2.29	0.51
1:B:67:ASN:ND2	1:B:69:GLU:H	2.08	0.51
1:A:45:ARG:CG	1:C:136:PRO:HB3	2.36	0.51
1:A:93:HIS:O	1:A:146:GLY:HA2	2.11	0.51
1:C:161:MET:HE3	1:C:165:LYS:HE2	1.92	0.51
1:D:46:LEU:HA	1:D:49:ARG:HH12	1.75	0.50
1:D:67:ASN:ND2	1:D:69:GLU:N	2.59	0.50
1:D:259:TYR:HB2	1:E:256:ASP:OD2	2.11	0.50
1:A:198:ALA:O	1:A:202:ILE:HG23	2.10	0.50
1:A:14:GLY:O	3:A:301:NAD:O3B	2.30	0.50
1:B:161:MET:HE3	1:B:165:LYS:HE2	1.94	0.50
1:B:41:PHE:CD1	1:B:41:PHE:C	2.90	0.50
1:F:47:ILE:HG13	1:F:60:LEU:HD11	1.93	0.50
1:B:40:GLY:HA3	1:B:47:ILE:HD13	1.93	0.50
1:C:46:LEU:O	1:C:46:LEU:HD23	2.12	0.50
1:C:153:ARG:NH2	1:E:153:ARG:NH2	2.60	0.50
1:D:122:ILE:HD13	3:D:304:NAD:H61A	1.75	0.50
1:B:172:ASN:CG	1:B:188:LEU:HD13	2.37	0.50
1:F:40:GLY:HA3	1:F:47:ILE:CD1	2.41	0.50
1:F:47:ILE:HD11	1:F:60:LEU:HD21	1.94	0.50
1:C:147:MET:HE1	1:C:242:VAL:CG2	2.41	0.49
1:C:236:THR:HB	1:C:237:PRO:HD3	1.94	0.49
1:F:93:HIS:O	1:F:146:GLY:HA2	2.11	0.49
1:F:165:LYS:NZ	3:F:306:NAD:O2D	2.38	0.49
1:B:219:GLU:OE2	1:B:232:MET:CB	2.60	0.49
1:F:147:MET:HE1	1:F:242:VAL:HG22	1.93	0.49
1:A:148:ASP:OD2	1:A:169:GLU:OE2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:HIS:HB2	1:B:113:TYR:CE2	2.48	0.49
1:C:258:ILE:N	1:C:258:ILE:HD12	2.27	0.49
1:E:24:HIS:CD2	1:E:27:ARG:HH21	2.31	0.49
1:C:241:THR:HG23	1:F:250:LEU:HD23	1.95	0.49
1:F:67:ASN:HD22	1:F:68:GLU:N	2.10	0.49
1:E:102:GLY:O	1:E:160:TRP:HB2	2.13	0.49
1:B:258:ILE:HD12	1:B:258:ILE:N	2.28	0.48
1:D:135:LEU:HD13	1:D:144:ILE:HD11	1.94	0.48
1:D:147:MET:HE1	1:D:242:VAL:HG22	1.95	0.48
1:E:40:GLY:HA3	1:E:47:ILE:CD1	2.43	0.48
1:E:250:LEU:N	1:E:251:PRO:CD	2.76	0.48
1:B:67:ASN:C	1:B:67:ASN:ND2	2.71	0.48
1:F:155:MET:HB2	1:F:156:PRO:HD2	1.93	0.48
1:A:41:PHE:CD1	1:A:41:PHE:C	2.90	0.48
1:E:11:LEU:HA	1:E:37:VAL:O	2.13	0.48
1:F:145:VAL:HA	1:F:187:ASN:O	2.12	0.48
1:F:236:THR:HB	1:F:237:PRO:HD3	1.94	0.48
1:D:67:ASN:HD22	1:D:69:GLU:N	2.10	0.48
1:A:258:ILE:N	1:A:258:ILE:HD12	2.29	0.48
1:B:67:ASN:HD22	1:B:69:GLU:N	2.12	0.48
1:C:67:ASN:HD21	1:C:69:GLU:HB2	1.77	0.48
1:E:159:ASN:HA	1:F:174:PHE:CE2	2.49	0.48
1:B:14:GLY:O	3:B:302:NAD:O3B	2.27	0.48
1:C:158:TYR:HD2	1:C:162:THR:OG1	1.97	0.48
1:E:172:ASN:CG	1:E:188:LEU:HD13	2.38	0.48
1:C:241:THR:HG23	1:F:250:LEU:CD2	2.44	0.48
1:F:43:ARG:CZ	1:F:46:LEU:HD13	2.44	0.48
1:C:60:LEU:C	1:C:60:LEU:CD2	2.87	0.48
1:F:2:THR:HB	1:F:6:ASP:OD2	2.13	0.48
1:F:46:LEU:HD23	1:F:46:LEU:O	2.13	0.48
1:D:46:LEU:HD23	1:D:46:LEU:O	2.14	0.48
1:E:147:MET:HE1	1:E:242:VAL:CG2	2.43	0.47
1:C:66:GLN:HG2	1:C:121:HIS:CE1	2.50	0.47
1:E:74:LEU:HD13	1:E:134:LEU:HD21	1.97	0.47
1:E:67:ASN:HD21	1:E:69:GLU:HB2	1.78	0.47
1:E:165:LYS:O	1:E:169:GLU:HG3	2.14	0.47
1:C:155:MET:HB2	1:C:156:PRO:HD2	1.95	0.47
1:C:269:LEU:HD23	1:E:218:LEU:HD12	1.95	0.47
1:D:41:PHE:CD1	1:D:41:PHE:C	2.92	0.47
1:C:65:VAL:HB	1:C:126:SER:HB2	1.97	0.47
1:D:67:ASN:HD22	1:D:68:GLU:N	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:ILE:HD13	1:F:246:LEU:HD13	1.95	0.47
1:B:67:ASN:ND2	1:B:69:GLU:N	2.63	0.47
1:E:27:ARG:HG2	1:E:31:GLU:OE2	2.15	0.47
1:E:155:MET:HB2	1:E:156:PRO:HD2	1.97	0.47
1:A:222:TRP:HE1	1:A:261:ASP:HB2	1.80	0.47
1:C:259:TYR:HB2	1:F:256:ASP:OD2	2.15	0.47
1:D:153:ARG:NH2	1:F:153:ARG:NH2	2.63	0.47
1:D:265:HIS:O	1:F:153:ARG:NH1	2.47	0.47
1:F:113:TYR:CE2	1:F:117:SER:HB2	2.49	0.47
1:B:4:LEU:HD22	1:B:247:SER:HB2	1.97	0.46
1:B:93:HIS:O	1:B:146:GLY:HA2	2.15	0.46
1:C:172:ASN:CG	1:C:188:LEU:HD13	2.40	0.46
1:D:153:ARG:HE	1:F:153:ARG:HH21	1.60	0.46
1:F:64:ASP:H	1:F:70:HIS:CD2	2.33	0.46
1:F:90:GLY:HA2	1:F:143:SER:O	2.16	0.46
1:A:135:LEU:HD13	1:A:144:ILE:HD11	1.97	0.46
1:A:250:LEU:N	1:A:251:PRO:CD	2.79	0.46
1:B:66:GLN:HG2	1:B:121:HIS:CE1	2.50	0.46
1:F:67:ASN:OD1	1:F:70:HIS:CE1	2.68	0.46
1:C:93:HIS:HA	1:C:130:MET:HE1	1.97	0.46
1:B:216:GLN:OE1	1:B:216:GLN:N	2.49	0.46
1:D:153:ARG:CZ	1:F:153:ARG:HH21	2.28	0.46
1:A:153:ARG:HG2	1:A:153:ARG:HH11	1.80	0.46
1:C:40:GLY:HA3	1:C:47:ILE:CD1	2.46	0.46
1:C:74:LEU:HD13	1:C:134:LEU:HD21	1.96	0.46
1:A:202:ILE:HD12	1:A:202:ILE:O	2.14	0.46
1:B:74:LEU:HD13	1:B:134:LEU:HD21	1.97	0.46
1:E:44:LEU:HA	1:E:47:ILE:HG12	1.97	0.46
1:A:144:ILE:O	1:A:186:SER:HA	2.15	0.46
1:F:158:TYR:HD2	1:F:162:THR:OG1	1.99	0.46
1:A:40:GLY:HA3	1:A:47:ILE:CD1	2.46	0.46
1:D:16:ILE:HG23	1:D:17:THR:HG23	1.98	0.46
1:D:256:ASP:OD2	1:E:259:TYR:HB2	2.16	0.45
1:E:18:ASP:HB3	1:E:53:ARG:HH21	1.81	0.45
1:E:135:LEU:N	1:E:136:PRO:CD	2.79	0.45
1:C:159:ASN:HA	1:D:174:PHE:CE2	2.51	0.45
1:A:63:LEU:O	3:A:301:NAD:H2A	2.17	0.45
1:D:67:ASN:HD22	1:D:69:GLU:H	1.63	0.45
1:E:79:THR:O	1:E:83:GLY:N	2.47	0.45
1:A:210:GLU:CD	1:A:210:GLU:H	2.23	0.45
1:E:46:LEU:HG	1:E:49:ARG:HH12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:GLY:O	1:C:160:TRP:HB2	2.16	0.45
1:D:250:LEU:N	1:D:251:PRO:CD	2.80	0.45
1:F:46:LEU:HA	1:F:49:ARG:HH12	1.82	0.45
1:A:67:ASN:ND2	1:A:69:GLU:H	2.15	0.45
1:B:8:LYS:HA	1:B:89:ASP:OD2	2.17	0.45
1:E:158:TYR:HD2	1:E:162:THR:OG1	2.00	0.45
1:A:161:MET:HE3	1:A:165:LYS:HE2	1.99	0.45
1:C:156:PRO:O	1:C:158:TYR:N	2.41	0.45
1:E:148:ASP:O	1:E:190:ALA:HA	2.17	0.45
1:D:45:ARG:O	1:D:48:GLN:HB2	2.17	0.45
1:E:9:ARG:HA	1:E:35:GLN:O	2.17	0.45
1:F:44:LEU:HD11	1:F:62:GLU:HB2	1.98	0.45
1:F:249:TRP:O	1:F:250:LEU:HG	2.17	0.45
1:E:93:HIS:CE1	1:E:95:ILE:HB	2.52	0.44
1:E:93:HIS:O	1:E:146:GLY:HA2	2.17	0.44
1:F:41:PHE:CD1	1:F:41:PHE:C	2.93	0.44
1:D:11:LEU:HA	1:D:37:VAL:O	2.17	0.44
1:A:145:VAL:HA	1:A:187:ASN:O	2.17	0.44
1:D:8:LYS:HA	1:D:89:ASP:OD2	2.17	0.44
1:E:66:GLN:HG2	1:E:121:HIS:CE1	2.52	0.44
1:F:67:ASN:HD21	1:F:69:GLU:HB2	1.81	0.44
1:A:39:THR:HA	1:A:61:LEU:O	2.17	0.44
1:C:194:ILE:N	3:C:303:NAD:O7N	2.36	0.44
1:D:147:MET:HE1	1:D:242:VAL:HG21	1.99	0.44
1:F:4:LEU:HD22	1:F:247:SER:HB2	1.99	0.44
1:F:250:LEU:N	1:F:251:PRO:CD	2.81	0.44
1:A:113:TYR:CZ	1:B:121:HIS:HB2	2.52	0.44
1:B:90:GLY:HA2	1:B:143:SER:O	2.17	0.44
1:B:207:LEU:HD13	1:B:211:ALA:HB1	2.00	0.44
1:C:250:LEU:N	1:C:251:PRO:HD3	2.32	0.44
1:D:65:VAL:HB	1:D:126:SER:HB2	1.99	0.44
1:E:121:HIS:HB2	1:F:113:TYR:CE2	2.53	0.44
1:F:78:VAL:O	1:F:82:ILE:HG12	2.18	0.44
1:B:219:GLU:OE2	1:B:232:MET:HB2	2.18	0.43
1:E:10:ILE:HB	1:E:36:LEU:CD2	2.47	0.43
1:F:147:MET:HE1	1:F:242:VAL:HG21	2.00	0.43
1:E:40:GLY:HA3	1:E:47:ILE:HD13	2.00	0.43
1:E:220:GLU:HG2	1:E:224:GLN:HE21	1.83	0.43
1:B:144:ILE:O	1:B:186:SER:HA	2.17	0.43
1:A:159:ASN:HA	1:B:174:PHE:CE2	2.53	0.43
1:A:196:THR:HG21	3:A:301:NAD:O2A	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:VAL:HA	1:E:187:ASN:O	2.18	0.43
1:A:83:GLY:O	1:A:84:ALA:C	2.62	0.43
1:A:18:ASP:CB	1:A:53:ARG:HH21	2.31	0.43
1:C:4:LEU:O	1:C:5:LEU:HD13	2.19	0.43
1:C:250:LEU:N	1:C:251:PRO:CD	2.82	0.43
1:D:269:LEU:O	1:E:177:ARG:NH2	2.51	0.43
1:A:64:ASP:H	1:A:70:HIS:HD2	1.65	0.43
1:E:63:LEU:HD22	1:E:74:LEU:HD11	1.99	0.43
1:F:69:GLU:O	1:F:70:HIS:C	2.62	0.43
1:A:67:ASN:HD22	1:A:69:GLU:H	1.67	0.43
1:B:147:MET:HE1	1:B:242:VAL:CG2	2.49	0.43
1:F:24:HIS:O	1:F:28:VAL:HG23	2.19	0.43
1:F:105:ILE:O	1:F:105:ILE:HG13	2.19	0.43
1:F:266:THR:OG1	1:F:267:GLN:NE2	2.45	0.43
1:C:113:TYR:CE2	1:D:121:HIS:HB2	2.54	0.43
1:C:74:LEU:O	1:C:78:VAL:HG23	2.19	0.42
1:D:90:GLY:HA2	1:D:143:SER:O	2.18	0.42
1:F:67:ASN:CG	1:F:70:HIS:ND1	2.77	0.42
1:A:18:ASP:HB3	1:A:53:ARG:HH21	1.84	0.42
1:A:24:HIS:CD2	1:A:27:ARG:HH21	2.37	0.42
1:A:24:HIS:HD2	1:A:27:ARG:HH21	1.66	0.42
1:D:44:LEU:HA	1:D:47:ILE:HG12	2.01	0.42
1:D:60:LEU:HD23	1:D:60:LEU:C	2.43	0.42
1:E:8:LYS:HA	1:E:89:ASP:OD2	2.20	0.42
1:F:67:ASN:ND2	1:F:69:GLU:H	2.17	0.42
1:B:102:GLY:O	1:B:160:TRP:HB2	2.19	0.42
1:C:177:ARG:NH2	1:F:269:LEU:O	2.52	0.42
1:F:8:LYS:HA	1:F:89:ASP:OD2	2.18	0.42
1:A:155:MET:HB2	1:A:156:PRO:HD2	2.01	0.42
1:A:185:ARG:HG3	1:A:185:ARG:HH11	1.84	0.42
1:C:93:HIS:CD2	1:C:127:TYR:HA	2.54	0.42
1:D:60:LEU:C	1:D:60:LEU:CD2	2.92	0.42
1:A:208:GLY:HA3	1:A:210:GLU:OE2	2.20	0.42
1:B:106:ASN:OD1	1:B:107:PRO:HD2	2.19	0.42
1:C:135:LEU:HD13	1:C:144:ILE:HD11	2.02	0.42
1:D:18:ASP:CB	1:D:53:ARG:HH21	2.31	0.42
1:E:10:ILE:HD13	1:E:246:LEU:HD13	2.01	0.42
1:E:258:ILE:HD12	1:E:258:ILE:N	2.35	0.42
1:E:67:ASN:ND2	1:E:69:GLU:H	2.18	0.42
1:C:46:LEU:HD23	1:C:46:LEU:C	2.45	0.42
1:D:155:MET:HB2	1:D:156:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:LEU:O	1:E:46:LEU:HD23	2.19	0.42
1:E:250:LEU:N	1:E:251:PRO:HD3	2.35	0.42
1:A:41:PHE:HB2	3:A:301:NAD:N3A	2.35	0.42
1:B:44:LEU:HD11	1:B:62:GLU:HB2	2.01	0.42
1:B:93:HIS:HA	1:B:130:MET:HE1	2.00	0.42
1:F:158:TYR:O	1:F:159:ASN:C	2.62	0.42
1:F:46:LEU:HG	1:F:49:ARG:HH12	1.84	0.42
1:B:82:ILE:O	1:B:86:ASN:ND2	2.38	0.41
1:D:44:LEU:HD11	1:D:62:GLU:HB2	2.02	0.41
1:F:83:GLY:O	1:F:84:ALA:C	2.62	0.41
1:B:250:LEU:HB3	1:B:253:THR:CG2	2.49	0.41
1:C:142:GLY:C	1:C:184:VAL:HG13	2.45	0.41
1:D:93:HIS:O	1:D:146:GLY:HA2	2.20	0.41
1:D:93:HIS:CE1	1:D:95:ILE:HB	2.55	0.41
1:F:215:ILE:HD12	1:F:215:ILE:O	2.21	0.41
1:A:27:ARG:O	1:A:31:GLU:HG3	2.21	0.41
1:C:67:ASN:HD22	1:C:69:GLU:N	2.18	0.41
1:E:58:ALA:HA	1:E:59:PRO:HD3	1.94	0.41
1:E:113:TYR:CE2	1:E:117:SER:HB2	2.55	0.41
1:E:156:PRO:CG	1:E:214:GLN:HB3	2.50	0.41
1:A:90:GLY:HA2	1:A:143:SER:O	2.21	0.41
1:C:44:LEU:HA	1:C:47:ILE:HG12	2.02	0.41
1:D:197:LEU:C	1:D:199:MET:H	2.29	0.41
1:A:210:GLU:C	1:A:211:ALA:O	2.61	0.41
1:C:4:LEU:C	1:C:5:LEU:HD13	2.45	0.41
1:C:231:ASN:ND2	1:C:234:ASP:HB2	2.36	0.41
1:D:116:VAL:HG11	1:D:160:TRP:CE3	2.55	0.41
1:C:41:PHE:CD1	1:C:41:PHE:C	2.99	0.41
1:C:153:ARG:NH2	1:E:153:ARG:CZ	2.83	0.41
1:D:153:ARG:CZ	1:F:153:ARG:NH2	2.84	0.41
1:C:18:ASP:HB3	1:C:53:ARG:HH21	1.85	0.41
1:C:144:ILE:O	1:C:186:SER:HA	2.19	0.41
1:F:67:ASN:C	1:F:67:ASN:ND2	2.77	0.41
1:C:149:PHE:O	1:C:150:ASP:C	2.64	0.41
1:D:187:ASN:OD1	1:D:254:THR:HA	2.21	0.41
1:E:227:PRO:HD3	1:E:267:GLN:HG3	2.03	0.41
1:E:41:PHE:CD1	1:E:41:PHE:C	2.98	0.40
1:E:250:LEU:HB3	1:E:253:THR:CG2	2.51	0.40
1:F:218:LEU:O	1:F:220:GLU:N	2.55	0.40
1:A:216:GLN:HA	1:A:219:GLU:OE1	2.22	0.40
1:D:24:HIS:HD2	1:D:27:ARG:HH21	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:ILE:HD11	1:F:43:ARG:HH21	1.87	0.40
1:F:102:GLY:O	1:F:160:TRP:HB2	2.22	0.40
1:F:215:ILE:HB	1:F:218:LEU:HD11	2.03	0.40
1:E:27:ARG:O	1:E:31:GLU:HG3	2.22	0.40
1:E:67:ASN:HD22	1:E:68:GLU:N	2.20	0.40
1:B:18:ASP:HB3	1:B:53:ARG:HH21	1.86	0.40
1:C:67:ASN:HD22	1:C:68:GLU:N	2.19	0.40
1:F:149:PHE:CD2	3:F:306:NAD:H5N	2.57	0.40
1:F:172:ASN:CG	1:F:188:LEU:HD13	2.46	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:NH1	1:A:265:HIS:O[2_555]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	266/269 (99%)	240 (90%)	21 (8%)	5 (2%)	6	22
1	B	255/269 (95%)	239 (94%)	15 (6%)	1 (0%)	30	60
1	C	244/269 (91%)	227 (93%)	17 (7%)	0	100	100
1	D	244/269 (91%)	223 (91%)	19 (8%)	2 (1%)	16	44
1	E	250/269 (93%)	234 (94%)	15 (6%)	1 (0%)	30	60
1	F	247/269 (92%)	220 (89%)	26 (10%)	1 (0%)	30	60
All	All	1506/1614 (93%)	1383 (92%)	113 (8%)	10 (1%)	18	47

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	ALA
1	A	212	GLY
1	A	203	VAL
1	D	159	ASN
1	E	159	ASN
1	A	205	GLY
1	B	247	SER
1	F	219	GLU
1	A	84	ALA
1	D	65	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/205 (100%)	187 (92%)	17 (8%)	10	32
1	B	199/205 (97%)	181 (91%)	18 (9%)	9	28
1	C	193/205 (94%)	178 (92%)	15 (8%)	11	35
1	D	192/205 (94%)	178 (93%)	14 (7%)	13	38
1	E	196/205 (96%)	179 (91%)	17 (9%)	9	30
1	F	196/205 (96%)	177 (90%)	19 (10%)	8	25
All	All	1180/1230 (96%)	1080 (92%)	100 (8%)	10	31

All (100) residues with a non-rotameric sidechain are listed below:

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

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Mol	Chain	Res	Type
1	A	145	VAL
1	A	168	LEU
1	A	202	ILE
1	A	210	GLU
1	A	232	MET
1	A	245	LEU
1	A	253	THR
1	A	269	LEU
1	B	4	LEU
1	B	5	LEU
1	B	6	ASP
1	B	60	LEU
1	B	67	ASN
1	B	69	GLU
1	B	71	LEU
1	B	74	LEU
1	B	101	THR
1	B	135	LEU
1	B	145	VAL
1	B	162	THR
1	B	168	LEU
1	B	216	GLN
1	B	232	MET
1	B	245	LEU
1	B	253	THR
1	B	269	LEU
1	C	4	LEU
1	C	5	LEU
1	C	6	ASP
1	C	60	LEU
1	C	67	ASN
1	C	69	GLU
1	C	71	LEU
1	C	74	LEU
1	C	135	LEU
1	C	145	VAL
1	C	168	LEU
1	C	232	MET
1	C	253	THR
1	C	258	ILE
1	C	269	LEU
1	D	4	LEU

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Mol	Chain	Res	Type
1	D	5	LEU
1	D	60	LEU
1	D	67	ASN
1	D	69	GLU
1	D	71	LEU
1	D	74	LEU
1	D	135	LEU
1	D	145	VAL
1	D	168	LEU
1	D	197	LEU
1	D	232	MET
1	D	253	THR
1	D	269	LEU
1	E	4	LEU
1	E	5	LEU
1	E	6	ASP
1	E	60	LEU
1	E	67	ASN
1	E	69	GLU
1	E	71	LEU
1	E	74	LEU
1	E	135	LEU
1	E	145	VAL
1	E	162	THR
1	E	168	LEU
1	E	218	LEU
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	60	LEU
1	F	67	ASN
1	F	69	GLU
1	F	71	LEU
1	F	74	LEU
1	F	101	THR
1	F	135	LEU
1	F	145	VAL
1	F	168	LEU

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Mol	Chain	Res	Type
1	F	215	ILE
1	F	216	GLN
1	F	217	LEU
1	F	218	LEU
1	F	232	MET
1	F	253	THR
1	F	269	LEU

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

Mol	Chain	Res	Type
1	A	24	HIS
1	A	67	ASN
1	A	70	HIS
1	A	139	ASN
1	A	172	ASN
1	A	224	GLN
1	B	35	GLN
1	B	67	ASN
1	B	139	ASN
1	B	214	GLN
1	C	67	ASN
1	C	139	ASN
1	C	172	ASN
1	D	35	GLN
1	D	66	GLN
1	D	67	ASN
1	D	121	HIS
1	D	139	ASN
1	E	66	GLN
1	E	67	ASN
1	E	70	HIS
1	E	121	HIS
1	E	139	ASN
1	E	159	ASN
1	E	172	ASN
1	E	214	GLN
1	E	224	GLN
1	F	66	GLN
1	F	67	ASN
1	F	121	HIS
1	F	139	ASN

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Mol	Chain	Res	Type
1	F	214	GLN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
2	5PP	E	294	-	20,20,20	1.21	1 (5%)	25,25,25	1.13	2 (8%)
3	NAD	E	305	-	46,48,48	1.89	6 (13%)	64,73,73	1.91	14 (21%)
2	5PP	B	291	-	20,20,20	1.10	2 (10%)	25,25,25	1.07	1 (4%)
3	NAD	F	306	-	46,48,48	1.65	5 (10%)	64,73,73	1.81	13 (20%)
3	NAD	C	303	-	46,48,48	1.69	6 (13%)	64,73,73	1.64	12 (18%)
3	NAD	B	302	-	46,48,48	1.63	4 (8%)	64,73,73	1.84	13 (20%)
2	5PP	C	292	-	20,20,20	1.22	1 (5%)	25,25,25	1.53	4 (16%)
3	NAD	D	304	-	46,48,48	1.65	3 (6%)	64,73,73	1.79	12 (18%)
2	5PP	D	293	-	20,20,20	1.07	3 (15%)	25,25,25	1.31	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5PP	A	290	-	20,20,20	0.99	2 (10%)	25,25,25	1.06	2 (8%)
2	5PP	F	295	-	20,20,20	1.28	1 (5%)	25,25,25	1.55	5 (20%)
3	NAD	A	301	-	46,48,48	1.66	7 (15%)	64,73,73	2.07	18 (28%)

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	5PP	E	294	-	-	3/9/9/9	0/2/2/2
3	NAD	E	305	-	-	4/30/62/62	0/5/5/5
2	5PP	B	291	-	-	4/9/9/9	0/2/2/2
3	NAD	F	306	-	-	6/30/62/62	0/5/5/5
3	NAD	C	303	-	-	2/30/62/62	0/5/5/5
3	NAD	B	302	-	-	6/30/62/62	0/5/5/5
2	5PP	C	292	-	-	2/9/9/9	0/2/2/2
3	NAD	D	304	-	-	2/30/62/62	0/5/5/5
2	5PP	D	293	-	-	3/9/9/9	0/2/2/2
2	5PP	A	290	-	-	4/9/9/9	0/2/2/2
2	5PP	F	295	-	-	2/9/9/9	0/2/2/2
3	NAD	A	301	-	-	3/30/62/62	0/5/5/5

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	305	NAD	O7N-C7N	9.88	1.42	1.24
3	C	303	NAD	O7N-C7N	8.57	1.40	1.24
3	F	306	NAD	O7N-C7N	8.46	1.39	1.24
3	D	304	NAD	O7N-C7N	8.17	1.39	1.24
3	B	302	NAD	O7N-C7N	8.11	1.39	1.24
3	A	301	NAD	O7N-C7N	7.73	1.38	1.24
2	F	295	5PP	C6-C5	4.18	1.47	1.40
2	C	292	5PP	C6-C5	4.11	1.47	1.40
2	E	294	5PP	C6-C5	3.86	1.47	1.40
2	B	291	5PP	C6-C5	3.72	1.46	1.40
3	A	301	NAD	C2A-N3A	3.64	1.40	1.33
3	F	306	NAD	C2A-N1A	3.31	1.39	1.33
3	A	301	NAD	C2A-N1A	2.88	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	304	NAD	C5A-N7A	-2.87	1.33	1.39
3	E	305	NAD	PN-O3	2.86	1.62	1.59
3	E	305	NAD	C2A-N1A	2.78	1.38	1.33
3	A	301	NAD	PN-O3	2.76	1.62	1.59
2	A	290	5PP	C6-C5	2.75	1.45	1.40
2	D	293	5PP	C6-C5	2.70	1.45	1.40
3	C	303	NAD	C2A-N1A	2.61	1.38	1.33
3	D	304	NAD	C2A-N3A	2.55	1.38	1.33
3	B	302	NAD	C8A-N7A	2.55	1.36	1.31
3	E	305	NAD	C8A-N7A	2.55	1.36	1.31
3	F	306	NAD	C2A-N3A	2.54	1.38	1.33
3	E	305	NAD	C2A-N3A	2.49	1.38	1.33
2	D	293	5PP	O17-C6	-2.43	1.31	1.36
3	F	306	NAD	C2N-N1N	2.40	1.37	1.35
2	B	291	5PP	O17-C6	-2.39	1.31	1.36
3	B	302	NAD	PN-O3	2.37	1.62	1.59
3	C	303	NAD	O4D-C1D	2.35	1.44	1.40
3	C	303	NAD	C2A-N3A	2.32	1.38	1.33
3	C	303	NAD	C8A-N7A	2.24	1.36	1.31
2	A	290	5PP	O17-C6	-2.24	1.31	1.36
3	A	301	NAD	C5A-N7A	-2.24	1.35	1.39
3	F	306	NAD	C8A-N7A	2.19	1.35	1.31
3	B	302	NAD	O4D-C1D	2.17	1.43	1.40
3	E	305	NAD	C4A-N3A	2.15	1.38	1.34
2	D	293	5PP	C13-C8	2.11	1.42	1.38
3	C	303	NAD	C5A-N7A	-2.04	1.35	1.39
3	A	301	NAD	C8A-N7A	2.01	1.35	1.31
3	A	301	NAD	C3N-C7N	-2.00	1.47	1.50

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	305	NAD	N3A-C2A-N1A	-6.72	118.42	128.58
3	F	306	NAD	N3A-C2A-N1A	-6.56	118.65	128.58
3	C	303	NAD	N3A-C2A-N1A	-6.41	118.87	128.58
3	A	301	NAD	C5A-C4A-N3A	-5.90	118.59	126.72
3	B	302	NAD	N3A-C2A-N1A	-5.80	119.80	128.58
3	D	304	NAD	N3A-C2A-N1A	-5.80	119.81	128.58
3	A	301	NAD	N3A-C2A-N1A	-5.35	120.49	128.58
2	F	295	5PP	C5-O7-C8	5.30	130.78	117.95
3	E	305	NAD	N9A-C8A-N7A	-5.12	106.67	113.94
3	B	302	NAD	N9A-C8A-N7A	-4.88	107.02	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	292	5PP	C5-O7-C8	4.61	129.11	117.95
3	A	301	NAD	N9A-C8A-N7A	-4.59	107.42	113.94
3	A	301	NAD	N3A-C4A-N9A	4.53	134.87	127.17
3	C	303	NAD	N9A-C8A-N7A	-4.44	107.63	113.94
3	F	306	NAD	N9A-C8A-N7A	-4.41	107.68	113.94
3	D	304	NAD	O4B-C1B-N9A	4.32	116.38	108.09
3	A	301	NAD	C5A-N7A-C8A	4.27	110.16	103.45
3	D	304	NAD	N9A-C8A-N7A	-4.24	107.92	113.94
3	D	304	NAD	C5A-C4A-N3A	-4.15	121.00	126.72
3	A	301	NAD	C2A-N3A-C4A	4.00	121.60	111.83
3	B	302	NAD	C5A-C4A-N3A	-3.92	121.33	126.72
3	E	305	NAD	C5A-N7A-C8A	3.87	109.53	103.45
3	E	305	NAD	O4B-C1B-N9A	3.83	115.44	108.09
3	F	306	NAD	C5A-C4A-N3A	-3.81	121.46	126.72
3	E	305	NAD	C4A-N9A-C8A	3.63	109.55	105.74
3	F	306	NAD	C2A-N3A-C4A	3.60	120.63	111.83
3	B	302	NAD	C4A-N9A-C8A	3.54	109.45	105.74
3	B	302	NAD	C5A-N7A-C8A	3.53	109.00	103.45
3	D	304	NAD	C6N-N1N-C2N	-3.48	118.91	121.88
3	E	305	NAD	C2A-N3A-C4A	3.46	120.27	111.83
3	D	304	NAD	C2A-N3A-C4A	3.44	120.22	111.83
2	E	294	5PP	C5-O7-C8	3.39	126.15	117.95
3	F	306	NAD	C5A-N7A-C8A	3.37	108.75	103.45
3	C	303	NAD	C5A-N7A-C8A	3.34	108.69	103.45
3	E	305	NAD	C5A-C4A-N3A	-3.32	122.15	126.72
3	F	306	NAD	C6N-N1N-C2N	-3.30	119.07	121.88
3	B	302	NAD	O3-PN-O1N	-3.26	100.90	110.70
3	E	305	NAD	C4B-O4B-C1B	-3.24	102.31	109.47
2	C	292	5PP	C3-C2-C1	3.23	123.00	118.55
3	B	302	NAD	N3A-C4A-N9A	3.20	132.61	127.17
3	B	302	NAD	C2A-N3A-C4A	3.19	119.63	111.83
3	A	301	NAD	O2N-PN-O1N	3.19	127.26	112.44
3	D	304	NAD	C5A-N7A-C8A	3.18	108.45	103.45
3	D	304	NAD	N3A-C4A-N9A	3.16	132.55	127.17
3	C	303	NAD	C2A-N3A-C4A	3.02	119.21	111.83
3	F	306	NAD	C4A-N9A-C8A	3.01	108.89	105.74
3	A	301	NAD	O3-PA-O1A	-2.99	101.72	110.70
3	C	303	NAD	C4A-N9A-C8A	2.98	108.86	105.74
3	C	303	NAD	C5A-C4A-N3A	-2.88	122.75	126.72
3	A	301	NAD	C5A-C6A-N6A	-2.84	116.26	123.29
3	D	304	NAD	C4A-N9A-C8A	2.80	108.68	105.74
3	A	301	NAD	C2N-C3N-C4N	2.78	121.50	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	NAD	C4A-C5A-N7A	-2.76	107.42	110.58
3	E	305	NAD	C4A-C5A-N7A	-2.75	107.44	110.58
3	E	305	NAD	C4A-N9A-C1B	-2.69	120.33	126.63
3	F	306	NAD	C2N-C3N-C4N	2.69	121.39	118.26
2	B	291	5PP	C3-C2-C1	2.66	122.22	118.55
2	A	290	5PP	O17-C6-C5	-2.65	113.91	120.13
3	B	302	NAD	O3-PA-O1A	-2.65	102.74	110.70
3	F	306	NAD	N3A-C4A-N9A	2.62	131.62	127.17
3	A	301	NAD	C4A-N9A-C8A	2.58	108.45	105.74
3	A	301	NAD	C6N-N1N-C2N	-2.58	119.68	121.88
3	E	305	NAD	C4D-O4D-C1D	-2.52	107.62	109.92
3	C	303	NAD	C4A-N9A-C1B	-2.49	120.82	126.63
3	A	301	NAD	O4B-C1B-C2B	-2.48	101.31	106.62
3	F	306	NAD	C4A-C5A-N7A	-2.47	107.75	110.58
3	E	305	NAD	O2A-PA-O3	-2.47	100.60	107.27
2	D	293	5PP	C3-C2-C1	2.45	121.92	118.55
2	C	292	5PP	C15-C14-C2	-2.44	104.57	113.67
3	A	301	NAD	C6A-C5A-C4A	2.39	120.44	117.18
3	B	302	NAD	C4B-O4B-C1B	-2.38	104.22	109.47
3	D	304	NAD	C5A-C6A-N6A	-2.31	117.57	123.29
3	A	301	NAD	O4B-C4B-C5B	2.29	116.67	109.33
3	C	303	NAD	C4A-C5A-N7A	-2.28	107.97	110.58
3	E	305	NAD	N3A-C4A-N9A	2.27	131.03	127.17
3	A	301	NAD	O3-PN-O1N	-2.27	103.87	110.70
3	A	301	NAD	O3B-C3B-C4B	-2.26	104.59	111.08
3	C	303	NAD	C4D-O4D-C1D	-2.26	107.86	109.92
2	F	295	5PP	C9-C8-C13	-2.25	116.87	120.16
3	C	303	NAD	C4B-O4B-C1B	-2.23	104.55	109.47
3	B	302	NAD	O7N-C7N-N7N	-2.21	119.42	122.62
3	F	306	NAD	C2N-N1N-C1D	2.21	124.01	119.13
3	D	304	NAD	C5N-C4N-C3N	-2.21	118.20	120.36
2	C	292	5PP	C6-C1-C2	-2.18	118.55	120.81
2	D	293	5PP	C9-C8-C13	-2.18	116.98	120.16
3	E	305	NAD	O7N-C7N-C3N	-2.16	116.96	119.60
2	F	295	5PP	C14-C2-C3	-2.16	115.67	121.18
3	B	302	NAD	O2N-PN-O3	2.14	113.05	107.27
3	F	306	NAD	C3N-C7N-N7N	2.13	120.37	117.74
2	D	293	5PP	C6-C1-C2	-2.13	118.60	120.81
3	C	303	NAD	C2N-C3N-C4N	2.11	120.71	118.26
3	F	306	NAD	C4N-C3N-C7N	-2.10	115.35	121.06
2	A	290	5PP	C3-C2-C1	2.07	121.40	118.55
3	C	303	NAD	C2A-N1A-C6A	2.06	122.11	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	304	NAD	O2N-PN-O1N	2.05	121.96	112.44
2	E	294	5PP	C4-C5-C6	-2.04	117.45	119.87
2	F	295	5PP	C4-C5-C6	-2.04	117.45	119.87
2	D	293	5PP	C12-C13-C8	2.03	122.05	118.98
2	F	295	5PP	C10-C9-C8	2.03	122.05	118.98
3	B	302	NAD	O4B-C1B-N9A	2.02	111.96	108.09

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	NAD	O4D-C1D-N1N-C2N
3	C	303	NAD	O4D-C1D-N1N-C2N
3	D	304	NAD	O4D-C1D-N1N-C2N
3	E	305	NAD	C5B-O5B-PA-O1A
3	E	305	NAD	C5B-O5B-PA-O3
3	F	306	NAD	C2N-C3N-C7N-O7N
2	E	294	5PP	C2-C14-C15-C16
2	A	290	5PP	C2-C14-C15-C16
2	F	295	5PP	C2-C14-C15-C16
2	B	291	5PP	C2-C14-C15-C16
3	F	306	NAD	C2N-C3N-C7N-N7N
2	D	293	5PP	C2-C14-C15-C16
2	B	291	5PP	C14-C15-C16-C17
2	E	294	5PP	C14-C15-C16-C17
2	C	292	5PP	C14-C15-C16-C17
2	F	295	5PP	C14-C15-C16-C17
2	A	290	5PP	C15-C16-C17-C18
2	D	293	5PP	C15-C16-C17-C18
2	A	290	5PP	C14-C15-C16-C17
2	C	292	5PP	C15-C16-C17-C18
2	E	294	5PP	C15-C16-C17-C18
3	F	306	NAD	PN-O3-PA-O1A
2	D	293	5PP	C14-C15-C16-C17
3	A	301	NAD	O4D-C4D-C5D-O5D
3	B	302	NAD	PA-O3-PN-O2N
3	F	306	NAD	PN-O3-PA-O2A
2	B	291	5PP	C15-C16-C17-C18
3	F	306	NAD	C4N-C3N-C7N-N7N
3	B	302	NAD	O4D-C1D-N1N-C6N
3	C	303	NAD	O4D-C1D-N1N-C6N
3	D	304	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	A	301	NAD	PN-O3-PA-O1A
3	F	306	NAD	C4N-C3N-C7N-O7N
2	B	291	5PP	C6-C5-O7-C8
2	A	290	5PP	C6-C5-O7-C8
3	B	302	NAD	PA-O3-PN-O1N
3	E	305	NAD	O4B-C4B-C5B-O5B
3	B	302	NAD	O4D-C4D-C5D-O5D
3	A	301	NAD	PA-O3-PN-O1N
3	E	305	NAD	PN-O3-PA-O2A
3	B	302	NAD	O4B-C4B-C5B-O5B

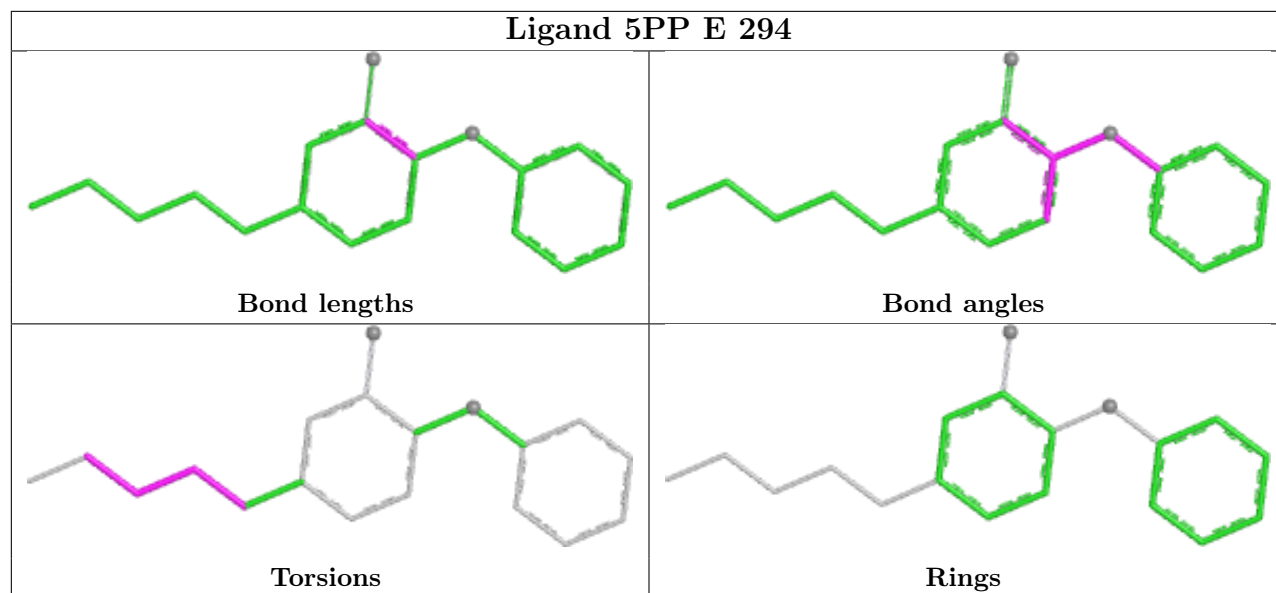
There are no ring outliers.

5 monomers are involved in 10 short contacts:

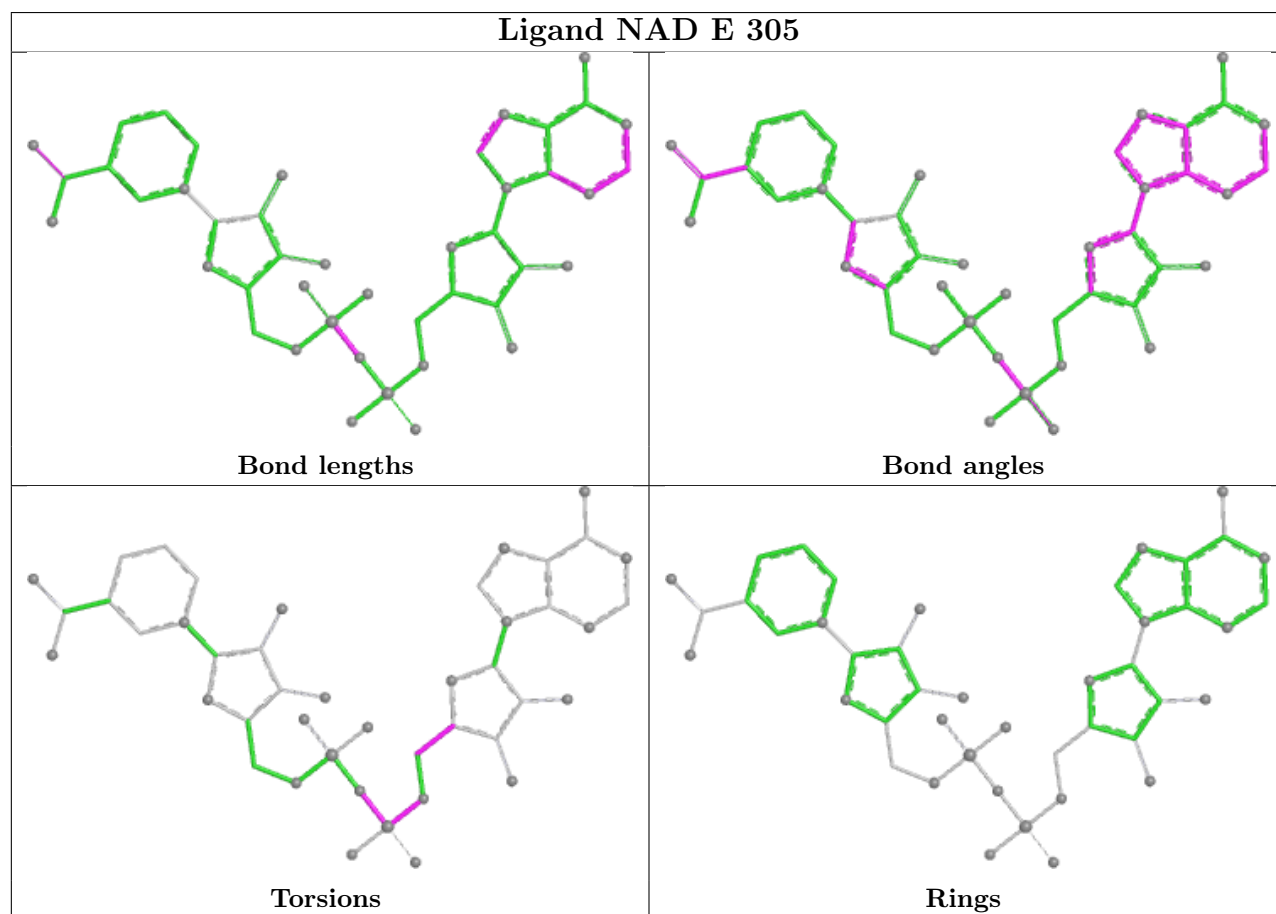
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	306	NAD	3	0
3	C	303	NAD	1	0
3	B	302	NAD	1	0
3	D	304	NAD	1	0
3	A	301	NAD	4	0

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

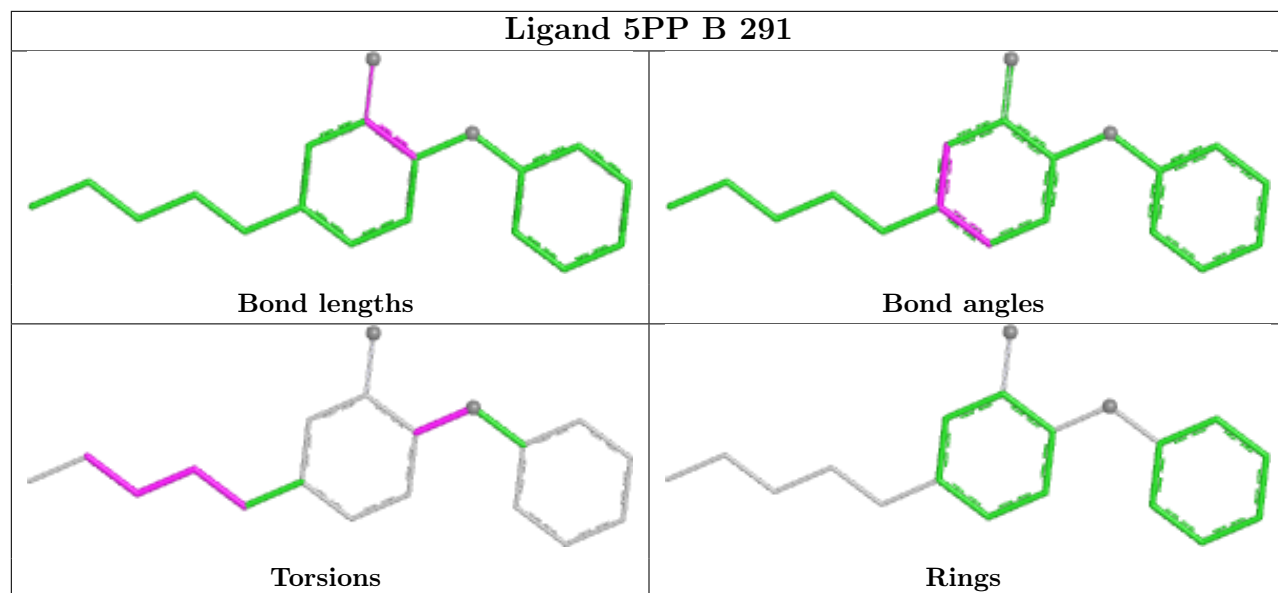
Ligand 5PP E 294



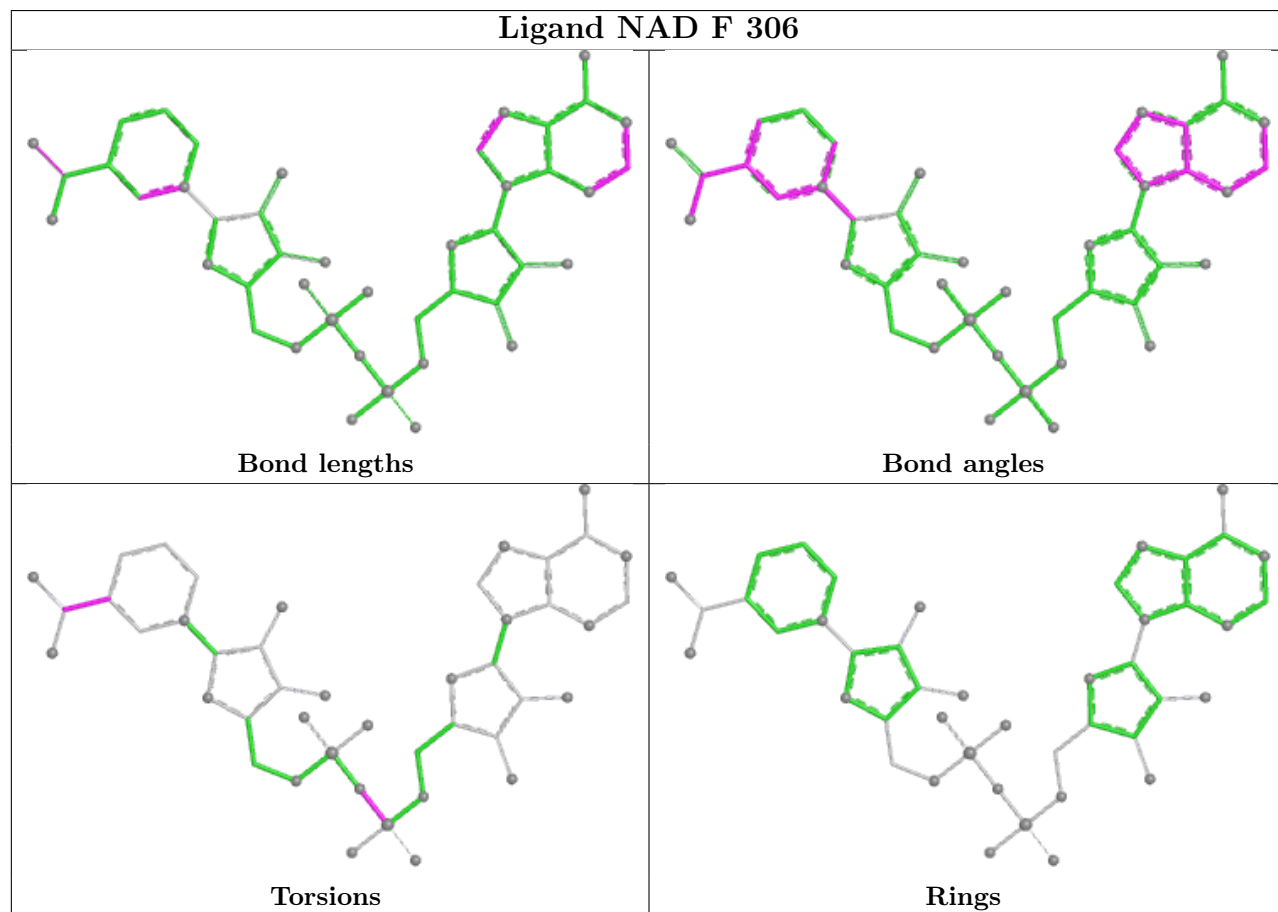
Ligand NAD E 305

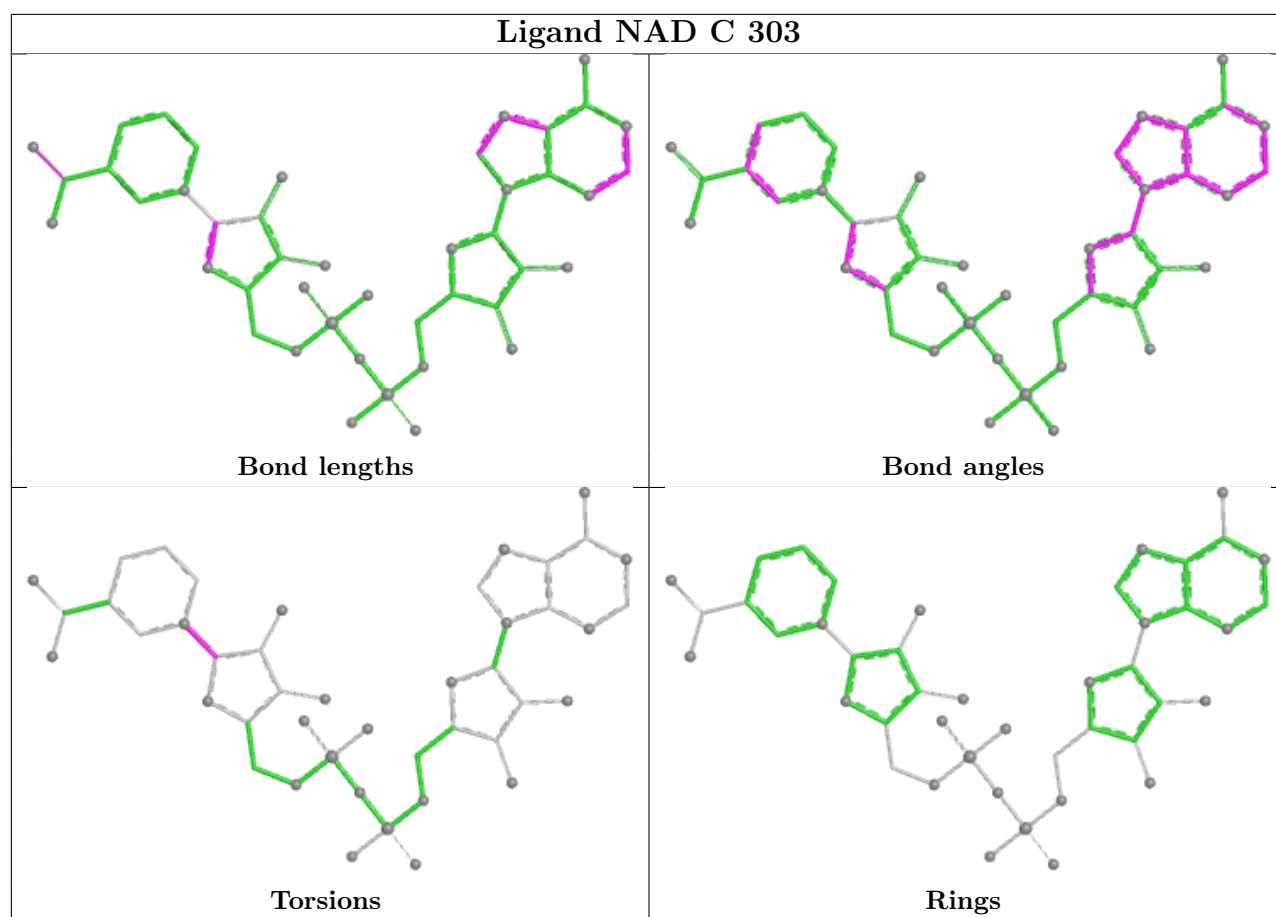


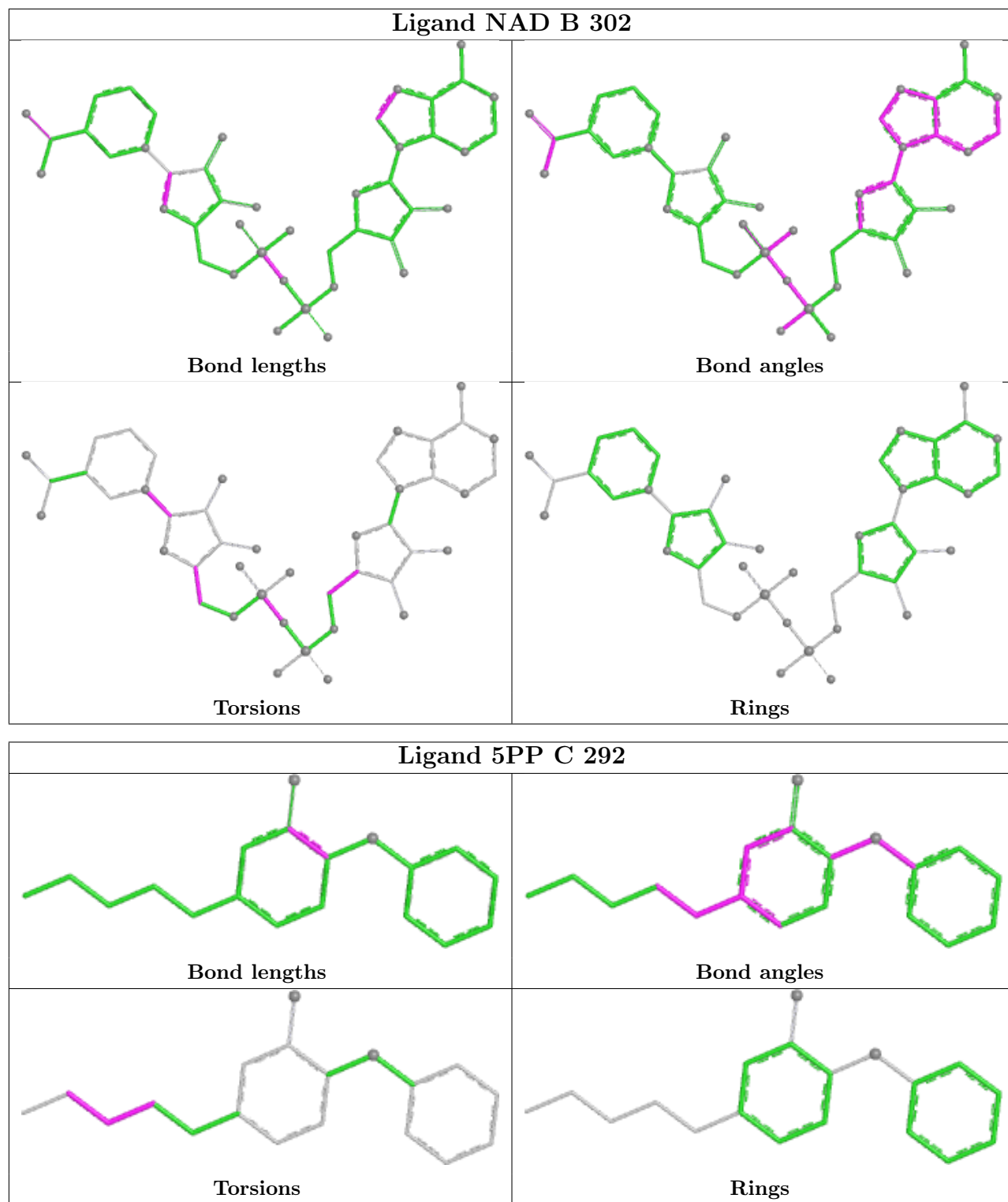
Ligand 5PP B 291

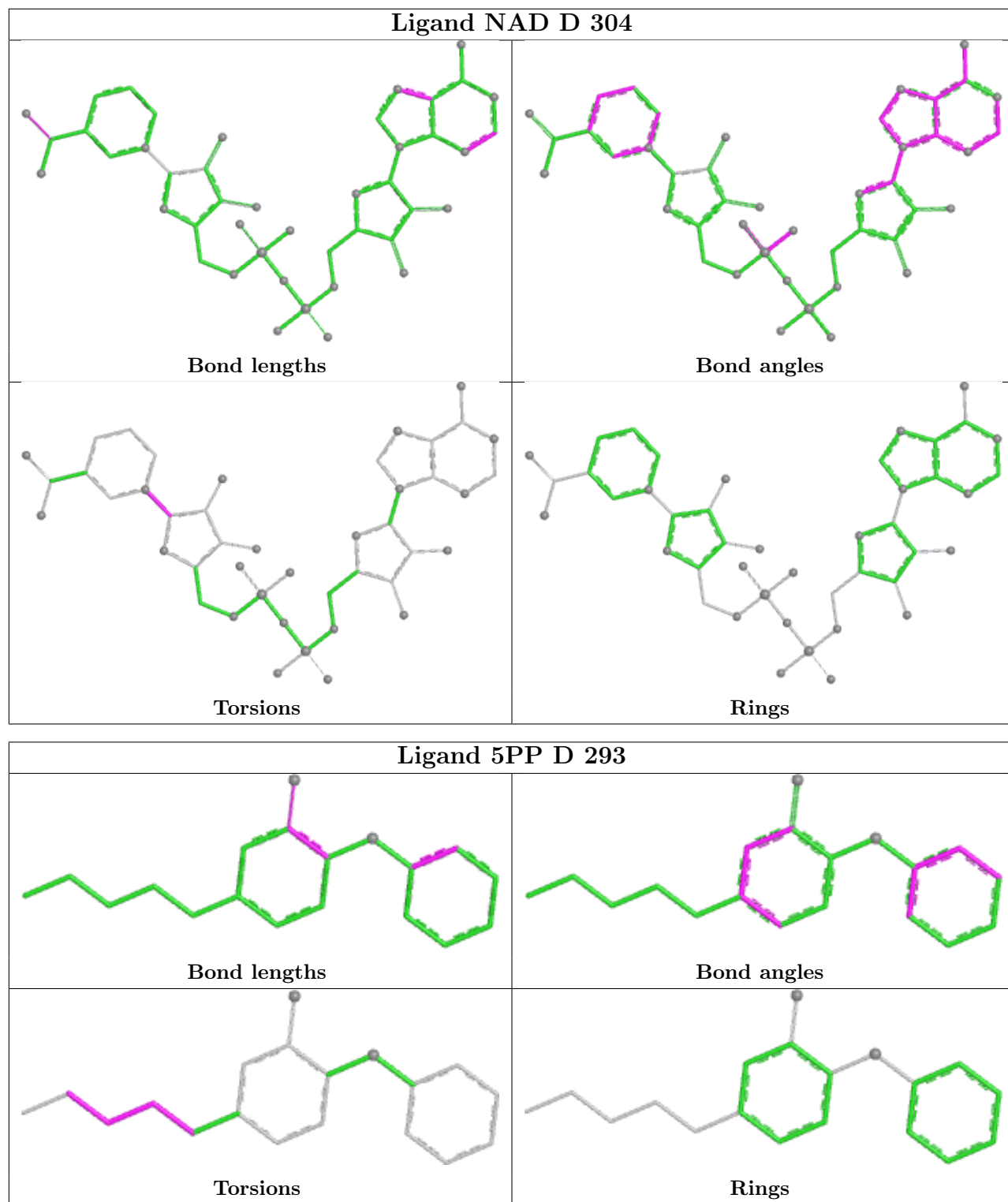


Ligand NAD F 306

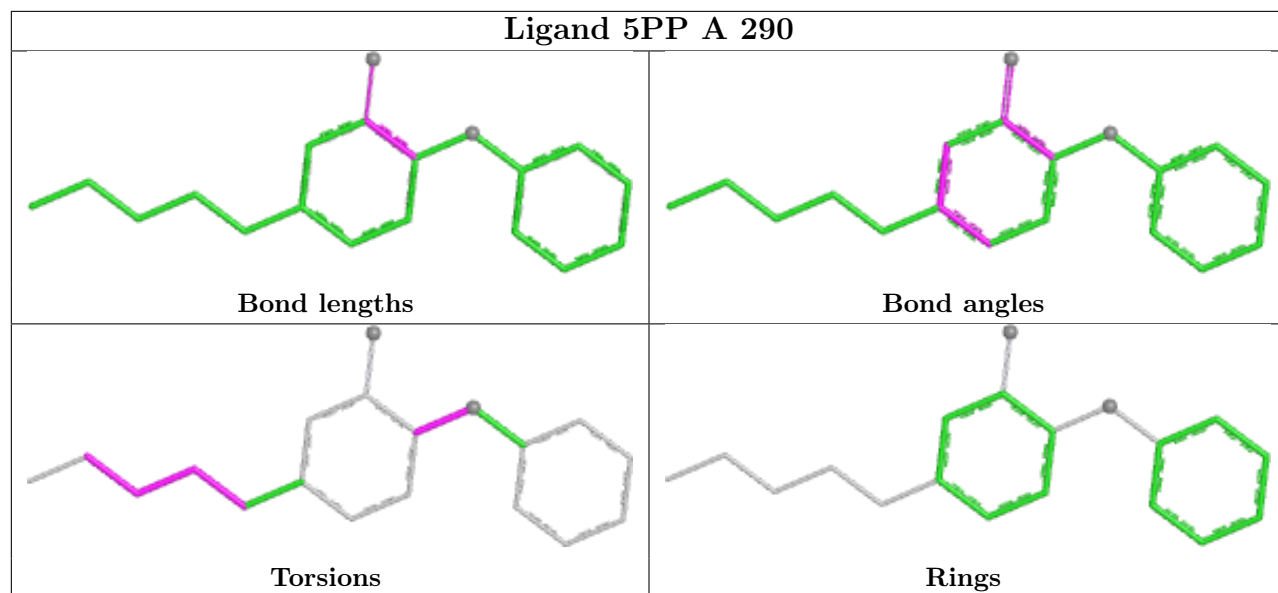




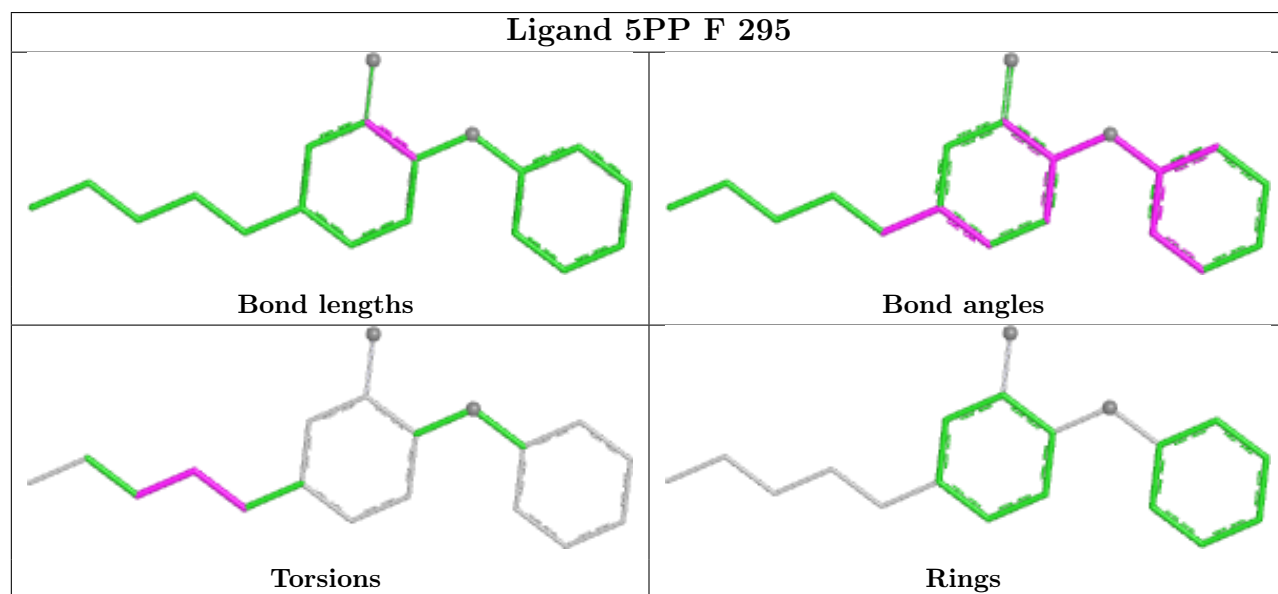


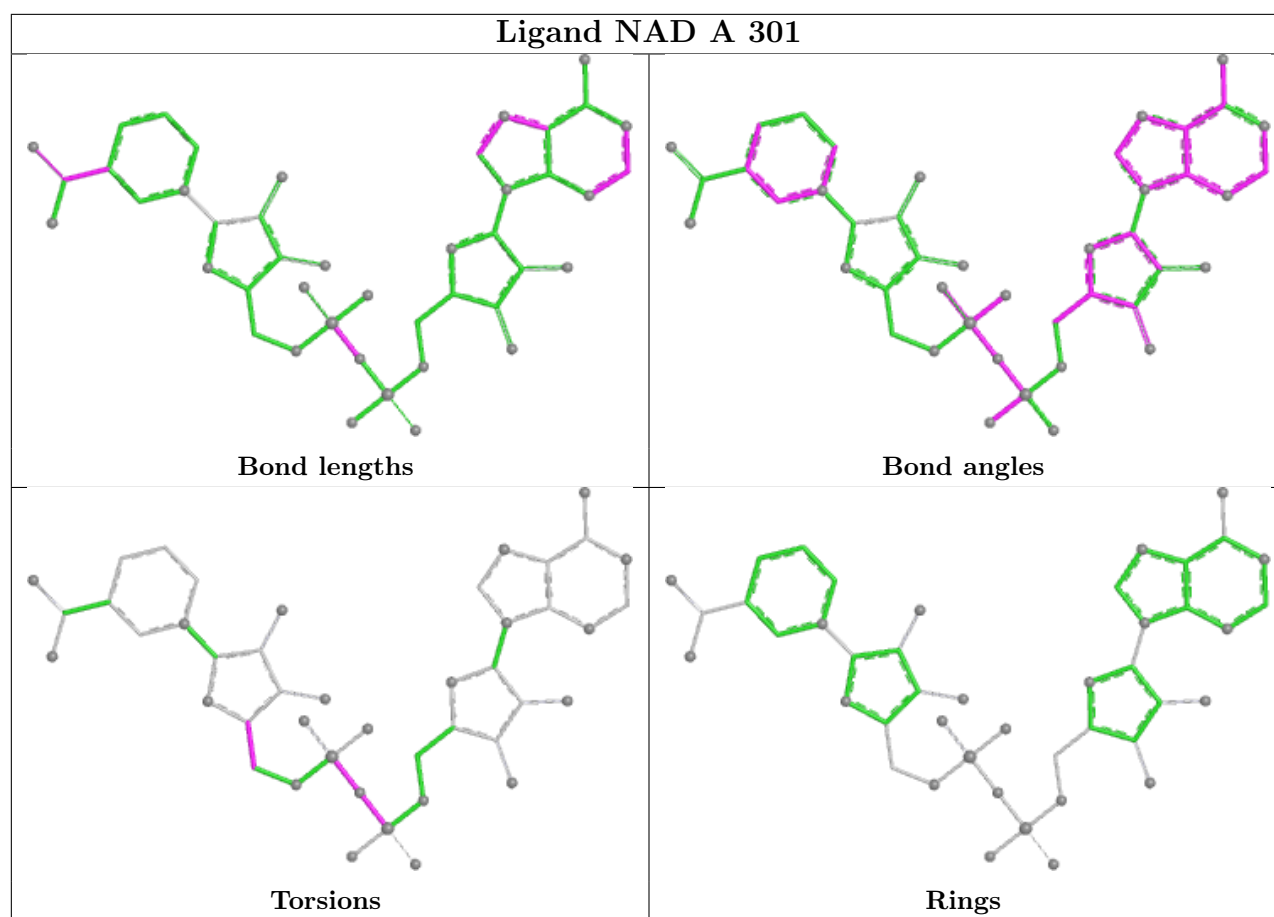


Ligand 5PP A 290



Ligand 5PP F 295





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	268/269 (99%)	-0.06	10 (3%) 45 36	6, 22, 55, 80	0
1	B	259/269 (96%)	-0.11	3 (1%) 76 68	4, 21, 48, 63	0
1	C	248/269 (92%)	0.19	3 (1%) 76 68	18, 35, 59, 64	0
1	D	248/269 (92%)	0.35	15 (6%) 27 21	19, 35, 58, 66	0
1	E	254/269 (94%)	0.09	2 (0%) 82 75	16, 33, 52, 63	0
1	F	251/269 (93%)	0.24	11 (4%) 39 31	14, 33, 57, 68	0
All	All	1528/1614 (94%)	0.11	44 (2%) 53 43	4, 31, 56, 80	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	SER	4.7
1	A	197	LEU	4.5
1	D	106	ASN	4.3
1	A	46	LEU	3.9
1	F	44	LEU	3.8
1	D	197	LEU	3.6
1	D	196	THR	3.2
1	A	204	GLY	3.2
1	A	198	ALA	3.0
1	A	199	MET	3.0
1	F	220	GLU	3.0
1	A	52	ASP	2.9
1	A	196	THR	2.9
1	B	76	GLY	2.8
1	F	57	LYS	2.8
1	A	201	ALA	2.7
1	F	50	ILE	2.7
1	F	79	THR	2.7
1	A	202	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	53	ARG	2.6
1	F	41	PHE	2.5
1	D	195	ARG	2.5
1	B	47	ILE	2.4
1	B	105	ILE	2.4
1	C	33	GLY	2.4
1	D	157	ALA	2.4
1	F	71	LEU	2.4
1	F	221	GLY	2.3
1	D	198	ALA	2.3
1	E	2	THR	2.2
1	D	50	ILE	2.2
1	C	220	GLU	2.2
1	D	103	MET	2.1
1	F	46	LEU	2.1
1	D	19	SER	2.1
1	D	70	HIS	2.1
1	D	83	GLY	2.1
1	D	180	GLY	2.1
1	F	49	ARG	2.1
1	C	3	GLY	2.1
1	D	46	LEU	2.0
1	E	158	TYR	2.0
1	D	86	ASN	2.0
1	F	76	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

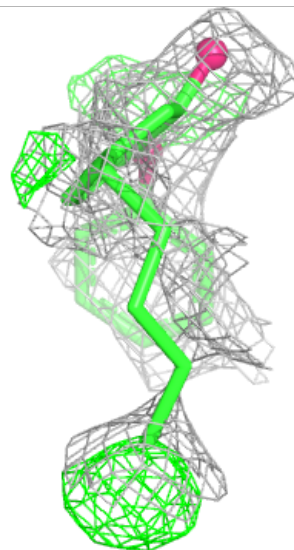
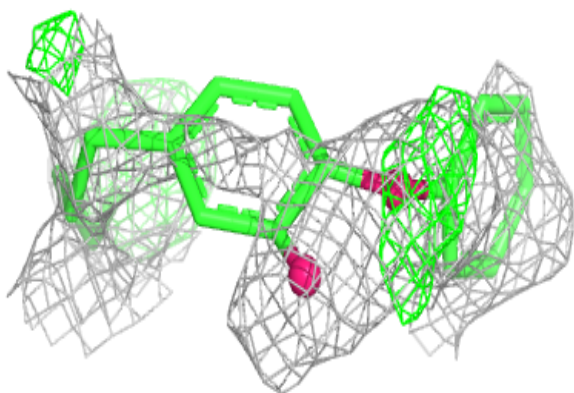
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	5PP	F	295	19/19	0.28	0.26	46,50,51,51	19
2	5PP	E	294	19/19	0.39	0.24	59,60,61,61	19
2	5PP	C	292	19/19	0.63	0.20	20,23,27,27	19
2	5PP	B	291	19/19	0.77	0.22	26,29,30,31	19
2	5PP	D	293	19/19	0.78	0.17	18,20,21,21	19
2	5PP	A	290	19/19	0.82	0.16	22,25,27,27	19
3	NAD	C	303	44/44	0.88	0.10	24,39,46,49	0
3	NAD	D	304	44/44	0.90	0.09	22,36,45,46	0
3	NAD	F	306	44/44	0.92	0.09	22,34,49,50	0
3	NAD	E	305	44/44	0.93	0.08	19,23,27,29	0
3	NAD	B	302	44/44	0.95	0.07	4,11,18,21	0
3	NAD	A	301	44/44	0.97	0.06	2,11,19,20	0

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

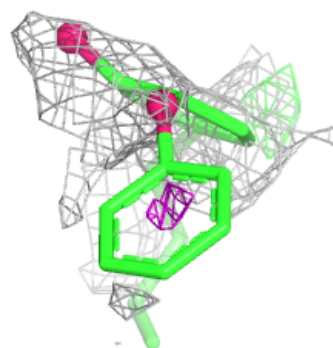
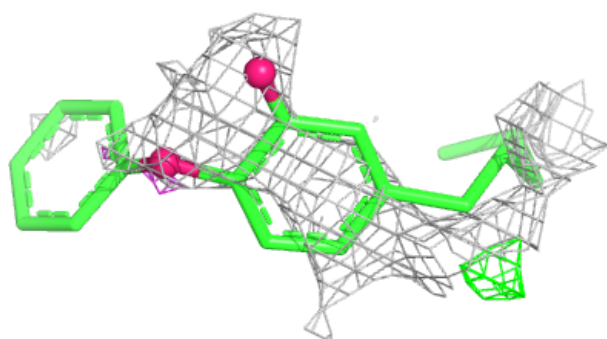
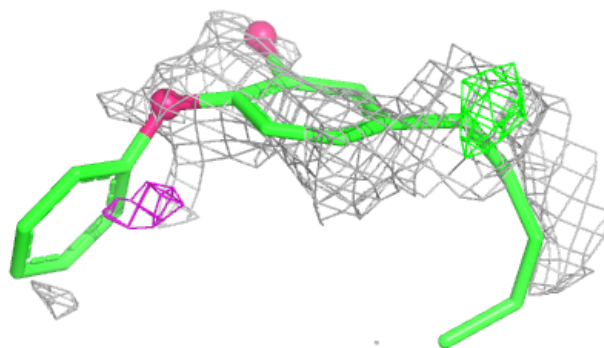
Electron density around 5PP F 295:

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

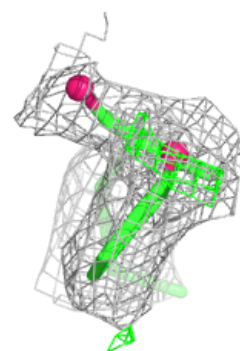
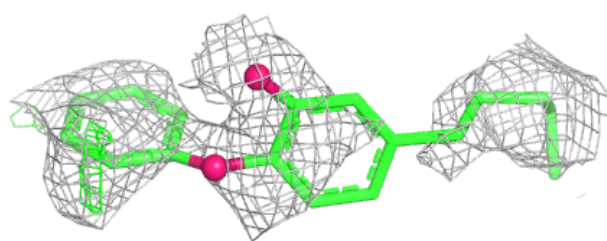
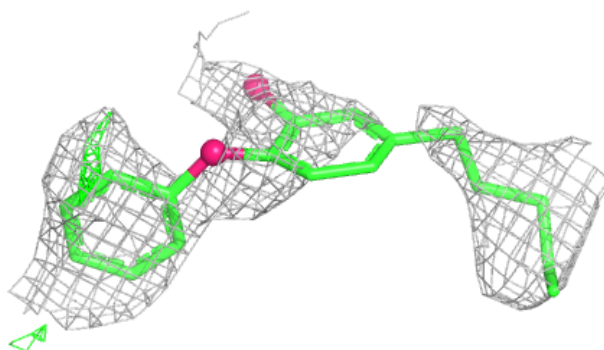


Electron density around 5PP E 294:

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

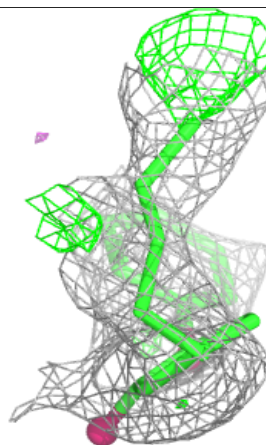
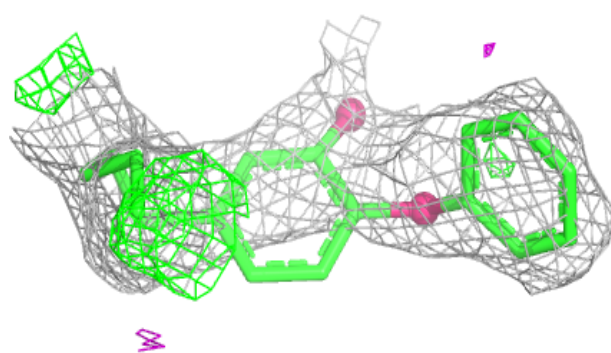
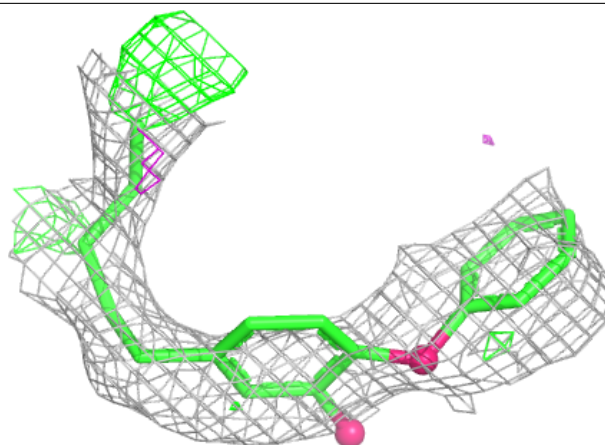
**Electron density around 5PP C 292:**

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



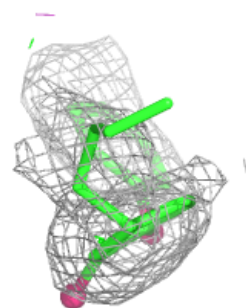
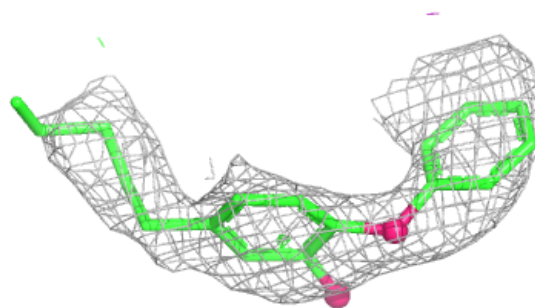
Electron density around 5PP B 291:

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



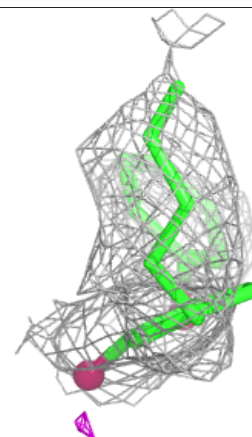
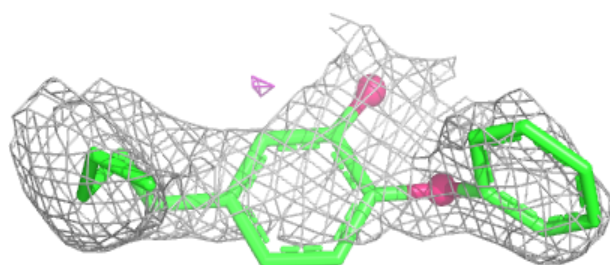
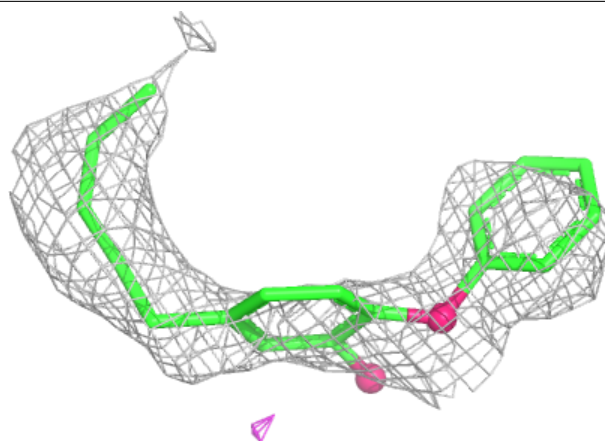
Electron density around 5PP D 293:

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

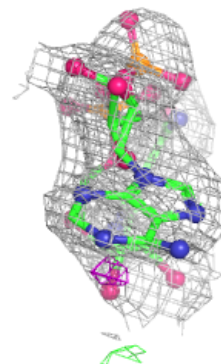
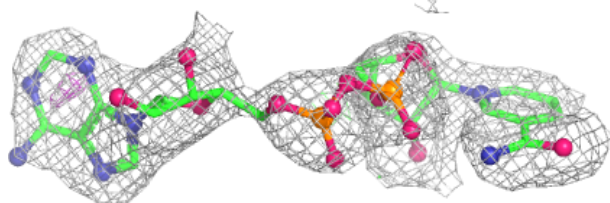
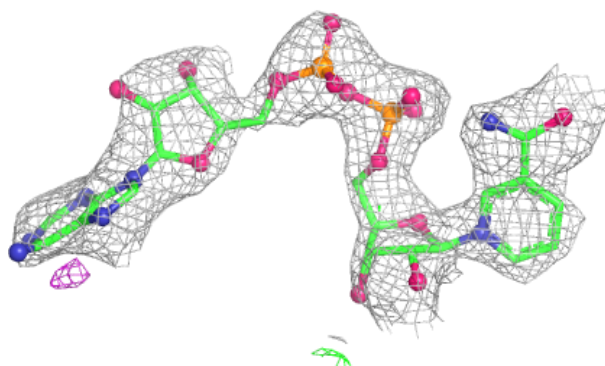


Electron density around 5PP A 290:

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

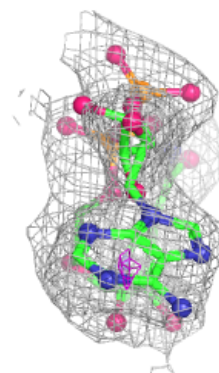
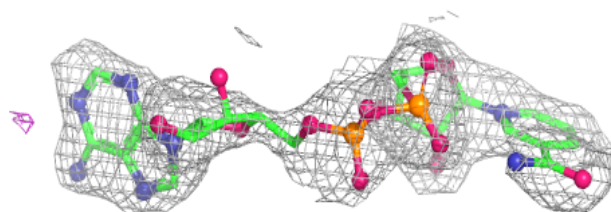
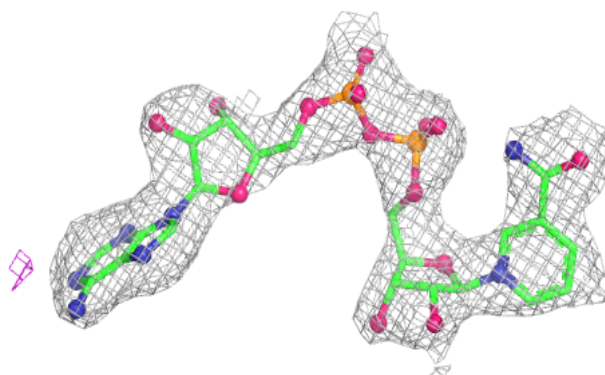
**Electron density around NAD C 303:**

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

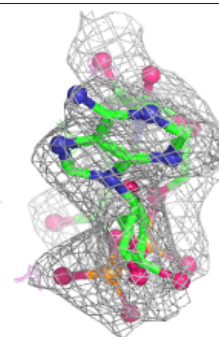
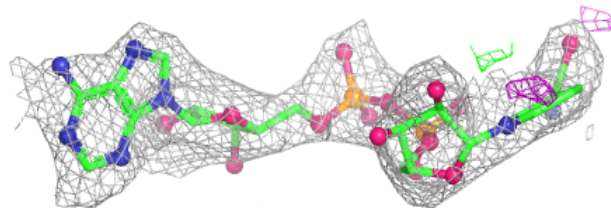
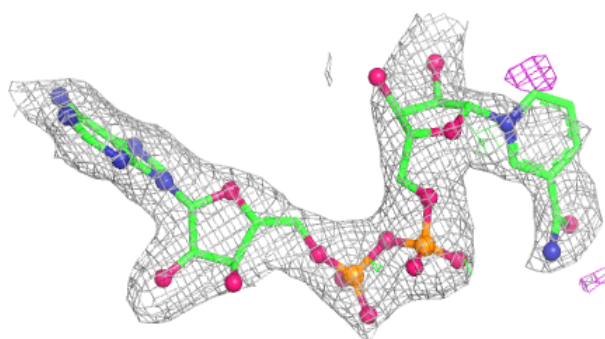


Electron density around NAD D 304:

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

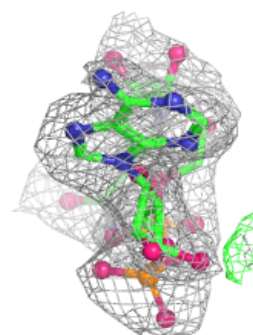
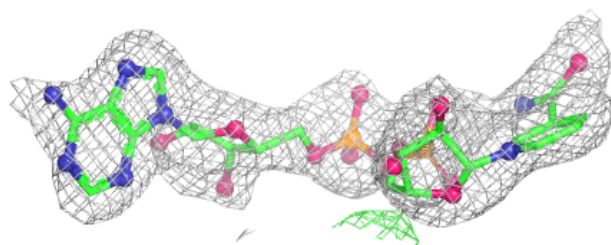
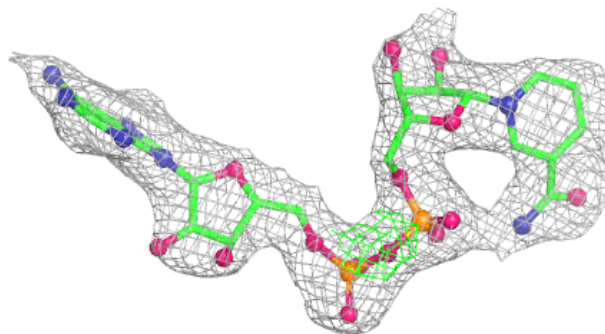
**Electron density around NAD F 306:**

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

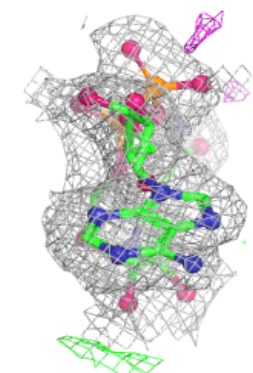
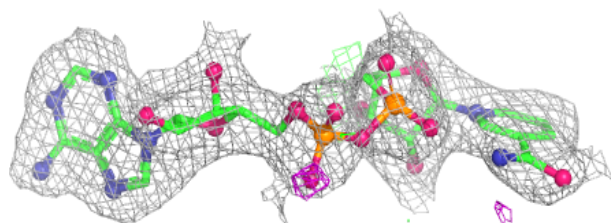
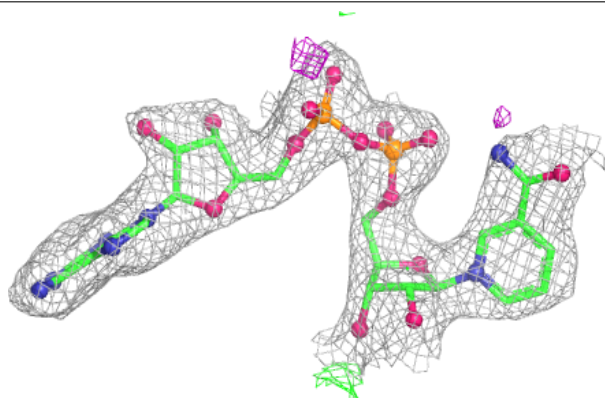


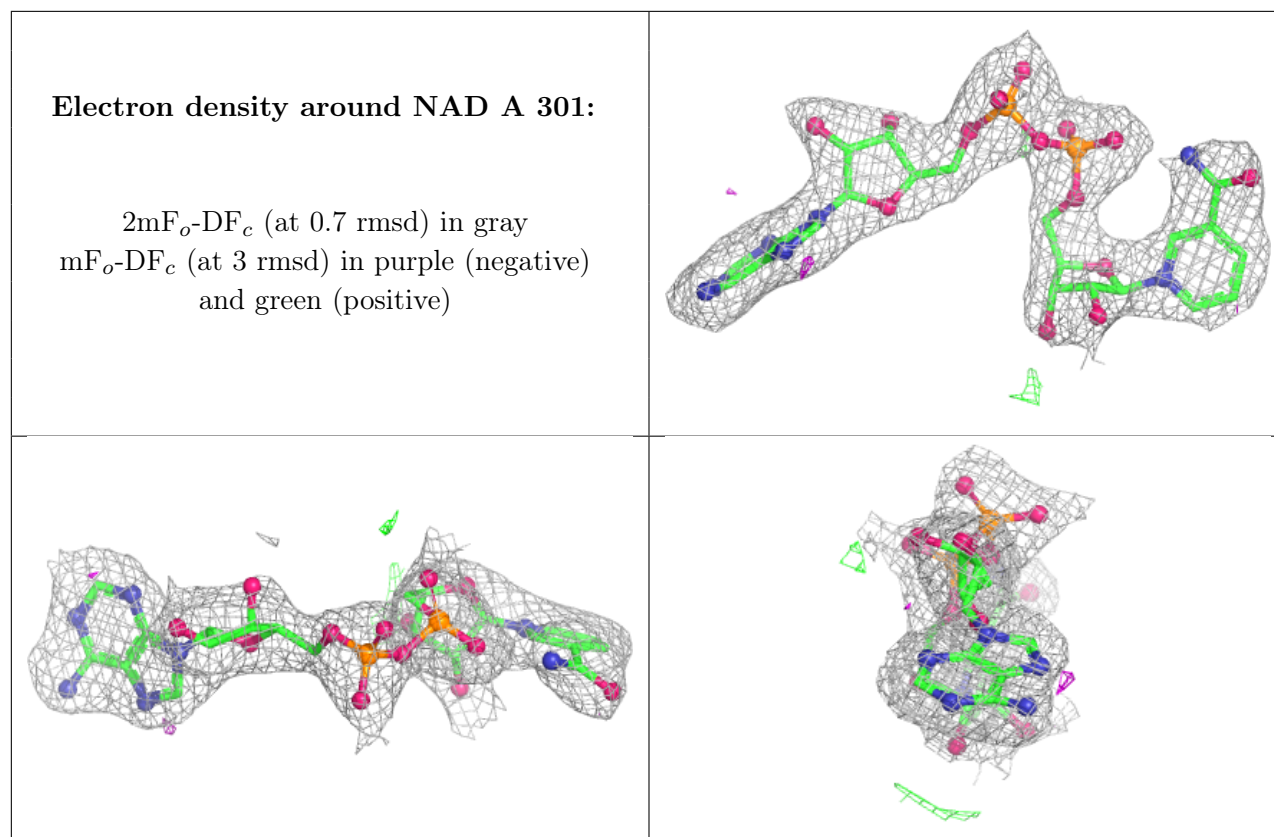
Electron density around NAD E 305:

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

**Electron density around NAD B 302:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.