



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:56 PM UTC

PDB ID : 1E6W / pdb_00001e6w
Title : Rat brain 3-hydroxyacyl-CoA dehydrogenase binary complex with NADH and estradiol
Authors : Read, J.A.; Powell, A.J.; Brady, R.L.
Deposited on : 2000-08-23
Resolution : 1.70 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

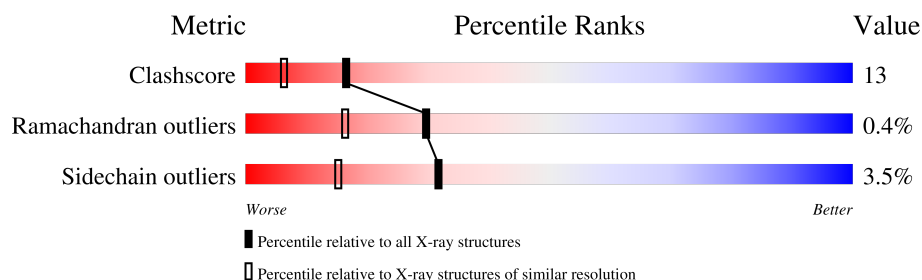
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	260	
1	B	260	
1	C	260	
1	D	260	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EST	C	302	X	-	X	-

2 Entry composition ⓘ

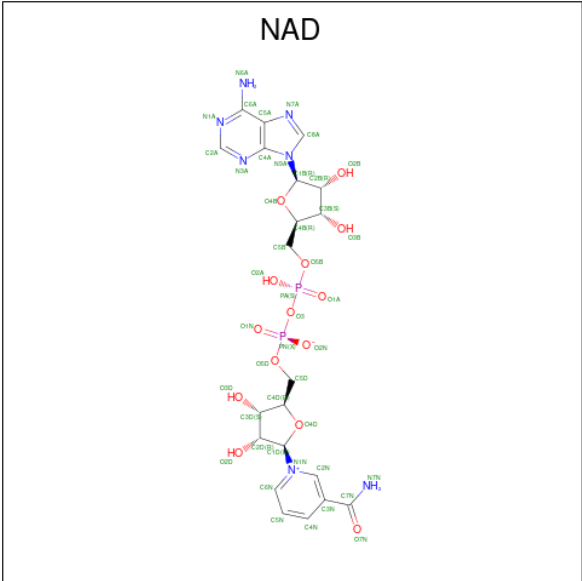
There are 4 unique types of molecules in this entry. The entry contains 8106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SHORT CHAIN 3-HYDROXYACYL-COA DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	8	0
			1841	1160	323	351	7			
1	B	247	Total	C	N	O	S	0	11	0
			1848	1167	328	347	6			
1	C	248	Total	C	N	O	S	0	5	0
			1820	1147	324	342	7			
1	D	255	Total	C	N	O	S	0	2	0
			1856	1172	329	349	6			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



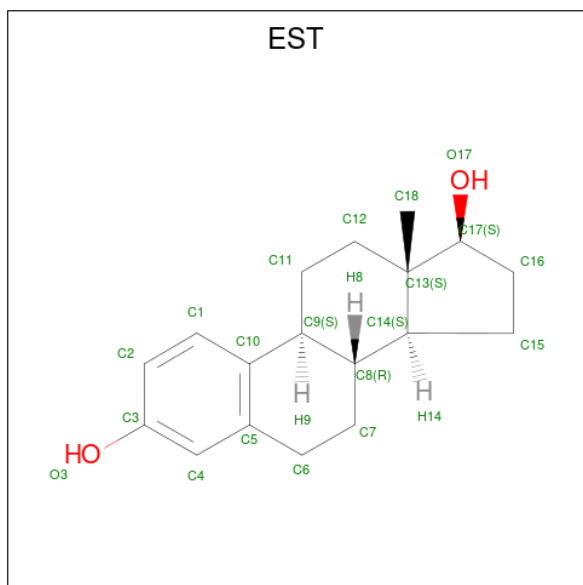
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

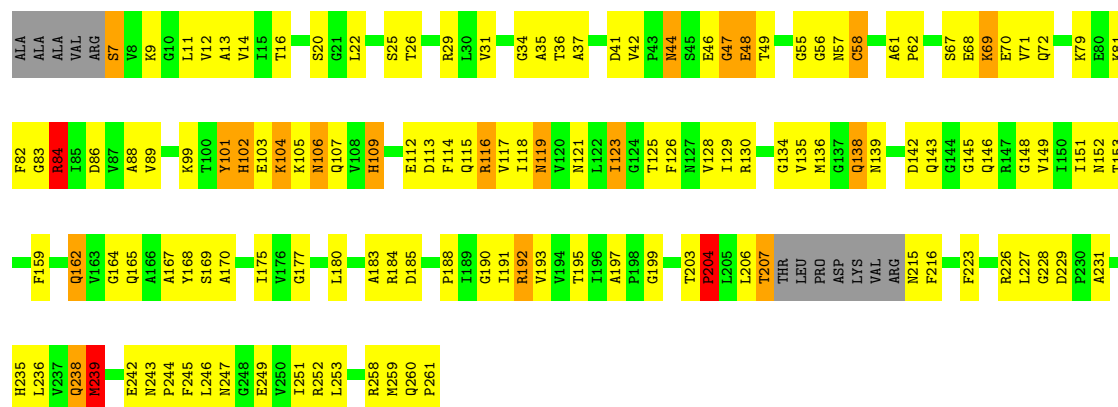
- Molecule 3 is ESTRADIOL (CCD ID: EST) (formula: $C_{18}H_{24}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			20	18	2		

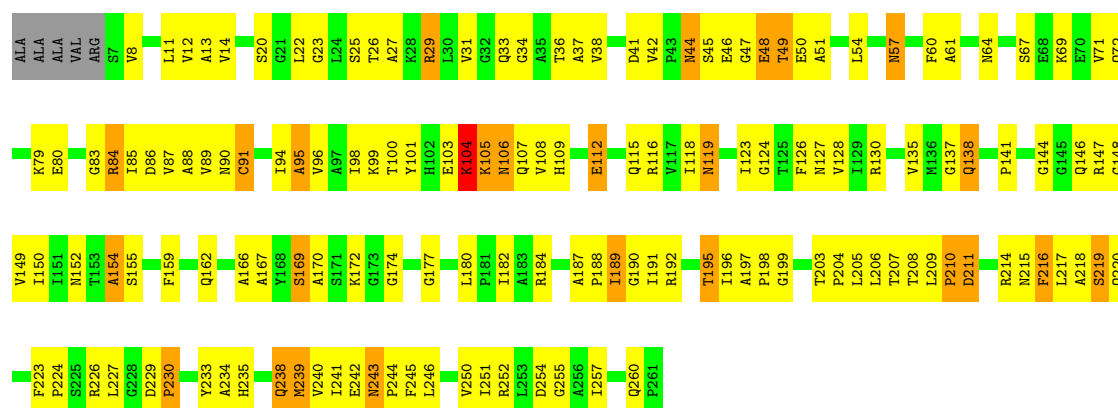
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	146	Total	O	0	0
			146	146		
4	B	128	Total	O	0	0
			128	128		
4	C	143	Total	O	0	0
			143	143		
4	D	128	Total	O	0	0
			128	128		



• Molecule 1: SHORT CHAIN 3-HYDROXYACYL-COA DEHYDROGENASE

Chain D: 40% 48% 10%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.60 Å 67.43 Å 67.50 Å 65.22° 73.27° 75.67°	Depositor
Resolution (Å)	30.00 – 1.70	Depositor
% Data completeness (in resolution range)	94.4 (30.00-1.70)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.184 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8106	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.92	29/1906 (1.5%)	2.69	143/2589 (5.5%)
1	B	1.78	21/1928 (1.1%)	2.47	130/2612 (5.0%)
1	C	2.03	45/1869 (2.4%)	2.75	153/2534 (6.0%)
1	D	1.91	34/1895 (1.8%)	2.66	144/2574 (5.6%)
All	All	1.91	129/7598 (1.7%)	2.64	570/10309 (5.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	10
1	C	0	12
1	D	0	10
All	All	0	41

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	31	VAL	N-CA	8.65	1.56	1.46
1	A	221	VAL	N-CA	8.22	1.52	1.46
1	C	112	GLU	CA-CB	8.17	1.66	1.53
1	D	50	GLU	C-O	7.96	1.33	1.24
1	C	41	ASP	CA-C	7.90	1.62	1.52
1	C	70	GLU	C-N	7.63	1.43	1.33
1	B	239	MET	SD-CE	7.57	1.98	1.79
1	A	84	ARG	N-CA	7.48	1.55	1.46
1	C	193	VAL	N-CA	7.47	1.55	1.46
1	C	101	TYR	N-CA	7.34	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	109	HIS	CA-CB	7.00	1.64	1.53
1	B	114	PHE	C-O	6.99	1.32	1.24
1	A	199	GLY	CA-C	6.90	1.61	1.51
1	C	114	PHE	N-CA	6.86	1.54	1.46
1	D	255	GLY	N-CA	6.83	1.55	1.45
1	D	26	THR	CA-C	6.80	1.61	1.52
1	D	64	ASN	C-N	6.80	1.41	1.33
1	C	14	VAL	N-CA	6.79	1.54	1.46
1	B	176	VAL	N-CA	6.79	1.54	1.46
1	D	235	HIS	C-O	6.78	1.32	1.24
1	D	184	ARG	NE-CZ	6.71	1.40	1.33
1	D	235	HIS	CE1-NE2	6.66	1.39	1.32
1	D	85	ILE	N-CA	6.59	1.54	1.46
1	C	148	GLY	N-CA	6.53	1.53	1.45
1	D	252	ARG	CD-NE	6.51	1.55	1.46
1	C	47	GLY	C-O	6.49	1.31	1.23
1	A	202	ALA	N-CA	6.42	1.54	1.46
1	C	129	ILE	CA-CB	6.36	1.61	1.54
1	C	48	GLU	C-O	6.35	1.31	1.24
1	D	241	ILE	N-CA	6.31	1.53	1.46
1	D	12	VAL	CA-C	6.30	1.60	1.52
1	C	180	LEU	C-N	-6.28	1.26	1.34
1	C	117	VAL	C-O	6.26	1.31	1.24
1	B	114	PHE	N-CA	6.24	1.54	1.46
1	A	41	ASP	CA-C	6.22	1.60	1.52
1	D	95	ALA	N-CA	6.21	1.53	1.45
1	A	16	THR	C-N	6.18	1.41	1.33
1	C	62	PRO	N-CA	-6.13	1.39	1.47
1	B	236	LEU	N-CA	6.12	1.53	1.46
1	D	260	GLN	CA-C	6.10	1.59	1.52
1	C	20	SER	C-O	-6.09	1.16	1.23
1	B	233	TYR	C-N	6.06	1.41	1.33
1	B	235	HIS	CE1-NE2	6.06	1.38	1.32
1	D	148	GLY	CA-C	6.03	1.59	1.51
1	D	167	ALA	N-CA	6.00	1.53	1.46
1	C	11	LEU	N-CA	6.00	1.53	1.45
1	B	251	ILE	C-O	5.98	1.30	1.24
1	C	239[A]	MET	N-CA	5.97	1.53	1.46
1	C	239[B]	MET	N-CA	5.97	1.53	1.46
1	C	35	ALA	N-CA	5.96	1.52	1.45
1	C	235	HIS	CE1-NE2	5.95	1.38	1.32
1	B	134	GLY	N-CA	5.93	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	261	PRO	N-CD	5.91	1.56	1.47
1	C	261	PRO	N-CD	5.88	1.55	1.47
1	A	174	GLY	N-CA	5.85	1.53	1.45
1	C	162	GLN	C-N	5.82	1.41	1.33
1	D	88	ALA	CA-C	5.82	1.59	1.52
1	A	163	VAL	N-CA	5.82	1.53	1.46
1	A	245	PHE	N-CA	5.80	1.53	1.45
1	B	258	ARG	NE-CZ	5.79	1.39	1.33
1	C	16	THR	N-CA	5.78	1.53	1.46
1	A	109	HIS	C-O	-5.76	1.16	1.23
1	C	114	PHE	C-O	5.73	1.30	1.24
1	D	67	SER	N-CA	5.72	1.53	1.46
1	C	109	HIS	CE1-NE2	5.71	1.38	1.32
1	A	92	ALA	CA-CB	5.71	1.62	1.53
1	D	13	ALA	C-O	5.70	1.30	1.24
1	C	116	ARG	CD-NE	-5.70	1.38	1.46
1	B	38	VAL	C-O	5.69	1.30	1.24
1	B	180	LEU	N-CA	5.67	1.51	1.46
1	A	241	ILE	CA-CB	5.67	1.61	1.54
1	B	29	ARG	N-CA	5.66	1.53	1.46
1	D	195	THR	CB-OG1	5.65	1.52	1.43
1	D	130	ARG	NE-CZ	5.65	1.39	1.33
1	D	25	SER	CA-CB	5.64	1.62	1.53
1	C	183	ALA	N-CA	5.62	1.53	1.46
1	C	184	ARG	NE-CZ	5.60	1.39	1.33
1	A	243	ASN	N-CA	5.58	1.52	1.46
1	D	34	GLY	N-CA	5.58	1.52	1.45
1	C	101	TYR	C-O	-5.55	1.17	1.23
1	C	252	ARG	CZ-NH2	5.49	1.40	1.33
1	D	90	ASN	C-O	5.48	1.30	1.24
1	C	123	ILE	C-O	5.46	1.31	1.24
1	B	109	HIS	CA-CB	5.45	1.62	1.53
1	B	261	PRO	N-CD	5.44	1.55	1.47
1	D	72	GLN	C-N	-5.44	1.26	1.33
1	A	251	ILE	CA-CB	5.43	1.61	1.54
1	A	40	LEU	C-N	5.42	1.40	1.33
1	C	184	ARG	CA-C	5.42	1.60	1.52
1	B	257	ILE	N-CA	5.42	1.53	1.46
1	C	243	ASN	N-CA	5.42	1.54	1.46
1	A	232	GLU	N-CA	5.38	1.52	1.46
1	D	177	GLY	N-CA	5.37	1.52	1.45
1	A	47	GLY	CA-C	5.36	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	LEU	N-CA	5.36	1.52	1.46
1	D	87	VAL	N-CA	5.35	1.52	1.46
1	C	130	ARG	CZ-NH2	5.35	1.40	1.33
1	A	57	ASN	N-CA	5.30	1.52	1.46
1	D	233	TYR	C-O	-5.29	1.18	1.24
1	D	126	PHE	CA-C	5.28	1.59	1.52
1	A	85	ILE	C-O	5.26	1.29	1.24
1	A	90	ASN	C-O	5.22	1.30	1.24
1	C	153	THR	C-O	5.22	1.30	1.24
1	C	175	ILE	CA-CB	-5.21	1.48	1.54
1	B	132	VAL	C-O	5.19	1.30	1.24
1	D	191	ILE	CA-C	5.19	1.59	1.52
1	B	90	ASN	N-CA	5.18	1.52	1.46
1	C	152	ASN	C-N	5.17	1.40	1.33
1	D	187	ALA	CA-C	5.15	1.58	1.52
1	D	89	VAL	C-N	5.15	1.40	1.33
1	A	29	ARG	CZ-NH2	5.13	1.40	1.33
1	C	125	THR	N-CA	5.13	1.52	1.46
1	D	109	HIS	CA-CB	5.12	1.61	1.53
1	B	196	ILE	N-CA	5.10	1.52	1.46
1	C	235	HIS	N-CA	5.10	1.52	1.46
1	D	174	GLY	C-O	5.09	1.29	1.23
1	A	246	LEU	N-CA	5.08	1.52	1.46
1	A	125	THR	N-CA	5.07	1.52	1.46
1	D	87	VAL	C-N	5.07	1.40	1.33
1	B	58	CYS	C-O	5.06	1.29	1.23
1	A	127	ASN	N-CA	5.05	1.52	1.46
1	A	193	VAL	N-CA	5.04	1.52	1.46
1	A	16	THR	N-CA	5.04	1.52	1.45
1	C	34	GLY	C-N	5.03	1.41	1.33
1	C	193	VAL	CA-CB	-5.02	1.47	1.54
1	A	76	THR	CA-CB	5.02	1.61	1.53
1	A	164	GLY	C-N	5.01	1.40	1.33
1	C	67	SER	CA-CB	5.01	1.60	1.53
1	C	249	GLU	CA-C	5.00	1.58	1.52

All (570) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ARG	CD-NE-CZ	25.67	160.34	124.40
1	C	44	ASN	CA-CB-CG	19.33	131.93	112.60
1	C	116	ARG	CD-NE-CZ	18.09	149.73	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ASN	OD1-CG-ND2	16.50	139.10	122.60
1	D	119	ASN	OD1-CG-ND2	-13.91	108.69	122.60
1	C	215	ASN	CA-CB-CG	13.74	126.34	112.60
1	C	138	GLN	OE1-CD-NE2	-12.97	109.63	122.60
1	B	80	GLU	CA-C-O	-12.94	107.37	120.70
1	C	215	ASN	OD1-CG-ND2	-12.27	110.33	122.60
1	C	44	ASN	CB-CG-ND2	-11.91	98.54	116.40
1	B	106	ASN	OD1-CG-ND2	-11.77	110.83	122.60
1	D	162	GLN	OE1-CD-NE2	11.69	134.29	122.60
1	A	121	ASN	OD1-CG-ND2	-11.51	111.09	122.60
1	D	150	ILE	CA-C-O	-11.18	108.65	120.39
1	C	84[A]	ARG	CD-NE-CZ	11.15	140.01	124.40
1	C	84[B]	ARG	CD-NE-CZ	11.15	140.01	124.40
1	D	49	THR	CA-CB-OG1	-10.85	93.33	109.60
1	A	116	ARG	NE-CZ-NH2	-10.71	109.56	119.20
1	D	138	GLN	OE1-CD-NE2	-10.57	112.03	122.60
1	B	205	LEU	CA-C-O	-10.50	106.47	119.38
1	C	72	GLN	CG-CD-NE2	10.49	132.14	116.40
1	C	243	ASN	OD1-CG-ND2	10.37	132.97	122.60
1	C	72	GLN	CB-CG-CD	10.13	129.83	112.60
1	A	226	ARG	O-C-N	10.11	133.40	123.29
1	A	107	GLN	OE1-CD-NE2	-10.04	112.56	122.60
1	A	220	GLN	CA-C-N	-10.04	115.36	122.59
1	A	220	GLN	C-N-CA	-10.04	115.36	122.59
1	C	44	ASN	CB-CG-OD1	9.95	140.71	120.80
1	D	226	ARG	NE-CZ-NH2	-9.93	110.27	119.20
1	C	191	ILE	O-C-N	9.83	133.62	123.20
1	A	226	ARG	CA-C-O	-9.75	110.84	121.28
1	A	243	ASN	CA-C-O	9.73	125.62	119.29
1	D	29	ARG	NE-CZ-NH1	9.71	131.21	121.50
1	A	241	ILE	N-CA-CB	-9.66	99.25	110.55
1	D	126	PHE	CA-C-O	-9.59	110.26	120.42
1	D	44	ASN	CA-CB-CG	-9.57	103.03	112.60
1	A	116	ARG	NH1-CZ-NH2	9.56	131.73	119.30
1	D	126	PHE	O-C-N	9.47	132.95	122.15
1	D	252	ARG	NE-CZ-NH1	9.46	130.96	121.50
1	C	109	HIS	CB-CG-CD2	-9.44	118.92	131.20
1	C	130	ARG	NE-CZ-NH2	-9.41	110.73	119.20
1	A	243	ASN	O-C-N	-9.39	113.62	121.23
1	A	149	VAL	O-C-N	9.27	133.08	123.07
1	D	191	ILE	O-C-N	9.22	132.85	122.99
1	D	180	LEU	CA-C-O	-9.19	110.35	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	184	ARG	NE-CZ-NH1	-9.13	112.37	121.50
1	C	243	ASN	O-C-N	-9.07	113.01	121.35
1	C	84[A]	ARG	NE-CZ-NH2	9.04	127.33	119.20
1	C	84[B]	ARG	NE-CZ-NH2	9.04	127.33	119.20
1	D	150	ILE	O-C-N	8.94	132.92	123.26
1	A	57	ASN	OD1-CG-ND2	8.93	131.53	122.60
1	D	107	GLN	CA-CB-CG	8.92	131.94	114.10
1	D	239	MET	CG-SD-CE	8.73	120.11	100.90
1	D	57	ASN	CA-CB-CG	8.70	121.30	112.60
1	A	205	LEU	CA-C-O	-8.47	112.11	121.00
1	A	82	PHE	CA-CB-CG	-8.34	105.46	113.80
1	D	50	GLU	CA-C-O	-8.28	111.78	120.55
1	D	38	VAL	CA-C-O	-8.25	111.60	120.59
1	A	24	LEU	O-C-N	-8.25	113.38	122.12
1	A	101	TYR	OH-CZ-CE2	-8.24	95.17	119.90
1	B	8	VAL	CA-C-O	8.21	127.44	119.97
1	C	82	PHE	O-C-N	-8.19	112.28	122.35
1	D	41	ASP	CA-C-O	-8.18	112.71	121.38
1	D	84	ARG	NE-CZ-NH1	-8.14	113.36	121.50
1	D	238[A]	GLN	CA-C-O	-8.14	111.92	120.55
1	D	238[B]	GLN	CA-C-O	-8.14	111.92	120.55
1	D	86	ASP	CA-C-O	-8.10	110.08	119.24
1	B	121	ASN	CA-CB-CG	8.10	120.70	112.60
1	D	215	ASN	O-C-N	-8.06	112.79	122.22
1	D	243	ASN	CA-CB-CG	-8.03	104.57	112.60
1	A	103	GLU	CA-C-O	-8.02	112.05	120.55
1	D	191	ILE	CA-C-O	-8.01	111.67	120.48
1	D	188	PRO	O-C-N	-7.96	112.54	122.17
1	D	33	GLN	CG-CD-NE2	-7.96	104.47	116.40
1	A	50	GLU	O-C-N	7.94	130.54	122.12
1	D	115	GLN	CB-CG-CD	7.93	126.09	112.60
1	B	193	VAL	CA-C-O	-7.93	112.26	120.27
1	D	226	ARG	NE-CZ-NH1	7.91	129.41	121.50
1	C	109	HIS	O-C-N	-7.84	113.22	122.95
1	A	226	ARG	CB-CA-C	-7.84	96.83	110.95
1	D	240	VAL	O-C-N	7.82	129.46	121.87
1	C	113	ASP	O-C-N	7.81	131.05	122.15
1	C	109	HIS	CB-CG-ND1	7.76	134.34	122.70
1	A	101	TYR	CE1-CZ-OH	7.73	143.10	119.90
1	A	202	ALA	N-CA-CB	-7.71	99.52	110.46
1	B	260	GLN	CA-C-O	7.69	129.35	120.96
1	C	244	PRO	CA-C-N	-7.67	110.63	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	244	PRO	C-N-CA	-7.67	110.63	122.60
1	D	84	ARG	NE-CZ-NH2	7.67	126.11	119.20
1	D	169	SER	O-C-N	-7.67	113.41	122.15
1	D	88	ALA	CA-C-O	-7.67	112.42	120.70
1	D	45	SER	CA-C-O	-7.63	112.59	121.82
1	B	12	VAL	CA-C-O	-7.63	112.37	120.53
1	B	29	ARG	CD-NE-CZ	-7.63	113.72	124.40
1	D	29	ARG	NE-CZ-NH2	-7.60	112.36	119.20
1	A	31	VAL	O-C-N	-7.58	114.52	121.87
1	C	48	GLU	CA-CB-CG	-7.57	98.97	114.10
1	C	129	ILE	O-C-N	7.55	129.31	121.91
1	B	104	LYS	CA-C-O	-7.53	112.57	120.55
1	A	103	GLU	N-CA-C	7.42	119.37	111.28
1	B	153	THR	CA-C-O	7.41	128.23	120.30
1	B	252	ARG	NE-CZ-NH2	7.40	125.86	119.20
1	D	170	ALA	N-CA-C	-7.38	103.18	111.07
1	B	146	GLN	OE1-CD-NE2	7.37	129.97	122.60
1	B	72	GLN	CB-CA-C	-7.37	98.55	110.79
1	D	84	ARG	O-C-N	7.37	130.66	123.29
1	A	215	ASN	OD1-CG-ND2	7.36	129.96	122.60
1	D	88	ALA	O-C-N	7.36	132.80	123.23
1	A	205	LEU	N-CA-CB	-7.34	99.20	109.91
1	A	15	ILE	O-C-N	7.29	130.93	123.20
1	A	226	ARG	NE-CZ-NH2	-7.29	112.64	119.20
1	A	143	GLN	OE1-CD-NE2	-7.28	115.32	122.60
1	B	80	GLU	CA-C-N	7.22	129.96	120.28
1	B	80	GLU	C-N-CA	7.22	129.96	120.28
1	C	197	ALA	CA-C-O	7.22	127.17	120.09
1	C	229	ASP	N-CA-C	-7.22	100.35	110.31
1	A	201	PHE	O-C-N	7.18	132.08	123.24
1	A	70	GLU	CA-C-N	-7.16	111.39	120.56
1	A	70	GLU	C-N-CA	-7.16	111.39	120.56
1	A	102	HIS	CA-CB-CG	7.16	120.96	113.80
1	D	60	PHE	CA-CB-CG	7.16	120.96	113.80
1	A	81	LYS	CA-C-O	7.15	128.33	120.82
1	D	215	ASN	CA-C-N	7.14	134.65	121.52
1	D	215	ASN	C-N-CA	7.14	134.65	121.52
1	D	230	PRO	O-C-N	-7.10	114.07	122.24
1	A	135	VAL	O-C-N	-7.10	114.52	121.90
1	C	89	VAL	O-C-N	7.09	130.55	123.18
1	A	195	THR	CA-CB-OG1	-7.05	99.03	109.60
1	C	247	ASN	OD1-CG-ND2	-7.02	115.58	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	216	PHE	CA-C-O	7.01	126.15	118.65
1	B	176	VAL	O-C-N	-6.96	115.09	121.91
1	D	72	GLN	OE1-CD-NE2	-6.96	115.64	122.60
1	A	112	GLU	CA-CB-CG	-6.96	100.19	114.10
1	D	41	ASP	O-C-N	6.94	130.55	123.26
1	A	134	GLY	O-C-N	-6.94	114.71	122.28
1	A	102	HIS	O-C-N	-6.94	114.33	122.87
1	D	219	SER	CA-C-O	-6.93	113.14	120.63
1	C	83	GLY	N-CA-C	6.93	124.54	115.40
1	A	70	GLU	O-C-N	6.90	130.76	122.27
1	D	166	ALA	CA-C-N	-6.90	110.49	120.29
1	D	166	ALA	C-N-CA	-6.90	110.49	120.29
1	C	259	MET	O-C-N	6.90	131.11	123.04
1	C	167	ALA	O-C-N	6.87	129.98	122.15
1	C	7	SER	CA-CB-OG	6.87	124.83	111.10
1	B	84[A]	ARG	NE-CZ-NH2	6.86	125.38	119.20
1	B	84[B]	ARG	NE-CZ-NH2	6.86	125.38	119.20
1	C	207	THR	N-CA-CB	6.86	123.16	111.50
1	A	44	ASN	O-C-N	-6.86	113.24	122.43
1	B	103	GLU	CA-C-O	-6.86	113.15	120.42
1	B	140	GLU	N-CA-C	-6.86	101.12	109.83
1	D	167	ALA	N-CA-C	6.84	118.82	111.36
1	A	15	ILE	CA-C-O	-6.84	113.27	120.39
1	C	204	PRO	CA-C-N	6.83	130.35	120.38
1	C	204	PRO	C-N-CA	6.83	130.35	120.38
1	D	127	ASN	OD1-CG-ND2	6.81	129.41	122.60
1	A	96	VAL	CA-C-O	-6.76	114.58	121.67
1	C	113	ASP	CA-C-N	-6.76	110.70	120.29
1	C	113	ASP	C-N-CA	-6.76	110.70	120.29
1	D	106	ASN	CA-CB-CG	6.75	119.35	112.60
1	B	205	LEU	CA-CB-CG	6.74	139.89	116.30
1	C	260[A]	GLN	CA-C-O	6.74	130.97	121.27
1	C	260[B]	GLN	CA-C-O	6.74	130.97	121.27
1	C	207	THR	CA-CB-OG1	6.74	119.70	109.60
1	B	9	LYS	CA-C-O	6.73	128.30	120.96
1	B	205	LEU	CA-C-N	6.73	132.53	122.17
1	B	205	LEU	C-N-CA	6.73	132.53	122.17
1	C	89	VAL	CA-C-O	-6.71	113.49	120.27
1	D	128	VAL	O-C-N	-6.71	114.92	121.83
1	C	118	ILE	O-C-N	-6.70	115.37	121.87
1	A	132	VAL	CA-C-O	-6.70	111.47	119.58
1	D	197	ALA	CA-C-O	6.70	125.82	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ASP	CA-C-O	-6.70	114.28	121.38
1	D	239	MET	CB-CG-SD	6.68	132.74	112.70
1	B	173	GLY	O-C-N	6.67	130.00	122.34
1	C	72	GLN	CG-CD-OE1	-6.66	107.47	120.80
1	C	151	ILE	O-C-N	6.63	130.22	123.20
1	C	107	GLN	O-C-N	6.62	130.95	123.27
1	A	98	ILE	O-C-N	-6.62	115.92	123.07
1	D	37	ALA	CA-C-O	6.62	128.27	120.66
1	A	138	GLN	OE1-CD-NE2	-6.61	115.99	122.60
1	D	86	ASP	O-C-N	6.59	131.19	122.36
1	D	144	GLY	O-C-N	-6.59	114.76	122.27
1	A	100	THR	O-C-N	6.54	128.90	122.09
1	C	112	GLU	CA-CB-CG	-6.53	101.04	114.10
1	D	119	ASN	CB-CG-OD1	6.53	133.86	120.80
1	C	223	PHE	CA-CB-CG	-6.53	107.28	113.80
1	C	242	GLU	CA-C-O	-6.52	112.47	119.97
1	B	88	ALA	CA-C-O	-6.51	113.09	120.32
1	D	184	ARG	NH1-CZ-NH2	6.51	127.77	119.30
1	D	239	MET	CA-CB-CG	6.51	127.12	114.10
1	B	130	ARG	CA-C-N	-6.50	109.57	121.52
1	B	130	ARG	C-N-CA	-6.50	109.57	121.52
1	D	86	ASP	N-CA-C	-6.48	105.91	113.88
1	C	20	SER	N-CA-CB	-6.47	101.34	111.56
1	A	44	ASN	CA-CB-CG	-6.46	106.14	112.60
1	C	123	ILE	CA-C-O	-6.45	113.51	120.47
1	B	76	THR	CA-C-O	-6.45	113.72	120.55
1	D	23	GLY	O-C-N	6.42	128.42	122.19
1	C	121	ASN	CA-C-O	-6.42	114.09	120.70
1	A	147	ARG	NE-CZ-NH2	6.41	124.97	119.20
1	A	56	GLY	CA-C-N	-6.41	112.02	122.65
1	A	56	GLY	C-N-CA	-6.41	112.02	122.65
1	D	61	ALA	CA-C-O	6.39	125.55	119.99
1	D	220	GLN	OE1-CD-NE2	6.39	128.99	122.60
1	B	179	THR	O-C-N	6.36	128.62	122.07
1	D	37	ALA	O-C-N	-6.36	115.51	123.27
1	C	119	ASN	CA-C-O	-6.36	113.81	120.55
1	C	130	ARG	NH1-CZ-NH2	6.34	127.55	119.30
1	C	170	ALA	N-CA-C	-6.34	104.28	111.07
1	A	135	VAL	CA-C-O	6.34	128.09	121.05
1	C	258	ARG	CA-C-O	-6.32	113.54	120.24
1	A	249	GLU	CA-C-O	-6.32	114.07	121.46
1	D	152	ASN	CA-C-O	-6.31	113.93	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	56	GLY	O-C-N	6.31	131.57	122.68
1	A	12	VAL	CA-C-O	-6.30	113.78	120.53
1	A	112	GLU	CB-CG-CD	6.30	123.32	112.60
1	D	48	GLU	O-C-N	-6.29	115.46	122.12
1	B	26	THR	O-C-N	6.28	128.54	122.07
1	D	198	PRO	N-CD-CG	-6.28	93.78	103.20
1	B	158	ALA	O-C-N	6.27	130.84	122.43
1	D	229	ASP	N-CA-C	-6.27	101.88	109.72
1	B	38	VAL	O-C-N	6.27	129.69	122.99
1	B	239	MET	CB-CA-C	6.26	122.69	110.67
1	A	104	LYS	CA-CB-CG	6.25	126.59	114.10
1	B	38	VAL	CA-C-O	-6.24	113.61	120.48
1	D	260	GLN	CA-C-O	6.23	130.62	121.46
1	D	98	ILE	CA-C-O	-6.23	114.08	120.25
1	A	243	ASN	CA-CB-CG	-6.22	106.38	112.60
1	D	167	ALA	CA-C-O	6.21	127.01	120.42
1	C	231	ALA	CA-C-O	-6.21	113.08	120.10
1	A	90	ASN	CA-C-O	-6.18	113.96	120.58
1	B	137	GLY	O-C-N	6.18	130.01	122.84
1	A	91	CYS	N-CA-CB	6.18	119.41	110.88
1	B	247	ASN	CA-CB-CG	-6.17	106.43	112.60
1	C	109	HIS	CA-C-O	6.17	127.96	120.92
1	A	44	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	D	91	CYS	O-C-N	-6.14	114.96	122.20
1	B	162	GLN	CG-CD-NE2	6.13	125.60	116.40
1	B	68	GLU	CA-CB-CG	-6.13	101.84	114.10
1	A	222	PRO	N-CA-CB	6.13	109.69	103.25
1	A	149	VAL	CA-C-N	-6.13	115.59	123.19
1	A	149	VAL	C-N-CA	-6.13	115.59	123.19
1	C	135	VAL	O-C-N	-6.12	115.52	121.83
1	C	169	SER	CA-C-O	6.12	127.04	120.55
1	A	50	GLU	CB-CG-CD	6.12	123.01	112.60
1	C	245	PHE	CA-C-N	-6.12	113.56	122.19
1	C	245	PHE	C-N-CA	-6.12	113.56	122.19
1	D	48	GLU	CA-CB-CG	-6.11	101.88	114.10
1	B	93	GLY	O-C-N	6.11	130.64	122.70
1	C	41	ASP	CA-C-O	-6.11	114.91	121.38
1	A	149	VAL	CA-C-O	-6.10	113.78	120.43
1	A	186	LEU	O-C-N	6.10	129.97	122.34
1	D	27	ALA	O-C-N	6.10	129.10	122.15
1	B	178	MET	CA-C-N	6.10	128.37	120.44
1	B	178	MET	C-N-CA	6.10	128.37	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	42	VAL	CA-C-O	6.07	128.09	119.95
1	B	29	ARG	NE-CZ-NH2	-6.07	113.74	119.20
1	C	31	VAL	N-CA-CB	-6.07	102.28	110.54
1	A	235	HIS	CA-C-O	-6.07	113.99	120.42
1	A	110	THR	CA-C-O	-6.05	114.97	121.56
1	B	94	ILE	CB-CG1-CD1	6.05	126.50	113.80
1	B	68	GLU	CB-CA-C	-6.04	100.76	110.79
1	D	146	GLN	OE1-CD-NE2	6.04	128.64	122.60
1	B	68	GLU	CB-CG-CD	6.04	122.87	112.60
1	D	104	LYS	CA-CB-CG	6.03	126.17	114.10
1	C	35	ALA	O-C-N	6.03	130.02	122.43
1	D	146	GLN	CA-C-N	6.03	131.70	122.24
1	D	146	GLN	C-N-CA	6.03	131.70	122.24
1	B	50	GLU	CB-CG-CD	6.03	122.84	112.60
1	A	24	LEU	CA-C-O	6.02	126.93	120.55
1	D	14	VAL	CA-C-N	-6.02	115.07	123.13
1	D	14	VAL	C-N-CA	-6.02	115.07	123.13
1	B	155	SER	O-C-N	6.01	130.59	122.59
1	C	184	ARG	CA-C-O	-6.01	113.06	119.97
1	D	112	GLU	CB-CG-CD	6.01	122.81	112.60
1	B	83	GLY	N-CA-C	6.00	121.83	114.69
1	B	189	ILE	CA-C-O	-6.00	113.58	120.42
1	B	110	THR	CA-C-O	-5.99	114.59	121.47
1	A	109	HIS	CA-C-N	-5.98	111.55	120.94
1	A	109	HIS	C-N-CA	-5.98	111.55	120.94
1	C	191	ILE	CA-C-O	-5.98	114.17	120.39
1	A	8	VAL	CB-CA-C	-5.97	104.18	112.36
1	D	61	ALA	O-C-N	-5.96	114.51	120.83
1	B	235	HIS	O-C-N	5.95	128.43	122.12
1	A	49	THR	CA-CB-OG1	-5.95	100.67	109.60
1	C	227	LEU	CA-C-N	5.95	125.75	120.10
1	C	227	LEU	C-N-CA	5.95	125.75	120.10
1	D	238[A]	GLN	O-C-N	5.95	128.43	122.12
1	D	238[B]	GLN	O-C-N	5.95	128.43	122.12
1	C	82	PHE	CA-C-N	5.95	132.14	122.09
1	C	82	PHE	C-N-CA	5.95	132.14	122.09
1	A	252	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	A	123	ILE	CA-C-O	-5.94	114.77	120.95
1	D	217	LEU	CA-C-N	5.92	129.02	120.79
1	D	217	LEU	C-N-CA	5.92	129.02	120.79
1	C	146	GLN	OE1-CD-NE2	5.92	128.51	122.60
1	A	235	HIS	N-CA-CB	-5.91	101.42	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	PHE	O-C-N	-5.91	116.49	123.22
1	B	8	VAL	CB-CA-C	-5.90	104.45	111.65
1	C	119	ASN	O-C-N	5.90	128.37	122.12
1	A	165	GLN	O-C-N	-5.89	114.67	122.20
1	C	226	ARG	O-C-N	5.89	129.44	123.26
1	C	184	ARG	NE-CZ-NH2	-5.88	113.90	119.20
1	B	176	VAL	N-CA-CB	-5.88	103.67	110.55
1	D	215	ASN	CA-C-O	5.88	126.74	120.10
1	C	68	GLU	N-CA-CB	-5.87	101.49	110.01
1	C	226	ARG	CA-C-O	-5.87	115.15	121.38
1	C	22	LEU	O-C-N	5.87	129.49	122.27
1	A	128	VAL	O-C-N	-5.87	115.78	121.83
1	D	148	GLY	CA-C-N	-5.87	114.26	122.71
1	D	148	GLY	C-N-CA	-5.87	114.26	122.71
1	B	173	GLY	N-CA-C	-5.86	105.08	113.86
1	D	89	VAL	CA-C-O	5.86	126.05	120.31
1	B	9	LYS	CA-C-N	-5.86	113.37	122.86
1	B	9	LYS	C-N-CA	-5.86	113.37	122.86
1	B	127	ASN	OD1-CG-ND2	5.85	128.45	122.60
1	B	179	THR	CA-C-O	-5.85	114.67	120.82
1	A	258	ARG	NE-CZ-NH2	-5.84	113.94	119.20
1	B	154	ALA	CA-C-O	-5.83	112.17	120.51
1	D	20	SER	N-CA-CB	-5.83	102.35	111.56
1	C	168	TYR	O-C-N	5.83	128.79	122.15
1	C	62	PRO	N-CA-CB	5.83	108.49	103.36
1	C	121	ASN	O-C-N	5.82	128.38	122.09
1	A	152	ASN	CA-C-N	-5.82	114.57	123.07
1	A	152	ASN	C-N-CA	-5.82	114.57	123.07
1	D	216	PHE	CA-CB-CG	-5.82	107.98	113.80
1	A	29	ARG	CA-C-O	-5.81	114.72	120.82
1	A	44	ASN	CA-C-O	5.81	126.53	119.38
1	B	36[A]	THR	CA-C-N	-5.81	113.32	122.73
1	B	36[A]	THR	C-N-CA	-5.81	113.32	122.73
1	B	36[B]	THR	CA-C-N	-5.81	113.32	122.73
1	B	36[B]	THR	C-N-CA	-5.81	113.32	122.73
1	B	70	GLU	CG-CD-OE1	5.81	131.75	118.40
1	C	112	GLU	N-CA-CB	-5.80	101.28	110.22
1	A	50	GLU	CA-C-O	-5.79	114.41	120.55
1	B	72	GLN	CA-C-O	-5.79	114.41	120.55
1	D	11	LEU	O-C-N	-5.79	116.42	122.96
1	C	193	VAL	CA-CB-CG2	5.78	120.22	110.40
1	B	34	GLY	CA-C-O	5.78	125.20	118.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ASN	OD1-CG-ND2	5.75	128.35	122.60
1	C	48	GLU	OE1-CD-OE2	5.75	136.71	122.90
1	A	150	ILE	CA-C-O	-5.75	114.38	120.48
1	B	43	PRO	O-C-N	-5.74	114.52	122.27
1	C	82	PHE	CA-C-O	5.74	125.36	119.05
1	C	123	ILE	CB-CA-C	-5.74	102.97	112.26
1	B	83	GLY	CA-C-O	5.73	125.41	119.27
1	D	242	GLU	N-CA-C	5.73	119.53	112.54
1	C	190	GLY	CA-C-N	-5.72	115.49	123.10
1	C	190	GLY	C-N-CA	-5.72	115.49	123.10
1	B	202	ALA	O-C-N	-5.72	114.98	122.59
1	B	144	GLY	O-C-N	-5.71	115.27	122.70
1	B	26	THR	CA-CB-CG2	5.71	120.21	110.50
1	A	17	GLY	CA-C-O	5.71	127.00	119.58
1	B	28	LYS	CA-C-N	-5.70	113.03	120.44
1	B	28	LYS	C-N-CA	-5.70	113.03	120.44
1	B	140	GLU	CG-CD-OE1	5.70	131.50	118.40
1	C	71	VAL	CA-C-O	-5.68	114.33	120.47
1	D	116	ARG	NH1-CZ-NH2	5.68	126.68	119.30
1	D	25	SER	O-C-N	-5.67	115.29	122.27
1	A	42	VAL	CA-CB-CG2	5.67	120.04	110.40
1	C	184	ARG	CA-CB-CG	-5.67	102.76	114.10
1	B	217	LEU	O-C-N	5.67	127.91	122.07
1	D	149	VAL	CA-C-O	-5.66	114.53	120.76
1	C	56	GLY	CA-C-N	-5.66	112.83	122.56
1	C	56	GLY	C-N-CA	-5.66	112.83	122.56
1	C	185	ASP	CB-CA-C	-5.65	101.41	110.79
1	A	173	GLY	N-CA-C	-5.65	105.80	113.37
1	C	243	ASN	CA-C-O	5.65	123.50	119.32
1	B	113	ASP	CA-C-N	-5.65	112.27	120.29
1	B	113	ASP	C-N-CA	-5.65	112.27	120.29
1	A	80	GLU	CA-C-O	-5.65	114.88	120.70
1	A	160	GLU	CG-CD-OE2	-5.64	105.42	118.40
1	C	149	VAL	O-C-N	5.64	129.17	123.07
1	C	61	ALA	O-C-N	-5.63	114.86	120.83
1	C	151	ILE	CA-C-N	-5.63	113.01	122.92
1	C	151	ILE	C-N-CA	-5.63	113.01	122.92
1	B	123	ILE	CB-CG1-CD1	-5.62	102.00	113.80
1	D	155	SER	CA-C-O	-5.62	114.82	121.06
1	C	106	ASN	OD1-CG-ND2	5.62	128.22	122.60
1	B	106	ASN	CB-CG-ND2	5.61	124.82	116.40
1	D	71	VAL	CA-CB-CG2	-5.61	100.87	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	GLN	CG-CD-OE1	-5.60	109.60	120.80
1	C	130	ARG	CG-CD-NE	-5.60	99.68	112.00
1	B	151	ILE	O-C-N	5.60	129.13	123.20
1	A	19	ALA	N-CA-C	5.57	119.92	113.18
1	D	147	ARG	N-CA-CB	5.57	118.31	110.90
1	A	158	ALA	CA-C-O	5.56	126.22	119.38
1	A	12	VAL	O-C-N	5.56	129.60	123.10
1	D	196	ILE	CA-C-O	5.56	127.06	120.72
1	B	43	PRO	CA-C-O	5.56	127.51	119.34
1	C	243	ASN	CA-CB-CG	-5.56	107.04	112.60
1	D	227	LEU	N-CA-C	-5.56	103.19	110.53
1	B	91	CYS	N-CA-C	-5.55	106.34	114.39
1	D	44	ASN	CB-CA-C	5.55	120.62	110.36
1	B	71	VAL	O-C-N	5.55	127.54	121.83
1	C	57	ASN	CA-CB-CG	-5.54	107.06	112.60
1	C	236	LEU	N-CA-C	-5.54	105.32	111.36
1	C	162	GLN	CA-C-O	5.54	128.14	121.88
1	B	133	ALA	CA-C-N	-5.54	113.36	120.34
1	B	133	ALA	C-N-CA	-5.54	113.36	120.34
1	A	61	ALA	O-C-N	-5.53	115.62	121.04
1	A	112	GLU	CG-CD-OE2	-5.52	105.70	118.40
1	C	168	TYR	CA-C-O	-5.52	114.57	120.42
1	A	254	ASP	N-CA-CB	-5.52	101.16	110.49
1	C	195	THR	CA-C-N	-5.51	116.00	123.10
1	C	195	THR	C-N-CA	-5.51	116.00	123.10
1	D	31	VAL	CA-C-N	5.50	126.09	119.98
1	D	31	VAL	C-N-CA	5.50	126.09	119.98
1	B	151	ILE	CA-C-O	-5.49	114.68	120.39
1	A	76	THR	CA-C-N	5.48	127.56	120.44
1	A	76	THR	C-N-CA	5.48	127.56	120.44
1	C	126	PHE	O-C-N	5.47	128.62	122.22
1	B	252	ARG	NH1-CZ-NH2	-5.47	112.19	119.30
1	B	71	VAL	CA-C-N	-5.46	112.96	120.28
1	B	71	VAL	C-N-CA	-5.46	112.96	120.28
1	D	141	PRO	CA-C-O	-5.46	115.12	121.34
1	C	136	MET	N-CA-C	-5.45	105.89	112.54
1	A	147	ARG	NH1-CZ-NH2	-5.45	112.22	119.30
1	D	86	ASP	CA-CB-CG	-5.45	107.15	112.60
1	C	13	ALA	N-CA-CB	-5.44	101.54	110.68
1	B	130	ARG	O-C-N	5.44	128.35	122.15
1	D	119	ASN	N-CA-CB	-5.43	102.10	110.20
1	A	107	GLN	CA-C-O	-5.43	114.84	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	ASN	OD1-CG-ND2	5.43	128.03	122.60
1	A	44	ASN	CB-CA-C	5.42	121.65	110.31
1	A	242	GLU	CA-C-N	-5.42	114.58	121.74
1	A	242	GLU	C-N-CA	-5.42	114.58	121.74
1	C	142	ASP	CA-CB-CG	5.42	118.02	112.60
1	C	239[A]	MET	CB-CA-C	-5.42	100.60	110.63
1	C	239[B]	MET	CB-CA-C	-5.42	100.60	110.63
1	A	119	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	C	118	ILE	CA-C-N	5.42	127.54	120.28
1	C	118	ILE	C-N-CA	5.42	127.54	120.28
1	D	124	GLY	O-C-N	-5.42	116.94	122.19
1	D	103	GLU	CA-C-O	-5.41	115.31	121.00
1	B	107	GLN	CA-C-O	-5.41	114.37	120.32
1	B	140	GLU	O-C-N	5.41	127.49	121.43
1	B	168	TYR	N-CA-CB	-5.41	102.17	110.12
1	B	64	ASN	N-CA-CB	-5.40	101.48	110.23
1	D	218	ALA	O-C-N	5.40	127.85	122.08
1	D	8	VAL	N-CA-C	-5.39	107.73	112.90
1	A	20	SER	N-CA-CB	-5.39	103.05	111.56
1	A	64	ASN	N-CA-CB	-5.38	101.27	110.16
1	B	88	ALA	O-C-N	5.38	129.61	123.31
1	D	162	GLN	O-C-N	-5.37	115.55	122.20
1	D	96	VAL	O-C-N	5.36	128.66	122.82
1	B	72	GLN	N-CA-CB	5.35	117.99	110.12
1	D	83	GLY	N-CA-C	5.35	122.16	115.21
1	D	189	ILE	CA-C-O	-5.35	113.12	119.54
1	D	234	ALA	O-C-N	5.34	127.78	122.12
1	C	238[A]	GLN	CA-C-N	-5.34	112.59	120.28
1	C	238[A]	GLN	C-N-CA	-5.34	112.59	120.28
1	C	238[B]	GLN	CA-C-N	-5.34	112.59	120.28
1	C	238[B]	GLN	C-N-CA	-5.34	112.59	120.28
1	B	14	VAL	CA-C-O	-5.33	114.83	120.48
1	C	252	ARG	CB-CA-C	-5.33	100.74	109.53
1	A	141	PRO	CA-C-O	-5.32	115.28	121.34
1	D	100	THR	N-CA-C	-5.32	105.48	111.28
1	A	225[A]	SER	N-CA-C	5.31	117.84	109.39
1	A	225[B]	SER	N-CA-C	5.31	117.84	109.39
1	A	247	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	C	226	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	C	184	ARG	NH1-CZ-NH2	5.30	126.19	119.30
1	B	184	ARG	N-CA-CB	5.30	117.70	110.01
1	C	169	SER	N-CA-C	5.30	117.06	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	216	PHE	CA-C-N	5.30	131.66	121.54
1	D	216	PHE	C-N-CA	5.30	131.66	121.54
1	B	38	VAL	CA-C-N	-5.30	114.04	121.72
1	B	38	VAL	C-N-CA	-5.30	114.04	121.72
1	B	202	ALA	CA-C-O	5.30	128.08	120.51
1	C	188	PRO	N-CA-CB	5.29	108.78	103.48
1	A	241	ILE	CA-CB-CG2	-5.29	101.51	110.50
1	A	24	LEU	N-CA-C	5.29	117.05	111.28
1	B	71	VAL	CA-C-O	-5.29	115.24	120.85
1	B	175	ILE	CA-C-N	-5.29	113.90	120.56
1	B	175	ILE	C-N-CA	-5.29	113.90	120.56
1	D	22	LEU	CA-C-O	5.29	126.16	120.55
1	A	241	ILE	CA-C-O	-5.29	115.57	121.17
1	A	252	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	C	26	THR	CA-CB-OG1	-5.27	101.70	109.60
1	D	46	GLU	CA-CB-CG	5.26	124.62	114.10
1	A	164	GLY	CA-C-N	-5.25	114.82	122.86
1	A	164	GLY	C-N-CA	-5.25	114.82	122.86
1	C	183	ALA	CA-C-O	-5.25	114.86	120.42
1	B	141	PRO	CB-CA-C	-5.24	104.52	111.23
1	A	80	GLU	N-CA-CB	5.24	117.66	110.07
1	D	105	LYS	CA-C-N	5.24	129.84	122.46
1	D	105	LYS	C-N-CA	5.24	129.84	122.46
1	D	192	ARG	CD-NE-CZ	5.24	131.73	124.40
1	C	34	GLY	CA-C-O	5.23	124.61	118.96
1	C	126	PHE	CG-CD2-CE2	-5.23	111.81	120.70
1	C	25	SER	N-CA-C	-5.23	105.66	111.36
1	B	82	PHE	O-C-N	-5.22	116.16	122.48
1	B	220	GLN	OE1-CD-NE2	5.22	127.82	122.60
1	A	78	ALA	O-C-N	-5.22	116.69	122.07
1	C	128	VAL	N-CA-C	-5.21	105.63	110.53
1	C	61	ALA	CA-C-O	5.21	124.53	119.99
1	B	46	GLU	CG-CD-OE2	5.21	130.38	118.40
1	A	52	LYS	O-C-N	-5.21	116.47	122.09
1	D	106	ASN	CA-C-N	5.19	130.31	122.99
1	D	106	ASN	C-N-CA	5.19	130.31	122.99
1	C	177	GLY	CA-C-O	-5.18	114.80	120.40
1	C	192	ARG	CA-CB-CG	-5.18	103.74	114.10
1	B	96	VAL	CA-C-O	-5.18	116.51	121.63
1	A	143	GLN	CG-CD-OE1	5.17	131.15	120.80
1	B	219	SER	N-CA-C	5.17	118.69	112.38
1	B	14	VAL	CA-CB-CG2	-5.17	101.61	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	ILE	CA-C-O	5.17	126.33	120.95
1	A	192	ARG	CA-CB-CG	-5.17	103.77	114.10
1	B	96	VAL	N-CA-CB	5.16	121.91	112.36
1	A	77	LEU	CA-C-N	-5.16	113.73	120.44
1	A	77	LEU	C-N-CA	-5.16	113.73	120.44
1	A	102	HIS	CA-C-O	5.16	126.41	120.84
1	C	145	GLY	CA-C-N	-5.16	114.45	122.09
1	C	145	GLY	C-N-CA	-5.16	114.45	122.09
1	D	154	ALA	O-C-N	5.16	125.34	121.47
1	A	114	PHE	N-CA-C	5.14	116.69	111.14
1	C	159	PHE	N-CA-C	-5.12	106.98	113.43
1	B	15	ILE	CA-CB-CG2	5.12	119.20	110.50
1	D	94	ILE	CA-C-N	-5.12	113.92	122.21
1	D	94	ILE	C-N-CA	-5.12	113.92	122.21
1	A	127	ASN	CB-CG-ND2	-5.12	108.73	116.40
1	D	252	ARG	NH1-CZ-NH2	-5.11	112.65	119.30
1	D	245	PHE	CA-C-N	-5.10	114.20	121.50
1	D	245	PHE	C-N-CA	-5.10	114.20	121.50
1	B	236	LEU	O-C-N	-5.10	116.33	122.15
1	C	70	GLU	CA-C-O	5.10	125.83	120.42
1	B	50	GLU	O-C-N	5.10	127.52	122.12
1	A	258	ARG	N-CA-CB	5.09	119.60	110.80
1	B	52	LYS	CG-CD-CE	5.09	123.00	111.30
1	C	55	GLY	O-C-N	-5.08	117.78	122.86
1	A	226	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	A	96	VAL	N-CA-CB	5.08	120.97	112.44
1	B	140	GLU	CB-CG-CD	5.08	121.23	112.60
1	C	102	HIS	CA-CB-CG	-5.07	108.73	113.80
1	D	118	ILE	CA-C-O	5.07	125.95	120.47
1	C	88	ALA	CA-C-N	-5.07	115.78	122.98
1	C	88	ALA	C-N-CA	-5.07	115.78	122.98
1	C	164	GLY	O-C-N	5.07	128.64	122.60
1	B	49	THR	N-CA-C	5.07	116.81	111.28
1	C	197	ALA	O-C-N	-5.07	115.29	121.02
1	A	249	GLU	CA-CB-CG	5.06	124.22	114.10
1	B	194	VAL	CA-C-N	-5.06	115.34	122.94
1	B	194	VAL	C-N-CA	-5.06	115.34	122.94
1	B	103	GLU	N-CA-C	5.06	116.87	111.36
1	C	9	LYS	N-CA-CB	-5.05	102.32	109.85
1	C	113	ASP	CA-C-O	-5.04	115.08	120.42
1	A	55	GLY	O-C-N	-5.04	117.81	123.10
1	D	159	PHE	CA-C-O	-5.04	113.64	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	190	GLY	CA-C-N	-5.04	116.38	123.13
1	D	190	GLY	C-N-CA	-5.04	116.38	123.13
1	A	106	ASN	CA-C-N	-5.04	115.39	122.94
1	A	106	ASN	C-N-CA	-5.04	115.39	122.94
1	A	228	GLY	CA-C-O	-5.04	115.97	121.71
1	C	253	LEU	CA-C-N	-5.03	111.93	121.54
1	C	253	LEU	C-N-CA	-5.03	111.93	121.54
1	B	112[A]	GLU	CA-C-O	-5.03	115.22	120.55
1	B	112[B]	GLU	CA-C-O	-5.03	115.22	120.55
1	D	14	VAL	CA-C-O	-5.03	115.19	120.57
1	A	213	VAL	N-CA-C	-5.03	106.25	111.58
1	D	167	ALA	N-CA-CB	-5.03	102.72	110.16
1	B	20	SER	N-CA-CB	-5.02	103.28	111.66
1	D	162	GLN	CA-C-O	5.02	127.90	121.82
1	D	147	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	A	16	THR	N-CA-CB	5.02	117.91	110.29
1	A	242	GLU	CA-C-O	-5.01	114.21	119.97
1	B	166	ALA	CA-C-O	-5.01	115.56	120.82
1	A	222	PRO	O-C-N	-5.00	115.89	122.64
1	A	260[A]	GLN	CA-C-O	5.00	126.41	120.96
1	A	260[B]	GLN	CA-C-O	5.00	126.41	120.96

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	HIS	Mainchain
1	A	105	LYS	Mainchain
1	A	120	VAL	Mainchain
1	A	139	ASN	Mainchain
1	A	144	GLY	Mainchain
1	A	199	GLY	Mainchain
1	A	217	LEU	Mainchain
1	A	24	LEU	Mainchain
1	A	7	SER	Mainchain
1	B	10	GLY	Mainchain
1	B	144	GLY	Mainchain
1	B	17	GLY	Mainchain
1	B	189	ILE	Mainchain
1	B	205	LEU	Mainchain
1	B	222	PRO	Mainchain
1	B	61	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	B	64	ASN	Mainchain
1	B	80	GLU	Mainchain
1	B	81	LYS	Mainchain
1	C	123	ILE	Mainchain
1	C	138	GLN	Mainchain
1	C	143	GLN	Mainchain
1	C	199	GLY	Mainchain
1	C	203	THR	Mainchain
1	C	228	GLY	Mainchain
1	C	251	ILE	Mainchain
1	C	47	GLY	Mainchain
1	C	58	CYS	Mainchain
1	C	81	LYS	Mainchain
1	C	84[A]	ARG	Mainchain
1	C	84[B]	ARG	Mainchain
1	D	135	VAL	Mainchain
1	D	137	GLY	Mainchain
1	D	169	SER	Mainchain
1	D	199	GLY	Mainchain
1	D	205	LEU	Mainchain
1	D	211	ASP	Mainchain
1	D	42	VAL	Mainchain
1	D	47	GLY	Mainchain
1	D	51	ALA	Mainchain
1	D	91	CYS	Mainchain

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	1841	0	1864	57	2
1	B	1848	0	1916	50	4
1	C	1820	0	1872	59	2
1	D	1856	0	1889	45	6
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	2	0
2	D	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	20	0	21	11	0
4	A	146	0	0	16	1
4	B	128	0	0	12	3
4	C	143	0	0	14	3
4	D	128	0	0	11	1
All	All	8106	0	7666	197	11

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (197) 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:D:239:MET:HG2	4:D:515:HOH:O	1.63	0.98
1:A:29:ARG:HE	1:A:238[B]:GLN:NE2	1.62	0.95
1:D:29:ARG:HE	1:D:238[B]:GLN:NE2	1.64	0.94
1:D:29:ARG:HH21	1:D:238[B]:GLN:HE22	0.96	0.94
1:D:29:ARG:HE	1:D:238[B]:GLN:HE21	0.94	0.93
1:A:239[A]:MET:CG	1:C:239[A]:MET:HG3	2.01	0.91
1:C:101:TYR:HE2	4:C:407:HOH:O	1.52	0.91
1:B:141:PRO:CD	4:B:519:HOH:O	2.19	0.90
1:A:239[A]:MET:HG3	1:C:239[A]:MET:HG3	1.54	0.89
1:B:29:ARG:HH21	1:B:238[B]:GLN:HE22	1.12	0.89
1:D:29:ARG:HH21	1:D:238[B]:GLN:NE2	1.72	0.87
1:C:206:LEU:HD23	3:C:302:EST:H151	1.55	0.87
1:B:29:ARG:NH2	1:B:238[B]:GLN:HE22	1.73	0.86
1:C:29:ARG:HH21	1:C:238[B]:GLN:HE22	1.20	0.85
1:D:29:ARG:NE	1:D:238[B]:GLN:HE21	1.77	0.82
1:A:103:GLU:OE2	1:B:188:PRO:HB2	1.81	0.81
1:B:29:ARG:HE	1:B:238[B]:GLN:HE21	1.28	0.81
1:C:12:VAL:HG23	1:C:84[A]:ARG:NH1	1.96	0.81
1:A:29:ARG:HE	1:A:238[B]:GLN:HE21	1.24	0.80
1:B:29:ARG:HH21	1:B:238[B]:GLN:NE2	1.80	0.80
1:D:29:ARG:NH2	1:D:238[B]:GLN:HE22	1.78	0.80
1:D:79:LYS:HE3	4:D:496:HOH:O	1.83	0.79
1:B:141:PRO:CG	4:B:519:HOH:O	2.30	0.79
1:B:29:ARG:HE	1:B:238[B]:GLN:NE2	1.81	0.78
1:B:46:GLU:HG2	4:B:522:HOH:O	1.82	0.78
1:C:29:ARG:HE	1:C:238[B]:GLN:NE2	1.81	0.78
1:C:46:GLU:HG3	4:C:426:HOH:O	1.84	0.77
1:C:101:TYR:CE2	4:C:407:HOH:O	2.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LYS:HA	4:A:405:HOH:O	1.85	0.76
1:C:29:ARG:HE	1:C:238[B]:GLN:HE21	1.33	0.74
1:A:36[A]:THR:HG23	4:A:464:HOH:O	1.90	0.71
1:A:239[A]:MET:HG3	1:C:239[A]:MET:CG	2.20	0.71
1:C:99:LYS:HD3	4:D:513:HOH:O	1.90	0.70
1:D:36:THR:HG23	4:D:468:HOH:O	1.91	0.70
1:A:106:ASN:HB3	4:A:517:HOH:O	1.92	0.70
1:A:29:ARG:HH21	1:A:238[B]:GLN:HE22	1.42	0.67
1:C:44:ASN:HB2	4:C:502:HOH:O	1.94	0.67
1:B:260:GLN:NE2	4:B:402:HOH:O	2.28	0.66
1:A:29:ARG:NE	1:A:238[B]:GLN:NE2	2.41	0.66
1:B:29:ARG:NE	1:B:238[B]:GLN:HE21	1.94	0.66
1:B:116[A]:ARG:HH11	1:B:116[A]:ARG:HB3	1.60	0.65
1:D:29:ARG:NE	1:D:238[B]:GLN:NE2	2.40	0.65
1:B:29:ARG:NE	1:B:238[B]:GLN:NE2	2.43	0.65
1:B:220:GLN:HB3	4:B:402:HOH:O	1.96	0.64
1:B:207:THR:HG21	4:B:465:HOH:O	1.97	0.64
1:A:115[B]:GLN:NE2	1:B:123:ILE:HD13	2.13	0.64
1:A:239[A]:MET:HB2	1:C:239[A]:MET:HG3	1.79	0.64
1:C:206:LEU:CD2	3:C:302:EST:H151	2.27	0.63
2:C:301:NAD:O7N	3:C:302:EST:H162	1.98	0.63
1:B:68:GLU:OE2	1:B:72:GLN:NE2	2.31	0.63
1:A:239[B]:MET:CG	1:C:239[B]:MET:HG3	2.29	0.63
3:C:302:EST:H112	4:C:462:HOH:O	1.98	0.62
1:C:29:ARG:HH21	1:C:238[B]:GLN:NE2	1.96	0.61
1:B:239:MET:CB	1:D:239:MET:HG3	2.30	0.61
1:A:105:LYS:HD3	1:A:107:GLN:NE2	2.16	0.61
3:C:302:EST:H1	4:C:462:HOH:O	1.99	0.61
1:A:207:THR:HA	4:A:542:HOH:O	1.99	0.61
1:B:29:ARG:NH2	1:B:238[B]:GLN:NE2	2.44	0.60
1:C:116:ARG:HD3	4:C:410:HOH:O	2.00	0.60
1:A:33[B]:GLN:HE22	1:A:238[B]:GLN:NE2	1.98	0.60
1:B:104:LYS:HG3	1:B:105:LYS:HD2	1.83	0.60
1:D:105:LYS:HG3	4:D:485:HOH:O	2.00	0.60
1:B:68:GLU:O	1:B:72:GLN:HG3	2.02	0.59
1:B:260:GLN:HG2	4:B:449:HOH:O	2.02	0.59
1:C:49:THR:HG23	4:C:520:HOH:O	2.01	0.59
1:A:239[B]:MET:HG2	1:C:239[B]:MET:CG	2.32	0.59
1:C:165:GLN:HE22	3:C:302:EST:H121	1.67	0.59
1:C:165:GLN:NE2	3:C:302:EST:H121	2.19	0.58
1:C:29:ARG:NH2	1:C:238[B]:GLN:HE22	1.97	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239[B]:MET:HE1	1:C:246:LEU:HD21	1.86	0.58
1:C:84[A]:ARG:CZ	1:C:86:ASP:OD2	2.52	0.58
1:B:116[A]:ARG:HB3	1:B:116[A]:ARG:NH1	2.19	0.58
1:A:99:LYS:HD3	4:A:407:HOH:O	2.03	0.57
1:B:217:LEU:HB2	4:B:405:HOH:O	2.04	0.57
1:D:69:LYS:HG3	4:D:404:HOH:O	2.05	0.57
1:C:204:PRO:O	1:C:207:THR:N	2.38	0.56
1:A:142:ASP:HB2	4:A:438:HOH:O	2.05	0.56
2:C:301:NAD:C7N	3:C:302:EST:H162	2.36	0.56
1:A:239[B]:MET:CG	1:C:239[B]:MET:CG	2.85	0.55
1:A:44:ASN:HB2	4:A:417:HOH:O	2.06	0.55
1:A:223:PHE:CD1	1:A:224:PRO:HA	2.41	0.55
1:B:216:PHE:N	4:B:404:HOH:O	2.40	0.55
1:A:108:VAL:HG12	4:A:489:HOH:O	2.08	0.54
1:B:200:LEU:HD13	1:B:217:LEU:HB3	1.89	0.54
1:A:239[A]:MET:CG	1:C:239[A]:MET:CG	2.79	0.54
1:A:239[B]:MET:HG2	1:C:239[B]:MET:HG3	1.87	0.54
1:A:201:PHE:O	1:A:206:LEU:HD22	2.07	0.53
1:C:102:HIS:CD2	1:C:105:LYS:HG3	2.43	0.53
1:D:29:ARG:NH2	1:D:238[B]:GLN:NE2	2.45	0.53
1:A:33[B]:GLN:HE22	1:A:238[B]:GLN:CD	2.17	0.53
1:C:36:THR:HG23	4:C:463:HOH:O	2.08	0.53
1:B:102:HIS:CD2	1:B:104:LYS:HG2	2.44	0.52
1:D:254:ASP:HB2	1:D:257:ILE:HG22	1.91	0.52
1:A:12:VAL:HG23	1:A:84:ARG:NH1	2.23	0.52
1:A:12:VAL:HG23	1:A:84:ARG:HH11	1.74	0.52
1:D:203:THR:HB	1:D:204:PRO:CD	2.40	0.52
1:A:143:GLN:HG3	4:A:438:HOH:O	2.10	0.51
1:B:68:GLU:HG2	1:B:72:GLN:HE21	1.74	0.51
1:B:84[A]:ARG:NH1	1:B:86:ASP:OD2	2.43	0.51
1:B:102:HIS:NE2	1:B:104:LYS:HG2	2.25	0.51
1:A:44:ASN:ND2	4:A:402:HOH:O	2.35	0.51
1:C:115[A]:GLN:OE1	1:D:123[A]:ILE:HD13	2.10	0.51
1:A:29:ARG:NH2	1:A:238[B]:GLN:HE22	2.09	0.51
1:C:103:GLU:O	1:C:106:ASN:N	2.37	0.51
1:D:216:PHE:CD1	1:D:216:PHE:N	2.79	0.51
1:C:29:ARG:NE	1:C:238[B]:GLN:NE2	2.55	0.50
1:C:29:ARG:NE	1:C:238[B]:GLN:HE21	2.06	0.50
1:C:101:TYR:OH	1:C:106:ASN:ND2	2.41	0.50
1:C:134:GLY:HA2	4:C:403:HOH:O	2.11	0.50
1:D:216:PHE:O	1:D:219:SER:OG	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:VAL:HG21	4:A:479:HOH:O	2.12	0.50
1:D:95:ALA:HB3	1:D:208:THR:HG21	1.92	0.50
1:B:227:LEU:N	4:B:401:HOH:O	1.77	0.50
1:C:103:GLU:O	1:C:104:LYS:C	2.51	0.50
1:C:105:LYS:O	1:C:106:ASN:C	2.54	0.50
1:A:33[B]:GLN:NE2	1:A:238[B]:GLN:NE2	2.60	0.49
1:A:52:LYS:CD	4:A:420:HOH:O	2.60	0.49
1:A:187:ALA:N	1:A:188:PRO:HD2	2.26	0.49
1:A:195:THR:HB	1:A:250:VAL:HG22	1.94	0.49
1:D:119:ASN:HB3	4:D:509:HOH:O	2.12	0.48
1:D:154:ALA:HA	1:D:172:LYS:HD2	1.94	0.48
3:C:302:EST:H122	4:C:464:HOH:O	2.13	0.48
1:D:36:THR:HG22	1:D:57:ASN:HB3	1.95	0.48
1:B:68:GLU:HG3	1:B:130:ARG:NH2	2.28	0.48
1:D:101:TYR:HD1	1:D:108:VAL:HG22	1.78	0.48
1:A:37:ALA:O	1:A:58:CYS:HA	2.13	0.48
1:A:260[B]:GLN:HG2	4:A:474:HOH:O	2.14	0.48
1:C:115[A]:GLN:CD	1:D:123[A]:ILE:HD13	2.39	0.48
1:C:206:LEU:O	1:C:207:THR:C	2.56	0.48
1:A:44:ASN:CB	4:A:417:HOH:O	2.61	0.47
1:A:239[A]:MET:SD	1:A:246:LEU:CD2	3.02	0.47
1:A:12:VAL:HG22	1:A:36[A]:THR:OG1	2.15	0.47
1:B:239:MET:HG3	1:D:239:MET:HG3	1.96	0.47
1:C:12:VAL:HG23	1:C:84[A]:ARG:HH12	1.76	0.47
1:C:239[B]:MET:SD	1:C:246:LEU:CD2	3.03	0.47
1:B:201:PHE:O	1:B:206:LEU:HD12	2.15	0.46
1:A:187:ALA:N	1:A:188:PRO:CD	2.78	0.46
1:A:239[B]:MET:HG2	1:C:239[B]:MET:HG2	1.96	0.46
1:B:36[B]:THR:HG21	1:B:82:PHE:CE1	2.50	0.46
1:D:84:ARG:HH11	1:D:84:ARG:HD2	1.49	0.46
1:D:239:MET:SD	4:D:515:HOH:O	2.61	0.46
1:D:119:ASN:CB	4:D:509:HOH:O	2.64	0.46
1:B:217:LEU:N	4:B:405:HOH:O	2.49	0.46
1:D:223:PHE:CD1	1:D:224:PRO:HA	2.51	0.45
1:C:69:LYS:HE3	4:C:531:HOH:O	2.16	0.45
1:A:105:LYS:HE2	1:A:107:GLN:NE2	2.31	0.45
1:D:79:LYS:NZ	1:D:138:GLN:OE1	2.35	0.45
1:B:68:GLU:HG2	1:B:72:GLN:NE2	2.30	0.45
1:D:246:LEU:HD21	1:D:251:ILE:HD11	1.99	0.45
1:A:29:ARG:NE	1:A:238[B]:GLN:HE21	2.04	0.45
1:A:138:GLN:OE1	1:A:138:GLN:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ARG:HD2	1:C:246:LEU:O	2.17	0.45
1:A:102:HIS:NE2	1:A:104:LYS:HE2	2.33	0.44
1:C:84[B]:ARG:NH2	1:C:139:ASN:HB3	2.32	0.44
1:D:182:ILE:HD13	1:D:182:ILE:HG21	1.78	0.44
1:D:101:TYR:CD1	1:D:108:VAL:HG22	2.52	0.44
1:D:195:THR:HB	1:D:250:VAL:HG22	1.99	0.44
4:C:455:HOH:O	1:D:99:LYS:HD3	2.18	0.44
1:D:195:THR:O	1:D:250:VAL:HA	2.18	0.44
1:C:84[B]:ARG:HH21	1:C:139:ASN:HB3	1.83	0.43
1:C:44:ASN:O	1:C:44:ASN:ND2	2.51	0.43
1:A:123:ILE:HD13	1:B:115[B]:GLN:OE1	2.18	0.43
1:C:115[A]:GLN:HG3	1:C:119:ASN:ND2	2.33	0.43
1:B:257:ILE:HG21	1:B:257:ILE:HD13	1.82	0.43
1:C:46:GLU:CG	4:C:426:HOH:O	2.56	0.43
1:B:99[B]:LYS:HD2	1:B:102:HIS:ND1	2.33	0.43
1:C:37:ALA:O	1:C:58:CYS:HA	2.19	0.43
1:D:204:PRO:HD2	2:D:301:NAD:O2A	2.19	0.43
1:A:200:LEU:HB2	4:A:479:HOH:O	2.18	0.43
1:D:243:ASN:HA	1:D:244:PRO:HD3	1.90	0.43
1:C:206:LEU:CD2	3:C:302:EST:H72	2.49	0.42
1:D:112:GLU:HB3	4:D:435:HOH:O	2.20	0.42
1:A:61:ALA:HA	1:A:62:PRO:HD2	1.91	0.42
1:A:103:GLU:H	1:A:103:GLU:HG3	1.28	0.42
1:B:16:THR:HG21	1:B:128:VAL:HG21	2.02	0.42
1:B:187:ALA:HB3	1:B:188:PRO:HD3	2.01	0.42
1:B:187:ALA:N	1:B:188:PRO:CD	2.82	0.42
1:D:54:LEU:HD23	1:D:54:LEU:HA	1.88	0.42
1:D:239:MET:CG	4:D:515:HOH:O	2.40	0.42
1:C:99:LYS:O	1:C:109:HIS:HB2	2.19	0.42
1:C:206:LEU:HD23	3:C:302:EST:C15	2.38	0.41
1:B:36[B]:THR:HG21	1:B:82:PHE:CZ	2.55	0.41
1:C:12:VAL:HG23	1:C:84[A]:ARG:HH11	1.82	0.41
1:A:44:ASN:C	4:A:417:HOH:O	2.64	0.41
1:D:79:LYS:HZ2	1:D:138:GLN:CD	2.26	0.40
1:A:115[B]:GLN:CD	1:B:123:ILE:HD13	2.44	0.40
1:D:209:LEU:O	1:D:210:PRO:C	2.63	0.40
1:B:37:ALA:O	1:B:58:CYS:HA	2.22	0.40
1:B:12:VAL:HG22	1:B:36[A]:THR:OG1	2.21	0.40
1:B:141:PRO:HD2	4:B:519:HOH:O	2.04	0.40
1:B:239:MET:HB3	1:D:239:MET:HE2	2.03	0.40

All (11) 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:B:44:ASN:ND2	1:D:49:THR:OG1[1_565]	1.39	0.81
1:B:44:ASN:CG	1:D:49:THR:OG1[1_565]	1.90	0.30
4:B:521:HOH:O	4:C:426:HOH:O[1_564]	1.93	0.27
1:D:44:ASN:CB	4:B:477:HOH:O[1_545]	1.94	0.26
1:B:44:ASN:ND2	1:D:49:THR:CB[1_565]	2.01	0.19
1:A:69:LYS:CG	4:D:406:HOH:O[1_565]	2.03	0.17
1:A:215:ASN:ND2	1:B:227:LEU:CD1[1_455]	2.03	0.17
4:B:489:HOH:O	4:C:502:HOH:O[1_564]	2.05	0.15
1:C:103:GLU:OE2	1:D:104:LYS:CB[1_655]	2.09	0.11
1:C:104:LYS:O	1:D:106:ASN:CB[1_655]	2.17	0.03
4:A:545:HOH:O	4:C:433:HOH:O[1_565]	2.19	0.01

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	255/260 (98%)	245 (96%)	10 (4%)	0	100	100
1	B	254/260 (98%)	241 (95%)	13 (5%)	0	100	100
1	C	249/260 (96%)	237 (95%)	12 (5%)	0	100	100
1	D	255/260 (98%)	239 (94%)	12 (5%)	4 (2%)	7	1
All	All	1013/1040 (97%)	962 (95%)	47 (5%)	4 (0%)	30	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	211	ASP
1	D	207	THR
1	D	210	PRO
1	D	206	LEU

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	193/199 (97%)	186 (96%)	7 (4%)	31	14
1	B	199/199 (100%)	192 (96%)	7 (4%)	32	15
1	C	191/199 (96%)	183 (96%)	8 (4%)	26	11
1	D	192/199 (96%)	186 (97%)	6 (3%)	35	18
All	All	775/796 (97%)	747 (96%)	28 (4%)	32	14

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	80	GLU
1	A	84	ARG
1	A	103	GLU
1	A	132	VAL
1	A	205	LEU
1	A	206	LEU
1	B	116[A]	ARG
1	B	116[B]	ARG
1	B	125	THR
1	B	205	LEU
1	B	216	PHE
1	B	220	GLN
1	B	230	PRO
1	C	7	SER
1	C	48	GLU
1	C	69	LYS
1	C	79	LYS
1	C	104	LYS
1	C	204	PRO
1	C	239[A]	MET
1	C	239[B]	MET
1	D	48	GLU
1	D	80	GLU

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Mol	Chain	Res	Type
1	D	104	LYS
1	D	189	ILE
1	D	214	ARG
1	D	230	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	106	ASN
1	A	107	GLN
1	A	143	GLN
1	B	72	GLN
1	B	106	ASN
1	B	220	GLN
1	C	44	ASN
1	C	90	ASN
1	C	102	HIS
1	C	106	ASN
1	C	138	GLN
1	D	44	ASN
1	D	215	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	C	301	-	46,48,48	2.00	14 (30%)	64,73,73	2.41	21 (32%)
2	NAD	D	301	-	46,48,48	1.90	9 (19%)	64,73,73	2.12	16 (25%)
2	NAD	A	301	-	46,48,48	1.83	13 (28%)	64,73,73	2.92	23 (35%)
2	NAD	B	301	-	46,48,48	1.57	8 (17%)	64,73,73	2.32	16 (25%)
3	EST	C	302	-	23,23,23	2.64	6 (26%)	36,36,36	2.81	17 (47%)

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	C	301	-	-	8/30/62/62	0/5/5/5
2	NAD	D	301	-	-	7/30/62/62	0/5/5/5
2	NAD	A	301	-	-	5/30/62/62	0/5/5/5
2	NAD	B	301	-	-	6/30/62/62	0/5/5/5
3	EST	C	302	-	2/2/5/5	-	0/4/4/4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	EST	O17-C17	-10.86	1.25	1.43
2	C	301	NAD	O4D-C1D	5.92	1.48	1.40
2	D	301	NAD	PN-O3	5.78	1.65	1.59
2	B	301	NAD	C6N-N1N	4.75	1.46	1.35
2	C	301	NAD	C3N-C7N	4.63	1.57	1.50
2	D	301	NAD	O4D-C1D	4.62	1.47	1.40
2	A	301	NAD	C4N-C3N	4.41	1.46	1.39
2	D	301	NAD	C4N-C3N	4.27	1.45	1.39
2	D	301	NAD	C2N-N1N	4.09	1.39	1.35
2	B	301	NAD	C3N-C7N	4.09	1.56	1.50
2	C	301	NAD	PA-O3	3.92	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAD	C6N-N1N	3.73	1.43	1.35
2	C	301	NAD	C5N-C4N	3.73	1.45	1.38
2	A	301	NAD	O2B-C2B	3.68	1.52	1.43
2	A	301	NAD	C2A-N1A	3.52	1.40	1.33
2	A	301	NAD	PN-O3	3.31	1.63	1.59
2	A	301	NAD	C4A-N9A	3.16	1.44	1.37
2	C	301	NAD	C4A-N9A	3.14	1.44	1.37
2	A	301	NAD	C6N-N1N	3.08	1.42	1.35
3	C	302	EST	C9-C8	3.04	1.57	1.54
2	D	301	NAD	C3N-C7N	3.00	1.55	1.50
2	D	301	NAD	O2B-C2B	2.93	1.50	1.43
2	A	301	NAD	O4B-C4B	-2.92	1.38	1.45
2	B	301	NAD	O3D-C3D	2.92	1.50	1.43
2	C	301	NAD	C2A-N1A	2.80	1.38	1.33
3	C	302	EST	C10-C9	2.78	1.56	1.52
2	B	301	NAD	C2A-N1A	2.77	1.38	1.33
2	C	301	NAD	C3D-C4D	2.77	1.60	1.53
2	A	301	NAD	O2D-C2D	2.77	1.49	1.43
2	C	301	NAD	C4A-N3A	-2.76	1.29	1.34
2	B	301	NAD	C7N-N7N	2.63	1.37	1.33
2	A	301	NAD	C3B-C4B	2.57	1.59	1.53
2	D	301	NAD	C8A-N7A	2.46	1.36	1.31
2	A	301	NAD	PA-O3	2.44	1.62	1.59
2	C	301	NAD	O2B-C2B	2.41	1.48	1.43
2	A	301	NAD	O4B-C1B	2.38	1.47	1.42
2	B	301	NAD	C4N-C3N	2.37	1.43	1.39
2	D	301	NAD	O4B-C1B	2.35	1.47	1.42
2	A	301	NAD	O3B-C3B	2.28	1.48	1.43
2	C	301	NAD	C4N-C3N	2.21	1.42	1.39
2	C	301	NAD	PN-O3	2.19	1.61	1.59
2	C	301	NAD	C2N-C3N	-2.19	1.35	1.39
3	C	302	EST	C18-C13	2.17	1.57	1.54
2	D	301	NAD	PA-O3	2.17	1.61	1.59
2	A	301	NAD	C3N-C7N	2.15	1.53	1.50
2	B	301	NAD	C5A-C4A	-2.14	1.35	1.39
2	B	301	NAD	C2B-C1B	2.12	1.60	1.53
3	C	302	EST	C12-C11	2.10	1.57	1.53
3	C	302	EST	C6-C5	2.09	1.54	1.51
2	C	301	NAD	PA-O2A	-2.05	1.45	1.55

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NAD	C5N-C4N-C3N	-11.72	108.84	120.36
2	C	301	NAD	C5N-C4N-C3N	-8.68	111.83	120.36
2	A	301	NAD	C6N-C5N-C4N	8.50	131.69	119.45
2	B	301	NAD	C5N-C4N-C3N	-7.69	112.81	120.36
2	D	301	NAD	C5N-C4N-C3N	-7.57	112.93	120.36
2	C	301	NAD	C2N-C3N-C4N	7.54	127.03	118.26
2	A	301	NAD	C5N-C6N-N1N	-7.28	110.46	120.38
3	C	302	EST	C15-C14-C8	6.93	130.15	119.10
2	B	301	NAD	C2N-C3N-C4N	6.14	125.40	118.26
2	D	301	NAD	C2N-C3N-C4N	5.94	125.17	118.26
2	A	301	NAD	C2N-C3N-C4N	5.54	124.70	118.26
3	C	302	EST	C9-C8-C14	5.50	116.33	108.68
2	A	301	NAD	C6N-N1N-C2N	5.47	126.53	121.88
2	B	301	NAD	O7N-C7N-C3N	5.46	126.28	119.60
3	C	302	EST	C13-C14-C8	5.45	122.16	114.41
3	C	302	EST	O17-C17-C13	5.43	126.17	114.80
2	B	301	NAD	C6N-C5N-C4N	5.30	127.09	119.45
2	C	301	NAD	C4N-C3N-C7N	-5.22	106.85	121.06
2	A	301	NAD	C4N-C3N-C7N	-4.70	108.25	121.06
2	D	301	NAD	C4N-C3N-C7N	-4.64	108.42	121.06
2	B	301	NAD	C6N-N1N-C1D	-4.58	110.73	119.73
2	B	301	NAD	C5N-C6N-N1N	-4.44	114.33	120.38
2	A	301	NAD	C6N-N1N-C1D	-4.27	111.34	119.73
3	C	302	EST	C15-C16-C17	-4.24	101.14	105.76
2	B	301	NAD	C4N-C3N-C7N	-4.18	109.69	121.06
2	A	301	NAD	C3N-C7N-N7N	-4.17	112.61	117.74
2	D	301	NAD	C6N-C5N-C4N	4.03	125.25	119.45
2	B	301	NAD	O4B-C1B-C2B	-3.92	98.22	106.62
3	C	302	EST	C11-C9-C10	3.91	119.68	113.84
2	D	301	NAD	C6N-N1N-C2N	3.91	125.20	121.88
2	A	301	NAD	C1B-N9A-C8A	3.89	135.73	127.09
2	D	301	NAD	C3N-C7N-N7N	-3.87	112.97	117.74
2	C	301	NAD	C5A-C4A-N3A	3.85	132.01	126.72
2	B	301	NAD	C3N-C7N-N7N	-3.73	113.15	117.74
2	C	301	NAD	C4D-O4D-C1D	-3.71	106.53	109.92
2	C	301	NAD	O7N-C7N-N7N	3.71	127.97	122.62
2	C	301	NAD	C5N-C6N-N1N	-3.69	115.35	120.38
2	C	301	NAD	C6N-C5N-C4N	3.66	124.73	119.45
2	C	301	NAD	N3A-C2A-N1A	-3.61	123.12	128.58
3	C	302	EST	C14-C13-C17	3.54	102.86	99.25
2	A	301	NAD	O4B-C1B-C2B	-3.42	99.29	106.62
2	C	301	NAD	C6N-N1N-C1D	-3.42	113.02	119.73
3	C	302	EST	C18-C13-C17	-3.38	104.41	109.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	EST	O17-C17-C16	3.38	120.49	111.69
2	B	301	NAD	C6N-N1N-C2N	3.37	124.75	121.88
3	C	302	EST	C5-C10-C9	-3.36	117.18	121.00
2	A	301	NAD	O3B-C3B-C4B	-3.36	101.44	111.08
3	C	302	EST	C15-C14-C13	3.26	107.67	103.84
2	C	301	NAD	O3-PA-O1A	-3.20	101.07	110.70
2	D	301	NAD	O4D-C4D-C5D	-3.15	99.26	109.33
2	D	301	NAD	O2N-PN-O1N	3.14	127.04	112.44
2	A	301	NAD	C4A-N9A-C1B	-3.10	119.39	126.63
2	D	301	NAD	C4D-O4D-C1D	-3.06	107.12	109.92
2	A	301	NAD	C4D-O4D-C1D	3.04	112.71	109.92
2	A	301	NAD	C5B-C4B-C3B	-3.03	104.31	115.21
2	D	301	NAD	O7N-C7N-N7N	3.02	126.97	122.62
2	D	301	NAD	C5N-C6N-N1N	-2.99	116.30	120.38
2	D	301	NAD	O4B-C1B-C2B	-2.97	100.25	106.62
2	B	301	NAD	C4D-O4D-C1D	-2.93	107.24	109.92
2	B	301	NAD	O3D-C3D-C4D	-2.92	102.69	111.08
3	C	302	EST	C7-C8-C14	2.90	116.90	112.08
2	B	301	NAD	O2N-PN-O3	2.84	114.94	107.27
2	C	301	NAD	C6N-N1N-C2N	2.78	124.24	121.88
2	C	301	NAD	O4B-C1B-C2B	-2.78	100.67	106.62
3	C	302	EST	C18-C13-C14	2.75	116.66	111.68
2	D	301	NAD	C4A-N9A-C1B	-2.74	120.22	126.63
2	A	301	NAD	O3-PN-O1N	-2.74	102.47	110.70
3	C	302	EST	C7-C6-C5	2.67	117.94	112.87
2	C	301	NAD	C3N-C7N-N7N	-2.66	114.46	117.74
2	A	301	NAD	O2N-PN-O3	2.64	114.42	107.27
2	A	301	NAD	C2N-C3N-C7N	2.63	127.04	119.46
2	A	301	NAD	N3A-C2A-N1A	-2.60	124.65	128.58
2	C	301	NAD	O3-PN-O1N	-2.59	102.92	110.70
2	A	301	NAD	C2B-C1B-N9A	-2.59	106.88	113.30
2	C	301	NAD	C2A-N1A-C6A	2.55	122.92	118.73
3	C	302	EST	C11-C9-C8	2.50	114.72	111.45
2	D	301	NAD	N3A-C2A-N1A	-2.48	124.83	128.58
2	D	301	NAD	O3-PA-O1A	-2.47	103.28	110.70
2	C	301	NAD	N3A-C4A-N9A	-2.45	123.00	127.17
2	B	301	NAD	O4D-C4D-C3D	2.43	109.97	105.15
2	B	301	NAD	C2N-N1N-C1D	2.41	124.45	119.13
2	D	301	NAD	C2N-C3N-C7N	2.40	126.40	119.46
3	C	302	EST	C16-C15-C14	-2.40	100.44	105.14
2	B	301	NAD	O2B-C2B-C1B	-2.37	101.94	110.10
2	C	301	NAD	O4B-C4B-C5B	-2.32	101.89	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAD	C2N-C3N-C7N	2.30	126.10	119.46
2	A	301	NAD	O4B-C4B-C5B	-2.27	102.05	109.33
3	C	302	EST	C16-C17-C13	2.23	106.28	104.52
2	C	301	NAD	O3D-C3D-C2D	-2.22	104.71	111.82
2	C	301	NAD	O3B-C3B-C2B	2.17	118.76	111.82
2	A	301	NAD	O7N-C7N-C3N	2.14	122.22	119.60
2	A	301	NAD	C5A-C6A-N6A	2.14	128.58	123.29
2	A	301	NAD	C3B-C2B-C1B	2.03	105.31	101.46

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	302	EST	C14
3	C	302	EST	C17

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAD	C5D-O5D-PN-O3
2	A	301	NAD	C5D-O5D-PN-O1N
2	A	301	NAD	C5D-O5D-PN-O2N
2	B	301	NAD	C5D-O5D-PN-O3
2	B	301	NAD	O4D-C1D-N1N-C2N
2	C	301	NAD	C5D-O5D-PN-O3
2	C	301	NAD	C5D-O5D-PN-O1N
2	C	301	NAD	C5D-O5D-PN-O2N
2	D	301	NAD	C5D-O5D-PN-O3
2	D	301	NAD	C5D-O5D-PN-O1N
2	C	301	NAD	PN-O3-PA-O5B
2	A	301	NAD	PA-O3-PN-O2N
2	B	301	NAD	PA-O3-PN-O2N
2	B	301	NAD	C5D-O5D-PN-O1N
2	D	301	NAD	C5D-O5D-PN-O2N
2	C	301	NAD	PA-O3-PN-O2N
2	D	301	NAD	PA-O3-PN-O2N
2	C	301	NAD	O4D-C1D-N1N-C6N
2	C	301	NAD	PA-O3-PN-O1N
2	D	301	NAD	PN-O3-PA-O5B
2	D	301	NAD	C2B-C1B-N9A-C8A
2	B	301	NAD	O4D-C4D-C5D-O5D
2	C	301	NAD	O4B-C4B-C5B-O5B
2	A	301	NAD	PA-O3-PN-O1N

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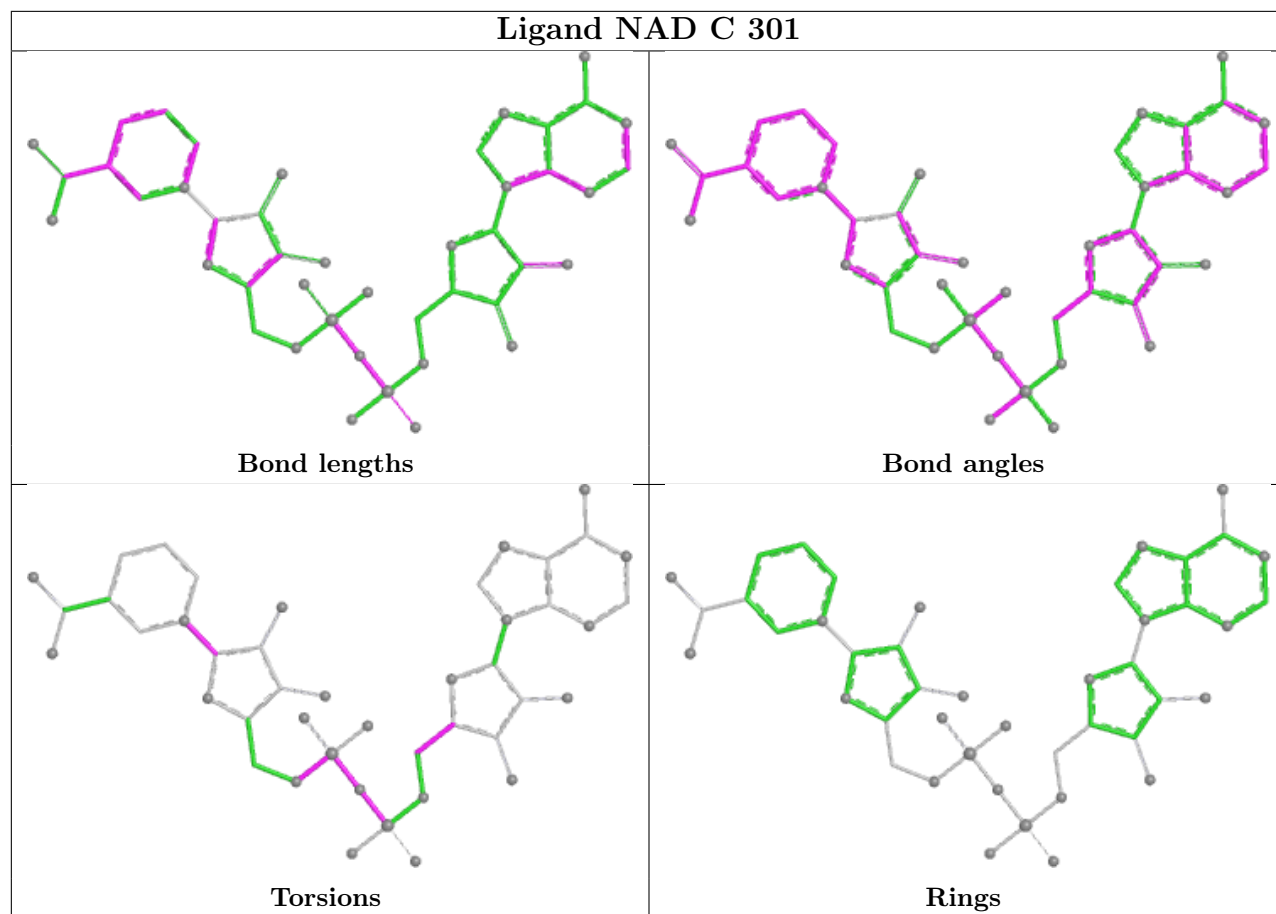
Mol	Chain	Res	Type	Atoms
2	B	301	NAD	PA-O3-PN-O1N
2	D	301	NAD	PA-O3-PN-O1N

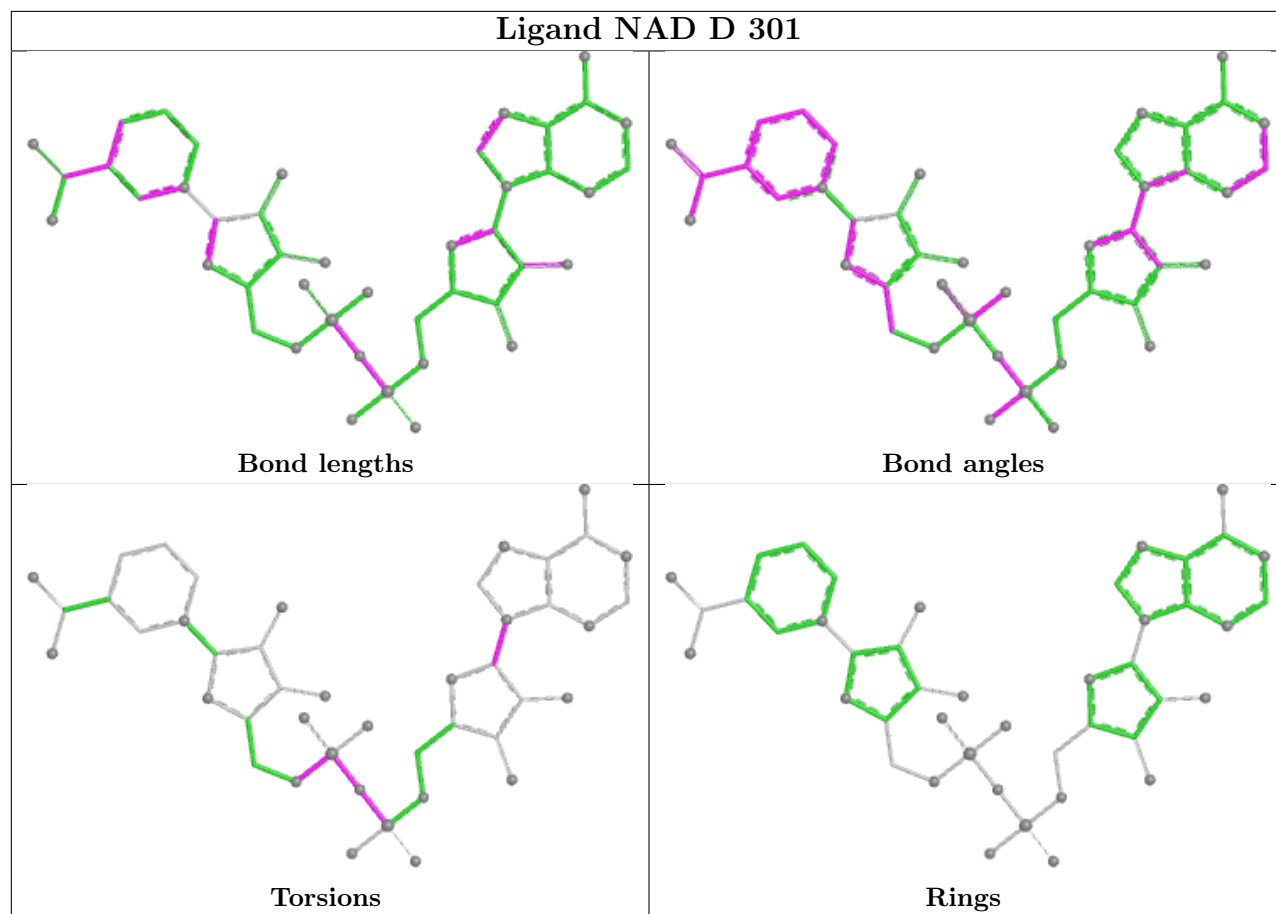
There are no ring outliers.

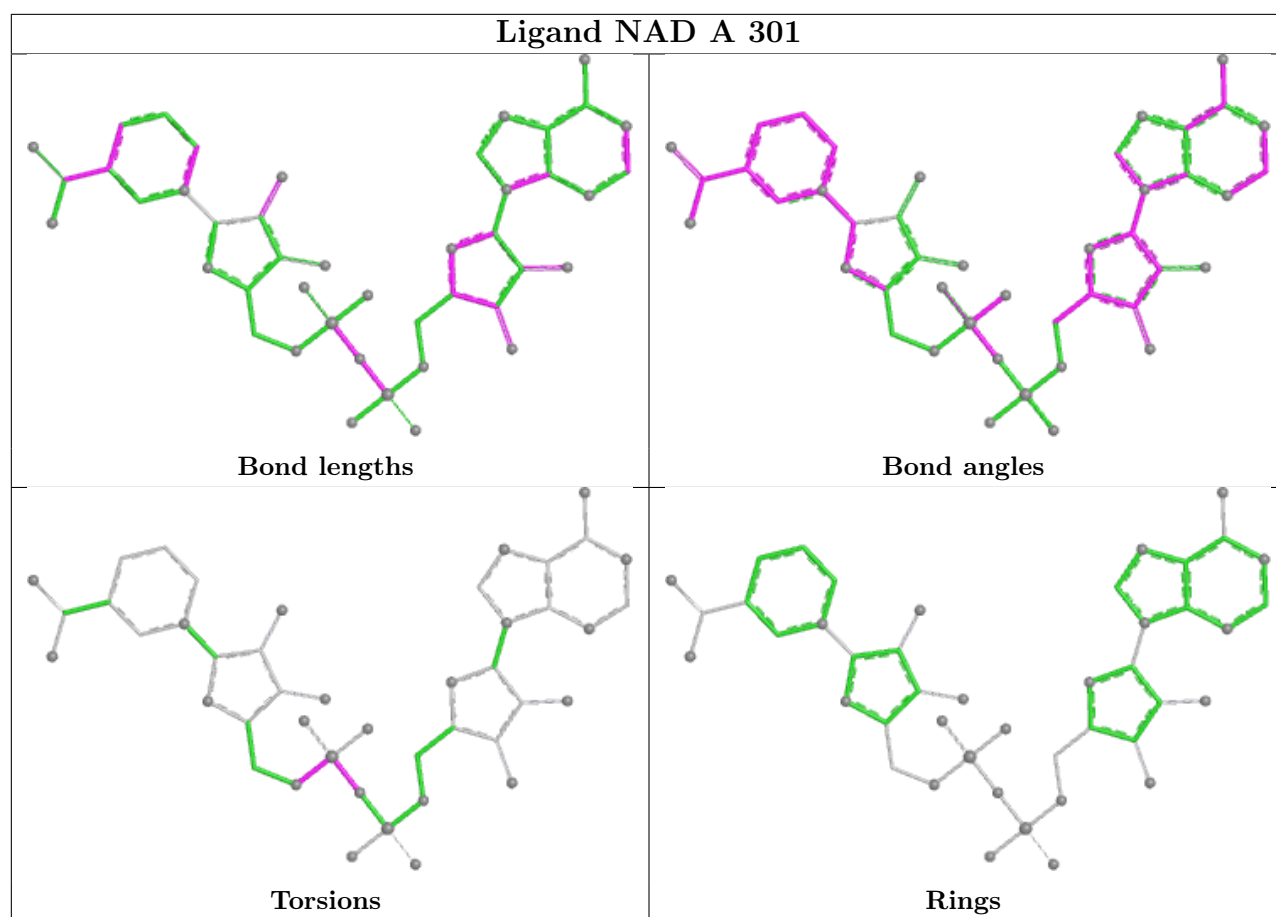
3 monomers are involved in 12 short contacts:

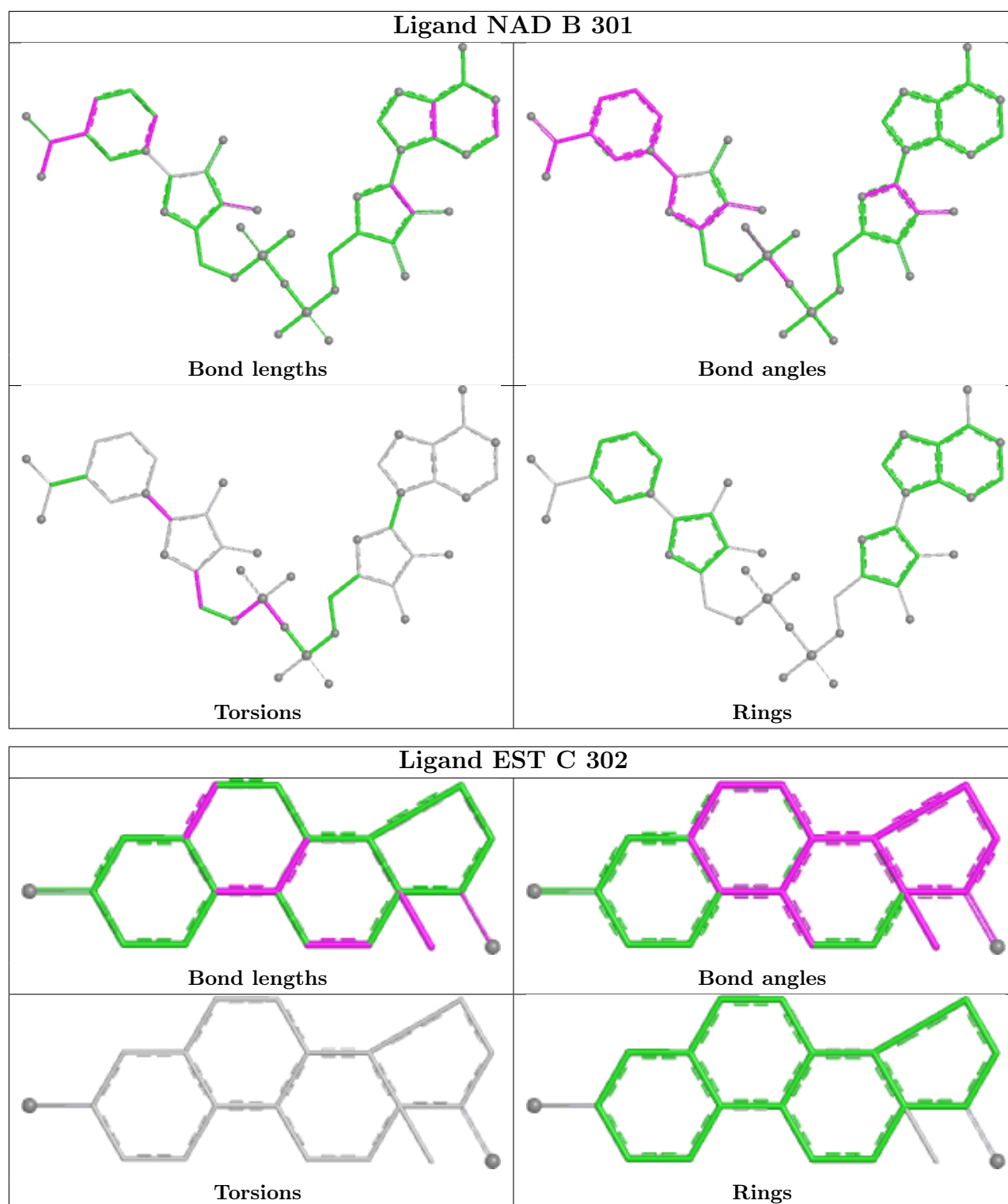
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	NAD	2	0
2	D	301	NAD	1	0
3	C	302	EST	11	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.