



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:42 AM UTC

PDB ID : 9LDT / pdb_00009ldt
Title : DESIGN AND SYNTHESIS OF NEW ENZYMES BASED ON THE LACTATE DEHYDROGENASE FRAMEWORK
Authors : Dunn, C.R.; Holbrook, J.J.; Muirhead, H.
Deposited on : 1991-11-26
Resolution : 2.00 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

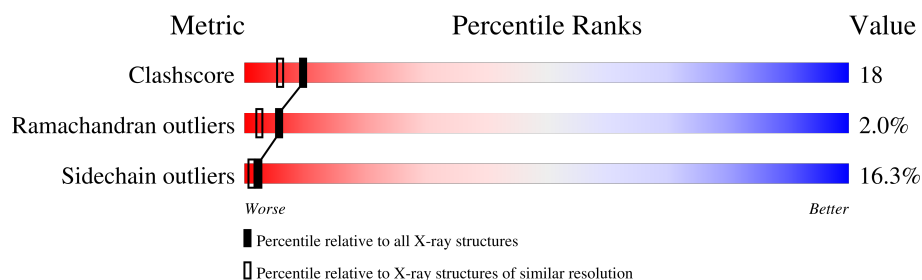
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	332	
1	B	332	

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
4	OXM	A	402	-	X	-	-

2 Entry composition [i](#)

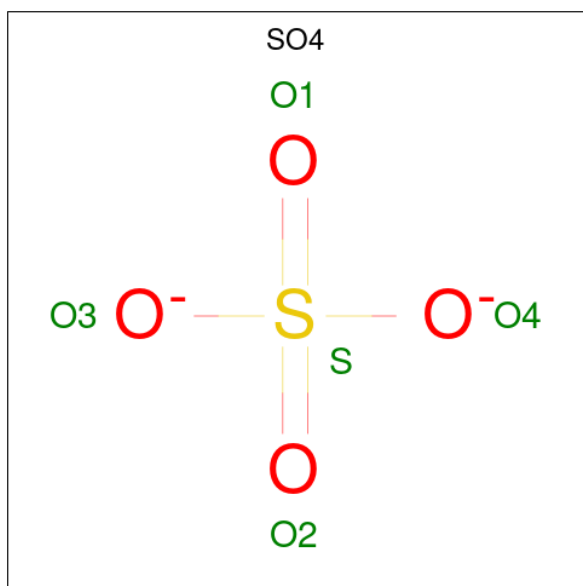
There are 5 unique types of molecules in this entry. The entry contains 5399 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LACTATE DEHYDROGENASE.

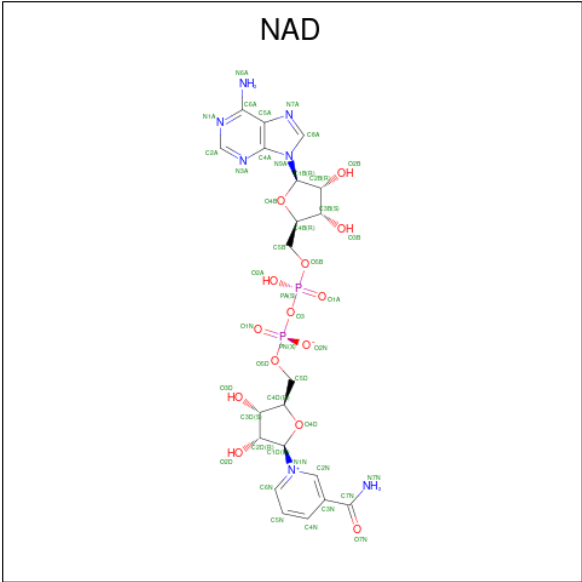
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2568	1640	445	470	13			
1	B	332	Total	C	N	O	S	0	0	0
			2568	1640	445	470	13			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



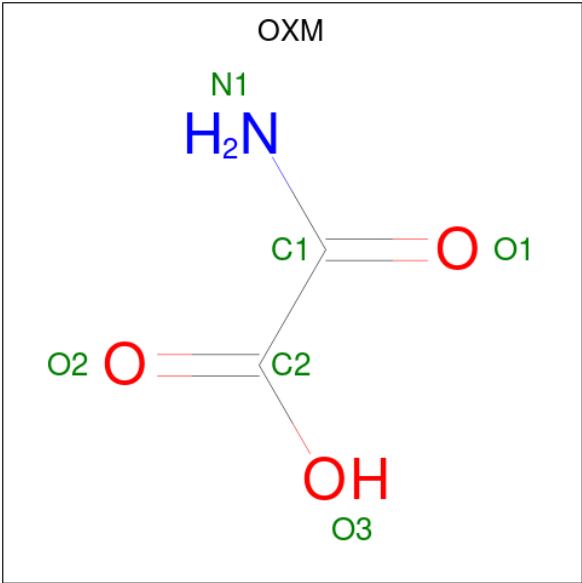
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 4 is OXAMIC ACID (CCD ID: OXM) (formula: C₂H₃NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			6	2	1	3		
4	B	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 5 is water.

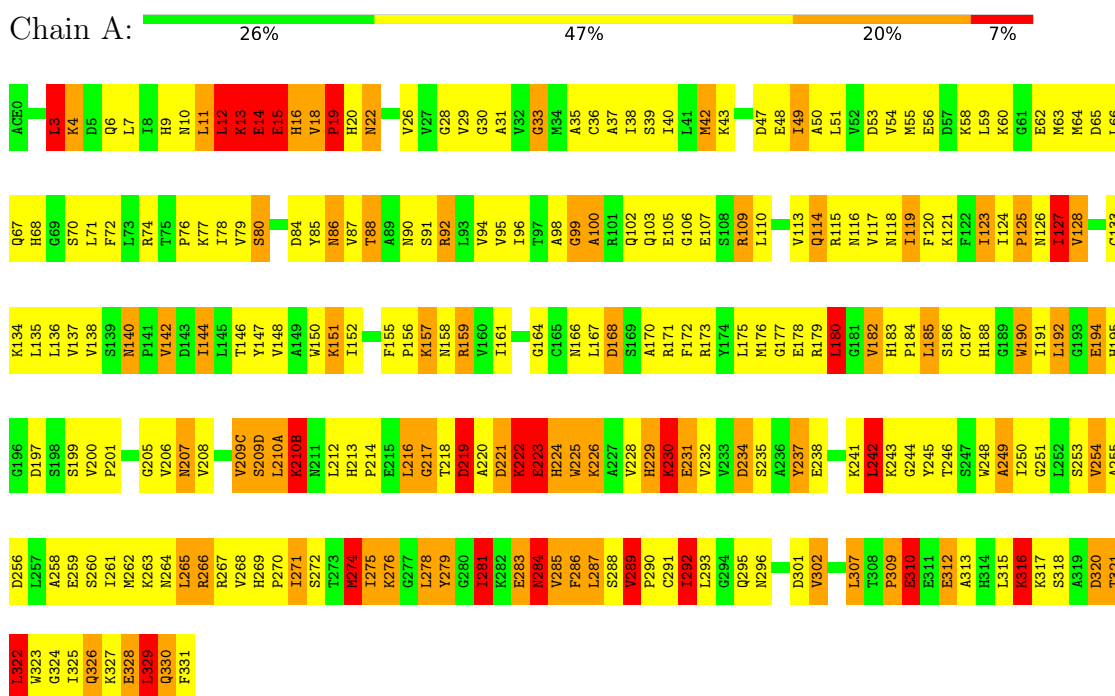
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total 76	O 76	0	0
5	B	77	Total 77	O 77	0	0

3 Residue-property plots

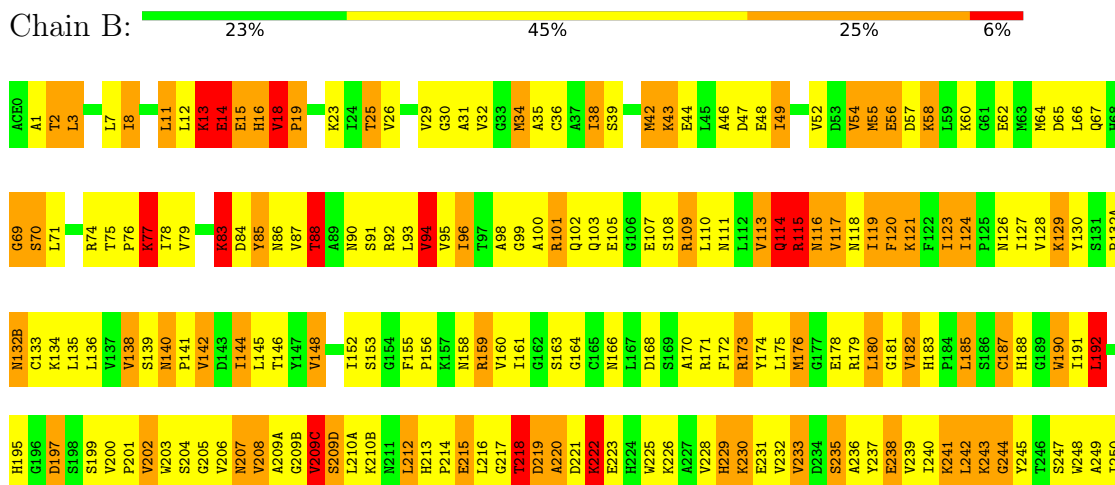
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

● Molecule 1: LACTATE DEHYDROGENASE



● Molecule 1: LACTATE DEHYDROGENASE



K316	K317	S318	A319	D320	T321	L322	W323	G324	I325	Q326	K327	E328	L329	Q330	F331
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	60.30Å 136.39Å 86.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.233 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5399	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: ACE, OXM, NAD, SO4

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	1.41	9/2615 (0.3%)	3.40	459/3541 (13.0%)
1	B	1.39	4/2615 (0.2%)	3.62	462/3541 (13.0%)
All	All	1.40	13/5230 (0.2%)	3.51	921/7082 (13.0%)

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	1
1	B	0	2
All	All	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	VAL	N-CA	5.86	1.52	1.46
1	B	171	ARG	NE-CZ	5.77	1.39	1.33
1	B	297	GLY	C-N	-5.62	1.27	1.33
1	B	261	ILE	CA-CB	5.56	1.60	1.54
1	A	289	VAL	C-O	5.50	1.28	1.24
1	A	140	ASN	CA-C	5.47	1.59	1.53
1	A	96	ILE	CA-CB	5.42	1.60	1.53
1	A	88	THR	CA-CB	5.13	1.62	1.53
1	A	30	GLY	CA-C	5.08	1.57	1.51
1	B	200	VAL	N-CA	5.06	1.51	1.46
1	A	238	GLU	CD-OE2	5.05	1.34	1.25
1	A	170	ALA	C-O	5.05	1.30	1.24
1	A	96	ILE	N-CA	5.02	1.52	1.46

All (921) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	ASP	CA-C-N	30.58	179.95	121.54
1	B	221	ASP	C-N-CA	30.58	179.95	121.54
1	B	115	ARG	NE-CZ-NH2	22.96	139.87	119.20
1	B	109	ARG	CD-NE-CZ	22.53	155.94	124.40
1	B	101	ARG	CD-NE-CZ	21.20	154.08	124.40
1	B	289	VAL	CB-CA-C	20.27	129.20	109.33
1	A	320	ASP	CA-CB-CG	18.61	131.21	112.60
1	A	159	ARG	NE-CZ-NH1	18.57	140.07	121.50
1	A	159	ARG	NE-CZ-NH2	-17.75	103.23	119.20
1	B	221	ASP	CA-CB-CG	17.31	129.91	112.60
1	B	15	GLU	CA-CB-CG	16.93	147.97	114.10
1	A	86	ASN	CA-CB-CG	16.90	129.50	112.60
1	B	289	VAL	N-CA-CB	-16.68	93.79	111.64
1	B	14	GLU	CA-C-O	16.66	144.33	120.51
1	B	292	ILE	CA-CB-CG2	16.33	138.26	110.50
1	A	312	GLU	CA-CB-CG	16.20	146.50	114.10
1	B	243	LYS	CA-C-O	-15.68	100.68	119.18
1	A	179	ARG	NE-CZ-NH1	-15.25	106.25	121.50
1	B	101	ARG	CG-CD-NE	15.22	145.48	112.00
1	A	289	VAL	N-CA-CB	-15.21	95.14	111.87
1	B	290	PRO	CB-CA-C	14.63	127.51	111.56
1	B	284	ASN	CA-CB-CG	14.57	127.17	112.60
1	B	221	ASP	O-C-N	-14.47	105.94	123.01
1	A	219	ASP	CA-CB-CG	14.28	126.88	112.60
1	B	220	ALA	CA-C-N	14.06	141.52	121.42
1	B	220	ALA	C-N-CA	14.06	141.52	121.42
1	B	16	HIS	CA-CB-CG	-13.96	99.84	113.80
1	B	86	ASN	OD1-CG-ND2	-13.89	108.71	122.60
1	B	317	LYS	CA-CB-CG	13.75	141.60	114.10
1	B	166	ASN	CB-CG-ND2	13.69	136.93	116.40
1	B	119	ILE	CA-CB-CG2	13.50	133.45	110.50
1	B	166	ASN	OD1-CG-ND2	-13.42	109.18	122.60
1	A	13	LYS	CA-C-O	13.39	137.11	121.44
1	A	289	VAL	CB-CA-C	13.34	124.30	109.89
1	A	16	HIS	O-C-N	13.23	140.18	122.59
1	A	221	ASP	CA-CB-CG	13.22	125.82	112.60
1	A	65	ASP	CA-C-O	-12.71	107.47	120.82
1	B	43	LYS	CA-C-N	12.63	141.24	122.68
1	B	43	LYS	C-N-CA	12.63	141.24	122.68
1	B	249	ALA	CA-C-O	-12.44	108.09	120.90
1	A	292	ILE	CA-CB-CG2	12.34	131.48	110.50
1	B	118	ASN	CA-CB-CG	-12.33	100.27	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209(B)	GLY	CA-C-O	-12.25	106.53	119.27
1	A	178	GLU	CB-CG-CD	12.21	133.35	112.60
1	B	287	LEU	CA-C-O	-12.19	108.46	121.38
1	A	33	GLY	CA-C-O	-11.99	108.05	121.00
1	B	271	ILE	CA-C-O	-11.99	108.97	121.67
1	A	222	LYS	CA-C-O	11.93	137.56	120.51
1	B	267	ARG	NE-CZ-NH1	-11.84	109.66	121.50
1	A	255	ALA	CA-C-N	11.79	135.76	120.44
1	A	255	ALA	C-N-CA	11.79	135.76	120.44
1	B	292	ILE	CB-CA-C	11.77	127.11	110.98
1	B	118	ASN	OD1-CG-ND2	-11.76	110.84	122.60
1	A	220	ALA	CA-C-O	-11.71	103.77	120.51
1	A	217	GLY	CA-C-N	11.52	143.54	121.54
1	A	217	GLY	C-N-CA	11.52	143.54	121.54
1	B	179	ARG	CD-NE-CZ	11.50	140.50	124.40
1	A	67	GLN	CA-C-N	11.48	136.81	120.28
1	A	67	GLN	C-N-CA	11.48	136.81	120.28
1	A	278	LEU	CA-C-O	-11.37	106.89	119.40
1	A	77	LYS	O-C-N	11.24	136.31	123.27
1	B	86	ASN	CB-CG-ND2	11.19	133.19	116.40
1	B	209(C)	VAL	CA-C-O	11.11	133.26	120.71
1	B	292	ILE	CB-CG1-CD1	-11.09	90.52	113.80
1	A	330	GLN	CA-C-N	11.07	141.63	121.70
1	A	330	GLN	C-N-CA	11.07	141.63	121.70
1	B	11	LEU	CA-CB-CG	11.02	154.87	116.30
1	B	238	GLU	CA-C-O	-10.89	109.48	120.70
1	B	266	ARG	CD-NE-CZ	10.85	139.59	124.40
1	B	84	ASP	N-CA-C	10.81	124.36	111.82
1	A	292	ILE	CB-CA-C	10.78	124.00	110.96
1	B	65	ASP	CA-CB-CG	10.66	123.26	112.60
1	B	111	ASN	CA-C-O	-10.66	106.59	119.49
1	B	115	ARG	NE-CZ-NH1	-10.53	110.97	121.50
1	A	176	MET	CA-C-N	10.52	131.88	119.99
1	A	176	MET	C-N-CA	10.52	131.88	119.99
1	B	155	PHE	O-C-N	10.51	133.09	121.53
1	A	272	SER	N-CA-CB	10.45	126.91	109.87
1	A	310	GLU	CB-CG-CD	10.40	130.29	112.60
1	B	242	LEU	CA-C-O	-10.39	107.21	119.78
1	A	58	LYS	CA-C-N	10.37	134.34	120.65
1	A	58	LYS	C-N-CA	10.37	134.34	120.65
1	B	243	LYS	O-C-N	10.37	134.44	122.20
1	A	237	TYR	O-C-N	10.32	133.06	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ARG	O-C-N	-10.32	108.62	122.97
1	B	233	VAL	CA-C-N	10.27	137.87	120.72
1	B	233	VAL	C-N-CA	10.27	137.87	120.72
1	A	207	ASN	CA-CB-CG	10.23	122.83	112.60
1	B	86	ASN	CA-CB-CG	10.15	122.75	112.60
1	A	289	VAL	O-C-N	10.13	128.81	121.72
1	A	157	LYS	CA-CB-CG	10.04	134.17	114.10
1	B	256	ASP	CA-C-O	9.92	131.24	120.82
1	B	67	GLN	OE1-CD-NE2	-9.91	112.69	122.60
1	A	207	ASN	O-C-N	9.82	133.93	123.42
1	A	267	ARG	CD-NE-CZ	-9.76	110.73	124.40
1	B	70	SER	CA-CB-OG	-9.68	91.75	111.10
1	B	195	HIS	CB-CG-CD2	-9.65	118.65	131.20
1	A	147	TYR	CA-C-O	9.63	131.20	120.90
1	B	103	GLN	OE1-CD-NE2	9.60	132.20	122.60
1	B	249	ALA	O-C-N	9.60	132.40	122.03
1	B	328	GLU	CB-CG-CD	9.59	128.90	112.60
1	A	47	ASP	CA-CB-CG	9.58	122.18	112.60
1	A	289	VAL	CA-C-O	-9.54	109.40	121.13
1	A	78	ILE	CA-C-O	-9.49	110.52	120.39
1	A	302	VAL	O-C-N	-9.45	113.50	123.14
1	A	274	MET	CA-CB-CG	-9.43	95.25	114.10
1	B	272	SER	O-C-N	9.41	133.95	123.13
1	A	179	ARG	NE-CZ-NH2	9.39	127.65	119.20
1	B	2	THR	CA-CB-CG2	9.39	126.46	110.50
1	A	223	GLU	CA-C-N	9.38	139.45	121.54
1	A	223	GLU	C-N-CA	9.38	139.45	121.54
1	A	113	VAL	CA-C-O	-9.35	111.54	121.27
1	B	144	ILE	CA-C-O	-9.35	110.94	120.85
1	A	281	ILE	CB-CA-C	9.33	124.58	110.96
1	B	35	ALA	O-C-N	9.32	131.67	122.07
1	B	323	TRP	CA-C-N	9.31	130.51	119.99
1	B	323	TRP	C-N-CA	9.31	130.51	119.99
1	B	173	ARG	CA-C-O	9.31	130.28	120.42
1	A	59	LEU	O-C-N	9.27	131.67	122.03
1	B	119	ILE	CB-CG1-CD1	-9.25	94.37	113.80
1	B	57	ASP	CA-C-O	-9.25	111.38	120.90
1	B	123	ILE	CA-C-O	-9.23	111.06	120.85
1	B	263	LYS	CA-C-O	-9.23	108.55	119.35
1	B	103	GLN	N-CA-C	-9.20	96.84	110.46
1	A	234	ASP	CA-CB-CG	9.17	121.77	112.60
1	B	219	ASP	CB-CA-C	9.14	126.24	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	THR	N-CA-CB	-9.11	96.51	110.44
1	B	174	TYR	CA-C-N	9.07	132.23	120.44
1	B	174	TYR	C-N-CA	9.07	132.23	120.44
1	B	91	SER	CA-C-O	-9.04	111.03	121.16
1	A	267	ARG	CA-C-O	-9.04	111.05	121.72
1	A	126	ASN	CA-C-O	-9.04	111.39	120.70
1	B	221	ASP	N-CA-CB	-9.04	96.42	110.06
1	A	186	SER	CA-C-O	-9.03	108.36	119.28
1	A	222	LYS	CA-C-N	9.02	137.01	122.67
1	A	222	LYS	C-N-CA	9.02	137.01	122.67
1	A	86	ASN	CB-CG-ND2	9.00	129.91	116.40
1	B	180	LEU	N-CA-CB	-8.99	95.75	110.40
1	B	321	THR	CA-C-O	-8.99	110.89	120.42
1	A	113	VAL	N-CA-CB	-8.99	100.54	110.51
1	B	46	ALA	CA-C-O	-8.98	110.70	121.56
1	B	260	SER	N-CA-CB	8.97	123.30	110.12
1	B	289	VAL	N-CA-C	-8.96	101.84	109.19
1	A	123	ILE	CA-C-O	-8.96	110.57	120.25
1	A	264	ASN	CA-CB-CG	8.96	121.56	112.60
1	B	132(B)	ASN	CA-CB-CG	-8.92	103.68	112.60
1	A	328	GLU	CA-CB-CG	8.91	131.91	114.10
1	A	103	GLN	CB-CG-CD	8.89	127.72	112.60
1	B	174	TYR	O-C-N	-8.88	112.80	122.03
1	B	13	LYS	CA-C-O	8.87	133.20	120.51
1	B	105	GLU	CG-CD-OE1	8.86	138.78	118.40
1	A	267	ARG	NH1-CZ-NH2	8.86	130.81	119.30
1	A	223	GLU	CA-C-O	8.80	130.34	119.95
1	A	197	ASP	CA-CB-CG	8.78	121.38	112.60
1	A	221	ASP	N-CA-C	8.77	123.46	110.48
1	B	190	TRP	O-C-N	8.77	134.63	123.23
1	A	55	MET	CG-SD-CE	-8.76	81.63	100.90
1	A	296	ASN	CA-C-O	-8.76	109.11	119.35
1	B	267	ARG	NH1-CZ-NH2	8.76	130.68	119.30
1	B	307	LEU	O-C-N	8.76	133.32	123.16
1	B	105	GLU	CG-CD-OE2	-8.73	98.31	118.40
1	B	241	LYS	CA-CB-CG	8.73	131.56	114.10
1	A	86	ASN	CB-CG-OD1	-8.70	103.40	120.80
1	B	153	SER	O-C-N	8.69	131.33	122.12
1	A	115	ARG	CA-C-O	-8.65	111.38	120.55
1	B	219	ASP	CA-C-O	8.62	129.88	120.32
1	B	161	ILE	N-CA-C	8.58	120.52	107.99
1	B	287	LEU	O-C-N	8.57	132.25	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	ILE	CA-C-N	8.54	131.72	120.28
1	B	261	ILE	C-N-CA	8.54	131.72	120.28
1	A	60	LYS	CA-C-N	8.53	129.44	119.98
1	A	60	LYS	C-N-CA	8.53	129.44	119.98
1	B	152	ILE	CA-CB-CG1	8.52	124.88	110.40
1	B	96	ILE	CA-C-O	8.51	130.62	120.66
1	B	85	TYR	N-CA-CB	8.50	124.85	110.49
1	A	70	SER	CA-CB-OG	-8.49	94.13	111.10
1	A	63	MET	CA-C-O	-8.47	111.76	121.07
1	B	191	ILE	N-CA-CB	8.46	122.34	111.67
1	A	225	TRP	O-C-N	8.46	132.68	122.27
1	A	113	VAL	CB-CA-C	8.42	122.66	111.88
1	B	203	TRP	N-CA-CB	8.42	124.37	110.39
1	A	78	ILE	O-C-N	8.42	132.12	123.20
1	A	56	GLU	N-CA-C	8.40	120.06	111.07
1	A	6	GLN	OE1-CD-NE2	8.40	131.00	122.60
1	B	14	GLU	CA-C-N	8.38	137.55	121.54
1	B	14	GLU	C-N-CA	8.38	137.55	121.54
1	B	209(C)	VAL	CB-CA-C	8.37	121.29	110.91
1	B	98	ALA	CA-C-O	8.36	130.39	121.19
1	A	281	ILE	N-CA-C	-8.36	95.68	107.80
1	B	12	LEU	CA-CB-CG	8.35	145.51	116.30
1	B	138	VAL	CA-C-O	-8.34	112.46	120.30
1	B	208	VAL	CA-CB-CG2	8.33	124.56	110.40
1	A	253	SER	CA-C-O	-8.32	111.60	120.42
1	A	328	GLU	CB-CG-CD	8.32	126.75	112.60
1	A	13	LYS	CA-C-N	8.30	137.40	121.54
1	A	13	LYS	C-N-CA	8.30	137.40	121.54
1	B	327	LYS	CA-C-N	8.30	137.39	121.54
1	B	327	LYS	C-N-CA	8.30	137.39	121.54
1	A	310	GLU	CA-C-N	8.28	131.71	120.54
1	A	310	GLU	C-N-CA	8.28	131.71	120.54
1	B	2	THR	CA-CB-OG1	-8.26	97.21	109.60
1	A	222	LYS	N-CA-C	8.25	128.37	110.80
1	B	306	THR	CA-C-N	8.24	134.28	122.09
1	B	306	THR	C-N-CA	8.24	134.28	122.09
1	A	9	HIS	CA-C-O	8.23	129.27	120.46
1	A	77	LYS	N-CA-CB	8.20	123.45	110.65
1	B	269	HIS	O-C-N	8.16	129.72	121.72
1	A	221	ASP	CA-C-O	8.15	130.85	121.47
1	B	243	LYS	N-CA-C	-8.15	101.39	113.61
1	A	329	LEU	CA-C-O	8.12	129.33	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	PRO	CB-CA-C	8.12	120.41	111.56
1	B	326	GLN	CA-C-O	-8.12	110.93	120.10
1	A	92	ARG	N-CA-C	-8.11	101.51	111.40
1	B	78	ILE	O-C-N	-8.10	114.76	123.18
1	B	221	ASP	N-CA-C	8.07	122.94	110.20
1	A	251	GLY	CA-C-O	-8.05	112.45	120.75
1	B	158	ASN	CA-CB-CG	8.05	120.65	112.60
1	B	244	GLY	N-CA-C	8.05	124.66	115.08
1	A	29	VAL	O-C-N	-8.04	112.53	122.57
1	B	26	VAL	O-C-N	8.01	131.69	123.20
1	A	68	HIS	N-CA-C	-8.01	102.50	111.71
1	A	237	TYR	CA-C-O	-8.00	112.07	120.55
1	B	290	PRO	O-C-N	-8.00	114.55	123.03
1	B	48	GLU	CA-CB-CG	8.00	130.09	114.10
1	A	42	MET	CG-SD-CE	-7.99	83.32	100.90
1	B	232	VAL	CA-CB-CG1	7.99	123.97	110.40
1	A	183	HIS	CA-C-N	7.96	128.39	119.32
1	A	183	HIS	C-N-CA	7.96	128.39	119.32
1	A	261	ILE	O-C-N	-7.92	113.66	121.90
1	B	302	VAL	CA-C-O	-7.91	112.08	120.39
1	B	327	LYS	O-C-N	-7.91	111.50	122.41
1	B	115	ARG	NH1-CZ-NH2	-7.88	109.05	119.30
1	A	256	ASP	CA-CB-CG	7.87	120.47	112.60
1	A	100	ALA	O-C-N	7.86	132.29	123.01
1	B	118	ASN	CA-C-O	-7.86	112.22	120.55
1	B	222	LYS	N-CA-C	7.85	127.52	110.80
1	B	133	CYS	CA-C-N	7.83	133.53	122.72
1	B	133	CYS	C-N-CA	7.83	133.53	122.72
1	A	148	VAL	N-CA-CB	7.83	119.71	110.55
1	A	301	ASP	CA-C-O	-7.83	112.22	120.99
1	B	114	GLN	CB-CG-CD	7.83	125.91	112.60
1	B	146	THR	N-CA-C	-7.83	102.69	111.14
1	B	318	SER	O-C-N	-7.83	113.23	122.15
1	B	253	SER	N-CA-CB	7.81	121.34	110.01
1	A	221	ASP	O-C-N	-7.80	114.14	122.96
1	B	127	ILE	CA-C-N	7.79	133.40	120.62
1	B	127	ILE	C-N-CA	7.79	133.40	120.62
1	A	53	ASP	CA-C-O	-7.78	112.91	121.23
1	B	108	SER	CA-C-O	-7.77	113.09	121.56
1	B	195	HIS	CB-CG-ND1	7.77	134.35	122.70
1	A	272	SER	CB-CA-C	-7.75	97.58	110.29
1	B	99	GLY	N-CA-C	7.71	121.10	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ARG	CD-NE-CZ	7.70	135.18	124.40
1	A	168	ASP	CA-C-O	-7.69	112.67	120.90
1	A	33	GLY	N-CA-C	-7.68	103.59	112.50
1	A	88	THR	CA-CB-OG1	-7.68	98.08	109.60
1	B	232	VAL	N-CA-CB	7.68	120.40	110.57
1	A	219	ASP	N-CA-C	7.67	127.13	110.80
1	B	243	LYS	N-CA-CB	7.67	122.22	110.80
1	A	90	ASN	CA-C-O	7.65	130.60	121.65
1	A	326	GLN	O-C-N	7.65	130.22	122.12
1	B	241	LYS	CG-CD-CE	7.64	128.88	111.30
1	A	152	ILE	N-CA-C	7.64	117.71	110.53
1	A	74	ARG	CD-NE-CZ	7.61	135.06	124.40
1	A	276	LYS	CA-CB-CG	7.61	129.32	114.10
1	A	47	ASP	N-CA-C	-7.59	103.85	113.72
1	A	307	LEU	CA-C-O	-7.59	112.66	120.71
1	B	250	ILE	CA-C-O	-7.58	112.46	120.57
1	B	195	HIS	CA-CB-CG	-7.57	106.23	113.80
1	B	261	ILE	O-C-N	-7.57	113.84	121.94
1	A	123	ILE	N-CA-C	7.57	121.58	111.44
1	A	230	LYS	CA-C-O	-7.56	112.88	120.82
1	B	270	PRO	CA-C-O	-7.56	106.85	120.60
1	A	64	MET	CA-C-N	7.54	130.25	120.44
1	A	64	MET	C-N-CA	7.54	130.25	120.44
1	A	192	LEU	O-C-N	-7.53	112.94	122.43
1	B	200	VAL	N-CA-C	7.53	116.31	107.73
1	A	65	ASP	N-CA-C	-7.52	103.02	111.07
1	A	18	VAL	CA-C-O	7.51	130.02	119.95
1	B	84	ASP	CA-C-O	-7.50	111.34	119.97
1	B	85	TYR	CA-C-O	-7.49	109.80	120.51
1	A	156	PRO	CB-CA-C	7.49	121.17	111.21
1	A	87	VAL	CA-CB-CG2	7.47	123.11	110.40
1	B	176	MET	CA-C-O	7.47	128.46	120.55
1	B	153	SER	CA-C-O	-7.46	112.64	120.55
1	A	99	GLY	O-C-N	7.45	130.14	123.06
1	B	223	GLU	CA-C-N	7.44	135.76	121.54
1	B	223	GLU	C-N-CA	7.44	135.76	121.54
1	B	54	VAL	CB-CA-C	-7.43	101.17	111.65
1	B	179	ARG	CA-C-O	-7.41	113.04	120.82
1	B	170	ALA	CA-C-O	7.39	128.61	120.63
1	A	137	VAL	O-C-N	7.37	131.35	122.95
1	B	47	ASP	CA-CB-CG	7.36	119.96	112.60
1	B	94	VAL	CA-C-N	7.34	132.55	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	VAL	C-N-CA	7.34	132.55	122.93
1	B	123	ILE	O-C-N	7.34	129.39	121.83
1	B	223	GLU	CA-C-O	7.34	127.84	119.18
1	B	216	LEU	CA-C-O	7.33	129.28	120.92
1	B	161	ILE	CA-C-N	-7.32	114.47	122.38
1	B	161	ILE	C-N-CA	-7.32	114.47	122.38
1	A	146	THR	N-CA-C	-7.32	103.23	111.14
1	B	75	THR	O-C-N	7.32	127.98	121.32
1	A	100	ALA	CA-C-O	-7.30	112.73	121.05
1	A	95	VAL	CA-C-O	-7.30	112.11	120.65
1	A	177	GLY	N-CA-C	-7.30	103.81	112.64
1	B	305	VAL	CB-CA-C	7.30	121.70	111.34
1	A	114	GLN	N-CA-CB	7.29	120.55	109.91
1	B	132(B)	ASN	OD1-CG-ND2	7.28	129.88	122.60
1	A	90	ASN	CA-CB-CG	7.26	119.86	112.60
1	A	208	VAL	CA-C-O	-7.26	112.76	120.39
1	A	307	LEU	O-C-N	7.26	132.43	123.21
1	B	205	GLY	CA-C-O	-7.24	107.97	120.57
1	B	285	VAL	O-C-N	7.24	130.51	122.98
1	A	315	LEU	CA-C-N	7.21	129.94	120.28
1	A	315	LEU	C-N-CA	7.21	129.94	120.28
1	B	77	LYS	CG-CD-CE	7.20	127.87	111.30
1	B	152	ILE	CB-CA-C	-7.19	102.30	112.22
1	B	259	GLU	CB-CG-CD	7.19	124.82	112.60
1	A	220	ALA	O-C-N	7.18	132.14	122.59
1	A	80	SER	O-C-N	7.17	131.09	123.42
1	B	179	ARG	NE-CZ-NH2	7.17	125.65	119.20
1	B	39	SER	N-CA-C	-7.17	103.16	110.97
1	B	218	THR	CA-C-N	7.16	133.77	122.74
1	B	218	THR	C-N-CA	7.16	133.77	122.74
1	A	199	SER	CA-C-O	7.12	129.10	121.55
1	A	67	GLN	O-C-N	-7.12	114.58	122.12
1	A	96	ILE	CB-CG1-CD1	7.09	128.69	113.80
1	A	210(B)	LYS	O-C-N	-7.07	114.09	122.15
1	A	119	ILE	CA-C-O	-7.07	113.21	121.05
1	A	64	MET	CA-C-O	-7.06	113.41	120.82
1	A	38	ILE	CA-CB-CG2	7.06	122.50	110.50
1	A	35	ALA	N-CA-C	-7.05	103.64	111.82
1	B	130	TYR	CA-C-N	7.03	130.19	122.74
1	B	130	TYR	C-N-CA	7.03	130.19	122.74
1	B	247	SER	CA-C-O	-7.03	110.45	120.51
1	B	168	ASP	O-C-N	7.02	130.91	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	ILE	N-CA-C	7.01	117.92	108.11
1	A	187	CYS	N-CA-C	-7.00	97.80	109.07
1	A	151	LYS	O-C-N	-6.99	114.82	122.09
1	B	232	VAL	O-C-N	6.99	129.17	121.90
1	A	166	ASN	N-CA-C	-6.98	103.60	111.07
1	A	292	ILE	N-CA-C	-6.97	97.57	108.23
1	A	329	LEU	CA-C-N	6.96	134.84	121.54
1	A	329	LEU	C-N-CA	6.96	134.84	121.54
1	A	18	VAL	CA-C-N	6.94	127.11	120.31
1	A	18	VAL	C-N-CA	6.94	127.11	120.31
1	B	118	ASN	CB-CG-ND2	6.94	126.81	116.40
1	B	48	GLU	N-CA-CB	6.94	122.30	110.57
1	B	222	LYS	N-CA-CB	6.92	122.19	110.49
1	B	197	ASP	CA-CB-CG	6.92	119.52	112.60
1	B	317	LYS	N-CA-C	-6.92	103.79	111.82
1	A	86	ASN	CA-C-N	6.91	131.39	120.47
1	A	86	ASN	C-N-CA	6.91	131.39	120.47
1	B	236	ALA	O-C-N	6.91	129.55	122.09
1	A	65	ASP	CA-C-N	6.91	129.42	120.44
1	A	65	ASP	C-N-CA	6.91	129.42	120.44
1	B	266	ARG	NE-CZ-NH2	6.90	125.41	119.20
1	A	296	ASN	O-C-N	6.89	130.96	122.34
1	A	192	LEU	N-CA-CB	-6.89	99.42	110.51
1	A	121	LYS	CA-CB-CG	6.88	127.87	114.10
1	A	266	ARG	NE-CZ-NH2	-6.88	113.01	119.20
1	B	176	MET	CA-C-N	6.88	134.90	121.41
1	B	176	MET	C-N-CA	6.88	134.90	121.41
1	B	188	HIS	CA-CB-CG	-6.88	106.92	113.80
1	A	22	ASN	OD1-CG-ND2	6.86	129.46	122.60
1	A	224	HIS	CA-CB-CG	-6.86	106.94	113.80
1	A	248	TRP	CA-C-O	-6.86	113.63	120.70
1	B	26	VAL	N-CA-CB	6.84	120.54	111.64
1	A	251	GLY	O-C-N	6.83	128.75	122.19
1	A	155	PHE	CA-CB-CG	6.83	120.63	113.80
1	B	327	LYS	CA-C-O	6.83	129.65	121.66
1	B	67	GLN	CG-CD-NE2	6.82	126.63	116.40
1	A	253	SER	N-CA-C	-6.82	103.93	111.36
1	A	207	ASN	N-CA-CB	-6.81	101.01	111.56
1	B	219	ASP	CA-CB-CG	-6.80	105.80	112.60
1	B	113	VAL	CA-C-O	6.80	128.34	121.27
1	B	229	HIS	ND1-CE1-NE2	-6.79	101.61	108.40
1	B	12	LEU	O-C-N	6.78	130.68	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ARG	CB-CG-CD	6.78	126.89	111.30
1	A	172	PHE	CA-CB-CG	6.77	120.57	113.80
1	B	32	VAL	N-CA-C	-6.77	104.25	110.82
1	B	272	SER	N-CA-CB	6.77	121.55	110.17
1	A	123	ILE	O-C-N	6.75	131.07	121.82
1	A	58	LYS	CA-CB-CG	6.75	127.60	114.10
1	B	14	GLU	CA-CB-CG	6.75	127.60	114.10
1	B	55	MET	CG-SD-CE	-6.74	86.07	100.90
1	A	295	GLN	CG-CD-NE2	-6.74	106.30	116.40
1	B	93	LEU	CA-C-N	-6.74	112.98	122.75
1	B	93	LEU	C-N-CA	-6.74	112.98	122.75
1	A	329	LEU	N-CA-C	6.73	119.93	111.24
1	A	267	ARG	CB-CG-CD	-6.73	95.82	111.30
1	A	289	VAL	CA-CB-CG1	6.73	121.84	110.40
1	A	117	VAL	N-CA-C	-6.73	103.76	110.62
1	A	66	LEU	O-C-N	-6.72	115.15	122.07
1	A	200	VAL	CA-C-O	-6.72	114.30	119.20
1	B	70	SER	CB-CA-C	-6.71	99.61	110.74
1	B	239	VAL	CA-C-N	6.70	129.64	120.46
1	B	239	VAL	C-N-CA	6.70	129.64	120.46
1	B	132(B)	ASN	N-CA-C	6.68	121.50	112.88
1	B	232	VAL	N-CA-C	-6.68	104.25	110.53
1	B	32	VAL	CB-CA-C	6.67	120.78	112.04
1	B	57	ASP	O-C-N	6.67	129.24	122.03
1	A	65	ASP	CA-CB-CG	6.67	119.27	112.60
1	B	78	ILE	CA-C-N	6.66	132.44	122.58
1	B	78	ILE	C-N-CA	6.66	132.44	122.58
1	A	251	GLY	CA-C-N	6.66	129.49	120.44
1	A	251	GLY	C-N-CA	6.66	129.49	120.44
1	B	16	HIS	CA-C-O	-6.65	113.88	121.66
1	B	179	ARG	NH1-CZ-NH2	-6.65	110.66	119.30
1	B	115	ARG	O-C-N	6.64	130.44	122.27
1	A	201	PRO	CA-C-O	-6.63	113.21	120.97
1	A	269	HIS	CA-C-O	-6.63	112.87	120.03
1	B	47	ASP	N-CA-C	-6.63	105.11	113.72
1	A	235	SER	CA-C-O	-6.61	113.88	120.82
1	A	275	ILE	CA-C-O	-6.61	112.98	120.26
1	B	67	GLN	CA-C-O	6.61	127.55	120.55
1	B	296	ASN	CA-C-O	-6.60	111.80	119.59
1	A	322	LEU	O-C-N	-6.59	115.28	122.07
1	B	312	GLU	CA-C-N	6.58	129.43	120.54
1	B	312	GLU	C-N-CA	6.58	129.43	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ASN	CB-CG-ND2	6.57	126.26	116.40
1	A	265	LEU	CA-C-O	-6.57	111.30	119.38
1	B	75	THR	CA-C-O	-6.56	112.48	120.74
1	B	130	TYR	CA-C-O	-6.56	111.68	119.15
1	A	135	LEU	CA-C-O	-6.55	113.14	120.54
1	B	87	VAL	CA-C-N	6.54	134.22	122.38
1	B	87	VAL	C-N-CA	6.54	134.22	122.38
1	A	254	VAL	CA-C-O	-6.53	114.16	120.95
1	B	263	LYS	N-CA-C	-6.53	104.94	113.17
1	B	3	LEU	N-CA-C	-6.52	104.26	111.82
1	A	261	ILE	CA-C-O	6.52	128.29	121.05
1	A	293	LEU	O-C-N	-6.52	115.60	123.29
1	A	15	GLU	CA-C-N	-6.51	109.10	121.54
1	A	15	GLU	C-N-CA	-6.51	109.10	121.54
1	B	121	LYS	CA-C-O	-6.51	113.65	120.55
1	B	78	ILE	CA-C-O	6.51	126.85	120.27
1	A	290	PRO	CA-C-O	-6.50	113.32	120.92
1	A	87	VAL	N-CA-CB	6.49	121.75	110.65
1	A	164	GLY	N-CA-C	6.47	123.12	111.34
1	B	111	ASN	CA-CB-CG	-6.47	106.13	112.60
1	B	181	GLY	CA-C-N	6.47	131.94	122.94
1	B	181	GLY	C-N-CA	6.47	131.94	122.94
1	A	98	ALA	N-CA-CB	-6.47	100.85	110.17
1	A	212	LEU	CA-CB-CG	6.47	138.95	116.30
1	A	268	VAL	CA-CB-CG1	6.47	121.40	110.40
1	A	267	ARG	CA-CB-CG	-6.46	101.18	114.10
1	B	48	GLU	O-C-N	6.46	130.78	123.42
1	B	19	PRO	CB-CA-C	6.46	119.95	110.85
1	B	174	TYR	CA-CB-CG	-6.46	102.28	113.90
1	B	258	ALA	N-CA-C	-6.45	104.25	111.28
1	B	212	LEU	CA-C-N	6.45	132.17	123.46
1	B	212	LEU	C-N-CA	6.45	132.17	123.46
1	A	231	GLU	CA-CB-CG	6.45	126.99	114.10
1	B	171	ARG	N-CA-C	-6.45	104.18	111.14
1	A	326	GLN	CA-C-O	-6.44	113.67	120.63
1	B	235	SER	CB-CA-C	6.43	121.47	110.79
1	A	172	PHE	CA-C-N	6.43	128.79	120.44
1	A	172	PHE	C-N-CA	6.43	128.79	120.44
1	A	229	HIS	N-CA-CB	6.42	119.32	110.01
1	A	20	HIS	O-C-N	6.41	130.95	122.36
1	A	176	MET	CA-C-O	6.41	127.55	120.82
1	B	35	ALA	N-CA-CB	6.40	119.29	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	LYS	CB-CG-CD	-6.40	96.57	111.30
1	A	16	HIS	CG-CD2-NE2	6.39	113.59	107.20
1	A	70	SER	CB-CA-C	-6.38	100.61	110.81
1	B	116	ASN	CB-CA-C	6.37	123.37	110.38
1	B	328	GLU	CA-CB-CG	6.37	126.83	114.10
1	A	321	THR	CA-C-N	6.36	128.71	120.44
1	A	321	THR	C-N-CA	6.36	128.71	120.44
1	A	313	ALA	CA-C-O	-6.36	112.29	119.79
1	A	320	ASP	N-CA-C	-6.35	102.89	112.04
1	A	103	GLN	N-CA-C	-6.35	101.38	110.59
1	A	144	ILE	CA-CB-CG1	-6.33	99.64	110.40
1	B	237	TYR	CA-C-O	6.33	127.46	120.82
1	B	229	HIS	CE1-NE2-CD2	6.32	115.32	109.00
1	B	209(A)	ALA	CA-C-O	6.32	128.64	120.81
1	B	13	LYS	CA-CB-CG	6.31	126.73	114.10
1	B	192	LEU	N-CA-CB	-6.31	101.01	110.60
1	A	279	TYR	CB-CA-C	6.31	119.64	111.50
1	A	267	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	A	31	ALA	O-C-N	6.30	128.82	122.08
1	A	222	LYS	N-CA-CB	-6.28	99.87	110.49
1	B	25	THR	CA-CB-OG1	-6.28	100.18	109.60
1	A	16	HIS	N-CA-C	-6.26	97.46	110.80
1	B	170	ALA	CA-C-N	6.25	128.95	120.44
1	B	170	ALA	C-N-CA	6.25	128.95	120.44
1	A	207	ASN	N-CA-C	6.25	118.36	108.79
1	B	70	SER	CA-C-O	-6.25	113.92	120.92
1	B	3	LEU	CA-C-O	6.24	127.15	119.97
1	A	68	HIS	CB-CG-ND1	6.24	132.06	122.70
1	B	158	ASN	O-C-N	6.24	129.52	122.22
1	B	200	VAL	N-CA-CB	-6.24	103.53	111.39
1	B	208	VAL	N-CA-CB	6.24	120.08	112.10
1	A	216	LEU	CA-C-O	-6.24	113.81	120.92
1	B	117	VAL	N-CA-C	-6.23	104.27	110.62
1	A	244	GLY	CA-C-O	6.23	125.56	119.27
1	B	242	LEU	CA-C-N	-6.22	112.59	122.29
1	B	242	LEU	C-N-CA	-6.22	112.59	122.29
1	A	222	LYS	O-C-N	-6.20	114.35	122.59
1	B	172	PHE	CA-CB-CG	6.20	120.00	113.80
1	A	19	PRO	CA-C-O	-6.19	114.44	122.12
1	A	283	GLU	O-C-N	6.19	131.60	122.81
1	B	2	THR	CB-CA-C	6.17	123.65	110.19
1	A	155	PHE	O-C-N	6.16	128.52	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ARG	CA-C-O	-6.16	113.89	120.42
1	B	222	LYS	CB-CA-C	-6.16	98.16	110.42
1	A	194	GLU	CB-CG-CD	6.16	123.07	112.60
1	A	310	GLU	O-C-N	-6.14	115.50	122.08
1	B	187	CYS	N-CA-CB	6.13	120.18	110.55
1	B	225	TRP	CA-C-N	6.13	129.10	120.28
1	B	225	TRP	C-N-CA	6.13	129.10	120.28
1	B	90	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	A	102	GLN	OE1-CD-NE2	6.12	128.72	122.60
1	A	249	ALA	N-CA-CB	-6.12	101.12	110.12
1	A	36	CYS	CA-C-N	6.12	128.80	120.54
1	A	36	CYS	C-N-CA	6.12	128.80	120.54
1	B	114	GLN	CB-CA-C	6.12	120.49	110.88
1	A	195	HIS	N-CA-C	-6.12	97.88	108.52
1	B	228	VAL	CA-C-N	6.10	128.38	120.44
1	B	228	VAL	C-N-CA	6.10	128.38	120.44
1	A	183	HIS	CE1-NE2-CD2	-6.10	102.90	109.00
1	A	3	LEU	CB-CA-C	6.10	120.62	110.92
1	A	110	LEU	CB-CA-C	6.09	122.36	110.67
1	B	101	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	A	115	ARG	NE-CZ-NH1	-6.09	115.41	121.50
1	B	101	ARG	CA-C-N	6.09	130.50	120.94
1	B	101	ARG	C-N-CA	6.09	130.50	120.94
1	B	49	ILE	CA-C-O	-6.08	114.00	120.39
1	B	134	LYS	N-CA-C	-6.08	99.33	109.24
1	B	124	ILE	CA-C-O	-6.08	114.62	118.69
1	A	266	ARG	NH1-CZ-NH2	6.07	127.20	119.30
1	A	317	LYS	CG-CD-CE	6.07	125.26	111.30
1	B	209(B)	GLY	N-CA-C	-6.06	107.86	115.08
1	B	258	ALA	O-C-N	6.06	128.55	122.12
1	A	142	VAL	CA-C-O	-6.05	114.66	120.95
1	B	275	ILE	CA-CB-CG1	-6.05	100.11	110.40
1	A	158	ASN	CA-C-O	-6.05	112.65	119.79
1	B	305	VAL	N-CA-C	-6.05	100.98	109.21
1	A	29	VAL	CA-C-O	6.04	128.33	120.78
1	B	163	SER	O-C-N	-6.04	115.16	122.22
1	A	63	MET	CA-C-N	6.03	128.28	120.44
1	A	63	MET	C-N-CA	6.03	128.28	120.44
1	A	178	GLU	CA-C-O	6.03	126.91	119.97
1	A	16	HIS	CB-CA-C	6.03	122.42	110.42
1	B	94	VAL	CB-CA-C	6.03	119.80	110.28
1	B	251	GLY	CA-C-N	6.03	130.77	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	GLY	C-N-CA	6.03	130.77	120.71
1	B	182	VAL	CA-C-O	6.02	127.41	120.67
1	A	117	VAL	O-C-N	-6.02	116.03	121.87
1	B	67	GLN	O-C-N	-6.01	115.75	122.12
1	A	31	ALA	CA-C-O	-6.01	114.46	121.07
1	A	92	ARG	CD-NE-CZ	-6.01	115.99	124.40
1	B	142	VAL	CA-C-N	6.01	128.25	120.44
1	B	142	VAL	C-N-CA	6.01	128.25	120.44
1	B	156	PRO	CB-CA-C	6.00	118.84	110.98
1	B	281	ILE	O-C-N	6.00	129.22	122.68
1	B	176	MET	CG-SD-CE	-5.99	87.72	100.90
1	B	292	ILE	CA-CB-CG1	-5.98	100.24	110.40
1	B	160	VAL	CA-C-N	5.97	130.54	122.90
1	B	160	VAL	C-N-CA	5.97	130.54	122.90
1	B	263	LYS	CA-CB-CG	-5.97	102.16	114.10
1	B	323	TRP	CA-C-O	-5.97	114.09	120.42
1	A	312	GLU	OE1-CD-OE2	-5.96	108.58	122.90
1	B	330	GLN	CA-C-N	-5.96	110.96	121.70
1	B	330	GLN	C-N-CA	-5.96	110.96	121.70
1	A	13	LYS	CA-CB-CG	5.96	126.02	114.10
1	A	127	ILE	CA-CB-CG2	5.96	120.63	110.50
1	B	293	LEU	O-C-N	-5.96	116.43	123.22
1	B	321	THR	CA-CB-OG1	-5.96	100.67	109.60
1	B	314	HIS	N-CA-CB	5.94	119.49	110.28
1	B	32	VAL	CA-C-O	-5.93	113.90	120.96
1	A	291	CYS	O-C-N	5.93	130.51	123.33
1	A	157	LYS	CA-C-O	5.93	128.99	120.51
1	B	36	CYS	CA-C-O	5.93	127.04	120.82
1	A	173	ARG	CA-C-O	5.92	127.04	120.82
1	B	235	SER	CA-CB-OG	-5.92	99.26	111.10
1	B	218	THR	CB-CA-C	5.92	122.19	110.42
1	B	220	ALA	CB-CA-C	5.92	121.72	109.95
1	A	191	ILE	N-CA-CB	5.91	119.12	111.67
1	B	209(D)	SER	CA-CB-OG	-5.91	99.29	111.10
1	B	328	GLU	CB-CA-C	-5.91	98.67	110.42
1	A	15	GLU	N-CA-C	-5.91	98.22	110.80
1	B	256	ASP	O-C-N	-5.90	115.99	122.07
1	A	106	GLY	CA-C-O	5.89	125.60	119.00
1	B	244	GLY	CA-C-O	5.89	125.40	119.27
1	B	329	LEU	O-C-N	-5.89	114.75	122.59
1	B	75	THR	CA-CB-OG1	-5.89	100.77	109.60
1	A	87	VAL	CA-C-O	-5.89	114.27	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	SER	CB-CA-C	5.88	119.47	109.53
1	B	242	LEU	O-C-N	5.88	130.79	122.20
1	B	291	CYS	CA-C-N	-5.88	115.37	122.90
1	B	291	CYS	C-N-CA	-5.88	115.37	122.90
1	B	146	THR	CA-CB-OG1	5.88	118.42	109.60
1	B	92	ARG	NH1-CZ-NH2	-5.87	111.67	119.30
1	A	7	LEU	CA-C-N	5.87	130.83	123.14
1	A	7	LEU	C-N-CA	5.87	130.83	123.14
1	A	249	ALA	CA-C-O	-5.87	114.33	120.55
1	A	77	LYS	CB-CA-C	-5.87	100.42	110.16
1	B	323	TRP	CB-CG-CD1	5.86	135.69	126.90
1	B	136	LEU	CA-C-N	5.84	129.67	122.37
1	B	136	LEU	C-N-CA	5.84	129.67	122.37
1	B	187	CYS	CB-CA-C	-5.84	100.62	110.19
1	A	117	VAL	CA-C-N	5.83	129.18	120.31
1	A	117	VAL	C-N-CA	5.83	129.18	120.31
1	A	9	HIS	O-C-N	-5.83	115.79	123.13
1	B	319	ALA	CA-C-O	-5.82	113.28	119.97
1	A	105	GLU	CA-C-O	5.82	127.55	120.92
1	B	2	THR	N-CA-CB	-5.82	102.41	110.38
1	A	243	LYS	CA-C-O	-5.80	112.67	119.05
1	A	267	ARG	NE-CZ-NH2	-5.80	113.98	119.20
1	A	86	ASN	N-CA-CB	-5.80	101.30	110.28
1	A	148	VAL	CA-C-O	-5.80	115.03	121.17
1	B	257	LEU	CA-C-N	5.79	128.04	120.28
1	B	257	LEU	C-N-CA	5.79	128.04	120.28
1	A	269	HIS	CE1-NE2-CD2	-5.79	103.22	109.00
1	A	318	SER	CA-C-N	5.79	130.38	120.72
1	A	318	SER	C-N-CA	5.79	130.38	120.72
1	B	121	LYS	N-CA-CB	5.78	118.62	110.12
1	B	275	ILE	CA-CB-CG2	5.78	120.32	110.50
1	B	323	TRP	CE2-CD2-CE3	5.77	124.57	118.80
1	B	202	VAL	O-C-N	-5.77	115.36	122.57
1	A	36	CYS	N-CA-C	-5.77	104.91	111.14
1	A	92	ARG	CA-C-O	-5.77	114.38	120.55
1	A	259	GLU	CG-CD-OE1	5.76	131.64	118.40
1	B	179	ARG	O-C-N	5.75	128.00	122.07
1	B	210(A)	LEU	CB-CA-C	5.75	121.28	110.63
1	A	140	ASN	OD1-CG-ND2	5.75	128.35	122.60
1	B	140	ASN	CB-CG-OD1	5.75	132.30	120.80
1	A	12	LEU	O-C-N	5.74	130.81	122.94
1	A	156	PRO	O-C-N	-5.74	116.21	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	PRO	N-CA-C	5.74	121.40	113.65
1	B	274	MET	CG-SD-CE	-5.74	88.27	100.90
1	A	9	HIS	CB-CA-C	5.74	120.15	110.79
1	B	148	VAL	N-CA-CB	5.74	117.26	110.55
1	A	316	LYS	CA-C-N	5.74	127.89	120.44
1	A	316	LYS	C-N-CA	5.74	127.89	120.44
1	B	26	VAL	CA-CB-CG2	5.74	120.15	110.40
1	A	178	GLU	O-C-N	-5.73	115.22	122.27
1	B	248	TRP	CA-C-O	-5.73	114.48	120.55
1	A	293	LEU	CA-C-N	5.72	132.63	121.41
1	A	293	LEU	C-N-CA	5.72	132.63	121.41
1	B	48	GLU	CA-C-N	-5.72	115.64	123.14
1	B	48	GLU	C-N-CA	-5.72	115.64	123.14
1	B	83	LYS	N-CA-CB	5.72	119.11	110.30
1	A	263	LYS	CG-CD-CE	5.72	124.45	111.30
1	A	66	LEU	CA-C-N	5.71	127.94	120.28
1	A	66	LEU	C-N-CA	5.71	127.94	120.28
1	B	71	LEU	CA-C-O	-5.71	112.34	120.51
1	B	34	MET	CA-C-N	5.71	127.86	120.44
1	B	34	MET	C-N-CA	5.71	127.86	120.44
1	B	90	ASN	CA-CB-CG	5.71	118.31	112.60
1	B	159	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	A	264	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	B	38	ILE	CA-CB-CG2	5.70	120.19	110.50
1	B	174	TYR	CA-C-O	5.70	126.98	121.00
1	A	135	LEU	CA-C-N	5.70	131.39	123.07
1	A	135	LEU	C-N-CA	5.70	131.39	123.07
1	A	79	VAL	CA-CB-CG1	5.70	120.08	110.40
1	B	93	LEU	CA-C-O	-5.69	114.45	121.11
1	B	111	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	B	128	VAL	CA-C-N	5.69	128.37	120.29
1	B	128	VAL	C-N-CA	5.69	128.37	120.29
1	A	209(D)	SER	CB-CA-C	5.68	119.31	110.67
1	B	58	LYS	CB-CA-C	-5.68	101.42	110.84
1	B	116	ASN	CB-CG-ND2	5.68	124.91	116.40
1	B	31	ALA	CA-C-O	5.67	126.56	120.55
1	A	312	GLU	CG-CD-OE1	5.67	131.45	118.40
1	A	244	GLY	N-CA-C	5.66	121.50	114.37
1	B	146	THR	N-CA-CB	5.66	118.27	110.07
1	A	159	ARG	CA-CB-CG	5.65	125.40	114.10
1	A	114	GLN	O-C-N	5.65	127.90	122.03
1	A	77	LYS	CA-C-N	-5.64	115.59	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	LYS	C-N-CA	-5.64	115.59	123.10
1	A	272	SER	O-C-N	5.64	129.96	123.02
1	A	309	PRO	CA-C-O	-5.64	110.34	120.60
1	A	200	VAL	N-CA-C	5.63	114.08	107.77
1	A	9	HIS	CA-CB-CG	-5.63	108.17	113.80
1	A	292	ILE	CA-C-O	5.62	127.23	120.65
1	B	129	LYS	CA-C-O	-5.62	114.46	120.42
1	B	307	LEU	CA-C-O	-5.62	114.46	120.92
1	A	148	VAL	N-CA-C	-5.62	105.03	110.42
1	A	179	ARG	CA-C-O	-5.62	114.01	120.24
1	B	315	LEU	O-C-N	5.62	128.55	122.15
1	A	176	MET	N-CA-CB	-5.61	101.87	110.01
1	A	3	LEU	O-C-N	-5.60	116.09	122.08
1	A	271	ILE	CB-CA-C	5.60	119.06	110.55
1	A	74	ARG	NE-CZ-NH2	-5.60	114.16	119.20
1	A	256	ASP	N-CA-CB	5.59	118.11	110.01
1	A	284	ASN	CA-C-O	-5.58	111.66	120.37
1	B	49	ILE	CB-CA-C	5.58	118.89	110.63
1	B	235	SER	CA-C-O	-5.58	114.63	120.55
1	B	266	ARG	N-CA-C	-5.58	104.20	111.74
1	B	92	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	A	264	ASN	CB-CG-OD1	5.58	131.95	120.80
1	B	319	ALA	N-CA-CB	5.58	118.92	110.28
1	A	115	ARG	N-CA-C	5.57	117.36	111.28
1	A	232	VAL	O-C-N	-5.57	116.45	121.91
1	B	178	GLU	CB-CG-CD	-5.57	103.14	112.60
1	B	173	ARG	O-C-N	-5.56	115.81	122.15
1	A	50	ALA	CA-C-O	5.56	126.37	120.36
1	B	304	LYS	CA-C-O	-5.56	115.36	121.58
1	A	168	ASP	N-CA-CB	5.54	118.20	109.94
1	B	271	ILE	N-CA-C	5.54	116.82	108.96
1	B	230	LYS	CD-CE-NZ	5.53	129.61	111.90
1	B	71	LEU	CA-C-N	-5.53	113.80	122.65
1	B	71	LEU	C-N-CA	-5.53	113.80	122.65
1	A	54	VAL	N-CA-C	-5.52	105.50	113.07
1	B	328	GLU	CA-C-N	5.52	132.09	121.54
1	B	328	GLU	C-N-CA	5.52	132.09	121.54
1	A	242	LEU	CA-C-O	-5.51	114.65	120.55
1	B	201	PRO	CA-C-O	-5.51	114.74	121.03
1	B	197	ASP	CB-CG-OD2	-5.51	105.72	118.40
1	B	12	LEU	CB-CA-C	-5.51	100.38	110.62
1	B	132(B)	ASN	N-CA-CB	-5.50	102.20	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASP	N-CA-CB	5.50	118.74	110.65
1	A	286	PHE	CA-C-O	-5.50	114.41	120.30
1	A	267	ARG	CG-CD-NE	-5.50	99.90	112.00
1	B	92	ARG	CA-C-O	5.50	126.34	120.24
1	B	204	SER	O-C-N	-5.50	115.79	122.22
1	A	102	GLN	CB-CG-CD	-5.49	103.26	112.60
1	B	118	ASN	O-C-N	5.48	127.93	122.12
1	A	171	ARG	N-CA-C	-5.48	105.38	111.36
1	A	118	ASN	CA-CB-CG	5.48	118.08	112.60
1	A	84	ASP	N-CA-CB	5.48	119.10	110.23
1	B	121	LYS	CA-CB-CG	5.47	125.04	114.10
1	B	18	VAL	O-C-N	5.46	126.58	121.61
1	B	118	ASN	N-CA-CB	5.46	118.15	110.12
1	A	152	ILE	N-CA-CB	-5.46	103.58	110.57
1	B	291	CYS	CA-C-O	-5.46	114.95	121.11
1	B	274	MET	N-CA-CB	-5.45	100.66	109.60
1	B	319	ALA	N-CA-C	-5.45	105.50	111.82
1	A	261	ILE	CA-C-N	5.45	128.13	120.28
1	A	261	ILE	C-N-CA	5.45	128.13	120.28
1	B	25	THR	CA-C-N	-5.45	115.85	123.10
1	B	25	THR	C-N-CA	-5.45	115.85	123.10
1	A	16	HIS	CE1-NE2-CD2	-5.45	103.56	109.00
1	A	54	VAL	O-C-N	5.45	128.44	122.12
1	A	288	SER	CA-CB-OG	-5.45	100.21	111.10
1	A	258	ALA	N-CA-C	-5.44	105.35	111.28
1	A	114	GLN	CG-CD-NE2	5.44	124.56	116.40
1	A	324	GLY	N-CA-C	-5.44	106.08	113.37
1	B	209(D)	SER	O-C-N	5.44	129.82	122.59
1	A	231	GLU	CA-C-O	-5.43	113.96	120.10
1	A	254	VAL	O-C-N	5.43	127.14	121.87
1	B	145	LEU	CA-C-N	5.43	127.82	120.44
1	B	145	LEU	C-N-CA	5.43	127.82	120.44
1	A	118	ASN	CB-CG-ND2	5.42	124.53	116.40
1	B	213	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	B	233	VAL	N-CA-C	5.42	115.62	110.42
1	A	59	LEU	CA-C-O	-5.41	115.32	121.00
1	A	183	HIS	CG-CD2-NE2	5.41	112.61	107.20
1	A	285	VAL	O-C-N	5.41	129.24	122.59
1	B	56	GLU	CA-C-O	-5.41	115.12	120.90
1	B	207	ASN	N-CA-CB	-5.40	102.29	111.69
1	B	64	MET	N-CA-CB	5.40	118.06	110.12
1	B	191	ILE	CB-CG1-CD1	-5.40	102.47	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	LEU	CA-C-O	5.39	127.35	120.07
1	B	110	LEU	N-CA-CB	-5.39	101.91	110.22
1	A	26	VAL	O-C-N	5.38	128.25	123.03
1	A	302	VAL	CA-C-N	5.38	129.79	122.90
1	A	302	VAL	C-N-CA	5.38	129.79	122.90
1	B	47	ASP	CB-CA-C	5.38	118.59	109.55
1	B	274	MET	CB-CA-C	5.38	118.85	110.67
1	A	185	LEU	O-C-N	5.38	128.33	122.20
1	B	140	ASN	CB-CA-C	5.38	116.84	108.61
1	B	329	LEU	CA-C-O	5.37	128.19	120.51
1	A	166	ASN	CA-CB-CG	-5.37	107.23	112.60
1	A	96	ILE	N-CA-C	5.37	115.51	107.51
1	A	126	ASN	OD1-CG-ND2	5.37	127.97	122.60
1	A	180	LEU	N-CA-CB	-5.37	101.65	110.40
1	A	246	THR	CA-CB-OG1	-5.37	101.55	109.60
1	A	226	LYS	CA-C-N	5.36	129.67	120.72
1	A	226	LYS	C-N-CA	5.36	129.67	120.72
1	A	263	LYS	CB-CA-C	5.36	118.97	109.65
1	A	159	ARG	CA-C-O	5.35	125.90	119.43
1	B	66	LEU	CA-C-N	5.35	127.45	120.28
1	B	66	LEU	C-N-CA	5.35	127.45	120.28
1	B	69	GLY	N-CA-C	-5.35	106.74	115.46
1	A	120	PHE	CA-C-O	-5.34	114.76	120.42
1	A	209(C)	VAL	CA-CB-CG1	5.34	119.48	110.40
1	A	42	MET	O-C-N	5.33	128.83	122.27
1	A	113	VAL	CA-C-N	5.33	127.69	120.65
1	A	113	VAL	C-N-CA	5.33	127.69	120.65
1	B	142	VAL	CB-CA-C	5.33	119.02	112.04
1	B	220	ALA	O-C-N	-5.33	114.65	122.43
1	B	11	LEU	CB-CA-C	5.32	117.96	109.02
1	A	62	GLU	CA-C-N	5.32	128.18	120.79
1	A	62	GLU	C-N-CA	5.32	128.18	120.79
1	B	219	ASP	CB-CG-OD1	5.32	130.62	118.40
1	B	127	ILE	CB-CG1-CD1	-5.31	102.64	113.80
1	A	92	ARG	NE-CZ-NH2	5.31	123.97	119.20
1	A	221	ASP	N-CA-CB	-5.30	102.23	110.29
1	A	190	TRP	CB-CG-CD2	5.30	134.22	126.80
1	A	68	HIS	N-CA-CB	5.29	118.37	110.22
1	A	209(D)	SER	CA-CB-OG	5.29	121.69	111.10
1	A	88	THR	OG1-CB-CG2	5.29	119.88	109.30
1	B	252	LEU	CA-C-O	5.29	126.20	120.55
1	B	3	LEU	CA-C-N	5.28	127.36	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	LEU	C-N-CA	5.28	127.36	120.28
1	A	102	GLN	O-C-N	5.28	129.33	122.89
1	B	107	GLU	O-C-N	5.28	129.24	123.22
1	A	241	LYS	CA-C-O	-5.28	114.95	120.55
1	A	235	SER	CA-CB-OG	-5.27	100.56	111.10
1	B	170	ALA	O-C-N	-5.27	116.53	122.12
1	A	151	LYS	CA-C-N	5.27	127.30	120.56
1	A	151	LYS	C-N-CA	5.27	127.30	120.56
1	B	95	VAL	O-C-N	5.26	130.50	122.76
1	A	184	PRO	O-C-N	5.26	128.29	122.24
1	A	256	ASP	CB-CG-OD2	-5.26	106.30	118.40
1	B	267	ARG	CA-C-N	5.26	129.63	122.90
1	B	267	ARG	C-N-CA	5.26	129.63	122.90
1	A	90	ASN	OD1-CG-ND2	5.25	127.85	122.60
1	A	127	ILE	O-C-N	-5.25	116.42	121.83
1	B	178	GLU	CB-CA-C	-5.25	102.41	110.81
1	B	330	GLN	O-C-N	5.25	129.28	121.72
1	A	29	VAL	CB-CA-C	5.24	119.89	111.29
1	A	109	ARG	CG-CD-NE	5.24	123.53	112.00
1	A	207	ASN	CA-C-N	-5.24	116.27	123.14
1	A	207	ASN	C-N-CA	-5.24	116.27	123.14
1	B	164	GLY	O-C-N	5.24	129.51	122.70
1	A	259	GLU	CB-CG-CD	-5.23	103.70	112.60
1	A	78	ILE	CA-C-N	-5.23	115.39	122.92
1	A	78	ILE	C-N-CA	-5.23	115.39	122.92
1	A	248	TRP	O-C-N	5.23	127.74	122.09
1	A	179	ARG	NH1-CZ-NH2	5.23	126.10	119.30
1	A	219	ASP	CA-C-O	5.22	127.98	120.51
1	B	71	LEU	O-C-N	5.22	129.53	122.59
1	B	230	LYS	CB-CA-C	5.22	119.07	110.88
1	A	231	GLU	CB-CG-CD	5.21	121.45	112.60
1	B	153	SER	CB-CA-C	-5.21	102.14	110.79
1	A	3	LEU	N-CA-C	-5.21	104.67	111.02
1	B	116	ASN	N-CA-CB	-5.21	102.28	110.30
1	A	115	ARG	CD-NE-CZ	-5.20	117.11	124.40
1	A	260	SER	N-CA-CB	5.20	118.34	110.28
1	A	200	VAL	N-CA-CB	-5.18	104.85	111.23
1	A	55	MET	O-C-N	-5.18	115.62	122.57
1	A	241	LYS	CA-CB-CG	5.18	124.46	114.10
1	A	54	VAL	CA-C-N	-5.18	113.78	122.17
1	A	54	VAL	C-N-CA	-5.18	113.78	122.17
1	A	9	HIS	CA-C-N	5.17	128.82	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	HIS	C-N-CA	5.17	128.82	121.42
1	B	102	GLN	CG-CD-NE2	5.17	124.16	116.40
1	B	327	LYS	N-CA-CB	5.17	117.80	110.46
1	B	239	VAL	O-C-N	-5.16	116.66	121.87
1	A	58	LYS	O-C-N	-5.16	116.17	122.11
1	B	312	GLU	CG-CD-OE2	-5.16	106.53	118.40
1	A	327	LYS	CA-CB-CG	5.16	124.42	114.10
1	B	74	ARG	CA-C-N	5.16	130.04	122.98
1	B	74	ARG	C-N-CA	5.16	130.04	122.98
1	B	323	TRP	CB-CG-CD2	-5.15	119.59	126.80
1	A	64	MET	N-CA-CB	5.14	117.47	110.01
1	B	232	VAL	CA-C-O	-5.14	115.34	121.05
1	B	12	LEU	N-CA-C	5.14	116.65	108.79
1	A	3	LEU	CA-C-N	5.14	131.35	121.54
1	A	3	LEU	C-N-CA	5.14	131.35	121.54
1	A	20	HIS	ND1-CE1-NE2	-5.14	103.26	108.40
1	A	269	HIS	CG-CD2-NE2	5.13	112.33	107.20
1	A	281	ILE	CA-C-O	-5.13	115.04	120.53
1	A	228	VAL	CA-C-O	-5.13	115.41	120.85
1	A	301	ASP	CB-CG-OD1	5.13	130.19	118.40
1	B	101	ARG	CA-C-O	5.12	128.34	121.78
1	A	107	GLU	N-CA-C	5.12	117.91	109.76
1	B	140	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	B	123	ILE	N-CA-C	5.12	115.89	110.72
1	B	26	VAL	N-CA-C	-5.12	100.28	107.75
1	B	225	TRP	N-CA-C	-5.12	105.78	112.23
1	A	134	LYS	N-CA-CB	5.11	118.76	110.42
1	B	192	LEU	CA-C-N	5.11	131.42	121.41
1	B	192	LEU	C-N-CA	5.11	131.42	121.41
1	B	329	LEU	CB-CA-C	5.11	120.59	110.42
1	B	126	ASN	CB-CG-OD1	-5.11	110.59	120.80
1	B	152	ILE	CA-C-N	5.11	127.12	120.28
1	B	152	ILE	C-N-CA	5.11	127.12	120.28
1	A	40	ILE	O-C-N	-5.11	116.92	121.87
1	A	125	PRO	N-CA-CB	5.11	108.95	103.33
1	A	221	ASP	CB-CG-OD1	5.09	130.12	118.40
1	B	139	SER	CA-CB-OG	-5.09	100.91	111.10
1	B	175	LEU	CA-C-O	-5.09	115.47	120.82
1	A	269	HIS	O-C-N	5.09	127.28	121.94
1	A	205	GLY	CA-C-N	5.09	127.90	120.98
1	A	205	GLY	C-N-CA	5.09	127.90	120.98
1	B	54	VAL	CA-C-O	-5.08	114.58	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ARG	CG-CD-NE	5.08	123.17	112.00
1	A	49	ILE	O-C-N	5.07	128.74	123.26
1	A	150	TRP	CA-C-N	5.07	127.39	120.54
1	A	150	TRP	C-N-CA	5.07	127.39	120.54
1	A	72	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	48	GLU	O-C-N	5.07	129.20	123.42
1	B	279	TYR	CA-C-O	-5.06	115.67	121.54
1	A	90	ASN	N-CA-C	5.06	118.60	111.52
1	B	46	ALA	CA-C-N	5.06	130.30	122.26
1	B	46	ALA	C-N-CA	5.06	130.30	122.26
1	A	201	PRO	CB-CA-C	5.05	117.02	111.11
1	A	225	TRP	CA-C-O	-5.05	114.16	119.97
1	A	283	GLU	CB-CG-CD	5.05	121.19	112.60
1	B	44	GLU	O-C-N	5.05	129.07	122.86
1	A	147	TYR	O-C-N	-5.05	116.84	122.09
1	A	243	LYS	O-C-N	5.04	128.56	122.35
1	A	62	GLU	N-CA-C	-5.04	105.48	111.69
1	A	178	GLU	CG-CD-OE1	5.04	129.99	118.40
1	A	253	SER	O-C-N	-5.04	116.41	122.15
1	B	120	PHE	CA-C-N	5.04	127.03	120.28
1	B	120	PHE	C-N-CA	5.04	127.03	120.28
1	B	320	ASP	OD1-CG-OD2	-5.04	110.81	122.90
1	B	111	ASN	CA-C-N	5.04	131.40	121.58
1	B	111	ASN	C-N-CA	5.04	131.40	121.58
1	A	219	ASP	OD1-CG-OD2	5.03	134.97	122.90
1	A	264	ASN	O-C-N	-5.03	115.67	122.41
1	B	42	MET	CA-CB-CG	-5.03	104.04	114.10
1	B	94	VAL	CA-CB-CG1	5.03	118.95	110.40
1	A	188	HIS	CE1-NE2-CD2	5.03	114.03	109.00
1	A	293	LEU	N-CA-CB	-5.02	102.69	110.57
1	A	262	MET	O-C-N	-5.02	116.35	122.22
1	A	157	LYS	N-CA-CB	-5.02	102.01	110.49
1	A	159	ARG	CG-CD-NE	5.01	123.03	112.00
1	B	229	HIS	N-CA-CB	5.01	117.28	110.01
1	A	192	LEU	CA-C-N	5.01	131.22	121.41
1	A	192	LEU	C-N-CA	5.01	131.22	121.41
1	A	245	TYR	O-C-N	5.00	128.29	123.29
1	A	37	ALA	O-C-N	5.00	127.29	122.09
1	A	328	GLU	CG-CD-OE1	5.00	129.90	118.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	LEU	Mainchain
1	B	220	ALA	Mainchain
1	B	38	ILE	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	2568	0	2642	96	0
1	B	2568	0	2641	97	1
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	44	0	26	1	0
3	B	44	0	26	3	0
4	A	6	0	2	0	0
4	B	6	0	2	0	0
5	A	76	0	0	6	0
5	B	77	0	0	11	0
All	All	5399	0	5339	187	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 18.

All (187) 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:4:LYS:HG2	5:B:406:HOH:O	1.45	1.14
1:A:221:ASP:O	1:A:222:LYS:HB2	1.48	1.09
1:B:217:GLY:O	1:B:219:ASP:N	1.93	1.01
1:A:39:SER:HA	1:B:42:MET:HE1	1.43	1.01
1:A:100:ALA:H	1:A:116:ASN:HD21	1.04	0.95
1:B:176:MET:HE1	1:B:206:VAL:HG11	1.53	0.90
1:A:18:VAL:HG23	1:A:19:PRO:HD2	1.53	0.90
1:A:43:LYS:HE3	5:A:474:HOH:O	1.69	0.90
1:B:100:ALA:H	1:B:116:ASN:HD21	1.20	0.90
5:A:479:HOH:O	1:B:2:THR:HG22	1.73	0.86
1:B:13:LYS:CG	1:B:14:GLU:H	1.83	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:HG23	1:A:271:ILE:HD12	1.58	0.85
1:A:18:VAL:CG2	1:A:19:PRO:HD2	2.08	0.84
1:B:217:GLY:C	1:B:219:ASP:H	1.85	0.83
1:A:85:TYR:O	1:A:88:THR:HB	1.78	0.82
1:B:114:GLN:HG3	1:B:330:GLN:HE22	1.45	0.81
1:B:132(A):PRO:O	1:B:159:ARG:NH1	2.13	0.80
1:B:55:MET:HE3	3:B:401:NAD:O2B	1.87	0.75
1:A:4:LYS:HE3	5:A:439:HOH:O	1.87	0.74
1:A:10:ASN:ND2	1:A:12:LEU:O	2.20	0.73
1:A:14:GLU:C	1:A:15:GLU:O	2.28	0.73
1:B:77:LYS:HE3	5:B:456:HOH:O	1.88	0.72
1:B:266:ARG:HB3	1:B:292:ILE:HD11	1.71	0.72
1:A:274:MET:HG3	1:A:286:PHE:CE2	2.26	0.71
1:A:221:ASP:O	1:A:222:LYS:CB	2.32	0.70
1:B:290:PRO:HG2	1:B:305:VAL:HG11	1.74	0.70
1:A:222:LYS:HG2	1:A:223:GLU:H	1.55	0.70
1:B:238:GLU:O	1:B:242:LEU:HD12	1.91	0.69
1:B:114:GLN:HG3	1:B:330:GLN:NE2	2.07	0.68
1:B:123:ILE:HG13	1:B:124:ILE:N	2.09	0.68
1:A:217:GLY:H	1:A:222:LYS:HZ2	1.39	0.68
1:A:266:ARG:HB3	1:A:292:ILE:HD13	1.77	0.67
1:B:329:LEU:HA	1:B:331:PHE:CE1	2.29	0.67
1:B:132(B):ASN:HA	1:B:159:ARG:NH1	2.10	0.67
1:A:175:LEU:HD13	1:A:231:GLU:HG3	1.76	0.67
1:A:289:VAL:HG13	1:A:302:VAL:HG13	1.77	0.66
1:A:242:LEU:HD21	1:B:60:LYS:HD3	1.76	0.66
1:B:243:LYS:HE2	1:B:245:TYR:O	1.96	0.65
1:A:281:ILE:C	1:A:281:ILE:HD13	2.21	0.65
1:B:13:LYS:HG3	1:B:14:GLU:H	1.61	0.65
1:A:230:LYS:HE3	5:A:421:HOH:O	1.97	0.65
1:A:210(A):LEU:HD11	1:B:7:LEU:HD22	1.77	0.65
1:B:88:THR:CG2	5:B:453:HOH:O	2.45	0.64
1:A:217:GLY:H	1:A:222:LYS:NZ	1.94	0.64
1:A:100:ALA:N	1:A:116:ASN:HD21	1.87	0.63
1:B:261:ILE:HG13	1:B:293:LEU:HD13	1.81	0.63
1:B:275:ILE:CD1	1:B:281:ILE:HG13	2.30	0.62
1:A:138:VAL:O	3:A:401:NAD:H2N	2.00	0.62
1:B:100:ALA:N	1:B:116:ASN:HD21	1.94	0.61
1:A:210(A):LEU:HG	1:B:3:LEU:HD21	1.82	0.60
1:B:329:LEU:HA	1:B:331:PHE:HE1	1.66	0.60
1:B:13:LYS:CD	1:B:14:GLU:H	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:HD12	1:A:281:ILE:HG21	1.83	0.60
1:B:199:SER:OG	1:B:229:HIS:HE1	1.85	0.59
1:A:161:ILE:CG2	1:A:271:ILE:HD12	2.30	0.59
1:B:176:MET:CE	1:B:206:VAL:HG11	2.30	0.59
1:A:94:VAL:HG21	1:A:127:ILE:HD13	1.84	0.59
1:A:316:LYS:HE3	1:A:316:LYS:HA	1.85	0.58
1:A:190:TRP:CZ3	1:A:270:PRO:HD3	2.37	0.58
1:A:289:VAL:HG13	1:A:302:VAL:CG1	2.34	0.58
1:A:222:LYS:CG	1:A:223:GLU:H	2.10	0.58
1:B:274:MET:CG	1:B:286:PHE:CE2	2.87	0.58
1:B:117:VAL:HG22	1:B:148:VAL:HG21	1.86	0.57
1:A:292:ILE:C	1:A:292:ILE:HD12	2.29	0.57
1:B:58:LYS:NZ	5:B:472:HOH:O	2.18	0.57
1:A:127:ILE:HD11	1:A:133:CYS:SG	2.44	0.57
1:A:14:GLU:O	1:A:15:GLU:O	2.22	0.56
1:B:190:TRP:HB3	1:B:192:LEU:HD13	1.86	0.56
1:B:16:HIS:O	1:B:16:HIS:CG	2.55	0.56
1:A:13:LYS:O	1:A:15:GLU:N	2.39	0.56
1:A:289:VAL:CG1	1:A:302:VAL:HG13	2.35	0.55
1:A:4:LYS:CG	5:B:406:HOH:O	2.24	0.55
1:A:309:PRO:O	1:A:310:GLU:C	2.46	0.55
1:B:182:VAL:HG23	1:B:187:CYS:SG	2.46	0.55
1:B:96:ILE:HD11	1:B:135:LEU:HD22	1.88	0.55
1:A:287:LEU:C	1:A:287:LEU:HD12	2.31	0.54
1:B:182:VAL:CG2	1:B:187:CYS:SG	2.95	0.54
1:A:22:ASN:HD22	1:A:92:ARG:HH21	1.54	0.54
1:B:16:HIS:O	1:B:16:HIS:ND1	2.41	0.54
1:B:88:THR:HG22	5:B:453:HOH:O	2.07	0.54
1:B:271:ILE:O	1:B:288:SER:HA	2.07	0.53
1:B:274:MET:HG3	1:B:286:PHE:CE2	2.43	0.53
1:B:7:LEU:HG	1:B:8:ILE:HG13	1.91	0.53
1:B:308:THR:HG22	1:B:311:GLU:HG3	1.90	0.53
1:A:4:LYS:HD3	5:B:406:HOH:O	2.09	0.53
1:B:328:GLU:O	1:B:328:GLU:HG2	2.08	0.53
1:B:29:VAL:HG12	1:B:62:GLU:HG3	1.91	0.53
1:B:77:LYS:CE	5:B:456:HOH:O	2.52	0.52
1:A:194:GLU:HG3	1:A:322:LEU:CD1	2.40	0.52
1:B:56:GLU:OE1	1:B:83:LYS:HE2	2.09	0.52
1:B:120:PHE:HA	1:B:123:ILE:HG12	1.92	0.52
1:B:285:VAL:HG21	1:B:319:ALA:HB1	1.92	0.52
1:A:4:LYS:CD	5:B:406:HOH:O	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ILE:HG12	1:B:287:LEU:HG	1.90	0.52
1:B:115:ARG:HD3	5:B:420:HOH:O	2.10	0.51
1:B:16:HIS:CD2	1:B:16:HIS:C	2.87	0.51
1:A:222:LYS:HD2	1:A:225:TRP:H	1.75	0.51
1:B:266:ARG:HB3	1:B:292:ILE:CD1	2.39	0.51
1:A:180:LEU:HB3	1:A:182:VAL:HG23	1.93	0.51
1:B:183:HIS:ND1	1:B:185:LEU:HB2	2.26	0.51
1:A:51:LEU:O	1:A:80:SER:HA	2.11	0.50
1:B:215:GLU:O	1:B:219:ASP:HB2	2.11	0.50
1:A:127:ILE:HG13	1:A:128:VAL:N	2.27	0.50
1:B:231:GLU:O	1:B:235:SER:HB3	2.12	0.50
1:B:18:VAL:HG23	1:B:19:PRO:HD2	1.92	0.49
1:A:22:ASN:ND2	1:A:92:ARG:HH21	2.10	0.49
1:A:316:LYS:HA	1:A:316:LYS:CE	2.42	0.49
1:B:29:VAL:CG1	1:B:62:GLU:HG3	2.43	0.49
1:A:85:TYR:CE2	1:A:127:ILE:HG22	2.48	0.49
1:A:15:GLU:O	1:A:16:HIS:CD2	2.65	0.49
1:B:192:LEU:HD22	1:B:202:VAL:HG21	1.93	0.49
1:A:144:ILE:HD13	1:A:325:ILE:HG21	1.95	0.49
1:A:210(B):LYS:NZ	1:A:214:PRO:O	2.42	0.48
1:B:328:GLU:O	1:B:330:GLN:N	2.46	0.48
1:A:124:ILE:HB	1:A:125:PRO:HD3	1.96	0.48
1:A:14:GLU:O	1:A:16:HIS:HD2	1.97	0.48
1:A:167:LEU:HD11	1:A:249:ALA:HB1	1.96	0.48
1:A:99:GLY:HA2	1:A:119:ILE:HD13	1.95	0.48
1:B:274:MET:HG2	1:B:286:PHE:CE2	2.49	0.47
1:A:71:LEU:HD12	1:B:185:LEU:HD13	1.96	0.47
1:A:210(A):LEU:CD1	1:B:7:LEU:HD22	2.44	0.47
1:A:217:GLY:N	1:A:222:LYS:NZ	2.62	0.47
1:B:285:VAL:HG12	1:B:326:GLN:NE2	2.30	0.46
1:A:217:GLY:O	1:A:219:ASP:OD2	2.33	0.46
1:A:123:ILE:O	1:A:127:ILE:HG23	2.15	0.46
1:A:206:VAL:HG12	1:A:210(A):LEU:HD22	1.97	0.46
1:A:159:ARG:HH21	1:A:159:ARG:HG3	1.81	0.46
1:A:279:TYR:H	1:A:281:ILE:HG22	1.81	0.46
1:A:289:VAL:CG1	1:A:302:VAL:CG1	2.94	0.46
1:B:183:HIS:CE1	1:B:185:LEU:HD22	2.51	0.46
1:A:28:GLY:O	1:A:33:GLY:HA3	2.16	0.46
1:A:194:GLU:HG3	1:A:322:LEU:HD13	1.97	0.46
1:A:285:VAL:HG22	1:A:323:TRP:HB2	1.98	0.46
1:B:109:ARG:HD3	1:B:140:ASN:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:MET:HB3	1:A:42:MET:HE2	1.80	0.45
1:B:190:TRP:HE3	1:B:270:PRO:HB3	1.82	0.45
1:B:240:ILE:O	1:B:244:GLY:N	2.49	0.44
1:B:173:ARG:NE	1:B:187:CYS:O	2.49	0.44
1:B:308:THR:HG23	1:B:310:GLU:OE1	2.18	0.44
1:B:208:VAL:O	1:B:209(C):VAL:HG13	2.17	0.44
1:A:3:LEU:C	1:A:3:LEU:HD12	2.41	0.44
1:A:234:ASP:HA	1:A:237:TYR:HD1	1.83	0.44
1:A:320:ASP:O	1:A:321:THR:C	2.61	0.44
1:B:19:PRO:HB2	1:B:23:LYS:HB2	2.00	0.44
1:A:216:LEU:HA	1:A:222:LYS:HD3	2.00	0.44
1:A:307:LEU:HD13	1:A:312:GLU:HA	1.99	0.44
1:B:140:ASN:HA	1:B:141:PRO:C	2.42	0.44
1:A:19:PRO:O	1:A:19:PRO:HG2	2.17	0.44
1:B:243:LYS:HE3	1:B:245:TYR:CE2	2.52	0.44
1:A:217:GLY:O	1:A:219:ASP:CG	2.61	0.43
1:A:283:GLU:HB3	1:A:284:ASN:H	1.60	0.43
1:B:289:VAL:HA	1:B:290:PRO:HD3	1.71	0.43
1:A:109:ARG:HG3	5:A:408:HOH:O	2.17	0.43
1:A:222:LYS:HB3	1:A:224:HIS:H	1.84	0.43
1:A:250:ILE:O	1:A:254:VAL:HG23	2.19	0.43
1:B:25:THR:HB	1:B:94:VAL:HB	2.00	0.43
1:B:30:GLY:HA3	3:B:401:NAD:O5B	2.19	0.43
1:B:140:ASN:HA	1:B:142:VAL:N	2.34	0.43
1:A:326:GLN:HA	1:A:329:LEU:HD22	1.99	0.43
1:A:13:LYS:CB	1:A:14:GLU:HG3	2.49	0.43
1:A:276:LYS:HB2	1:A:283:GLU:O	2.18	0.43
1:B:273:THR:HB	1:B:298:ILE:HD12	2.00	0.42
1:A:190:TRP:HB3	1:A:192:LEU:HD13	2.01	0.42
1:A:279:TYR:N	1:A:281:ILE:HG22	2.33	0.42
1:B:115:ARG:CD	5:B:420:HOH:O	2.65	0.42
1:B:113:VAL:O	1:B:117:VAL:HG23	2.18	0.42
1:A:140:ASN:HA	1:A:142:VAL:N	2.34	0.42
1:B:210(B):LYS:NZ	1:B:214:PRO:O	2.52	0.42
1:B:217:GLY:C	1:B:219:ASP:N	2.60	0.42
1:B:85:TYR:O	1:B:88:THR:HB	2.20	0.41
1:A:229:HIS:HD2	5:A:419:HOH:O	2.03	0.41
1:A:316:LYS:CE	1:A:316:LYS:CA	2.98	0.41
1:B:215:GLU:HG2	1:B:222:LYS:HZ2	1.83	0.41
1:B:138:VAL:O	3:B:401:NAD:H2N	2.21	0.41
1:B:190:TRP:HB3	1:B:192:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ILE:HD12	1:B:281:ILE:HG21	2.02	0.41
1:B:282:LYS:H	1:B:282:LYS:HG3	1.49	0.41
1:A:213:HIS:HD2	1:A:216:LEU:HB2	1.86	0.41
1:B:264:ASN:HB2	1:B:295:GLN:HB3	2.02	0.41
1:B:215:GLU:HG2	1:B:222:LYS:NZ	2.36	0.40
1:B:282:LYS:HD2	1:B:283:GLU:OE1	2.21	0.40
1:B:69:GLY:O	1:B:70:SER:C	2.65	0.40
1:A:85:TYR:HE2	1:A:127:ILE:HG22	1.86	0.40
1:B:29:VAL:HG13	1:B:34:MET:SD	2.61	0.40
1:B:197:ASP:HA	1:B:233:VAL:HG13	2.04	0.40
1:A:194:GLU:HG3	1:A:322:LEU:HD11	2.04	0.40
1:A:13:LYS:HB2	1:A:14:GLU:HG3	2.02	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:B:132(B):ASN:OD1	1:B:132(B):ASN:OD1[2_655]	1.53	0.67

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	330/332 (99%)	301 (91%)	23 (7%)	6 (2%)	6	3
1	B	330/332 (99%)	304 (92%)	19 (6%)	7 (2%)	5	2
All	All	660/664 (99%)	605 (92%)	42 (6%)	13 (2%)	6	2

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	GLU

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Mol	Chain	Res	Type
1	A	218	THR
1	A	222	LYS
1	A	330	GLN
1	B	1	ALA
1	B	14	GLU
1	B	218	THR
1	B	222	LYS
1	B	329	LEU
1	A	15	GLU
1	B	15	GLU
1	A	219	ASP
1	B	284	ASN

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	285/285 (100%)	241 (85%)	44 (15%)	2	1
1	B	285/285 (100%)	236 (83%)	49 (17%)	2	1
All	All	570/570 (100%)	477 (84%)	93 (16%)	2	1

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	4	LYS
1	A	11	LEU
1	A	12	LEU
1	A	13	LYS
1	A	14	GLU
1	A	15	GLU
1	A	19	PRO
1	A	49	ILE
1	A	76	PRO
1	A	86	ASN

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Mol	Chain	Res	Type
1	A	114	GLN
1	A	127	ILE
1	A	128	VAL
1	A	136	LEU
1	A	151	LYS
1	A	157	LYS
1	A	168	ASP
1	A	180	LEU
1	A	182	VAL
1	A	185	LEU
1	A	207	ASN
1	A	209(C)	VAL
1	A	209(D)	SER
1	A	210(A)	LEU
1	A	210(B)	LYS
1	A	222	LYS
1	A	223	GLU
1	A	226	LYS
1	A	230	LYS
1	A	242	LEU
1	A	274	MET
1	A	278	LEU
1	A	281	ILE
1	A	284	ASN
1	A	287	LEU
1	A	289	VAL
1	A	292	ILE
1	A	310	GLU
1	A	316	LYS
1	A	322	LEU
1	A	328	GLU
1	A	329	LEU
1	A	331	PHE
1	B	11	LEU
1	B	13	LYS
1	B	18	VAL
1	B	43	LYS
1	B	49	ILE
1	B	52	VAL
1	B	54	VAL
1	B	77	LYS
1	B	79	VAL

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Mol	Chain	Res	Type
1	B	83	LYS
1	B	88	THR
1	B	94	VAL
1	B	101	ARG
1	B	114	GLN
1	B	115	ARG
1	B	119	ILE
1	B	121	LYS
1	B	129	LYS
1	B	144	ILE
1	B	180	LEU
1	B	185	LEU
1	B	192	LEU
1	B	207	ASN
1	B	209(C)	VAL
1	B	209(D)	SER
1	B	212	LEU
1	B	215	GLU
1	B	218	THR
1	B	226	LYS
1	B	230	LYS
1	B	241	LYS
1	B	271	ILE
1	B	272	SER
1	B	274	MET
1	B	275	ILE
1	B	282	LYS
1	B	289	VAL
1	B	292	ILE
1	B	293	LEU
1	B	298	ILE
1	B	308	THR
1	B	316	LYS
1	B	317	LYS
1	B	323	TRP
1	B	325	ILE
1	B	327	LYS
1	B	328	GLU
1	B	329	LEU
1	B	331	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	16	HIS
1	A	22	ASN
1	A	111	ASN
1	A	116	ASN
1	A	126	ASN
1	A	207	ASN
1	A	229	HIS
1	A	284	ASN
1	B	10	ASN
1	B	114	GLN
1	B	116	ASN
1	B	126	ASN
1	B	207	ASN
1	B	211	ASN
1	B	229	HIS
1	B	284	ASN
1	B	326	GLN

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](#)

6 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	SO4	A	403	-	4,4,4	0.90	0	6,6,6	1.29	1 (16%)
4	OXM	B	402	-	5,5,5	8.05	4 (80%)	2,6,6	1.31	0
4	OXM	A	402	-	5,5,5	8.32	4 (80%)	2,6,6	11.10	2 (100%)
3	NAD	A	401	-	46,48,48	3.00	8 (17%)	64,73,73	3.84	32 (50%)
3	NAD	B	401	-	46,48,48	2.14	8 (17%)	64,73,73	2.31	20 (31%)
2	SO4	B	403	-	4,4,4	0.92	0	6,6,6	1.04	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	401	-	-	4/30/62/62	0/5/5/5
4	OXM	A	402	-	-	3/4/4/4	-
3	NAD	B	401	-	-	4/30/62/62	0/5/5/5
4	OXM	B	402	-	-	0/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NAD	C3N-C7N	14.63	1.72	1.50
4	B	402	OXM	C1-C2	-13.27	1.39	1.55
4	A	402	OXM	C1-C2	-13.26	1.39	1.55
4	A	402	OXM	C1-N1	10.60	1.64	1.33
4	B	402	OXM	C1-N1	9.82	1.61	1.33
3	B	401	NAD	O7N-C7N	-8.54	1.08	1.24
3	A	401	NAD	C2N-N1N	8.12	1.43	1.35
3	A	401	NAD	C6N-N1N	7.61	1.52	1.35
4	A	402	OXM	O1-C1	6.66	1.40	1.24
3	B	401	NAD	PA-O3	5.77	1.65	1.59
4	B	402	OXM	O1-C1	5.23	1.36	1.24
3	B	401	NAD	C3N-C7N	5.18	1.58	1.50
4	B	402	OXM	O2-C2	4.93	1.34	1.22
3	B	401	NAD	C5N-C4N	-4.46	1.31	1.38
3	A	401	NAD	C5N-C4N	-4.02	1.32	1.38
3	B	401	NAD	C6N-N1N	3.78	1.44	1.35
4	A	402	OXM	O2-C2	3.64	1.31	1.22
3	A	401	NAD	C2N-C3N	-2.62	1.34	1.39
3	B	401	NAD	C7N-N7N	-2.59	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	NAD	C2A-N3A	-2.54	1.29	1.33
3	B	401	NAD	C2A-N3A	-2.17	1.30	1.33
3	A	401	NAD	C6N-C5N	2.09	1.43	1.38
3	B	401	NAD	PA-O1A	-2.04	1.43	1.50
3	A	401	NAD	PN-O3	2.00	1.61	1.59

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAD	O7N-C7N-N7N	16.40	146.31	122.62
4	A	402	OXM	O1-C1-N1	-11.77	96.50	122.89
3	A	401	NAD	O7N-C7N-C3N	-11.66	105.34	119.60
4	A	402	OXM	O3-C2-O2	10.38	148.62	123.90
3	A	401	NAD	C2N-C3N-C4N	8.34	127.95	118.26
3	A	401	NAD	C3N-C7N-N7N	-7.64	108.33	117.74
3	A	401	NAD	N6A-C6A-N1A	-7.01	102.77	118.38
3	B	401	NAD	O7N-C7N-N7N	6.92	132.61	122.62
3	A	401	NAD	C5N-C6N-N1N	-6.63	111.33	120.38
3	A	401	NAD	C5A-C6A-N6A	6.42	139.19	123.29
3	B	401	NAD	C6N-N1N-C2N	-5.62	117.10	121.88
3	B	401	NAD	C5N-C4N-C3N	-5.36	115.09	120.36
3	B	401	NAD	C3N-C7N-N7N	-5.14	111.40	117.74
3	B	401	NAD	C2N-C3N-C4N	4.72	123.75	118.26
3	A	401	NAD	C2N-N1N-C1D	-4.34	109.54	119.13
3	A	401	NAD	C4A-C5A-N7A	-4.25	105.72	110.58
3	A	401	NAD	C5A-N7A-C8A	4.21	110.07	103.45
3	B	401	NAD	O7N-C7N-C3N	-3.88	114.86	119.60
3	A	401	NAD	C6A-C5A-N7A	3.73	139.28	132.09
3	A	401	NAD	O2D-C2D-C3D	3.70	123.68	111.82
3	B	401	NAD	O2A-PA-O1A	3.64	129.40	112.44
3	A	401	NAD	C1B-N9A-C8A	3.51	134.89	127.09
3	B	401	NAD	O4B-C4B-C3B	3.43	111.96	105.15
3	A	401	NAD	O2B-C2B-C1B	3.38	121.74	110.10
3	A	401	NAD	O2A-PA-O3	3.30	116.20	107.27
3	B	401	NAD	C2B-C3B-C4B	-3.28	96.27	102.61
3	B	401	NAD	O4B-C1B-C2B	-3.28	99.60	106.62
3	A	401	NAD	C6N-C5N-C4N	3.27	124.17	119.45
3	B	401	NAD	C1B-N9A-C8A	3.20	134.21	127.09
3	A	401	NAD	C4A-N9A-C1B	-3.13	119.32	126.63
3	A	401	NAD	C4N-C3N-C7N	-3.07	112.70	121.06
3	A	401	NAD	N9A-C8A-N7A	-3.04	109.62	113.94
3	B	401	NAD	C4N-C3N-C7N	-3.03	112.80	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAD	O2B-C2B-C3B	3.00	121.44	111.82
3	A	401	NAD	O5D-PN-O1N	2.98	120.75	108.94
3	B	401	NAD	O5D-PN-O1N	2.96	120.66	108.94
3	A	401	NAD	O4B-C1B-N9A	2.96	113.77	108.09
3	A	401	NAD	O3-PN-O1N	-2.77	102.37	110.70
3	A	401	NAD	C5N-C4N-C3N	-2.76	117.65	120.36
3	A	401	NAD	O2B-C2B-C3B	2.68	120.42	111.82
3	B	401	NAD	O3D-C3D-C4D	-2.68	103.37	111.08
3	B	401	NAD	C4A-N9A-C8A	-2.62	102.99	105.74
3	A	401	NAD	C5A-C4A-N9A	2.58	108.62	105.81
3	A	401	NAD	O2N-PN-O5D	2.57	119.19	107.57
3	A	401	NAD	C4D-O4D-C1D	-2.53	107.61	109.92
3	A	401	NAD	C4B-O4B-C1B	-2.52	103.91	109.47
3	B	401	NAD	O4D-C4D-C5D	-2.48	101.39	109.33
3	A	401	NAD	C5B-C4B-C3B	-2.41	106.53	115.21
3	A	401	NAD	C6N-N1N-C2N	-2.35	119.88	121.88
2	A	403	SO4	O3-S-O1	2.31	121.66	109.56
3	B	401	NAD	C4D-O4D-C1D	-2.31	107.81	109.92
3	B	401	NAD	O2N-PN-O3	-2.31	101.04	107.27
3	B	401	NAD	C5A-C4A-N9A	2.07	108.07	105.81
3	A	401	NAD	N3A-C4A-N9A	-2.06	123.67	127.17
3	A	401	NAD	O2N-PN-O3	-2.01	101.84	107.27

There are no chirality outliers.

All (11) torsion outliers are listed below:

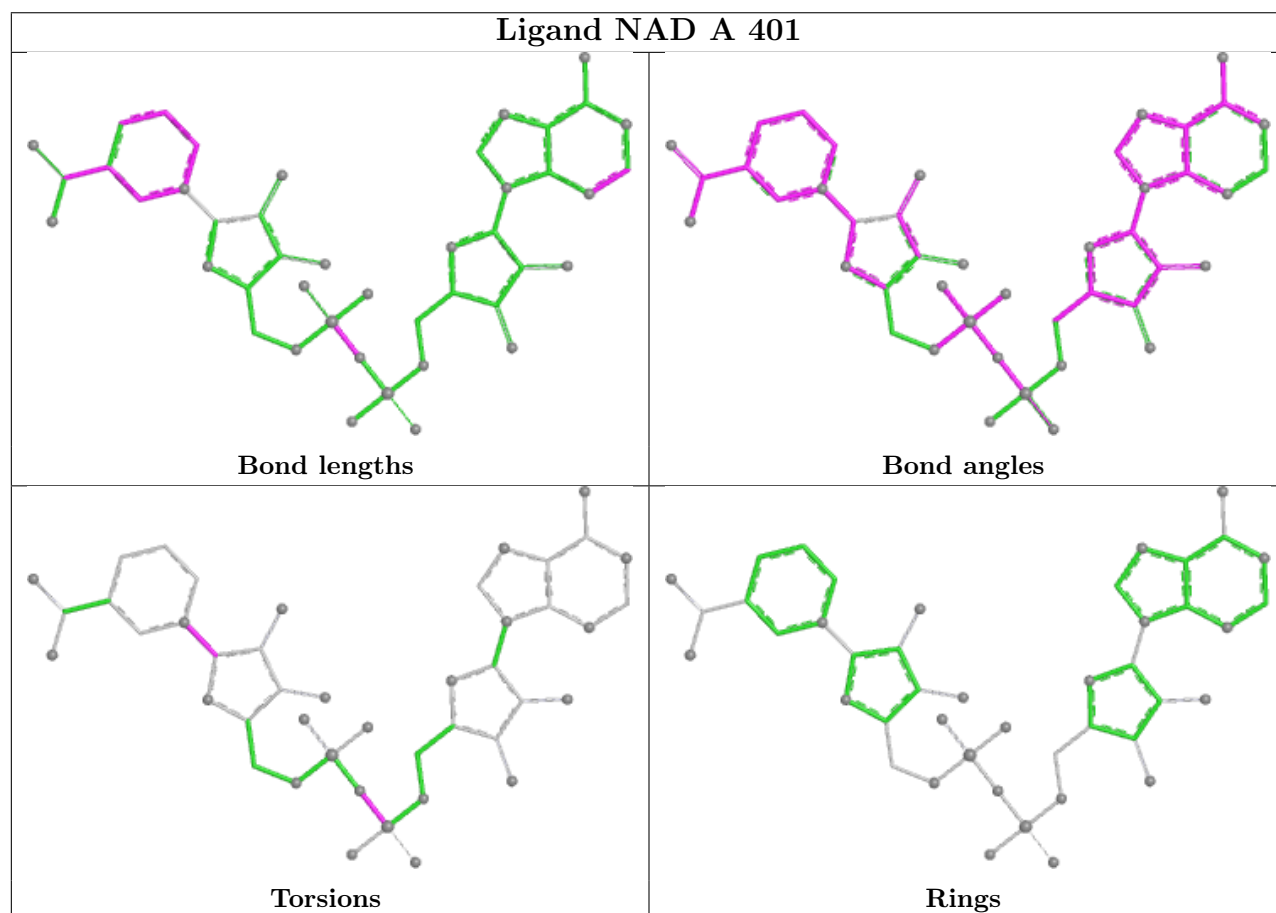
Mol	Chain	Res	Type	Atoms
3	A	401	NAD	O4D-C1D-N1N-C2N
3	A	401	NAD	O4D-C1D-N1N-C6N
3	A	401	NAD	C2D-C1D-N1N-C2N
3	B	401	NAD	O4D-C1D-N1N-C6N
3	B	401	NAD	C2D-C1D-N1N-C6N
4	A	402	OXM	N1-C1-C2-O3
4	A	402	OXM	O1-C1-C2-O3
3	B	401	NAD	C2D-C1D-N1N-C2N
4	A	402	OXM	N1-C1-C2-O2
3	B	401	NAD	O4D-C1D-N1N-C2N
3	A	401	NAD	PN-O3-PA-O2A

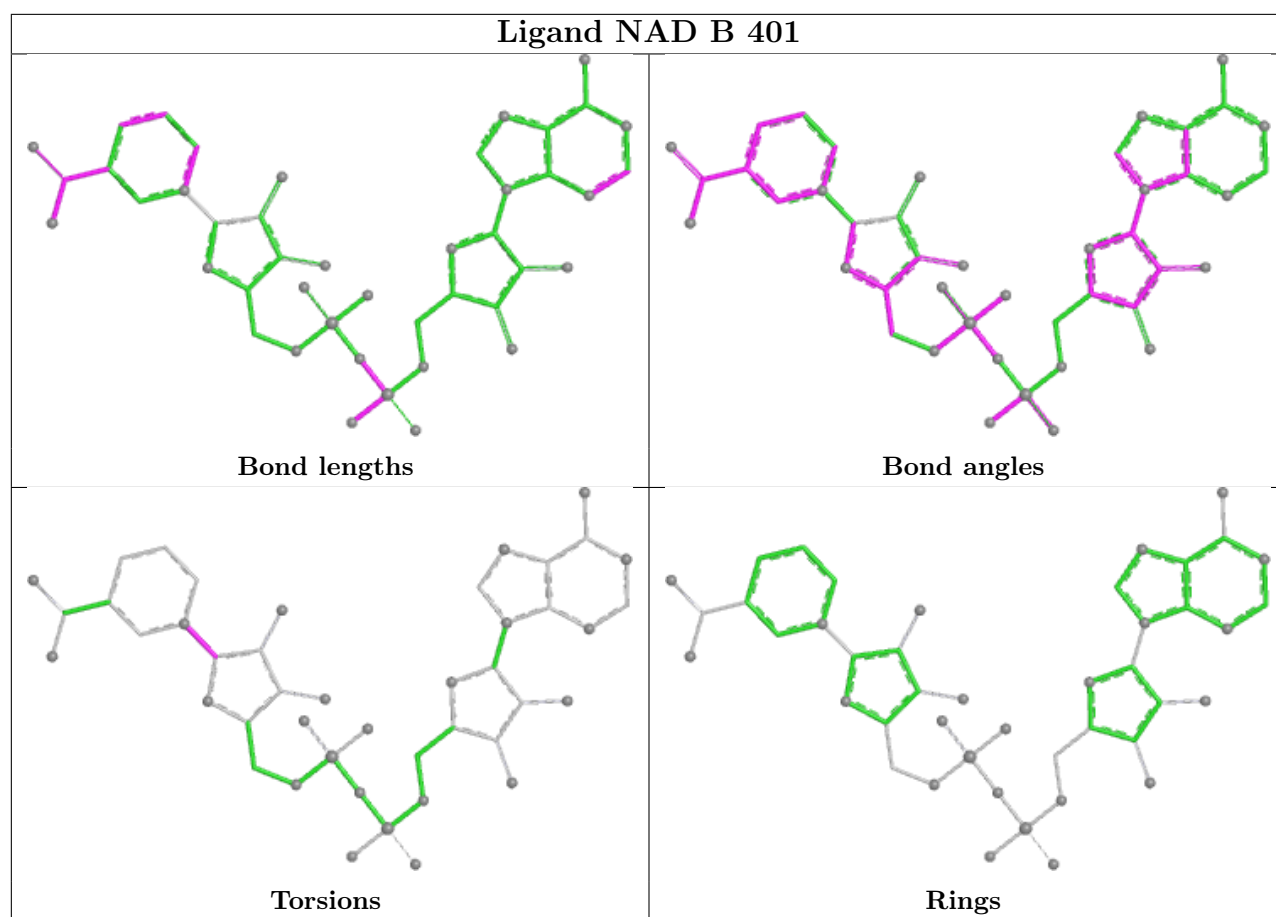
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAD	1	0
3	B	401	NAD	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.