



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 10:04 PM UTC

PDB ID : 9LDB / pdb_00009ldb
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 : 2.20 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

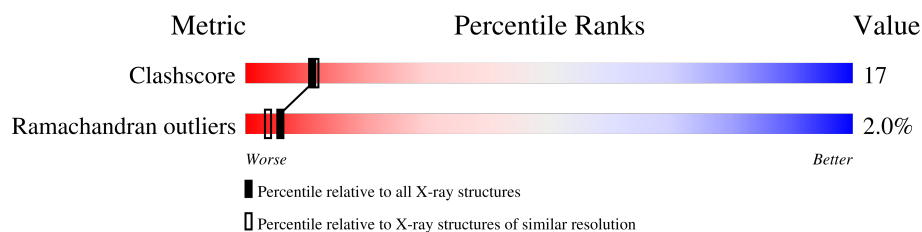
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)

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	 34% 46% 18% .
1	B	332	 31% 52% 17% .

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
2	SO4	A	402	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5396 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).



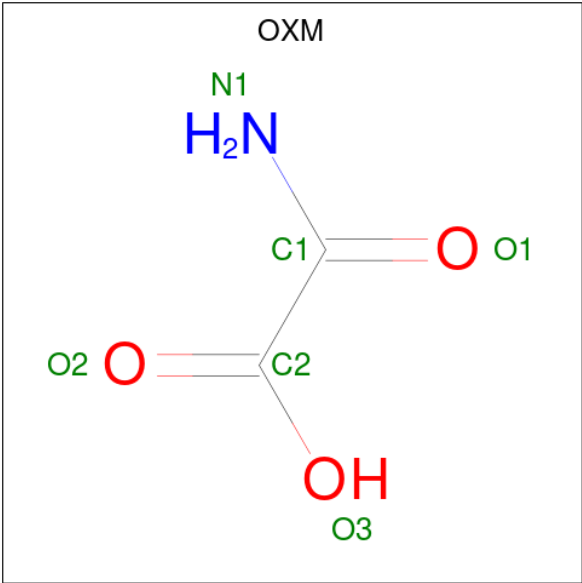
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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



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

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



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

- Molecule 5 is water.

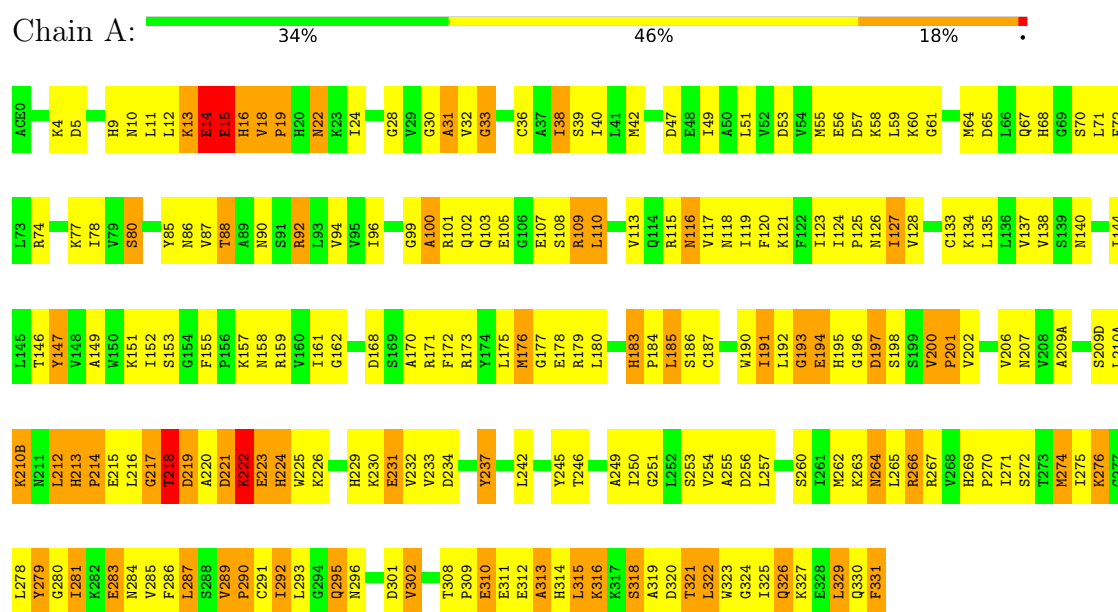
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total 81	O 81	0	0
5	B	70	Total 70	O 70	0	0

3 Residue-property plots

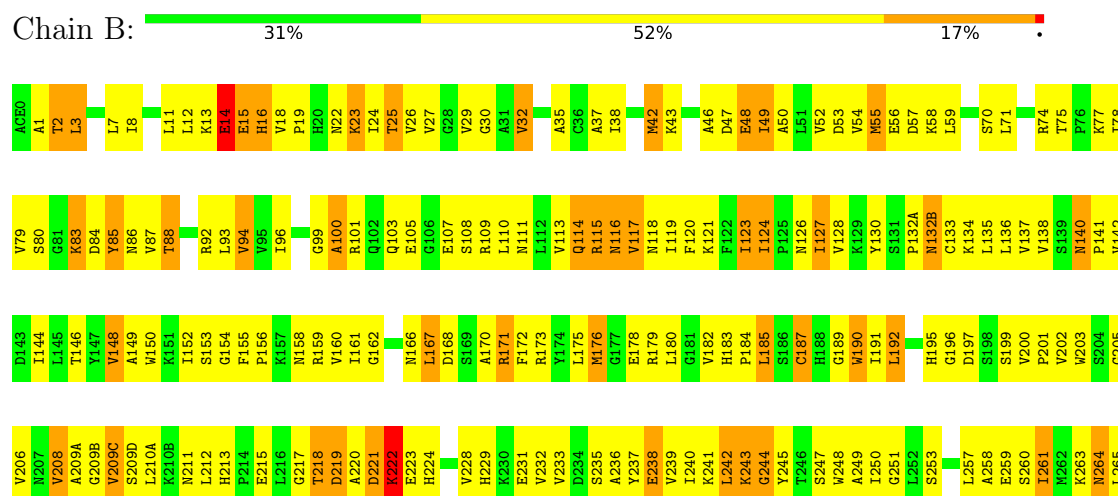
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



R266	R267	P270	I271	S272	T273	M274	I275	K276	G277	G280	I281	N284	V285	F286	L287	S288	V289	P290	C291	I292	L293	G294	Q295	N296	D301	V302	V303	K304	V305	T306	L307	T308	P309	E310	E311	E312	L315	K316	K317	S318	A319	D320	W323	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 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5396	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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, NAD, OXM, 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	1.48	6/2615 (0.2%)	3.02	348/3541 (9.8%)
1	B	1.47	11/2615 (0.4%)	3.22	357/3541 (10.1%)
All	All	1.48	17/5230 (0.3%)	3.12	705/7082 (10.0%)

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	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	289	VAL	C-O	7.05	1.29	1.24
1	A	74	ARG	CZ-NH2	6.88	1.42	1.33
1	A	217	GLY	N-CA	6.64	1.52	1.45
1	B	37	ALA	C-N	-6.62	1.25	1.33
1	B	101	ARG	CD-NE	-6.01	1.37	1.46
1	B	162	GLY	CA-C	5.81	1.56	1.52
1	B	201	PRO	C-O	5.80	1.29	1.23
1	B	124	ILE	CA-CB	5.56	1.56	1.54
1	B	170	ALA	N-CA	5.40	1.52	1.46
1	B	253	SER	C-N	-5.24	1.27	1.33
1	B	258	ALA	C-N	-5.19	1.27	1.33
1	A	250	ILE	CA-CB	5.07	1.60	1.54
1	B	261	ILE	C-N	-5.06	1.27	1.33
1	B	166	ASN	C-O	5.05	1.29	1.24
1	A	196	GLY	N-CA	-5.03	1.38	1.45
1	A	61	GLY	CA-C	5.03	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	267	ARG	CZ-NH1	5.00	1.39	1.32

All (705) 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	17.68	135.11	119.20
1	B	15	GLU	CA-CB-CG	17.47	149.04	114.10
1	B	109	ARG	CD-NE-CZ	17.38	148.74	124.40
1	B	292	ILE	CA-CB-CG2	17.36	140.01	110.50
1	A	159	ARG	NE-CZ-NH1	17.17	138.67	121.50
1	B	284	ASN	CA-CB-CG	16.01	128.61	112.60
1	B	101	ARG	CD-NE-CZ	15.90	146.66	124.40
1	B	221	ASP	O-C-N	-15.80	104.37	123.01
1	B	101	ARG	CG-CD-NE	15.54	146.19	112.00
1	A	105	GLU	CB-CG-CD	15.22	138.48	112.60
1	A	86	ASN	CA-CB-CG	13.77	126.37	112.60
1	A	289	VAL	N-CA-CB	-13.52	96.99	111.87
1	B	84	ASP	N-CA-C	13.51	126.08	111.36
1	A	178	GLU	CB-CG-CD	12.63	134.08	112.60
1	B	14	GLU	CA-C-O	12.58	138.50	120.51
1	A	197	ASP	CA-CB-CG	12.55	125.15	112.60
1	A	159	ARG	NE-CZ-NH2	-12.50	107.95	119.20
1	B	179	ARG	CD-NE-CZ	12.26	141.57	124.40
1	B	243	LYS	CA-C-O	-12.26	104.71	119.18
1	A	65	ASP	CA-C-O	-12.20	108.01	120.82
1	B	267	ARG	NE-CZ-NH1	-12.09	109.41	121.50
1	A	331	PHE	CB-CA-C	12.07	133.04	110.10
1	B	241	LYS	CA-CB-CG	11.72	137.53	114.10
1	B	166	ASN	OD1-CG-ND2	-11.60	111.00	122.60
1	B	292	ILE	CB-CA-C	11.42	126.62	110.98
1	B	86	ASN	OD1-CG-ND2	-11.12	111.48	122.60
1	A	289	VAL	CB-CA-C	11.09	121.87	109.89
1	B	43	LYS	CA-C-N	11.04	138.04	122.36
1	B	43	LYS	C-N-CA	11.04	138.04	122.36
1	B	221	ASP	CA-CB-CG	11.02	123.62	112.60
1	B	233	VAL	CA-C-N	10.90	140.22	121.14
1	B	233	VAL	C-N-CA	10.90	140.22	121.14
1	A	272	SER	N-CA-CB	10.81	126.70	109.95
1	B	328	GLU	CB-CG-CD	10.77	130.91	112.60
1	A	67	GLN	CA-C-N	10.69	135.67	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	GLN	C-N-CA	10.69	135.67	120.28
1	B	14	GLU	CB-CG-CD	10.67	130.74	112.60
1	A	281	ILE	CB-CA-C	10.66	126.53	110.96
1	B	119	ILE	CA-CB-CG2	10.46	128.28	110.50
1	A	60	LYS	CA-C-N	10.43	131.51	119.94
1	A	60	LYS	C-N-CA	10.43	131.51	119.94
1	A	220	ALA	CA-C-O	-10.37	105.68	120.51
1	B	11	LEU	CA-CB-CG	10.35	152.52	116.30
1	B	317	LYS	CA-CB-CG	10.27	134.63	114.10
1	B	118	ASN	OD1-CG-ND2	-10.24	112.36	122.60
1	B	35	ALA	O-C-N	10.19	133.77	122.15
1	B	88	THR	N-CA-CB	-10.19	94.85	110.44
1	B	277	GLY	CA-C-O	10.14	128.38	119.56
1	A	278	LEU	CA-C-O	-10.13	108.26	119.40
1	A	13	LYS	CA-C-O	10.11	133.27	121.44
1	B	272	SER	O-C-N	10.11	134.75	123.13
1	B	166	ASN	CB-CG-ND2	10.04	131.46	116.40
1	B	219	ASP	CA-CB-CG	-10.02	102.58	112.60
1	A	219	ASP	CA-CB-CG	9.96	122.56	112.60
1	A	331	PHE	CA-CB-CG	-9.96	103.84	113.80
1	B	249	ALA	CA-C-O	-9.82	110.50	120.82
1	A	326	GLN	CA-C-O	-9.81	109.22	120.20
1	A	222	LYS	CA-C-O	9.69	134.37	120.51
1	A	221	ASP	CA-CB-CG	9.56	122.16	112.60
1	B	292	ILE	CB-CG1-CD1	-9.54	93.76	113.80
1	B	132(B)	ASN	OD1-CG-ND2	9.53	132.13	122.60
1	B	86	ASN	CB-CG-ND2	9.46	130.60	116.40
1	A	196	GLY	N-CA-C	9.46	135.60	113.18
1	B	16	HIS	CA-CB-CG	-9.46	104.34	113.80
1	B	138	VAL	CA-C-O	-9.46	111.41	120.30
1	B	103	GLN	N-CA-C	-9.38	96.99	110.59
1	B	115	ARG	NE-CZ-NH1	-9.29	112.20	121.50
1	B	209(C)	VAL	CB-CA-C	9.29	122.21	110.96
1	B	289	VAL	N-CA-CB	-9.26	98.25	111.21
1	A	123	ILE	N-CA-C	9.24	122.64	111.09
1	A	33	GLY	CA-C-O	-9.23	111.03	121.00
1	B	12	LEU	CA-CB-CG	9.21	148.52	116.30
1	A	77	LYS	N-CA-CB	9.15	124.92	110.65
1	B	220	ALA	CA-C-N	9.15	134.50	121.42
1	B	220	ALA	C-N-CA	9.15	134.50	121.42
1	B	290	PRO	CB-CA-C	9.06	123.49	111.71
1	B	114	GLN	CB-CG-CD	9.02	127.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	VAL	N-CA-C	9.00	117.99	107.73
1	A	59	LEU	O-C-N	8.97	131.31	122.07
1	A	292	ILE	CB-CA-C	8.97	121.81	110.96
1	B	267	ARG	NH1-CZ-NH2	8.95	130.94	119.30
1	A	70	SER	CA-CB-OG	-8.94	93.21	111.10
1	A	179	ARG	NE-CZ-NH2	8.94	127.24	119.20
1	A	221	ASP	N-CA-C	8.93	123.69	110.48
1	A	171	ARG	NE-CZ-NH1	-8.92	112.58	121.50
1	B	161	ILE	N-CA-C	8.91	120.65	108.17
1	B	92	ARG	CD-NE-CZ	-8.88	111.96	124.40
1	A	231	GLU	CA-CB-CG	8.88	131.85	114.10
1	A	117	VAL	CA-C-N	8.84	132.85	120.29
1	A	117	VAL	C-N-CA	8.84	132.85	120.29
1	A	301	ASP	CA-C-O	-8.82	111.11	120.99
1	B	238	GLU	CA-C-O	-8.81	111.62	120.70
1	A	212	LEU	CA-CB-CG	8.81	147.13	116.30
1	B	263	LYS	CA-C-O	-8.79	109.07	119.35
1	B	84	ASP	CA-C-O	-8.74	111.15	120.42
1	A	64	MET	CA-C-N	8.70	131.75	120.44
1	A	64	MET	C-N-CA	8.70	131.75	120.44
1	B	168	ASP	O-C-N	8.68	132.38	122.22
1	B	266	ARG	CD-NE-CZ	8.62	136.47	124.40
1	B	261	ILE	CA-C-N	8.61	131.82	120.28
1	B	261	ILE	C-N-CA	8.61	131.82	120.28
1	A	217	GLY	CA-C-N	8.58	137.93	121.54
1	A	217	GLY	C-N-CA	8.58	137.93	121.54
1	A	330	GLN	CA-C-O	8.57	130.56	119.16
1	B	170	ALA	CA-C-O	8.57	129.63	120.55
1	B	243	LYS	O-C-N	8.57	132.31	122.20
1	B	144	ILE	CA-C-O	-8.55	111.79	120.85
1	A	276	LYS	CA-CB-CG	8.53	131.17	114.10
1	B	191	ILE	N-CA-CB	8.46	122.33	111.67
1	A	302	VAL	O-C-N	-8.38	114.59	123.14
1	B	75	THR	O-C-N	8.37	128.93	121.32
1	A	292	ILE	CA-CB-CG2	8.37	124.72	110.50
1	B	219	ASP	CA-C-O	8.35	129.59	120.32
1	A	108	SER	CB-CA-C	8.28	123.14	109.89
1	B	289	VAL	CB-CA-C	8.27	126.41	111.36
1	A	179	ARG	NE-CZ-NH1	-8.26	113.24	121.50
1	A	115	ARG	CA-C-O	-8.25	111.81	120.55
1	A	77	LYS	O-C-N	8.23	132.82	123.27
1	A	279	TYR	CB-CA-C	8.20	121.31	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	ILE	CB-CG1-CD1	-8.21	96.57	113.80
1	B	78	ILE	CA-C-O	8.20	128.55	120.27
1	A	186	SER	CA-C-O	-8.17	109.46	119.18
1	B	261	ILE	O-C-N	-8.16	113.21	121.94
1	B	118	ASN	CA-CB-CG	-8.14	104.46	112.60
1	B	328	GLU	CA-CB-CG	8.11	130.33	114.10
1	B	94	VAL	CA-C-N	8.09	133.53	122.93
1	B	94	VAL	C-N-CA	8.09	133.53	122.93
1	A	207	ASN	O-C-N	8.04	132.48	123.48
1	B	136	LEU	CA-C-N	8.02	132.40	122.37
1	B	136	LEU	C-N-CA	8.02	132.40	122.37
1	A	107	GLU	CA-C-O	8.01	130.03	120.81
1	A	264	ASN	OD1-CG-ND2	-8.00	114.60	122.60
1	B	219	ASP	CB-CA-C	7.95	124.08	109.70
1	A	38	ILE	CA-CB-CG2	7.95	124.01	110.50
1	B	48	GLU	CA-CB-CG	7.93	129.96	114.10
1	B	192	LEU	N-CA-CB	-7.93	98.55	110.60
1	B	57	ASP	CA-C-O	-7.91	112.75	120.90
1	B	307	LEU	O-C-N	7.89	132.22	123.22
1	B	232	VAL	O-C-N	7.88	129.63	121.91
1	B	221	ASP	N-CA-CB	-7.88	98.17	110.06
1	B	301	ASP	CA-CB-CG	7.87	120.47	112.60
1	A	223	GLU	CA-C-N	7.85	136.53	121.54
1	A	223	GLU	C-N-CA	7.85	136.53	121.54
1	A	197	ASP	N-CA-CB	-7.82	100.09	110.88
1	A	281	ILE	N-CA-C	-7.82	96.47	107.80
1	B	172	PHE	CA-CB-CG	7.80	121.61	113.80
1	B	270	PRO	CA-C-O	-7.79	106.42	120.60
1	B	221	ASP	N-CA-C	7.79	122.51	110.20
1	A	127	ILE	CA-CB-CG2	7.79	123.74	110.50
1	B	85	TYR	N-CA-CB	7.77	123.62	110.49
1	A	92	ARG	CD-NE-CZ	-7.76	113.53	124.40
1	B	111	ASN	CA-CB-CG	-7.75	104.85	112.60
1	A	15	GLU	N-CA-C	-7.75	97.74	109.60
1	A	16	HIS	O-C-N	7.75	132.90	122.59
1	A	118	ASN	CB-CG-ND2	7.73	128.00	116.40
1	A	237	TYR	O-C-N	7.69	129.99	122.07
1	A	192	LEU	CA-C-N	7.68	129.10	120.42
1	A	192	LEU	C-N-CA	7.68	129.10	120.42
1	A	155	PHE	CA-CB-CG	7.67	121.47	113.80
1	A	200	VAL	O-C-N	7.67	126.20	121.37
1	B	251	GLY	CA-C-N	7.65	130.85	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	GLY	C-N-CA	7.65	130.85	120.44
1	B	242	LEU	CA-C-O	-7.63	110.69	120.00
1	B	203	TRP	N-CA-CB	7.61	122.08	110.28
1	A	231	GLU	CB-CG-CD	7.59	125.50	112.60
1	A	152	ILE	N-CA-C	7.58	117.66	110.53
1	B	14	GLU	CA-C-N	7.54	135.94	121.54
1	B	14	GLU	C-N-CA	7.54	135.94	121.54
1	A	274	MET	CA-CB-CG	-7.52	99.06	114.10
1	B	123	ILE	CA-C-O	-7.50	112.72	121.05
1	A	13	LYS	CA-CB-CG	7.50	129.09	114.10
1	B	327	LYS	CA-C-N	7.50	135.86	121.54
1	B	327	LYS	C-N-CA	7.50	135.86	121.54
1	A	223	GLU	CA-C-O	7.49	128.79	119.95
1	B	218	THR	CA-C-N	7.49	134.27	122.74
1	B	218	THR	C-N-CA	7.49	134.27	122.74
1	A	171	ARG	CD-NE-CZ	-7.46	113.95	124.40
1	A	267	ARG	NE-CZ-NH1	-7.46	114.04	121.50
1	A	267	ARG	CD-NE-CZ	-7.42	114.02	124.40
1	B	103	GLN	OE1-CD-NE2	7.41	130.01	122.60
1	A	18	VAL	CA-C-N	7.40	127.56	120.31
1	A	18	VAL	C-N-CA	7.40	127.56	120.31
1	A	311	GLU	CB-CG-CD	7.40	125.17	112.60
1	B	83	LYS	N-CA-CB	7.39	121.68	110.30
1	B	167	LEU	CA-C-O	-7.37	113.11	120.70
1	B	292	ILE	CA-C-N	7.37	132.58	122.19
1	B	292	ILE	C-N-CA	7.37	132.58	122.19
1	A	315	LEU	CA-C-O	-7.34	112.09	120.24
1	B	121	LYS	CA-CB-CG	7.34	128.78	114.10
1	A	224	HIS	CA-CB-CG	-7.34	106.46	113.80
1	A	225	TRP	O-C-N	7.33	131.29	122.27
1	B	305	VAL	CB-CA-C	7.33	121.74	111.63
1	A	55	MET	CG-SD-CE	-7.33	84.78	100.90
1	A	92	ARG	N-CA-C	-7.32	102.69	111.69
1	A	308	THR	CB-CA-C	7.31	122.69	109.45
1	A	157	LYS	CA-CB-CG	7.30	128.70	114.10
1	B	35	ALA	N-CA-CB	7.30	120.96	110.16
1	B	35	ALA	CA-C-O	-7.30	112.69	120.42
1	A	42	MET	CG-SD-CE	-7.29	84.86	100.90
1	A	179	ARG	CD-NE-CZ	7.29	134.61	124.40
1	B	108	SER	CA-C-O	-7.28	113.63	121.56
1	B	152	ILE	CB-CA-C	-7.26	102.67	111.97
1	A	99	GLY	O-C-N	7.26	129.95	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ARG	NH1-CZ-NH2	7.24	128.72	119.30
1	B	155	PHE	O-C-N	7.24	129.49	121.53
1	B	124	ILE	CA-C-O	-7.23	113.22	118.71
1	A	262	MET	CA-C-O	7.21	128.25	120.10
1	B	99	GLY	N-CA-C	7.16	120.44	111.85
1	B	70	SER	CA-CB-OG	-7.15	96.80	111.10
1	B	290	PRO	O-C-N	-7.13	115.21	122.98
1	B	133	CYS	CA-C-N	7.13	132.56	122.72
1	B	133	CYS	C-N-CA	7.13	132.56	122.72
1	B	105	GLU	CG-CD-OE2	-7.12	102.03	118.40
1	B	228	VAL	CA-C-N	7.12	129.69	120.44
1	B	228	VAL	C-N-CA	7.12	129.69	120.44
1	B	176	MET	CA-C-O	7.11	128.09	120.55
1	B	288	SER	CA-C-O	7.07	128.53	120.54
1	A	207	ASN	CA-CB-CG	7.06	119.66	112.60
1	B	209(B)	GLY	CA-C-O	-7.05	111.94	119.27
1	A	77	LYS	CA-CB-CG	7.03	128.16	114.10
1	B	247	SER	CA-C-O	-7.02	110.47	120.51
1	B	100	ALA	O-C-N	7.02	131.14	122.86
1	B	130	TYR	CA-C-N	7.02	130.18	122.74
1	B	130	TYR	C-N-CA	7.02	130.18	122.74
1	B	123	ILE	O-C-N	7.00	129.18	121.90
1	B	249	ALA	O-C-N	7.00	129.28	122.07
1	B	222	LYS	N-CA-C	6.97	125.65	110.80
1	A	135	LEU	CA-C-O	-6.96	112.67	120.54
1	B	232	VAL	CA-CB-CG1	6.96	122.24	110.40
1	B	232	VAL	N-CA-CB	6.95	118.69	110.55
1	A	264	ASN	CA-CB-CG	6.95	119.55	112.60
1	B	8	ILE	N-CA-C	6.95	117.84	108.11
1	B	327	LYS	CA-C-O	6.95	129.79	121.66
1	A	267	ARG	CA-C-O	-6.94	113.53	121.72
1	A	124	ILE	O-C-N	6.94	124.86	120.42
1	A	59	LEU	CA-C-O	-6.93	113.54	120.82
1	A	121	LYS	CA-CB-CG	6.93	127.97	114.10
1	A	107	GLU	CA-C-N	6.93	130.65	120.95
1	A	107	GLU	C-N-CA	6.93	130.65	120.95
1	B	241	LYS	CG-CD-CE	6.92	127.22	111.30
1	B	170	ALA	O-C-N	-6.90	114.81	122.12
1	A	144	ILE	O-C-N	6.89	128.92	121.83
1	B	75	THR	CA-C-O	-6.89	112.06	120.74
1	B	3	LEU	N-CA-C	-6.88	103.83	111.82
1	A	326	GLN	OE1-CD-NE2	-6.88	115.72	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	LYS	N-CA-CB	6.88	121.61	110.40
1	A	108	SER	CA-CB-OG	6.87	124.84	111.10
1	B	126	ASN	OD1-CG-ND2	6.86	129.46	122.60
1	A	123	ILE	CA-C-O	-6.85	113.07	120.47
1	B	153	SER	O-C-N	6.85	129.13	122.07
1	A	56	GLU	N-CA-C	6.83	118.38	111.07
1	B	48	GLU	N-CA-CB	6.82	122.09	110.57
1	A	246	THR	CA-CB-OG1	-6.82	99.38	109.60
1	B	315	LEU	CA-C-N	6.81	129.30	120.44
1	B	315	LEU	C-N-CA	6.81	129.30	120.44
1	A	87	VAL	CA-CB-CG2	6.81	121.98	110.40
1	A	134	LYS	N-CA-CB	6.81	121.52	110.42
1	A	264	ASN	CB-CG-OD1	6.81	134.42	120.80
1	B	160	VAL	O-C-N	6.81	129.31	122.71
1	A	195	HIS	N-CA-C	-6.79	98.59	109.39
1	B	260	SER	N-CA-CB	6.78	120.08	110.12
1	A	32	VAL	O-C-N	6.77	128.81	121.83
1	B	54	VAL	CB-CA-C	-6.77	102.10	111.65
1	B	16	HIS	CA-C-O	-6.77	113.74	121.66
1	A	146	THR	N-CA-C	-6.75	103.85	111.14
1	A	58	LYS	CA-C-N	6.75	129.21	120.44
1	A	58	LYS	C-N-CA	6.75	129.21	120.44
1	B	94	VAL	CB-CA-C	6.75	120.94	110.28
1	A	67	GLN	O-C-N	-6.73	114.99	122.12
1	A	187	CYS	N-CA-C	-6.71	98.26	109.07
1	A	77	LYS	CB-CG-CD	6.70	126.72	111.30
1	A	229	HIS	N-CA-CB	6.70	119.96	110.12
1	A	110	LEU	CB-CA-C	6.68	123.96	109.99
1	A	9	HIS	CA-C-O	6.68	127.61	120.46
1	A	256	ASP	CA-CB-CG	6.67	119.27	112.60
1	A	47	ASP	CA-CB-CG	6.67	119.27	112.60
1	B	70	SER	CB-CA-C	-6.67	99.68	110.74
1	B	113	VAL	CB-CA-C	6.66	120.41	111.88
1	A	193	GLY	CA-C-O	6.66	128.95	120.89
1	A	65	ASP	CA-C-N	6.66	129.09	120.44
1	A	65	ASP	C-N-CA	6.66	129.09	120.44
1	B	190	TRP	O-C-N	6.65	131.87	123.23
1	A	330	GLN	CA-C-N	6.65	133.66	121.70
1	A	330	GLN	C-N-CA	6.65	133.66	121.70
1	A	212	LEU	CA-C-O	6.62	127.61	119.79
1	B	124	ILE	N-CA-CB	6.62	114.96	110.52
1	A	253	SER	CA-C-O	-6.62	113.40	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	THR	N-CA-CB	6.60	119.65	110.07
1	B	18	VAL	O-C-N	6.60	127.61	121.61
1	B	53	ASP	CA-C-O	-6.60	114.20	121.33
1	A	249	ALA	CB-CA-C	6.59	121.23	110.88
1	A	116	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	A	87	VAL	CA-C-N	6.58	134.20	121.18
1	A	87	VAL	C-N-CA	6.58	134.20	121.18
1	A	100	ALA	O-C-N	6.55	130.74	123.01
1	A	249	ALA	N-CA-CB	-6.54	100.52	110.01
1	A	158	ASN	CA-C-O	-6.54	112.07	119.79
1	A	105	GLU	CA-C-O	6.54	128.08	120.96
1	A	296	ASN	O-C-N	6.53	130.17	122.34
1	A	115	ARG	NH1-CZ-NH2	6.52	127.78	119.30
1	A	183	HIS	CA-C-N	6.51	126.75	119.32
1	A	183	HIS	C-N-CA	6.51	126.75	119.32
1	B	239	VAL	O-C-N	-6.51	115.29	121.87
1	B	171	ARG	CA-C-O	-6.51	113.99	120.70
1	B	179	ARG	CA-C-O	-6.51	113.98	120.82
1	A	260	SER	CA-C-O	-6.50	112.50	119.97
1	B	111	ASN	CA-C-O	-6.50	111.39	119.38
1	B	203	TRP	CA-C-O	-6.50	112.50	119.97
1	B	209(C)	VAL	CA-C-O	6.49	128.25	120.65
1	B	201	PRO	CB-CA-C	6.49	117.30	111.40
1	B	127	ILE	CA-C-N	6.48	131.24	120.62
1	B	127	ILE	C-N-CA	6.48	131.24	120.62
1	B	2	THR	CB-CA-C	6.46	124.27	110.19
1	A	269	HIS	CA-CB-CG	6.45	120.25	113.80
1	B	175	LEU	O-C-N	6.45	128.95	122.12
1	A	266	ARG	NH1-CZ-NH2	6.43	127.66	119.30
1	A	118	ASN	CA-CB-CG	6.43	119.03	112.60
1	B	232	VAL	N-CA-C	-6.43	104.25	110.42
1	A	78	ILE	CA-C-O	-6.42	113.41	120.48
1	A	237	TYR	CA-C-O	-6.42	114.08	120.82
1	B	114	GLN	CA-CB-CG	6.42	126.95	114.10
1	B	304	LYS	CB-CG-CD	6.42	126.07	111.30
1	B	271	ILE	CA-C-O	-6.42	114.86	121.67
1	A	86	ASN	CA-C-N	6.42	130.61	120.47
1	A	86	ASN	C-N-CA	6.42	130.61	120.47
1	A	86	ASN	CB-CG-OD1	-6.42	107.96	120.80
1	B	132(B)	ASN	N-CA-C	6.42	121.16	112.88
1	B	243	LYS	N-CA-CB	6.41	120.36	110.80
1	A	176	MET	N-CA-CB	-6.40	100.66	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	VAL	N-CA-CB	6.40	117.34	110.62
1	A	318	SER	CA-C-N	6.40	130.03	120.31
1	A	318	SER	C-N-CA	6.40	130.03	120.31
1	A	249	ALA	CA-C-O	-6.39	114.11	120.82
1	A	213	HIS	N-CA-CB	-6.38	103.04	111.40
1	A	90	ASN	CA-CB-CG	6.38	118.97	112.60
1	A	68	HIS	N-CA-CB	6.37	120.03	110.22
1	B	307	LEU	CA-C-O	-6.37	113.35	120.54
1	A	253	SER	O-C-N	-6.36	114.90	122.15
1	B	158	ASN	CA-CB-CG	6.35	118.95	112.60
1	A	253	SER	N-CA-C	-6.34	104.45	111.36
1	A	187	CYS	N-CA-CB	6.33	120.51	110.57
1	B	78	ILE	O-C-N	-6.33	116.60	123.18
1	A	172	PHE	CA-CB-CG	6.32	120.12	113.80
1	A	65	ASP	N-CA-C	-6.32	104.31	111.07
1	B	184	PRO	CA-C-N	6.32	129.38	120.28
1	B	184	PRO	C-N-CA	6.32	129.38	120.28
1	B	47	ASP	N-CA-C	-6.31	105.51	113.72
1	A	260	SER	N-CA-CB	6.30	120.05	110.28
1	A	191	ILE	N-CA-CB	6.30	119.61	111.67
1	A	219	ASP	N-CA-C	6.30	124.21	110.80
1	B	211	ASN	CA-C-O	-6.30	112.36	119.79
1	A	127	ILE	O-C-N	-6.29	115.35	121.83
1	A	180	LEU	N-CA-CB	-6.28	100.16	110.40
1	A	275	ILE	CA-C-O	-6.27	113.36	120.26
1	B	116	ASN	CB-CA-C	6.27	123.16	110.38
1	A	222	LYS	N-CA-C	6.24	124.08	110.80
1	A	251	GLY	CA-C-O	-6.23	114.27	121.00
1	A	115	ARG	O-C-N	6.22	128.72	122.12
1	A	309	PRO	O-C-N	6.22	130.76	122.30
1	B	105	GLU	CG-CD-OE1	6.22	132.71	118.40
1	B	317	LYS	CA-C-N	6.22	129.12	120.29
1	B	317	LYS	C-N-CA	6.22	129.12	120.29
1	A	47	ASP	N-CA-C	-6.21	105.65	113.72
1	B	78	ILE	CA-C-N	6.21	131.50	122.69
1	B	78	ILE	C-N-CA	6.21	131.50	122.69
1	A	123	ILE	CB-CG1-CD1	-6.21	100.77	113.80
1	B	218	THR	CB-CA-C	6.20	122.77	110.42
1	B	74	ARG	CG-CD-NE	6.20	125.64	112.00
1	B	55	MET	CG-SD-CE	-6.20	87.26	100.90
1	B	16	HIS	CA-C-N	-6.19	117.34	123.04
1	B	16	HIS	C-N-CA	-6.19	117.34	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	GLU	CA-CB-CG	6.19	126.48	114.10
1	B	197	ASP	CB-CG-OD2	-6.18	104.19	118.40
1	A	209(D)	SER	CA-CB-OG	6.17	123.45	111.10
1	B	223	GLU	CA-C-O	6.16	126.45	119.18
1	A	126	ASN	CA-CB-CG	6.16	118.76	112.60
1	B	29	VAL	CA-CB-CG1	6.16	120.87	110.40
1	A	185	LEU	O-C-N	6.16	128.65	122.12
1	B	179	ARG	O-C-N	6.16	128.41	122.07
1	A	57	ASP	CA-C-N	6.15	130.05	120.82
1	A	57	ASP	C-N-CA	6.15	130.05	120.82
1	A	176	MET	CA-C-N	6.15	126.94	119.99
1	A	176	MET	C-N-CA	6.15	126.94	119.99
1	B	58	LYS	O-C-N	6.15	129.18	122.11
1	B	293	LEU	N-CA-C	6.13	119.64	109.46
1	A	321	THR	CA-C-N	6.13	128.41	120.44
1	A	321	THR	C-N-CA	6.13	128.41	120.44
1	B	152	ILE	CA-CB-CG1	6.13	120.82	110.40
1	B	2	THR	CA-CB-OG1	-6.12	100.42	109.60
1	A	316	LYS	N-CA-C	-6.11	105.08	112.54
1	A	88	THR	CA-CB-OG1	-6.11	100.44	109.60
1	A	289	VAL	CA-C-O	-6.11	113.62	121.13
1	A	218	THR	CA-C-O	6.11	129.24	120.51
1	B	26	VAL	N-CA-CB	6.10	119.57	111.64
1	A	191	ILE	N-CA-C	-6.10	98.35	107.37
1	B	205	GLY	CA-C-O	-6.10	109.96	120.57
1	B	248	TRP	O-C-N	6.09	128.35	122.07
1	B	327	LYS	O-C-N	-6.09	114.00	122.41
1	B	74	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	A	234	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	47	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	48	GLU	O-C-N	6.08	130.35	123.42
1	B	123	ILE	N-CA-C	6.08	116.25	110.53
1	A	276	LYS	CA-C-O	6.08	127.62	120.69
1	B	248	TRP	CA-C-O	-6.08	114.44	120.82
1	B	86	ASN	N-CA-C	-6.07	104.78	111.82
1	B	274	MET	CA-C-O	-6.07	114.04	121.02
1	B	101	ARG	O-C-N	-6.07	114.27	122.94
1	B	153	SER	CA-C-O	-6.06	114.45	120.82
1	A	151	LYS	O-C-N	-6.06	115.79	122.09
1	A	176	MET	CB-CA-C	6.04	121.75	110.70
1	B	200	VAL	N-CA-CB	-6.04	103.78	111.39
1	A	177	GLY	N-CA-C	-6.04	105.34	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	LEU	CA-C-O	-6.03	114.16	120.55
1	A	201	PRO	CA-C-O	-6.02	113.92	120.97
1	B	209(A)	ALA	CA-C-O	6.02	128.27	120.81
1	A	100	ALA	CA-C-O	-5.99	114.22	121.05
1	B	296	ASN	CA-C-O	-5.99	112.55	119.56
1	A	53	ASP	CA-C-O	-5.99	114.86	121.33
1	B	49	ILE	CB-CA-C	5.98	119.48	110.63
1	A	291	CYS	O-C-N	5.97	130.59	123.24
1	B	287	LEU	CB-CA-C	5.97	121.69	110.95
1	B	134	LYS	N-CA-C	-5.96	99.52	109.24
1	B	176	MET	CG-SD-CE	-5.96	87.79	100.90
1	A	119	ILE	CA-C-N	5.96	128.26	120.28
1	A	119	ILE	C-N-CA	5.96	128.26	120.28
1	A	295	GLN	CG-CD-NE2	-5.94	107.48	116.40
1	A	296	ASN	CA-C-O	-5.94	112.61	119.56
1	B	2	THR	CA-CB-CG2	5.94	120.59	110.50
1	A	312	GLU	CA-CB-CG	5.93	125.96	114.10
1	A	251	GLY	O-C-N	5.93	127.87	122.18
1	B	290	PRO	CA-C-N	5.92	132.11	122.81
1	B	290	PRO	C-N-CA	5.92	132.11	122.81
1	A	312	GLU	CB-CG-CD	5.92	122.66	112.60
1	A	14	GLU	CG-CD-OE2	-5.92	104.80	118.40
1	B	74	ARG	CA-C-O	-5.91	114.26	121.89
1	B	138	VAL	O-C-N	5.91	128.21	122.07
1	A	88	THR	CA-CB-CG2	5.91	120.54	110.50
1	A	262	MET	O-C-N	-5.89	115.32	122.22
1	A	103	GLN	N-CA-C	-5.89	101.80	110.52
1	A	267	ARG	CB-CG-CD	-5.89	97.75	111.30
1	A	120	PHE	O-C-N	5.89	128.36	122.12
1	B	306	THR	CA-C-N	5.89	130.49	122.19
1	B	306	THR	C-N-CA	5.89	130.49	122.19
1	A	289	VAL	CA-CB-CG1	5.88	120.40	110.40
1	B	132(B)	ASN	CA-CB-CG	-5.88	106.72	112.60
1	B	210(A)	LEU	CB-CA-C	5.87	120.84	110.85
1	B	296	ASN	CA-CB-CG	5.87	118.47	112.60
1	A	262	MET	N-CA-C	5.86	118.45	111.71
1	A	310	GLU	CG-CD-OE2	-5.85	104.95	118.40
1	B	328	GLU	CB-CA-C	-5.85	98.78	110.42
1	A	253	SER	CB-CA-C	5.85	120.79	110.85
1	A	173	ARG	NH1-CZ-NH2	5.84	126.90	119.30
1	A	255	ALA	CA-C-N	5.84	128.04	120.44
1	A	255	ALA	C-N-CA	5.84	128.04	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	VAL	CA-C-N	5.82	128.44	120.46
1	B	239	VAL	C-N-CA	5.82	128.44	120.46
1	A	137	VAL	O-C-N	5.82	129.49	123.03
1	A	101	ARG	N-CA-CB	5.82	119.81	110.85
1	A	125	PRO	N-CA-CB	5.81	109.72	103.33
1	A	155	PHE	O-C-N	5.79	128.02	121.53
1	B	2	THR	N-CA-CB	-5.78	102.46	110.38
1	A	283	GLU	CB-CA-C	-5.78	100.45	111.48
1	B	152	ILE	N-CA-CB	5.76	117.29	110.55
1	B	161	ILE	CA-C-N	-5.76	116.77	122.36
1	B	161	ILE	C-N-CA	-5.76	116.77	122.36
1	B	212	LEU	CA-C-O	5.76	126.58	119.79
1	A	65	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	259	GLU	CB-CG-CD	5.75	122.38	112.60
1	B	212	LEU	N-CA-CB	-5.75	101.45	110.30
1	B	323	TRP	CA-C-O	-5.74	114.33	120.42
1	A	108	SER	N-CA-C	-5.74	101.35	109.96
1	B	35	ALA	CA-C-N	5.74	127.90	120.44
1	B	35	ALA	C-N-CA	5.74	127.90	120.44
1	A	214	PRO	CB-CA-C	5.73	120.05	111.68
1	B	23	LYS	CA-C-N	-5.73	115.63	123.14
1	B	23	LYS	C-N-CA	-5.73	115.63	123.14
1	B	150	TRP	O-C-N	5.73	127.98	122.03
1	B	195	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	A	101	ARG	CD-NE-CZ	5.72	132.40	124.40
1	A	13	LYS	CA-C-N	5.71	132.45	121.54
1	A	13	LYS	C-N-CA	5.71	132.45	121.54
1	A	200	VAL	N-CA-C	5.71	113.20	107.55
1	A	86	ASN	CB-CA-C	5.71	121.63	110.67
1	B	132(B)	ASN	N-CA-CB	-5.70	101.90	110.73
1	B	222	LYS	CB-CA-C	-5.69	99.10	110.42
1	A	16	HIS	N-CA-C	-5.68	98.69	110.80
1	B	233	VAL	N-CA-C	5.67	116.32	110.36
1	B	134	LYS	N-CA-CB	5.67	119.68	110.43
1	A	272	SER	O-C-N	5.67	129.67	123.04
1	B	168	ASP	CA-C-O	-5.67	113.70	120.10
1	A	210(B)	LYS	CD-CE-NZ	5.67	130.03	111.90
1	B	154	GLY	CA-C-N	5.67	129.29	120.68
1	B	154	GLY	C-N-CA	5.67	129.29	120.68
1	B	271	ILE	N-CA-C	5.66	117.00	108.96
1	B	244	GLY	N-CA-C	5.66	121.81	115.08
1	A	323	TRP	CA-C-N	5.66	126.38	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	TRP	C-N-CA	5.66	126.38	119.99
1	A	92	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	A	113	VAL	CA-C-O	-5.64	115.40	121.27
1	A	113	VAL	N-CA-C	5.64	116.28	110.36
1	A	209(A)	ALA	CA-C-O	-5.63	115.45	122.03
1	B	323	TRP	CA-C-N	5.63	126.33	120.03
1	B	323	TRP	C-N-CA	5.63	126.33	120.03
1	A	5	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	117	VAL	N-CA-C	-5.62	104.89	110.62
1	A	290	PRO	CB-CA-C	5.61	117.67	111.56
1	A	222	LYS	CA-C-N	5.61	131.58	122.67
1	A	222	LYS	C-N-CA	5.61	131.58	122.67
1	B	93	LEU	CA-C-N	-5.60	114.63	122.75
1	B	93	LEU	C-N-CA	-5.60	114.63	122.75
1	B	208	VAL	N-CA-CB	5.60	119.26	112.10
1	A	80	SER	O-C-N	5.58	129.39	123.42
1	A	86	ASN	CB-CG-ND2	5.58	124.76	116.40
1	B	121	LYS	N-CA-CB	5.58	118.81	110.22
1	B	293	LEU	O-C-N	-5.58	116.86	123.22
1	A	40	ILE	CA-C-O	-5.57	114.95	120.85
1	A	118	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	A	237	TYR	CB-CG-CD2	-5.56	112.46	120.80
1	A	9	HIS	CA-C-N	5.56	129.37	121.42
1	A	9	HIS	C-N-CA	5.56	129.37	121.42
1	A	117	VAL	CA-C-O	-5.56	114.47	120.47
1	A	254	VAL	CA-C-O	-5.56	115.17	120.95
1	A	318	SER	CB-CA-C	-5.55	99.37	110.42
1	B	236	ALA	O-C-N	5.55	128.48	122.15
1	A	272	SER	CB-CA-C	-5.55	100.79	109.84
1	B	232	VAL	CA-C-O	-5.55	115.29	121.17
1	A	283	GLU	OE1-CD-OE2	5.54	136.21	122.90
1	A	220	ALA	O-C-N	5.54	129.96	122.59
1	B	303	VAL	CA-C-O	-5.54	114.45	120.71
1	A	42	MET	O-C-N	5.53	129.85	122.43
1	A	31	ALA	CA-C-O	-5.53	114.98	120.90
1	A	147	TYR	CA-C-O	5.53	126.63	120.82
1	A	176	MET	CG-SD-CE	-5.53	88.73	100.90
1	B	32	VAL	CB-CA-C	5.53	119.28	112.04
1	B	84	ASP	N-CA-CB	-5.53	101.98	110.16
1	B	209(D)	SER	CA-CB-OG	-5.52	100.06	111.10
1	A	324	GLY	CA-C-N	5.51	127.58	120.70
1	A	324	GLY	C-N-CA	5.51	127.58	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	B	43	LYS	CB-CG-CD	-5.50	98.66	111.30
1	B	196	GLY	CA-C-O	-5.49	116.70	121.04
1	A	281	ILE	N-CA-CB	-5.49	104.55	111.46
1	A	285	VAL	CA-CB-CG1	5.49	119.73	110.40
1	B	222	LYS	N-CA-CB	5.48	119.76	110.49
1	A	16	HIS	CG-CD2-NE2	5.48	112.68	107.20
1	B	123	ILE	CA-CB-CG2	5.48	119.82	110.50
1	A	22	ASN	OD1-CG-ND2	5.48	128.08	122.60
1	A	55	MET	CA-C-N	5.48	127.56	120.44
1	A	55	MET	C-N-CA	5.48	127.56	120.44
1	A	312	GLU	CG-CD-OE1	5.48	131.01	118.40
1	A	149	ALA	CA-C-N	5.47	127.88	120.65
1	A	149	ALA	C-N-CA	5.47	127.88	120.65
1	A	221	ASP	N-CA-CB	-5.46	101.98	110.29
1	A	42	MET	CA-CB-CG	-5.46	103.19	114.10
1	B	2	THR	CA-C-N	5.45	128.59	120.31
1	B	2	THR	C-N-CA	5.45	128.59	120.31
1	A	292	ILE	N-CA-C	-5.44	99.91	108.23
1	B	197	ASP	N-CA-C	5.43	117.96	111.71
1	B	19	PRO	CB-CA-C	5.43	118.50	110.85
1	B	80	SER	N-CA-CB	-5.42	102.60	111.66
1	A	207	ASN	N-CA-C	5.42	117.33	108.76
1	B	87	VAL	CA-C-N	5.42	132.19	122.38
1	B	87	VAL	C-N-CA	5.42	132.19	122.38
1	B	274	MET	N-CA-CB	-5.42	101.31	109.88
1	A	16	HIS	CB-CA-C	5.42	121.20	110.42
1	B	47	ASP	CB-CA-C	5.41	118.64	109.55
1	B	213	HIS	O-C-N	5.40	126.23	121.37
1	B	261	ILE	CA-C-O	-5.39	114.92	121.18
1	A	153	SER	CA-C-O	-5.39	114.84	120.55
1	B	121	LYS	CA-C-O	-5.39	114.01	120.10
1	A	120	PHE	CA-C-O	-5.38	114.84	120.55
1	A	215	GLU	CA-C-N	5.38	128.99	121.02
1	A	215	GLU	C-N-CA	5.38	128.99	121.02
1	B	189	GLY	O-C-N	5.38	129.69	122.70
1	B	209(A)	ALA	N-CA-C	5.38	119.12	112.24
1	A	283	GLU	N-CA-CB	5.38	118.77	110.60
1	B	178	GLU	CB-CG-CD	-5.37	103.47	112.60
1	A	192	LEU	N-CA-CB	-5.36	102.15	110.46
1	B	153	SER	N-CA-C	5.36	116.80	111.07
1	B	156	PRO	N-CA-C	-5.36	103.37	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	CYS	CA-C-N	5.36	127.46	120.28
1	A	36	CYS	C-N-CA	5.36	127.46	120.28
1	A	310	GLU	CA-C-N	5.36	127.46	120.28
1	A	310	GLU	C-N-CA	5.36	127.46	120.28
1	B	224	HIS	CB-CG-CD2	-5.35	124.24	131.20
1	B	253	SER	N-CA-C	-5.35	105.45	111.28
1	A	313	ALA	N-CA-C	-5.34	105.37	111.14
1	A	276	LYS	CB-CA-C	5.34	118.54	109.84
1	B	211	ASN	O-C-N	5.33	129.48	122.33
1	B	94	VAL	CA-C-O	5.33	126.24	120.43
1	B	187	CYS	CA-C-N	-5.32	115.22	122.93
1	B	187	CYS	C-N-CA	-5.32	115.22	122.93
1	B	11	LEU	CB-CA-C	5.31	117.99	109.07
1	A	121	LYS	N-CA-CB	5.31	118.39	110.22
1	B	29	VAL	N-CA-CB	-5.31	102.47	111.23
1	B	128	VAL	CA-C-N	5.30	127.82	120.29
1	B	128	VAL	C-N-CA	5.30	127.82	120.29
1	A	263	LYS	CG-CD-CE	5.30	123.50	111.30
1	A	68	HIS	N-CA-C	-5.30	105.61	111.71
1	B	149	ALA	CA-C-N	5.30	127.64	120.65
1	B	149	ALA	C-N-CA	5.30	127.64	120.65
1	A	72	PHE	O-C-N	5.30	129.93	122.41
1	B	38	ILE	CA-CB-CG2	5.30	119.50	110.50
1	A	109	ARG	NE-CZ-NH2	5.29	123.97	119.20
1	B	317	LYS	N-CA-C	-5.29	105.62	111.71
1	A	293	LEU	N-CA-CB	-5.28	102.28	110.57
1	B	264	ASN	CB-CG-ND2	-5.28	108.48	116.40
1	B	118	ASN	N-CA-CB	5.27	118.34	110.22
1	B	86	ASN	N-CA-CB	5.27	118.45	110.28
1	B	110	LEU	N-CA-CB	-5.27	102.10	110.22
1	B	274	MET	CG-SD-CE	-5.26	89.32	100.90
1	A	170	ALA	N-CA-C	-5.26	105.63	111.36
1	B	170	ALA	CA-C-N	5.26	127.59	120.44
1	B	170	ALA	C-N-CA	5.26	127.59	120.44
1	A	72	PHE	CA-C-O	-5.25	112.93	119.18
1	B	32	VAL	CA-C-O	-5.25	114.71	120.96
1	B	320	ASP	CB-CA-C	5.24	119.75	110.85
1	A	327	LYS	CB-CG-CD	5.23	123.32	111.30
1	A	11	LEU	CA-C-O	5.22	125.92	119.81
1	A	96	ILE	CB-CG1-CD1	5.22	124.75	113.80
1	B	272	SER	CA-C-N	-5.22	114.01	122.36
1	B	272	SER	C-N-CA	-5.22	114.01	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	LEU	N-CA-C	5.21	117.87	111.82
1	B	197	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	166	ASN	CA-C-O	5.21	126.29	120.82
1	A	202	VAL	CA-C-N	5.19	127.76	120.28
1	A	202	VAL	C-N-CA	5.19	127.76	120.28
1	B	312	GLU	CG-CD-OE2	-5.19	106.46	118.40
1	B	253	SER	O-C-N	-5.19	116.62	122.12
1	A	267	ARG	CA-CB-CG	-5.19	103.72	114.10
1	B	25	THR	CA-CB-OG1	-5.18	101.82	109.60
1	A	232	VAL	CA-C-N	5.18	127.56	120.46
1	A	232	VAL	C-N-CA	5.18	127.56	120.46
1	A	179	ARG	O-C-N	5.18	127.68	122.09
1	B	250	ILE	CA-C-O	-5.18	115.56	120.95
1	B	309	PRO	CB-CA-C	5.18	121.65	112.64
1	A	74	ARG	NH1-CZ-NH2	5.18	126.03	119.30
1	B	3	LEU	CA-C-O	5.16	125.91	119.97
1	A	184	PRO	CA-C-N	5.16	127.45	120.38
1	A	184	PRO	C-N-CA	5.16	127.45	120.38
1	B	42	MET	CA-CB-CG	-5.16	103.78	114.10
1	A	87	VAL	N-CA-CB	5.16	119.47	110.65
1	A	242	LEU	N-CA-CB	-5.16	102.50	110.13
1	A	287	LEU	CB-CA-C	5.16	122.80	111.09
1	A	301	ASP	CB-CG-OD1	5.16	130.26	118.40
1	A	276	LYS	CA-C-N	5.15	128.96	122.00
1	A	276	LYS	C-N-CA	5.15	128.96	122.00
1	B	115	ARG	NH1-CZ-NH2	-5.15	112.60	119.30
1	B	85	TYR	CA-C-O	-5.15	113.15	120.51
1	B	137	VAL	O-C-N	5.15	129.22	122.94
1	A	123	ILE	O-C-N	5.14	127.60	121.80
1	B	83	LYS	CA-CB-CG	5.13	124.37	114.10
1	B	46	ALA	CA-C-O	-5.13	115.36	121.56
1	A	168	ASP	CA-C-O	-5.12	115.42	120.90
1	A	275	ILE	N-CA-CB	5.12	118.93	112.22
1	B	171	ARG	N-CA-CB	5.12	117.50	110.07
1	A	64	MET	O-C-N	-5.12	116.77	122.09
1	A	74	ARG	CA-C-N	5.12	129.99	122.98
1	A	74	ARG	C-N-CA	5.12	129.99	122.98
1	B	30	GLY	O-C-N	-5.12	117.50	122.77
1	B	280	GLY	CA-C-N	5.12	129.28	122.01
1	B	280	GLY	C-N-CA	5.12	129.28	122.01
1	A	171	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	58	LYS	CB-CG-CD	5.11	123.05	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	PRO	CA-CB-CG	-5.10	94.81	104.50
1	A	257	LEU	O-C-N	5.10	127.96	122.15
1	B	22	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	B	57	ASP	CA-C-N	5.09	128.46	120.82
1	B	57	ASP	C-N-CA	5.09	128.46	120.82
1	B	243	LYS	N-CA-C	-5.09	105.97	113.61
1	A	230	LYS	CA-C-O	-5.09	115.48	120.82
1	B	257	LEU	O-C-N	5.09	127.51	122.12
1	A	58	LYS	CA-CB-CG	5.08	124.25	114.10
1	B	55	MET	CA-C-N	5.07	127.39	120.54
1	B	55	MET	C-N-CA	5.07	127.39	120.54
1	A	322	LEU	CB-CA-C	5.07	118.84	110.88
1	A	296	ASN	OD1-CG-ND2	5.07	127.67	122.60
1	A	31	ALA	O-C-N	5.06	127.35	122.09
1	B	59	LEU	N-CA-C	5.06	117.18	111.11
1	B	185	LEU	CA-C-O	-5.06	114.38	120.10
1	A	53	ASP	CA-C-N	-5.05	113.39	121.02
1	A	53	ASP	C-N-CA	-5.05	113.39	121.02
1	B	187	CYS	N-CA-CB	5.05	118.49	110.55
1	B	140	ASN	CB-CG-OD1	5.05	130.90	120.80
1	A	292	ILE	N-CA-CB	5.05	116.75	111.00
1	B	201	PRO	N-CA-CB	-5.05	99.85	103.23
1	A	245	TYR	O-C-N	5.05	128.34	123.29
1	B	180	LEU	N-CA-C	5.05	119.29	113.18
1	B	237	TYR	CA-C-N	5.05	127.30	120.44
1	B	237	TYR	C-N-CA	5.05	127.30	120.44
1	B	296	ASN	O-C-N	5.05	128.40	122.34
1	A	172	PHE	CA-C-N	5.04	127.00	120.44
1	A	172	PHE	C-N-CA	5.04	127.00	120.44
1	B	71	LEU	CA-C-O	-5.04	114.55	120.20
1	A	218	THR	CA-CB-CG2	5.04	119.07	110.50
1	A	101	ARG	NE-CZ-NH2	-5.04	114.66	119.20
1	A	105	GLU	O-C-N	-5.03	117.02	123.06
1	A	162	GLY	N-CA-C	-5.03	101.76	110.71
1	B	223	GLU	CA-C-N	5.01	131.11	121.54
1	B	223	GLU	C-N-CA	5.01	131.11	121.54
1	A	308	THR	CA-C-N	5.00	124.61	119.56
1	A	308	THR	C-N-CA	5.00	124.61	119.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	TYR	Sidechain
1	A	265	LEU	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	89	0
1	B	2568	0	2641	92	1
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	44	0	26	3	0
3	B	44	0	26	2	0
4	B	6	0	2	0	0
5	A	81	0	0	6	1
5	B	70	0	0	9	1
All	All	5396	0	5337	175	2

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 17.

All (175) 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:B:217:GLY:O	1:B:219:ASP:N	1.93	1.01
1:A:221:ASP:O	1:A:222:LYS:HB2	1.58	0.99
1:A:39:SER:HA	1:B:42:MET:HE1	1.47	0.93
1:B:13:LYS:CG	1:B:14:GLU:H	1.82	0.91
1:B:176:MET:HE1	1:B:206:VAL:HG11	1.52	0.91
1:B:290:PRO:HG2	1:B:305:VAL:HG11	1.53	0.90
1:B:100:ALA:H	1:B:116:ASN:HD21	1.18	0.89
1:A:100:ALA:H	1:A:116:ASN:HD21	0.93	0.88
1:A:100:ALA:N	1:A:116:ASN:HD21	1.75	0.84
1:B:217:GLY:C	1:B:219:ASP:H	1.86	0.82
1:B:114:GLN:HG3	1:B:330:GLN:HE22	1.45	0.82
1:B:308:THR:HG22	1:B:311:GLU:HG3	1.60	0.82
1:A:161:ILE:HG23	1:A:271:ILE:HD12	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ILE:CD1	1:B:281:ILE:HG13	2.13	0.79
1:B:13:LYS:HG3	1:B:14:GLU:H	1.48	0.77
1:A:210(A):LEU:HD11	1:B:7:LEU:HD22	1.67	0.76
1:A:222:LYS:HG2	1:A:223:GLU:H	1.51	0.76
1:A:100:ALA:H	1:A:116:ASN:ND2	1.77	0.75
1:B:132(B):ASN:HA	1:B:159:ARG:NH1	2.02	0.75
1:A:193:GLY:HA2	1:A:287:LEU:HD13	1.70	0.74
1:A:276:LYS:HB2	1:A:283:GLU:O	1.89	0.73
1:B:266:ARG:HB3	1:B:292:ILE:HD11	1.69	0.73
1:A:85:TYR:O	1:A:88:THR:HB	1.88	0.73
1:B:55:MET:HE3	3:B:401:NAD:O2B	1.89	0.73
1:B:238:GLU:O	1:B:242:LEU:HD12	1.88	0.72
1:B:77:LYS:HE3	5:B:454:HOH:O	1.90	0.71
1:A:4:LYS:HG2	5:B:406:HOH:O	1.91	0.70
1:B:132(A):PRO:O	1:B:159:ARG:NH1	2.23	0.70
1:A:4:LYS:CG	5:B:406:HOH:O	2.39	0.69
5:A:481:HOH:O	1:B:2:THR:HG22	1.93	0.69
1:A:4:LYS:HE3	5:A:439:HOH:O	1.91	0.69
1:A:161:ILE:CG2	1:A:271:ILE:HD12	2.23	0.68
1:B:285:VAL:HG21	1:B:319:ALA:HB1	1.75	0.68
1:A:14:GLU:C	1:A:15:GLU:O	2.35	0.68
1:B:274:MET:HG2	1:B:286:PHE:CE2	2.28	0.67
1:A:289:VAL:HG13	1:A:302:VAL:HG13	1.76	0.67
1:A:10:ASN:ND2	1:A:12:LEU:O	2.29	0.66
1:A:281:ILE:C	1:A:281:ILE:HD13	2.21	0.66
1:B:271:ILE:O	1:B:288:SER:HA	1.96	0.65
1:B:114:GLN:HG3	1:B:330:GLN:NE2	2.11	0.65
1:B:290:PRO:HG2	1:B:305:VAL:CG1	2.25	0.65
1:B:123:ILE:HG13	1:B:124:ILE:N	2.12	0.64
1:B:117:VAL:HG22	1:B:148:VAL:HG21	1.79	0.64
1:B:243:LYS:HE2	1:B:245:TYR:O	1.97	0.64
1:A:221:ASP:O	1:A:222:LYS:CB	2.43	0.63
1:B:100:ALA:N	1:B:116:ASN:HD21	1.94	0.63
1:A:329:LEU:C	1:A:331:PHE:H	2.06	0.62
1:A:175:LEU:HD13	1:A:231:GLU:HG3	1.82	0.61
1:A:198:SER:O	1:A:318:SER:OG	2.17	0.61
1:A:266:ARG:HB3	1:A:292:ILE:HD13	1.82	0.61
1:A:264:ASN:HB2	1:A:295:GLN:HB3	1.83	0.61
1:A:190:TRP:CZ3	1:A:270:PRO:HD3	2.35	0.61
1:B:88:THR:CG2	5:B:451:HOH:O	2.48	0.60
1:B:190:TRP:HB3	1:B:192:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ASN:ND2	1:A:92:ARG:HH21	2.01	0.59
1:A:22:ASN:HD22	1:A:92:ARG:HH21	1.50	0.59
1:A:314:HIS:HB3	5:A:414:HOH:O	2.02	0.58
1:A:289:VAL:CG1	1:A:302:VAL:HG13	2.32	0.58
1:B:183:HIS:ND1	1:B:185:LEU:HB2	2.19	0.58
1:A:127:ILE:HD11	1:A:133:CYS:SG	2.43	0.58
1:A:289:VAL:HG13	1:A:302:VAL:CG1	2.34	0.58
1:A:94:VAL:HG21	1:A:127:ILE:HD13	1.85	0.58
1:B:266:ARG:HB3	1:B:292:ILE:CD1	2.33	0.57
1:A:140:ASN:HB2	3:A:401:NAD:O2D	2.06	0.56
1:B:274:MET:CG	1:B:286:PHE:CE2	2.89	0.56
1:A:197:ASP:HA	1:A:233:VAL:HG13	1.88	0.55
1:B:275:ILE:HG12	1:B:287:LEU:CD1	2.37	0.55
1:B:328:GLU:O	1:B:330:GLN:N	2.39	0.55
1:B:182:VAL:HG23	1:B:187:CYS:SG	2.47	0.55
1:A:183:HIS:ND1	1:A:185:LEU:HB2	2.22	0.55
1:B:120:PHE:HA	1:B:123:ILE:HG12	1.88	0.55
1:B:329:LEU:HA	1:B:331:PHE:CE1	2.42	0.55
1:A:71:LEU:HD12	1:B:185:LEU:HD13	1.89	0.54
1:B:182:VAL:CG2	1:B:187:CYS:SG	2.96	0.54
1:B:16:HIS:CG	1:B:16:HIS:O	2.60	0.54
1:A:210(B):LYS:NZ	1:A:214:PRO:O	2.41	0.54
1:B:13:LYS:CD	1:B:14:GLU:H	2.21	0.53
1:A:320:ASP:O	1:A:321:THR:C	2.50	0.53
1:A:109:ARG:HG3	5:A:408:HOH:O	2.08	0.53
1:B:25:THR:HB	1:B:94:VAL:HB	1.90	0.53
1:B:127:ILE:HG21	1:B:135:LEU:HD21	1.91	0.52
1:A:51:LEU:O	1:A:80:SER:HA	2.09	0.52
1:B:275:ILE:HG12	1:B:287:LEU:HD11	1.92	0.52
1:A:15:GLU:OE1	1:A:18:VAL:HG12	2.10	0.52
1:B:199:SER:OG	1:B:229:HIS:HE1	1.93	0.52
1:A:138:VAL:O	3:A:401:NAD:H2N	2.10	0.51
1:A:213:HIS:HD2	1:A:216:LEU:HB2	1.75	0.51
1:A:213:HIS:NE2	1:A:222:LYS:HG3	2.25	0.51
1:A:222:LYS:HB3	1:A:224:HIS:H	1.75	0.51
1:A:279:TYR:N	1:A:281:ILE:HG22	2.25	0.51
1:B:32:VAL:HG21	3:B:401:NAD:C6N	2.40	0.51
1:B:115:ARG:HD3	5:B:419:HOH:O	2.11	0.51
1:B:275:ILE:HD12	1:B:281:ILE:HG13	1.91	0.51
1:A:4:LYS:HB3	5:B:406:HOH:O	2.11	0.51
1:A:222:LYS:CG	1:A:223:GLU:H	2.01	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:TYR:H	1:A:281:ILE:HG22	1.75	0.51
1:B:27:VAL:HG22	1:B:52:VAL:HG22	1.93	0.50
1:B:215:GLU:O	1:B:219:ASP:HB2	2.11	0.50
1:A:292:ILE:C	1:A:292:ILE:HD12	2.37	0.50
1:A:210(A):LEU:HD11	1:B:7:LEU:CD2	2.38	0.50
1:A:13:LYS:HB2	1:A:14:GLU:HG3	1.94	0.50
1:A:310:GLU:O	1:A:313:ALA:HB3	2.12	0.50
1:B:221:ASP:HB3	1:B:222:LYS:HD2	1.93	0.50
1:B:192:LEU:HD22	1:B:202:VAL:HG21	1.93	0.49
1:B:88:THR:HG23	5:B:451:HOH:O	2.10	0.49
1:B:13:LYS:HG3	1:B:14:GLU:N	2.25	0.49
1:A:289:VAL:CG1	1:A:302:VAL:CG1	2.91	0.48
1:A:206:VAL:HG12	1:A:210(A):LEU:HD22	1.94	0.48
1:B:243:LYS:HE3	1:B:245:TYR:CE2	2.49	0.48
1:B:140:ASN:HA	1:B:142:VAL:N	2.29	0.48
1:A:14:GLU:O	1:A:16:HIS:HD2	1.97	0.48
1:B:275:ILE:HD12	1:B:281:ILE:HG21	1.96	0.48
1:B:275:ILE:HD13	1:B:281:ILE:HG13	1.93	0.48
1:A:38:ILE:HA	1:A:38:ILE:HD12	1.75	0.47
1:B:329:LEU:HA	1:B:331:PHE:HE1	1.79	0.47
1:A:110:LEU:HD13	1:A:325:ILE:CD1	2.44	0.47
1:B:13:LYS:CG	1:B:14:GLU:N	2.60	0.47
1:A:13:LYS:O	1:A:15:GLU:N	2.48	0.47
1:B:96:ILE:HD11	1:B:135:LEU:HD22	1.96	0.46
1:B:275:ILE:HG12	1:B:287:LEU:HG	1.97	0.46
1:A:30:GLY:O	1:A:31:ALA:C	2.57	0.46
1:A:127:ILE:HG13	1:A:128:VAL:N	2.30	0.46
1:B:85:TYR:O	1:B:88:THR:HB	2.14	0.46
1:A:280:GLY:O	1:A:316:LYS:HE2	2.15	0.46
1:A:15:GLU:O	1:A:16:HIS:CD2	2.68	0.46
1:A:218:THR:HA	1:A:226:LYS:HE3	1.98	0.46
1:A:284:ASN:HB2	5:A:477:HOH:O	2.15	0.45
1:B:308:THR:CG2	1:B:311:GLU:HG3	2.40	0.45
1:A:18:VAL:CG2	1:A:19:PRO:HD2	2.45	0.45
1:A:213:HIS:HB2	1:B:3:LEU:HD13	1.98	0.45
1:A:102:GLN:CD	1:A:109:ARG:HG2	2.41	0.45
1:B:56:GLU:OE1	1:B:83:LYS:HE2	2.17	0.45
1:A:210(A):LEU:CD1	1:B:7:LEU:HD22	2.41	0.44
1:A:274:MET:HG3	1:A:286:PHE:CE2	2.52	0.44
1:B:50:ALA:HA	1:B:79:VAL:O	2.18	0.44
1:B:176:MET:CE	1:B:206:VAL:HG11	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:MET:HE3	1:A:176:MET:HB2	1.62	0.44
1:B:190:TRP:HB3	1:B:192:LEU:CD1	2.47	0.44
1:B:289:VAL:HA	1:B:290:PRO:HD3	1.78	0.44
1:B:173:ARG:NE	1:B:187:CYS:O	2.50	0.44
1:A:197:ASP:HA	1:A:233:VAL:CG1	2.47	0.44
1:B:140:ASN:HA	1:B:141:PRO:C	2.43	0.44
1:B:23:LYS:HE3	1:B:48:GLU:OE2	2.18	0.43
1:A:287:LEU:HD21	1:A:319:ALA:HB2	2.00	0.43
1:A:329:LEU:C	1:A:331:PHE:N	2.75	0.43
1:B:208:VAL:O	1:B:209(C):VAL:HG13	2.19	0.43
1:A:281:ILE:HD13	1:A:283:GLU:H	1.84	0.42
3:A:401:NAD:H6N	5:A:413:HOH:O	2.17	0.42
1:A:24:ILE:O	1:A:49:ILE:HA	2.19	0.42
1:A:28:GLY:O	1:A:33:GLY:HA3	2.19	0.42
1:B:24:ILE:O	1:B:49:ILE:HA	2.18	0.42
1:B:240:ILE:O	1:B:244:GLY:N	2.49	0.42
1:B:231:GLU:O	1:B:235:SER:HB3	2.20	0.42
1:B:77:LYS:HE2	5:B:455:HOH:O	2.20	0.41
1:B:286:PHE:O	1:B:287:LEU:HB3	2.19	0.41
1:A:281:ILE:C	1:A:281:ILE:CD1	2.91	0.41
1:B:271:ILE:CD1	1:B:293:LEU:HG	2.50	0.41
1:B:217:GLY:C	1:B:219:ASP:N	2.61	0.41
1:B:261:ILE:HG13	1:B:293:LEU:HD13	2.03	0.41
1:A:14:GLU:O	1:A:16:HIS:CD2	2.72	0.41
1:A:200:VAL:HG21	1:A:315:LEU:HD12	2.01	0.41
1:A:289:VAL:HA	1:A:290:PRO:HD3	1.91	0.41
1:B:285:VAL:HG12	1:B:326:GLN:NE2	2.36	0.41
1:B:264:ASN:HB2	1:B:295:GLN:HB3	2.01	0.41
1:B:167:LEU:O	1:B:171:ARG:HG3	2.20	0.41
1:A:194:GLU:HG3	1:A:322:LEU:HD22	2.01	0.41
1:A:191:ILE:CD1	1:A:201:PRO:HA	2.52	0.41
1:B:266:ARG:CB	1:B:292:ILE:HD11	2.45	0.41
1:B:107:GLU:OE1	5:B:473:HOH:O	2.22	0.40
1:A:85:TYR:CE2	1:A:127:ILE:HG22	2.56	0.40
1:A:147:TYR:CD2	1:A:326:GLN:HG2	2.56	0.40
1:A:212:LEU:HD12	1:B:3:LEU:HD12	2.04	0.40
1:A:217:GLY:H	1:A:222:LYS:NZ	2.19	0.40
1:A:279:TYR:H	1:A:281:ILE:CG2	2.35	0.40
1:B:23:LYS:HE3	1:B:48:GLU:CD	2.46	0.40

All (2) 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)
5:A:483:HOH:O	5:B:473:HOH:O[4_455]	1.28	0.92
1:B:132(B):ASN:OD1	1:B:132(B):ASN:OD1[2_655]	1.63	0.57

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/332 (96%)	293 (92%)	21 (7%)	6 (2%)	6	4
1	B	330/332 (99%)	309 (94%)	14 (4%)	7 (2%)	5	3
All	All	650/664 (98%)	602 (93%)	35 (5%)	13 (2%)	6	4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	218	THR
1	A	222	LYS
1	B	1	ALA
1	B	14	GLU
1	B	218	THR
1	B	222	LYS
1	B	329	LEU
1	A	219	ASP
1	A	329	LEU
1	A	15	GLU
1	B	15	GLU
1	B	328	GLU

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
4	OXM	B	402	-	5,5,5	8.90	4 (80%)	2,6,6	1.67	1 (50%)
2	SO4	A	402	-	4,4,4	0.79	0	6,6,6	2.31	4 (66%)
3	NAD	A	401	-	46,48,48	1.61	5 (10%)	64,73,73	2.33	25 (39%)
2	SO4	A	403	-	4,4,4	0.94	0	6,6,6	0.73	0
3	NAD	B	401	-	46,48,48	1.78	6 (13%)	64,73,73	2.29	18 (28%)
2	SO4	B	403	-	4,4,4	0.78	0	6,6,6	0.86	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
3	NAD	B	401	-	-	5/30/62/62	0/5/5/5
4	OXM	B	402	-	-	0/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	402	OXM	C1-C2	-15.25	1.37	1.55
4	B	402	OXM	C1-N1	10.91	1.65	1.33
3	B	401	NAD	PA-O3	7.80	1.67	1.59
3	A	401	NAD	C3N-C7N	5.81	1.59	1.50
4	B	402	OXM	O1-C1	5.29	1.36	1.24
3	B	401	NAD	C3N-C7N	4.74	1.57	1.50
3	A	401	NAD	PN-O3	4.10	1.63	1.59
4	B	402	OXM	O2-C2	4.03	1.32	1.22
3	B	401	NAD	C6N-N1N	3.69	1.43	1.35
3	A	401	NAD	C6N-N1N	3.53	1.43	1.35
3	A	401	NAD	C2A-N3A	-3.49	1.27	1.33
3	B	401	NAD	O7N-C7N	-3.47	1.17	1.24
3	B	401	NAD	PN-O3	2.66	1.62	1.59
3	B	401	NAD	C2A-N3A	-2.31	1.29	1.33
3	A	401	NAD	C4A-N9A	2.17	1.42	1.37

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAD	C5N-C4N-C3N	-9.51	111.01	120.36
3	A	401	NAD	C5N-C4N-C3N	-6.41	114.07	120.36
3	B	401	NAD	C2N-C3N-C4N	6.25	125.53	118.26
3	B	401	NAD	C6N-C5N-C4N	5.98	128.07	119.45
3	A	401	NAD	O4B-C1B-N9A	5.05	117.79	108.09
3	A	401	NAD	N6A-C6A-N1A	-4.96	107.33	118.38
3	A	401	NAD	C5A-C6A-N6A	4.89	135.39	123.29
3	A	401	NAD	O7N-C7N-N7N	4.42	129.01	122.62
3	A	401	NAD	C6N-C5N-C4N	4.39	125.78	119.45
3	A	401	NAD	C2N-C3N-C4N	4.08	123.00	118.26
3	B	401	NAD	O2B-C2B-C3B	3.98	124.56	111.82
2	A	402	SO4	O4-S-O1	3.87	129.80	109.56
3	B	401	NAD	C5N-C6N-N1N	-3.62	115.45	120.38
3	A	401	NAD	C5A-N7A-C8A	3.41	108.80	103.45
3	B	401	NAD	O2A-PA-O1A	3.34	127.96	112.44
3	B	401	NAD	C6N-N1N-C2N	-3.31	119.06	121.88
3	A	401	NAD	C4N-C3N-C7N	-3.23	112.27	121.06
3	B	401	NAD	O4B-C1B-C2B	-3.22	99.73	106.62
3	A	401	NAD	C3N-C7N-N7N	-3.10	113.92	117.74
3	A	401	NAD	C4A-C5A-N7A	-3.01	107.14	110.58
3	B	401	NAD	O5B-C5B-C4B	-2.95	98.95	108.99
3	A	401	NAD	C5N-C6N-N1N	-2.92	116.40	120.38
3	B	401	NAD	O7N-C7N-N7N	2.92	126.83	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	NAD	O5D-PN-O1N	2.87	120.30	108.94
3	A	401	NAD	O2B-C2B-C3B	2.87	121.01	111.82
3	A	401	NAD	C6A-C5A-N7A	2.79	137.47	132.09
3	A	401	NAD	O2N-PN-O5D	2.78	120.17	107.57
3	A	401	NAD	O2A-PA-O3	2.77	114.76	107.27
3	A	401	NAD	C1B-N9A-C8A	2.72	133.13	127.09
3	A	401	NAD	C4A-N9A-C1B	-2.58	120.60	126.63
3	B	401	NAD	C4D-O4D-C1D	-2.48	107.65	109.92
3	A	401	NAD	O5D-PN-O1N	2.44	118.62	108.94
3	A	401	NAD	N9A-C8A-N7A	-2.42	110.50	113.94
3	A	401	NAD	C6N-N1N-C2N	-2.42	119.82	121.88
3	B	401	NAD	C1B-N9A-C8A	2.39	132.41	127.09
2	A	402	SO4	O3-S-O2	2.36	121.92	109.56
3	B	401	NAD	C4N-C3N-C7N	-2.36	114.64	121.06
2	A	402	SO4	O3-S-O1	-2.32	97.40	109.56
3	A	401	NAD	O7N-C7N-C3N	-2.31	116.77	119.60
4	B	402	OXM	O3-C2-O2	-2.27	118.50	123.90
2	A	402	SO4	O4-S-O3	-2.24	96.17	108.54
3	A	401	NAD	C5B-C4B-C3B	-2.20	107.31	115.21
3	B	401	NAD	O4D-C4D-C5D	-2.19	102.33	109.33
3	A	401	NAD	N3A-C2A-N1A	-2.13	125.35	128.58
3	B	401	NAD	O3D-C3D-C4D	-2.13	104.96	111.08
3	A	401	NAD	O2D-C2D-C3D	2.10	118.53	111.82
3	B	401	NAD	O7N-C7N-C3N	-2.05	117.09	119.60
3	B	401	NAD	O5D-C5D-C4D	-2.00	102.17	108.99

There are no chirality outliers.

All (9) torsion outliers are listed below:

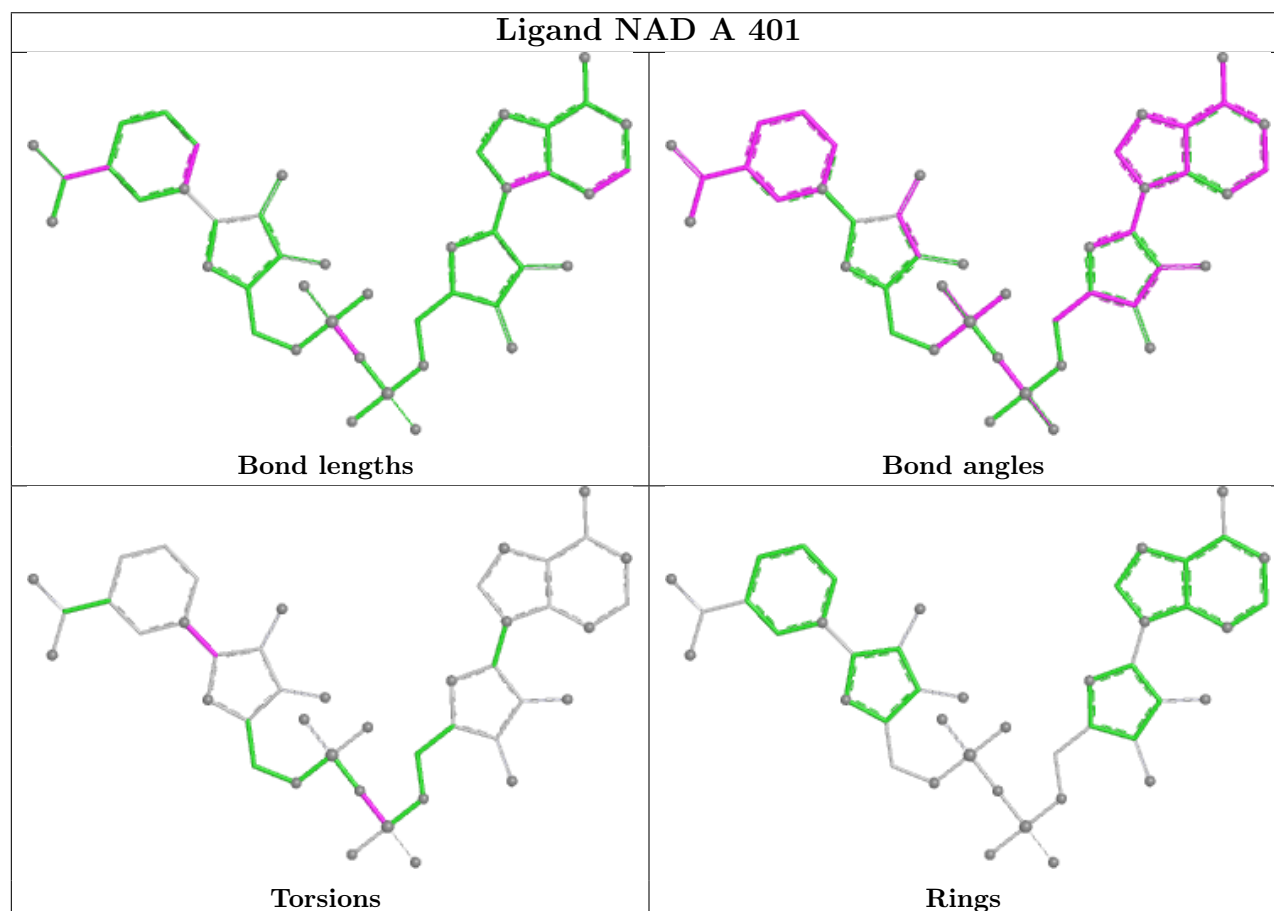
Mol	Chain	Res	Type	Atoms
3	A	401	NAD	O4D-C1D-N1N-C2N
3	A	401	NAD	O4D-C1D-N1N-C6N
3	B	401	NAD	O4D-C1D-N1N-C6N
3	B	401	NAD	C2D-C1D-N1N-C6N
3	A	401	NAD	C2D-C1D-N1N-C2N
3	B	401	NAD	C2D-C1D-N1N-C2N
3	B	401	NAD	O4D-C1D-N1N-C2N
3	A	401	NAD	PN-O3-PA-O2A
3	B	401	NAD	O4B-C4B-C5B-O5B

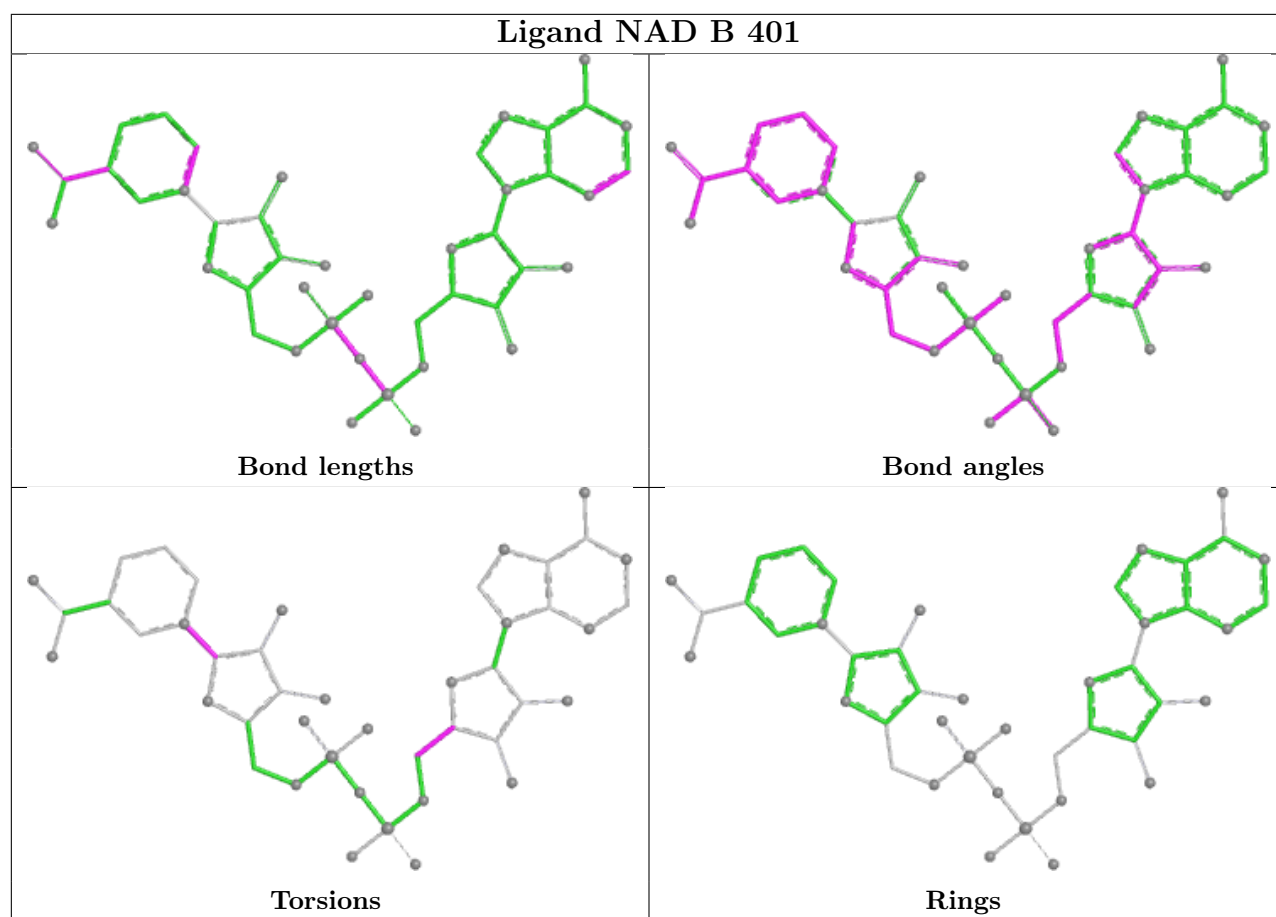
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAD	3	0
3	B	401	NAD	2	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.