



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:49 AM UTC

PDB ID : 4TLN / pdb_00004tln
Title : BINDING OF HYDROXAMIC ACID INHIBITORS TO CRYSTALLINE THERMOLYSIN SUGGESTS A PENTACOORDINATE ZINC INTERMEDIATE IN CATALYSIS
Authors : Matthews, B.W.; Holmes, M.A.
Deposited on : 1982-02-08
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

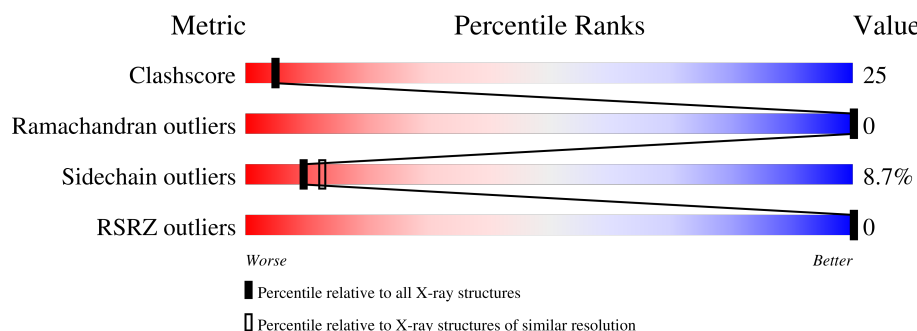
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

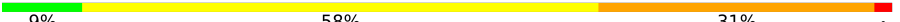
The reported resolution of this entry is 2.30 Å.

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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	316	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2597 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 THERMOLYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2432	1528	408	494	2			

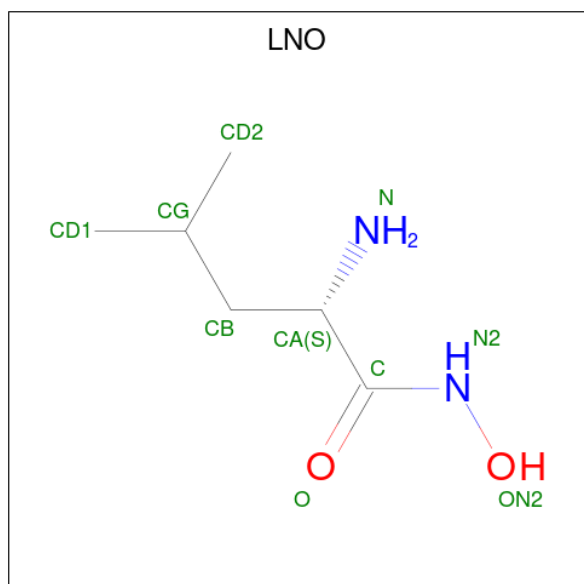
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is L-LEUCYL-HYDROXYLAMINE (CCD ID: LNO) (formula: C₆H₁₄N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	6	2	2		

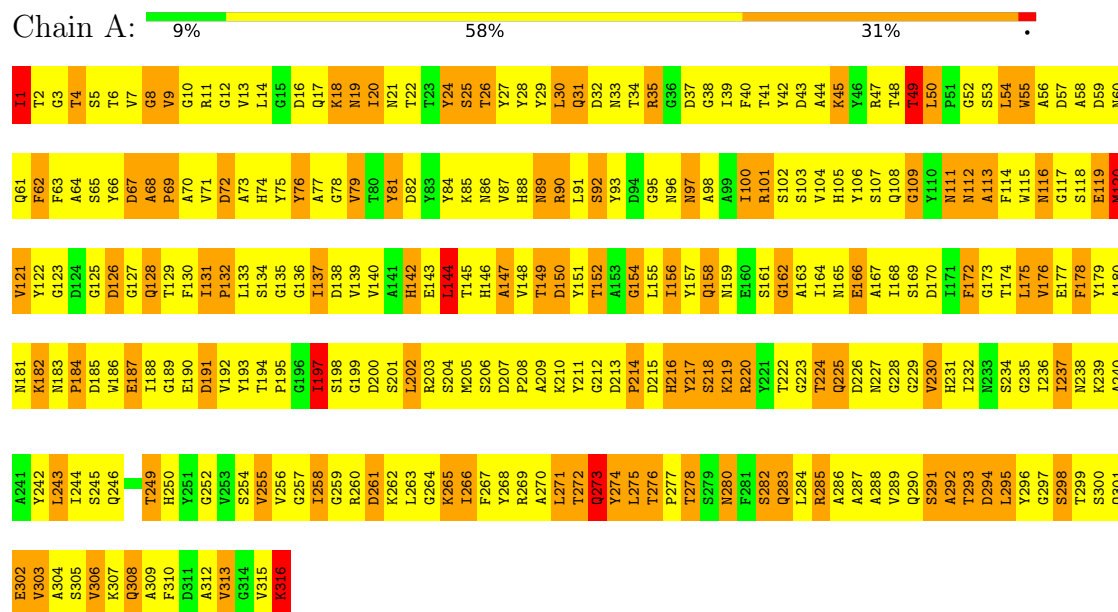
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	150	Total	O	0	0
			150	150		

3 Residue-property plots

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

• Molecule 1: THERMOLYSIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	94.20Å 94.20Å 131.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30 10.00 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 75.0 (10.00-2.31)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	114125.00 (at 2.31Å)	Xtriage
Refinement program	TNT, PROLSQ	Depositor
R, R_{free}	0.169 , (Not available) 0.156 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2597	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, LNO, ZN

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	2.92	219/2491 (8.8%)	3.90	570/3391 (16.8%)

All (219) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	GLY	N-CA	16.73	1.60	1.44
1	A	260	ARG	C-N	-13.55	1.15	1.33
1	A	35	ARG	C-N	-12.79	1.15	1.33
1	A	256	VAL	N-CA	11.48	1.60	1.46
1	A	108	GLN	C-O	11.29	1.36	1.24
1	A	20	ILE	C-O	10.93	1.35	1.23
1	A	77	ALA	C-O	-10.64	1.11	1.24
1	A	163	ALA	C-N	-10.38	1.21	1.33
1	A	267	PHE	C-O	10.33	1.36	1.24
1	A	216	HIS	CG-ND1	-10.18	1.27	1.38
1	A	101	ARG	CG-CD	9.95	1.82	1.52
1	A	285	ARG	C-N	9.65	1.46	1.33
1	A	39	ILE	CA-CB	9.29	1.65	1.54
1	A	11	ARG	NE-CZ	9.19	1.43	1.33
1	A	162	GLY	C-O	9.12	1.34	1.24
1	A	4	THR	C-O	9.11	1.35	1.23
1	A	53	SER	CA-CB	9.03	1.69	1.53
1	A	47	ARG	C-N	-9.01	1.21	1.33
1	A	10	GLY	C-O	8.94	1.33	1.23
1	A	173	GLY	CA-C	-8.90	1.40	1.51
1	A	185	ASP	C-O	8.84	1.32	1.24
1	A	235	GLY	C-O	8.78	1.35	1.23
1	A	10	GLY	C-N	-8.70	1.21	1.33
1	A	278	THR	CB-OG1	8.57	1.57	1.43
1	A	295	LEU	N-CA	-8.55	1.35	1.46
1	A	174	THR	C-O	8.54	1.34	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	LYS	CA-CB	-8.52	1.39	1.53
1	A	101	ARG	NE-CZ	-8.52	1.23	1.33
1	A	144	LEU	C-O	8.48	1.34	1.24
1	A	288	ALA	C-O	8.47	1.34	1.24
1	A	224	THR	CA-CB	8.39	1.66	1.53
1	A	297	GLY	C-N	-8.31	1.22	1.33
1	A	256	VAL	C-N	-8.26	1.24	1.33
1	A	39	ILE	C-N	-8.20	1.22	1.33
1	A	194	THR	CB-OG1	8.08	1.56	1.43
1	A	255	VAL	C-O	8.06	1.32	1.24
1	A	183	ASN	N-CA	7.93	1.57	1.46
1	A	4	THR	N-CA	7.85	1.56	1.46
1	A	303	VAL	C-N	-7.81	1.23	1.33
1	A	260	ARG	CA-C	-7.77	1.41	1.52
1	A	88	HIS	CA-C	-7.76	1.42	1.52
1	A	43	ASP	CA-C	7.71	1.62	1.52
1	A	52	GLY	C-O	7.62	1.34	1.23
1	A	265	LYS	N-CA	7.51	1.55	1.46
1	A	95	GLY	C-O	7.47	1.34	1.24
1	A	25	SER	CB-OG	7.44	1.57	1.42
1	A	213	ASP	CG-OD2	7.44	1.39	1.25
1	A	139	VAL	N-CA	7.36	1.55	1.46
1	A	108	GLN	CA-C	7.33	1.61	1.52
1	A	166	GLU	C-O	-7.33	1.15	1.24
1	A	85	LYS	N-CA	-7.18	1.37	1.46
1	A	26	THR	CA-CB	7.11	1.65	1.53
1	A	145	THR	N-CA	7.10	1.55	1.46
1	A	278	THR	C-N	-7.04	1.24	1.33
1	A	91	LEU	CA-CB	-6.99	1.44	1.53
1	A	274	TYR	C-N	-6.94	1.24	1.33
1	A	11	ARG	C-N	-6.92	1.24	1.33
1	A	186	TRP	CG-CD2	6.92	1.56	1.43
1	A	252	GLY	C-O	6.92	1.33	1.24
1	A	65	SER	C-O	6.92	1.32	1.24
1	A	9	VAL	C-O	6.91	1.30	1.24
1	A	116	ASN	CG-ND2	-6.91	1.18	1.33
1	A	259	GLY	C-O	-6.89	1.15	1.23
1	A	119	GLU	CD-OE1	-6.87	1.12	1.25
1	A	164	ILE	C-O	6.86	1.31	1.24
1	A	250	HIS	ND1-CE1	-6.86	1.25	1.32
1	A	316	LYS	C-OXT	6.86	1.37	1.23
1	A	44	ALA	C-O	6.83	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	HIS	CB-CG	-6.80	1.40	1.50
1	A	192	VAL	CA-CB	6.75	1.62	1.54
1	A	101	ARG	CZ-NH2	6.75	1.42	1.33
1	A	265	LYS	CE-NZ	6.70	1.69	1.49
1	A	306	VAL	C-O	6.69	1.32	1.24
1	A	47	ARG	NE-CZ	-6.69	1.25	1.33
1	A	98	ALA	C-O	6.66	1.32	1.23
1	A	5	SER	C-O	-6.64	1.15	1.23
1	A	27	TYR	C-N	-6.63	1.23	1.33
1	A	45	LYS	C-O	6.62	1.32	1.23
1	A	300	SER	C-O	6.60	1.32	1.23
1	A	245	SER	C-O	6.58	1.31	1.24
1	A	290	GLN	C-O	6.58	1.31	1.24
1	A	3	GLY	C-O	6.57	1.31	1.23
1	A	216	HIS	ND1-CE1	6.57	1.39	1.32
1	A	148	VAL	C-O	6.55	1.31	1.24
1	A	208	PRO	N-CA	-6.54	1.38	1.47
1	A	166	GLU	CD-OE1	-6.54	1.12	1.25
1	A	190	GLU	C-O	6.53	1.31	1.24
1	A	226	ASP	C-N	-6.52	1.24	1.33
1	A	308	GLN	CD-NE2	6.51	1.47	1.33
1	A	50	LEU	C-O	-6.47	1.16	1.24
1	A	222	THR	CA-CB	6.44	1.64	1.53
1	A	115	TRP	NE1-CE2	6.43	1.44	1.37
1	A	169	SER	C-O	6.42	1.31	1.24
1	A	293	THR	CA-C	6.42	1.61	1.52
1	A	133	LEU	C-O	6.41	1.32	1.24
1	A	151	TYR	C-O	6.38	1.32	1.24
1	A	284	LEU	C-N	-6.35	1.25	1.33
1	A	96	ASN	CG-OD1	6.31	1.35	1.23
1	A	35	ARG	CA-C	-6.29	1.45	1.52
1	A	88	HIS	CG-ND1	-6.28	1.31	1.38
1	A	9	VAL	C-N	-6.25	1.25	1.33
1	A	180	ALA	N-CA	6.20	1.54	1.46
1	A	203	ARG	N-CA	-6.20	1.38	1.45
1	A	114	PHE	C-O	-6.16	1.16	1.23
1	A	168	ILE	C-O	6.14	1.30	1.24
1	A	105	HIS	ND1-CE1	6.13	1.38	1.32
1	A	25	SER	C-N	-6.12	1.25	1.33
1	A	111	ASN	N-CA	-6.11	1.38	1.46
1	A	308	GLN	CA-C	6.08	1.60	1.52
1	A	200	ASP	C-O	6.07	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	TYR	C-N	-6.07	1.25	1.33
1	A	19	ASN	C-O	6.04	1.31	1.23
1	A	216	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	174	THR	CA-CB	6.04	1.62	1.53
1	A	188	ILE	CA-CB	6.03	1.61	1.54
1	A	157	TYR	C-N	-6.03	1.26	1.33
1	A	137	ILE	CB-CG1	6.03	1.65	1.53
1	A	30	LEU	CA-CB	6.02	1.60	1.52
1	A	105	HIS	CG-CD2	6.01	1.42	1.35
1	A	278	THR	CA-CB	6.00	1.62	1.53
1	A	146	HIS	CE1-NE2	-6.00	1.26	1.32
1	A	288	ALA	CA-C	-6.00	1.45	1.52
1	A	61	GLN	CA-C	6.00	1.59	1.52
1	A	78	GLY	CA-C	5.99	1.60	1.51
1	A	98	ALA	CA-C	-5.97	1.45	1.52
1	A	14	LEU	C-O	-5.95	1.16	1.24
1	A	191	ASP	C-O	-5.94	1.16	1.24
1	A	258	ILE	C-N	5.93	1.41	1.33
1	A	182	LYS	N-CA	5.89	1.54	1.46
1	A	243	LEU	N-CA	-5.88	1.39	1.46
1	A	198	SER	N-CA	5.87	1.53	1.45
1	A	131	ILE	CA-C	5.86	1.59	1.52
1	A	271	LEU	C-O	5.86	1.30	1.24
1	A	21	ASN	CG-ND2	-5.85	1.21	1.33
1	A	295	LEU	CA-CB	5.84	1.62	1.53
1	A	12	GLY	C-N	-5.84	1.26	1.34
1	A	190	GLU	N-CA	-5.83	1.39	1.46
1	A	260	ARG	C-O	5.80	1.31	1.24
1	A	178	PHE	N-CA	-5.79	1.39	1.46
1	A	223	GLY	CA-C	5.79	1.60	1.51
1	A	98	ALA	C-N	-5.79	1.25	1.33
1	A	225	GLN	CD-OE1	5.78	1.34	1.23
1	A	238	ASN	N-CA	5.78	1.53	1.46
1	A	210	LYS	C-O	5.78	1.30	1.24
1	A	297	GLY	C-O	-5.77	1.17	1.24
1	A	152	THR	N-CA	5.77	1.53	1.45
1	A	302	GLU	CA-CB	5.76	1.62	1.53
1	A	38	GLY	CA-C	-5.75	1.44	1.52
1	A	150	ASP	N-CA	-5.74	1.39	1.46
1	A	292	ALA	C-O	-5.74	1.17	1.24
1	A	73	ALA	N-CA	5.68	1.53	1.46
1	A	232	ILE	CA-CB	5.68	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	GLY	C-O	5.65	1.31	1.24
1	A	296	TYR	C-O	5.63	1.30	1.23
1	A	114	PHE	N-CA	-5.63	1.39	1.46
1	A	142	HIS	C-O	-5.62	1.17	1.24
1	A	184	PRO	CA-CB	-5.62	1.46	1.53
1	A	58	ALA	C-N	-5.62	1.24	1.33
1	A	24	TYR	C-O	5.61	1.30	1.24
1	A	74	HIS	C-O	5.61	1.30	1.24
1	A	214	PRO	CA-CB	-5.61	1.45	1.53
1	A	168	ILE	CA-C	-5.56	1.46	1.52
1	A	102	SER	C-O	5.55	1.30	1.23
1	A	71	VAL	CA-CB	5.55	1.60	1.54
1	A	69	PRO	C-N	5.53	1.41	1.33
1	A	53	SER	CA-C	-5.53	1.46	1.52
1	A	282	SER	CA-CB	-5.51	1.44	1.53
1	A	126	ASP	C-N	-5.50	1.25	1.33
1	A	297	GLY	N-CA	-5.50	1.38	1.45
1	A	260	ARG	CD-NE	5.49	1.53	1.46
1	A	206	SER	C-N	-5.48	1.27	1.33
1	A	275	LEU	CA-CB	5.48	1.62	1.53
1	A	175	LEU	C-O	-5.47	1.17	1.24
1	A	310	PHE	N-CA	5.47	1.53	1.46
1	A	79	VAL	C-N	-5.46	1.26	1.33
1	A	44	ALA	CA-CB	-5.46	1.44	1.53
1	A	246	GLN	C-O	5.45	1.31	1.24
1	A	79	VAL	C-O	5.45	1.30	1.24
1	A	58	ALA	CA-CB	5.45	1.62	1.53
1	A	261	ASP	C-N	-5.42	1.26	1.33
1	A	307	LYS	N-CA	5.42	1.52	1.46
1	A	22	THR	C-N	-5.41	1.26	1.33
1	A	98	ALA	N-CA	5.36	1.52	1.46
1	A	315	VAL	C-N	5.35	1.40	1.33
1	A	304	ALA	C-O	-5.31	1.18	1.24
1	A	132	PRO	N-CD	5.30	1.55	1.47
1	A	115	TRP	C-O	5.29	1.30	1.24
1	A	305	SER	C-O	5.29	1.30	1.24
1	A	245	SER	C-N	-5.29	1.25	1.33
1	A	250	HIS	N-CA	5.29	1.52	1.46
1	A	93	TYR	CA-C	-5.28	1.45	1.52
1	A	2	THR	N-CA	5.28	1.52	1.46
1	A	4	THR	CA-CB	5.26	1.61	1.53
1	A	107	SER	CA-CB	-5.26	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	ASN	C-N	-5.25	1.26	1.33
1	A	299	THR	N-CA	-5.21	1.39	1.46
1	A	64	ALA	C-N	-5.20	1.26	1.33
1	A	68	ALA	C-O	5.20	1.30	1.24
1	A	259	GLY	CA-C	-5.20	1.47	1.52
1	A	65	SER	N-CA	5.20	1.52	1.46
1	A	212	GLY	C-N	-5.18	1.22	1.33
1	A	184	PRO	CA-C	-5.17	1.46	1.52
1	A	55	TRP	C-O	5.17	1.30	1.24
1	A	136	GLY	C-O	5.14	1.30	1.23
1	A	182	LYS	C-O	5.12	1.31	1.23
1	A	201	SER	C-O	-5.12	1.18	1.23
1	A	9	VAL	CA-CB	5.09	1.62	1.54
1	A	289	VAL	CA-C	5.09	1.59	1.52
1	A	55	TRP	NE1-CE2	5.08	1.43	1.37
1	A	34	THR	CA-CB	5.06	1.62	1.53
1	A	285	ARG	CZ-NH2	-5.06	1.26	1.33
1	A	182	LYS	CE-NZ	5.04	1.64	1.49
1	A	166	GLU	N-CA	5.03	1.52	1.46
1	A	297	GLY	CA-C	5.03	1.58	1.52
1	A	11	ARG	CZ-NH2	5.03	1.40	1.33
1	A	38	GLY	N-CA	-5.02	1.39	1.45
1	A	270	ALA	N-CA	-5.01	1.40	1.46
1	A	168	ILE	CA-CB	5.01	1.60	1.54
1	A	237	ILE	C-N	-5.01	1.27	1.33

All (570) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	LYS	CG-CD-CE	22.52	163.09	111.30
1	A	47	ARG	CD-NE-CZ	22.22	155.50	124.40
1	A	101	ARG	CD-NE-CZ	22.19	155.47	124.40
1	A	168	ILE	CB-CG1-CD1	21.47	158.89	113.80
1	A	264	GLY	CA-C-O	20.23	140.63	120.80
1	A	38	GLY	CA-C-O	-16.51	107.38	122.57
1	A	56	ALA	CA-C-O	14.78	136.32	120.36
1	A	66	TYR	CA-C-N	14.34	142.11	120.31
1	A	66	TYR	C-N-CA	14.34	142.11	120.31
1	A	37	ASP	CA-C-N	13.62	141.82	122.06
1	A	37	ASP	C-N-CA	13.62	141.82	122.06
1	A	260	ARG	CA-C-N	13.62	138.96	120.44
1	A	260	ARG	C-N-CA	13.62	138.96	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	GLY	O-C-N	-13.56	111.79	123.59
1	A	101	ARG	CA-CB-CG	13.54	141.19	114.10
1	A	113	ALA	CA-C-N	13.38	146.10	121.62
1	A	113	ALA	C-N-CA	13.38	146.10	121.62
1	A	270	ALA	CA-C-O	13.34	134.44	120.70
1	A	206	SER	CA-C-N	13.25	134.69	122.37
1	A	206	SER	C-N-CA	13.25	134.69	122.37
1	A	301	GLN	OE1-CD-NE2	-12.78	109.82	122.60
1	A	300	SER	CA-C-N	12.39	137.29	120.44
1	A	300	SER	C-N-CA	12.39	137.29	120.44
1	A	103	SER	CA-C-O	-12.37	106.44	120.66
1	A	312	ALA	CA-C-N	12.27	141.34	121.09
1	A	312	ALA	C-N-CA	12.27	141.34	121.09
1	A	227	ASN	O-C-N	12.12	138.64	122.41
1	A	11	ARG	CD-NE-CZ	-12.10	107.46	124.40
1	A	308	GLN	CG-CD-OE1	12.09	144.97	120.80
1	A	53	SER	CA-C-O	-12.03	107.96	120.71
1	A	70	ALA	CA-C-O	11.99	133.13	120.42
1	A	263	LEU	O-C-N	-11.49	110.23	122.07
1	A	308	GLN	CG-CD-NE2	-11.47	99.19	116.40
1	A	261	ASP	CA-CB-CG	-11.18	101.42	112.60
1	A	297	GLY	CA-C-N	11.17	142.87	121.54
1	A	297	GLY	C-N-CA	11.17	142.87	121.54
1	A	101	ARG	CB-CA-C	11.16	131.46	109.35
1	A	288	ALA	CA-C-N	11.10	134.55	120.56
1	A	288	ALA	C-N-CA	11.10	134.55	120.56
1	A	197	ILE	CA-C-O	11.09	135.56	121.48
1	A	47	ARG	NE-CZ-NH1	11.05	132.56	121.50
1	A	223	GLY	CA-C-N	10.99	141.26	122.36
1	A	223	GLY	C-N-CA	10.99	141.26	122.36
1	A	44	ALA	CA-C-N	10.97	137.76	122.07
1	A	44	ALA	C-N-CA	10.97	137.76	122.07
1	A	39	ILE	CA-C-N	10.96	138.13	123.00
1	A	39	ILE	C-N-CA	10.96	138.13	123.00
1	A	204	SER	CA-C-O	-10.94	109.11	120.71
1	A	236	ILE	CA-C-N	10.85	135.83	120.42
1	A	236	ILE	C-N-CA	10.85	135.83	120.42
1	A	163	ALA	CA-C-N	10.78	134.15	120.56
1	A	163	ALA	C-N-CA	10.78	134.15	120.56
1	A	101	ARG	CG-CD-NE	-10.74	88.36	112.00
1	A	264	GLY	O-C-N	-10.69	111.80	122.17
1	A	224	THR	N-CA-C	10.65	126.97	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	VAL	O-C-N	10.60	135.02	122.62
1	A	119	GLU	N-CA-CB	-10.57	95.49	111.56
1	A	18	LYS	O-C-N	10.50	134.66	123.42
1	A	9	VAL	CA-C-O	-10.47	108.94	120.67
1	A	270	ALA	O-C-N	-10.45	110.80	122.09
1	A	242	TYR	CA-C-N	10.40	135.06	120.29
1	A	242	TYR	C-N-CA	10.40	135.06	120.29
1	A	148	VAL	CA-C-O	-10.36	110.21	121.29
1	A	112	ASN	OD1-CG-ND2	-10.33	112.27	122.60
1	A	166	GLU	CA-C-O	-10.30	109.50	120.42
1	A	56	ALA	O-C-N	-10.09	111.29	123.30
1	A	120	MET	CG-SD-CE	10.06	123.03	100.90
1	A	113	ALA	CA-C-O	-10.05	110.47	121.33
1	A	218	SER	CA-C-N	10.05	139.64	122.26
1	A	218	SER	C-N-CA	10.05	139.64	122.26
1	A	88	HIS	CA-CB-CG	-9.99	103.81	113.80
1	A	169	SER	O-C-N	-9.96	111.56	122.12
1	A	45	LYS	CB-CA-C	-9.95	97.28	111.80
1	A	61	GLN	O-C-N	9.92	134.78	123.27
1	A	101	ARG	CA-C-N	9.87	139.35	122.37
1	A	101	ARG	C-N-CA	9.87	139.35	122.37
1	A	148	VAL	N-CA-CB	9.83	121.34	110.62
1	A	103	SER	O-C-N	9.81	135.24	123.27
1	A	220	ARG	O-C-N	-9.79	111.38	123.12
1	A	257	GLY	CA-C-O	-9.79	112.64	121.64
1	A	49	THR	CA-C-O	-9.78	109.15	120.49
1	A	115	TRP	CA-C-O	-9.70	109.64	120.32
1	A	164	ILE	N-CA-C	-9.69	101.12	110.42
1	A	282	SER	CB-CA-C	9.69	127.31	110.85
1	A	256	VAL	CA-C-O	-9.67	109.78	120.71
1	A	143	GLU	CG-CD-OE1	9.62	140.53	118.40
1	A	306	VAL	CA-C-O	9.61	130.85	120.47
1	A	39	ILE	CB-CG1-CD1	9.57	133.90	113.80
1	A	73	ALA	CA-C-O	9.55	130.85	120.82
1	A	238	ASN	CA-C-N	9.52	132.82	120.44
1	A	238	ASN	C-N-CA	9.52	132.82	120.44
1	A	136	GLY	O-C-N	-9.49	117.37	123.35
1	A	38	GLY	O-C-N	9.45	133.54	122.68
1	A	126	ASP	CA-C-O	-9.35	108.06	119.18
1	A	260	ARG	NE-CZ-NH2	-9.31	110.82	119.20
1	A	198	SER	CB-CA-C	9.27	127.59	109.33
1	A	49	THR	O-C-N	9.26	134.41	123.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	VAL	CA-C-N	9.23	132.99	120.44
1	A	303	VAL	C-N-CA	9.23	132.99	120.44
1	A	38	GLY	N-CA-C	9.20	126.43	112.81
1	A	116	ASN	CA-C-O	-9.19	108.81	119.56
1	A	254	SER	CA-CB-OG	9.17	129.44	111.10
1	A	165	ASN	OD1-CG-ND2	-9.16	113.44	122.60
1	A	127	GLY	O-C-N	9.10	133.09	122.45
1	A	184	PRO	CA-C-O	-9.08	110.86	122.12
1	A	261	ASP	N-CA-CB	-9.05	96.94	110.07
1	A	9	VAL	CB-CA-C	-8.99	96.65	110.50
1	A	295	LEU	N-CA-C	8.99	122.75	111.69
1	A	140	VAL	O-C-N	-8.99	113.10	121.91
1	A	258	ILE	O-C-N	-8.98	113.43	122.14
1	A	227	ASN	CA-C-O	-8.93	110.65	121.28
1	A	49	THR	CA-CB-OG1	-8.90	96.24	109.60
1	A	262	LYS	CA-C-O	-8.83	111.06	120.42
1	A	162	GLY	O-C-N	-8.82	111.59	122.71
1	A	149	THR	CA-C-O	8.78	130.12	120.63
1	A	7	VAL	CA-C-O	-8.78	111.05	120.36
1	A	116	ASN	OD1-CG-ND2	-8.78	113.82	122.60
1	A	142	HIS	CA-C-N	8.72	132.68	120.29
1	A	142	HIS	C-N-CA	8.72	132.68	120.29
1	A	130	PHE	CA-C-O	-8.71	111.56	121.40
1	A	89	ASN	CA-CB-CG	-8.71	103.89	112.60
1	A	291	SER	O-C-N	8.66	132.02	122.15
1	A	260	ARG	N-CA-C	8.62	123.58	112.89
1	A	294	ASP	CA-C-N	8.59	135.26	120.58
1	A	294	ASP	C-N-CA	8.59	135.26	120.58
1	A	70	ALA	O-C-N	-8.57	112.38	122.15
1	A	184	PRO	O-C-N	8.57	133.60	123.14
1	A	30	LEU	CA-C-N	8.56	135.01	122.86
1	A	30	LEU	C-N-CA	8.56	135.01	122.86
1	A	84	TYR	CA-C-O	8.53	129.59	120.55
1	A	288	ALA	CB-CA-C	8.52	124.94	110.79
1	A	18	LYS	CG-CD-CE	8.49	130.83	111.30
1	A	159	ASN	OD1-CG-ND2	-8.47	114.13	122.60
1	A	78	GLY	CA-C-O	-8.46	105.84	120.57
1	A	156	ILE	CA-CB-CG2	8.45	124.86	110.50
1	A	225	GLN	CB-CA-C	8.45	128.61	110.19
1	A	45	LYS	CA-C-O	-8.42	111.77	121.54
1	A	301	GLN	CG-CD-OE1	8.40	137.61	120.80
1	A	170	ASP	CA-CB-CG	8.40	121.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	ALA	CA-C-O	8.35	129.40	120.55
1	A	131	ILE	N-CA-CB	8.33	122.88	111.21
1	A	96	ASN	O-C-N	8.31	133.65	122.26
1	A	259	GLY	CA-C-O	8.29	129.01	122.29
1	A	101	ARG	CB-CG-CD	8.28	130.35	111.30
1	A	197	ILE	O-C-N	-8.27	113.26	122.69
1	A	174	THR	CA-C-N	8.27	131.36	120.28
1	A	174	THR	C-N-CA	8.27	131.36	120.28
1	A	158	GLN	OE1-CD-NE2	8.26	130.86	122.60
1	A	71	VAL	CA-C-N	8.24	132.00	120.29
1	A	71	VAL	C-N-CA	8.24	132.00	120.29
1	A	265	LYS	O-C-N	-8.24	111.51	122.23
1	A	301	GLN	N-CA-C	-8.24	102.24	111.14
1	A	142	HIS	CA-C-O	8.24	129.28	120.55
1	A	224	THR	CA-C-N	-8.23	105.60	121.06
1	A	224	THR	C-N-CA	-8.23	105.60	121.06
1	A	45	LYS	O-C-N	8.22	133.17	122.40
1	A	17	GLN	CA-C-O	8.19	129.89	120.80
1	A	82	ASP	CA-C-O	-8.19	111.74	120.42
1	A	209	ALA	CA-C-N	8.18	131.59	120.38
1	A	209	ALA	C-N-CA	8.18	131.59	120.38
1	A	271	LEU	CA-C-O	-8.17	111.89	120.55
1	A	133	LEU	CA-C-O	-8.10	109.69	119.49
1	A	89	ASN	OD1-CG-ND2	8.06	130.66	122.60
1	A	229	GLY	CA-C-N	8.06	131.50	120.46
1	A	229	GLY	C-N-CA	8.06	131.50	120.46
1	A	108	GLN	CG-CD-OE1	-8.05	104.70	120.80
1	A	293	THR	CA-C-O	-8.02	111.92	120.42
1	A	270	ALA	N-CA-C	-8.02	102.48	111.14
1	A	283	GLN	CA-CB-CG	-8.01	98.08	114.10
1	A	177	GLU	O-C-N	-7.97	113.68	122.12
1	A	121	VAL	CA-CB-CG2	-7.94	96.91	110.40
1	A	139	VAL	N-CA-C	-7.93	102.97	110.42
1	A	108	GLN	O-C-N	7.92	132.46	123.27
1	A	170	ASP	N-CA-C	-7.90	101.97	111.69
1	A	89	ASN	CA-C-N	-7.89	111.48	122.93
1	A	89	ASN	C-N-CA	-7.89	111.48	122.93
1	A	133	LEU	N-CA-C	7.89	122.01	112.38
1	A	138	ASP	CA-C-N	7.89	130.35	120.72
1	A	138	ASP	C-N-CA	7.89	130.35	120.72
1	A	166	GLU	CB-CG-CD	-7.86	99.25	112.60
1	A	2	THR	O-C-N	-7.80	114.16	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SER	N-CA-CB	-7.78	97.77	111.08
1	A	96	ASN	CA-CB-CG	-7.77	104.83	112.60
1	A	90	ARG	NE-CZ-NH1	7.73	129.23	121.50
1	A	130	PHE	O-C-N	7.71	132.49	123.17
1	A	229	GLY	N-CA-C	7.69	127.61	113.76
1	A	145	THR	O-C-N	-7.68	113.24	122.22
1	A	263	LEU	CA-C-N	7.67	128.62	120.03
1	A	263	LEU	C-N-CA	7.67	128.62	120.03
1	A	96	ASN	OD1-CG-ND2	7.60	130.20	122.60
1	A	174	THR	OG1-CB-CG2	7.54	124.39	109.30
1	A	149	THR	CA-C-N	7.51	130.34	120.28
1	A	149	THR	C-N-CA	7.51	130.34	120.28
1	A	75	TYR	N-CA-C	7.48	119.51	111.36
1	A	93	TYR	CA-C-O	7.47	128.67	119.11
1	A	21	ASN	CA-CB-CG	-7.46	105.14	112.60
1	A	53	SER	CA-CB-OG	-7.45	96.19	111.10
1	A	201	SER	CA-C-O	-7.45	113.31	121.28
1	A	76	TYR	CA-C-O	-7.43	111.42	119.97
1	A	79	VAL	CA-C-O	-7.42	112.63	120.57
1	A	7	VAL	CA-C-N	-7.41	114.52	122.67
1	A	7	VAL	C-N-CA	-7.41	114.52	122.67
1	A	293	THR	CB-CA-C	-7.40	98.28	110.85
1	A	231	HIS	N-CA-CB	7.39	121.43	110.49
1	A	96	ASN	CA-C-O	-7.39	111.20	119.78
1	A	5	SER	N-CA-CB	7.38	121.21	110.06
1	A	265	LYS	N-CA-CB	-7.37	99.22	110.20
1	A	11	ARG	CA-C-O	-7.36	112.91	120.71
1	A	234	SER	O-C-N	-7.32	113.66	122.22
1	A	20	ILE	CA-C-O	-7.31	113.53	121.28
1	A	123	GLY	N-CA-C	-7.30	101.35	112.89
1	A	96	ASN	CB-CA-C	-7.29	98.89	110.85
1	A	205	MET	N-CA-CB	7.29	121.26	110.33
1	A	25	SER	CA-CB-OG	-7.28	96.54	111.10
1	A	161	SER	N-CA-C	-7.27	103.39	111.82
1	A	114	PHE	CA-C-O	7.25	128.99	121.23
1	A	11	ARG	NE-CZ-NH2	-7.25	112.67	119.20
1	A	53	SER	CB-CA-C	-7.24	96.35	109.38
1	A	81	TYR	N-CA-C	-7.22	103.48	111.36
1	A	211	TYR	CA-CB-CG	-7.22	100.91	113.90
1	A	105	HIS	O-C-N	7.22	131.24	122.58
1	A	154	GLY	CA-C-N	7.21	132.73	121.26
1	A	154	GLY	C-N-CA	7.21	132.73	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	PHE	N-CA-C	7.21	119.14	111.28
1	A	37	ASP	CA-CB-CG	7.20	119.80	112.60
1	A	290	GLN	CA-CB-CG	-7.19	99.72	114.10
1	A	178	PHE	CA-C-N	7.19	130.22	120.38
1	A	178	PHE	C-N-CA	7.19	130.22	120.38
1	A	290	GLN	CA-C-N	7.19	130.50	120.29
1	A	290	GLN	C-N-CA	7.19	130.50	120.29
1	A	220	ARG	NH1-CZ-NH2	7.17	128.62	119.30
1	A	162	GLY	CA-C-O	7.15	127.89	119.45
1	A	156	ILE	CB-CG1-CD1	-7.15	98.79	113.80
1	A	122	TYR	O-C-N	7.13	131.66	123.31
1	A	68	ALA	O-C-N	-7.12	113.13	121.32
1	A	235	GLY	CA-C-N	7.12	129.53	120.56
1	A	235	GLY	C-N-CA	7.12	129.53	120.56
1	A	101	ARG	N-CA-CB	-7.07	98.20	111.00
1	A	261	ASP	N-CA-C	-7.04	103.53	111.14
1	A	163	ALA	N-CA-C	-7.04	103.03	111.69
1	A	198	SER	CA-C-O	7.04	129.06	121.11
1	A	297	GLY	O-C-N	7.04	129.02	122.47
1	A	50	LEU	CA-C-O	-7.01	111.91	120.54
1	A	219	LYS	CB-CG-CD	7.01	127.43	111.30
1	A	211	TYR	CB-CA-C	-7.01	98.88	110.72
1	A	98	ALA	CA-C-O	-7.00	114.13	121.55
1	A	273	GLN	OE1-CD-NE2	-6.99	115.61	122.60
1	A	182	LYS	CB-CA-C	6.98	121.72	111.88
1	A	307	LYS	CA-C-N	6.98	129.97	120.54
1	A	307	LYS	C-N-CA	6.98	129.97	120.54
1	A	308	GLN	OE1-CD-NE2	-6.98	115.62	122.60
1	A	167	ALA	O-C-N	-6.97	114.06	122.22
1	A	146	HIS	ND1-CG-CD2	-6.97	99.13	106.10
1	A	190	GLU	CA-C-N	6.97	132.53	120.68
1	A	190	GLU	C-N-CA	6.97	132.53	120.68
1	A	129	THR	N-CA-C	-6.97	103.12	111.69
1	A	172	PHE	CA-CB-CG	-6.97	106.83	113.80
1	A	11	ARG	NH1-CZ-NH2	6.97	128.36	119.30
1	A	35	ARG	CA-C-O	-6.95	112.86	120.30
1	A	293	THR	O-C-N	6.95	130.07	122.15
1	A	209	ALA	N-CA-C	6.93	120.84	112.38
1	A	108	GLN	CG-CD-NE2	6.93	126.80	116.40
1	A	5	SER	CA-C-O	-6.92	113.16	121.05
1	A	225	GLN	OE1-CD-NE2	-6.92	115.69	122.60
1	A	212	GLY	CA-C-O	-6.91	110.46	119.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	SER	CA-C-N	6.90	134.72	121.54
1	A	25	SER	C-N-CA	6.90	134.72	121.54
1	A	175	LEU	CA-C-O	6.89	127.86	120.55
1	A	305	SER	CA-C-O	-6.88	112.33	120.10
1	A	101	ARG	NE-CZ-NH1	6.88	128.38	121.50
1	A	194	THR	O-C-N	6.88	129.23	121.32
1	A	223	GLY	O-C-N	6.88	131.64	122.70
1	A	58	ALA	CA-C-N	6.87	132.71	121.99
1	A	58	ALA	C-N-CA	6.87	132.71	121.99
1	A	16	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	298	SER	N-CA-CB	-6.86	98.89	110.49
1	A	104	VAL	CA-C-O	-6.86	113.89	121.92
1	A	161	SER	O-C-N	-6.85	113.84	122.27
1	A	275	LEU	CA-C-O	-6.84	113.61	121.47
1	A	100	ILE	CA-C-O	-6.80	113.30	120.57
1	A	105	HIS	CB-CA-C	-6.79	102.76	111.86
1	A	126	ASP	N-CA-CB	6.79	121.11	110.46
1	A	181	ASN	CA-C-O	6.78	129.38	120.98
1	A	35	ARG	O-C-N	6.78	131.13	123.27
1	A	282	SER	N-CA-CB	-6.77	100.14	110.16
1	A	282	SER	N-CA-C	-6.76	103.99	111.36
1	A	93	TYR	N-CA-C	6.75	121.35	113.18
1	A	302	GLU	CA-C-O	6.74	127.69	120.55
1	A	21	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	A	290	GLN	CA-C-O	-6.73	113.42	120.55
1	A	128	GLN	CA-CB-CG	-6.72	100.65	114.10
1	A	197	ILE	CA-C-N	-6.72	112.26	122.81
1	A	197	ILE	C-N-CA	-6.72	112.26	122.81
1	A	147	ALA	N-CA-CB	-6.72	100.27	110.01
1	A	181	ASN	CA-CB-CG	6.72	119.32	112.60
1	A	149	THR	O-C-N	-6.71	115.01	122.12
1	A	287	ALA	CA-C-O	-6.71	113.79	120.70
1	A	272	THR	N-CA-C	6.67	121.50	113.23
1	A	65	SER	CB-CA-C	6.65	122.16	110.85
1	A	61	GLN	CA-CB-CG	-6.65	100.80	114.10
1	A	259	GLY	O-C-N	-6.65	114.94	122.78
1	A	217	TYR	CA-C-O	6.64	127.60	120.10
1	A	41	THR	CA-CB-OG1	-6.63	99.66	109.60
1	A	130	PHE	CB-CA-C	-6.62	95.50	110.07
1	A	48	THR	CA-C-O	6.62	127.20	119.32
1	A	57	ASP	CA-CB-CG	-6.62	105.98	112.60
1	A	176	VAL	N-CA-C	-6.62	104.31	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	A	288	ALA	O-C-N	-6.59	115.14	122.12
1	A	86	ASN	CA-C-N	6.58	131.39	121.65
1	A	86	ASN	C-N-CA	6.58	131.39	121.65
1	A	85	LYS	CA-CB-CG	-6.57	100.96	114.10
1	A	245	SER	CA-C-N	6.57	133.61	121.52
1	A	245	SER	C-N-CA	6.57	133.61	121.52
1	A	266	ILE	O-C-N	-6.55	115.09	121.83
1	A	146	HIS	CA-C-N	6.54	128.94	120.44
1	A	146	HIS	C-N-CA	6.54	128.94	120.44
1	A	147	ALA	CB-CA-C	6.54	121.14	110.88
1	A	117	GLY	N-CA-C	-6.53	106.92	114.69
1	A	147	ALA	O-C-N	6.52	128.79	122.07
1	A	82	ASP	O-C-N	6.52	129.58	122.15
1	A	275	LEU	O-C-N	6.51	130.32	122.96
1	A	117	GLY	CA-C-N	-6.49	110.12	120.70
1	A	117	GLY	C-N-CA	-6.49	110.12	120.70
1	A	126	ASP	O-C-N	6.48	131.61	122.41
1	A	266	ILE	N-CA-C	-6.48	104.18	110.72
1	A	85	LYS	CA-C-O	6.48	127.43	120.24
1	A	138	ASP	OD1-CG-OD2	-6.47	107.36	122.90
1	A	268	TYR	O-C-N	-6.46	114.32	122.27
1	A	75	TYR	N-CA-CB	-6.46	100.60	110.16
1	A	48	THR	O-C-N	-6.45	114.43	122.24
1	A	179	TYR	O-C-N	6.45	128.96	122.12
1	A	309	ALA	CB-CA-C	6.43	120.98	110.88
1	A	302	GLU	O-C-N	-6.43	115.31	122.12
1	A	106	TYR	N-CA-CB	-6.42	99.56	110.16
1	A	158	GLN	O-C-N	6.42	130.66	123.48
1	A	117	GLY	CA-C-O	6.40	126.12	119.27
1	A	146	HIS	N-CA-CB	6.39	119.51	110.12
1	A	237	ILE	CA-CB-CG1	-6.39	99.54	110.40
1	A	4	THR	CB-CA-C	6.37	120.05	109.53
1	A	169	SER	CA-C-N	6.37	131.47	120.58
1	A	169	SER	C-N-CA	6.37	131.47	120.58
1	A	239	LYS	N-CA-C	-6.35	104.28	111.07
1	A	143	GLU	CG-CD-OE2	-6.34	103.83	118.40
1	A	295	LEU	CA-C-N	6.32	132.48	122.11
1	A	295	LEU	C-N-CA	6.32	132.48	122.11
1	A	115	TRP	N-CA-C	-6.32	98.22	108.52
1	A	188	ILE	N-CA-C	6.31	116.94	107.80
1	A	27	TYR	CB-CG-CD2	-6.30	111.35	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	THR	CA-C-N	6.30	130.85	121.72
1	A	48	THR	C-N-CA	6.30	130.85	121.72
1	A	33	ASN	N-CA-C	6.29	120.95	113.28
1	A	313	VAL	CA-C-O	6.28	127.21	119.43
1	A	165	ASN	CA-CB-CG	6.26	118.86	112.60
1	A	120	MET	CA-C-N	6.24	131.67	122.99
1	A	120	MET	C-N-CA	6.24	131.67	122.99
1	A	87	VAL	CA-C-N	-6.23	112.88	122.60
1	A	87	VAL	C-N-CA	-6.23	112.88	122.60
1	A	114	PHE	CA-C-N	6.23	131.77	123.05
1	A	114	PHE	C-N-CA	6.23	131.77	123.05
1	A	130	PHE	CA-CB-CG	-6.21	107.59	113.80
1	A	135	GLY	CA-C-O	6.21	129.25	119.31
1	A	55	TRP	CA-C-N	6.17	131.69	122.99
1	A	55	TRP	C-N-CA	6.17	131.69	122.99
1	A	199	GLY	CA-C-O	-6.16	112.18	119.02
1	A	289	VAL	N-CA-CB	6.15	117.74	110.55
1	A	115	TRP	CD2-CE3-CZ3	6.14	126.58	118.60
1	A	265	LYS	CB-CG-CD	-6.12	97.22	111.30
1	A	62	PHE	CA-CB-CG	-6.11	107.69	113.80
1	A	220	ARG	CA-C-N	6.10	131.14	122.72
1	A	220	ARG	C-N-CA	6.10	131.14	122.72
1	A	27	TYR	CZ-CE2-CD2	-6.08	108.66	119.60
1	A	242	TYR	CA-C-O	-6.08	113.98	120.42
1	A	215	ASP	N-CA-C	-6.07	103.98	113.02
1	A	306	VAL	O-C-N	-6.07	114.94	121.80
1	A	121	VAL	N-CA-CB	-6.06	102.68	111.52
1	A	155	LEU	CA-C-O	-6.05	114.26	120.80
1	A	126	ASP	CA-CB-CG	-6.05	106.55	112.60
1	A	224	THR	CA-CB-OG1	-6.05	100.53	109.60
1	A	60	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	A	119	GLU	CA-C-O	-6.03	114.47	121.10
1	A	265	LYS	CA-CB-CG	6.03	126.16	114.10
1	A	273	GLN	CA-CB-CG	6.03	126.16	114.10
1	A	114	PHE	N-CA-C	6.01	117.99	108.79
1	A	116	ASN	CB-CG-ND2	6.01	125.42	116.40
1	A	211	TYR	CB-CG-CD2	-6.01	111.79	120.80
1	A	159	ASN	CB-CG-OD1	6.01	132.81	120.80
1	A	142	HIS	O-C-N	-5.98	115.78	122.12
1	A	219	LYS	CA-C-O	5.98	125.97	119.15
1	A	274	TYR	N-CA-CB	-5.97	101.87	110.65
1	A	278	THR	CA-C-N	5.96	129.31	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	THR	C-N-CA	5.96	129.31	120.90
1	A	67	ASP	CB-CG-OD1	5.92	132.03	118.40
1	A	26	THR	CB-CA-C	5.92	122.20	110.42
1	A	64	ALA	O-C-N	-5.92	116.10	122.85
1	A	111	ASN	CA-CB-CG	5.92	118.52	112.60
1	A	304	ALA	CA-C-O	-5.91	114.61	120.70
1	A	85	LYS	N-CA-CB	-5.91	101.39	110.20
1	A	273	GLN	CB-CG-CD	5.91	122.64	112.60
1	A	260	ARG	CA-C-O	-5.90	111.99	119.31
1	A	90	ARG	CG-CD-NE	-5.90	99.03	112.00
1	A	183	ASN	N-CA-CB	-5.89	99.88	110.37
1	A	119	GLU	CB-CG-CD	5.89	122.61	112.60
1	A	72	ASP	CA-C-O	-5.88	114.18	120.42
1	A	119	GLU	CA-C-N	5.88	131.41	122.65
1	A	119	GLU	C-N-CA	5.88	131.41	122.65
1	A	250	HIS	ND1-CG-CD2	-5.88	100.22	106.10
1	A	138	ASP	CA-C-O	-5.86	113.48	120.10
1	A	263	LEU	N-CA-C	-5.86	104.80	111.07
1	A	47	ARG	CA-C-N	5.85	131.56	122.49
1	A	47	ARG	C-N-CA	5.85	131.56	122.49
1	A	214	PRO	CA-C-O	-5.84	114.79	121.56
1	A	173	GLY	N-CA-C	-5.83	105.55	113.37
1	A	108	GLN	OE1-CD-NE2	5.81	128.41	122.60
1	A	191	ASP	CA-C-N	5.79	129.45	122.16
1	A	191	ASP	C-N-CA	5.79	129.45	122.16
1	A	47	ARG	NH1-CZ-NH2	-5.79	111.78	119.30
1	A	190	GLU	CB-CG-CD	-5.77	102.79	112.60
1	A	1	ILE	CA-CB-CG1	-5.77	100.60	110.40
1	A	170	ASP	CA-C-O	-5.76	113.84	120.24
1	A	275	LEU	CB-CA-C	5.75	120.04	109.46
1	A	193	TYR	N-CA-C	5.75	119.29	110.20
1	A	291	SER	CB-CA-C	-5.75	101.08	110.85
1	A	101	ARG	N-CA-C	-5.75	99.64	109.24
1	A	165	ASN	N-CA-C	5.74	117.21	111.07
1	A	126	ASP	N-CA-C	-5.74	106.28	113.28
1	A	182	LYS	CB-CG-CD	5.74	124.49	111.30
1	A	262	LYS	N-CA-CB	5.73	118.64	110.16
1	A	237	ILE	CB-CG1-CD1	-5.71	101.81	113.80
1	A	103	SER	CA-CB-OG	5.70	122.51	111.10
1	A	45	LYS	CB-CG-CD	5.70	124.41	111.30
1	A	261	ASP	OD1-CG-OD2	5.70	136.57	122.90
1	A	268	TYR	CA-C-O	5.68	126.50	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ALA	CB-CA-C	-5.67	101.94	110.90
1	A	236	ILE	O-C-N	-5.67	116.36	121.91
1	A	154	GLY	O-C-N	-5.67	116.29	122.41
1	A	244	ILE	N-CA-C	5.66	116.40	110.62
1	A	174	THR	CA-CB-OG1	-5.66	101.11	109.60
1	A	288	ALA	N-CA-CB	-5.65	101.82	110.12
1	A	236	ILE	CB-CG1-CD1	5.64	125.64	113.80
1	A	260	ARG	CA-CB-CG	5.63	125.37	114.10
1	A	265	LYS	CD-CE-NZ	-5.63	93.88	111.90
1	A	276	THR	CA-C-O	5.62	126.62	120.94
1	A	19	ASN	CA-CB-CG	-5.62	106.98	112.60
1	A	292	ALA	N-CA-CB	5.61	118.15	110.01
1	A	240	ALA	CA-C-O	-5.61	114.93	120.82
1	A	17	GLN	CG-CD-OE1	5.59	131.98	120.80
1	A	54	LEU	N-CA-C	-5.58	102.14	110.23
1	A	18	LYS	CA-C-O	-5.57	115.27	121.23
1	A	260	ARG	NH1-CZ-NH2	5.56	126.53	119.30
1	A	174	THR	O-C-N	-5.56	115.81	122.15
1	A	180	ALA	CB-CA-C	5.56	120.40	109.72
1	A	266	ILE	CA-C-N	5.56	127.73	120.28
1	A	266	ILE	C-N-CA	5.56	127.73	120.28
1	A	285	ARG	O-C-N	5.55	127.78	122.07
1	A	45	LYS	N-CA-CB	5.53	120.08	111.84
1	A	24	TYR	CG-CD1-CE1	5.53	129.49	121.20
1	A	85	LYS	O-C-N	-5.53	115.04	122.23
1	A	240	ALA	CB-CA-C	-5.52	102.22	110.88
1	A	227	ASN	CB-CG-ND2	5.51	124.67	116.40
1	A	245	SER	CA-C-O	-5.51	115.01	120.80
1	A	18	LYS	CA-C-N	5.51	130.25	122.09
1	A	18	LYS	C-N-CA	5.51	130.25	122.09
1	A	106	TYR	CA-C-N	5.50	132.05	121.54
1	A	106	TYR	C-N-CA	5.50	132.05	121.54
1	A	149	THR	CA-CB-CG2	5.50	119.84	110.50
1	A	101	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	A	65	SER	CA-CB-OG	-5.48	100.13	111.10
1	A	201	SER	O-C-N	5.47	128.76	123.29
1	A	129	THR	O-C-N	-5.47	115.12	122.23
1	A	96	ASN	CA-C-N	-5.46	115.11	123.47
1	A	96	ASN	C-N-CA	-5.46	115.11	123.47
1	A	39	ILE	CA-C-O	-5.46	114.71	120.39
1	A	289	VAL	CB-CA-C	-5.46	104.98	111.97
1	A	90	ARG	NE-CZ-NH2	-5.45	114.30	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	A	97	ASN	CA-CB-CG	-5.43	107.17	112.60
1	A	97	ASN	OD1-CG-ND2	5.42	128.02	122.60
1	A	67	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	49	THR	N-CA-CB	-5.41	101.05	109.87
1	A	240	ALA	N-CA-CB	5.41	117.85	110.01
1	A	293	THR	N-CA-CB	5.40	118.16	110.16
1	A	76	TYR	CA-C-N	5.40	127.96	120.29
1	A	76	TYR	C-N-CA	5.40	127.96	120.29
1	A	207	ASP	CA-C-O	-5.40	116.27	121.34
1	A	291	SER	CA-CB-OG	-5.39	100.32	111.10
1	A	33	ASN	N-CA-CB	-5.38	102.01	110.46
1	A	75	TYR	CA-C-N	5.38	128.50	120.31
1	A	75	TYR	C-N-CA	5.38	128.50	120.31
1	A	114	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	294	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	298	SER	CA-C-O	5.38	128.20	120.51
1	A	145	THR	CA-C-N	5.36	127.46	120.28
1	A	145	THR	C-N-CA	5.36	127.46	120.28
1	A	22	THR	CA-CB-CG2	5.35	119.59	110.50
1	A	202	LEU	CA-C-N	5.33	130.85	122.21
1	A	202	LEU	C-N-CA	5.33	130.85	122.21
1	A	28	TYR	N-CA-C	-5.33	100.03	108.73
1	A	213	ASP	CB-CA-C	5.32	116.37	108.87
1	A	92	SER	CA-C-N	-5.32	111.21	121.58
1	A	92	SER	C-N-CA	-5.32	111.21	121.58
1	A	292	ALA	N-CA-C	-5.31	105.39	111.07
1	A	228	GLY	O-C-N	5.30	128.53	122.33
1	A	178	PHE	N-CA-C	-5.29	105.60	111.36
1	A	234	SER	N-CA-C	-5.29	105.63	111.71
1	A	216	HIS	CB-CG-CD2	-5.28	124.34	131.20
1	A	210	LYS	CA-C-N	5.26	130.81	122.60
1	A	210	LYS	C-N-CA	5.26	130.81	122.60
1	A	305	SER	CA-C-N	5.26	128.92	120.30
1	A	305	SER	C-N-CA	5.26	128.92	120.30
1	A	238	ASN	CA-C-O	-5.25	114.98	120.55
1	A	290	GLN	CG-CD-OE1	5.22	131.23	120.80
1	A	249	THR	CA-CB-OG1	-5.21	101.78	109.60
1	A	187	GLU	CG-CD-OE1	5.21	130.37	118.40
1	A	133	LEU	CA-C-N	5.20	133.69	121.52
1	A	133	LEU	C-N-CA	5.20	133.69	121.52
1	A	224	THR	N-CA-CB	-5.20	103.68	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	47	ARG	N-CA-C	-5.19	102.48	109.95
1	A	224	THR	CA-CB-CG2	5.19	119.32	110.50
1	A	203	ARG	O-C-N	5.18	129.44	123.17
1	A	26	THR	CA-CB-CG2	5.18	119.30	110.50
1	A	47	ARG	NE-CZ-NH2	-5.17	114.55	119.20
1	A	189	GLY	N-CA-C	5.16	122.72	115.30
1	A	237	ILE	CA-C-O	-5.16	115.39	120.85
1	A	170	ASP	N-CA-CB	5.15	117.88	110.20
1	A	47	ARG	CA-C-O	-5.15	114.78	121.73
1	A	122	TYR	CA-C-N	-5.13	113.91	121.30
1	A	122	TYR	C-N-CA	-5.13	113.91	121.30
1	A	192	VAL	CA-CB-CG2	5.13	119.13	110.40
1	A	276	THR	N-CA-CB	5.13	119.37	110.09
1	A	296	TYR	CA-C-N	5.12	136.25	121.60
1	A	296	TYR	C-N-CA	5.12	136.25	121.60
1	A	242	TYR	O-C-N	-5.12	116.31	122.15
1	A	216	HIS	N-CA-C	5.12	117.50	108.75
1	A	255	VAL	CA-C-N	-5.11	115.78	122.37
1	A	255	VAL	C-N-CA	-5.11	115.78	122.37
1	A	202	LEU	O-C-N	5.11	127.33	122.07
1	A	179	TYR	N-CA-CB	5.10	117.71	110.06
1	A	163	ALA	CA-C-O	-5.09	114.59	120.24
1	A	187	GLU	N-CA-C	5.09	117.86	109.72
1	A	296	TYR	O-C-N	-5.09	116.32	122.48
1	A	316	LYS	N-CA-CB	-5.08	101.86	110.50
1	A	237	ILE	N-CA-C	-5.08	105.59	110.72
1	A	282	SER	CA-CB-OG	5.08	121.25	111.10
1	A	47	ARG	CG-CD-NE	-5.07	100.84	112.00
1	A	105	HIS	CA-C-N	-5.07	115.05	122.19
1	A	105	HIS	C-N-CA	-5.07	115.05	122.19
1	A	112	ASN	CB-CG-OD1	5.06	130.93	120.80
1	A	40	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	309	ALA	O-C-N	-5.06	116.86	122.07
1	A	175	LEU	O-C-N	-5.05	116.76	122.12
1	A	63	PHE	O-C-N	-5.04	116.29	122.34
1	A	89	ASN	CB-CG-OD1	-5.04	110.72	120.80
1	A	93	TYR	N-CA-CB	-5.04	101.95	110.41
1	A	42	TYR	CA-C-N	5.04	129.39	122.84
1	A	42	TYR	C-N-CA	5.04	129.39	122.84
1	A	109	GLY	O-C-N	5.04	129.25	122.70
1	A	86	ASN	CA-C-O	-5.03	114.65	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ASP	O-C-N	5.03	128.51	122.72
1	A	48	THR	CB-CA-C	5.03	118.67	110.17
1	A	40	PHE	CA-C-O	-5.03	114.90	120.38
1	A	185	ASP	CA-C-O	-5.02	115.78	121.05
1	A	75	TYR	CE1-CZ-CE2	5.01	130.33	120.30
1	A	31	GLN	CG-CD-NE2	5.01	123.92	116.40
1	A	128	GLN	O-C-N	-5.01	115.93	122.59
1	A	214	PRO	N-CD-CG	-5.00	95.70	103.20
1	A	112	ASN	N-CA-CB	-5.00	102.04	110.49
1	A	230	VAL	CB-CA-C	5.00	118.89	112.14
1	A	244	ILE	CB-CA-C	-5.00	105.39	112.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2432	0	2263	116	2
2	A	4	0	0	0	0
3	A	1	0	0	0	0
4	A	10	0	13	4	0
5	A	150	0	0	35	10
All	All	2597	0	2276	119	10

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 25.

All (119) 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:265:LYS:CE	1:A:265:LYS:NZ	1.69	1.56
1:A:101:ARG:CD	1:A:101:ARG:CG	1.82	1.54
4:A:322:LNO:N	4:A:322:LNO:HD13	1.45	1.18
1:A:308:GLN:HG2	5:A:388:HOH:O	1.44	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:SER:HB3	5:A:435:HOH:O	1.43	1.14
1:A:118:SER:N	5:A:442:HOH:O	1.78	1.11
1:A:216:HIS:ND1	5:A:435:HOH:O	1.88	1.04
4:A:322:LNO:N	4:A:322:LNO:CD1	2.15	1.02
1:A:116:ASN:OD1	5:A:442:HOH:O	1.78	1.01
1:A:92:SER:HA	5:A:451:HOH:O	1.61	0.99
1:A:101:ARG:CG	1:A:101:ARG:NE	2.29	0.96
1:A:280:ASN:HD22	1:A:280:ASN:C	1.72	0.96
4:A:322:LNO:HD13	4:A:322:LNO:HN1	1.04	0.95
1:A:137:ILE:HG22	1:A:182:LYS:NZ	1.83	0.94
1:A:219:LYS:HE2	5:A:391:HOH:O	1.71	0.90
1:A:219:LYS:CE	5:A:391:HOH:O	2.22	0.85
1:A:100:ILE:HD11	5:A:451:HOH:O	1.79	0.83
1:A:265:LYS:NZ	1:A:265:LYS:CD	2.40	0.83
1:A:137:ILE:HG22	1:A:182:LYS:HZ3	1.43	0.81
1:A:119:GLU:OE1	5:A:447:HOH:O	1.97	0.81
1:A:273:GLN:CG	5:A:372:HOH:O	2.29	0.81
1:A:216:HIS:CE1	5:A:435:HOH:O	2.31	0.81
1:A:278:THR:HG22	1:A:278:THR:O	1.79	0.80
1:A:269:ARG:NH1	1:A:294:ASP:OD2	2.18	0.77
1:A:111:ASN:O	1:A:112:ASN:HB2	1.86	0.75
1:A:92:SER:OG	5:A:451:HOH:O	2.04	0.74
1:A:116:ASN:C	5:A:442:HOH:O	2.32	0.73
1:A:191:ASP:HB2	5:A:350:HOH:O	1.90	0.71
1:A:92:SER:CB	5:A:451:HOH:O	2.37	0.71
1:A:1:ILE:HD13	1:A:29:TYR:CE2	2.26	0.71
1:A:280:ASN:ND2	1:A:283:GLN:H	1.89	0.70
1:A:137:ILE:HG22	1:A:182:LYS:HZ2	1.57	0.68
1:A:144:LEU:O	1:A:147:ALA:HB3	1.93	0.68
1:A:126:ASP:OD2	1:A:128:GLN:N	2.25	0.67
1:A:273:GLN:HB3	5:A:372:HOH:O	1.94	0.67
1:A:131:ILE:HB	1:A:132:PRO:CD	2.24	0.67
1:A:120:MET:HE3	5:A:408:HOH:O	1.95	0.66
1:A:172:PHE:O	1:A:176:VAL:HG23	1.96	0.66
1:A:162:GLY:O	1:A:230:VAL:HG13	1.94	0.66
1:A:101:ARG:NE	1:A:101:ARG:HG3	2.12	0.65
1:A:273:GLN:CB	5:A:372:HOH:O	2.45	0.65
1:A:120:MET:C	1:A:121:VAL:HG23	2.21	0.64
1:A:278:THR:O	1:A:278:THR:CG2	2.46	0.64
1:A:280:ASN:C	1:A:280:ASN:ND2	2.47	0.62
1:A:30:LEU:HB2	1:A:55:TRP:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:MET:SD	1:A:144:LEU:HD23	2.40	0.62
1:A:152:THR:HG21	1:A:272:THR:HG22	1.82	0.62
1:A:150:ASP:HA	5:A:379:HOH:O	2.00	0.61
1:A:187:GLU:OE1	5:A:411:HOH:O	2.16	0.61
1:A:197:ILE:HD13	1:A:197:ILE:N	2.16	0.61
1:A:154:GLY:HA2	5:A:379:HOH:O	2.01	0.60
1:A:137:ILE:H	1:A:182:LYS:HZ2	1.49	0.60
1:A:131:ILE:HG23	1:A:195:PRO:HG3	1.84	0.59
1:A:217:TYR:O	1:A:220:ARG:HB2	2.02	0.59
1:A:50:LEU:HD12	5:A:336:HOH:O	2.04	0.58
1:A:178:PHE:CE1	1:A:184:PRO:HB2	2.39	0.58
1:A:308:GLN:CG	5:A:388:HOH:O	2.22	0.58
1:A:218:SER:N	5:A:435:HOH:O	2.30	0.57
1:A:68:ALA:HB3	1:A:69:PRO:HD3	1.86	0.57
1:A:273:GLN:HG3	5:A:372:HOH:O	1.99	0.56
1:A:280:ASN:HD21	1:A:283:GLN:H	1.52	0.56
1:A:273:GLN:CD	5:A:372:HOH:O	2.49	0.55
1:A:128:GLN:O	1:A:195:PRO:HD2	2.09	0.53
1:A:131:ILE:HB	1:A:132:PRO:HD2	1.90	0.53
1:A:166:GLU:HG3	1:A:230:VAL:HG12	1.91	0.52
1:A:1:ILE:N	1:A:31:GLN:HE22	2.10	0.50
1:A:137:ILE:H	1:A:182:LYS:NZ	2.08	0.50
1:A:45:LYS:NZ	5:A:412:HOH:O	2.45	0.50
1:A:4:THR:HG22	1:A:24:TYR:HB3	1.93	0.49
1:A:265:LYS:HE2	5:A:446:HOH:O	2.13	0.49
1:A:285:ARG:HD3	1:A:316:LYS:HD3	1.94	0.49
1:A:298:SER:HB2	5:A:424:HOH:O	2.12	0.49
1:A:282:SER:HA	1:A:316:LYS:HD2	1.94	0.48
1:A:276:THR:HB	1:A:277:PRO:CD	2.43	0.48
1:A:13:VAL:CG1	1:A:131:ILE:HD12	2.43	0.48
1:A:149:THR:O	1:A:154:GLY:N	2.41	0.48
1:A:116:ASN:CG	5:A:442:HOH:O	2.43	0.48
1:A:178:PHE:CD1	1:A:184:PRO:HB2	2.49	0.48
1:A:218:SER:CB	5:A:435:HOH:O	2.26	0.48
1:A:49:THR:O	1:A:49:THR:HG22	2.15	0.47
1:A:156:ILE:HD13	1:A:156:ILE:HG21	1.70	0.47
1:A:291:SER:O	1:A:295:LEU:HD12	2.13	0.47
1:A:62:PHE:HA	1:A:67:ASP:OD2	2.14	0.47
1:A:113:ALA:O	4:A:322:LNO:HB1	2.14	0.47
1:A:162:GLY:C	1:A:230:VAL:HG13	2.40	0.47
1:A:271:LEU:HA	1:A:275:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:TYR:OH	1:A:182:LYS:HE3	2.15	0.46
1:A:81:TYR:HD1	5:A:451:HOH:O	1.97	0.46
1:A:293:THR:HA	1:A:303:VAL:HG21	1.97	0.46
1:A:249:THR:HG22	5:A:454:HOH:O	2.16	0.46
1:A:32:ASP:OD1	1:A:35:ARG:NH1	2.48	0.45
1:A:92:SER:HB2	1:A:97:ASN:HA	1.99	0.45
1:A:137:ILE:HG22	1:A:137:ILE:H	1.37	0.45
1:A:120:MET:C	1:A:121:VAL:CG2	2.85	0.45
1:A:1:ILE:HD13	1:A:29:TYR:CZ	2.52	0.44
1:A:258:ILE:HG21	1:A:302:GLU:HA	1.99	0.44
1:A:302:GLU:O	1:A:306:VAL:HG23	2.17	0.44
1:A:166:GLU:CG	1:A:230:VAL:HG12	2.47	0.44
1:A:237:ILE:HG23	1:A:237:ILE:HD12	1.80	0.43
1:A:280:ASN:ND2	1:A:282:SER:H	2.17	0.43
1:A:265:LYS:HE3	1:A:265:LYS:HB2	1.83	0.43
1:A:269:ARG:HD2	1:A:295:LEU:HD11	2.01	0.43
1:A:197:ILE:N	1:A:197:ILE:CD1	2.82	0.42
1:A:109:GLY:HA2	1:A:125:GLY:O	2.20	0.42
1:A:202:LEU:HA	1:A:202:LEU:HD12	1.61	0.42
1:A:214:PRO:HB3	1:A:219:LYS:HB3	2.00	0.42
1:A:131:ILE:O	1:A:132:PRO:C	2.60	0.42
1:A:72:ASP:HB3	1:A:134:SER:O	2.19	0.42
1:A:142:HIS:CD2	1:A:142:HIS:C	2.97	0.42
1:A:274:TYR:OH	1:A:294:ASP:OD2	2.28	0.42
1:A:131:ILE:HD13	1:A:131:ILE:HG21	1.90	0.41
1:A:266:ILE:HG12	1:A:292:ALA:HA	2.01	0.41
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.78	0.41
1:A:255:VAL:HG22	1:A:308:GLN:HB3	2.02	0.41
1:A:285:ARG:CD	1:A:316:LYS:HD3	2.50	0.41
1:A:158:GLN:OE1	5:A:375:HOH:O	2.21	0.41
1:A:219:LYS:O	1:A:220:ARG:C	2.62	0.41
1:A:8:GLY:O	1:A:19:ASN:HA	2.20	0.41
1:A:90:ARG:NH1	1:A:90:ARG:HG3	2.36	0.40

All (10) 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:372:HOH:O	5:A:409:HOH:O[5_564]	0.93	1.27
5:A:369:HOH:O	5:A:407:HOH:O[5_564]	1.42	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:333:HOH:O	5:A:337:HOH:O[10_664]	1.74	0.46
5:A:332:HOH:O	5:A:336:HOH:O[10_664]	1.75	0.45
5:A:418:HOH:O	5:A:418:HOH:O[12_565]	1.75	0.45
5:A:485:HOH:O	5:A:485:HOH:O[7_555]	1.80	0.40
5:A:379:HOH:O	5:A:396:HOH:O[10_664]	2.01	0.19
1:A:6:THR:CB	5:A:473:HOH:O[12_565]	2.03	0.17
1:A:116:ASN:O	5:A:336:HOH:O[10_664]	2.11	0.09
5:A:372:HOH:O	5:A:463:HOH:O[5_564]	2.14	0.06

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	314/316 (99%)	299 (95%)	15 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	252/252 (100%)	230 (91%)	22 (9%)	9	12

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	9	VAL
1	A	18	LYS
1	A	20	ILE
1	A	25	SER
1	A	26	THR
1	A	49	THR
1	A	54	LEU
1	A	79	VAL
1	A	89	ASN
1	A	120	MET
1	A	144	LEU
1	A	175	LEU
1	A	197	ILE
1	A	224	THR
1	A	225	GLN
1	A	243	LEU
1	A	261	ASP
1	A	273	GLN
1	A	280	ASN
1	A	313	VAL
1	A	316	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	31	GLN
1	A	33	ASN
1	A	97	ASN
1	A	159	ASN
1	A	246	GLN
1	A	280	ASN
1	A	290	GLN
1	A	301	GLN
1	A	308	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

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	LNO	A	322	3	7,9,9	1.02	1 (14%)	6,11,11	2.48	4 (66%)

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
4	LNO	A	322	3	-	4/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	322	LNO	O-C	2.35	1.27	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	322	LNO	O-C-CA	3.54	127.74	120.28
4	A	322	LNO	CA-C-N2	-2.88	111.37	115.93
4	A	322	LNO	CD1-CG-CB	-2.58	101.80	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	322	LNO	C-CA-N	2.19	117.62	109.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	322	LNO	N-CA-CB-CG
4	A	322	LNO	C-CA-CB-CG
4	A	322	LNO	O-C-CA-CB
4	A	322	LNO	N2-C-CA-CB

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	322	LNO	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	35:ARG	C	36:GLY	N	1.15
1	A	260:ARG	C	261:ASP	N	1.15

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	316/316 (100%)	-0.88	0 100 100	2, 9, 20, 29	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LNO	A	322	10/10	0.92	0.12	23,27,29,29	0
2	CA	A	319	1/1	0.96	0.02	11,11,11,11	0
3	ZN	A	321	1/1	0.98	0.04	14,14,14,14	0
2	CA	A	320	1/1	0.99	0.02	14,14,14,14	0
2	CA	A	318	1/1	0.99	0.02	13,13,13,13	0
2	CA	A	317	1/1	0.99	0.01	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.