



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:11 AM UTC

PDB ID : 5TLN / pdb_00005tlN
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

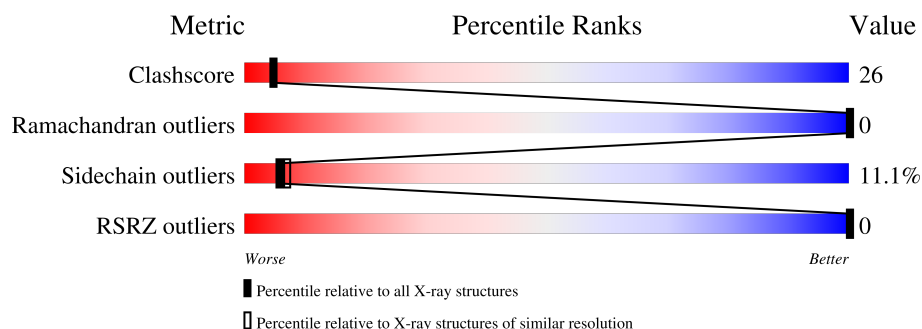
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

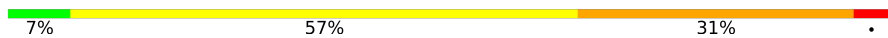
The reported resolution of this entry is 2.30 Å.

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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BAN	A	322	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2606 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			

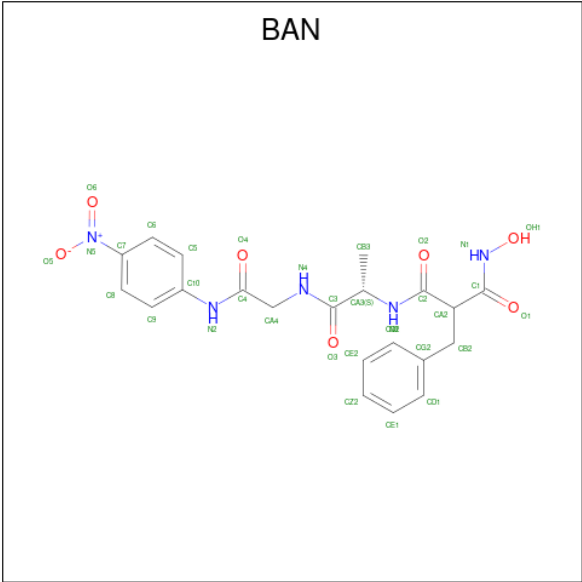
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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 HONH-BENZYLALONYL-L-ALANYLGLYCINE-P-NITROANILIDE (CCD ID: BAN) (formula: C₂₁H₂₃N₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			23	15	3	5		

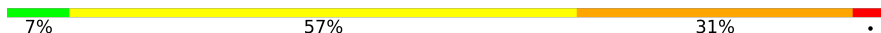
- Molecule 5 is water.

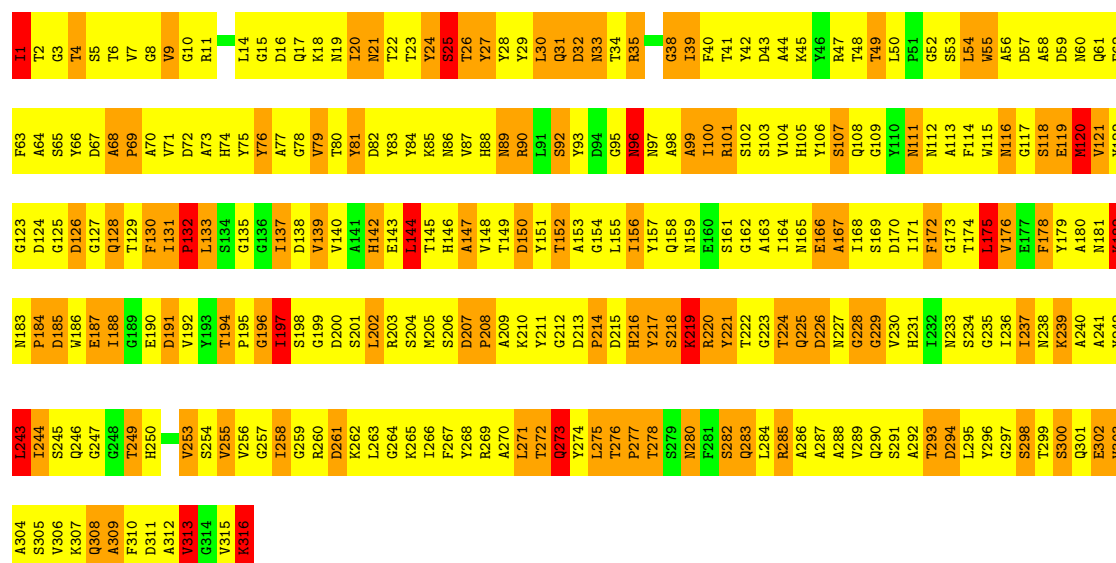
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	146	Total	O	0	0
			146	146		

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

Chain A: 



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) 75.2 (10.00-2.31)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	88777.78 (at 2.31Å)	Xtriage
Refinement program	TNT, PROLSQ	Depositor
R, R_{free}	0.179 , (Not available) 0.164 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2606	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 4.12% 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, ZN, BAN

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	2.99	252/2491 (10.1%)	3.99	615/3391 (18.1%)

All (252) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	ILE	C-O	13.91	1.38	1.23
1	A	144	LEU	C-O	13.19	1.39	1.24
1	A	35	ARG	C-N	-12.99	1.15	1.33
1	A	10	GLY	C-N	-12.12	1.17	1.33
1	A	260	ARG	C-N	-11.75	1.18	1.33
1	A	108	GLN	C-O	11.26	1.36	1.24
1	A	65	SER	C-O	11.26	1.38	1.24
1	A	9	VAL	C-O	11.18	1.35	1.24
1	A	152	THR	N-CA	10.99	1.58	1.45
1	A	265	LYS	CA-CB	-10.88	1.35	1.53
1	A	267	PHE	C-O	10.67	1.36	1.24
1	A	88	HIS	CA-C	-10.65	1.37	1.52
1	A	38	GLY	CA-C	-10.34	1.40	1.52
1	A	44	ALA	C-O	10.24	1.37	1.24
1	A	101	ARG	CG-CD	10.01	1.82	1.52
1	A	39	ILE	CA-CB	9.84	1.66	1.54
1	A	98	ALA	C-O	9.41	1.35	1.23
1	A	95	GLY	C-O	9.36	1.36	1.24
1	A	198	SER	N-CA	9.29	1.57	1.45
1	A	214	PRO	CA-CB	-9.15	1.41	1.53
1	A	297	GLY	C-N	-9.14	1.20	1.33
1	A	303	VAL	C-N	-9.12	1.22	1.33
1	A	163	ALA	C-N	-9.01	1.22	1.33
1	A	278	THR	CB-OG1	8.96	1.58	1.43
1	A	10	GLY	C-O	8.93	1.33	1.23
1	A	39	ILE	C-N	-8.85	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	THR	C-N	-8.82	1.21	1.33
1	A	4	THR	N-CA	8.78	1.57	1.46
1	A	76	TYR	C-N	-8.74	1.22	1.33
1	A	93	TYR	N-CA	8.66	1.57	1.46
1	A	11	ARG	NE-CZ	8.54	1.42	1.33
1	A	10	GLY	N-CA	8.49	1.53	1.45
1	A	93	TYR	CA-C	-8.40	1.41	1.52
1	A	168	ILE	C-O	8.39	1.33	1.24
1	A	8	GLY	N-CA	8.34	1.57	1.45
1	A	173	GLY	CA-C	-8.30	1.42	1.52
1	A	295	LEU	N-CA	-8.24	1.35	1.46
1	A	224	THR	CA-CB	8.23	1.65	1.53
1	A	105	HIS	C-N	-8.16	1.22	1.33
1	A	101	ARG	NE-CZ	-8.13	1.24	1.33
1	A	260	ARG	CA-C	-8.12	1.41	1.52
1	A	186	TRP	CG-CD2	8.08	1.58	1.43
1	A	4	THR	C-O	8.07	1.33	1.23
1	A	265	LYS	N-CA	8.06	1.56	1.46
1	A	99	ALA	C-N	-8.05	1.22	1.33
1	A	290	GLN	C-O	7.96	1.33	1.24
1	A	148	VAL	C-O	7.92	1.32	1.24
1	A	264	GLY	CA-C	-7.86	1.42	1.52
1	A	194	THR	CB-OG1	7.82	1.56	1.43
1	A	98	ALA	N-CA	7.79	1.55	1.46
1	A	54	LEU	CA-C	7.78	1.62	1.52
1	A	215	ASP	N-CA	7.66	1.55	1.46
1	A	225	GLN	C-O	7.61	1.34	1.23
1	A	307	LYS	C-O	-7.61	1.15	1.24
1	A	217	TYR	C-O	7.58	1.33	1.24
1	A	5	SER	C-O	-7.50	1.14	1.23
1	A	24	TYR	C-O	7.45	1.33	1.24
1	A	306	VAL	C-O	7.44	1.33	1.24
1	A	149	THR	C-O	7.44	1.32	1.24
1	A	292	ALA	C-O	-7.44	1.15	1.24
1	A	139	VAL	N-CA	7.40	1.55	1.46
1	A	208	PRO	N-CA	-7.38	1.37	1.47
1	A	116	ASN	CG-ND2	-7.37	1.17	1.33
1	A	184	PRO	CA-CB	-7.37	1.43	1.53
1	A	35	ARG	CA-C	-7.32	1.44	1.52
1	A	64	ALA	C-N	-7.30	1.24	1.34
1	A	308	GLN	CA-C	7.29	1.62	1.52
1	A	137	ILE	N-CA	-7.24	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	SER	CA-CB	-7.24	1.41	1.53
1	A	162	GLY	C-O	7.23	1.32	1.24
1	A	255	VAL	C-O	7.22	1.31	1.24
1	A	242	TYR	C-N	-7.21	1.24	1.33
1	A	96	ASN	CG-OD1	7.20	1.37	1.23
1	A	3	GLY	C-O	7.16	1.31	1.23
1	A	273	GLN	C-O	7.13	1.33	1.23
1	A	44	ALA	CA-CB	-7.09	1.41	1.53
1	A	4	THR	CA-CB	7.08	1.64	1.53
1	A	210	LYS	C-O	7.08	1.32	1.24
1	A	297	GLY	C-O	-7.04	1.14	1.23
1	A	74	HIS	C-O	7.03	1.32	1.24
1	A	9	VAL	C-N	-7.01	1.25	1.33
1	A	142	HIS	C-O	-6.98	1.15	1.24
1	A	247	GLY	N-CA	6.95	1.52	1.45
1	A	131	ILE	N-CA	-6.94	1.38	1.46
1	A	117	GLY	C-N	6.92	1.43	1.33
1	A	47	ARG	C-N	-6.91	1.24	1.33
1	A	34	THR	CA-CB	6.85	1.65	1.53
1	A	180	ALA	N-CA	6.85	1.55	1.46
1	A	275	LEU	N-CA	6.83	1.54	1.45
1	A	85	LYS	N-CA	-6.79	1.37	1.46
1	A	11	ARG	C-N	-6.76	1.23	1.33
1	A	308	GLN	CD-NE2	6.75	1.47	1.33
1	A	282	SER	C-O	6.75	1.32	1.24
1	A	127	GLY	C-O	6.71	1.32	1.24
1	A	199	GLY	CA-C	-6.70	1.42	1.51
1	A	212	GLY	C-O	6.69	1.32	1.24
1	A	274	TYR	C-N	-6.66	1.24	1.33
1	A	166	GLU	C-O	-6.64	1.16	1.24
1	A	126	ASP	C-N	-6.63	1.24	1.33
1	A	315	VAL	C-N	6.62	1.42	1.33
1	A	159	ASN	C-O	-6.62	1.17	1.24
1	A	295	LEU	CA-CB	6.62	1.64	1.53
1	A	192	VAL	CA-CB	6.60	1.61	1.54
1	A	151	TYR	C-N	-6.59	1.26	1.34
1	A	115	TRP	NE1-CE2	6.58	1.44	1.37
1	A	250	HIS	C-N	-6.57	1.24	1.33
1	A	79	VAL	C-O	6.54	1.32	1.24
1	A	222	THR	CA-CB	6.52	1.64	1.53
1	A	200	ASP	C-N	6.51	1.41	1.33
1	A	22	THR	C-N	-6.47	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	HIS	CA-CB	6.45	1.64	1.53
1	A	203	ARG	N-CA	-6.40	1.37	1.45
1	A	43	ASP	CA-C	6.38	1.61	1.52
1	A	157	TYR	C-N	-6.37	1.25	1.33
1	A	145	THR	N-CA	6.34	1.54	1.46
1	A	216	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	310	PHE	C-O	6.31	1.31	1.24
1	A	131	ILE	CA-CB	-6.30	1.46	1.54
1	A	101	ARG	CZ-NH2	6.30	1.41	1.33
1	A	50	LEU	C-O	-6.27	1.17	1.24
1	A	263	LEU	N-CA	-6.26	1.39	1.46
1	A	128	GLN	C-N	-6.24	1.25	1.33
1	A	47	ARG	NE-CZ	-6.23	1.26	1.33
1	A	305	SER	CA-C	6.21	1.61	1.52
1	A	116	ASN	C-O	6.19	1.32	1.24
1	A	178	PHE	C-O	-6.19	1.16	1.24
1	A	297	GLY	N-CA	-6.18	1.36	1.45
1	A	223	GLY	CA-C	6.17	1.59	1.51
1	A	185	ASP	C-O	6.16	1.29	1.24
1	A	137	ILE	C-O	6.16	1.32	1.24
1	A	221	TYR	CA-CB	-6.16	1.44	1.53
1	A	175	LEU	C-O	-6.12	1.16	1.24
1	A	287	ALA	C-O	-6.11	1.17	1.24
1	A	59	ASP	CA-C	-6.07	1.44	1.52
1	A	62	PHE	C-O	-6.06	1.16	1.24
1	A	120	MET	CA-CB	-6.06	1.44	1.53
1	A	55	TRP	NE1-CE2	6.05	1.44	1.37
1	A	118	SER	CA-CB	-6.03	1.43	1.53
1	A	296	TYR	C-O	6.03	1.31	1.23
1	A	243	LEU	C-O	-6.03	1.17	1.24
1	A	278	THR	CA-C	-6.03	1.45	1.52
1	A	98	ALA	CA-C	-6.02	1.45	1.52
1	A	69	PRO	C-O	6.01	1.31	1.24
1	A	133	LEU	C-O	6.01	1.31	1.24
1	A	68	ALA	CA-CB	6.01	1.60	1.53
1	A	52	GLY	C-O	5.96	1.33	1.23
1	A	25	SER	CB-OG	5.96	1.54	1.42
1	A	137	ILE	CB-CG1	5.96	1.65	1.53
1	A	77	ALA	C-O	-5.95	1.17	1.24
1	A	108	GLN	CA-C	5.94	1.59	1.52
1	A	96	ASN	CA-CB	5.91	1.62	1.53
1	A	250	HIS	CE1-NE2	-5.91	1.26	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	SER	CA-CB	5.90	1.63	1.53
1	A	260	ARG	C-O	5.89	1.31	1.24
1	A	119	GLU	C-N	-5.88	1.25	1.33
1	A	256	VAL	N-CA	5.88	1.53	1.46
1	A	305	SER	C-O	5.88	1.31	1.24
1	A	211	TYR	N-CA	-5.87	1.39	1.46
1	A	169	SER	C-N	-5.87	1.25	1.33
1	A	105	HIS	CG-CD2	5.86	1.42	1.35
1	A	209	ALA	C-N	-5.85	1.26	1.33
1	A	169	SER	C-O	5.84	1.31	1.24
1	A	302	GLU	CA-CB	5.84	1.62	1.53
1	A	288	ALA	CA-C	-5.82	1.45	1.52
1	A	58	ALA	CA-CB	5.79	1.63	1.53
1	A	78	GLY	CA-C	5.78	1.60	1.51
1	A	226	ASP	C-N	-5.78	1.25	1.33
1	A	148	VAL	C-N	-5.78	1.26	1.33
1	A	313	VAL	CA-C	-5.78	1.45	1.52
1	A	184	PRO	CA-C	-5.77	1.45	1.52
1	A	58	ALA	C-N	-5.77	1.25	1.33
1	A	197	ILE	C-O	-5.76	1.16	1.24
1	A	258	ILE	C-O	5.76	1.32	1.24
1	A	190	GLU	N-CA	-5.76	1.39	1.46
1	A	2	THR	N-CA	5.73	1.53	1.46
1	A	187	GLU	C-N	-5.72	1.26	1.33
1	A	297	GLY	CA-C	5.70	1.58	1.51
1	A	156	ILE	N-CA	5.69	1.52	1.46
1	A	156	ILE	C-O	5.68	1.30	1.24
1	A	266	ILE	C-O	-5.68	1.17	1.24
1	A	229	GLY	CA-C	-5.67	1.45	1.51
1	A	26	THR	CA-CB	5.67	1.63	1.53
1	A	171	ILE	C-O	-5.63	1.17	1.24
1	A	258	ILE	C-N	5.61	1.41	1.32
1	A	227	ASN	N-CA	-5.59	1.38	1.46
1	A	120	MET	C-O	-5.59	1.17	1.23
1	A	172	PHE	N-CA	5.59	1.53	1.46
1	A	96	ASN	CG-ND2	5.58	1.45	1.33
1	A	113	ALA	CA-C	-5.58	1.45	1.52
1	A	170	ASP	CG-OD2	-5.58	1.14	1.25
1	A	300	SER	C-O	5.58	1.31	1.23
1	A	200	ASP	N-CA	5.57	1.52	1.45
1	A	2	THR	CB-OG1	5.55	1.52	1.43
1	A	61	GLN	CA-C	5.54	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	GLN	CA-C	5.53	1.59	1.52
1	A	259	GLY	C-O	-5.52	1.16	1.23
1	A	216	HIS	CG-ND1	-5.51	1.32	1.38
1	A	47	ARG	CA-C	5.48	1.60	1.53
1	A	140	VAL	CA-CB	-5.47	1.47	1.54
1	A	158	GLN	C-O	-5.47	1.17	1.23
1	A	103	SER	C-O	5.46	1.30	1.24
1	A	187	GLU	N-CA	5.46	1.52	1.45
1	A	102	SER	CA-CB	5.46	1.67	1.53
1	A	194	THR	N-CA	5.46	1.53	1.46
1	A	315	VAL	CA-CB	-5.46	1.47	1.53
1	A	11	ARG	CZ-NH2	5.45	1.40	1.33
1	A	256	VAL	C-N	-5.44	1.27	1.33
1	A	132	PRO	N-CD	5.42	1.55	1.47
1	A	265	LYS	CB-CG	-5.39	1.36	1.52
1	A	90	ARG	C-N	-5.39	1.24	1.33
1	A	255	VAL	CA-CB	5.38	1.61	1.54
1	A	260	ARG	CD-NE	5.37	1.53	1.46
1	A	185	ASP	N-CA	-5.36	1.38	1.46
1	A	174	THR	C-O	5.35	1.30	1.24
1	A	231	HIS	CG-ND1	-5.35	1.32	1.38
1	A	130	PHE	C-O	5.35	1.30	1.23
1	A	121	VAL	C-O	5.31	1.29	1.24
1	A	316	LYS	C-OXT	5.29	1.34	1.23
1	A	203	ARG	CZ-NH2	5.28	1.40	1.33
1	A	70	ALA	CA-CB	-5.27	1.45	1.53
1	A	14	LEU	C-O	-5.27	1.17	1.24
1	A	313	VAL	CA-CB	5.25	1.61	1.54
1	A	78	GLY	C-O	5.23	1.30	1.23
1	A	233	ASN	C-O	5.22	1.30	1.24
1	A	18	LYS	C-O	-5.22	1.17	1.23
1	A	40	PHE	C-N	-5.21	1.26	1.33
1	A	262	LYS	C-O	-5.20	1.18	1.24
1	A	182	LYS	N-CA	5.20	1.53	1.46
1	A	285	ARG	C-N	5.19	1.40	1.33
1	A	245	SER	C-N	-5.17	1.25	1.33
1	A	70	ALA	C-O	5.17	1.30	1.24
1	A	139	VAL	C-N	5.17	1.40	1.33
1	A	113	ALA	N-CA	-5.16	1.39	1.45
1	A	151	TYR	C-O	5.15	1.30	1.24
1	A	192	VAL	C-N	-5.15	1.25	1.33
1	A	224	THR	N-CA	-5.13	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	ASN	CG-ND2	-5.13	1.22	1.33
1	A	54	LEU	C-O	5.13	1.29	1.23
1	A	304	ALA	CA-CB	5.12	1.61	1.53
1	A	101	ARG	CZ-NH1	5.09	1.39	1.32
1	A	120	MET	CB-CG	-5.09	1.37	1.52
1	A	283	GLN	C-O	5.07	1.30	1.24
1	A	214	PRO	N-CA	5.07	1.53	1.47
1	A	166	GLU	CD-OE1	-5.06	1.15	1.25
1	A	235	GLY	C-O	5.05	1.31	1.23
1	A	133	LEU	CA-C	-5.04	1.45	1.52
1	A	221	TYR	CA-C	5.04	1.59	1.52
1	A	142	HIS	CA-C	5.03	1.59	1.52
1	A	278	THR	CB-CG2	-5.03	1.35	1.52
1	A	288	ALA	CA-CB	5.03	1.61	1.53
1	A	270	ALA	C-O	-5.01	1.18	1.24
1	A	26	THR	N-CA	5.00	1.52	1.46

All (615) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	GLY	CA-C-O	-22.79	106.51	122.23
1	A	47	ARG	CD-NE-CZ	22.13	155.38	124.40
1	A	101	ARG	CD-NE-CZ	21.81	154.93	124.40
1	A	264	GLY	CA-C-O	19.34	139.75	120.80
1	A	227	ASN	O-C-N	17.60	145.46	122.40
1	A	182	LYS	CG-CD-CE	16.84	150.04	111.30
1	A	53	SER	CA-C-O	-16.11	103.64	120.71
1	A	66	TYR	CA-C-N	15.78	144.30	120.31
1	A	66	TYR	C-N-CA	15.78	144.30	120.31
1	A	270	ALA	CA-C-O	15.36	136.52	120.70
1	A	297	GLY	CA-C-N	15.05	150.29	121.54
1	A	297	GLY	C-N-CA	15.05	150.29	121.54
1	A	163	ALA	CA-C-N	14.48	138.80	120.56
1	A	163	ALA	C-N-CA	14.48	138.80	120.56
1	A	315	VAL	O-C-N	14.41	139.48	122.62
1	A	56	ALA	CA-C-O	13.99	135.47	120.36
1	A	39	ILE	CB-CG1-CD1	13.78	142.74	113.80
1	A	113	ALA	CA-C-N	13.71	146.72	121.62
1	A	113	ALA	C-N-CA	13.71	146.72	121.62
1	A	101	ARG	CA-CB-CG	13.50	141.09	114.10
1	A	38	GLY	N-CA-C	13.35	127.24	112.29
1	A	85	LYS	CA-C-O	12.97	134.64	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	GLY	CA-C-O	-12.81	103.50	119.13
1	A	288	ALA	CA-C-N	12.71	136.58	120.56
1	A	288	ALA	C-N-CA	12.71	136.58	120.56
1	A	301	GLN	OE1-CD-NE2	-12.67	109.93	122.60
1	A	242	TYR	CA-C-N	12.62	136.84	120.44
1	A	242	TYR	C-N-CA	12.62	136.84	120.44
1	A	257	GLY	CA-C-O	-12.61	110.04	121.64
1	A	101	ARG	CA-C-N	12.50	142.97	122.73
1	A	101	ARG	C-N-CA	12.50	142.97	122.73
1	A	113	ALA	CA-C-O	-12.32	106.77	121.06
1	A	224	THR	N-CA-C	12.27	128.97	113.88
1	A	143	GLU	CG-CD-OE1	12.11	146.26	118.40
1	A	308	GLN	CG-CD-NE2	-12.03	98.36	116.40
1	A	166	GLU	CA-C-O	-11.97	107.73	120.42
1	A	11	ARG	CD-NE-CZ	-11.87	107.78	124.40
1	A	227	ASN	CA-C-O	-11.83	107.82	121.54
1	A	264	GLY	O-C-N	-11.77	110.75	122.17
1	A	88	HIS	CA-CB-CG	-11.43	102.37	113.80
1	A	21	ASN	CA-CB-CG	-11.43	101.17	112.60
1	A	162	GLY	O-C-N	-11.42	109.20	122.34
1	A	184	PRO	CA-C-O	-11.36	108.04	122.12
1	A	260	ARG	CA-C-N	11.32	135.83	120.44
1	A	260	ARG	C-N-CA	11.32	135.83	120.44
1	A	101	ARG	CB-CA-C	11.31	131.74	109.35
1	A	265	LYS	CA-CB-CG	11.25	136.59	114.10
1	A	47	ARG	NE-CZ-NH1	11.24	132.74	121.50
1	A	206	SER	CA-C-N	11.20	132.14	122.28
1	A	206	SER	C-N-CA	11.20	132.14	122.28
1	A	148	VAL	CA-C-O	-11.20	109.31	121.29
1	A	103	SER	CA-C-O	-11.06	108.04	120.32
1	A	18	LYS	O-C-N	10.98	135.17	123.42
1	A	96	ASN	OD1-CG-ND2	10.89	133.49	122.60
1	A	270	ALA	O-C-N	-10.88	110.34	122.09
1	A	258	ILE	O-C-N	-10.84	111.62	122.14
1	A	101	ARG	CG-CD-NE	-10.82	88.20	112.00
1	A	312	ALA	CA-C-N	10.77	138.37	121.35
1	A	312	ALA	C-N-CA	10.77	138.37	121.35
1	A	282	SER	CB-CA-C	10.70	129.03	110.85
1	A	103	SER	O-C-N	10.62	135.73	123.31
1	A	234	SER	O-C-N	-10.53	109.90	122.22
1	A	164	ILE	N-CA-C	-10.53	100.32	110.42
1	A	168	ILE	CB-CG1-CD1	10.49	135.83	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	VAL	O-C-N	-10.38	111.80	121.87
1	A	261	ASP	N-CA-CB	-10.33	95.09	110.07
1	A	104	VAL	CA-C-O	-10.31	109.86	121.92
1	A	7	VAL	CA-C-O	-10.28	109.47	120.36
1	A	209	ALA	CA-C-N	10.24	134.36	120.54
1	A	209	ALA	C-N-CA	10.24	134.36	120.54
1	A	229	GLY	CA-C-N	10.18	134.41	120.46
1	A	229	GLY	C-N-CA	10.18	134.41	120.46
1	A	308	GLN	CG-CD-OE1	10.14	141.08	120.80
1	A	165	ASN	CA-CB-CG	10.11	122.71	112.60
1	A	286	ALA	CA-C-O	10.09	131.24	120.55
1	A	115	TRP	CA-C-O	-10.04	109.28	120.32
1	A	259	GLY	O-C-N	-9.97	111.09	122.56
1	A	187	GLU	CA-C-O	-9.92	109.90	121.11
1	A	89	ASN	CA-CB-CG	-9.82	102.78	112.60
1	A	211	TYR	CB-CG-CD2	-9.77	106.15	120.80
1	A	211	TYR	CA-C-O	-9.68	108.53	119.95
1	A	181	ASN	CA-CB-CG	9.66	122.26	112.60
1	A	56	ALA	O-C-N	-9.62	111.85	123.30
1	A	138	ASP	CA-C-N	9.59	132.41	120.72
1	A	138	ASP	C-N-CA	9.59	132.41	120.72
1	A	73	ALA	CA-C-O	9.57	130.87	120.82
1	A	76	TYR	CA-C-O	-9.57	108.97	119.97
1	A	167	ALA	O-C-N	-9.55	111.26	122.15
1	A	263	LEU	O-C-N	-9.55	112.24	122.07
1	A	146	HIS	CA-C-N	9.50	132.79	120.44
1	A	146	HIS	C-N-CA	9.50	132.79	120.44
1	A	119	GLU	N-CA-CB	-9.48	96.86	111.56
1	A	197	ILE	CA-C-O	9.44	134.63	121.51
1	A	49	THR	CA-CB-OG1	-9.40	95.50	109.60
1	A	50	LEU	CA-C-O	-9.38	110.46	120.87
1	A	306	VAL	CA-C-O	9.26	130.47	120.47
1	A	47	ARG	CA-C-N	9.24	136.82	122.49
1	A	47	ARG	C-N-CA	9.24	136.82	122.49
1	A	148	VAL	N-CA-CB	9.24	120.69	110.62
1	A	300	SER	CA-C-O	9.24	132.56	121.94
1	A	48	THR	CA-C-O	9.21	130.28	119.32
1	A	142	HIS	CA-C-N	9.19	132.94	120.44
1	A	142	HIS	C-N-CA	9.19	132.94	120.44
1	A	260	ARG	NE-CZ-NH2	-9.17	110.94	119.20
1	A	122	TYR	CA-C-N	-9.15	111.03	121.83
1	A	122	TYR	C-N-CA	-9.15	111.03	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	GLN	CA-CB-CG	9.15	132.40	114.10
1	A	181	ASN	OD1-CG-ND2	-9.13	113.47	122.60
1	A	198	SER	N-CA-CB	-9.09	94.82	111.37
1	A	259	GLY	CA-C-O	9.08	130.14	122.24
1	A	219	LYS	CB-CG-CD	9.04	132.09	111.30
1	A	238	ASN	CA-C-N	9.02	132.16	120.44
1	A	238	ASN	C-N-CA	9.02	132.16	120.44
1	A	239	LYS	CB-CG-CD	8.97	131.94	111.30
1	A	84	TYR	CA-C-O	8.95	130.03	120.55
1	A	122	TYR	O-C-N	8.95	133.78	123.31
1	A	170	ASP	N-CA-C	-8.92	100.72	111.69
1	A	231	HIS	N-CA-CB	8.88	123.63	110.49
1	A	290	GLN	CA-CB-CG	-8.82	96.46	114.10
1	A	15	GLY	CA-C-O	8.81	129.94	119.19
1	A	30	LEU	CA-C-N	8.80	135.36	122.86
1	A	30	LEU	C-N-CA	8.80	135.36	122.86
1	A	93	TYR	CA-C-O	8.79	130.36	119.11
1	A	293	THR	CA-C-O	-8.77	109.89	119.97
1	A	260	ARG	N-CA-C	8.76	123.75	112.89
1	A	293	THR	O-C-N	8.75	133.03	122.27
1	A	211	TYR	O-C-N	8.74	133.01	122.26
1	A	226	ASP	CA-CB-CG	8.70	121.30	112.60
1	A	48	THR	O-C-N	-8.66	111.76	122.24
1	A	61	GLN	O-C-N	8.66	133.31	123.27
1	A	82	ASP	CA-C-O	-8.65	111.25	120.42
1	A	311	ASP	CA-C-O	8.63	129.56	120.42
1	A	21	ASN	OD1-CG-ND2	-8.62	113.98	122.60
1	A	9	VAL	CB-CA-C	-8.61	97.24	110.50
1	A	243	LEU	O-C-N	-8.56	113.25	122.07
1	A	184	PRO	O-C-N	8.55	133.57	123.14
1	A	236	ILE	CA-C-N	8.51	134.16	120.55
1	A	236	ILE	C-N-CA	8.51	134.16	120.55
1	A	170	ASP	CA-CB-CG	8.49	121.09	112.60
1	A	198	SER	CB-CA-C	8.45	127.04	109.38
1	A	139	VAL	N-CA-C	-8.44	102.48	110.42
1	A	158	GLN	OE1-CD-NE2	8.44	131.04	122.60
1	A	165	ASN	OD1-CG-ND2	-8.42	114.18	122.60
1	A	120	MET	CG-SD-CE	8.40	119.39	100.90
1	A	178	PHE	CA-C-N	8.40	131.88	120.54
1	A	178	PHE	C-N-CA	8.40	131.88	120.54
1	A	78	GLY	CA-C-O	-8.40	105.95	120.57
1	A	85	LYS	O-C-N	-8.37	111.35	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	SER	CA-C-O	-8.37	110.64	120.10
1	A	284	LEU	CA-C-O	8.35	129.40	120.55
1	A	108	GLN	O-C-N	8.33	132.93	123.27
1	A	211	TYR	CB-CA-C	-8.31	97.63	111.02
1	A	267	PHE	N-CA-C	8.31	120.34	111.28
1	A	101	ARG	CB-CG-CD	8.27	130.31	111.30
1	A	111	ASN	OD1-CG-ND2	-8.23	114.37	122.60
1	A	201	SER	CA-CB-OG	-8.17	94.75	111.10
1	A	54	LEU	O-C-N	8.14	132.88	122.87
1	A	117	GLY	CA-C-O	8.13	128.18	119.07
1	A	262	LYS	CA-C-O	-8.11	111.83	120.42
1	A	261	ASP	N-CA-C	-8.09	102.40	111.14
1	A	2	THR	O-C-N	-8.08	113.84	123.13
1	A	74	HIS	CA-C-O	8.08	129.30	120.82
1	A	204	SER	CA-C-O	-8.07	111.64	120.36
1	A	77	ALA	O-C-N	8.07	131.35	122.15
1	A	212	GLY	O-C-N	8.04	132.46	122.41
1	A	70	ALA	CA-C-O	8.04	128.94	120.42
1	A	143	GLU	CG-CD-OE2	-8.03	99.93	118.40
1	A	33	ASN	N-CA-C	8.03	123.07	113.28
1	A	288	ALA	O-C-N	-8.03	113.00	122.15
1	A	32	ASP	CA-CB-CG	8.01	120.61	112.60
1	A	45	LYS	O-C-N	8.01	133.24	122.59
1	A	224	THR	CA-CB-OG1	-8.01	97.59	109.60
1	A	228	GLY	O-C-N	7.99	131.68	122.33
1	A	223	GLY	CA-C-N	7.98	136.09	122.36
1	A	223	GLY	C-N-CA	7.98	136.09	122.36
1	A	170	ASP	CA-C-O	-7.95	111.42	120.24
1	A	211	TYR	CA-CB-CG	-7.93	99.62	113.90
1	A	35	ARG	CA-C-O	-7.93	111.81	120.30
1	A	75	TYR	N-CA-C	7.89	119.66	111.14
1	A	301	GLN	N-CA-C	-7.86	102.65	111.14
1	A	169	SER	O-C-N	-7.86	113.03	122.22
1	A	121	VAL	N-CA-CB	-7.83	100.09	111.52
1	A	149	THR	CA-C-N	7.80	130.58	120.44
1	A	149	THR	C-N-CA	7.80	130.58	120.44
1	A	39	ILE	CA-C-N	7.79	133.97	122.99
1	A	39	ILE	C-N-CA	7.79	133.97	122.99
1	A	156	ILE	CA-CB-CG2	7.79	123.74	110.50
1	A	261	ASP	OD1-CG-OD2	7.77	141.55	122.90
1	A	165	ASN	CA-C-N	7.75	131.30	120.29
1	A	165	ASN	C-N-CA	7.75	131.30	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ALA	N-CA-C	7.75	121.84	112.38
1	A	49	THR	CA-C-O	-7.74	111.51	120.49
1	A	282	SER	N-CA-C	-7.71	102.95	111.36
1	A	45	LYS	CB-CG-CD	7.71	129.03	111.30
1	A	17	GLN	CA-C-O	7.70	129.34	120.80
1	A	85	LYS	CA-CB-CG	-7.67	98.77	114.10
1	A	117	GLY	N-CA-C	-7.64	104.98	114.92
1	A	133	LEU	N-CA-C	7.63	121.69	112.38
1	A	298	SER	N-CA-CB	-7.63	97.59	110.49
1	A	227	ASN	CB-CG-ND2	7.61	127.81	116.40
1	A	174	THR	CA-C-N	7.57	131.04	120.29
1	A	174	THR	C-N-CA	7.57	131.04	120.29
1	A	263	LEU	CA-C-N	7.54	128.48	120.03
1	A	263	LEU	C-N-CA	7.54	128.48	120.03
1	A	303	VAL	CA-C-N	7.53	130.59	120.65
1	A	303	VAL	C-N-CA	7.53	130.59	120.65
1	A	98	ALA	CA-C-N	7.53	131.40	120.71
1	A	98	ALA	C-N-CA	7.53	131.40	120.71
1	A	235	GLY	CA-C-N	7.52	130.04	120.56
1	A	235	GLY	C-N-CA	7.52	130.04	120.56
1	A	275	LEU	CA-C-O	-7.51	113.38	121.56
1	A	254	SER	CA-CB-OG	7.50	126.10	111.10
1	A	53	SER	CB-CA-C	-7.47	95.92	109.38
1	A	309	ALA	CB-CA-C	7.46	122.60	110.88
1	A	90	ARG	NE-CZ-NH1	7.46	128.96	121.50
1	A	170	ASP	N-CA-CB	7.46	121.31	110.20
1	A	186	TRP	O-C-N	7.46	132.19	122.20
1	A	164	ILE	N-CA-CB	7.44	119.26	110.55
1	A	45	LYS	CB-CA-C	-7.44	95.61	110.42
1	A	261	ASP	CA-CB-CG	-7.43	105.17	112.60
1	A	129	THR	O-C-N	-7.43	112.28	122.30
1	A	81	TYR	CA-C-O	7.42	128.41	120.55
1	A	89	ASN	OD1-CG-ND2	7.41	130.01	122.60
1	A	233	ASN	O-C-N	7.39	132.26	122.43
1	A	275	LEU	O-C-N	7.39	131.58	122.86
1	A	70	ALA	O-C-N	-7.38	113.73	122.15
1	A	147	ALA	CB-CA-C	7.38	122.46	110.88
1	A	18	LYS	CG-CD-CE	7.37	128.25	111.30
1	A	135	GLY	CA-C-O	7.36	131.08	119.31
1	A	11	ARG	CA-C-O	-7.35	112.92	120.71
1	A	271	LEU	CA-C-O	-7.33	113.12	120.82
1	A	194	THR	O-C-N	7.33	129.75	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	TYR	CA-C-N	7.33	130.69	120.29
1	A	76	TYR	C-N-CA	7.33	130.69	120.29
1	A	96	ASN	CA-C-N	-7.32	112.19	122.74
1	A	96	ASN	C-N-CA	-7.32	112.19	122.74
1	A	225	GLN	CB-CA-C	7.32	124.68	109.68
1	A	158	GLN	N-CA-CB	7.31	122.89	111.56
1	A	311	ASP	O-C-N	-7.31	113.82	122.15
1	A	172	PHE	CA-CB-CG	-7.30	106.50	113.80
1	A	274	TYR	N-CA-C	7.30	123.31	113.97
1	A	300	SER	CA-C-N	7.28	130.34	120.44
1	A	300	SER	C-N-CA	7.28	130.34	120.44
1	A	85	LYS	N-CA-CB	-7.27	99.37	110.20
1	A	116	ASN	CA-C-O	-7.25	111.08	119.56
1	A	44	ALA	CA-C-N	7.23	135.35	121.54
1	A	44	ALA	C-N-CA	7.23	135.35	121.54
1	A	131	ILE	N-CA-CB	7.23	121.33	111.21
1	A	233	ASN	CA-CB-CG	-7.22	105.38	112.60
1	A	101	ARG	NE-CZ-NH1	7.22	128.72	121.50
1	A	162	GLY	CA-C-O	7.21	127.80	120.09
1	A	226	ASP	CA-C-N	7.18	132.34	122.07
1	A	226	ASP	C-N-CA	7.18	132.34	122.07
1	A	156	ILE	CB-CG1-CD1	-7.18	98.73	113.80
1	A	282	SER	N-CA-CB	-7.16	99.57	110.16
1	A	236	ILE	CB-CG1-CD1	7.15	128.82	113.80
1	A	68	ALA	O-C-N	-7.14	113.77	120.55
1	A	250	HIS	CA-C-O	-7.13	112.60	120.38
1	A	25	SER	CA-CB-OG	-7.13	96.84	111.10
1	A	73	ALA	CA-C-N	7.12	129.69	120.44
1	A	73	ALA	C-N-CA	7.12	129.69	120.44
1	A	183	ASN	CA-CB-CG	7.11	119.71	112.60
1	A	108	GLN	CG-CD-NE2	7.11	127.06	116.40
1	A	52	GLY	CA-C-O	-7.11	114.39	120.64
1	A	253	VAL	CA-C-O	7.11	128.34	120.59
1	A	301	GLN	CA-C-O	7.10	128.01	120.70
1	A	8	GLY	O-C-N	-7.09	113.49	122.70
1	A	274	TYR	N-CA-CB	-7.08	100.83	110.67
1	A	276	THR	CA-C-O	7.08	128.09	120.94
1	A	92	SER	CA-C-N	-7.07	107.79	121.58
1	A	92	SER	C-N-CA	-7.07	107.79	121.58
1	A	198	SER	CA-CB-OG	7.07	125.24	111.10
1	A	71	VAL	CA-C-N	7.07	130.33	120.29
1	A	71	VAL	C-N-CA	7.07	130.33	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	SER	CB-CA-C	-7.02	98.91	110.85
1	A	93	TYR	N-CA-C	7.01	121.66	113.18
1	A	179	TYR	O-C-N	7.00	129.37	122.09
1	A	26	THR	CA-CB-CG2	6.99	122.39	110.50
1	A	60	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	A	79	VAL	CA-C-O	-6.98	113.10	120.57
1	A	11	ARG	NE-CZ-NH2	-6.96	112.93	119.20
1	A	227	ASN	OD1-CG-ND2	-6.94	115.66	122.60
1	A	270	ALA	N-CA-C	-6.91	103.68	111.14
1	A	224	THR	CA-C-N	-6.90	108.41	120.97
1	A	224	THR	C-N-CA	-6.90	108.41	120.97
1	A	236	ILE	O-C-N	-6.90	115.15	121.91
1	A	35	ARG	O-C-N	6.89	131.26	123.27
1	A	167	ALA	CA-C-O	6.89	127.72	120.42
1	A	255	VAL	CA-C-O	6.89	127.66	120.36
1	A	119	GLU	CG-CD-OE2	-6.88	102.57	118.40
1	A	220	ARG	NH1-CZ-NH2	6.86	128.22	119.30
1	A	11	ARG	NH1-CZ-NH2	6.86	128.22	119.30
1	A	191	ASP	CA-C-N	6.84	130.78	122.16
1	A	191	ASP	C-N-CA	6.84	130.78	122.16
1	A	239	LYS	CG-CD-CE	6.84	127.03	111.30
1	A	224	THR	CA-CB-CG2	6.83	122.11	110.50
1	A	283	GLN	CA-CB-CG	-6.83	100.44	114.10
1	A	101	ARG	N-CA-CB	-6.83	98.64	111.00
1	A	211	TYR	CB-CG-CD1	6.76	130.94	120.80
1	A	218	SER	CA-C-N	6.75	133.94	122.26
1	A	218	SER	C-N-CA	6.75	133.94	122.26
1	A	33	ASN	N-CA-CB	-6.75	99.87	110.46
1	A	138	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	313	VAL	CA-C-O	6.72	127.29	119.36
1	A	48	THR	CA-C-N	6.71	131.44	121.72
1	A	48	THR	C-N-CA	6.71	131.44	121.72
1	A	123	GLY	N-CA-C	-6.68	102.38	112.60
1	A	96	ASN	O-C-N	6.68	131.41	122.26
1	A	14	LEU	CA-C-N	6.67	131.65	121.51
1	A	14	LEU	C-N-CA	6.67	131.65	121.51
1	A	55	TRP	CA-C-O	-6.67	113.03	120.70
1	A	129	THR	N-CA-C	-6.65	102.47	112.04
1	A	98	ALA	CA-C-O	-6.64	114.51	121.55
1	A	41	THR	O-C-N	6.63	131.19	123.30
1	A	268	TYR	O-C-N	-6.63	114.12	122.27
1	A	58	ALA	CA-C-O	-6.62	111.11	119.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	LEU	CA-C-N	-6.61	111.24	121.02
1	A	54	LEU	C-N-CA	-6.61	111.24	121.02
1	A	120	MET	CA-C-N	6.60	132.16	122.99
1	A	120	MET	C-N-CA	6.60	132.16	122.99
1	A	138	ASP	OD1-CG-OD2	-6.60	107.06	122.90
1	A	256	VAL	N-CA-C	-6.58	99.10	108.58
1	A	214	PRO	CA-C-O	-6.58	113.93	121.56
1	A	272	THR	N-CA-C	6.57	121.37	113.23
1	A	275	LEU	CB-CA-C	6.56	121.60	109.54
1	A	165	ASN	CB-CG-ND2	6.52	126.18	116.40
1	A	86	ASN	CA-C-O	-6.48	113.04	120.24
1	A	226	ASP	CB-CA-C	-6.48	102.69	111.89
1	A	179	TYR	N-CA-CB	6.48	119.59	109.94
1	A	89	ASN	CA-C-N	-6.47	113.54	122.93
1	A	89	ASN	C-N-CA	-6.47	113.54	122.93
1	A	185	ASP	O-C-N	6.45	130.14	122.72
1	A	197	ILE	O-C-N	-6.43	114.57	122.61
1	A	41	THR	CA-CB-OG1	-6.40	100.00	109.60
1	A	256	VAL	CA-C-O	-6.40	113.48	120.71
1	A	77	ALA	N-CA-CB	6.38	119.61	110.16
1	A	9	VAL	CA-CB-CG1	6.38	121.25	110.40
1	A	220	ARG	O-C-N	-6.38	115.47	123.12
1	A	1	ILE	CA-CB-CG1	-6.36	99.59	110.40
1	A	117	GLY	CA-C-N	-6.35	109.41	121.54
1	A	117	GLY	C-N-CA	-6.35	109.41	121.54
1	A	197	ILE	CA-C-N	-6.35	112.71	122.62
1	A	197	ILE	C-N-CA	-6.35	112.71	122.62
1	A	153	ALA	O-C-N	-6.35	115.39	122.12
1	A	105	HIS	CB-CA-C	-6.34	103.37	111.86
1	A	93	TYR	N-CA-CB	-6.33	99.77	110.41
1	A	99	ALA	CA-C-N	6.33	131.00	122.90
1	A	99	ALA	C-N-CA	6.33	131.00	122.90
1	A	201	SER	CA-C-O	-6.32	114.51	121.28
1	A	114	PHE	CA-CB-CG	6.32	120.12	113.80
1	A	216	HIS	N-CA-C	6.30	119.52	108.75
1	A	234	SER	CA-C-N	6.28	128.04	120.13
1	A	234	SER	C-N-CA	6.28	128.04	120.13
1	A	183	ASN	CB-CG-ND2	6.28	125.82	116.40
1	A	243	LEU	N-CA-CB	-6.27	100.92	110.01
1	A	207	ASP	CA-C-O	-6.26	115.06	121.32
1	A	265	LYS	O-C-N	-6.25	114.10	122.23
1	A	96	ASN	CB-CA-C	-6.25	100.59	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	GLN	OE1-CD-NE2	6.25	128.85	122.60
1	A	273	GLN	OE1-CD-NE2	-6.25	116.35	122.60
1	A	287	ALA	CB-CA-C	-6.25	101.03	110.90
1	A	242	TYR	O-C-N	-6.22	115.66	122.07
1	A	188	ILE	N-CA-C	6.22	116.88	108.17
1	A	33	ASN	CA-C-O	6.21	126.57	119.18
1	A	163	ALA	N-CA-C	-6.20	104.07	111.69
1	A	174	THR	CA-CB-OG1	-6.19	100.32	109.60
1	A	150	ASP	O-C-N	6.18	128.44	122.07
1	A	128	GLN	CA-CB-CG	-6.17	101.77	114.10
1	A	103	SER	CA-CB-OG	6.16	123.43	111.10
1	A	236	ILE	CA-CB-CG2	-6.16	100.04	110.50
1	A	101	ARG	NE-CZ-NH2	-6.15	113.66	119.20
1	A	126	ASP	CA-C-O	-6.14	111.87	119.18
1	A	263	LEU	N-CA-C	-6.14	104.50	111.07
1	A	114	PHE	N-CA-C	6.13	118.17	108.79
1	A	73	ALA	O-C-N	-6.12	115.76	122.07
1	A	101	ARG	O-C-N	-6.12	115.80	123.27
1	A	67	ASP	CB-CG-OD1	6.12	132.47	118.40
1	A	229	GLY	N-CA-C	6.11	124.76	113.76
1	A	7	VAL	O-C-N	6.11	129.80	123.20
1	A	245	SER	CA-C-N	6.11	132.75	121.52
1	A	245	SER	C-N-CA	6.11	132.75	121.52
1	A	54	LEU	N-CA-C	-6.10	101.38	110.23
1	A	5	SER	CA-CB-OG	6.08	123.26	111.10
1	A	167	ALA	CB-CA-C	6.07	121.17	110.85
1	A	21	ASN	CB-CG-OD1	6.03	132.86	120.80
1	A	117	GLY	O-C-N	-6.02	115.43	122.60
1	A	168	ILE	CA-C-O	6.02	127.55	121.17
1	A	247	GLY	O-C-N	-6.01	115.76	122.68
1	A	238	ASN	CA-C-O	-6.01	114.05	120.42
1	A	47	ARG	NH1-CZ-NH2	-5.99	111.51	119.30
1	A	187	GLU	N-CA-C	5.99	119.30	109.72
1	A	50	LEU	N-CA-C	5.98	119.59	110.50
1	A	90	ARG	CG-CD-NE	-5.98	98.84	112.00
1	A	306	VAL	O-C-N	-5.98	115.04	121.80
1	A	256	VAL	CA-C-N	-5.97	113.96	120.71
1	A	256	VAL	C-N-CA	-5.97	113.96	120.71
1	A	231	HIS	CA-C-N	5.97	132.72	121.97
1	A	231	HIS	C-N-CA	5.97	132.72	121.97
1	A	224	THR	N-CA-CB	-5.97	102.65	110.59
1	A	131	ILE	CB-CG1-CD1	-5.97	101.27	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	TRP	N-CA-C	-5.96	98.80	108.52
1	A	260	ARG	CA-C-O	-5.96	111.92	119.31
1	A	65	SER	CB-CA-C	5.96	121.65	110.63
1	A	144	LEU	CD1-CG-CD2	-5.96	97.70	110.80
1	A	179	TYR	CA-C-O	-5.95	114.53	120.90
1	A	191	ASP	O-C-N	-5.95	114.95	122.27
1	A	96	ASN	CA-CB-CG	-5.95	106.66	112.60
1	A	130	PHE	CA-CB-CG	-5.95	107.86	113.80
1	A	221	TYR	CA-C-O	5.94	127.25	120.54
1	A	127	GLY	O-C-N	5.94	129.40	122.45
1	A	64	ALA	O-C-N	-5.93	116.26	122.96
1	A	40	PHE	CA-C-N	5.93	131.35	122.99
1	A	40	PHE	C-N-CA	5.93	131.35	122.99
1	A	178	PHE	CE1-CZ-CE2	-5.93	109.33	120.00
1	A	80	THR	CA-CB-OG1	-5.92	100.72	109.60
1	A	101	ARG	N-CA-C	-5.91	99.37	109.24
1	A	16	ASP	O-C-N	5.89	130.00	123.16
1	A	182	LYS	CB-CA-C	5.88	120.17	111.88
1	A	242	TYR	CA-C-O	-5.88	114.65	120.82
1	A	161	SER	N-CA-C	-5.87	105.02	111.82
1	A	5	SER	N-CA-CB	5.86	118.91	110.06
1	A	133	LEU	CA-C-O	-5.85	112.41	119.49
1	A	166	GLU	CA-C-N	5.82	128.55	120.29
1	A	166	GLU	C-N-CA	5.82	128.55	120.29
1	A	202	LEU	CB-CA-C	5.82	120.02	110.88
1	A	29	TYR	CB-CG-CD2	5.81	129.52	120.80
1	A	222	THR	CA-C-N	-5.81	115.10	122.19
1	A	222	THR	C-N-CA	-5.81	115.10	122.19
1	A	148	VAL	CA-C-N	5.80	128.33	120.38
1	A	148	VAL	C-N-CA	5.80	128.33	120.38
1	A	18	LYS	CA-C-O	-5.80	115.02	121.23
1	A	4	THR	CA-CB-CG2	5.79	120.35	110.50
1	A	104	VAL	O-C-N	5.79	128.78	122.76
1	A	38	GLY	O-C-N	5.79	129.35	122.64
1	A	241	ALA	CA-C-N	5.79	127.96	120.44
1	A	241	ALA	C-N-CA	5.79	127.96	120.44
1	A	45	LYS	N-CA-CB	5.78	120.27	110.49
1	A	151	TYR	N-CA-CB	5.78	119.29	110.44
1	A	289	VAL	N-CA-CB	5.78	117.31	110.55
1	A	295	LEU	N-CA-C	5.78	120.48	112.45
1	A	57	ASP	CA-CB-CG	-5.78	106.82	112.60
1	A	108	GLN	CG-CD-OE1	-5.78	109.24	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	ILE	CA-C-N	5.78	130.24	120.88
1	A	244	ILE	C-N-CA	5.78	130.24	120.88
1	A	89	ASN	CB-CG-OD1	-5.77	109.26	120.80
1	A	87	VAL	O-C-N	-5.76	115.36	122.57
1	A	188	ILE	CA-CB-CG1	-5.76	100.61	110.40
1	A	256	VAL	O-C-N	5.75	129.51	122.95
1	A	289	VAL	CB-CA-C	-5.75	104.61	111.97
1	A	258	ILE	N-CA-C	-5.75	107.14	112.83
1	A	294	ASP	CA-C-N	5.74	133.86	121.64
1	A	294	ASP	C-N-CA	5.74	133.86	121.64
1	A	212	GLY	N-CA-C	5.74	123.27	115.30
1	A	3	GLY	CA-C-N	-5.72	113.62	122.09
1	A	3	GLY	C-N-CA	-5.72	113.62	122.09
1	A	205	MET	N-CA-CB	5.72	118.92	110.33
1	A	249	THR	CA-CB-OG1	-5.72	101.02	109.60
1	A	130	PHE	CB-CA-C	-5.71	97.51	110.07
1	A	196	GLY	CA-C-N	5.71	132.76	122.43
1	A	196	GLY	C-N-CA	5.71	132.76	122.43
1	A	273	GLN	CG-CD-NE2	5.71	124.96	116.40
1	A	313	VAL	O-C-N	-5.70	115.50	122.12
1	A	265	LYS	CB-CG-CD	-5.70	98.19	111.30
1	A	149	THR	CA-CB-CG2	5.70	120.19	110.50
1	A	1	ILE	O-C-N	-5.69	113.89	123.00
1	A	120	MET	CA-C-O	-5.69	114.48	120.80
1	A	27	TYR	CZ-CE2-CD2	-5.68	109.37	119.60
1	A	265	LYS	N-CA-CB	-5.68	101.74	110.20
1	A	215	ASP	N-CA-C	-5.68	104.56	113.02
1	A	192	VAL	CA-C-O	-5.67	113.57	118.96
1	A	83	TYR	O-C-N	5.67	128.13	122.12
1	A	28	TYR	N-CA-CB	5.67	119.45	110.55
1	A	61	GLN	CA-CB-CG	-5.66	102.78	114.10
1	A	107	SER	CA-CB-OG	5.66	122.41	111.10
1	A	114	PHE	CA-C-O	5.65	127.28	121.23
1	A	301	GLN	CG-CD-OE1	5.65	132.10	120.80
1	A	209	ALA	O-C-N	-5.64	115.06	122.39
1	A	288	ALA	N-CA-CB	-5.64	101.82	110.16
1	A	234	SER	N-CA-C	-5.63	105.24	111.71
1	A	190	GLU	CA-C-N	5.62	128.86	120.31
1	A	190	GLU	C-N-CA	5.62	128.86	120.31
1	A	174	THR	OG1-CB-CG2	5.62	120.54	109.30
1	A	176	VAL	N-CA-C	-5.61	105.05	110.72
1	A	161	SER	CA-CB-OG	-5.60	99.91	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	ILE	CA-CB-CG1	-5.59	100.89	110.40
1	A	9	VAL	O-C-N	-5.59	117.12	123.10
1	A	90	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	A	146	HIS	N-CA-C	-5.59	105.19	111.28
1	A	145	THR	CA-C-N	5.57	127.75	120.28
1	A	145	THR	C-N-CA	5.57	127.75	120.28
1	A	267	PHE	CA-C-N	5.57	128.77	120.31
1	A	267	PHE	C-N-CA	5.57	128.77	120.31
1	A	76	TYR	N-CA-C	-5.57	105.36	111.82
1	A	124	ASP	CA-C-N	5.57	128.75	121.85
1	A	124	ASP	C-N-CA	5.57	128.75	121.85
1	A	316	LYS	N-CA-CB	-5.57	101.04	110.50
1	A	299	THR	N-CA-CB	5.56	118.98	110.70
1	A	150	ASP	CA-C-O	-5.55	114.99	120.82
1	A	249	THR	CA-C-O	-5.55	114.53	120.46
1	A	138	ASP	CB-CG-OD1	5.54	131.15	118.40
1	A	135	GLY	O-C-N	-5.54	114.86	122.68
1	A	119	GLU	CA-C-N	5.54	130.90	122.65
1	A	119	GLU	C-N-CA	5.54	130.90	122.65
1	A	260	ARG	CA-CB-CG	5.53	125.16	114.10
1	A	147	ALA	N-CA-C	-5.53	105.16	111.07
1	A	283	GLN	O-C-N	-5.52	115.86	122.15
1	A	31	GLN	O-C-N	-5.51	115.85	123.12
1	A	298	SER	CA-C-O	5.51	128.39	120.51
1	A	254	SER	CA-C-N	5.51	130.65	122.99
1	A	254	SER	C-N-CA	5.51	130.65	122.99
1	A	284	LEU	O-C-N	-5.50	116.29	122.12
1	A	47	ARG	N-CA-C	-5.49	102.04	109.95
1	A	306	VAL	N-CA-C	-5.49	104.23	111.09
1	A	20	ILE	CA-C-O	-5.48	115.47	121.28
1	A	27	TYR	CB-CG-CD1	5.48	129.02	120.80
1	A	34	THR	CA-C-N	-5.47	115.29	123.00
1	A	34	THR	C-N-CA	-5.47	115.29	123.00
1	A	146	HIS	N-CA-CB	5.46	118.15	110.12
1	A	292	ALA	N-CA-C	-5.46	105.22	111.07
1	A	29	TYR	N-CA-C	5.46	118.71	109.76
1	A	223	GLY	O-C-N	5.46	128.39	122.77
1	A	213	ASP	CB-CA-C	5.46	116.56	108.87
1	A	287	ALA	N-CA-C	-5.45	105.26	111.14
1	A	63	PHE	O-C-N	-5.44	115.54	122.34
1	A	155	LEU	CD1-CG-CD2	-5.43	98.85	110.80
1	A	216	HIS	CA-C-N	-5.43	112.46	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	HIS	C-N-CA	-5.43	112.46	120.28
1	A	260	ARG	NH1-CZ-NH2	5.43	126.36	119.30
1	A	4	THR	O-C-N	-5.40	116.90	123.16
1	A	308	GLN	O-C-N	5.38	127.68	122.09
1	A	309	ALA	O-C-N	-5.37	116.53	122.07
1	A	210	LYS	CA-C-N	5.37	131.21	122.67
1	A	210	LYS	C-N-CA	5.37	131.21	122.67
1	A	28	TYR	N-CA-C	-5.35	99.81	108.52
1	A	4	THR	CB-CA-C	5.35	118.35	109.53
1	A	119	GLU	OE1-CD-OE2	5.35	135.73	122.90
1	A	268	TYR	CA-C-O	5.34	126.11	119.97
1	A	293	THR	CB-CA-C	-5.34	100.42	110.67
1	A	9	VAL	CA-C-O	-5.32	114.71	120.67
1	A	40	PHE	CA-C-O	-5.32	114.62	120.36
1	A	237	ILE	CB-CG1-CD1	-5.31	102.66	113.80
1	A	82	ASP	O-C-N	5.31	128.20	122.15
1	A	28	TYR	CA-CB-CG	-5.30	104.36	113.90
1	A	83	TYR	CA-C-O	-5.29	114.94	120.55
1	A	106	TYR	N-CA-CB	-5.29	101.28	110.17
1	A	15	GLY	O-C-N	-5.28	116.10	122.38
1	A	200	ASP	CB-CG-OD1	5.28	130.54	118.40
1	A	183	ASN	CB-CG-OD1	-5.27	110.27	120.80
1	A	215	ASP	CA-C-O	5.27	125.08	119.34
1	A	262	LYS	CB-CA-C	-5.26	101.91	110.85
1	A	150	ASP	CB-CA-C	-5.25	102.63	110.88
1	A	75	TYR	N-CA-CB	-5.25	102.45	110.07
1	A	186	TRP	CZ3-CH2-CZ2	-5.25	114.68	121.50
1	A	144	LEU	CA-C-O	5.24	125.97	120.42
1	A	191	ASP	N-CA-CB	-5.24	102.16	110.28
1	A	24	TYR	CA-C-O	5.23	125.96	120.36
1	A	157	TYR	CA-C-O	-5.23	113.03	120.51
1	A	183	ASN	N-CA-CB	-5.23	101.06	110.37
1	A	218	SER	CB-CA-C	-5.22	100.13	110.27
1	A	266	ILE	CA-C-N	5.22	127.27	120.28
1	A	266	ILE	C-N-CA	5.22	127.27	120.28
1	A	89	ASN	CA-C-O	-5.21	114.52	120.98
1	A	19	ASN	CA-CB-CG	-5.21	107.39	112.60
1	A	27	TYR	CB-CG-CD2	-5.20	113.00	120.80
1	A	73	ALA	N-CA-CB	-5.20	102.47	110.01
1	A	130	PHE	CB-CG-CD1	5.20	129.54	120.70
1	A	262	LYS	N-CA-CB	5.19	117.84	110.16
1	A	25	SER	CA-C-O	-5.19	115.18	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	TRP	CB-CG-CD1	5.18	134.68	126.90
1	A	291	SER	CA-CB-OG	-5.18	100.74	111.10
1	A	126	ASP	N-CA-C	-5.18	106.96	113.28
1	A	23	THR	O-C-N	5.18	129.68	123.36
1	A	114	PHE	CA-C-N	5.16	130.28	123.05
1	A	114	PHE	C-N-CA	5.16	130.28	123.05
1	A	146	HIS	ND1-CG-CD2	-5.16	100.94	106.10
1	A	126	ASP	O-C-N	5.16	129.73	122.41
1	A	131	ILE	CA-CB-CG2	5.16	119.27	110.50
1	A	184	PRO	CA-C-N	5.16	131.40	122.32
1	A	184	PRO	C-N-CA	5.16	131.40	122.32
1	A	22	THR	CA-C-N	5.15	130.98	122.33
1	A	22	THR	C-N-CA	5.15	130.98	122.33
1	A	239	LYS	N-CA-C	-5.14	105.56	111.07
1	A	96	ASN	CB-CG-ND2	-5.14	108.69	116.40
1	A	277	PRO	CA-C-N	-5.14	114.45	122.37
1	A	277	PRO	C-N-CA	-5.14	114.45	122.37
1	A	72	ASP	CA-C-O	-5.14	114.98	120.42
1	A	175	LEU	CA-C-O	5.14	125.86	120.42
1	A	149	THR	CA-C-O	5.13	126.17	120.63
1	A	261	ASP	CB-CG-OD1	-5.13	106.59	118.40
1	A	219	LYS	CA-C-O	5.13	125.00	119.15
1	A	42	TYR	CA-C-N	5.12	129.49	122.84
1	A	42	TYR	C-N-CA	5.12	129.49	122.84
1	A	115	TRP	CB-CA-C	5.12	118.59	110.19
1	A	209	ALA	CA-C-O	5.12	125.68	119.49
1	A	47	ARG	CA-C-O	-5.10	114.84	121.73
1	A	150	ASP	N-CA-CB	5.10	117.40	110.01
1	A	47	ARG	CG-CD-NE	-5.10	100.79	112.00
1	A	130	PHE	O-C-N	5.09	129.33	123.17
1	A	231	HIS	CB-CA-C	-5.08	101.60	110.09
1	A	253	VAL	N-CA-CB	5.07	117.14	111.21
1	A	307	LYS	CA-C-N	5.07	127.39	120.54
1	A	307	LYS	C-N-CA	5.07	127.39	120.54
1	A	58	ALA	N-CA-C	5.05	119.16	112.89
1	A	67	ASP	CA-C-N	5.05	128.44	120.97
1	A	67	ASP	C-N-CA	5.05	128.44	120.97
1	A	100	ILE	CB-CA-C	5.05	117.89	110.98
1	A	276	THR	O-C-N	-5.04	117.03	121.32
1	A	35	ARG	N-CA-CB	-5.04	102.78	110.65
1	A	115	TRP	CD2-CE3-CZ3	5.04	125.14	118.60
1	A	290	GLN	CB-CG-CD	-5.04	104.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ILE	CA-C-O	-5.03	115.10	120.59
1	A	316	LYS	CB-CA-C	5.03	119.65	110.10
1	A	297	GLY	CA-C-O	-5.03	117.87	122.24
1	A	263	LEU	N-CA-CB	5.02	117.29	110.01
1	A	53	SER	CA-CB-OG	-5.01	101.08	111.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2264	120	1
2	A	4	0	0	0	0
3	A	1	0	0	0	0
4	A	23	0	15	3	0
5	A	146	0	0	36	10
All	All	2606	0	2279	120	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 26.

All (120) 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:101:ARG:CD	1:A:101:ARG:CG	1.82	1.54
1:A:92:SER:CB	5:A:451:HOH:O	1.88	1.19
1:A:92:SER:OG	5:A:451:HOH:O	1.65	1.12
1:A:118:SER:N	5:A:442:HOH:O	1.78	1.11
1:A:228:GLY:C	5:A:382:HOH:O	1.94	1.10
1:A:92:SER:HA	5:A:451:HOH:O	1.53	1.09
1:A:308:GLN:HG2	5:A:388:HOH:O	1.52	1.08
1:A:218:SER:HB3	5:A:435:HOH:O	1.54	1.04
1:A:101:ARG:CG	1:A:101:ARG:NE	2.29	0.96
1:A:119:GLU:OE1	5:A:447:HOH:O	1.85	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:HE2	5:A:391:HOH:O	1.72	0.88
1:A:278:THR:HG22	1:A:278:THR:O	1.82	0.80
1:A:228:GLY:CA	5:A:382:HOH:O	2.26	0.80
1:A:219:LYS:CE	5:A:391:HOH:O	2.26	0.80
1:A:111:ASN:O	1:A:112:ASN:HB2	1.83	0.79
1:A:116:ASN:OD1	5:A:442:HOH:O	2.02	0.78
1:A:216:HIS:ND1	5:A:435:HOH:O	2.17	0.78
1:A:137:ILE:HG22	1:A:182:LYS:NZ	2.00	0.77
1:A:269:ARG:NH1	1:A:294:ASP:OD2	2.18	0.76
1:A:228:GLY:HA2	5:A:382:HOH:O	1.85	0.75
1:A:197:ILE:HD13	1:A:197:ILE:N	2.05	0.71
1:A:273:GLN:CG	5:A:372:HOH:O	2.38	0.70
1:A:131:ILE:HB	1:A:132:PRO:CD	2.21	0.69
1:A:280:ASN:ND2	1:A:283:GLN:H	1.90	0.69
1:A:280:ASN:HD22	1:A:280:ASN:C	2.00	0.69
1:A:216:HIS:CE1	5:A:435:HOH:O	2.46	0.68
1:A:150:ASP:HA	5:A:379:HOH:O	1.94	0.67
1:A:273:GLN:HG3	5:A:372:HOH:O	1.94	0.67
1:A:1:ILE:N	1:A:31:GLN:HE22	1.92	0.67
1:A:120:MET:HE3	5:A:408:HOH:O	1.95	0.66
1:A:128:GLN:O	1:A:195:PRO:HD2	1.96	0.66
1:A:191:ASP:HB2	5:A:350:HOH:O	1.94	0.66
1:A:101:ARG:NE	1:A:101:ARG:HG3	2.12	0.65
1:A:144:LEU:O	1:A:147:ALA:HB3	1.96	0.65
1:A:278:THR:O	1:A:278:THR:CG2	2.45	0.65
1:A:273:GLN:HB3	5:A:372:HOH:O	1.97	0.64
1:A:120:MET:SD	1:A:144:LEU:HD23	2.38	0.63
1:A:217:TYR:O	1:A:220:ARG:HB2	1.97	0.63
1:A:187:GLU:OE1	5:A:411:HOH:O	2.15	0.63
1:A:137:ILE:HG22	1:A:182:LYS:HZ3	1.62	0.62
1:A:30:LEU:HB2	1:A:55:TRP:HB3	1.81	0.62
1:A:131:ILE:HG23	1:A:195:PRO:HG3	1.82	0.61
1:A:152:THR:HG21	1:A:272:THR:HG22	1.84	0.59
1:A:126:ASP:OD2	1:A:128:GLN:N	2.31	0.59
1:A:172:PHE:O	1:A:176:VAL:HG23	2.04	0.57
1:A:120:MET:C	1:A:121:VAL:HG23	2.28	0.57
1:A:33:ASN:ND2	5:A:459:HOH:O	2.37	0.56
1:A:137:ILE:H	1:A:182:LYS:HZ2	1.54	0.56
1:A:137:ILE:HG22	1:A:182:LYS:HZ2	1.70	0.56
1:A:188:ILE:HG22	4:A:322:BAN:H15	1.89	0.55
1:A:276:THR:HB	1:A:277:PRO:CD	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLY:N	5:A:382:HOH:O	2.26	0.55
1:A:282:SER:HA	1:A:316:LYS:HD2	1.88	0.55
1:A:92:SER:CA	5:A:451:HOH:O	2.07	0.54
1:A:218:SER:CB	5:A:435:HOH:O	2.30	0.54
1:A:207:ASP:OD1	5:A:361:HOH:O	2.18	0.54
1:A:240:ALA:O	1:A:244:ILE:HG13	2.08	0.53
1:A:308:GLN:CG	5:A:388:HOH:O	2.31	0.53
1:A:285:ARG:HD3	1:A:316:LYS:HD3	1.92	0.51
1:A:271:LEU:HA	1:A:275:LEU:HD12	1.93	0.51
1:A:100:ILE:HD11	5:A:451:HOH:O	2.10	0.51
1:A:273:GLN:CB	5:A:372:HOH:O	2.53	0.51
1:A:4:THR:HG22	1:A:24:TYR:HB3	1.93	0.50
1:A:131:ILE:HB	1:A:132:PRO:HD2	1.93	0.50
1:A:35:ARG:HD2	1:A:39:ILE:HD12	1.92	0.50
1:A:214:PRO:HB3	1:A:219:LYS:HB3	1.92	0.50
1:A:111:ASN:O	1:A:112:ASN:CB	2.56	0.49
1:A:1:ILE:H2	1:A:31:GLN:HE22	1.61	0.48
1:A:32:ASP:OD1	1:A:35:ARG:NH1	2.42	0.48
1:A:298:SER:CB	5:A:424:HOH:O	2.61	0.48
1:A:249:THR:HA	1:A:253:VAL:O	2.14	0.47
1:A:133:LEU:H	1:A:133:LEU:HD12	1.80	0.47
1:A:116:ASN:C	5:A:442:HOH:O	2.57	0.47
1:A:298:SER:HB3	5:A:424:HOH:O	2.14	0.47
1:A:1:ILE:N	1:A:31:GLN:NE2	2.61	0.47
1:A:178:PHE:CD1	1:A:184:PRO:HB2	2.49	0.47
1:A:300:SER:HB2	1:A:302:GLU:OE1	2.15	0.46
1:A:243:LEU:HD12	1:A:243:LEU:HA	1.70	0.46
1:A:258:ILE:HG21	1:A:302:GLU:HA	1.97	0.46
1:A:202:LEU:HD12	1:A:202:LEU:HA	1.78	0.45
1:A:178:PHE:CE1	1:A:184:PRO:HB2	2.51	0.45
1:A:185:ASP:OD2	1:A:187:GLU:HB2	2.17	0.45
1:A:21:ASN:HD22	1:A:21:ASN:HA	1.49	0.44
1:A:139:VAL:HG22	4:A:322:BAN:CZ2	2.47	0.44
1:A:68:ALA:HB3	1:A:69:PRO:HD3	1.98	0.44
1:A:109:GLY:HA2	1:A:125:GLY:O	2.18	0.44
1:A:96:ASN:O	1:A:97:ASN:HB2	2.17	0.43
1:A:217:TYR:N	1:A:313:VAL:O	2.44	0.43
1:A:92:SER:HB2	1:A:97:ASN:HA	1.99	0.43
1:A:166:GLU:HG3	1:A:230:VAL:HG12	2.00	0.43
1:A:167:ALA:CB	1:A:237:ILE:HB	2.49	0.43
1:A:285:ARG:CD	1:A:316:LYS:HD3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLY:C	1:A:197:ILE:HD13	2.43	0.43
1:A:32:ASP:O	1:A:38:GLY:HA2	2.19	0.43
1:A:237:ILE:HA	1:A:237:ILE:HD13	1.71	0.42
1:A:30:LEU:HA	1:A:30:LEU:HD23	1.75	0.42
1:A:221:TYR:CD2	5:A:382:HOH:O	2.71	0.42
1:A:269:ARG:HG3	1:A:273:GLN:HG2	2.00	0.42
1:A:81:TYR:CD2	1:A:81:TYR:C	2.97	0.42
1:A:194:THR:HA	1:A:195:PRO:HD2	1.92	0.42
1:A:76:TYR:OH	1:A:182:LYS:HE3	2.20	0.42
1:A:221:TYR:CE2	5:A:382:HOH:O	2.57	0.42
1:A:21:ASN:HB2	1:A:32:ASP:CG	2.45	0.42
1:A:99:ALA:CB	1:A:101:ARG:NH1	2.82	0.42
1:A:25:SER:O	1:A:27:TYR:N	2.46	0.42
1:A:280:ASN:ND2	1:A:280:ASN:C	2.69	0.42
1:A:130:PHE:HZ	1:A:202:LEU:HD22	1.84	0.42
1:A:156:ILE:HD13	1:A:156:ILE:HG21	1.91	0.42
1:A:197:ILE:N	1:A:197:ILE:CD1	2.75	0.42
1:A:285:ARG:HD3	1:A:316:LYS:NZ	2.35	0.42
1:A:154:GLY:HA2	5:A:379:HOH:O	2.19	0.41
1:A:293:THR:HA	1:A:303:VAL:HG21	2.02	0.41
1:A:142:HIS:CD2	1:A:142:HIS:C	2.99	0.41
1:A:255:VAL:HG11	1:A:309:ALA:HB2	2.03	0.41
1:A:255:VAL:HG22	1:A:308:GLN:HB3	2.03	0.41
1:A:175:LEU:HD12	1:A:175:LEU:HA	1.78	0.41
1:A:120:MET:C	1:A:121:VAL:CG2	2.90	0.41
1:A:90:ARG:NH1	1:A:90:ARG:HG3	2.36	0.41
1:A:226:ASP:OD1	4:A:322:BAN:H29	2.21	0.41
1:A:131:ILE:HG21	1:A:131:ILE:HD13	1.47	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]	1.17	1.03
5:A:369:HOH:O	5:A:407:HOH:O[5_564]	1.19	1.01
5:A:332:HOH:O	5:A:336:HOH:O[10_664]	1.34	0.86
5:A:485:HOH:O	5:A:485:HOH:O[7_555]	1.54	0.66
5:A:436:HOH:O	5:A:447:HOH:O[10_664]	1.78	0.42
5:A:372:HOH:O	5:A:463:HOH:O[5_564]	1.92	0.28
5:A:418:HOH:O	5:A:418:HOH:O[12_565]	1.95	0.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:379:HOH:O	5:A:396:HOH:O[10_664]	1.99	0.21
5:A:333:HOH:O	5:A:337:HOH:O[10_664]	2.10	0.10
1:A:6:THR:CB	5:A:473:HOH:O[12_565]	2.12	0.08

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	314/316 (99%)	297 (95%)	17 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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%)	224 (89%)	28 (11%)	6	7

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

Mol	Chain	Res	Type
1	A	1	ILE
1	A	9	VAL
1	A	20	ILE
1	A	25	SER
1	A	26	THR

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Mol	Chain	Res	Type
1	A	49	THR
1	A	54	LEU
1	A	79	VAL
1	A	89	ASN
1	A	96	ASN
1	A	107	SER
1	A	120	MET
1	A	132	PRO
1	A	144	LEU
1	A	175	LEU
1	A	182	LYS
1	A	197	ILE
1	A	208	PRO
1	A	219	LYS
1	A	224	THR
1	A	225	GLN
1	A	239	LYS
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	31	GLN
1	A	33	ASN
1	A	61	GLN
1	A	97	ASN
1	A	159	ASN
1	A	225	GLN
1	A	227	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 ⓘ

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 ⓘ

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	BAN	A	322	3	20,23,34	4.25	12 (60%)	20,29,45	3.97	12 (60%)

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	BAN	A	322	3	-	9/25/26/35	0/1/1/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	322	BAN	CB2-CA2	-9.95	1.34	1.54
4	A	322	BAN	O1-C1	8.08	1.38	1.23
4	A	322	BAN	CA3-N3	7.28	1.59	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	322	BAN	CB3-CA3	-6.76	1.35	1.52
4	A	322	BAN	CA4-C4	5.38	1.68	1.49
4	A	322	BAN	CE2-CD2	-3.47	1.33	1.38
4	A	322	BAN	C2-N3	3.40	1.41	1.34
4	A	322	BAN	O3-C3	3.14	1.29	1.23
4	A	322	BAN	CE1-CD1	-2.99	1.33	1.38
4	A	322	BAN	O4-C4	2.72	1.35	1.20
4	A	322	BAN	OH1-N1	2.46	1.45	1.40
4	A	322	BAN	C3-N4	2.29	1.39	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	322	BAN	O4-C4-CA4	-10.07	90.53	125.17
4	A	322	BAN	CB3-CA3-C3	6.60	122.65	110.14
4	A	322	BAN	CG2-CB2-CA2	6.13	126.15	113.31
4	A	322	BAN	O3-C3-CA3	-5.74	107.91	120.57
4	A	322	BAN	O2-C2-N3	4.48	130.98	122.96
4	A	322	BAN	CB2-CG2-CD1	-3.91	113.64	120.90
4	A	322	BAN	CA3-C3-N4	3.49	124.51	116.47
4	A	322	BAN	CB3-CA3-N3	3.02	115.92	110.38
4	A	322	BAN	C3-CA3-N3	-2.99	104.18	111.59
4	A	322	BAN	CA3-N3-C2	-2.90	115.21	121.32
4	A	322	BAN	CD2-CG2-CD1	2.83	122.44	118.23
4	A	322	BAN	O3-C3-N4	2.16	127.54	122.98

There are no chirality outliers.

All (9) torsion outliers are listed below:

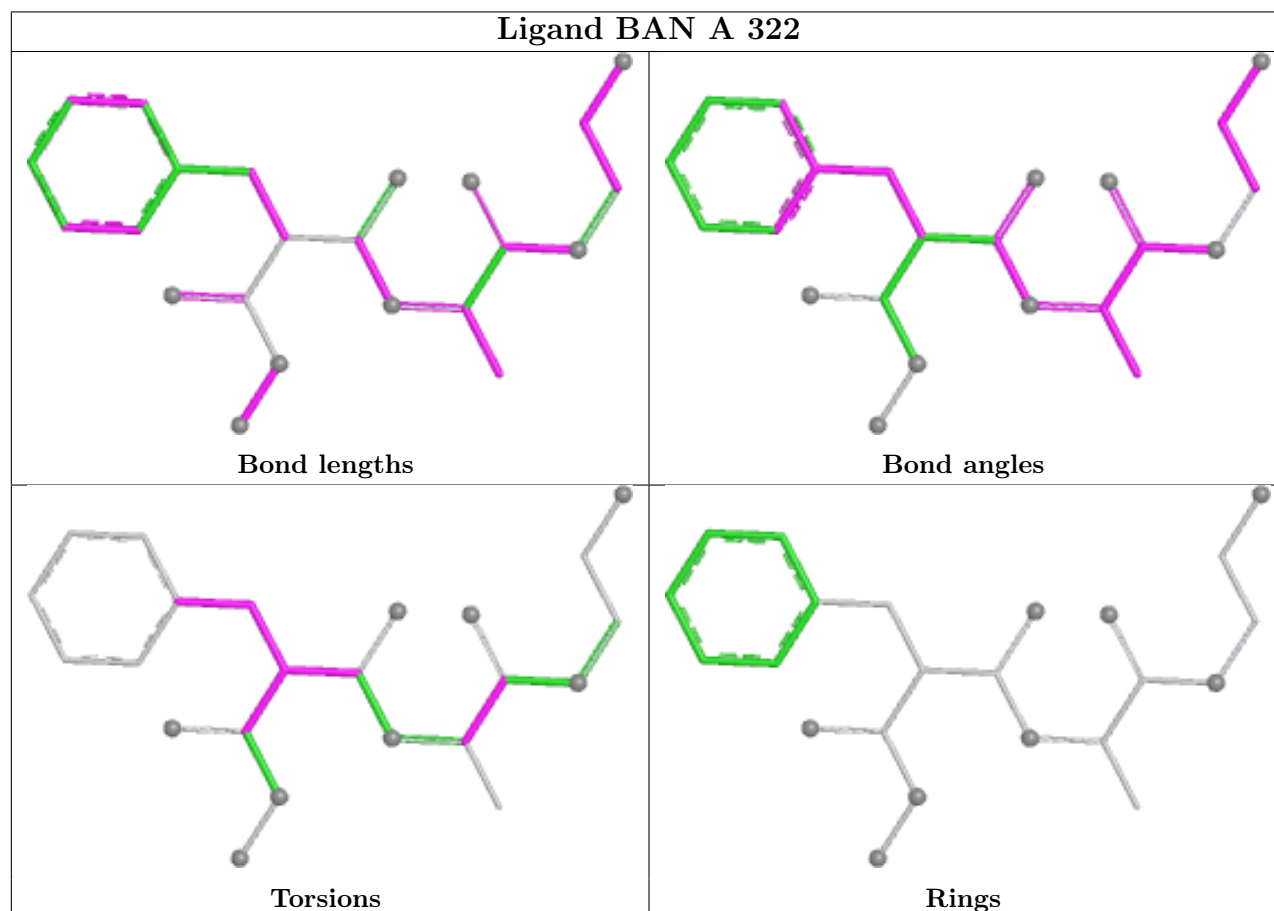
Mol	Chain	Res	Type	Atoms
4	A	322	BAN	N1-C1-CA2-CB2
4	A	322	BAN	O1-C1-CA2-CB2
4	A	322	BAN	C1-CA2-CB2-CG2
4	A	322	BAN	O3-C3-CA3-CB3
4	A	322	BAN	N3-C2-CA2-CB2
4	A	322	BAN	CA2-CB2-CG2-CD1
4	A	322	BAN	CA2-CB2-CG2-CD2
4	A	322	BAN	N4-C3-CA3-CB3
4	A	322	BAN	O2-C2-CA2-CB2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	322	BAN	3	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	260:ARG	C	261:ASP	N	1.18
1	A	10:GLY	C	11:ARG	N	1.16
1	A	35:ARG	C	36:GLY	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%)	-0.78	0 100 100	2, 10, 19, 27	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.

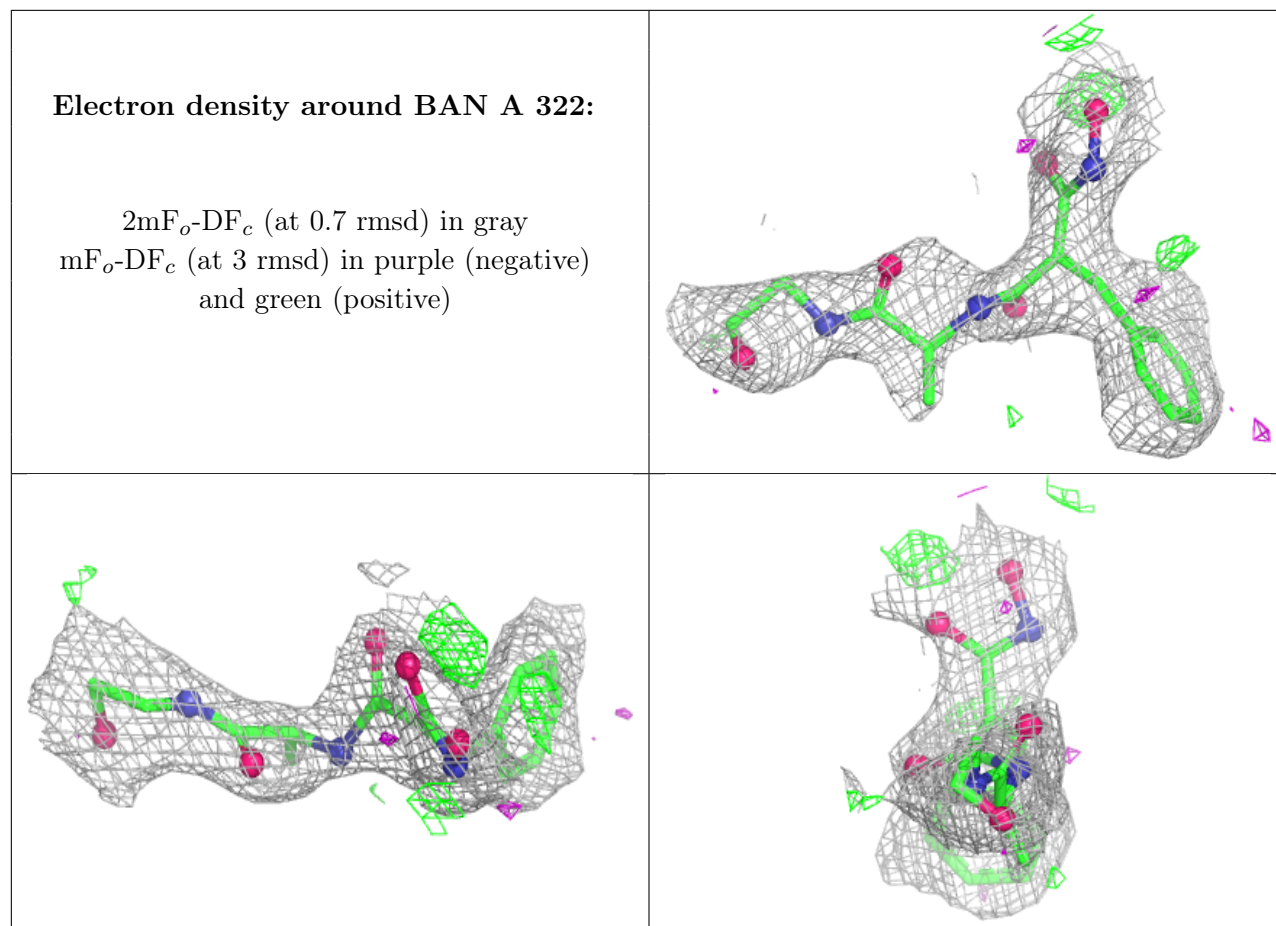
6.4 Ligands [i](#)

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	BAN	A	322	23/33	0.89	0.09	21,23,31,33	0
2	CA	A	319	1/1	0.98	0.02	11,11,11,11	0
2	CA	A	318	1/1	0.98	0.04	13,13,13,13	0
2	CA	A	320	1/1	0.99	0.02	13,13,13,13	0
3	ZN	A	321	1/1	0.99	0.06	16,16,16,16	0
2	CA	A	317	1/1	0.99	0.02	9,9,9,9	0

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

orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.