



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:18 AM UTC

PDB ID : 1IU4 / pdb_00001iu4
Title : Crystal Structure Analysis of the Microbial Transglutaminase
Authors : Kashiwagi, T.; Yokoyama, K.; Ishikawa, K.; Ono, K.; Ejima, D.; Matsui, H.; Suzuki, E.
Deposited on : 2002-02-27
Resolution : 2.40 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
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

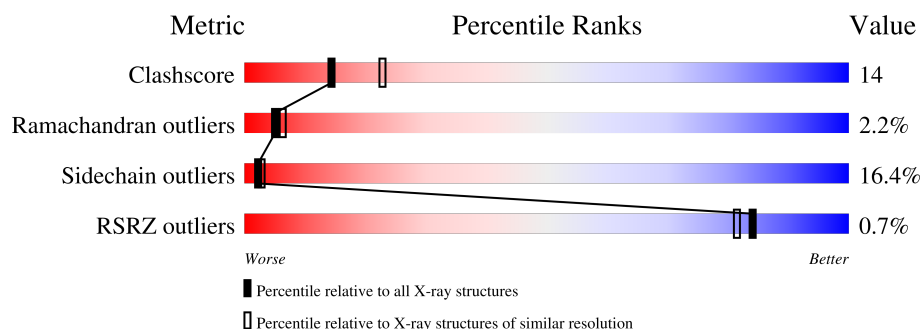
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	331	% 35% 39% 21% 5%
1	B	331	44% 34% 17% 5%
1	C	331	% 39% 40% 17% .
1	D	331	% 36% 38% 19% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11262 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 microbial transglutaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2678	1659	495	517	7			
1	B	331	Total	C	N	O	S	0	0	0
			2678	1659	495	517	7			
1	C	331	Total	C	N	O	S	0	0	0
			2678	1659	495	517	7			
1	D	331	Total	C	N	O	S	0	0	0
			2678	1659	495	517	7			

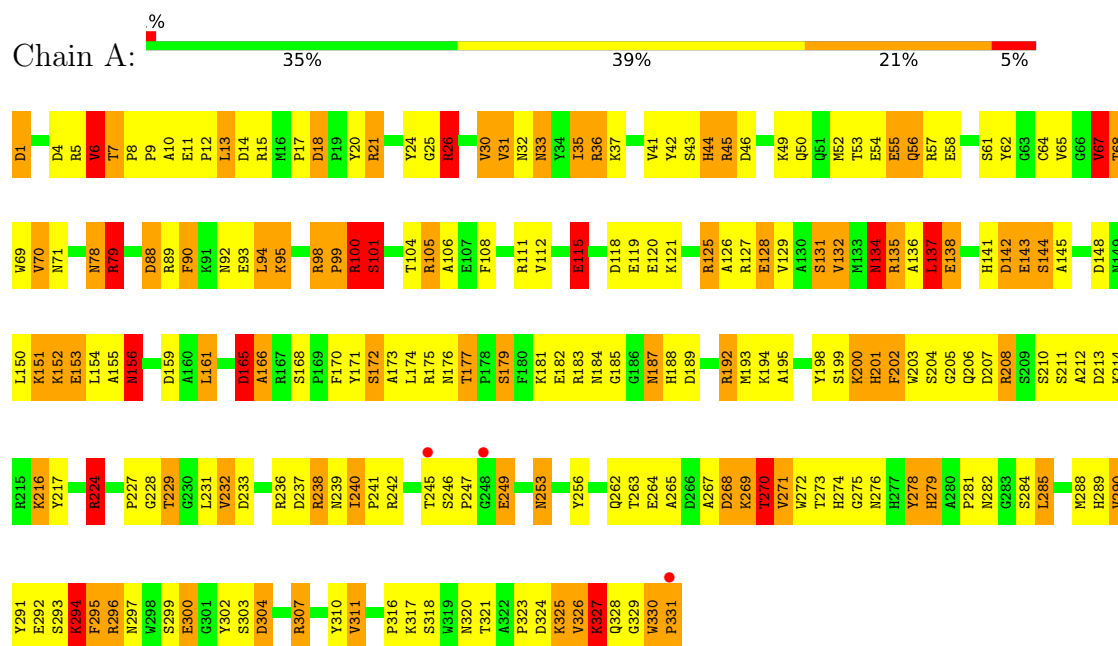
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	147	Total	O	0	0
			147	147		
2	B	157	Total	O	0	0
			157	157		
2	C	154	Total	O	0	0
			154	154		
2	D	92	Total	O	0	0
			92	92		

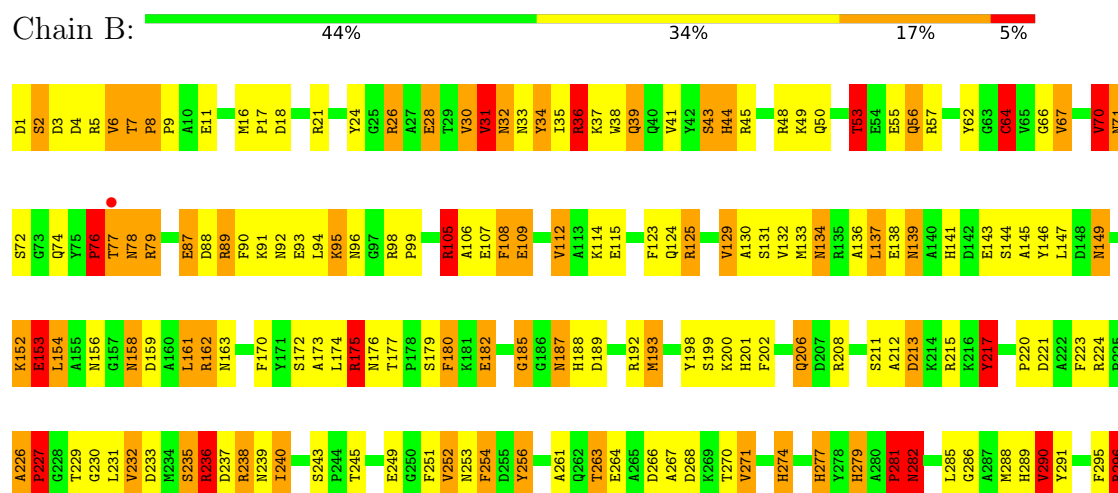
3 Residue-property plots

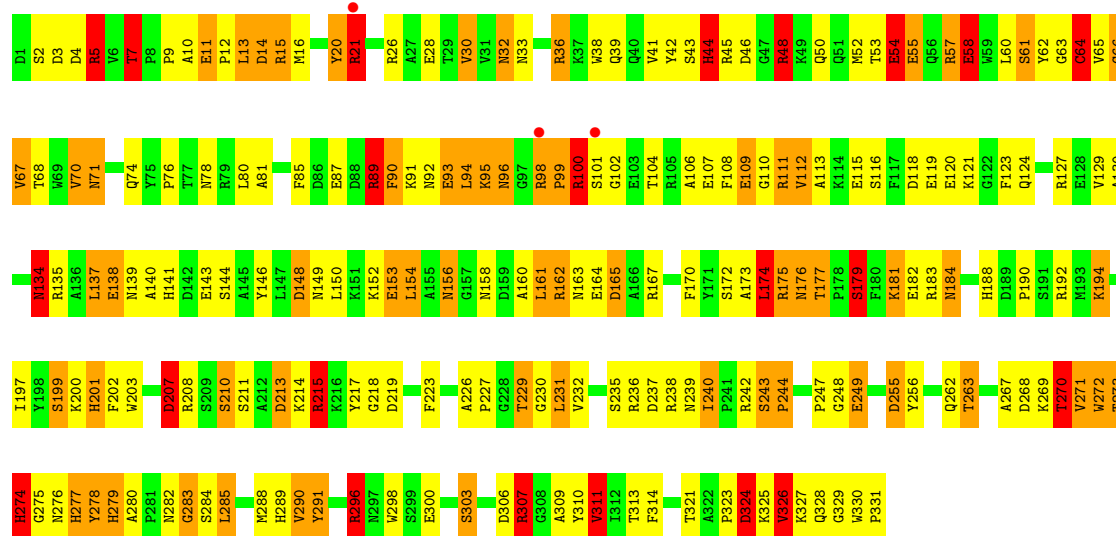
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: microbial transglutaminase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.41Å 117.12Å 85.74Å 90.00° 112.80° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 40.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (40.00-2.40) 98.0 (40.00-2.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.199 , 0.266 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 76.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11262	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.42	16/2755 (0.6%)	2.47	222/3726 (6.0%)
1	B	1.40	16/2755 (0.6%)	2.38	174/3726 (4.7%)
1	C	1.42	17/2755 (0.6%)	2.39	190/3726 (5.1%)
1	D	1.44	13/2755 (0.5%)	2.44	200/3726 (5.4%)
All	All	1.42	62/11020 (0.6%)	2.42	786/14904 (5.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	14
1	B	0	17
1	C	0	17
1	D	0	19
All	All	0	67

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	45	ARG	CA-C	-8.84	1.43	1.52
1	B	98	ARG	CA-C	8.14	1.59	1.52
1	B	45	ARG	NE-CZ	7.74	1.41	1.33
1	B	95	LYS	CA-C	-6.74	1.45	1.53
1	C	201	HIS	ND1-CE1	6.70	1.39	1.32
1	B	44	HIS	ND1-CE1	6.54	1.39	1.32
1	B	8	PRO	CA-C	6.54	1.55	1.51
1	C	277	HIS	CE1-NE2	6.46	1.39	1.32
1	B	277	HIS	CE1-NE2	6.43	1.39	1.32
1	C	64	CYS	CA-CB	6.23	1.63	1.53
1	A	201	HIS	CE1-NE2	6.22	1.38	1.32
1	D	277	HIS	CE1-NE2	6.22	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	HIS	CE1-NE2	6.16	1.38	1.32
1	B	201	HIS	ND1-CE1	6.14	1.38	1.32
1	D	141	HIS	CE1-NE2	6.08	1.38	1.32
1	C	141	HIS	CE1-NE2	6.06	1.38	1.32
1	A	289	HIS	CG-CD2	6.04	1.42	1.35
1	A	279	HIS	ND1-CE1	5.96	1.38	1.32
1	D	274	HIS	ND1-CE1	5.95	1.38	1.32
1	C	64	CYS	CB-SG	5.88	2.00	1.81
1	B	141	HIS	CE1-NE2	5.86	1.38	1.32
1	A	141	HIS	ND1-CE1	5.85	1.38	1.32
1	D	64	CYS	N-CA	5.82	1.53	1.46
1	C	64	CYS	CA-C	5.79	1.60	1.52
1	A	289	HIS	ND1-CE1	5.75	1.38	1.32
1	B	289	HIS	CE1-NE2	5.72	1.38	1.32
1	B	64	CYS	CA-CB	5.69	1.63	1.53
1	D	85	PHE	CA-C	5.68	1.59	1.52
1	C	197	ILE	CA-C	5.62	1.59	1.52
1	D	279	HIS	ND1-CE1	5.62	1.38	1.32
1	D	201	HIS	ND1-CE1	5.61	1.38	1.32
1	A	201	HIS	ND1-CE1	5.58	1.38	1.32
1	C	141	HIS	ND1-CE1	5.55	1.38	1.32
1	B	277	HIS	ND1-CE1	5.54	1.38	1.32
1	A	188	HIS	ND1-CE1	5.53	1.38	1.32
1	C	165	ASP	CA-C	5.51	1.59	1.52
1	D	289	HIS	CE1-NE2	5.50	1.38	1.32
1	A	289	HIS	CE1-NE2	5.43	1.38	1.32
1	A	188	HIS	CE1-NE2	5.42	1.38	1.32
1	C	31	VAL	CA-CB	-5.42	1.47	1.54
1	A	179	SER	CA-C	5.38	1.60	1.52
1	D	64	CYS	CA-C	5.34	1.59	1.52
1	B	245	THR	CA-C	5.32	1.57	1.53
1	D	274	HIS	CE1-NE2	5.32	1.37	1.32
1	C	148	ASP	CA-C	-5.31	1.46	1.52
1	A	31	VAL	CA-CB	-5.29	1.46	1.54
1	C	201	HIS	CG-CD2	5.29	1.41	1.35
1	B	279	HIS	CE1-NE2	5.28	1.37	1.32
1	D	98	ARG	CA-C	5.28	1.57	1.52
1	C	201	HIS	CE1-NE2	5.17	1.37	1.32
1	B	77	THR	CB-OG1	5.17	1.52	1.43
1	D	188	HIS	CE1-NE2	5.17	1.37	1.32
1	C	188	HIS	CE1-NE2	5.16	1.37	1.32
1	C	279	HIS	CE1-NE2	5.14	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	HIS	ND1-CE1	5.12	1.37	1.32
1	B	7	THR	C-N	5.09	1.38	1.33
1	A	231	LEU	CA-C	-5.08	1.46	1.52
1	A	56	GLN	CA-C	5.05	1.59	1.52
1	A	141	HIS	CE1-NE2	5.05	1.37	1.32
1	B	141	HIS	ND1-CE1	5.05	1.37	1.32
1	C	10	ALA	CA-C	-5.02	1.46	1.52
1	D	44	HIS	CE1-NE2	5.01	1.37	1.32

All (786) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	ASP	CA-CB-CG	-13.27	99.33	112.60
1	B	94	LEU	CA-C-N	-13.07	104.12	122.95
1	B	94	LEU	C-N-CA	-13.07	104.12	122.95
1	A	1	ASP	CA-CB-CG	-12.62	99.98	112.60
1	D	65	VAL	N-CA-C	12.27	126.43	111.09
1	D	207	ASP	CA-CB-CG	-11.42	101.18	112.60
1	A	143	GLU	N-CA-C	11.23	123.52	111.28
1	A	31	VAL	CB-CA-C	-11.13	95.81	112.05
1	D	13	LEU	N-CA-C	10.84	125.62	111.75
1	A	204	SER	N-CA-C	10.78	123.11	111.36
1	B	229	THR	N-CA-C	10.73	122.97	111.28
1	B	193	MET	N-CA-C	10.40	123.94	110.53
1	D	127	ARG	N-CA-C	10.24	122.03	111.07
1	B	145	ALA	N-CA-C	9.86	123.05	111.71
1	D	129	VAL	N-CA-C	9.34	120.16	110.36
1	D	215	ARG	N-CA-C	9.33	121.53	111.36
1	B	147	LEU	N-CA-C	9.30	121.02	111.07
1	D	62	TYR	CA-C-N	-9.25	113.10	122.63
1	D	62	TYR	C-N-CA	-9.25	113.10	122.63
1	A	271	VAL	N-CA-C	9.19	121.51	108.36
1	D	289	HIS	CA-C-N	-9.12	111.22	122.90
1	D	289	HIS	C-N-CA	-9.12	111.22	122.90
1	A	121	LYS	N-CA-C	9.04	121.95	111.11
1	D	119	GLU	N-CA-C	9.04	122.30	111.82
1	A	270	THR	N-CA-CB	-8.89	97.36	110.17
1	A	100	ARG	N-CA-C	8.85	123.72	108.76
1	B	56	GLN	N-CA-C	8.78	121.73	111.02
1	D	268	ASP	CA-CB-CG	-8.72	103.88	112.60
1	D	63	GLY	N-CA-C	8.67	120.22	111.21
1	C	64	CYS	CA-C-O	8.65	131.14	121.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	289	HIS	CA-C-N	-8.65	111.83	122.90
1	C	289	HIS	C-N-CA	-8.65	111.83	122.90
1	D	229	THR	CB-CA-C	8.64	122.73	109.34
1	C	156	ASN	N-CA-C	8.58	121.58	111.71
1	C	65	VAL	N-CA-C	8.50	121.67	111.05
1	C	92	ASN	N-CA-C	8.37	122.75	112.54
1	C	245	THR	CA-C-N	8.36	131.88	120.67
1	C	245	THR	C-N-CA	8.36	131.88	120.67
1	A	134	ASN	CA-CB-CG	-8.31	104.29	112.60
1	C	92	ASN	CA-CB-CG	-8.29	104.31	112.60
1	C	242	ARG	CD-NE-CZ	-8.02	113.17	124.40
1	D	98	ARG	CD-NE-CZ	-7.94	113.29	124.40
1	A	249	GLU	N-CA-C	7.90	121.82	108.23
1	C	45	ARG	CA-C-N	-7.88	106.49	121.54
1	C	45	ARG	C-N-CA	-7.88	106.49	121.54
1	A	237	ASP	CA-C-O	7.86	130.06	121.02
1	A	24	TYR	N-CA-C	7.85	121.97	111.30
1	A	179	SER	N-CA-C	7.84	121.78	111.75
1	B	282	ASN	N-CA-C	7.82	127.46	110.80
1	D	290	VAL	N-CA-C	7.79	119.37	107.99
1	A	88	ASP	N-CA-C	7.78	120.89	111.40
1	C	197	ILE	N-CA-C	7.77	119.80	108.53
1	B	271	VAL	N-CA-C	7.74	120.25	108.71
1	D	230	GLY	CA-C-O	7.73	126.28	119.56
1	A	237	ASP	CA-CB-CG	7.70	120.30	112.60
1	C	132	VAL	N-CA-C	7.69	117.80	110.42
1	A	242	ARG	N-CA-C	7.69	121.83	110.30
1	C	242	ARG	CA-C-N	-7.67	110.39	120.67
1	C	242	ARG	C-N-CA	-7.67	110.39	120.67
1	C	253	ASN	N-CA-C	7.67	121.89	112.23
1	B	123	PHE	N-CA-C	7.65	119.26	111.07
1	A	148	ASP	O-C-N	7.64	129.94	122.07
1	A	205	GLY	CA-C-N	-7.62	110.72	122.60
1	A	205	GLY	C-N-CA	-7.62	110.72	122.60
1	B	8	PRO	N-CA-C	7.61	117.78	110.47
1	D	70	VAL	N-CA-C	7.61	118.41	110.72
1	C	94	LEU	N-CA-C	7.61	120.24	111.11
1	C	145	ALA	N-CA-C	7.59	119.24	110.97
1	B	129	VAL	N-CA-C	7.59	117.70	110.42
1	D	271	VAL	N-CA-C	7.58	120.01	108.71
1	C	250	GLY	CA-C-N	-7.57	111.58	122.94
1	C	250	GLY	C-N-CA	-7.57	111.58	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	274	HIS	CA-CB-CG	7.57	121.37	113.80
1	C	215	ARG	N-CA-C	7.56	120.19	111.11
1	C	220	PRO	CA-C-N	-7.54	110.58	122.65
1	C	220	PRO	C-N-CA	-7.54	110.58	122.65
1	C	229	THR	N-CA-C	7.53	119.57	111.36
1	C	7	THR	N-CA-C	7.50	123.01	109.44
1	B	3	ASP	N-CA-C	7.47	122.08	113.19
1	A	88	ASP	CA-CB-CG	-7.44	105.16	112.60
1	B	79	ARG	O-C-N	7.44	130.13	122.09
1	B	296	ARG	N-CA-C	7.44	120.10	111.02
1	B	270	THR	N-CA-C	7.44	121.95	110.20
1	D	13	LEU	CA-C-N	7.42	135.87	122.06
1	D	13	LEU	C-N-CA	7.42	135.87	122.06
1	B	170	PHE	N-CA-C	7.42	119.01	111.07
1	A	269	LYS	CB-CA-C	-7.42	96.65	110.01
1	C	271	VAL	N-CA-C	7.42	119.28	108.53
1	A	328	GLN	CA-C-N	-7.40	109.84	122.21
1	A	328	GLN	C-N-CA	-7.40	109.84	122.21
1	A	303	SER	CA-C-O	7.36	128.26	119.06
1	A	106	ALA	CB-CA-C	-7.35	99.05	110.81
1	A	112	VAL	N-CA-C	7.35	120.24	111.05
1	A	70	VAL	N-CA-C	7.34	118.99	110.62
1	D	4	ASP	CA-C-N	-7.33	110.94	121.42
1	D	4	ASP	C-N-CA	-7.33	110.94	121.42
1	B	8	PRO	CA-C-O	7.31	126.16	120.90
1	B	158	ASN	CA-C-N	-7.31	112.64	122.72
1	B	158	ASN	C-N-CA	-7.31	112.64	122.72
1	C	243	SER	N-CA-C	7.29	120.22	109.50
1	D	283	GLY	CA-C-N	7.29	130.55	120.63
1	D	283	GLY	C-N-CA	7.29	130.55	120.63
1	B	55	GLU	CA-C-N	-7.29	110.66	120.79
1	B	55	GLU	C-N-CA	-7.29	110.66	120.79
1	B	79	ARG	CA-C-N	7.29	133.56	122.77
1	B	79	ARG	C-N-CA	7.29	133.56	122.77
1	C	114	LYS	CA-CB-CG	7.29	128.68	114.10
1	A	302	TYR	N-CA-C	7.29	121.38	109.94
1	A	329	GLY	N-CA-C	7.29	122.37	112.17
1	B	227	PRO	N-CA-C	7.27	127.45	112.47
1	D	285	LEU	CA-C-N	-7.26	108.32	121.32
1	D	285	LEU	C-N-CA	-7.26	108.32	121.32
1	A	328	GLN	N-CA-C	7.25	121.17	110.30
1	A	276	ASN	N-CA-C	7.24	119.17	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	HIS	N-CA-C	7.22	121.93	113.20
1	A	56	GLN	N-CA-C	7.21	119.77	111.11
1	B	36	ARG	NE-CZ-NH2	7.21	125.69	119.20
1	B	285	LEU	N-CA-C	7.19	122.44	112.45
1	D	81	ALA	N-CA-C	7.18	121.20	109.72
1	B	176	ASN	N-CA-C	7.17	120.14	111.82
1	A	299	SER	N-CA-C	7.14	121.81	113.18
1	A	65	VAL	N-CA-C	7.13	120.00	111.09
1	B	252	VAL	N-CA-C	7.12	120.77	110.09
1	A	136	ALA	CA-C-N	-7.08	111.24	122.29
1	A	136	ALA	C-N-CA	-7.08	111.24	122.29
1	C	238	ARG	CD-NE-CZ	7.08	134.31	124.40
1	C	289	HIS	CA-CB-CG	-7.07	106.73	113.80
1	C	129	VAL	N-CA-C	7.07	117.16	110.30
1	B	289	HIS	CA-C-N	-7.05	114.05	122.93
1	B	289	HIS	C-N-CA	-7.05	114.05	122.93
1	C	296	ARG	N-CA-C	7.04	119.56	111.11
1	C	39	GLN	N-CA-C	7.04	118.95	111.28
1	C	211	SER	CA-C-N	-7.01	108.88	121.14
1	C	211	SER	C-N-CA	-7.01	108.88	121.14
1	B	4	ASP	N-CA-C	6.99	119.86	110.35
1	B	162	ARG	CA-C-N	-6.98	111.48	122.65
1	B	162	ARG	C-N-CA	-6.98	111.48	122.65
1	A	43	SER	N-CA-C	6.96	121.79	113.16
1	A	14	ASP	N-CA-C	6.96	118.94	111.36
1	D	275	GLY	CA-C-O	6.96	127.31	121.88
1	B	134	ASN	N-CA-C	6.96	118.51	111.07
1	C	136	ALA	N-CA-C	6.95	119.71	111.71
1	B	26	ARG	N-CA-C	6.93	121.13	109.76
1	B	173	ALA	N-CA-C	6.93	119.68	111.71
1	D	270	THR	N-CA-C	6.93	120.35	109.96
1	B	175	ARG	CA-C-O	6.91	128.09	120.63
1	B	92	ASN	N-CA-C	6.90	121.94	112.90
1	C	57	ARG	N-CA-C	6.89	118.79	111.28
1	C	112	VAL	N-CA-C	6.89	117.65	110.62
1	B	156	ASN	N-CA-C	6.88	120.55	111.75
1	D	279	HIS	CA-C-N	-6.87	114.70	123.16
1	D	279	HIS	C-N-CA	-6.87	114.70	123.16
1	B	92	ASN	CA-C-N	-6.87	110.54	120.29
1	B	92	ASN	C-N-CA	-6.87	110.54	120.29
1	A	152	LYS	N-CA-C	6.84	118.53	111.14
1	A	300	GLU	N-CA-C	6.84	118.39	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	296	ARG	CD-NE-CZ	6.83	133.97	124.40
1	C	170	PHE	N-CA-C	6.83	118.38	111.07
1	C	116	SER	N-CA-C	6.81	121.33	112.89
1	C	48	ARG	CD-NE-CZ	-6.80	114.88	124.40
1	B	267	ALA	N-CA-C	6.80	119.55	111.33
1	A	106	ALA	N-CA-C	6.78	119.25	111.11
1	A	321	THR	CA-C-N	-6.78	115.14	123.21
1	A	321	THR	C-N-CA	-6.78	115.14	123.21
1	B	136	ALA	N-CA-C	6.78	121.01	112.87
1	D	48	ARG	CA-C-N	-6.78	110.30	120.94
1	D	48	ARG	C-N-CA	-6.78	110.30	120.94
1	D	161	LEU	N-CA-CB	-6.78	99.78	110.22
1	A	253	ASN	N-CA-C	6.78	119.68	111.82
1	D	175	ARG	N-CA-C	6.78	119.50	111.71
1	A	237	ASP	N-CA-C	6.74	119.41	108.63
1	B	177	THR	N-CA-C	6.73	119.26	109.71
1	A	206	GLN	N-CA-C	6.72	121.56	112.88
1	C	31	VAL	CB-CA-C	-6.72	100.26	111.29
1	A	262	GLN	N-CA-C	6.72	119.49	110.35
1	C	2	SER	N-CA-C	6.70	119.42	111.71
1	A	18	ASP	CA-CB-CG	6.70	119.30	112.60
1	A	182	GLU	N-CA-C	6.70	121.22	109.96
1	A	10	ALA	N-CA-C	6.68	119.42	109.59
1	D	290	VAL	CA-C-N	-6.68	110.64	122.07
1	D	290	VAL	C-N-CA	-6.68	110.64	122.07
1	A	156	ASN	N-CA-C	6.66	118.62	111.36
1	D	215	ARG	NE-CZ-NH1	6.66	128.16	121.50
1	D	4	ASP	CA-CB-CG	6.65	119.25	112.60
1	D	111	ARG	N-CA-C	6.65	121.61	112.90
1	B	72	SER	CA-C-O	6.65	126.92	119.41
1	B	215	ARG	N-CA-C	6.62	119.34	111.33
1	A	15	ARG	N-CA-C	6.59	120.24	109.76
1	C	268	ASP	N-CA-C	6.58	120.41	112.38
1	D	214	LYS	N-CA-C	6.55	122.18	111.37
1	D	273	THR	N-CA-C	6.55	119.20	108.52
1	A	268	ASP	N-CA-C	6.55	124.75	110.80
1	C	87	GLU	N-CA-C	6.54	120.86	113.01
1	A	240	ILE	CB-CG1-CD1	-6.54	100.06	113.80
1	D	96	ASN	CA-CB-CG	-6.53	106.07	112.60
1	A	270	THR	CA-CB-CG2	6.53	121.59	110.50
1	C	163	ASN	N-CA-C	6.52	120.84	113.02
1	C	26	ARG	CD-NE-CZ	-6.51	115.28	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	VAL	CA-C-O	-6.51	115.59	121.97
1	D	172	SER	N-CA-C	6.51	120.33	112.38
1	D	269	LYS	CA-C-N	6.51	130.07	120.95
1	D	269	LYS	C-N-CA	6.51	130.07	120.95
1	A	170	PHE	N-CA-C	6.51	118.46	111.36
1	B	34	TYR	N-CA-C	6.51	118.04	111.07
1	A	290	VAL	N-CA-C	6.50	117.27	108.17
1	B	290	VAL	N-CA-C	6.49	117.65	108.36
1	A	289	HIS	CA-C-N	-6.49	115.14	123.19
1	A	289	HIS	C-N-CA	-6.49	115.14	123.19
1	C	127	ARG	N-CA-C	6.49	118.36	111.28
1	C	194	LYS	CA-C-N	-6.48	113.55	122.30
1	C	194	LYS	C-N-CA	-6.48	113.55	122.30
1	A	201	HIS	CA-C-N	-6.48	110.72	121.80
1	A	201	HIS	C-N-CA	-6.48	110.72	121.80
1	D	188	HIS	CA-CB-CG	-6.47	107.33	113.80
1	D	313	THR	CA-C-N	-6.46	112.54	122.62
1	D	313	THR	C-N-CA	-6.46	112.54	122.62
1	A	137	LEU	CB-CA-C	6.45	121.21	109.99
1	D	5	ARG	N-CA-CB	6.45	119.80	110.06
1	B	231	LEU	N-CA-C	6.45	119.70	110.10
1	B	220	PRO	CB-CA-C	6.44	121.08	111.68
1	D	329	GLY	N-CA-C	6.43	124.21	112.37
1	D	130	ALA	CA-C-N	-6.42	111.70	120.44
1	D	130	ALA	C-N-CA	-6.42	111.70	120.44
1	D	161	LEU	N-CA-C	6.42	119.09	111.71
1	B	153	GLU	CA-CB-CG	6.42	126.94	114.10
1	C	264	GLU	N-CA-C	6.41	119.78	110.42
1	A	233	ASP	CB-CA-C	6.40	121.37	110.81
1	C	36	ARG	NE-CZ-NH1	6.38	127.88	121.50
1	D	307	ARG	CD-NE-CZ	-6.37	115.48	124.40
1	B	31	VAL	CB-CA-C	-6.37	100.85	111.29
1	A	115	GLU	CB-CA-C	-6.36	97.51	109.72
1	A	155	ALA	CA-C-O	6.36	127.50	120.63
1	B	324	ASP	CA-C-O	6.34	127.26	119.97
1	C	21	ARG	CA-C-O	6.34	124.54	119.59
1	C	165	ASP	CA-CB-CG	6.34	118.94	112.60
1	D	123	PHE	N-CA-C	6.33	117.85	111.07
1	D	284	SER	N-CA-C	6.33	118.06	111.03
1	A	105	ARG	N-CA-C	6.33	118.74	111.02
1	B	109	GLU	N-CA-C	6.32	119.15	111.82
1	C	148	ASP	O-C-N	6.32	129.81	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	LYS	CB-CA-C	-6.31	97.33	109.37
1	C	221	ASP	CB-CA-C	6.29	121.19	110.56
1	D	93	GLU	CA-C-N	-6.29	112.18	121.24
1	D	93	GLU	C-N-CA	-6.29	112.18	121.24
1	C	184	ASN	CA-CB-CG	-6.29	106.31	112.60
1	D	306	ASP	CA-C-O	6.28	125.91	118.69
1	C	121	LYS	CA-C-N	-6.27	112.44	120.34
1	C	121	LYS	C-N-CA	-6.27	112.44	120.34
1	B	286	GLY	CA-C-N	-6.27	111.29	120.75
1	B	286	GLY	C-N-CA	-6.27	111.29	120.75
1	C	85	PHE	N-CA-CB	-6.26	100.89	110.65
1	A	195	ALA	N-CA-C	6.25	119.33	109.96
1	C	36	ARG	CB-CG-CD	6.24	125.66	111.30
1	A	142	ASP	CA-C-N	-6.24	111.92	120.28
1	A	142	ASP	C-N-CA	-6.24	111.92	120.28
1	A	68	THR	N-CA-C	6.24	118.63	111.02
1	B	139	ASN	N-CA-C	6.23	124.08	110.80
1	A	295	PHE	N-CA-C	6.23	118.59	111.11
1	C	174	LEU	CA-C-O	6.22	127.02	120.42
1	A	239	ASN	CB-CA-C	-6.22	103.05	111.89
1	C	306	ASP	CA-C-O	6.22	126.93	119.59
1	D	139	ASN	CA-CB-CG	6.22	118.82	112.60
1	A	174	LEU	N-CA-C	6.21	117.85	111.14
1	A	240	ILE	CA-C-O	6.21	123.22	119.19
1	B	36	ARG	NE-CZ-NH1	-6.20	115.30	121.50
1	A	30	VAL	CB-CA-C	-6.18	103.28	111.13
1	B	32	ASN	CA-C-O	6.18	127.10	120.55
1	D	28	GLU	N-CA-C	6.17	118.69	108.99
1	D	158	ASN	CA-CB-CG	-6.17	106.43	112.60
1	A	125	ARG	N-CA-C	6.17	118.55	111.02
1	A	189	ASP	CB-CA-C	6.16	117.01	110.17
1	B	125	ARG	N-CA-C	6.15	117.65	111.07
1	A	35	ILE	N-CA-C	6.15	116.81	110.36
1	D	53	THR	N-CA-C	6.14	118.83	110.35
1	D	285	LEU	CA-C-O	6.14	126.48	119.18
1	B	202	PHE	N-CA-C	6.13	116.33	108.24
1	A	303	SER	CA-C-N	6.12	133.24	121.54
1	A	303	SER	C-N-CA	6.12	133.24	121.54
1	C	204	SER	N-CA-C	6.12	118.03	111.36
1	D	58	GLU	CA-C-N	6.12	128.80	120.54
1	D	58	GLU	C-N-CA	6.12	128.80	120.54
1	A	90	PHE	CA-C-N	-6.12	110.28	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	PHE	C-N-CA	-6.12	110.28	120.68
1	C	278	TYR	N-CA-C	6.11	118.22	110.33
1	B	176	ASN	CA-CB-CG	-6.11	106.49	112.60
1	A	229	THR	N-CA-C	6.11	118.02	111.36
1	B	230	GLY	CA-C-O	6.10	125.75	119.10
1	C	247	PRO	CA-C-N	-6.10	111.74	122.97
1	C	247	PRO	C-N-CA	-6.10	111.74	122.97
1	C	326	VAL	O-C-N	6.10	129.37	123.14
1	C	263	THR	N-CA-CB	-6.10	101.13	110.16
1	B	221	ASP	CA-C-N	-6.09	112.29	122.64
1	B	221	ASP	C-N-CA	-6.09	112.29	122.64
1	D	229	THR	N-CA-CB	-6.09	101.57	110.40
1	A	56	GLN	N-CA-CB	-6.09	100.87	109.94
1	B	212	ALA	N-CA-C	6.09	118.00	111.36
1	A	172	SER	N-CA-C	6.09	120.17	112.87
1	B	149	ASN	CA-C-O	6.08	126.97	119.97
1	A	132	VAL	N-CA-C	6.08	116.25	110.42
1	A	274	HIS	CA-C-N	-6.07	114.33	120.10
1	A	274	HIS	C-N-CA	-6.07	114.33	120.10
1	C	86	ASP	N-CA-C	6.06	118.33	108.63
1	D	138	GLU	N-CA-C	6.06	119.45	110.48
1	C	328	GLN	N-CA-C	6.06	119.01	110.23
1	B	131	SER	N-CA-C	6.05	118.37	111.11
1	B	285	LEU	CA-C-N	-6.05	112.11	122.21
1	B	285	LEU	C-N-CA	-6.05	112.11	122.21
1	A	148	ASP	CA-C-N	6.04	129.19	120.79
1	A	148	ASP	C-N-CA	6.04	129.19	120.79
1	B	36	ARG	N-CA-C	6.04	117.87	111.28
1	D	96	ASN	CA-C-O	6.04	126.42	119.35
1	C	202	PHE	N-CA-C	6.04	116.40	107.88
1	A	216	LYS	N-CA-C	6.04	121.31	113.88
1	D	90	PHE	N-CA-C	6.04	117.66	111.14
1	C	136	ALA	CA-C-N	-6.03	110.43	121.52
1	C	136	ALA	C-N-CA	-6.03	110.43	121.52
1	D	291	TYR	O-C-N	6.02	129.80	123.06
1	D	30	VAL	CB-CA-C	-6.02	101.42	111.29
1	D	14	ASP	CA-C-O	6.00	126.32	119.18
1	B	295	PHE	N-CA-C	6.00	118.59	111.33
1	D	174	LEU	N-CA-C	6.00	117.62	111.14
1	A	30	VAL	CG1-CB-CG2	5.99	123.99	110.80
1	C	224	ARG	CA-CB-CG	-5.99	102.12	114.10
1	B	251	PHE	CA-CB-CG	-5.99	107.81	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	327	LYS	N-CA-C	5.99	119.16	109.40
1	B	70	VAL	N-CA-C	5.99	116.77	110.72
1	C	64	CYS	CB-CA-C	5.99	120.78	110.84
1	D	30	VAL	CG1-CB-CG2	5.99	123.98	110.80
1	A	155	ALA	N-CA-C	5.98	118.57	111.33
1	A	232	VAL	N-CA-C	5.98	117.20	108.53
1	A	108	PHE	CA-C-N	5.98	128.54	120.65
1	A	108	PHE	C-N-CA	5.98	128.54	120.65
1	C	256	TYR	CB-CA-C	-5.98	99.19	109.65
1	B	8	PRO	CB-CA-C	5.95	116.98	111.39
1	B	227	PRO	N-CA-CB	-5.95	97.01	103.25
1	A	70	VAL	N-CA-CB	5.95	117.90	110.47
1	C	141	HIS	CA-C-O	5.95	126.61	119.59
1	C	161	LEU	N-CA-C	5.95	118.52	111.33
1	D	2	SER	CA-C-N	-5.94	112.83	122.34
1	D	2	SER	C-N-CA	-5.94	112.83	122.34
1	A	317	LYS	CA-CB-CG	5.94	125.98	114.10
1	D	194	LYS	CG-CD-CE	5.94	124.97	111.30
1	D	223	PHE	N-CA-C	5.94	123.45	110.80
1	A	129	VAL	N-CA-C	5.94	116.68	110.62
1	B	282	ASN	CA-CB-CG	5.94	118.54	112.60
1	A	165	ASP	N-CA-CB	-5.93	100.46	110.49
1	A	274	HIS	N-CA-C	5.93	118.05	108.32
1	D	248	GLY	N-CA-C	5.93	121.96	114.25
1	D	327	LYS	CA-C-O	5.93	127.11	120.70
1	C	192	ARG	CD-NE-CZ	-5.92	116.11	124.40
1	A	15	ARG	CD-NE-CZ	-5.92	116.11	124.40
1	A	92	ASN	N-CA-C	5.92	118.97	111.69
1	C	55	GLU	CA-C-O	5.91	127.02	120.63
1	C	238	ARG	CA-CB-CG	5.91	125.92	114.10
1	D	247	PRO	CA-C-N	-5.91	114.04	123.31
1	D	247	PRO	C-N-CA	-5.91	114.04	123.31
1	A	213	ASP	N-CA-C	5.90	118.47	111.33
1	C	279	HIS	CA-C-N	-5.90	116.19	123.21
1	C	279	HIS	C-N-CA	-5.90	116.19	123.21
1	A	227	PRO	CA-C-N	-5.90	109.85	121.41
1	A	227	PRO	C-N-CA	-5.90	109.85	121.41
1	A	293	SER	CB-CA-C	-5.90	100.02	109.75
1	B	231	LEU	CA-C-N	-5.90	115.88	123.19
1	B	231	LEU	C-N-CA	-5.90	115.88	123.19
1	A	1	ASP	CB-CA-C	5.89	121.29	110.10
1	A	175	ARG	CA-C-O	5.89	126.52	119.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	ASP	CA-C-O	5.89	124.30	119.36
1	D	309	ALA	N-CA-C	5.89	119.14	109.72
1	D	325	LYS	N-CA-C	5.89	118.50	108.90
1	D	134	ASN	N-CA-C	5.88	118.17	111.11
1	D	213	ASP	N-CA-C	5.88	117.68	111.28
1	D	5	ARG	CA-CB-CG	5.87	125.85	114.10
1	B	300	GLU	CA-C-O	5.87	126.98	120.82
1	D	9	PRO	CA-C-N	-5.87	113.03	121.42
1	D	9	PRO	C-N-CA	-5.87	113.03	121.42
1	C	20	TYR	N-CA-C	5.86	117.70	108.96
1	C	138	GLU	CA-C-N	-5.86	114.06	122.68
1	C	138	GLU	C-N-CA	-5.86	114.06	122.68
1	B	24	TYR	N-CA-C	5.86	119.48	111.39
1	C	269	LYS	CA-C-O	5.86	126.37	119.28
1	C	311	VAL	N-CA-C	5.86	117.79	108.89
1	B	224	ARG	NE-CZ-NH1	-5.85	115.65	121.50
1	B	162	ARG	CA-CB-CG	5.85	125.79	114.10
1	C	139	ASN	CA-CB-CG	5.85	118.45	112.60
1	A	21	ARG	CB-CA-C	5.84	117.92	109.45
1	A	269	LYS	CA-C-O	5.84	126.35	119.28
1	A	294	LYS	CA-CB-CG	-5.84	102.42	114.10
1	B	87	GLU	CA-C-O	5.83	126.60	120.42
1	A	151	LYS	CG-CD-CE	5.82	124.69	111.30
1	D	269	LYS	CA-C-O	5.82	126.11	119.18
1	D	215	ARG	NE-CZ-NH2	-5.82	113.97	119.20
1	D	112	VAL	N-CA-C	5.82	116.55	110.62
1	B	130	ALA	N-CA-C	5.81	118.36	111.33
1	A	127	ARG	CD-NE-CZ	5.81	132.53	124.40
1	B	185	GLY	CA-C-N	-5.81	110.03	121.41
1	B	185	GLY	C-N-CA	-5.81	110.03	121.41
1	C	84	SER	N-CA-C	5.81	118.42	109.07
1	C	297	ASN	CA-C-N	-5.80	112.90	120.44
1	C	297	ASN	C-N-CA	-5.80	112.90	120.44
1	B	172	SER	N-CA-C	5.80	119.97	113.01
1	B	137	LEU	CB-CA-C	5.79	119.47	109.15
1	A	224	ARG	CA-CB-CG	-5.79	102.51	114.10
1	C	55	GLU	N-CA-C	5.79	118.33	111.33
1	D	153	GLU	CA-C-O	5.79	126.88	120.63
1	A	98	ARG	CB-CA-C	5.78	117.16	109.65
1	D	255	ASP	CA-CB-CG	5.78	118.38	112.60
1	D	118	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	181	LYS	CA-CB-CG	-5.77	102.56	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	249	GLU	N-CA-CB	5.76	118.65	110.46
1	C	1	ASP	CA-CB-CG	-5.76	106.84	112.60
1	C	152	LYS	CA-C-O	5.76	126.64	120.70
1	D	324	ASP	CA-C-O	5.76	126.04	119.18
1	A	166	ALA	CA-C-O	5.76	125.38	119.05
1	B	311	VAL	CA-CB-CG2	5.76	120.19	110.40
1	C	297	ASN	CB-CA-C	-5.76	99.98	110.63
1	C	20	TYR	CA-C-N	5.75	130.26	122.56
1	C	20	TYR	C-N-CA	5.75	130.26	122.56
1	B	325	LYS	CG-CD-CE	5.74	124.51	111.30
1	C	203	TRP	CA-C-O	5.74	126.64	120.38
1	D	249	GLU	N-CA-C	5.74	118.79	108.17
1	D	203	TRP	N-CA-C	5.74	119.17	109.76
1	C	87	GLU	CA-CB-CG	-5.73	102.63	114.10
1	A	101	SER	CA-C-N	-5.73	113.51	122.51
1	A	101	SER	C-N-CA	-5.73	113.51	122.51
1	B	88	ASP	CA-CB-CG	-5.73	106.87	112.60
1	D	194	LYS	CA-CB-CG	5.73	125.55	114.10
1	A	31	VAL	CG1-CB-CG2	5.73	123.40	110.80
1	C	119	GLU	N-CA-C	5.72	117.60	111.36
1	B	7	THR	N-CA-C	5.72	116.86	109.65
1	A	12	PRO	CA-C-N	-5.71	110.44	121.58
1	A	12	PRO	C-N-CA	-5.71	110.44	121.58
1	A	176	ASN	CA-CB-CG	-5.71	106.89	112.60
1	B	45	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	B	187	ASN	CA-C-O	5.71	127.06	120.32
1	A	229	THR	O-C-N	5.71	128.66	122.15
1	D	213	ASP	CB-CA-C	5.70	120.26	110.79
1	A	126	ALA	N-CA-C	5.70	119.33	112.38
1	C	57	ARG	NE-CZ-NH2	-5.70	114.07	119.20
1	C	271	VAL	CB-CA-C	5.69	119.46	110.81
1	A	324	ASP	N-CA-C	5.69	117.56	111.36
1	B	147	LEU	N-CA-CB	-5.68	101.77	110.01
1	D	255	ASP	CB-CA-C	5.68	122.58	110.07
1	A	324	ASP	CA-C-N	-5.68	114.42	122.94
1	A	324	ASP	C-N-CA	-5.68	114.42	122.94
1	D	101	SER	N-CA-C	5.68	122.91	110.80
1	C	66	GLY	N-CA-C	5.68	121.03	114.16
1	C	311	VAL	CA-CB-CG2	5.68	120.06	110.40
1	D	311	VAL	CB-CA-C	5.68	119.88	111.31
1	A	189	ASP	CA-C-O	5.68	124.81	119.59
1	C	25	GLY	CA-C-O	5.67	125.32	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	GLY	CA-C-O	5.67	128.02	121.90
1	D	326	VAL	N-CA-C	5.67	116.64	108.48
1	A	273	THR	N-CA-C	5.67	118.86	109.46
1	C	208	ARG	CA-CB-CG	5.66	125.43	114.10
1	D	231	LEU	N-CA-C	5.66	118.79	110.30
1	D	244	PRO	CA-C-O	5.66	127.21	121.27
1	A	6	VAL	CA-C-N	-5.65	110.20	120.94
1	A	6	VAL	C-N-CA	-5.65	110.20	120.94
1	D	67	VAL	CA-CB-CG2	5.65	120.01	110.40
1	B	182	GLU	CA-CB-CG	5.65	125.40	114.10
1	D	110	GLY	N-CA-C	5.65	119.47	112.64
1	B	152	LYS	N-CA-C	5.64	117.88	111.11
1	C	36	ARG	N-CA-C	5.64	117.10	111.07
1	C	127	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	C	290	VAL	N-CA-C	5.63	116.21	107.99
1	D	94	LEU	N-CA-C	5.63	117.86	109.59
1	D	202	PHE	N-CA-C	5.62	115.97	108.38
1	A	144	SER	CB-CA-C	-5.62	101.52	110.84
1	A	128	GLU	N-CA-C	5.61	117.39	111.28
1	C	160	ALA	N-CA-C	5.61	118.16	111.71
1	C	158	ASN	CA-CB-CG	5.61	118.21	112.60
1	C	233	ASP	N-CA-C	5.61	117.87	108.23
1	B	281	PRO	CA-C-N	5.60	132.24	121.54
1	B	281	PRO	C-N-CA	5.60	132.24	121.54
1	C	216	LYS	N-CA-C	5.60	118.32	111.82
1	D	66	GLY	CA-C-N	-5.60	112.47	120.42
1	D	66	GLY	C-N-CA	-5.60	112.47	120.42
1	D	48	ARG	CA-CB-CG	5.60	125.29	114.10
1	A	13	LEU	N-CA-C	5.59	119.95	113.18
1	B	55	GLU	CA-C-O	5.59	126.69	120.82
1	D	54	GLU	N-CA-C	5.59	117.84	111.02
1	B	114	LYS	N-CA-C	5.59	120.59	111.37
1	D	36	ARG	CB-CG-CD	5.58	124.14	111.30
1	D	199	SER	CA-C-N	-5.58	115.24	123.05
1	D	199	SER	C-N-CA	-5.58	115.24	123.05
1	D	243	SER	N-CA-C	5.58	117.71	109.50
1	B	253	ASN	N-CA-C	5.58	119.26	112.23
1	C	249	GLU	N-CA-C	5.58	118.23	108.52
1	D	274	HIS	N-CA-C	5.58	119.77	112.13
1	D	170	PHE	CA-CB-CG	-5.58	108.22	113.80
1	D	41	VAL	N-CA-C	5.57	116.41	111.90
1	B	309	ALA	CA-C-N	-5.57	114.94	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	ALA	C-N-CA	-5.57	114.94	123.07
1	D	62	TYR	N-CA-C	5.57	119.92	113.18
1	D	107	GLU	CB-CA-C	5.57	120.89	110.70
1	D	175	ARG	CD-NE-CZ	-5.56	116.61	124.40
1	A	99	PRO	CA-C-N	-5.56	114.17	122.74
1	A	99	PRO	C-N-CA	-5.56	114.17	122.74
1	B	31	VAL	CG1-CB-CG2	5.56	123.03	110.80
1	C	303	SER	CA-C-N	5.56	128.28	120.28
1	C	303	SER	C-N-CA	5.56	128.28	120.28
1	D	146	TYR	N-CA-C	5.56	117.42	111.36
1	D	11	GLU	CB-CA-C	5.56	115.67	110.17
1	A	131	SER	N-CA-C	5.55	117.77	111.11
1	D	149	ASN	N-CA-C	5.55	117.33	111.28
1	A	79	ARG	CB-CG-CD	5.55	124.07	111.30
1	B	180	PHE	N-CA-CB	-5.54	101.69	110.28
1	D	32	ASN	N-CA-C	5.54	118.03	111.33
1	B	95	LYS	N-CA-CB	5.53	119.89	110.87
1	A	228	GLY	CA-C-O	5.53	130.19	120.57
1	B	92	ASN	CA-CB-CG	-5.53	107.07	112.60
1	D	98	ARG	N-CA-C	5.53	119.15	109.48
1	C	121	LYS	N-CA-C	5.52	118.06	111.71
1	C	149	ASN	CB-CA-C	-5.52	101.30	110.68
1	A	135	ARG	CB-CG-CD	5.52	123.99	111.30
1	A	203	TRP	N-CA-C	5.52	118.81	109.76
1	D	163	ASN	CA-C-N	-5.52	113.03	120.87
1	D	163	ASN	C-N-CA	-5.52	113.03	120.87
1	B	39	GLN	N-CA-C	5.51	118.81	111.75
1	B	98	ARG	N-CA-C	5.51	119.22	107.91
1	A	208	ARG	CB-CA-C	-5.51	101.64	110.79
1	A	270	THR	CB-CA-C	5.51	119.68	109.54
1	A	17	PRO	N-CA-C	5.51	119.34	111.13
1	D	272	TRP	CA-C-N	-5.50	115.34	123.05
1	D	272	TRP	C-N-CA	-5.50	115.34	123.05
1	C	326	VAL	CA-C-N	5.50	130.76	123.00
1	C	326	VAL	C-N-CA	5.50	130.76	123.00
1	C	25	GLY	CA-C-N	-5.50	112.29	121.64
1	C	25	GLY	C-N-CA	-5.50	112.29	121.64
1	D	89	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	B	306	ASP	CA-C-O	5.50	126.08	119.59
1	C	111	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	A	135	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	A	325	LYS	CA-C-N	-5.49	116.38	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	LYS	C-N-CA	-5.49	116.38	123.19
1	C	175	ARG	N-CA-CB	-5.49	101.76	110.22
1	C	165	ASP	CB-CA-C	5.49	119.36	109.64
1	A	325	LYS	N-CA-C	5.49	118.34	109.40
1	C	301	GLY	CA-C-O	5.48	130.11	120.57
1	C	43	SER	CB-CA-C	-5.48	99.05	109.95
1	B	311	VAL	CB-CA-C	5.48	119.58	111.31
1	D	174	LEU	CA-C-N	-5.48	112.39	120.28
1	D	174	LEU	C-N-CA	-5.48	112.39	120.28
1	B	175	ARG	N-CA-CB	-5.47	101.85	110.06
1	A	126	ALA	CA-C-O	5.47	126.11	119.49
1	A	310	TYR	CA-C-N	-5.46	114.49	122.68
1	A	310	TYR	C-N-CA	-5.46	114.49	122.68
1	C	5	ARG	CG-CD-NE	-5.46	99.98	112.00
1	D	98	ARG	CA-C-N	5.46	126.66	119.84
1	D	98	ARG	C-N-CA	5.46	126.66	119.84
1	C	189	ASP	N-CA-CB	-5.46	103.24	110.17
1	D	113	ALA	N-CA-C	5.46	116.91	111.07
1	A	184	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	108	PHE	CA-CB-CG	-5.45	108.35	113.80
1	D	192	ARG	CB-CG-CD	5.45	123.83	111.30
1	D	7	THR	N-CA-C	5.45	116.52	109.65
1	B	321	THR	N-CA-C	5.45	119.79	113.20
1	A	145	ALA	CA-C-O	5.44	126.51	120.63
1	C	192	ARG	CA-CB-CG	-5.44	103.22	114.10
1	D	93	GLU	CA-C-O	5.44	125.96	119.60
1	D	183	ARG	CA-C-O	5.43	127.04	121.07
1	D	230	GLY	CA-C-N	5.43	129.89	121.26
1	D	230	GLY	C-N-CA	5.43	129.89	121.26
1	D	98	ARG	CA-CB-CG	5.43	124.96	114.10
1	A	242	ARG	CA-C-O	5.42	126.66	120.80
1	D	229	THR	CA-CB-CG2	5.42	119.71	110.50
1	A	187	ASN	CA-CB-CG	5.42	118.02	112.60
1	D	106	ALA	N-CA-C	5.42	118.68	111.75
1	C	319	TRP	CA-C-N	-5.41	114.58	122.86
1	C	319	TRP	C-N-CA	-5.41	114.58	122.86
1	A	95	LYS	N-CA-C	5.41	119.66	112.30
1	B	108	PHE	CA-CB-CG	-5.41	108.39	113.80
1	B	53	THR	N-CA-C	5.40	117.66	110.53
1	D	240	ILE	N-CA-CB	-5.40	104.36	111.21
1	B	106	ALA	N-CA-C	5.39	117.91	111.71
1	A	10	ALA	CA-C-N	-5.39	113.45	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ALA	C-N-CA	-5.39	113.45	120.67
1	A	238	ARG	CA-CB-CG	5.39	124.87	114.10
1	C	138	GLU	N-CA-C	5.38	118.37	110.30
1	B	107	GLU	N-CA-C	5.38	116.95	111.14
1	C	56	GLN	CB-CG-CD	-5.37	103.46	112.60
1	D	120	GLU	N-CA-CB	5.37	118.02	110.12
1	A	318	SER	N-CA-C	5.37	119.00	112.23
1	D	42	TYR	CB-CA-C	-5.36	101.43	110.44
1	C	77	THR	CA-C-O	5.36	125.95	119.31
1	D	15	ARG	CA-C-N	5.36	128.80	120.60
1	D	15	ARG	C-N-CA	5.36	128.80	120.60
1	D	284	SER	CB-CA-C	-5.35	102.65	110.95
1	A	326	VAL	N-CA-C	5.35	115.66	108.17
1	B	7	THR	CB-CA-C	5.35	118.08	109.41
1	C	299	SER	N-CA-C	5.35	119.67	113.20
1	A	217	TYR	N-CA-C	5.35	119.96	113.38
1	A	78	ASN	N-CA-C	5.34	119.38	112.86
1	A	93	GLU	N-CA-CB	5.34	117.94	109.82
1	B	232	VAL	CB-CA-C	5.34	118.79	110.83
1	B	49	LYS	N-CA-CB	5.33	117.85	110.17
1	B	152	LYS	CA-C-O	-5.33	115.19	120.90
1	B	175	ARG	CA-CB-CG	5.33	124.77	114.10
1	B	307	ARG	CB-CG-CD	5.33	123.57	111.30
1	B	235	SER	N-CA-C	5.33	118.57	111.75
1	C	232	VAL	N-CA-C	5.33	116.25	108.58
1	D	244	PRO	N-CA-C	5.32	119.57	110.95
1	D	273	THR	CA-C-N	-5.32	114.58	122.56
1	D	273	THR	C-N-CA	-5.32	114.58	122.56
1	A	168	SER	O-C-N	5.32	127.38	121.43
1	B	43	SER	N-CA-C	5.32	119.03	112.54
1	C	282	ASN	CA-CB-CG	-5.31	107.29	112.60
1	A	176	ASN	CA-C-N	-5.31	112.57	121.17
1	A	176	ASN	C-N-CA	-5.31	112.57	121.17
1	B	329	GLY	N-CA-C	5.31	123.64	112.17
1	C	237	ASP	CA-C-N	-5.31	111.40	121.54
1	C	237	ASP	C-N-CA	-5.31	111.40	121.54
1	C	318	SER	N-CA-C	5.31	119.38	113.01
1	D	98	ARG	CB-CG-CD	-5.30	99.10	111.30
1	D	290	VAL	N-CA-CB	5.30	117.42	111.21
1	C	313	THR	CA-C-N	-5.30	114.99	122.94
1	C	313	THR	C-N-CA	-5.30	114.99	122.94
1	A	331	PRO	N-CA-C	5.30	125.34	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	LEU	N-CA-CB	5.30	118.72	109.72
1	C	14	ASP	N-CA-C	5.30	119.00	112.54
1	D	80	LEU	N-CA-C	5.29	117.94	107.98
1	A	304	ASP	O-C-N	5.29	129.63	122.59
1	C	242	ARG	N-CA-C	5.29	118.02	110.24
1	A	296	ARG	CD-NE-CZ	-5.29	117.00	124.40
1	A	31	VAL	N-CA-C	5.29	118.47	111.17
1	D	182	GLU	CA-C-N	-5.29	113.44	120.79
1	D	182	GLU	C-N-CA	-5.29	113.44	120.79
1	C	263	THR	N-CA-C	5.28	117.12	111.36
1	B	251	PHE	N-CA-C	5.27	117.32	108.73
1	D	68	THR	CA-C-N	5.27	127.66	120.54
1	D	68	THR	C-N-CA	5.27	127.66	120.54
1	D	71	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	A	67	VAL	CA-CB-CG2	5.27	119.36	110.40
1	B	134	ASN	CA-C-N	-5.27	113.43	120.54
1	B	134	ASN	C-N-CA	-5.27	113.43	120.54
1	C	199	SER	CA-C-N	-5.27	115.73	123.00
1	C	199	SER	C-N-CA	-5.27	115.73	123.00
1	A	20	TYR	N-CA-C	5.26	117.68	109.52
1	B	263	THR	N-CA-C	5.26	122.01	110.80
1	A	307	ARG	CA-CB-CG	5.26	124.62	114.10
1	D	179	SER	N-CA-C	5.26	122.00	110.80
1	B	289	HIS	CA-CB-CG	-5.26	108.54	113.80
1	C	31	VAL	CG1-CB-CG2	5.26	122.36	110.80
1	A	296	ARG	N-CA-C	5.25	118.47	111.75
1	C	304	ASP	N-CA-C	5.25	117.75	111.71
1	A	118	ASP	CA-C-N	-5.25	111.76	120.68
1	A	118	ASP	C-N-CA	-5.25	111.76	120.68
1	D	38	TRP	N-CA-C	5.25	116.69	110.97
1	D	303	SER	CB-CA-C	-5.25	100.93	110.63
1	B	213	ASP	N-CA-C	5.24	119.39	112.89
1	C	111	ARG	N-CA-C	5.24	118.14	111.69
1	A	263	THR	CA-C-O	5.24	124.90	119.14
1	A	32	ASN	CA-C-O	5.24	126.32	120.82
1	B	226	ALA	CA-C-N	5.24	126.38	119.84
1	B	226	ALA	C-N-CA	5.24	126.38	119.84
1	B	139	ASN	CA-C-N	-5.23	113.44	120.87
1	B	139	ASN	C-N-CA	-5.23	113.44	120.87
1	B	77	THR	N-CA-C	5.23	121.95	110.80
1	C	322	ALA	N-CA-C	5.23	118.16	109.79
1	A	26	ARG	CB-CA-C	-5.23	100.66	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ASN	CA-CB-CG	-5.23	107.37	112.60
1	A	328	GLN	CG-CD-NE2	-5.22	108.57	116.40
1	A	6	VAL	CA-CB-CG2	5.22	119.27	110.40
1	B	39	GLN	CA-C-N	-5.22	111.81	120.68
1	B	39	GLN	C-N-CA	-5.22	111.81	120.68
1	B	217	TYR	N-CA-C	5.22	121.04	114.31
1	B	254	PHE	CA-CB-CG	5.21	119.01	113.80
1	B	290	VAL	CB-CA-C	5.21	117.93	110.84
1	C	1	ASP	CA-C-N	-5.21	112.78	120.28
1	C	1	ASP	C-N-CA	-5.21	112.78	120.28
1	A	153	GLU	CA-C-O	5.21	126.29	120.82
1	A	172	SER	CB-CA-C	-5.21	98.81	110.21
1	C	106	ALA	N-CA-C	5.21	119.26	113.01
1	D	21	ARG	CB-CG-CD	5.21	123.28	111.30
1	C	238	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	B	67	VAL	N-CA-C	5.20	117.59	111.09
1	B	153	GLU	CA-C-O	5.20	125.76	119.11
1	A	33	ASN	N-CA-C	5.19	116.94	111.28
1	A	55	GLU	CA-C-N	-5.19	113.53	120.54
1	A	55	GLU	C-N-CA	-5.19	113.53	120.54
1	B	236	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	D	111	ARG	N-CA-CB	5.19	118.12	110.33
1	D	167	ARG	CA-C-O	5.19	126.07	119.95
1	A	193	MET	N-CA-C	5.19	117.75	109.81
1	B	3	ASP	CA-C-O	5.18	127.20	118.91
1	D	239	ASN	N-CA-C	5.18	118.58	111.54
1	D	109	GLU	N-CA-C	5.18	116.61	111.07
1	D	98	ARG	NE-CZ-NH2	-5.17	114.54	119.20
1	D	268	ASP	N-CA-C	5.17	119.44	113.18
1	A	49	LYS	CA-CB-CG	5.17	124.44	114.10
1	A	271	VAL	CA-CB-CG2	5.17	119.19	110.40
1	D	235	SER	CB-CA-C	-5.17	100.13	110.42
1	A	192	ARG	N-CA-C	5.17	119.30	113.15
1	B	99	PRO	CA-C-N	-5.16	113.34	121.86
1	B	99	PRO	C-N-CA	-5.16	113.34	121.86
1	D	236	ARG	N-CA-C	5.16	119.43	113.18
1	B	57	ARG	N-CA-C	5.16	118.36	111.75
1	D	211	SER	N-CA-C	5.16	117.72	110.14
1	A	265	ALA	N-CA-C	5.16	118.83	112.54
1	B	105	ARG	CG-CD-NE	5.16	123.34	112.00
1	C	4	ASP	CB-CA-C	-5.16	101.46	109.61
1	C	95	LYS	CA-CB-CG	5.15	124.41	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	VAL	CA-C-N	-5.15	111.15	120.94
1	B	6	VAL	C-N-CA	-5.15	111.15	120.94
1	C	206	GLN	CA-C-N	-5.15	112.05	121.52
1	C	206	GLN	C-N-CA	-5.15	112.05	121.52
1	D	173	ALA	N-CA-C	5.15	117.29	111.11
1	C	236	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	B	279	HIS	N-CA-CB	-5.14	101.98	109.95
1	A	213	ASP	CA-CB-CG	-5.13	107.47	112.60
1	B	162	ARG	CD-NE-CZ	5.13	131.58	124.40
1	D	116	SER	N-CA-C	5.13	119.59	113.23
1	A	327	LYS	N-CA-C	5.13	118.17	109.76
1	C	79	ARG	CA-C-O	5.13	125.67	119.31
1	C	184	ASN	CA-C-N	-5.13	111.36	121.41
1	C	184	ASN	C-N-CA	-5.13	111.36	121.41
1	C	83	ALA	CA-C-N	-5.13	115.92	123.00
1	C	83	ALA	C-N-CA	-5.13	115.92	123.00
1	A	46	ASP	N-CA-C	5.12	118.69	111.52
1	B	193	MET	CA-C-O	5.12	127.83	121.94
1	C	325	LYS	CG-CD-CE	5.12	123.08	111.30
1	C	142	ASP	CA-CB-CG	-5.12	107.48	112.60
1	C	172	SER	N-CA-C	5.12	119.28	113.19
1	C	112	VAL	N-CA-CB	5.12	117.50	110.54
1	A	231	LEU	CA-C-N	-5.11	116.50	123.10
1	A	231	LEU	C-N-CA	-5.11	116.50	123.10
1	D	183	ARG	N-CA-C	5.11	117.26	111.02
1	A	119	GLU	N-CA-C	5.11	118.67	112.23
1	B	163	ASN	N-CA-C	5.11	119.20	112.92
1	A	100	ARG	CA-C-O	5.09	125.97	120.32
1	A	330	TRP	CB-CA-C	5.09	116.93	110.16
1	C	326	VAL	N-CA-C	5.09	115.91	108.53
1	B	227	PRO	CA-N-CD	-5.09	104.88	112.00
1	A	127	ARG	N-CA-C	5.09	117.95	111.69
1	A	236	ARG	NE-CZ-NH2	5.08	123.78	119.20
1	C	320	ASN	N-CA-C	5.08	118.97	112.26
1	A	247	PRO	N-CA-C	5.08	120.21	113.86
1	B	88	ASP	CB-CA-C	5.08	120.75	110.38
1	B	206	GLN	CA-C-O	5.08	125.84	119.59
1	D	95	LYS	N-CA-C	5.08	121.62	110.80
1	A	138	GLU	CA-C-O	5.08	125.93	120.55
1	C	125	ARG	CA-C-N	-5.08	113.08	120.29
1	C	125	ARG	C-N-CA	-5.08	113.08	120.29
1	C	291	TYR	CA-C-N	5.08	130.26	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	291	TYR	C-N-CA	5.08	130.26	122.95
1	C	153	GLU	CA-CB-CG	-5.08	103.95	114.10
1	B	130	ALA	CA-C-O	5.07	126.11	120.63
1	A	94	LEU	N-CA-C	5.07	121.60	110.80
1	A	108	PHE	N-CA-C	5.07	117.19	111.11
1	C	5	ARG	NE-CZ-NH2	-5.06	114.64	119.20
1	C	252	VAL	N-CA-C	5.06	116.09	109.21
1	B	71	ASN	N-CA-C	5.06	117.69	111.82
1	D	33	ASN	N-CA-C	5.06	117.69	111.82
1	B	76	PRO	N-CA-C	5.06	122.89	112.47
1	A	61	SER	N-CA-C	5.05	121.56	110.80
1	C	44	HIS	CA-C-N	-5.05	114.20	122.79
1	C	44	HIS	C-N-CA	-5.05	114.20	122.79
1	D	188	HIS	N-CA-C	5.05	119.29	113.38
1	D	270	THR	CA-CB-CG2	5.05	119.08	110.50
1	A	165	ASP	N-CA-C	5.04	121.55	110.80
1	A	176	ASN	N-CA-C	5.04	119.58	113.38
1	B	114	LYS	CA-C-O	5.04	126.57	120.92
1	B	64	CYS	CA-C-O	5.04	127.71	120.51
1	C	179	SER	N-CA-C	5.04	118.53	112.38
1	D	239	ASN	CA-C-O	5.04	127.38	121.54
1	A	132	VAL	CB-CA-C	-5.04	105.53	111.97
1	A	292	GLU	CA-CB-CG	-5.03	104.03	114.10
1	D	181	LYS	CA-C-N	-5.03	114.64	122.09
1	D	181	LYS	C-N-CA	-5.03	114.64	122.09
1	D	111	ARG	CA-C-N	-5.02	113.58	120.46
1	D	111	ARG	C-N-CA	-5.02	113.58	120.46
1	C	192	ARG	N-CA-C	5.02	119.13	113.15
1	B	307	ARG	CB-CA-C	5.02	119.62	109.68
1	A	175	ARG	CA-C-N	-5.01	113.59	122.26
1	A	175	ARG	C-N-CA	-5.01	113.59	122.26
1	C	105	ARG	CA-C-N	-5.01	111.26	121.18
1	C	105	ARG	C-N-CA	-5.01	111.26	121.18
1	A	330	TRP	CA-C-O	5.01	124.28	119.72
1	B	124	GLN	N-CA-C	5.01	117.12	111.11
1	B	199	SER	CA-C-N	5.00	130.06	123.00
1	B	199	SER	C-N-CA	5.00	130.06	123.00
1	D	92	ASN	N-CA-C	5.00	117.47	111.71
1	A	43	SER	CA-C-O	5.00	125.33	119.28
1	B	30	VAL	CA-CB-CG1	5.00	118.90	110.40
1	C	285	LEU	N-CA-C	5.00	116.73	111.28
1	D	263	THR	CA-CB-CG2	5.00	119.00	110.50

There are no chirality outliers.

All (67) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	A	166	ALA	Peptide
1	A	183	ARG	Sidechain
1	A	202	PHE	Sidechain
1	A	224	ARG	Sidechain
1	A	238	ARG	Sidechain
1	A	26	ARG	Sidechain
1	A	278	TYR	Sidechain
1	A	282	ASN	Peptide
1	A	300	GLU	Peptide
1	A	36	ARG	Sidechain
1	A	42	TYR	Sidechain
1	A	45	ARG	Sidechain
1	A	62	TYR	Sidechain
1	B	105	ARG	Sidechain
1	B	175	ARG	Sidechain
1	B	198	TYR	Sidechain
1	B	208	ARG	Sidechain
1	B	217	TYR	Sidechain
1	B	226	ALA	Peptide
1	B	254	PHE	Sidechain
1	B	256	TYR	Sidechain
1	B	281	PRO	Peptide
1	B	296	ARG	Sidechain
1	B	307	ARG	Sidechain
1	B	34	TYR	Sidechain
1	B	36	ARG	Sidechain
1	B	5	ARG	Sidechain
1	B	62	TYR	Sidechain
1	B	76	PRO	Peptide
1	B	89	ARG	Sidechain
1	C	100	ARG	Peptide
1	C	105	ARG	Sidechain
1	C	162	ARG	Sidechain
1	C	175	ARG	Sidechain
1	C	192	ARG	Sidechain
1	C	20	TYR	Peptide
1	C	206	GLN	Peptide
1	C	208	ARG	Peptide
1	C	21	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	217	TYR	Sidechain
1	C	24	TYR	Sidechain
1	C	242	ARG	Sidechain
1	C	291	TYR	Sidechain
1	C	302	TYR	Sidechain
1	C	307	ARG	Sidechain
1	C	48	ARG	Sidechain
1	C	75	TYR	Sidechain
1	D	100	ARG	Peptide
1	D	102	GLY	Peptide
1	D	111	ARG	Sidechain
1	D	156	ASN	Peptide
1	D	20	TYR	Peptide
1	D	21	ARG	Sidechain
1	D	215	ARG	Sidechain
1	D	218	GLY	Peptide
1	D	238	ARG	Sidechain
1	D	274	HIS	Peptide
1	D	278	TYR	Sidechain
1	D	282	ASN	Peptide
1	D	307	ARG	Sidechain
1	D	310	TYR	Sidechain
1	D	324	ASP	Peptide
1	D	45	ARG	Peptide
1	D	57	ARG	Sidechain
1	D	95	LYS	Peptide
1	D	98	ARG	Sidechain

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	2678	0	2486	75	0
1	B	2678	0	2486	62	0
1	C	2678	0	2486	84	0
1	D	2678	0	2486	77	0
2	A	147	0	0	3	0
2	B	157	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	154	0	0	3	0
2	D	92	0	0	1	0
All	All	11262	0	9944	292	0

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 14.

All (292) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:THR:HG21	1:D:314:PHE:HB2	1.64	0.79
1:D:207:ASP:HB3	1:D:210:SER:HB3	1.66	0.78
1:C:242:ARG:HD2	1:C:251:PHE:CE1	2.21	0.75
1:D:5:ARG:HB3	1:D:278:TYR:HD1	1.53	0.74
1:D:39:GLN:HA	1:D:43:SER:HB3	1.69	0.73
1:C:31:VAL:HG22	1:C:288:MET:O	1.90	0.72
1:C:22:PRO:HA	1:C:26:ARG:O	1.90	0.71
1:D:262:GLN:HG2	1:D:326:VAL:HG13	1.73	0.71
1:D:280:ALA:O	1:D:283:GLY:HA2	1.89	0.70
1:C:25:GLY:HA2	1:C:294:LYS:HE3	1.73	0.70
1:C:155:ALA:HB2	1:C:162:ARG:HD3	1.74	0.69
1:D:267:ALA:O	1:D:270:THR:HB	1.93	0.69
1:C:148:ASP:HA	1:C:151:LYS:NZ	2.07	0.69
1:C:242:ARG:HB3	1:C:251:PHE:CD1	2.29	0.68
1:C:325:LYS:HE2	1:C:325:LYS:HA	1.75	0.67
1:A:90:PHE:O	1:A:94:LEU:HB2	1.95	0.67
1:D:20:TYR:HB2	1:D:21:ARG:HD3	1.78	0.66
1:D:64:CYS:HB3	1:D:255:ASP:HA	1.78	0.65
1:A:207:ASP:HB3	1:A:210:SER:HB2	1.79	0.65
1:A:330:TRP:HA	1:A:331:PRO:C	2.21	0.65
1:A:67:VAL:O	1:A:71:ASN:HB2	1.97	0.65
1:C:167:ARG:HH11	1:C:167:ARG:HB3	1.61	0.64
1:C:212:ALA:O	1:C:216:LYS:HG2	1.97	0.64
1:D:44:HIS:HA	1:D:48:ARG:O	1.97	0.64
1:B:159:ASP:OD1	1:B:161:LEU:HB2	1.97	0.64
1:A:267:ALA:O	1:A:270:THR:HB	1.98	0.63
1:D:199:SER:HB3	1:D:298:TRP:CZ2	2.33	0.63
1:B:279:HIS:HD2	1:B:288:MET:H	1.45	0.63
1:B:134:ASN:O	1:B:138:GLU:HG2	1.98	0.63
1:A:18:ASP:H	1:A:33:ASN:HD21	1.47	0.62
1:B:37:LYS:O	1:B:41:VAL:HG22	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ASN:HA	1:B:311:VAL:HG21	1.82	0.62
1:D:154:LEU:HB3	1:D:162:ARG:HG2	1.82	0.61
1:C:5:ARG:HH22	1:C:7:THR:HG22	1.65	0.61
1:C:267:ALA:O	1:C:270:THR:HB	2.00	0.61
1:C:185:GLY:HA3	1:C:316:PRO:HB3	1.83	0.61
1:A:53:THR:HB	1:A:56:GLN:HB2	1.82	0.60
1:A:279:HIS:HD2	1:A:288:MET:H	1.47	0.60
1:C:15:ARG:HG2	1:C:36:ARG:HD2	1.83	0.60
1:C:83:ALA:HB3	1:C:225:PRO:HG3	1.83	0.60
1:D:201:HIS:HE1	1:D:298:TRP:O	1.85	0.60
1:A:159:ASP:OD1	1:A:161:LEU:HB2	2.02	0.60
1:B:39:GLN:HA	1:B:43:SER:HB3	1.84	0.59
1:A:278:TYR:CE2	1:A:285:LEU:HD12	2.37	0.59
1:D:134:ASN:O	1:D:137:LEU:HB2	2.03	0.58
1:A:54:GLU:O	1:A:58:GLU:HG3	2.03	0.58
1:C:154:LEU:HB3	1:C:162:ARG:HB2	1.85	0.58
1:C:205:GLY:O	1:C:215:ARG:HD2	2.03	0.58
1:D:213:ASP:HB2	1:D:217:TYR:HD1	1.67	0.58
1:B:238:ARG:HB2	1:B:240:ILE:HG23	1.86	0.58
1:C:148:ASP:HA	1:C:151:LYS:HZ1	1.67	0.58
1:B:125:ARG:NH2	1:B:161:LEU:HD22	2.19	0.57
1:A:179:SER:OG	1:A:316:PRO:HD3	2.05	0.57
1:C:5:ARG:NH2	1:C:7:THR:HG22	2.19	0.57
1:D:135:ARG:HB2	1:D:153:GLU:OE1	2.04	0.57
1:B:87:GLU:HG3	1:B:91:LYS:HE3	1.87	0.57
1:A:111:ARG:O	1:A:115:GLU:HG3	2.05	0.56
1:B:277:HIS:O	1:B:288:MET:HG3	2.05	0.56
1:A:210:SER:OG	1:A:214:LYS:HB2	2.04	0.56
1:C:37:LYS:HG3	1:C:330:TRP:CE3	2.40	0.56
1:C:244:PRO:HB3	1:C:249:GLU:O	2.06	0.56
1:A:270:THR:CG2	1:A:272:TRP:HE1	2.17	0.56
1:D:60:LEU:O	1:D:288:MET:HE1	2.06	0.55
1:C:293:SER:HB3	1:C:297:ASN:HB2	1.88	0.55
1:D:93:GLU:HB3	1:D:112:VAL:HG11	1.88	0.55
1:D:307:ARG:HG2	2:D:334:HOH:O	2.07	0.55
1:C:85:PHE:CZ	1:C:224:ARG:HD3	2.42	0.54
1:A:152:LYS:O	1:A:156:ASN:HB2	2.07	0.54
1:A:327:LYS:HE2	1:A:331:PRO:OXT	2.06	0.54
1:D:256:TYR:O	1:D:274:HIS:HB3	2.08	0.54
1:D:330:TRP:HA	1:D:331:PRO:C	2.31	0.54
1:A:269:LYS:HE2	1:B:115:GLU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:HIS:HD2	1:C:288:MET:H	1.56	0.54
1:D:90:PHE:CZ	1:D:94:LEU:HD11	2.43	0.54
1:D:161:LEU:CD1	1:D:231:LEU:HD21	2.38	0.54
1:A:94:LEU:O	1:A:95:LYS:HD2	2.08	0.53
1:A:173:ALA:O	1:A:177:THR:HG22	2.09	0.53
1:D:279:HIS:HD2	1:D:288:MET:H	1.55	0.53
1:D:161:LEU:HD13	1:D:231:LEU:HD21	1.89	0.53
1:A:100:ARG:HG2	1:A:100:ARG:HH11	1.73	0.53
1:B:35:ILE:O	1:B:39:GLN:HG3	2.09	0.53
1:C:18:ASP:H	1:C:33:ASN:HD21	1.57	0.53
1:B:31:VAL:HG22	1:B:288:MET:O	2.09	0.53
1:C:206:GLN:HB2	1:C:238:ARG:NH1	2.23	0.53
1:C:12:PRO:HD2	1:C:15:ARG:CZ	2.39	0.53
1:A:330:TRP:HA	1:A:331:PRO:O	2.08	0.52
1:C:241:PRO:HB3	1:C:253:ASN:HA	1.92	0.52
1:D:277:HIS:ND1	1:D:285:LEU:HD13	2.24	0.52
1:C:270:THR:HG22	1:C:295:PHE:HB2	1.92	0.52
1:D:99:PRO:HA	1:D:108:PHE:CD2	2.43	0.52
1:A:53:THR:HG22	1:A:55:GLU:H	1.74	0.52
1:D:150:LEU:O	1:D:154:LEU:HB2	2.10	0.52
1:C:206:GLN:O	1:C:240:ILE:HD11	2.09	0.51
1:A:125:ARG:NH2	1:A:161:LEU:HD22	2.25	0.51
1:A:270:THR:HG22	1:A:295:PHE:HB2	1.92	0.51
1:A:44:HIS:CD2	1:A:44:HIS:H	2.27	0.51
1:C:296:ARG:HB3	1:D:296:ARG:CZ	2.39	0.51
1:D:5:ARG:HH22	1:D:7:THR:HG22	1.75	0.51
1:B:159:ASP:O	1:B:162:ARG:HB3	2.11	0.51
1:B:233:ASP:OD1	1:B:236:ARG:HD2	2.10	0.51
1:C:24:TYR:HA	1:D:300:GLU:HG2	1.92	0.51
1:C:28:GLU:OE1	1:C:289:HIS:HD2	1.93	0.51
1:C:31:VAL:O	1:C:35:ILE:HG13	2.10	0.51
1:B:256:TYR:O	1:B:274:HIS:HB3	2.11	0.51
1:A:187:ASN:HB2	1:A:192:ARG:HH21	1.75	0.51
1:B:288:MET:HE2	1:B:290:VAL:HG12	1.92	0.51
1:D:90:PHE:CE1	1:D:94:LEU:HD11	2.45	0.51
1:C:128:GLU:O	1:C:132:VAL:HG23	2.11	0.50
1:D:134:ASN:HA	1:D:137:LEU:HD22	1.92	0.50
1:D:270:THR:HG22	1:D:272:TRP:HE1	1.76	0.50
2:A:439:HOH:O	1:B:268:ASP:HB2	2.10	0.50
1:C:223:PHE:HB2	1:C:307:ARG:HD3	1.93	0.50
1:D:176:ASN:C	1:D:176:ASN:HD22	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PRO:HD3	1:A:253:ASN:HB3	1.94	0.50
1:B:44:HIS:H	1:B:44:HIS:CD2	2.29	0.50
1:B:206:GLN:NE2	1:B:238:ARG:H	2.10	0.50
1:C:7:THR:HG21	1:C:58:GLU:HG2	1.93	0.50
1:C:45:ARG:O	1:C:318:SER:O	2.29	0.50
1:D:270:THR:CG2	1:D:272:TRP:HE1	2.24	0.50
1:D:323:PRO:HG2	1:D:326:VAL:HG12	1.94	0.50
1:A:37:LYS:O	1:A:41:VAL:HG22	2.12	0.49
1:A:279:HIS:HD2	1:A:288:MET:N	2.11	0.49
1:B:316:PRO:HD2	1:B:319:TRP:CE2	2.48	0.49
1:C:206:GLN:HB2	1:C:238:ARG:HH11	1.76	0.49
1:B:133:MET:HE2	1:B:146:TYR:OH	2.13	0.49
1:A:330:TRP:CG	1:A:331:PRO:HA	2.48	0.49
1:C:67:VAL:HG13	2:C:338:HOH:O	2.11	0.49
1:A:53:THR:HG22	1:A:55:GLU:N	2.28	0.48
1:B:105:ARG:NH1	1:B:109:GLU:OE2	2.45	0.48
1:B:189:ASP:HB3	1:B:192:ARG:HG3	1.95	0.48
1:A:35:ILE:HG23	1:A:52:MET:HE3	1.94	0.48
1:B:18:ASP:H	1:B:33:ASN:HD21	1.60	0.48
1:C:303:SER:HB3	2:C:471:HOH:O	2.12	0.48
1:D:100:ARG:HE	1:D:100:ARG:HB3	1.54	0.48
1:B:6:VAL:HG21	1:B:281:PRO:HD2	1.95	0.48
1:B:200:LYS:NZ	1:B:237:ASP:OD1	2.45	0.48
1:C:148:ASP:HA	1:C:151:LYS:HZ3	1.76	0.48
1:D:213:ASP:HB2	1:D:217:TYR:CD1	2.47	0.48
1:D:60:LEU:HA	1:D:66:GLY:HA3	1.96	0.48
1:A:26:ARG:HG3	1:A:297:ASN:HD22	1.79	0.47
1:B:213:ASP:O	1:B:217:TYR:HB2	2.14	0.47
1:D:94:LEU:HD22	1:D:109:GLU:HG2	1.96	0.47
1:A:200:LYS:HE3	1:A:256:TYR:CZ	2.49	0.47
1:B:132:VAL:HG11	1:B:154:LEU:HD13	1.97	0.47
1:C:100:ARG:O	1:C:103:GLU:HB2	2.13	0.47
1:A:320:ASN:O	1:A:323:PRO:HD3	2.14	0.47
1:B:235:SER:OG	1:B:236:ARG:HG3	2.15	0.47
1:D:11:GLU:HA	1:D:12:PRO:HD3	1.78	0.47
1:A:25:GLY:HA2	1:A:294:LYS:HZ1	1.80	0.47
1:B:138:GLU:CD	1:B:317:LYS:HZ3	2.23	0.47
1:D:10:ALA:O	1:D:12:PRO:HD3	2.14	0.47
1:D:138:GLU:C	1:D:140:ALA:H	2.22	0.47
1:C:18:ASP:N	1:C:33:ASN:HD21	2.12	0.47
1:D:87:GLU:O	1:D:91:LYS:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ILE:HG21	1:A:240:ILE:HD13	1.64	0.46
1:B:206:GLN:HE22	1:B:238:ARG:H	1.64	0.46
1:C:184:ASN:O	1:C:185:GLY:O	2.34	0.46
1:C:262:GLN:CD	1:C:326:VAL:HG13	2.40	0.46
1:A:128:GLU:O	1:A:132:VAL:HG23	2.15	0.46
1:B:180:PHE:HB2	1:B:193:MET:HE2	1.97	0.46
1:A:100:ARG:HH11	1:A:100:ARG:CG	2.29	0.46
1:B:16:MET:HA	1:B:17:PRO:HD3	1.87	0.46
1:B:264:GLU:HG3	1:B:266:ASP:H	1.79	0.46
1:A:135:ARG:HH12	1:A:153:GLU:CD	2.23	0.46
1:B:179:SER:O	1:B:185:GLY:O	2.34	0.46
1:C:85:PHE:CE2	1:C:116:SER:HB2	2.50	0.46
1:C:296:ARG:HB3	1:D:296:ARG:NE	2.30	0.46
1:D:10:ALA:HB2	1:D:57:ARG:CZ	2.45	0.46
1:D:244:PRO:HB3	1:D:249:GLU:O	2.15	0.46
1:D:213:ASP:O	1:D:217:TYR:N	2.48	0.46
1:D:61:SER:HA	1:D:288:MET:HE1	1.98	0.46
1:C:32:ASN:H	1:C:32:ASN:ND2	2.13	0.46
1:C:120:GLU:HG3	1:C:295:PHE:HE1	1.81	0.46
1:C:196:VAL:HG11	1:C:315:ILE:HG12	1.98	0.46
1:B:90:PHE:CD2	1:B:112:VAL:HG23	2.51	0.45
1:B:8:PRO:HA	1:B:9:PRO:HD3	1.72	0.45
1:A:179:SER:O	1:A:185:GLY:O	2.34	0.45
1:C:195:ALA:HB2	1:C:314:PHE:CE2	2.52	0.45
1:C:243:SER:HA	1:C:244:PRO:HD3	1.80	0.45
1:C:30:VAL:HG22	1:C:289:HIS:CE1	2.52	0.45
1:A:78:ASN:HA	1:A:311:VAL:HG21	1.98	0.45
1:A:199:SER:HB2	1:A:272:TRP:CZ3	2.52	0.45
1:D:330:TRP:HA	1:D:331:PRO:O	2.16	0.45
1:B:187:ASN:O	1:B:188:HIS:HB2	2.17	0.45
1:D:10:ALA:HB2	1:D:57:ARG:NH2	2.32	0.45
1:B:143:GLU:OE2	1:B:175:ARG:HB2	2.17	0.45
1:C:15:ARG:HD2	2:C:454:HOH:O	2.16	0.45
1:C:147:LEU:O	1:C:151:LYS:HG3	2.17	0.45
1:C:207:ASP:CG	1:C:238:ARG:HH12	2.25	0.45
1:A:8:PRO:O	1:A:57:ARG:HD2	2.17	0.45
1:B:132:VAL:HG13	1:B:153:GLU:HG3	1.98	0.45
1:A:165:ASP:O	1:A:171:TYR:HD1	1.99	0.44
1:D:197:ILE:HG23	1:D:311:VAL:O	2.17	0.44
1:A:142:ASP:OD2	1:A:144:SER:HB2	2.18	0.44
1:B:125:ARG:O	1:B:129:VAL:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:TYR:O	1:C:35:ILE:C	2.60	0.44
1:A:8:PRO:HA	1:A:9:PRO:HD2	1.78	0.44
1:B:11:GLU:CD	1:B:36:ARG:HH11	2.25	0.44
1:A:291:TYR:CD1	1:A:291:TYR:N	2.86	0.44
1:D:55:GLU:O	1:D:58:GLU:HB3	2.17	0.44
1:A:270:THR:HG23	1:A:272:TRP:HE1	1.82	0.44
1:D:243:SER:HA	1:D:244:PRO:HD3	1.87	0.44
1:A:98:ARG:HA	1:A:99:PRO:HD3	1.70	0.44
1:D:148:ASP:CG	1:D:152:LYS:HZ2	2.24	0.44
1:C:270:THR:CG2	1:C:272:TRP:HE1	2.30	0.44
1:A:279:HIS:CD2	1:A:288:MET:H	2.32	0.43
1:C:216:LYS:NZ	1:C:244:PRO:O	2.43	0.43
1:B:66:GLY:O	1:B:70:VAL:HG13	2.17	0.43
1:C:187:ASN:O	1:C:188:HIS:HB2	2.17	0.43
1:D:89:ARG:HH21	1:D:115:GLU:HB3	1.83	0.43
1:A:211:SER:O	1:A:212:ALA:C	2.59	0.43
1:D:11:GLU:OE2	1:D:15:ARG:HD2	2.19	0.43
1:D:226:ALA:HA	1:D:227:PRO:HD3	1.80	0.43
1:A:198:TYR:CZ	1:A:311:VAL:HG22	2.53	0.43
1:A:200:LYS:HE3	1:A:256:TYR:OH	2.18	0.43
1:C:32:ASN:H	1:C:32:ASN:HD22	1.66	0.43
1:B:74:GLN:HE21	1:B:74:GLN:HB3	1.68	0.43
1:A:294:LYS:NZ	1:B:300:GLU:OE2	2.50	0.43
1:A:296:ARG:HB2	1:B:296:ARG:HB3	2.00	0.43
1:C:203:TRP:CZ2	1:C:218:GLY:N	2.87	0.43
1:A:79:ARG:HD3	2:A:435:HOH:O	2.17	0.43
1:A:161:LEU:HD13	1:A:229:THR:HG22	2.00	0.43
1:B:32:ASN:O	1:B:36:ARG:HG3	2.18	0.43
1:C:19:PRO:HA	1:C:330:TRP:O	2.19	0.43
1:D:148:ASP:OD1	1:D:152:LYS:NZ	2.52	0.43
1:A:199:SER:HB2	1:A:272:TRP:HZ3	1.84	0.43
1:A:275:GLY:HA3	1:A:288:MET:HE3	2.00	0.42
1:C:205:GLY:O	1:C:215:ARG:NH1	2.50	0.42
1:A:45:ARG:HD2	1:A:50:GLN:OE1	2.19	0.42
1:A:134:ASN:HA	1:A:137:LEU:HD22	2.00	0.42
1:A:201:HIS:O	1:A:202:PHE:HB3	2.18	0.42
1:C:26:ARG:HD3	1:C:291:TYR:CD2	2.53	0.42
1:C:125:ARG:NH2	1:C:161:LEU:HD22	2.34	0.42
1:D:54:GLU:OE1	1:D:57:ARG:NH1	2.51	0.42
1:D:194:LYS:NZ	1:D:324:ASP:OD2	2.52	0.42
1:C:176:ASN:HD22	1:C:176:ASN:HA	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ARG:HH11	1:D:5:ARG:HD3	1.71	0.42
1:A:18:ASP:H	1:A:33:ASN:ND2	2.14	0.42
1:B:53:THR:H	1:B:56:GLN:HE21	1.67	0.42
1:C:25:GLY:HA2	1:C:294:LYS:CE	2.45	0.42
1:C:223:PHE:HB2	1:C:307:ARG:CD	2.49	0.42
1:A:100:ARG:O	1:A:101:SER:C	2.63	0.42
1:A:327:LYS:HD2	1:A:327:LYS:O	2.20	0.42
1:B:28:GLU:C	1:B:28:GLU:OE2	2.63	0.42
1:C:59:TRP:CE3	1:C:69:TRP:CD1	3.08	0.42
1:A:6:VAL:HG13	1:A:281:PRO:HD2	2.02	0.42
1:C:206:GLN:HB3	1:C:240:ILE:HG12	2.02	0.42
1:C:216:LYS:O	1:C:242:ARG:NH2	2.49	0.42
1:C:17:PRO:HG3	1:C:37:LYS:N	2.35	0.42
1:A:150:LEU:O	1:A:151:LYS:C	2.61	0.41
1:B:26:ARG:HD3	1:B:291:TYR:CD2	2.55	0.41
1:C:35:ILE:O	1:C:39:GLN:HG3	2.20	0.41
1:C:84:SER:OG	1:C:118:ASP:HB3	2.19	0.41
1:D:39:GLN:HG2	1:D:52:MET:H	1.84	0.41
1:B:108:PHE:O	1:B:112:VAL:HG13	2.20	0.41
1:C:164:GLU:O	1:C:171:TYR:HE1	2.04	0.41
1:C:240:ILE:HA	1:C:241:PRO:HD3	1.93	0.41
1:D:184:ASN:OD1	1:D:184:ASN:N	2.53	0.41
1:D:200:LYS:NZ	1:D:237:ASP:OD2	2.52	0.41
1:A:5:ARG:HA	1:A:279:HIS:O	2.20	0.41
1:C:37:LYS:NZ	1:C:292:GLU:OE1	2.50	0.41
1:B:38:TRP:HE1	1:B:71:ASN:HD21	1.67	0.41
1:D:39:GLN:HE21	1:D:39:GLN:HB2	1.71	0.41
2:A:439:HOH:O	1:B:266:ASP:HB3	2.20	0.41
1:B:105:ARG:O	1:B:109:GLU:HG3	2.21	0.41
1:C:94:LEU:HD12	1:C:94:LEU:HA	1.73	0.41
1:C:330:TRP:HA	1:C:331:PRO:C	2.45	0.41
1:D:143:GLU:OE2	1:D:175:ARG:NH1	2.53	0.41
1:A:68:THR:O	1:A:69:TRP:C	2.62	0.41
1:B:2:SER:O	1:B:282:ASN:HB2	2.20	0.41
1:D:197:ILE:HG21	1:D:197:ILE:HD13	1.82	0.41
1:B:18:ASP:N	1:B:33:ASN:HD21	2.18	0.41
1:B:90:PHE:HD2	1:B:112:VAL:HG23	1.84	0.41
1:D:276:ASN:HB3	1:D:291:TYR:HE1	1.85	0.41
1:A:1:ASP:HB3	1:A:4:ASP:OD2	2.21	0.41
1:A:307:ARG:HH11	1:A:307:ARG:HD2	1.70	0.41
1:B:223:PHE:HB2	1:B:307:ARG:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:THR:O	1:B:264:GLU:C	2.63	0.41
1:C:207:ASP:HA	1:C:238:ARG:NH2	2.36	0.41
1:D:215:ARG:HH22	1:D:240:ILE:CG2	2.33	0.41
1:A:11:GLU:CD	1:A:36:ARG:HH11	2.29	0.41
1:B:53:THR:H	1:B:56:GLN:NE2	2.18	0.41
1:C:207:ASP:CG	1:C:236:ARG:HH11	2.28	0.41
1:D:164:GLU:O	1:D:165:ASP:C	2.63	0.41
1:D:174:LEU:HD11	1:D:190:PRO:HG3	2.02	0.41
1:A:5:ARG:HH22	1:A:7:THR:HG22	1.86	0.40
1:B:18:ASP:H	1:B:33:ASN:ND2	2.18	0.40
1:C:208:ARG:N	1:C:210:SER:H	2.19	0.40
1:D:71:ASN:HA	1:D:321:THR:HG21	2.02	0.40
1:D:276:ASN:HB3	1:D:291:TYR:CE1	2.56	0.40
1:D:26:ARG:HH11	1:D:26:ARG:HD2	1.77	0.40
1:D:242:ARG:NH1	1:D:303:SER:O	2.54	0.40

There are no symmetry-related clashes.

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	329/331 (99%)	298 (91%)	26 (8%)	5 (2%)	8	12
1	B	329/331 (99%)	294 (89%)	26 (8%)	9 (3%)	4	4
1	C	329/331 (99%)	300 (91%)	26 (8%)	3 (1%)	14	22
1	D	329/331 (99%)	281 (85%)	36 (11%)	12 (4%)	2	2
All	All	1316/1324 (99%)	1173 (89%)	114 (9%)	29 (2%)	5	6

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	ASP
1	B	227	PRO
1	B	249	GLU
1	C	185	GLY
1	D	44	HIS
1	D	100	ARG
1	A	101	SER
1	A	304	ASP
1	B	76	PRO
1	B	96	ASN
1	B	261	ALA
1	B	282	ASN
1	D	160	ALA
1	D	179	SER
1	D	210	SER
1	A	264	GLU
1	D	165	ASP
1	D	296	ARG
1	A	268	ASP
1	B	64	CYS
1	B	77	THR
1	D	36	ARG
1	C	261	ALA
1	D	46	ASP
1	D	76	PRO
1	D	99	PRO
1	B	78	ASN
1	C	301	GLY
1	D	64	CYS

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	279/279 (100%)	233 (84%)	46 (16%)	2	3
1	B	279/279 (100%)	230 (82%)	49 (18%)	2	2
1	C	279/279 (100%)	244 (88%)	35 (12%)	4	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	279/279 (100%)	226 (81%)	53 (19%)	1	2
All	All	1116/1116 (100%)	933 (84%)	183 (16%)	2	3

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	7	THR
1	A	13	LEU
1	A	21	ARG
1	A	30	VAL
1	A	31	VAL
1	A	64	CYS
1	A	67	VAL
1	A	70	VAL
1	A	79	ARG
1	A	88	ASP
1	A	89	ARG
1	A	100	ARG
1	A	101	SER
1	A	104	THR
1	A	115	GLU
1	A	120	GLU
1	A	131	SER
1	A	134	ASN
1	A	137	LEU
1	A	138	GLU
1	A	143	GLU
1	A	154	LEU
1	A	156	ASN
1	A	161	LEU
1	A	165	ASP
1	A	172	SER
1	A	177	THR
1	A	194	LYS
1	A	208	ARG
1	A	216	LYS
1	A	224	ARG
1	A	232	VAL
1	A	245	THR
1	A	246	SER
1	A	249	GLU

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Mol	Chain	Res	Type
1	A	270	THR
1	A	271	VAL
1	A	284	SER
1	A	285	LEU
1	A	290	VAL
1	A	294	LYS
1	A	311	VAL
1	A	325	LYS
1	A	326	VAL
1	A	327	LYS
1	B	1	ASP
1	B	2	SER
1	B	7	THR
1	B	21	ARG
1	B	28	GLU
1	B	30	VAL
1	B	31	VAL
1	B	48	ARG
1	B	50	GLN
1	B	53	THR
1	B	64	CYS
1	B	67	VAL
1	B	70	VAL
1	B	76	PRO
1	B	79	ARG
1	B	89	ARG
1	B	93	GLU
1	B	95	LYS
1	B	105	ARG
1	B	112	VAL
1	B	137	LEU
1	B	139	ASN
1	B	144	SER
1	B	149	ASN
1	B	152	LYS
1	B	153	GLU
1	B	154	LEU
1	B	158	ASN
1	B	161	LEU
1	B	174	LEU
1	B	182	GLU
1	B	211	SER

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Mol	Chain	Res	Type
1	B	227	PRO
1	B	232	VAL
1	B	236	ARG
1	B	238	ARG
1	B	239	ASN
1	B	240	ILE
1	B	243	SER
1	B	252	VAL
1	B	271	VAL
1	B	274	HIS
1	B	282	ASN
1	B	290	VAL
1	B	296	ARG
1	B	307	ARG
1	B	311	VAL
1	B	318	SER
1	B	325	LYS
1	C	5	ARG
1	C	7	THR
1	C	21	ARG
1	C	29	THR
1	C	31	VAL
1	C	32	ASN
1	C	64	CYS
1	C	67	VAL
1	C	87	GLU
1	C	94	LEU
1	C	112	VAL
1	C	114	LYS
1	C	120	GLU
1	C	154	LEU
1	C	161	LEU
1	C	167	ARG
1	C	174	LEU
1	C	187	ASN
1	C	208	ARG
1	C	210	SER
1	C	213	ASP
1	C	246	SER
1	C	252	VAL
1	C	263	THR
1	C	270	THR

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Mol	Chain	Res	Type
1	C	271	VAL
1	C	274	HIS
1	C	290	VAL
1	C	296	ARG
1	C	307	ARG
1	C	311	VAL
1	C	317	LYS
1	C	325	LYS
1	C	326	VAL
1	C	327	LYS
1	D	3	ASP
1	D	5	ARG
1	D	7	THR
1	D	13	LEU
1	D	14	ASP
1	D	16	MET
1	D	30	VAL
1	D	32	ASN
1	D	48	ARG
1	D	50	GLN
1	D	54	GLU
1	D	55	GLU
1	D	58	GLU
1	D	61	SER
1	D	64	CYS
1	D	67	VAL
1	D	70	VAL
1	D	74	GLN
1	D	78	ASN
1	D	89	ARG
1	D	96	ASN
1	D	104	THR
1	D	121	LYS
1	D	124	GLN
1	D	134	ASN
1	D	137	LEU
1	D	144	SER
1	D	148	ASP
1	D	154	LEU
1	D	156	ASN
1	D	162	ARG
1	D	174	LEU

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Mol	Chain	Res	Type
1	D	176	ASN
1	D	177	THR
1	D	179	SER
1	D	181	LYS
1	D	184	ASN
1	D	207	ASP
1	D	208	ARG
1	D	215	ARG
1	D	229	THR
1	D	232	VAL
1	D	263	THR
1	D	270	THR
1	D	271	VAL
1	D	273	THR
1	D	274	HIS
1	D	290	VAL
1	D	296	ARG
1	D	307	ARG
1	D	311	VAL
1	D	326	VAL
1	D	328	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	44	HIS
1	A	51	GLN
1	A	92	ASN
1	A	188	HIS
1	A	201	HIS
1	A	279	HIS
1	A	297	ASN
1	B	32	ASN
1	B	33	ASN
1	B	40	GLN
1	B	44	HIS
1	B	56	GLN
1	B	71	ASN
1	B	78	ASN
1	B	124	GLN
1	B	149	ASN

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Mol	Chain	Res	Type
1	B	206	GLN
1	B	279	HIS
1	B	328	GLN
1	C	32	ASN
1	C	33	ASN
1	C	44	HIS
1	C	50	GLN
1	C	51	GLN
1	C	78	ASN
1	C	96	ASN
1	C	176	ASN
1	C	187	ASN
1	C	279	HIS
1	C	328	GLN
1	D	32	ASN
1	D	50	GLN
1	D	71	ASN
1	D	74	GLN
1	D	92	ASN
1	D	158	ASN
1	D	176	ASN
1	D	187	ASN
1	D	201	HIS
1	D	279	HIS
1	D	320	ASN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	331/331 (100%)	-0.27	3 (0%) 81 78	7, 24, 48, 67	0
1	B	331/331 (100%)	-0.44	1 (0%) 90 88	5, 19, 38, 60	0
1	C	331/331 (100%)	-0.40	2 (0%) 85 83	7, 20, 41, 63	0
1	D	331/331 (100%)	0.03	3 (0%) 81 78	10, 31, 53, 71	0
All	All	1324/1324 (100%)	-0.27	9 (0%) 84 81	5, 23, 48, 71	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	THR	2.5
1	D	101	SER	2.5
1	A	331	PRO	2.3
1	C	21	ARG	2.3
1	D	21	ARG	2.2
1	C	245	THR	2.1
1	D	98	ARG	2.0
1	A	248	GLY	2.0
1	B	77	THR	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.