



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:45 PM UTC

PDB ID : 1T1U / pdb_00001t1u
Title : Structural Insights and Functional Implications of Choline Acetyltransferase
Authors : Govindasamy, L.; Pedersen, B.; Lian, W.; Kukar, T.; Gu, Y.; Jin, S.;
Agbandje-McKenna, M.; Wu, D.
Deposited on : 2004-04-18
Resolution : 1.55 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

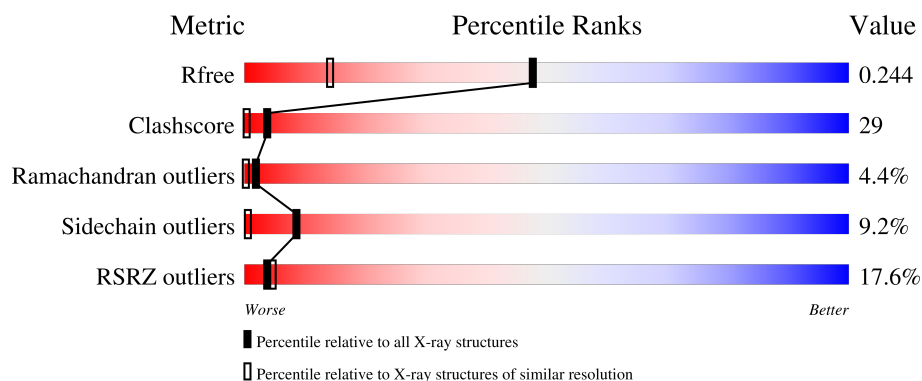
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	639	16% 17% 51% 18% 9% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5119 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 Choline O-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	597	4711	2975	817	880	39	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	377	TRP	LEU	see Remark 999	UNP P32738
A	499	GLN	HIS	see Remark 999	UNP P32738
A	500	THR	LYS	see Remark 999	UNP P32738
A	501	GLU	GLN	see Remark 999	UNP P32738
A	570	TYR	ASN	see Remark 999	UNP P32738

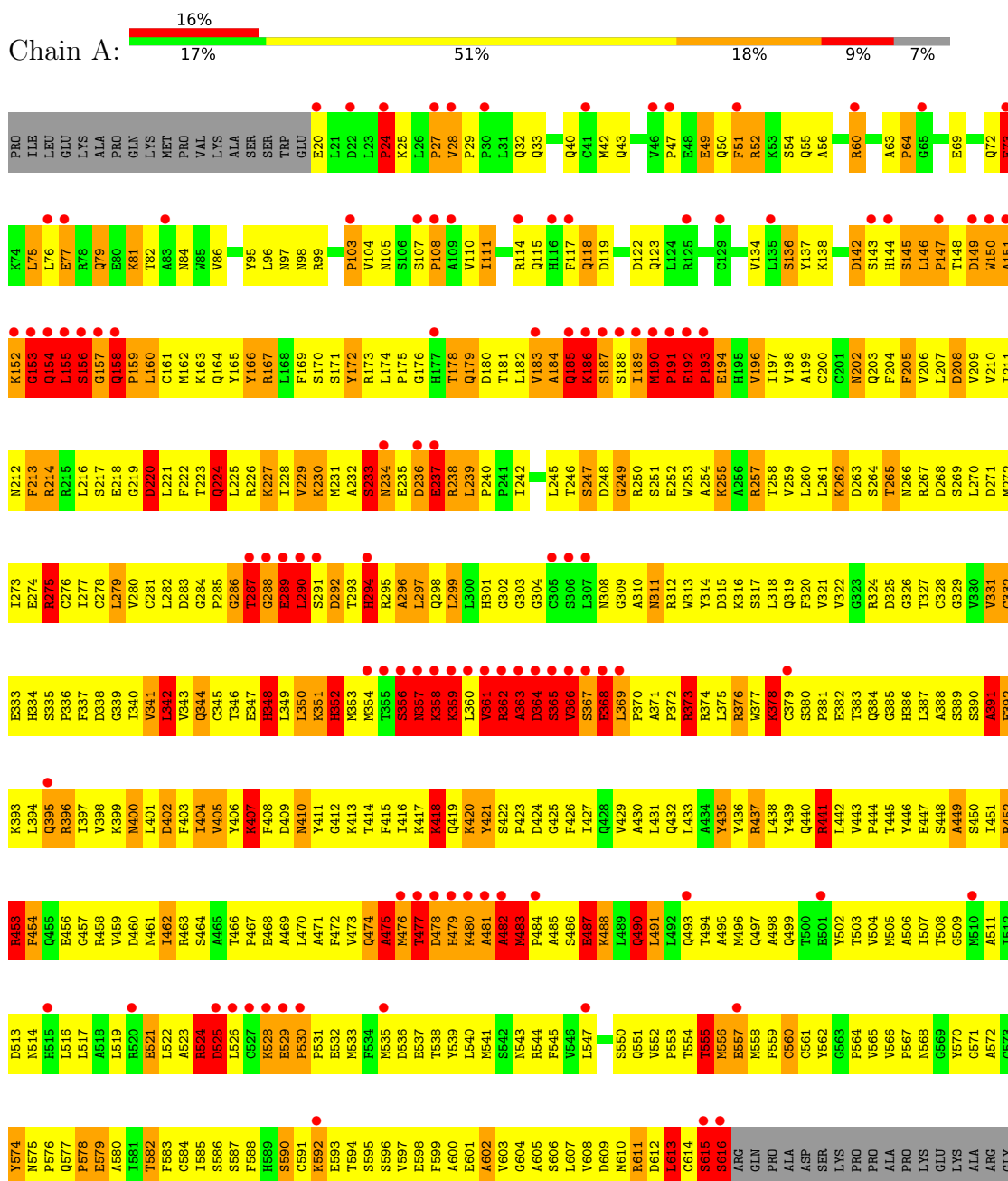
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	408	Total	O	0	0
			408	408		

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: Choline O-acetyltransferase



PRO
SER
GLN
ALA
LYS
GLN
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	138.95Å 77.50Å 59.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.55 30.00 – 1.55	Depositor EDS
% Data completeness (in resolution range)	5.0 (30.00-1.55) 77.4 (30.00-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.55Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.171 , 0.227 0.208 , 0.244	Depositor DCC
R_{free} test set	3646 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 43.6	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	0.94	EDS
Total number of atoms	5119	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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	4.08	869/4811 (18.1%)	3.61	887/6516 (13.6%)

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	53

All (869) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	ILE	C-O	-30.36	0.85	1.24
1	A	289	GLU	C-N	-24.44	0.99	1.33
1	A	240	PRO	CA-C	23.95	1.74	1.52
1	A	379	CYS	CA-CB	-23.41	1.22	1.53
1	A	267	ARG	NE-CZ	22.96	1.58	1.33
1	A	437	ARG	CZ-NH1	22.10	1.63	1.32
1	A	167	ARG	CD-NE	-19.76	1.18	1.46
1	A	470	LEU	C-O	18.34	1.45	1.24
1	A	189	ILE	C-N	-18.28	0.95	1.33
1	A	334	HIS	CE1-NE2	18.23	1.50	1.32
1	A	415	PHE	CA-C	-17.98	1.29	1.52
1	A	226	ARG	NE-CZ	-17.57	1.13	1.33
1	A	453	ARG	CA-CB	17.56	1.84	1.53
1	A	230	LYS	CA-C	-17.56	1.30	1.52
1	A	453	ARG	CD-NE	17.48	1.70	1.46
1	A	294	HIS	CB-CG	17.21	1.74	1.50
1	A	190	MET	N-CA	-17.16	1.22	1.46
1	A	615	SER	C-O	17.14	1.48	1.23
1	A	452	ARG	CD-NE	-17.13	1.22	1.46
1	A	441	ARG	CZ-NH1	16.63	1.56	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	GLU	N-CA	16.55	1.67	1.46
1	A	475	ALA	N-CA	16.39	1.68	1.46
1	A	600	ALA	CA-C	16.27	1.73	1.52
1	A	494	THR	CA-C	16.24	1.73	1.52
1	A	376	ARG	NE-CZ	16.08	1.50	1.33
1	A	209	VAL	CA-CB	-15.57	1.35	1.54
1	A	615	SER	CA-C	-15.57	1.30	1.53
1	A	348	HIS	C-O	15.41	1.42	1.24
1	A	267	ARG	N-CA	-15.38	1.27	1.46
1	A	226	ARG	N-CA	-15.26	1.28	1.46
1	A	437	ARG	CZ-NH2	15.11	1.53	1.33
1	A	415	PHE	C-N	14.86	1.52	1.33
1	A	494	THR	C-O	-14.82	1.07	1.24
1	A	487	GLU	CA-C	14.74	1.71	1.52
1	A	365	SER	N-CA	14.67	1.61	1.46
1	A	613	LEU	CB-CG	-14.66	1.24	1.53
1	A	522	LEU	C-O	14.66	1.42	1.24
1	A	344	GLN	CD-OE1	14.65	1.51	1.23
1	A	259	VAL	CA-CB	-14.59	1.36	1.54
1	A	216	LEU	N-CA	-14.33	1.27	1.45
1	A	266	ASN	CA-C	-14.22	1.33	1.52
1	A	448	SER	C-O	13.89	1.40	1.23
1	A	263	ASP	CA-CB	-13.85	1.32	1.53
1	A	578	PRO	C-O	13.81	1.40	1.24
1	A	258	THR	C-O	13.71	1.40	1.24
1	A	386	HIS	CA-CB	-13.71	1.32	1.53
1	A	611	ARG	NE-CZ	13.63	1.48	1.33
1	A	344	GLN	C-O	13.56	1.40	1.24
1	A	260	LEU	C-O	13.48	1.39	1.24
1	A	421	TYR	CE2-CZ	13.38	1.70	1.38
1	A	178	THR	CA-CB	13.38	1.76	1.53
1	A	417	LYS	CA-C	13.28	1.70	1.52
1	A	352	HIS	C-O	13.07	1.39	1.24
1	A	579	GLU	C-N	12.91	1.49	1.33
1	A	491	LEU	C-O	12.89	1.39	1.24
1	A	266	ASN	C-O	12.87	1.39	1.24
1	A	415	PHE	N-CA	-12.81	1.30	1.46
1	A	410	ASN	C-O	12.77	1.40	1.24
1	A	313	TRP	CA-CB	12.77	1.68	1.52
1	A	286	GLY	C-O	12.71	1.38	1.23
1	A	441	ARG	NE-CZ	12.70	1.47	1.33
1	A	362	ARG	N-CA	12.51	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	THR	CB-OG1	-12.51	1.23	1.43
1	A	190	MET	C-N	12.31	1.57	1.34
1	A	382	GLU	CA-CB	-12.31	1.34	1.53
1	A	555	THR	C-O	12.29	1.41	1.23
1	A	214	ARG	CA-CB	-12.28	1.33	1.53
1	A	292	ASP	C-O	-12.23	1.09	1.24
1	A	159	PRO	C-O	-12.20	1.10	1.23
1	A	373	ARG	CG-CD	12.18	1.89	1.52
1	A	379	CYS	CA-C	12.12	1.68	1.52
1	A	437	ARG	C-O	12.10	1.39	1.24
1	A	205	PHE	CA-C	-12.06	1.37	1.52
1	A	350	LEU	C-O	12.03	1.38	1.24
1	A	234	ASN	C-O	11.94	1.39	1.23
1	A	421	TYR	CZ-OH	11.93	1.63	1.38
1	A	496	MET	CA-C	-11.90	1.37	1.52
1	A	613	LEU	CG-CD1	11.88	1.91	1.52
1	A	218	GLU	CD-OE2	11.85	1.47	1.25
1	A	263	ASP	CA-C	-11.83	1.38	1.52
1	A	463	ARG	CA-CB	-11.81	1.37	1.52
1	A	344	GLN	CD-NE2	11.80	1.58	1.33
1	A	373	ARG	CD-NE	11.75	1.62	1.46
1	A	387	LEU	N-CA	11.75	1.60	1.46
1	A	456	GLU	CA-CB	-11.69	1.36	1.53
1	A	478	ASP	CA-C	-11.58	1.37	1.52
1	A	226	ARG	CZ-NH1	11.57	1.49	1.32
1	A	255	LYS	CD-CE	11.55	1.87	1.52
1	A	608	VAL	C-O	11.53	1.37	1.24
1	A	396	ARG	NE-CZ	11.52	1.45	1.33
1	A	531	PRO	N-CD	-11.52	1.31	1.47
1	A	196	VAL	CA-CB	-11.47	1.39	1.54
1	A	424	ASP	C-O	11.47	1.37	1.24
1	A	482	ALA	C-O	-11.39	1.09	1.24
1	A	429	VAL	C-O	11.37	1.36	1.24
1	A	267	ARG	CZ-NH2	-11.30	1.18	1.33
1	A	416	ILE	CA-CB	11.28	1.68	1.54
1	A	159	PRO	CA-C	11.27	1.64	1.52
1	A	530	PRO	CA-C	-11.27	1.41	1.52
1	A	277	ILE	CA-CB	11.26	1.69	1.54
1	A	418	LYS	CD-CE	11.16	1.85	1.52
1	A	351	LYS	CG-CD	11.05	1.85	1.52
1	A	169	PHE	CA-C	-11.02	1.38	1.52
1	A	474	GLN	N-CA	11.02	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	ASN	C-O	10.99	1.39	1.23
1	A	604	GLY	N-CA	10.96	1.59	1.45
1	A	418	LYS	CA-C	-10.95	1.37	1.52
1	A	349	LEU	CA-CB	10.92	1.70	1.53
1	A	421	TYR	N-CA	10.91	1.59	1.45
1	A	173	ARG	NE-CZ	-10.90	1.21	1.33
1	A	252	GLU	CD-OE2	10.90	1.46	1.25
1	A	483	MET	C-O	-10.87	1.10	1.24
1	A	381	PRO	N-CD	10.85	1.62	1.47
1	A	418	LYS	N-CA	10.85	1.60	1.46
1	A	378	LYS	CE-NZ	10.82	1.81	1.49
1	A	380	SER	CA-CB	-10.79	1.38	1.53
1	A	343	VAL	C-O	10.75	1.36	1.24
1	A	205	PHE	C-N	10.66	1.45	1.33
1	A	481	ALA	N-CA	-10.63	1.32	1.46
1	A	471	ALA	CA-C	10.60	1.66	1.52
1	A	321	VAL	CA-CB	-10.55	1.41	1.54
1	A	475	ALA	CA-C	-10.52	1.38	1.52
1	A	187	SER	C-O	10.50	1.37	1.24
1	A	261	LEU	CA-C	10.48	1.66	1.52
1	A	173	ARG	CD-NE	10.48	1.60	1.46
1	A	107	SER	CA-C	10.43	1.64	1.52
1	A	351	LYS	C-O	10.35	1.36	1.24
1	A	341	VAL	CA-C	-10.35	1.39	1.52
1	A	532	GLU	CA-C	10.32	1.66	1.52
1	A	303	GLY	C-O	10.31	1.39	1.24
1	A	179	GLN	CD-OE1	-10.27	1.04	1.23
1	A	261	LEU	C-O	-10.22	1.11	1.24
1	A	440	GLN	CD-OE1	10.20	1.43	1.23
1	A	576	PRO	C-N	-10.15	1.18	1.32
1	A	550	SER	CA-CB	-10.10	1.37	1.53
1	A	324	ARG	CD-NE	10.09	1.60	1.46
1	A	176	GLY	N-CA	10.08	1.55	1.44
1	A	224	GLN	CD-OE1	10.07	1.42	1.23
1	A	257	ARG	CZ-NH1	10.07	1.46	1.32
1	A	219	GLY	N-CA	-10.07	1.32	1.45
1	A	440	GLN	C-N	10.06	1.46	1.33
1	A	490	GLN	CD-NE2	10.04	1.54	1.33
1	A	285	PRO	CA-CB	10.03	1.66	1.53
1	A	604	GLY	CA-C	-9.95	1.41	1.52
1	A	269	SER	C-O	9.94	1.35	1.24
1	A	210	VAL	C-N	9.87	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	504	VAL	CA-CB	9.86	1.69	1.54
1	A	218	GLU	N-CA	9.80	1.58	1.46
1	A	185	GLN	CA-C	-9.75	1.39	1.52
1	A	370	PRO	CA-C	9.75	1.64	1.52
1	A	204	PHE	CE1-CZ	-9.74	1.09	1.38
1	A	475	ALA	CA-CB	9.73	1.70	1.53
1	A	497	GLN	CD-OE1	9.73	1.42	1.23
1	A	373	ARG	CZ-NH2	9.73	1.46	1.33
1	A	281	CYS	CA-C	-9.71	1.40	1.52
1	A	254	ALA	C-N	-9.68	1.21	1.33
1	A	269	SER	CA-C	9.67	1.65	1.52
1	A	490	GLN	N-CA	9.65	1.58	1.46
1	A	180	ASP	C-O	9.65	1.36	1.23
1	A	488	LYS	CA-CB	-9.64	1.38	1.53
1	A	448	SER	CA-CB	9.63	1.69	1.53
1	A	456	GLU	CD-OE1	9.63	1.43	1.25
1	A	214	ARG	NE-CZ	9.63	1.43	1.33
1	A	258	THR	CB-OG1	9.62	1.59	1.43
1	A	491	LEU	N-CA	9.60	1.57	1.46
1	A	452	ARG	CB-CG	-9.58	1.23	1.52
1	A	206	VAL	CA-CB	-9.57	1.42	1.54
1	A	444	PRO	N-CA	9.56	1.58	1.47
1	A	558	MET	N-CA	9.54	1.57	1.46
1	A	414	THR	N-CA	9.53	1.57	1.46
1	A	453	ARG	C-O	9.52	1.36	1.24
1	A	493	GLN	C-N	-9.49	1.21	1.33
1	A	179	GLN	CG-CD	9.47	1.75	1.52
1	A	592	LYS	C-N	-9.47	1.20	1.33
1	A	437	ARG	NE-CZ	9.46	1.43	1.33
1	A	503	THR	C-N	9.45	1.45	1.34
1	A	504	VAL	CA-C	-9.44	1.39	1.52
1	A	231	MET	CA-CB	-9.44	1.37	1.53
1	A	242	ILE	CA-C	9.44	1.65	1.52
1	A	173	ARG	CA-C	-9.43	1.40	1.53
1	A	257	ARG	NE-CZ	-9.43	1.22	1.33
1	A	407	LYS	N-CA	-9.41	1.34	1.46
1	A	396	ARG	CG-CD	9.39	1.80	1.52
1	A	437	ARG	CB-CG	-9.39	1.24	1.52
1	A	579	GLU	CD-OE1	9.38	1.43	1.25
1	A	304	GLY	CA-C	9.38	1.63	1.52
1	A	475	ALA	C-O	-9.37	1.11	1.24
1	A	270	LEU	C-O	9.37	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	LEU	C-O	9.35	1.35	1.24
1	A	600	ALA	N-CA	-9.32	1.35	1.46
1	A	472	PHE	N-CA	9.30	1.57	1.46
1	A	560	CYS	CA-C	9.30	1.63	1.52
1	A	440	GLN	CD-NE2	9.29	1.52	1.33
1	A	594	THR	C-O	9.28	1.35	1.23
1	A	423	PRO	C-O	9.27	1.36	1.24
1	A	216	LEU	CG-CD2	-9.27	1.22	1.52
1	A	376	ARG	CZ-NH1	9.27	1.45	1.32
1	A	493	GLN	C-O	9.23	1.34	1.24
1	A	262	LYS	CE-NZ	9.22	1.77	1.49
1	A	220	ASP	CB-CG	9.22	1.75	1.52
1	A	353	MET	C-O	9.18	1.35	1.24
1	A	454	PHE	C-N	9.17	1.46	1.33
1	A	166	TYR	CA-C	-9.17	1.39	1.52
1	A	536	ASP	C-N	9.17	1.46	1.33
1	A	396	ARG	N-CA	-9.15	1.34	1.46
1	A	414	THR	CB-OG1	9.13	1.58	1.43
1	A	612	ASP	C-O	9.13	1.34	1.24
1	A	303	GLY	CA-C	-9.12	1.38	1.51
1	A	230	LYS	CD-CE	9.12	1.79	1.52
1	A	233	SER	N-CA	-9.12	1.33	1.46
1	A	194	GLU	CD-OE1	9.07	1.42	1.25
1	A	381	PRO	CA-CB	9.05	1.67	1.53
1	A	521	GLU	CD-OE2	9.04	1.42	1.25
1	A	422	SER	CB-OG	9.00	1.60	1.42
1	A	593	GLU	C-O	-8.97	1.11	1.24
1	A	514	ASN	CA-C	8.94	1.64	1.52
1	A	218	GLU	C-N	8.89	1.46	1.33
1	A	226	ARG	CA-CB	8.88	1.67	1.53
1	A	554	THR	CA-CB	8.87	1.70	1.54
1	A	442	LEU	N-CA	8.86	1.56	1.45
1	A	499	GLN	C-O	8.86	1.34	1.24
1	A	556	MET	CA-C	-8.86	1.41	1.53
1	A	580	ALA	C-O	-8.86	1.13	1.23
1	A	532	GLU	CG-CD	8.84	1.74	1.52
1	A	344	GLN	CA-CB	-8.79	1.39	1.53
1	A	605	ALA	C-O	8.78	1.35	1.24
1	A	441	ARG	CA-C	8.77	1.63	1.52
1	A	456	GLU	CD-OE2	8.76	1.42	1.25
1	A	360	LEU	C-N	8.75	1.45	1.33
1	A	445	THR	N-CA	8.74	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	TYR	C-O	8.73	1.34	1.23
1	A	271	ASP	CB-CG	-8.71	1.30	1.52
1	A	396	ARG	CD-NE	-8.71	1.34	1.46
1	A	254	ALA	CA-C	8.70	1.63	1.52
1	A	466	THR	C-O	-8.70	1.12	1.23
1	A	566	VAL	C-O	-8.69	1.17	1.24
1	A	560	CYS	N-CA	8.67	1.56	1.45
1	A	487	GLU	N-CA	-8.64	1.36	1.46
1	A	29	PRO	C-N	-8.62	1.22	1.33
1	A	612	ASP	N-CA	8.62	1.56	1.46
1	A	446	TYR	N-CA	8.62	1.56	1.46
1	A	269	SER	CA-CB	-8.60	1.39	1.53
1	A	265	THR	CB-OG1	8.60	1.57	1.43
1	A	487	GLU	C-O	-8.60	1.14	1.24
1	A	444	PRO	CA-CB	-8.59	1.42	1.53
1	A	388	ALA	CA-C	8.59	1.64	1.52
1	A	236	ASP	N-CA	8.56	1.57	1.46
1	A	255	LYS	CE-NZ	8.56	1.75	1.49
1	A	611	ARG	CZ-NH1	8.55	1.44	1.32
1	A	259	VAL	N-CA	8.54	1.56	1.46
1	A	460	ASP	C-N	-8.52	1.21	1.33
1	A	378	LYS	N-CA	8.49	1.58	1.46
1	A	260	LEU	C-N	-8.47	1.21	1.33
1	A	568	ASN	C-O	-8.46	1.13	1.24
1	A	505	MET	N-CA	-8.45	1.36	1.46
1	A	386	HIS	N-CA	8.44	1.56	1.46
1	A	295	ARG	CZ-NH2	8.42	1.44	1.33
1	A	433	LEU	C-O	8.42	1.34	1.24
1	A	432	GLN	C-O	8.41	1.33	1.24
1	A	477	THR	C-N	-8.41	1.22	1.33
1	A	391	ALA	CA-C	-8.40	1.42	1.52
1	A	553	PRO	CA-C	8.40	1.62	1.52
1	A	450	SER	C-O	8.39	1.34	1.23
1	A	602	ALA	C-N	-8.39	1.23	1.33
1	A	213	PHE	CA-CB	8.39	1.66	1.53
1	A	496	MET	CB-CG	-8.37	1.27	1.52
1	A	482	ALA	CA-CB	8.37	1.67	1.53
1	A	586	SER	CA-CB	-8.36	1.34	1.53
1	A	521	GLU	C-N	-8.36	1.22	1.33
1	A	521	GLU	N-CA	8.35	1.57	1.46
1	A	483	MET	CA-CB	-8.33	1.40	1.53
1	A	308	ASN	CB-CG	-8.32	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	ILE	C-N	8.32	1.45	1.33
1	A	230	LYS	N-CA	8.31	1.56	1.46
1	A	497	GLN	CG-CD	8.31	1.72	1.52
1	A	467	PRO	CA-CB	8.30	1.65	1.53
1	A	494	THR	CA-CB	-8.30	1.40	1.53
1	A	544	ARG	NE-CZ	8.30	1.42	1.33
1	A	552	VAL	N-CA	8.24	1.56	1.46
1	A	576	PRO	CA-C	8.24	1.64	1.52
1	A	610	MET	N-CA	-8.22	1.36	1.46
1	A	601	GLU	N-CA	-8.22	1.36	1.46
1	A	508	THR	N-CA	8.20	1.55	1.46
1	A	259	VAL	CA-C	-8.19	1.42	1.52
1	A	317	SER	CA-C	-8.19	1.41	1.52
1	A	367	SER	N-CA	-8.19	1.35	1.46
1	A	562	TYR	CA-CB	-8.17	1.39	1.53
1	A	275	ARG	CD-NE	-8.16	1.34	1.46
1	A	235	GLU	CD-OE2	8.15	1.40	1.25
1	A	295	ARG	CA-C	8.15	1.63	1.52
1	A	275	ARG	NE-CZ	8.14	1.42	1.33
1	A	348	HIS	CD2-NE2	8.14	1.46	1.37
1	A	374	ARG	C-O	8.13	1.33	1.24
1	A	228	ILE	C-N	8.13	1.43	1.34
1	A	296	ALA	C-O	8.12	1.34	1.24
1	A	511	ALA	CA-CB	-8.12	1.41	1.53
1	A	531	PRO	CA-CB	-8.11	1.43	1.53
1	A	344	GLN	CA-C	-8.11	1.42	1.52
1	A	449	ALA	C-O	-8.11	1.15	1.24
1	A	166	TYR	CZ-OH	8.11	1.55	1.38
1	A	293	THR	C-N	8.11	1.44	1.33
1	A	228	ILE	C-O	8.09	1.33	1.24
1	A	598	GLU	CD-OE2	-8.09	1.09	1.25
1	A	267	ARG	C-O	-8.08	1.14	1.24
1	A	495	ALA	N-CA	8.08	1.56	1.46
1	A	280	VAL	CA-CB	8.07	1.64	1.53
1	A	577	GLN	CA-CB	-8.07	1.41	1.53
1	A	380	SER	CA-C	-8.07	1.42	1.52
1	A	555	THR	C-N	-8.06	1.22	1.33
1	A	498	ALA	C-N	-8.06	1.23	1.33
1	A	358	LYS	N-CA	8.04	1.56	1.45
1	A	436	TYR	CZ-OH	8.02	1.54	1.38
1	A	331	VAL	CA-CB	-8.02	1.44	1.54
1	A	328	CYS	CA-C	7.99	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	ILE	CA-C	-7.99	1.42	1.52
1	A	162	MET	C-O	7.99	1.34	1.24
1	A	574	TYR	C-O	7.99	1.33	1.23
1	A	384	GLN	CG-CD	7.97	1.72	1.52
1	A	223	THR	CB-OG1	7.97	1.56	1.43
1	A	223	THR	CA-C	7.96	1.63	1.52
1	A	343	VAL	N-CA	-7.96	1.36	1.46
1	A	474	GLN	C-O	7.96	1.34	1.24
1	A	174	LEU	CB-CG	-7.96	1.37	1.53
1	A	551	GLN	CD-OE1	7.96	1.38	1.23
1	A	308	ASN	CA-C	7.95	1.66	1.52
1	A	544	ARG	CA-C	7.93	1.62	1.53
1	A	553	PRO	N-CD	-7.93	1.36	1.47
1	A	452	ARG	C-O	7.92	1.34	1.24
1	A	357	ASN	N-CA	-7.90	1.35	1.46
1	A	387	LEU	CA-C	-7.90	1.42	1.52
1	A	217	SER	CA-C	7.89	1.64	1.53
1	A	550	SER	N-CA	7.88	1.55	1.46
1	A	299	LEU	CG-CD1	-7.88	1.26	1.52
1	A	167	ARG	NE-CZ	-7.87	1.24	1.33
1	A	562	TYR	CE2-CZ	-7.84	1.19	1.38
1	A	268	ASP	CG-OD2	7.84	1.40	1.25
1	A	249	GLY	CA-C	-7.82	1.45	1.52
1	A	435	TYR	C-O	7.80	1.33	1.24
1	A	409	ASP	CB-CG	-7.79	1.32	1.52
1	A	474	GLN	CB-CG	-7.79	1.29	1.52
1	A	222	PHE	N-CA	-7.78	1.37	1.46
1	A	426	PHE	CA-CB	7.75	1.65	1.53
1	A	251	SER	C-O	7.74	1.34	1.24
1	A	458	ARG	N-CA	7.73	1.55	1.45
1	A	340	ILE	C-N	-7.72	1.24	1.33
1	A	353	MET	SD-CE	-7.72	1.60	1.79
1	A	570	TYR	C-N	-7.72	1.26	1.33
1	A	164	GLN	CA-CB	-7.71	1.40	1.53
1	A	418	LYS	CE-NZ	7.71	1.72	1.49
1	A	504	VAL	N-CA	7.70	1.56	1.46
1	A	253	TRP	CZ2-CH2	-7.70	1.22	1.37
1	A	309	GLY	CA-C	-7.70	1.41	1.51
1	A	383	THR	C-N	7.70	1.43	1.33
1	A	608	VAL	N-CA	7.70	1.55	1.46
1	A	376	ARG	CA-C	7.69	1.63	1.53
1	A	484	PRO	N-CD	-7.69	1.36	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499	GLN	CA-CB	-7.68	1.41	1.53
1	A	408	PHE	N-CA	-7.68	1.36	1.46
1	A	446	TYR	CA-CB	-7.67	1.41	1.53
1	A	324	ARG	CZ-NH2	7.67	1.43	1.33
1	A	343	VAL	CA-CB	-7.67	1.44	1.54
1	A	174	LEU	N-CA	7.65	1.58	1.46
1	A	252	GLU	CA-CB	-7.64	1.41	1.53
1	A	327	THR	N-CA	7.62	1.55	1.46
1	A	409	ASP	N-CA	7.61	1.56	1.46
1	A	439	TYR	C-O	7.61	1.33	1.24
1	A	507	ILE	C-O	7.56	1.34	1.24
1	A	161	CYS	CA-C	-7.55	1.42	1.52
1	A	552	VAL	CA-CB	-7.55	1.44	1.54
1	A	343	VAL	CA-C	7.54	1.62	1.52
1	A	351	LYS	CD-CE	7.53	1.75	1.52
1	A	228	ILE	CA-C	-7.52	1.43	1.52
1	A	376	ARG	CD-NE	7.51	1.56	1.46
1	A	590	SER	CA-C	-7.51	1.42	1.52
1	A	225	LEU	C-O	-7.50	1.14	1.24
1	A	297	LEU	CA-C	-7.49	1.43	1.52
1	A	179	GLN	CD-NE2	-7.49	1.17	1.33
1	A	164	GLN	CG-CD	7.47	1.70	1.52
1	A	490	GLN	CA-C	7.46	1.62	1.52
1	A	346	THR	CA-CB	7.45	1.65	1.53
1	A	579	GLU	CA-C	-7.43	1.42	1.52
1	A	431	LEU	CA-CB	-7.42	1.41	1.53
1	A	613	LEU	CA-C	-7.41	1.42	1.52
1	A	418	LYS	C-O	7.41	1.33	1.24
1	A	564	PRO	N-CD	7.41	1.58	1.47
1	A	541	MET	SD-CE	7.40	1.98	1.79
1	A	218	GLU	CD-OE1	7.40	1.39	1.25
1	A	275	ARG	N-CA	7.39	1.55	1.46
1	A	463	ARG	CA-C	7.38	1.61	1.52
1	A	421	TYR	C-O	-7.38	1.14	1.23
1	A	152	LYS	CA-C	7.38	1.61	1.52
1	A	328	CYS	C-N	-7.38	1.25	1.33
1	A	386	HIS	CD2-NE2	-7.38	1.29	1.37
1	A	209	VAL	CA-C	7.37	1.63	1.52
1	A	422	SER	CA-C	-7.35	1.44	1.52
1	A	458	ARG	C-N	-7.35	1.24	1.33
1	A	530	PRO	CA-CB	-7.35	1.44	1.54
1	A	407	LYS	CG-CD	7.34	1.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	GLN	CD-OE1	7.34	1.37	1.23
1	A	415	PHE	CD2-CE2	7.33	1.60	1.38
1	A	271	ASP	CA-CB	7.32	1.64	1.53
1	A	423	PRO	N-CA	-7.31	1.38	1.47
1	A	613	LEU	CA-CB	7.31	1.65	1.53
1	A	483	MET	CA-C	7.30	1.62	1.52
1	A	601	GLU	CA-CB	7.30	1.64	1.53
1	A	591	CYS	N-CA	-7.29	1.37	1.46
1	A	505	MET	C-O	-7.28	1.15	1.24
1	A	213	PHE	C-N	7.28	1.43	1.33
1	A	496	MET	CA-CB	7.26	1.64	1.53
1	A	443	VAL	CA-C	7.26	1.59	1.52
1	A	407	LYS	C-N	-7.26	1.23	1.33
1	A	456	GLU	C-N	-7.24	1.27	1.33
1	A	267	ARG	CD-NE	-7.24	1.36	1.46
1	A	554	THR	CB-OG1	-7.21	1.32	1.43
1	A	344	GLN	CG-CD	-7.21	1.34	1.52
1	A	565	VAL	C-N	-7.19	1.27	1.33
1	A	175	PRO	C-O	7.16	1.31	1.23
1	A	587	SER	C-O	-7.16	1.15	1.23
1	A	387	LEU	CB-CG	-7.15	1.39	1.53
1	A	226	ARG	CA-C	-7.13	1.43	1.52
1	A	250	ARG	CZ-NH1	7.13	1.42	1.32
1	A	467	PRO	N-CA	7.12	1.56	1.47
1	A	503	THR	CA-C	7.10	1.61	1.52
1	A	414	THR	C-O	7.10	1.32	1.24
1	A	544	ARG	CZ-NH1	7.09	1.42	1.32
1	A	337	PHE	N-CA	-7.09	1.37	1.46
1	A	605	ALA	C-N	7.09	1.43	1.33
1	A	218	GLU	C-O	-7.06	1.15	1.24
1	A	222	PHE	C-N	7.05	1.42	1.33
1	A	158	GLN	N-CA	-7.05	1.35	1.45
1	A	167	ARG	N-CA	-7.04	1.36	1.46
1	A	478	ASP	C-N	-7.04	1.23	1.33
1	A	487	GLU	C-N	7.04	1.43	1.33
1	A	421	TYR	CD1-CE1	7.04	1.59	1.38
1	A	568	ASN	N-CA	-7.03	1.37	1.46
1	A	331	VAL	CB-CG1	-7.01	1.29	1.52
1	A	222	PHE	C-O	-7.01	1.16	1.24
1	A	611	ARG	CA-CB	6.99	1.64	1.53
1	A	541	MET	CG-SD	6.99	1.98	1.80
1	A	597	VAL	N-CA	6.98	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	ARG	CG-CD	6.97	1.73	1.52
1	A	369	LEU	N-CA	6.96	1.55	1.46
1	A	261	LEU	CA-CB	-6.95	1.41	1.53
1	A	229	VAL	N-CA	-6.94	1.37	1.46
1	A	554	THR	CA-C	-6.94	1.44	1.52
1	A	337	PHE	CA-CB	6.93	1.65	1.53
1	A	551	GLN	CD-NE2	-6.93	1.18	1.33
1	A	225	LEU	C-N	6.93	1.42	1.33
1	A	531	PRO	N-CA	-6.93	1.39	1.46
1	A	311	ASN	CG-OD1	6.92	1.36	1.23
1	A	390	SER	CA-CB	-6.92	1.42	1.53
1	A	570	TYR	CG-CD2	-6.92	1.24	1.39
1	A	444	PRO	N-CD	6.91	1.57	1.47
1	A	537	GLU	CD-OE2	6.91	1.38	1.25
1	A	342	LEU	CA-C	6.91	1.61	1.52
1	A	445	THR	CA-C	-6.91	1.44	1.52
1	A	351	LYS	C-N	-6.90	1.25	1.33
1	A	470	LEU	N-CA	6.90	1.54	1.46
1	A	324	ARG	NE-CZ	-6.89	1.25	1.33
1	A	370	PRO	N-CA	-6.89	1.39	1.46
1	A	374	ARG	NE-CZ	-6.88	1.25	1.33
1	A	543	ASN	N-CA	-6.87	1.37	1.46
1	A	498	ALA	CA-C	6.87	1.61	1.52
1	A	497	GLN	C-N	-6.86	1.24	1.33
1	A	259	VAL	C-N	6.84	1.43	1.33
1	A	217	SER	CB-OG	-6.84	1.28	1.42
1	A	419	GLN	C-N	-6.84	1.24	1.33
1	A	509	GLY	CA-C	-6.83	1.42	1.51
1	A	399	LYS	CG-CD	6.83	1.73	1.52
1	A	298	GLN	N-CA	6.82	1.54	1.46
1	A	388	ALA	C-N	-6.81	1.24	1.33
1	A	210	VAL	C-O	6.81	1.31	1.24
1	A	182	LEU	CB-CG	-6.80	1.39	1.53
1	A	172	TYR	CE2-CZ	6.80	1.54	1.38
1	A	385	GLY	CA-C	6.80	1.59	1.51
1	A	251	SER	C-N	-6.79	1.25	1.33
1	A	595	SER	C-N	-6.79	1.25	1.33
1	A	609	ASP	C-O	6.78	1.32	1.24
1	A	324	ARG	CZ-NH1	-6.78	1.23	1.32
1	A	564	PRO	N-CA	-6.77	1.39	1.47
1	A	438	LEU	N-CA	-6.75	1.37	1.46
1	A	197	ILE	CA-CB	6.75	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	PRO	CA-C	-6.75	1.44	1.52
1	A	361	VAL	C-N	6.75	1.43	1.33
1	A	272	MET	CA-CB	-6.74	1.42	1.53
1	A	609	ASP	CB-CG	-6.74	1.35	1.52
1	A	406	TYR	CG-CD2	-6.74	1.25	1.39
1	A	334	HIS	CG-ND1	6.73	1.45	1.38
1	A	350	LEU	N-CA	6.73	1.54	1.46
1	A	440	GLN	CB-CG	-6.72	1.32	1.52
1	A	496	MET	CG-SD	-6.72	1.64	1.80
1	A	577	GLN	C-N	6.71	1.42	1.34
1	A	265	THR	CA-CB	-6.71	1.42	1.53
1	A	433	LEU	CA-C	-6.70	1.43	1.52
1	A	554	THR	C-O	-6.70	1.15	1.23
1	A	579	GLU	CA-CB	6.70	1.64	1.53
1	A	352	HIS	CA-C	-6.69	1.44	1.52
1	A	426	PHE	CD1-CE1	6.69	1.58	1.38
1	A	490	GLN	C-O	-6.69	1.16	1.24
1	A	320	PHE	C-N	-6.68	1.24	1.33
1	A	588	PHE	N-CA	6.68	1.54	1.46
1	A	350	LEU	CG-CD1	6.67	1.74	1.52
1	A	472	PHE	C-O	-6.67	1.16	1.24
1	A	295	ARG	CA-CB	-6.66	1.42	1.53
1	A	282	LEU	C-N	-6.65	1.24	1.33
1	A	407	LYS	C-O	-6.65	1.16	1.24
1	A	426	PHE	N-CA	-6.64	1.38	1.46
1	A	218	GLU	CA-C	-6.63	1.43	1.52
1	A	394	LEU	C-O	6.63	1.31	1.24
1	A	214	ARG	CD-NE	-6.62	1.36	1.46
1	A	294	HIS	CG-CD2	6.61	1.43	1.35
1	A	616	SER	C-O	6.60	1.36	1.23
1	A	262	LYS	CA-C	-6.59	1.43	1.52
1	A	271	ASP	N-CA	-6.59	1.38	1.46
1	A	614	CYS	C-O	-6.57	1.15	1.24
1	A	255	LYS	CA-C	-6.57	1.44	1.52
1	A	213	PHE	CE1-CZ	6.55	1.58	1.38
1	A	533	MET	C-O	-6.55	1.16	1.24
1	A	261	LEU	C-N	-6.55	1.24	1.33
1	A	482	ALA	N-CA	-6.54	1.37	1.46
1	A	478	ASP	N-CA	-6.54	1.37	1.46
1	A	588	PHE	CB-CG	6.54	1.65	1.50
1	A	469	ALA	N-CA	6.53	1.54	1.46
1	A	337	PHE	CE2-CZ	6.53	1.58	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	LEU	CA-C	-6.52	1.45	1.52
1	A	352	HIS	N-CA	-6.52	1.38	1.46
1	A	245	LEU	C-O	-6.51	1.16	1.24
1	A	249	GLY	N-CA	-6.51	1.37	1.45
1	A	450	SER	CA-C	-6.50	1.44	1.52
1	A	612	ASP	CG-OD1	6.49	1.37	1.25
1	A	158	GLN	CA-C	-6.48	1.43	1.52
1	A	332	CYS	CA-CB	-6.48	1.43	1.53
1	A	507	ILE	N-CA	6.47	1.54	1.46
1	A	577	GLN	CG-CD	-6.47	1.35	1.52
1	A	200	CYS	C-O	6.46	1.31	1.23
1	A	609	ASP	C-N	6.46	1.42	1.33
1	A	326	GLY	C-N	6.45	1.42	1.33
1	A	397	ILE	N-CA	6.43	1.54	1.46
1	A	158	GLN	C-N	-6.42	1.25	1.33
1	A	178	THR	C-O	-6.42	1.15	1.24
1	A	257	ARG	CZ-NH2	6.42	1.41	1.33
1	A	610	MET	CG-SD	6.42	1.96	1.80
1	A	160	LEU	CA-CB	6.41	1.66	1.53
1	A	212	ASN	CA-C	-6.40	1.44	1.53
1	A	164	GLN	C-N	6.37	1.42	1.34
1	A	203	GLN	CA-CB	6.37	1.63	1.53
1	A	450	SER	N-CA	6.37	1.53	1.46
1	A	302	GLY	C-N	-6.36	1.23	1.33
1	A	487	GLU	CA-CB	-6.36	1.43	1.53
1	A	521	GLU	CD-OE1	6.36	1.37	1.25
1	A	537	GLU	CD-OE1	6.36	1.37	1.25
1	A	336	PRO	CA-CB	-6.35	1.43	1.53
1	A	430	ALA	N-CA	-6.35	1.38	1.46
1	A	284	GLY	CA-C	-6.35	1.42	1.51
1	A	593	GLU	CD-OE2	6.35	1.37	1.25
1	A	536	ASP	CG-OD1	6.34	1.37	1.25
1	A	280	VAL	CA-C	-6.34	1.44	1.52
1	A	373	ARG	CZ-NH1	6.33	1.41	1.32
1	A	540	LEU	CG-CD1	6.33	1.73	1.52
1	A	555	THR	N-CA	6.33	1.54	1.46
1	A	352	HIS	CE1-NE2	6.32	1.38	1.32
1	A	181	THR	CA-CB	-6.30	1.41	1.53
1	A	572	ALA	CA-C	6.30	1.59	1.52
1	A	398	VAL	CA-C	6.29	1.60	1.52
1	A	211	ILE	CA-CB	-6.29	1.46	1.54
1	A	403	PHE	CA-C	-6.28	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	427	ILE	CA-CB	-6.28	1.47	1.54
1	A	532	GLU	N-CA	-6.28	1.38	1.46
1	A	335	SER	CA-CB	-6.27	1.45	1.53
1	A	447	GLU	CA-CB	-6.26	1.43	1.53
1	A	229	VAL	CA-C	6.26	1.61	1.52
1	A	382	GLU	N-CA	-6.25	1.39	1.46
1	A	327	THR	C-N	-6.25	1.25	1.33
1	A	615	SER	CB-OG	6.25	1.54	1.42
1	A	205	PHE	N-CA	6.25	1.53	1.46
1	A	578	PRO	N-CA	6.25	1.55	1.47
1	A	462	ILE	CA-CB	-6.24	1.46	1.54
1	A	470	LEU	CA-C	-6.24	1.44	1.52
1	A	482	ALA	CA-C	-6.24	1.44	1.52
1	A	316	LYS	CG-CD	6.23	1.71	1.52
1	A	346	THR	CB-OG1	6.22	1.53	1.43
1	A	165	TYR	CG-CD2	-6.22	1.26	1.39
1	A	444	PRO	CG-CD	-6.21	1.29	1.50
1	A	297	LEU	N-CA	6.21	1.53	1.46
1	A	404	ILE	N-CA	6.20	1.53	1.46
1	A	404	ILE	CA-C	-6.20	1.44	1.52
1	A	496	MET	N-CA	6.19	1.53	1.46
1	A	415	PHE	CG-CD2	-6.19	1.25	1.38
1	A	264	SER	C-O	-6.19	1.16	1.24
1	A	298	GLN	CG-CD	6.18	1.67	1.52
1	A	322	VAL	C-O	-6.18	1.17	1.24
1	A	386	HIS	C-O	6.18	1.31	1.24
1	A	427	ILE	C-N	-6.18	1.25	1.33
1	A	246	THR	C-O	6.17	1.31	1.24
1	A	211	ILE	CA-C	6.17	1.60	1.52
1	A	207	LEU	C-O	-6.17	1.16	1.23
1	A	582	THR	CA-C	6.17	1.60	1.52
1	A	179	GLN	C-O	6.16	1.30	1.23
1	A	273	ILE	CA-C	-6.16	1.45	1.52
1	A	194	GLU	N-CA	-6.15	1.38	1.46
1	A	242	ILE	N-CA	-6.13	1.38	1.46
1	A	164	GLN	CA-C	-6.11	1.44	1.52
1	A	372	PRO	CA-C	6.10	1.59	1.52
1	A	247	SER	CA-C	6.10	1.61	1.52
1	A	285	PRO	CG-CD	6.10	1.71	1.50
1	A	575	ASN	N-CA	6.10	1.53	1.46
1	A	284	GLY	N-CA	6.09	1.53	1.44
1	A	279	LEU	C-O	6.09	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	MET	SD-CE	-6.08	1.64	1.79
1	A	524	ARG	CA-C	-6.08	1.44	1.52
1	A	220	ASP	CA-C	6.08	1.60	1.52
1	A	558	MET	CA-CB	-6.08	1.43	1.53
1	A	265	THR	C-O	6.07	1.31	1.24
1	A	285	PRO	C-O	-6.07	1.16	1.23
1	A	471	ALA	C-O	-6.05	1.17	1.24
1	A	560	CYS	C-O	-6.05	1.16	1.23
1	A	258	THR	C-N	-6.05	1.26	1.33
1	A	345	CYS	CA-C	6.04	1.60	1.52
1	A	381	PRO	C-O	6.03	1.31	1.24
1	A	334	HIS	N-CA	6.03	1.54	1.46
1	A	381	PRO	C-N	-6.03	1.26	1.33
1	A	411	TYR	CG-CD2	-6.02	1.26	1.39
1	A	562	TYR	CB-CG	-6.02	1.38	1.51
1	A	579	GLU	C-O	-6.02	1.16	1.24
1	A	347	GLU	N-CA	6.01	1.54	1.46
1	A	415	PHE	CD1-CE1	6.00	1.56	1.38
1	A	559	PHE	CB-CG	-6.00	1.36	1.50
1	A	204	PHE	C-N	-6.00	1.24	1.33
1	A	596	SER	CA-C	6.00	1.60	1.52
1	A	317	SER	C-N	6.00	1.41	1.33
1	A	344	GLN	N-CA	5.99	1.53	1.46
1	A	348	HIS	CE1-NE2	-5.99	1.26	1.32
1	A	196	VAL	C-N	5.99	1.41	1.33
1	A	200	CYS	CA-C	5.98	1.59	1.52
1	A	208	ASP	CG-OD2	5.98	1.36	1.25
1	A	147	PRO	C-N	-5.98	1.25	1.33
1	A	76	LEU	CA-C	5.97	1.60	1.52
1	A	496	MET	C-O	5.95	1.30	1.24
1	A	442	LEU	CA-C	-5.95	1.45	1.52
1	A	171	SER	N-CA	-5.95	1.38	1.45
1	A	265	THR	C-N	-5.94	1.26	1.33
1	A	423	PRO	CG-CD	-5.94	1.30	1.50
1	A	308	ASN	N-CA	-5.94	1.38	1.46
1	A	350	LEU	CG-CD2	-5.93	1.32	1.52
1	A	507	ILE	CA-C	-5.93	1.45	1.52
1	A	216	LEU	CA-C	5.93	1.60	1.52
1	A	606	SER	N-CA	-5.92	1.39	1.46
1	A	321	VAL	N-CA	5.92	1.53	1.46
1	A	479	HIS	CB-CG	5.92	1.58	1.50
1	A	185	GLN	C-N	-5.91	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	511	ALA	N-CA	5.90	1.52	1.46
1	A	613	LEU	C-O	5.90	1.31	1.24
1	A	469	ALA	C-O	5.89	1.31	1.24
1	A	552	VAL	CA-C	5.89	1.59	1.52
1	A	157	GLY	CA-C	5.88	1.60	1.51
1	A	285	PRO	C-N	-5.88	1.25	1.33
1	A	459	VAL	N-CA	5.88	1.52	1.46
1	A	268	ASP	CA-C	-5.88	1.45	1.52
1	A	537	GLU	CA-CB	5.88	1.63	1.53
1	A	189	ILE	N-CA	5.88	1.54	1.46
1	A	266	ASN	CA-CB	5.87	1.62	1.53
1	A	371	ALA	CA-C	5.87	1.60	1.53
1	A	570	TYR	CZ-OH	5.87	1.50	1.38
1	A	577	GLN	N-CA	5.87	1.53	1.45
1	A	284	GLY	C-N	-5.86	1.26	1.33
1	A	360	LEU	CA-C	5.86	1.60	1.52
1	A	265	THR	N-CA	-5.84	1.38	1.46
1	A	374	ARG	CZ-NH2	-5.83	1.25	1.33
1	A	196	VAL	N-CA	5.83	1.52	1.46
1	A	408	PHE	CG-CD1	5.82	1.51	1.38
1	A	161	CYS	C-O	5.81	1.30	1.24
1	A	472	PHE	C-N	5.80	1.40	1.33
1	A	178	THR	CA-C	-5.79	1.45	1.52
1	A	412	GLY	N-CA	5.78	1.51	1.46
1	A	178	THR	C-N	5.78	1.41	1.33
1	A	208	ASP	CA-CB	5.78	1.62	1.53
1	A	438	LEU	CA-CB	5.77	1.62	1.53
1	A	605	ALA	CA-C	-5.77	1.44	1.52
1	A	454	PHE	C-O	-5.77	1.16	1.23
1	A	488	LYS	N-CA	5.77	1.53	1.46
1	A	407	LYS	CD-CE	-5.77	1.35	1.52
1	A	220	ASP	CG-OD2	-5.76	1.14	1.25
1	A	378	LYS	C-O	-5.76	1.17	1.23
1	A	484	PRO	CG-CD	5.76	1.70	1.50
1	A	614	CYS	C-N	5.75	1.44	1.34
1	A	82	THR	N-CA	-5.75	1.38	1.45
1	A	610	MET	CA-C	5.75	1.60	1.52
1	A	457	GLY	C-O	5.74	1.29	1.24
1	A	464	SER	CB-OG	5.74	1.53	1.42
1	A	586	SER	CB-OG	5.74	1.53	1.42
1	A	166	TYR	CE1-CZ	-5.72	1.24	1.38
1	A	262	LYS	C-O	5.72	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286	GLY	CA-C	5.72	1.61	1.52
1	A	352	HIS	CB-CG	5.72	1.58	1.50
1	A	420	LYS	CA-CB	5.72	1.62	1.53
1	A	450	SER	CB-OG	5.72	1.53	1.42
1	A	516	LEU	CG-CD2	5.71	1.71	1.52
1	A	336	PRO	C-O	5.70	1.31	1.24
1	A	207	LEU	CB-CG	-5.70	1.42	1.53
1	A	564	PRO	CA-C	-5.68	1.46	1.52
1	A	430	ALA	C-O	5.68	1.30	1.24
1	A	503	THR	C-O	-5.67	1.17	1.24
1	A	325	ASP	CB-CG	-5.67	1.37	1.52
1	A	443	VAL	C-N	-5.67	1.26	1.33
1	A	402	ASP	CA-C	-5.66	1.45	1.53
1	A	228	ILE	CA-CB	-5.66	1.47	1.54
1	A	359	LYS	N-CA	5.65	1.53	1.46
1	A	446	TYR	CD2-CE2	-5.65	1.21	1.38
1	A	448	SER	N-CA	5.65	1.53	1.46
1	A	341	VAL	N-CA	5.64	1.53	1.46
1	A	164	GLN	N-CA	5.64	1.53	1.46
1	A	390	SER	CB-OG	5.63	1.53	1.42
1	A	171	SER	C-O	-5.63	1.16	1.23
1	A	372	PRO	N-CA	5.63	1.54	1.47
1	A	498	ALA	N-CA	-5.63	1.39	1.46
1	A	333	GLU	CA-CB	-5.62	1.45	1.53
1	A	373	ARG	NE-CZ	5.62	1.39	1.33
1	A	270	LEU	C-N	5.62	1.41	1.33
1	A	250	ARG	N-CA	5.61	1.53	1.46
1	A	603	VAL	C-N	-5.61	1.26	1.33
1	A	250	ARG	C-O	-5.61	1.17	1.24
1	A	204	PHE	CA-CB	5.60	1.63	1.53
1	A	576	PRO	CA-CB	-5.60	1.45	1.53
1	A	529	GLU	N-CA	5.59	1.54	1.46
1	A	273	ILE	CA-CB	-5.59	1.47	1.54
1	A	219	GLY	C-O	-5.59	1.17	1.23
1	A	211	ILE	N-CA	-5.59	1.39	1.46
1	A	295	ARG	C-N	5.59	1.41	1.34
1	A	333	GLU	CA-C	-5.58	1.46	1.52
1	A	469	ALA	CA-CB	5.58	1.62	1.53
1	A	367	SER	C-N	-5.57	1.25	1.33
1	A	231	MET	CB-CG	5.56	1.69	1.52
1	A	272	MET	N-CA	5.56	1.53	1.46
1	A	312	ARG	CD-NE	-5.55	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	486	SER	C-N	-5.55	1.26	1.33
1	A	317	SER	CB-OG	-5.54	1.31	1.42
1	A	598	GLU	C-N	-5.54	1.26	1.33
1	A	352	HIS	CA-CB	5.53	1.61	1.53
1	A	346	THR	CA-C	5.53	1.59	1.52
1	A	595	SER	N-CA	-5.52	1.39	1.46
1	A	220	ASP	CG-OD1	5.51	1.35	1.25
1	A	579	GLU	CD-OE2	-5.50	1.14	1.25
1	A	166	TYR	C-N	5.50	1.41	1.33
1	A	294	HIS	CD2-NE2	5.50	1.43	1.37
1	A	418	LYS	CG-CD	5.47	1.68	1.52
1	A	335	SER	N-CA	5.47	1.52	1.46
1	A	184	ALA	N-CA	-5.47	1.39	1.46
1	A	531	PRO	CA-C	-5.46	1.45	1.52
1	A	519	LEU	CB-CG	-5.45	1.42	1.53
1	A	318	LEU	CA-C	-5.45	1.46	1.52
1	A	282	LEU	CG-CD1	5.45	1.70	1.52
1	A	352	HIS	CG-CD2	-5.45	1.29	1.35
1	A	342	LEU	C-N	-5.44	1.27	1.33
1	A	321	VAL	C-O	-5.44	1.18	1.24
1	A	264	SER	CA-CB	5.43	1.62	1.53
1	A	278	CYS	CA-C	-5.43	1.46	1.52
1	A	593	GLU	CG-CD	-5.42	1.38	1.52
1	A	470	LEU	C-N	-5.42	1.27	1.33
1	A	262	LYS	CD-CE	5.42	1.68	1.52
1	A	242	ILE	CB-CG1	5.41	1.64	1.53
1	A	276	CYS	CA-CB	-5.41	1.45	1.53
1	A	425	GLY	CA-C	-5.41	1.46	1.52
1	A	64	PRO	N-CD	5.40	1.55	1.47
1	A	372	PRO	N-CD	5.40	1.55	1.47
1	A	47	PRO	N-CD	5.39	1.55	1.47
1	A	353	MET	CG-SD	5.39	1.94	1.80
1	A	285	PRO	CA-C	5.39	1.58	1.52
1	A	108	PRO	N-CD	5.39	1.55	1.47
1	A	176	GLY	C-O	-5.39	1.16	1.24
1	A	29	PRO	N-CD	5.38	1.55	1.47
1	A	497	GLN	CB-CG	-5.38	1.36	1.52
1	A	347	GLU	CA-C	5.38	1.60	1.52
1	A	580	ALA	C-N	5.38	1.40	1.33
1	A	52	ARG	N-CA	5.38	1.52	1.46
1	A	410	ASN	CA-C	-5.37	1.45	1.52
1	A	570	TYR	CD2-CE2	5.37	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	494	THR	N-CA	-5.37	1.40	1.46
1	A	197	ILE	C-N	-5.36	1.26	1.33
1	A	175	PRO	N-CD	5.36	1.55	1.47
1	A	28	VAL	C-N	5.36	1.39	1.33
1	A	497	GLN	C-O	5.35	1.30	1.24
1	A	304	GLY	N-CA	-5.35	1.37	1.45
1	A	273	ILE	C-O	-5.35	1.18	1.24
1	A	287	THR	CA-C	-5.34	1.45	1.52
1	A	213	PHE	CG-CD2	5.33	1.50	1.38
1	A	516	LEU	CA-CB	5.33	1.61	1.53
1	A	231	MET	CA-C	-5.31	1.45	1.52
1	A	376	ARG	CA-CB	5.31	1.62	1.53
1	A	76	LEU	C-N	5.30	1.40	1.33
1	A	172	TYR	CB-CG	-5.30	1.40	1.51
1	A	441	ARG	C-O	-5.30	1.17	1.23
1	A	221	LEU	CA-C	5.30	1.59	1.52
1	A	516	LEU	C-N	5.30	1.40	1.33
1	A	406	TYR	CA-CB	-5.29	1.45	1.53
1	A	423	PRO	N-CD	5.29	1.55	1.47
1	A	380	SER	N-CA	5.29	1.53	1.45
1	A	373	ARG	CA-CB	-5.28	1.45	1.53
1	A	579	GLU	CG-CD	5.28	1.65	1.52
1	A	181	THR	CA-C	5.26	1.58	1.52
1	A	615	SER	CA-CB	5.26	1.65	1.53
1	A	578	PRO	CA-CB	5.25	1.61	1.53
1	A	388	ALA	N-CA	-5.25	1.40	1.46
1	A	593	GLU	CA-CB	-5.25	1.45	1.53
1	A	356	SER	CA-C	-5.24	1.45	1.52
1	A	160	LEU	CG-CD2	-5.24	1.35	1.52
1	A	319	GLN	CD-OE1	5.22	1.33	1.23
1	A	390	SER	C-O	5.22	1.30	1.24
1	A	555	THR	CB-OG1	-5.22	1.35	1.43
1	A	166	TYR	N-CA	5.22	1.53	1.46
1	A	385	GLY	C-N	-5.22	1.27	1.33
1	A	436	TYR	CE2-CZ	-5.22	1.25	1.38
1	A	205	PHE	CD2-CE2	5.22	1.54	1.38
1	A	506	ALA	C-N	5.21	1.39	1.34
1	A	416	ILE	N-CA	-5.21	1.40	1.46
1	A	295	ARG	C-O	5.21	1.30	1.24
1	A	362	ARG	CA-C	5.20	1.59	1.52
1	A	610	MET	C-N	-5.20	1.27	1.33
1	A	227	LYS	CA-C	-5.19	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	454	PHE	CG-CD1	5.19	1.49	1.38
1	A	505	MET	CA-C	5.19	1.59	1.52
1	A	409	ASP	CA-C	-5.19	1.45	1.52
1	A	413	LYS	N-CA	-5.18	1.40	1.46
1	A	253	TRP	CA-CB	5.17	1.61	1.53
1	A	267	ARG	C-N	5.17	1.40	1.33
1	A	327	THR	C-O	-5.16	1.17	1.24
1	A	358	LYS	CA-C	5.16	1.59	1.52
1	A	231	MET	C-O	5.16	1.30	1.24
1	A	491	LEU	CA-C	5.15	1.59	1.52
1	A	157	GLY	C-N	-5.15	1.24	1.33
1	A	277	ILE	C-O	-5.14	1.17	1.24
1	A	597	VAL	C-O	-5.14	1.18	1.24
1	A	340	ILE	CA-C	5.14	1.59	1.52
1	A	198	VAL	C-O	5.14	1.29	1.24
1	A	221	LEU	N-CA	5.14	1.52	1.46
1	A	461	ASN	C-N	5.14	1.40	1.33
1	A	166	TYR	CG-CD1	-5.13	1.28	1.39
1	A	273	ILE	N-CA	5.13	1.52	1.46
1	A	229	VAL	CA-CB	-5.13	1.47	1.54
1	A	346	THR	N-CA	-5.13	1.40	1.46
1	A	313	TRP	N-CA	-5.12	1.40	1.47
1	A	108	PRO	C-N	-5.12	1.25	1.33
1	A	571	GLY	C-O	5.12	1.30	1.23
1	A	294	HIS	C-O	5.12	1.30	1.24
1	A	216	LEU	C-O	5.11	1.30	1.23
1	A	210	VAL	CB-CG1	5.11	1.69	1.52
1	A	51	PHE	CA-C	5.10	1.59	1.52
1	A	585	ILE	N-CA	-5.10	1.40	1.46
1	A	278	CYS	C-N	5.10	1.40	1.33
1	A	556	MET	SD-CE	5.10	1.92	1.79
1	A	446	TYR	CE1-CZ	-5.09	1.26	1.38
1	A	362	ARG	C-N	5.09	1.40	1.33
1	A	468	GLU	C-O	5.09	1.30	1.24
1	A	616	SER	CA-CB	-5.09	1.43	1.53
1	A	557	GLU	C-O	5.07	1.30	1.23
1	A	349	LEU	C-O	-5.07	1.18	1.24
1	A	267	ARG	CG-CD	5.06	1.67	1.52
1	A	275	ARG	CG-CD	5.05	1.67	1.52
1	A	530	PRO	CB-CG	5.05	1.74	1.49
1	A	609	ASP	CA-C	-5.05	1.46	1.52
1	A	380	SER	C-O	5.04	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	GLN	CB-CG	-5.03	1.37	1.52
1	A	560	CYS	C-N	5.03	1.40	1.33
1	A	610	MET	CA-CB	5.03	1.61	1.53
1	A	598	GLU	CG-CD	5.03	1.64	1.52
1	A	268	ASP	C-O	-5.02	1.18	1.24
1	A	331	VAL	C-N	5.02	1.40	1.33
1	A	371	ALA	CA-CB	-5.01	1.44	1.52
1	A	457	GLY	N-CA	5.01	1.51	1.45
1	A	165	TYR	CA-C	-5.00	1.46	1.52

All (887) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	GLU	O-C-N	-31.12	90.59	123.26
1	A	189	ILE	CA-C-O	-30.16	87.90	120.47
1	A	167	ARG	NE-CZ-NH2	-27.70	94.27	119.20
1	A	190	MET	O-C-N	-27.16	90.09	121.32
1	A	189	ILE	O-C-N	24.08	149.01	121.80
1	A	360	LEU	CA-C-N	19.71	157.45	121.97
1	A	360	LEU	C-N-CA	19.71	157.45	121.97
1	A	189	ILE	N-CA-C	19.13	135.00	111.09
1	A	226	ARG	NE-CZ-NH1	-18.92	102.58	121.50
1	A	415	PHE	CA-C-O	18.23	140.41	120.90
1	A	452	ARG	NE-CZ-NH2	18.12	135.51	119.20
1	A	267	ARG	NE-CZ-NH1	18.09	139.59	121.50
1	A	376	ARG	NE-CZ-NH1	18.07	139.57	121.50
1	A	267	ARG	NH1-CZ-NH2	-17.33	96.77	119.30
1	A	288	GLY	O-C-N	-16.74	100.94	122.70
1	A	286	GLY	CA-C-N	16.14	152.37	121.54
1	A	286	GLY	C-N-CA	16.14	152.37	121.54
1	A	526	LEU	N-CA-C	-15.95	93.76	113.38
1	A	526	LEU	N-CA-CB	-15.89	86.85	110.53
1	A	219	GLY	CA-C-O	15.71	136.20	120.80
1	A	185	GLN	CA-C-N	-15.69	97.81	122.29
1	A	185	GLN	C-N-CA	-15.69	97.81	122.29
1	A	267	ARG	CA-CB-CG	15.28	144.66	114.10
1	A	190	MET	N-CA-CB	15.15	137.33	110.37
1	A	219	GLY	N-CA-C	15.03	131.16	112.83
1	A	237	GLU	N-CA-CB	14.94	135.74	110.49
1	A	364	ASP	CA-C-N	-14.79	104.84	122.44
1	A	364	ASP	C-N-CA	-14.79	104.84	122.44
1	A	258	THR	CA-C-O	-14.38	105.31	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	GLN	CB-CG-CD	14.35	136.99	112.60
1	A	154	GLN	CA-C-N	-14.27	93.96	123.20
1	A	154	GLN	C-N-CA	-14.27	93.96	123.20
1	A	308	ASN	N-CA-C	14.16	128.78	112.93
1	A	415	PHE	O-C-N	-14.09	107.44	122.09
1	A	226	ARG	N-CA-C	13.96	127.86	111.11
1	A	254	ALA	CA-C-O	-13.90	106.22	120.82
1	A	494	THR	O-C-N	13.87	136.36	122.07
1	A	417	LYS	O-C-N	13.84	139.29	122.27
1	A	544	ARG	NE-CZ-NH2	-13.77	106.81	119.20
1	A	237	GLU	N-CA-C	-13.45	82.15	110.80
1	A	292	ASP	N-CA-C	-13.42	96.66	111.28
1	A	577	GLN	O-C-N	-13.40	111.50	121.14
1	A	612	ASP	O-C-N	-13.40	108.16	122.09
1	A	532	GLU	CG-CD-OE2	-13.16	88.14	118.40
1	A	365	SER	N-CA-C	13.12	130.96	111.02
1	A	616	SER	CA-C-O	-13.04	98.63	120.80
1	A	532	GLU	OE1-CD-OE2	13.04	154.20	122.90
1	A	607	LEU	O-C-N	13.00	135.90	122.12
1	A	383	THR	O-C-N	-12.93	106.36	122.27
1	A	496	MET	CG-SD-CE	-12.82	72.70	100.90
1	A	415	PHE	N-CA-C	12.60	126.23	111.11
1	A	478	ASP	CA-CB-CG	-12.57	100.03	112.60
1	A	226	ARG	NH1-CZ-NH2	12.53	135.58	119.30
1	A	598	GLU	N-CA-CB	12.40	128.02	109.91
1	A	367	SER	N-CA-C	12.35	127.61	107.73
1	A	236	ASP	CB-CA-C	-12.16	93.88	112.12
1	A	348	HIS	O-C-N	-12.01	108.46	122.15
1	A	167	ARG	CD-NE-CZ	11.97	141.17	124.40
1	A	220	ASP	O-C-N	11.94	136.95	122.27
1	A	411	TYR	O-C-N	11.82	134.37	123.26
1	A	383	THR	CA-C-N	11.67	136.29	120.54
1	A	383	THR	C-N-CA	11.67	136.29	120.54
1	A	288	GLY	CA-C-N	11.66	141.75	121.80
1	A	288	GLY	C-N-CA	11.66	141.75	121.80
1	A	222	PHE	CA-C-O	11.64	133.36	120.90
1	A	254	ALA	O-C-N	11.64	134.06	122.07
1	A	367	SER	N-CA-CB	-11.64	87.08	111.87
1	A	193	PRO	CA-C-N	-11.52	105.74	123.13
1	A	193	PRO	C-N-CA	-11.52	105.74	123.13
1	A	192	GLU	N-CA-C	11.50	135.23	109.81
1	A	261	LEU	O-C-N	11.42	137.78	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	PRO	CA-C-O	-11.41	107.94	121.86
1	A	260	LEU	CA-C-O	-11.39	108.47	120.55
1	A	608	VAL	CA-C-O	11.39	133.24	121.17
1	A	373	ARG	NE-CZ-NH1	-11.35	110.15	121.50
1	A	437	ARG	NH1-CZ-NH2	11.34	134.05	119.30
1	A	218	GLU	CA-C-O	11.31	133.59	120.92
1	A	212	ASN	OD1-CG-ND2	-11.30	111.30	122.60
1	A	214	ARG	NE-CZ-NH2	-11.29	109.04	119.20
1	A	266	ASN	O-C-N	-11.11	108.75	122.20
1	A	176	GLY	O-C-N	-11.07	113.66	123.29
1	A	391	ALA	O-C-N	-11.02	110.28	122.08
1	A	386	HIS	N-CA-C	-11.02	97.88	111.11
1	A	453	ARG	CA-CB-CG	11.01	136.13	114.10
1	A	577	GLN	CA-C-O	11.01	130.88	121.08
1	A	376	ARG	NE-CZ-NH2	-11.00	109.30	119.20
1	A	72	GLN	OE1-CD-NE2	-11.00	111.60	122.60
1	A	178	THR	OG1-CB-CG2	-10.99	87.31	109.30
1	A	458	ARG	CA-C-O	-10.99	112.84	119.55
1	A	395	GLN	OE1-CD-NE2	-10.95	111.65	122.60
1	A	267	ARG	CA-C-O	10.95	132.45	120.63
1	A	484	PRO	N-CA-CB	10.94	113.04	103.19
1	A	273	ILE	CA-C-O	10.92	132.31	120.95
1	A	491	LEU	CA-C-O	-10.90	108.99	120.55
1	A	609	ASP	O-C-N	-10.90	109.73	122.15
1	A	380	SER	CA-CB-OG	10.82	132.74	111.10
1	A	529	GLU	CA-C-N	-10.78	109.28	120.38
1	A	529	GLU	C-N-CA	-10.78	109.28	120.38
1	A	437	ARG	NE-CZ-NH1	-10.74	110.76	121.50
1	A	605	ALA	CA-C-N	10.71	135.50	120.29
1	A	605	ALA	C-N-CA	10.71	135.50	120.29
1	A	381	PRO	N-CD-CG	-10.71	87.14	103.20
1	A	493	GLN	CA-C-O	-10.70	109.58	120.82
1	A	417	LYS	CA-C-O	-10.64	107.73	119.97
1	A	258	THR	O-C-N	10.61	133.37	122.12
1	A	267	ARG	CG-CD-NE	-10.59	88.71	112.00
1	A	251	SER	CA-C-N	10.54	134.14	120.44
1	A	251	SER	C-N-CA	10.54	134.14	120.44
1	A	365	SER	N-CA-CB	-10.53	90.04	111.00
1	A	275	ARG	NE-CZ-NH2	-10.50	109.75	119.20
1	A	158	GLN	O-C-N	10.46	130.61	121.20
1	A	190	MET	N-CA-C	-10.42	86.78	109.81
1	A	608	VAL	O-C-N	-10.34	111.78	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	ASN	O-C-N	10.33	134.55	122.25
1	A	605	ALA	O-C-N	-10.32	108.21	122.46
1	A	400	ASN	CA-CB-CG	10.29	122.89	112.60
1	A	186	LYS	CA-C-N	10.27	141.15	121.54
1	A	186	LYS	C-N-CA	10.27	141.15	121.54
1	A	209	VAL	CA-CB-CG2	10.26	127.84	110.40
1	A	331	VAL	CA-CB-CG1	10.25	127.83	110.40
1	A	379	CYS	CB-CA-C	-10.21	94.44	110.78
1	A	377	TRP	O-C-N	10.19	135.34	123.41
1	A	378	LYS	CB-CG-CD	10.19	134.74	111.30
1	A	32	GLN	OE1-CD-NE2	-10.15	112.45	122.60
1	A	115	GLN	OE1-CD-NE2	-10.15	112.45	122.60
1	A	240	PRO	O-C-N	10.15	133.43	121.46
1	A	419	GLN	N-CA-C	10.14	125.21	113.15
1	A	220	ASP	CA-C-O	-10.06	108.41	119.97
1	A	209	VAL	O-C-N	10.00	132.20	122.20
1	A	222	PHE	N-CA-C	9.99	123.10	111.11
1	A	118	GLN	OE1-CD-NE2	-9.96	112.64	122.60
1	A	437	ARG	CD-NE-CZ	-9.95	110.47	124.40
1	A	544	ARG	NE-CZ-NH1	9.93	131.43	121.50
1	A	235	GLU	O-C-N	-9.88	110.94	122.20
1	A	33	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	A	493	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	A	43	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	A	401	LEU	O-C-N	-9.79	112.06	123.22
1	A	154	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	A	294	HIS	CA-CB-CG	-9.76	104.04	113.80
1	A	308	ASN	N-CA-CB	-9.74	97.11	110.56
1	A	611	ARG	CB-CA-C	-9.73	94.64	110.79
1	A	521	GLU	CG-CD-OE1	9.71	140.73	118.40
1	A	50	GLN	OE1-CD-NE2	-9.69	112.91	122.60
1	A	55	GLN	OE1-CD-NE2	-9.65	112.95	122.60
1	A	123	GLN	OE1-CD-NE2	-9.61	112.99	122.60
1	A	266	ASN	OD1-CG-ND2	-9.59	113.01	122.60
1	A	600	ALA	O-C-N	9.59	131.95	122.07
1	A	490	GLN	CA-C-O	-9.58	110.39	120.55
1	A	380	SER	N-CA-C	-9.56	96.12	110.07
1	A	79	GLN	OE1-CD-NE2	-9.54	113.06	122.60
1	A	107	SER	O-C-N	9.53	129.41	121.31
1	A	453	ARG	CG-CD-NE	9.52	132.94	112.00
1	A	301	HIS	ND1-CG-CD2	9.51	115.61	106.10
1	A	479	HIS	CA-C-N	9.51	138.72	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	HIS	C-N-CA	9.51	138.72	122.36
1	A	351	LYS	CA-C-O	-9.47	110.51	120.55
1	A	376	ARG	CD-NE-CZ	9.47	137.66	124.40
1	A	608	VAL	N-CA-CB	9.45	121.61	110.55
1	A	364	ASP	CA-CB-CG	9.44	122.04	112.60
1	A	167	ARG	NH1-CZ-NH2	9.44	131.56	119.30
1	A	452	ARG	NE-CZ-NH1	-9.38	112.12	121.50
1	A	567	PRO	O-C-N	9.37	134.92	122.27
1	A	473	VAL	O-C-N	9.30	132.31	121.80
1	A	487	GLU	N-CA-CB	9.29	123.48	110.01
1	A	373	ARG	N-CA-CB	-9.28	96.18	110.29
1	A	295	ARG	NE-CZ-NH2	-9.28	110.85	119.20
1	A	178	THR	CA-CB-OG1	-9.28	95.69	109.60
1	A	154	GLN	O-C-N	-9.23	110.32	122.59
1	A	432	GLN	CA-C-O	-9.21	111.15	120.82
1	A	255	LYS	O-C-N	-9.20	112.37	122.12
1	A	483	MET	N-CA-CB	9.20	126.74	110.37
1	A	491	LEU	N-CA-C	-9.19	101.26	111.28
1	A	273	ILE	O-C-N	-9.16	112.98	121.87
1	A	391	ALA	CA-C-O	9.16	131.15	121.07
1	A	350	LEU	O-C-N	9.12	131.47	122.07
1	A	209	VAL	CA-C-O	-9.11	109.55	119.20
1	A	40	GLN	OE1-CD-NE2	-9.09	113.51	122.60
1	A	335	SER	CA-C-O	-9.08	109.98	118.33
1	A	358	LYS	N-CA-CB	-9.08	98.05	110.67
1	A	293	THR	CA-C-O	9.05	130.32	120.82
1	A	490	GLN	N-CA-C	-9.03	101.44	111.28
1	A	187	SER	O-C-N	-9.02	110.60	122.59
1	A	601	GLU	CA-C-O	8.96	130.05	120.55
1	A	224	GLN	O-C-N	-8.93	112.88	122.07
1	A	158	GLN	OE1-CD-NE2	-8.91	113.69	122.60
1	A	429	VAL	O-C-N	-8.90	112.64	121.90
1	A	412	GLY	O-C-N	-8.86	116.40	123.14
1	A	396	ARG	CD-NE-CZ	-8.84	112.03	124.40
1	A	413	LYS	O-C-N	8.82	131.47	122.12
1	A	199	ALA	CA-C-O	8.82	130.04	120.43
1	A	350	LEU	CA-C-O	-8.80	111.58	120.82
1	A	429	VAL	N-CA-C	-8.80	102.26	110.53
1	A	365	SER	CA-C-N	-8.79	106.14	121.97
1	A	365	SER	C-N-CA	-8.79	106.14	121.97
1	A	396	ARG	NE-CZ-NH2	-8.79	111.29	119.20
1	A	299	LEU	N-CA-C	-8.77	101.80	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	ARG	CA-C-O	8.77	130.28	120.90
1	A	178	THR	CA-CB-CG2	-8.77	95.60	110.50
1	A	413	LYS	CA-C-N	-8.75	109.06	120.44
1	A	413	LYS	C-N-CA	-8.75	109.06	120.44
1	A	571	GLY	O-C-N	-8.73	115.76	123.80
1	A	407	LYS	CA-C-N	8.71	134.97	121.99
1	A	407	LYS	C-N-CA	8.71	134.97	121.99
1	A	219	GLY	O-C-N	-8.71	113.72	122.17
1	A	454	PHE	CD1-CG-CD2	-8.70	105.55	118.60
1	A	403	PHE	CA-C-O	-8.69	111.32	120.70
1	A	361	VAL	O-C-N	-8.68	111.72	122.57
1	A	185	GLN	OE1-CD-NE2	-8.67	113.93	122.60
1	A	452	ARG	CD-NE-CZ	8.67	136.53	124.40
1	A	218	GLU	CB-CG-CD	8.65	127.31	112.60
1	A	437	ARG	O-C-N	-8.64	110.54	122.46
1	A	603	VAL	O-C-N	8.61	130.85	121.90
1	A	166	TYR	CG-CD1-CE1	8.60	134.09	121.20
1	A	410	ASN	O-C-N	-8.56	110.65	122.46
1	A	532	GLU	O-C-N	8.55	131.18	122.12
1	A	453	ARG	CD-NE-CZ	-8.54	112.45	124.40
1	A	477	THR	CA-C-N	-8.52	105.26	121.54
1	A	477	THR	C-N-CA	-8.52	105.26	121.54
1	A	218	GLU	CG-CD-OE1	-8.51	98.83	118.40
1	A	205	PHE	CA-C-O	8.51	130.44	120.66
1	A	385	GLY	CA-C-N	8.50	132.01	120.54
1	A	385	GLY	C-N-CA	8.50	132.01	120.54
1	A	270	LEU	O-C-N	-8.48	113.13	122.12
1	A	424	ASP	N-CA-C	-8.47	102.00	111.07
1	A	611	ARG	NE-CZ-NH2	-8.46	111.58	119.20
1	A	614	CYS	O-C-N	8.46	133.76	122.43
1	A	275	ARG	NE-CZ-NH1	8.45	129.95	121.50
1	A	275	ARG	CD-NE-CZ	8.44	136.22	124.40
1	A	260	LEU	CA-C-N	8.42	137.62	121.54
1	A	260	LEU	C-N-CA	8.42	137.62	121.54
1	A	487	GLU	CA-C-N	-8.42	108.84	120.38
1	A	487	GLU	C-N-CA	-8.42	108.84	120.38
1	A	346	THR	O-C-N	8.41	131.03	122.12
1	A	597	VAL	CA-C-N	8.37	131.69	120.65
1	A	597	VAL	C-N-CA	8.37	131.69	120.65
1	A	411	TYR	CA-C-O	-8.36	111.90	121.26
1	A	344	GLN	CG-CD-NE2	-8.36	103.87	116.40
1	A	187	SER	CA-C-O	-8.35	108.57	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	559	PHE	CD1-CG-CD2	-8.35	106.08	118.60
1	A	376	ARG	N-CA-CB	-8.34	97.54	110.46
1	A	423	PRO	CA-CB-CG	-8.33	88.68	104.50
1	A	447	GLU	CA-C-O	8.33	130.52	120.28
1	A	556	MET	O-C-N	-8.31	113.37	122.85
1	A	466	THR	CA-C-N	-8.31	110.14	119.28
1	A	466	THR	C-N-CA	-8.31	110.14	119.28
1	A	230	LYS	CG-CD-CE	-8.30	92.21	111.30
1	A	233	SER	N-CA-CB	-8.30	97.68	110.46
1	A	517	LEU	O-C-N	8.29	130.61	122.07
1	A	299	LEU	CA-C-O	-8.23	111.70	120.42
1	A	211	ILE	O-C-N	8.22	131.95	123.07
1	A	601	GLU	N-CA-C	8.22	120.24	111.28
1	A	259	VAL	O-C-N	-8.20	113.92	121.87
1	A	484	PRO	CA-C-O	-8.20	112.38	121.32
1	A	403	PHE	N-CA-C	8.17	122.71	109.40
1	A	460	ASP	CA-C-O	-8.15	111.73	121.60
1	A	192	GLU	CA-C-N	-8.08	109.75	119.84
1	A	192	GLU	C-N-CA	-8.08	109.75	119.84
1	A	458	ARG	O-C-N	8.08	127.98	120.71
1	A	268	ASP	O-C-N	8.05	130.46	122.09
1	A	161	CYS	O-C-N	-8.03	112.33	123.01
1	A	588	PHE	CG-CD1-CE1	-8.03	107.05	120.70
1	A	257	ARG	NE-CZ-NH2	8.03	126.43	119.20
1	A	230	LYS	CB-CA-C	8.02	123.47	110.88
1	A	614	CYS	CA-C-O	-8.01	109.53	119.38
1	A	474	GLN	CA-C-O	-8.00	109.53	119.38
1	A	176	GLY	CA-C-O	8.00	130.97	121.77
1	A	151	ALA	N-CA-C	-8.00	103.32	113.23
1	A	274	GLU	N-CA-C	7.99	122.13	112.38
1	A	297	LEU	O-C-N	-7.99	113.04	122.15
1	A	612	ASP	CA-C-O	7.97	129.43	120.90
1	A	394	LEU	CA-C-O	7.97	128.99	120.55
1	A	578	PRO	N-CA-CB	-7.95	95.10	103.52
1	A	566	VAL	O-C-N	-7.95	116.16	121.72
1	A	207	LEU	CA-C-O	7.94	129.75	120.70
1	A	205	PHE	O-C-N	-7.93	113.59	123.27
1	A	156	SER	N-CA-C	7.92	127.67	110.80
1	A	525	ASP	CA-C-N	-7.92	108.56	122.26
1	A	525	ASP	C-N-CA	-7.92	108.56	122.26
1	A	261	LEU	CA-C-O	-7.91	109.19	120.51
1	A	450	SER	N-CA-CB	-7.90	98.35	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ALA	CA-C-O	-7.90	110.11	119.35
1	A	289	GLU	N-CA-C	7.90	120.13	108.60
1	A	392	GLU	N-CA-CB	7.90	121.71	109.94
1	A	363	ALA	CA-C-N	7.86	136.56	121.54
1	A	363	ALA	C-N-CA	7.86	136.56	121.54
1	A	459	VAL	CA-C-O	7.86	129.41	121.63
1	A	381	PRO	CA-CB-CG	-7.85	89.58	104.50
1	A	382	GLU	CB-CG-CD	7.83	125.92	112.60
1	A	553	PRO	CA-C-O	-7.82	112.32	121.86
1	A	282	LEU	CA-C-N	7.81	131.79	120.71
1	A	282	LEU	C-N-CA	7.81	131.79	120.71
1	A	472	PHE	O-C-N	-7.81	113.66	122.09
1	A	196	VAL	CB-CA-C	7.79	123.28	111.68
1	A	451	ILE	N-CA-C	-7.78	103.68	111.77
1	A	493	GLN	CA-C-N	7.78	130.55	120.44
1	A	493	GLN	C-N-CA	7.78	130.55	120.44
1	A	609	ASP	OD1-CG-OD2	-7.78	104.23	122.90
1	A	419	GLN	CB-CG-CD	7.77	125.80	112.60
1	A	441	ARG	NE-CZ-NH2	-7.77	112.21	119.20
1	A	376	ARG	CG-CD-NE	-7.76	94.92	112.00
1	A	73	GLU	CB-CA-C	7.75	123.21	110.81
1	A	431	LEU	N-CA-C	7.74	119.72	111.28
1	A	334	HIS	ND1-CE1-NE2	-7.74	100.66	108.40
1	A	613	LEU	CA-C-O	7.74	128.84	120.10
1	A	153	GLY	CA-C-N	-7.73	106.78	121.54
1	A	153	GLY	C-N-CA	-7.73	106.78	121.54
1	A	220	ASP	CA-C-N	-7.71	107.57	120.68
1	A	220	ASP	C-N-CA	-7.71	107.57	120.68
1	A	391	ALA	CA-C-N	7.68	130.91	120.54
1	A	391	ALA	C-N-CA	7.68	130.91	120.54
1	A	345	CYS	CA-C-O	7.68	128.61	120.70
1	A	191	PRO	CA-C-N	7.67	140.52	121.80
1	A	191	PRO	C-N-CA	7.67	140.52	121.80
1	A	348	HIS	CA-C-N	7.66	130.40	120.44
1	A	348	HIS	C-N-CA	7.66	130.40	120.44
1	A	433	LEU	O-C-N	-7.65	113.27	122.22
1	A	448	SER	CA-CB-OG	-7.64	95.81	111.10
1	A	286	GLY	O-C-N	7.61	132.89	122.84
1	A	437	ARG	CG-CD-NE	-7.61	95.25	112.00
1	A	247	SER	CA-C-O	-7.61	110.02	119.38
1	A	252	GLU	O-C-N	-7.61	114.23	122.07
1	A	218	GLU	OE1-CD-OE2	7.58	141.08	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ASP	CA-C-O	7.58	130.75	121.89
1	A	173	ARG	O-C-N	-7.57	113.56	122.87
1	A	227	LYS	N-CA-C	7.56	120.40	111.71
1	A	380	SER	CA-C-O	7.52	132.09	121.27
1	A	442	LEU	O-C-N	-7.51	114.55	123.03
1	A	370	PRO	O-C-N	7.51	132.59	123.13
1	A	332	CYS	CA-C-O	-7.49	112.21	120.38
1	A	387	LEU	N-CA-C	7.49	119.44	111.28
1	A	454	PHE	CB-CG-CD2	7.47	133.41	120.70
1	A	405	VAL	CA-C-O	-7.46	111.64	120.75
1	A	386	HIS	N-CA-CB	7.46	121.06	109.94
1	A	240	PRO	N-CA-C	-7.44	101.63	110.70
1	A	399	LYS	CA-CB-CG	-7.43	99.25	114.10
1	A	223	THR	O-C-N	7.42	129.81	122.09
1	A	483	MET	CA-CB-CG	-7.41	99.28	114.10
1	A	345	CYS	O-C-N	-7.36	114.14	122.09
1	A	267	ARG	N-CA-C	7.34	120.22	111.33
1	A	186	LYS	N-CA-C	-7.34	102.60	113.61
1	A	379	CYS	CA-CB-SG	-7.34	97.52	114.40
1	A	189	ILE	CA-C-N	7.34	139.71	121.80
1	A	189	ILE	C-N-CA	7.34	139.71	121.80
1	A	380	SER	O-C-N	-7.34	110.70	121.12
1	A	584	CYS	CA-C-O	-7.34	112.34	120.70
1	A	448	SER	CA-C-O	-7.30	112.59	120.92
1	A	338	ASP	CA-C-O	7.29	130.74	121.55
1	A	615	SER	CA-CB-OG	7.28	125.66	111.10
1	A	606	SER	CA-C-O	7.28	128.13	120.42
1	A	448	SER	N-CA-CB	7.27	120.81	109.69
1	A	522	LEU	N-CA-C	-7.27	102.75	111.69
1	A	242	ILE	CA-CB-CG1	-7.26	98.05	110.40
1	A	613	LEU	N-CA-C	7.26	120.06	111.71
1	A	255	LYS	CA-C-N	7.26	130.31	120.44
1	A	255	LYS	C-N-CA	7.26	130.31	120.44
1	A	196	VAL	N-CA-C	-7.26	97.66	109.12
1	A	199	ALA	O-C-N	-7.25	115.08	123.27
1	A	348	HIS	CB-CG-ND1	-7.25	111.83	122.70
1	A	343	VAL	CA-C-O	-7.25	113.17	120.85
1	A	456	GLU	CA-C-N	-7.24	112.76	120.43
1	A	456	GLU	C-N-CA	-7.24	112.76	120.43
1	A	181	THR	OG1-CB-CG2	-7.23	94.83	109.30
1	A	203	GLN	CG-CD-NE2	7.23	127.24	116.40
1	A	204	PHE	CG-CD2-CE2	-7.21	108.44	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	GLU	CA-C-O	7.21	128.39	120.82
1	A	295	ARG	NE-CZ-NH1	7.20	128.70	121.50
1	A	495	ALA	CA-C-O	-7.20	112.78	120.42
1	A	452	ARG	CB-CG-CD	7.17	127.78	111.30
1	A	605	ALA	N-CA-C	-7.16	104.01	112.89
1	A	185	GLN	CG-CD-NE2	7.15	127.13	116.40
1	A	603	VAL	CA-C-N	-7.14	112.05	119.98
1	A	603	VAL	C-N-CA	-7.14	112.05	119.98
1	A	303	GLY	O-C-N	-7.14	113.07	122.42
1	A	144	HIS	CA-CB-CG	-7.12	106.68	113.80
1	A	276	CYS	N-CA-C	7.12	119.51	110.33
1	A	606	SER	O-C-N	-7.12	114.03	122.15
1	A	315	ASP	CA-CB-CG	-7.12	105.48	112.60
1	A	317	SER	N-CA-C	7.11	120.07	111.82
1	A	325	ASP	N-CA-CB	7.09	122.32	110.41
1	A	494	THR	CA-C-N	-7.07	110.25	120.29
1	A	494	THR	C-N-CA	-7.07	110.25	120.29
1	A	231	MET	N-CA-C	7.07	120.02	111.82
1	A	513	ASP	N-CA-CB	7.05	120.30	110.07
1	A	282	LEU	CA-C-O	-7.04	114.27	122.37
1	A	40	GLN	CG-CD-NE2	7.04	126.96	116.40
1	A	375	LEU	O-C-N	-7.04	114.27	122.93
1	A	358	LYS	N-CA-C	7.03	122.97	113.97
1	A	487	GLU	CG-CD-OE2	-7.03	102.23	118.40
1	A	504	VAL	N-CA-CB	-7.03	98.63	110.65
1	A	396	ARG	NH1-CZ-NH2	7.03	128.44	119.30
1	A	583	PHE	CG-CD2-CE2	7.02	132.63	120.70
1	A	551	GLN	CG-CD-NE2	7.01	126.92	116.40
1	A	294	HIS	ND1-CG-CD2	-7.00	99.10	106.10
1	A	343	VAL	O-C-N	6.99	129.03	121.83
1	A	484	PRO	O-C-N	6.97	131.36	122.85
1	A	447	GLU	O-C-N	-6.96	114.87	123.36
1	A	275	ARG	N-CA-C	-6.94	104.84	113.38
1	A	240	PRO	N-CD-CG	-6.92	92.82	103.20
1	A	249	GLY	O-C-N	-6.91	114.41	122.91
1	A	441	ARG	O-C-N	6.91	130.52	123.26
1	A	258	THR	OG1-CB-CG2	-6.91	95.49	109.30
1	A	491	LEU	O-C-N	6.90	129.43	122.12
1	A	419	GLN	CB-CA-C	-6.88	97.63	110.36
1	A	229	VAL	O-C-N	6.88	128.82	121.87
1	A	175	PRO	CA-C-O	6.88	129.56	121.31
1	A	488	LYS	CD-CE-NZ	6.87	133.89	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	ARG	NE-CZ-NH2	6.87	125.38	119.20
1	A	401	LEU	CA-C-N	6.86	133.30	123.14
1	A	401	LEU	C-N-CA	6.86	133.30	123.14
1	A	585	ILE	O-C-N	-6.83	115.11	123.10
1	A	560	CYS	N-CA-C	-6.82	99.10	109.95
1	A	393	LYS	CD-CE-NZ	6.82	133.72	111.90
1	A	118	GLN	CG-CD-NE2	6.82	126.63	116.40
1	A	550	SER	CA-C-O	6.81	128.52	121.23
1	A	55	GLN	CG-CD-NE2	6.81	126.61	116.40
1	A	115	GLN	CG-CD-NE2	6.80	126.61	116.40
1	A	122	ASP	CA-CB-CG	-6.80	105.80	112.60
1	A	370	PRO	N-CD-CG	-6.79	93.01	103.20
1	A	528	LYS	N-CA-C	6.79	125.27	110.80
1	A	451	ILE	CA-CB-CG2	-6.79	98.96	110.50
1	A	196	VAL	O-C-N	-6.77	114.14	122.61
1	A	442	LEU	CA-C-O	6.77	129.92	121.66
1	A	446	TYR	N-CA-C	-6.76	98.18	109.07
1	A	283	ASP	CA-CB-CG	6.76	119.36	112.60
1	A	444	PRO	CA-N-CD	-6.75	102.55	112.00
1	A	414	THR	CA-C-O	-6.74	113.74	120.82
1	A	154	GLN	CG-CD-NE2	6.74	126.51	116.40
1	A	395	GLN	CG-CD-NE2	6.73	126.50	116.40
1	A	278	CYS	O-C-N	-6.73	116.56	123.29
1	A	493	GLN	CG-CD-NE2	6.72	126.48	116.40
1	A	352	HIS	O-C-N	-6.72	115.15	122.07
1	A	562	TYR	CA-CB-CG	6.71	125.98	113.90
1	A	384	GLN	N-CA-C	-6.71	103.06	111.11
1	A	208	ASP	CA-C-O	-6.70	113.11	120.81
1	A	333	GLU	CB-CA-C	6.70	121.40	110.22
1	A	298	GLN	O-C-N	6.69	128.96	122.07
1	A	315	ASP	CB-CA-C	-6.68	96.54	110.17
1	A	389	SER	CA-C-O	-6.68	113.34	120.42
1	A	479	HIS	O-C-N	6.68	131.47	122.59
1	A	463	ARG	O-C-N	6.66	131.09	122.43
1	A	470	LEU	CA-C-N	6.66	129.53	120.54
1	A	470	LEU	C-N-CA	6.66	129.53	120.54
1	A	151	ALA	CA-C-N	6.66	132.79	121.87
1	A	151	ALA	C-N-CA	6.66	132.79	121.87
1	A	185	GLN	N-CA-C	6.64	124.95	110.80
1	A	286	GLY	N-CA-C	-6.64	102.44	112.60
1	A	384	GLN	N-CA-CB	6.64	119.83	109.94
1	A	232	ALA	N-CA-C	6.63	120.59	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	406	TYR	O-C-N	-6.63	114.78	123.13
1	A	511	ALA	O-C-N	-6.63	113.09	121.78
1	A	24	PRO	CA-N-CD	-6.63	102.72	112.00
1	A	252	GLU	CG-CD-OE1	6.63	133.65	118.40
1	A	156	SER	CA-C-N	6.62	134.39	121.41
1	A	156	SER	C-N-CA	6.62	134.39	121.41
1	A	456	GLU	OE1-CD-OE2	-6.62	107.02	122.90
1	A	182	LEU	CA-C-O	6.61	127.41	120.54
1	A	397	ILE	CA-C-O	-6.61	113.85	120.85
1	A	456	GLU	CG-CD-OE1	6.60	133.58	118.40
1	A	72	GLN	CG-CD-NE2	6.60	126.30	116.40
1	A	178	THR	N-CA-CB	6.59	121.63	110.49
1	A	157	GLY	O-C-N	6.57	131.24	122.70
1	A	250	ARG	O-C-N	6.57	128.92	122.09
1	A	363	ALA	O-C-N	6.55	131.31	122.59
1	A	190	MET	C-N-CD	-6.55	106.19	120.60
1	A	597	VAL	O-C-N	-6.55	115.08	121.83
1	A	301	HIS	CB-CG-ND1	-6.54	112.89	122.70
1	A	551	GLN	CG-CD-OE1	-6.54	107.72	120.80
1	A	449	ALA	CA-C-N	-6.54	111.58	120.87
1	A	449	ALA	C-N-CA	-6.54	111.58	120.87
1	A	327	THR	N-CA-C	-6.52	99.39	109.76
1	A	394	LEU	O-C-N	-6.52	115.21	122.12
1	A	166	TYR	O-C-N	-6.51	112.75	122.39
1	A	322	VAL	CA-C-N	6.51	127.17	120.60
1	A	322	VAL	C-N-CA	6.51	127.17	120.60
1	A	587	SER	CA-C-N	-6.50	114.03	123.00
1	A	587	SER	C-N-CA	-6.50	114.03	123.00
1	A	373	ARG	CA-CB-CG	-6.48	101.13	114.10
1	A	577	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	A	188	SER	N-CA-C	6.48	124.60	110.80
1	A	271	ASP	OD1-CG-OD2	-6.47	107.36	122.90
1	A	599	PHE	CD1-CG-CD2	-6.47	108.89	118.60
1	A	263	ASP	N-CA-C	6.46	120.36	109.76
1	A	170	SER	N-CA-CB	-6.46	100.58	111.17
1	A	531	PRO	CA-C-N	6.44	129.21	120.38
1	A	531	PRO	C-N-CA	6.44	129.21	120.38
1	A	218	GLU	O-C-N	-6.44	114.70	122.11
1	A	478	ASP	CA-C-N	-6.44	109.24	121.54
1	A	478	ASP	C-N-CA	-6.44	109.24	121.54
1	A	347	GLU	O-C-N	6.44	130.19	122.27
1	A	530	PRO	N-CD-CG	-6.43	93.55	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	GLN	CG-CD-NE2	6.42	126.04	116.40
1	A	158	GLN	CG-CD-NE2	6.42	126.03	116.40
1	A	225	LEU	CA-C-O	6.42	127.35	120.10
1	A	298	GLN	OE1-CD-NE2	6.41	129.01	122.60
1	A	567	PRO	CA-C-O	-6.41	109.92	119.34
1	A	377	TRP	CA-C-O	-6.40	112.66	120.54
1	A	611	ARG	NH1-CZ-NH2	6.40	127.62	119.30
1	A	419	GLN	N-CA-CB	6.39	120.30	110.46
1	A	610	MET	CA-CB-CG	-6.39	101.32	114.10
1	A	271	ASP	N-CA-C	6.39	118.24	111.28
1	A	550	SER	N-CA-C	-6.38	99.02	108.79
1	A	579	GLU	CA-C-O	6.38	126.71	119.18
1	A	431	LEU	CA-C-O	6.38	127.31	120.55
1	A	420	LYS	CG-CD-CE	6.37	125.95	111.30
1	A	226	ARG	CG-CD-NE	-6.37	97.99	112.00
1	A	474	GLN	N-CA-C	-6.36	104.78	112.54
1	A	607	LEU	N-CA-C	6.36	118.22	111.28
1	A	348	HIS	N-CA-C	-6.36	104.43	111.36
1	A	173	ARG	CA-C-O	6.35	127.70	120.84
1	A	172	TYR	CD1-CG-CD2	-6.35	108.57	118.10
1	A	374	ARG	NE-CZ-NH2	-6.35	113.48	119.20
1	A	426	PHE	CA-CB-CG	6.35	120.15	113.80
1	A	570	TYR	CD1-CG-CD2	6.35	127.62	118.10
1	A	158	GLN	CA-C-O	6.34	127.91	120.87
1	A	580	ALA	CA-C-O	6.34	128.01	121.23
1	A	341	VAL	O-C-N	-6.33	115.31	121.83
1	A	149	ASP	CA-C-O	6.33	127.85	120.96
1	A	475	ALA	O-C-N	-6.32	113.73	122.46
1	A	266	ASN	CA-CB-CG	6.32	118.92	112.60
1	A	372	PRO	CA-N-CD	-6.32	103.16	112.00
1	A	522	LEU	O-C-N	-6.31	114.03	122.23
1	A	576	PRO	N-CA-CB	6.31	109.87	103.25
1	A	123	GLN	CG-CD-NE2	6.30	125.86	116.40
1	A	444	PRO	CA-C-O	6.30	128.19	121.32
1	A	216	LEU	CB-CG-CD2	6.29	129.57	110.70
1	A	376	ARG	NH1-CZ-NH2	-6.29	111.13	119.30
1	A	576	PRO	O-C-N	6.28	131.12	122.64
1	A	50	GLN	CG-CD-NE2	6.27	125.81	116.40
1	A	538	THR	CA-C-O	-6.27	113.77	120.42
1	A	413	LYS	N-CA-C	6.27	118.91	111.33
1	A	228	ILE	CB-CA-C	6.26	119.98	111.97
1	A	227	LYS	CA-C-O	6.25	127.17	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ARG	CD-NE-CZ	6.25	133.15	124.40
1	A	149	ASP	CB-CA-C	6.24	119.20	109.84
1	A	228	ILE	CA-CB-CG1	6.23	120.99	110.40
1	A	32	GLN	CG-CD-NE2	6.22	125.74	116.40
1	A	613	LEU	CB-CG-CD2	6.22	129.37	110.70
1	A	454	PHE	CG-CD2-CE2	6.21	131.26	120.70
1	A	222	PHE	O-C-N	-6.21	115.63	122.09
1	A	33	GLN	CG-CD-NE2	6.21	125.71	116.40
1	A	43	GLN	CG-CD-NE2	6.21	125.71	116.40
1	A	412	GLY	CA-C-N	6.19	128.87	120.38
1	A	412	GLY	C-N-CA	6.19	128.87	120.38
1	A	452	ARG	CA-C-O	-6.19	111.30	119.10
1	A	220	ASP	CB-CG-OD1	-6.19	104.17	118.40
1	A	297	LEU	CA-C-N	6.17	128.47	120.44
1	A	297	LEU	C-N-CA	6.17	128.47	120.44
1	A	433	LEU	CA-C-N	6.17	128.54	120.28
1	A	433	LEU	C-N-CA	6.17	128.54	120.28
1	A	223	THR	OG1-CB-CG2	-6.17	96.97	109.30
1	A	369	LEU	N-CA-CB	-6.17	99.40	110.37
1	A	167	ARG	O-C-N	-6.16	114.78	122.24
1	A	473	VAL	CA-C-O	-6.16	113.82	120.47
1	A	612	ASP	CB-CG-OD2	6.16	132.56	118.40
1	A	613	LEU	O-C-N	-6.16	115.02	122.22
1	A	248	ASP	CA-C-N	-6.15	114.25	120.10
1	A	248	ASP	C-N-CA	-6.15	114.25	120.10
1	A	254	ALA	N-CA-C	-6.15	104.49	111.07
1	A	404	ILE	O-C-N	-6.15	116.23	123.05
1	A	370	PRO	N-CA-C	6.15	121.94	111.68
1	A	253	TRP	CB-CA-C	6.14	121.28	110.85
1	A	432	GLN	N-CA-C	-6.13	104.51	111.07
1	A	298	GLN	CA-C-O	-6.13	114.38	120.82
1	A	169	PHE	N-CA-CB	-6.12	101.65	110.65
1	A	566	VAL	CB-CA-C	6.10	116.48	109.89
1	A	458	ARG	NH1-CZ-NH2	6.10	127.23	119.30
1	A	223	THR	CA-CB-OG1	-6.09	100.46	109.60
1	A	419	GLN	CG-CD-OE1	-6.09	108.61	120.80
1	A	478	ASP	CA-C-O	6.09	129.21	120.51
1	A	389	SER	CB-CA-C	6.08	121.18	110.85
1	A	456	GLU	N-CA-CB	6.08	123.06	113.15
1	A	331	VAL	O-C-N	-6.07	116.29	123.03
1	A	471	ALA	CA-C-N	-6.06	112.19	120.44
1	A	471	ALA	C-N-CA	-6.06	112.19	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	GLN	OE1-CD-NE2	-6.06	116.54	122.60
1	A	505	MET	CA-C-N	-6.06	112.20	120.44
1	A	505	MET	C-N-CA	-6.06	112.20	120.44
1	A	226	ARG	CD-NE-CZ	-6.05	115.92	124.40
1	A	384	GLN	CB-CG-CD	-6.05	102.31	112.60
1	A	265	THR	OG1-CB-CG2	-6.05	97.19	109.30
1	A	564	PRO	N-CD-CG	-6.04	94.14	103.20
1	A	425	GLY	O-C-N	-6.04	116.39	122.19
1	A	421	TYR	CG-CD2-CE2	-6.03	112.16	121.20
1	A	466	THR	CA-CB-CG2	-6.03	100.26	110.50
1	A	170	SER	N-CA-C	6.01	120.19	112.26
1	A	599	PHE	CA-CB-CG	-6.01	107.79	113.80
1	A	275	ARG	CA-C-O	-6.00	112.30	119.15
1	A	435	TYR	N-CA-CB	6.00	119.05	110.16
1	A	538	THR	O-C-N	5.99	128.97	122.15
1	A	495	ALA	N-CA-C	-5.99	104.84	111.36
1	A	152	LYS	N-CA-C	-5.98	100.05	108.96
1	A	374	ARG	N-CA-C	-5.98	99.54	109.46
1	A	96	LEU	N-CA-C	5.97	118.58	111.71
1	A	236	ASP	N-CA-C	5.97	118.58	109.62
1	A	418	LYS	CB-CA-C	-5.97	98.07	109.95
1	A	474	GLN	OE1-CD-NE2	5.97	128.57	122.60
1	A	350	LEU	CB-CA-C	5.96	120.24	110.88
1	A	416	ILE	N-CA-C	5.96	116.70	110.62
1	A	404	ILE	CA-C-N	5.95	129.93	122.43
1	A	404	ILE	C-N-CA	5.95	129.93	122.43
1	A	604	GLY	CA-C-O	-5.95	114.62	120.75
1	A	186	LYS	O-C-N	-5.95	115.18	122.20
1	A	469	ALA	CA-C-O	-5.95	114.24	120.55
1	A	172	TYR	CG-CD1-CE1	5.95	130.12	121.20
1	A	325	ASP	CA-C-N	-5.94	113.25	122.69
1	A	325	ASP	C-N-CA	-5.94	113.25	122.69
1	A	310	ALA	N-CA-C	-5.93	105.69	113.17
1	A	606	SER	N-CA-CB	5.93	118.93	110.16
1	A	414	THR	OG1-CB-CG2	-5.92	97.46	109.30
1	A	409	ASP	CB-CG-OD1	5.92	132.01	118.40
1	A	615	SER	N-CA-CB	-5.92	102.18	111.23
1	A	336	PRO	CB-CA-C	-5.91	101.79	111.31
1	A	426	PHE	N-CA-C	5.90	117.72	111.28
1	A	292	ASP	N-CA-CB	5.90	118.80	110.12
1	A	616	SER	N-CA-C	-5.90	94.48	111.00
1	A	291	SER	CA-C-N	5.88	128.16	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	SER	C-N-CA	5.88	128.16	120.28
1	A	353	MET	CA-C-O	-5.87	112.16	119.38
1	A	236	ASP	CA-C-O	-5.87	115.06	122.63
1	A	327	THR	N-CA-CB	-5.86	100.86	109.95
1	A	257	ARG	N-CA-C	5.86	117.67	111.28
1	A	209	VAL	N-CA-C	-5.86	106.02	113.22
1	A	616	SER	N-CA-CB	5.85	120.45	110.50
1	A	250	ARG	CB-CA-C	5.85	120.17	110.81
1	A	521	GLU	CA-C-O	-5.84	113.25	119.97
1	A	155	LEU	CB-CA-C	5.82	123.55	112.43
1	A	188	SER	O-C-N	-5.82	114.85	122.59
1	A	350	LEU	N-CA-C	-5.82	104.84	111.07
1	A	383	THR	CA-C-O	5.82	126.66	119.97
1	A	575	ASN	CA-C-O	-5.81	114.39	120.09
1	A	24	PRO	CA-C-N	-5.81	112.13	122.07
1	A	24	PRO	C-N-CA	-5.81	112.13	122.07
1	A	312	ARG	NE-CZ-NH2	-5.81	113.97	119.20
1	A	344	GLN	CA-CB-CG	-5.80	102.50	114.10
1	A	503	THR	CA-C-N	-5.80	111.31	120.47
1	A	503	THR	C-N-CA	-5.80	111.31	120.47
1	A	339	GLY	O-C-N	5.79	128.59	122.28
1	A	418	LYS	O-C-N	-5.78	113.99	122.43
1	A	42	MET	N-CA-C	5.78	120.05	112.89
1	A	370	PRO	CB-CA-C	-5.78	102.37	110.63
1	A	452	ARG	NH1-CZ-NH2	-5.78	111.79	119.30
1	A	418	LYS	CD-CE-NZ	5.77	130.35	111.90
1	A	351	LYS	CA-C-N	5.76	127.93	120.44
1	A	351	LYS	C-N-CA	5.76	127.93	120.44
1	A	388	ALA	CA-C-O	-5.76	114.44	120.55
1	A	437	ARG	CA-C-N	5.76	133.91	121.64
1	A	437	ARG	C-N-CA	5.76	133.91	121.64
1	A	223	THR	CA-CB-CG2	-5.76	100.71	110.50
1	A	532	GLU	N-CA-CB	5.75	118.69	110.06
1	A	320	PHE	CA-C-N	5.75	129.56	122.37
1	A	320	PHE	C-N-CA	5.75	129.56	122.37
1	A	331	VAL	CA-C-N	5.75	130.93	123.00
1	A	331	VAL	C-N-CA	5.75	130.93	123.00
1	A	411	TYR	CZ-CE2-CD2	-5.75	109.26	119.60
1	A	277	ILE	CA-CB-CG1	-5.74	100.64	110.40
1	A	378	LYS	CA-C-O	-5.74	111.27	120.85
1	A	210	VAL	O-C-N	-5.73	117.22	123.18
1	A	214	ARG	CG-CD-NE	-5.72	99.41	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	ASN	N-CA-C	5.72	119.98	112.89
1	A	437	ARG	NE-CZ-NH2	-5.71	114.06	119.20
1	A	553	PRO	O-C-N	5.71	130.33	123.13
1	A	334	HIS	CG-CD2-NE2	5.71	112.91	107.20
1	A	384	GLN	O-C-N	-5.71	116.16	122.09
1	A	280	VAL	N-CA-C	5.70	115.81	107.37
1	A	225	LEU	N-CA-C	5.69	118.25	111.71
1	A	76	LEU	CB-CA-C	5.69	121.59	110.67
1	A	570	TYR	CZ-CE2-CD2	-5.68	109.38	119.60
1	A	152	LYS	CA-C-O	-5.67	115.38	121.45
1	A	293	THR	O-C-N	-5.67	116.23	122.07
1	A	380	SER	CA-C-N	5.67	125.79	119.32
1	A	380	SER	C-N-CA	5.67	125.79	119.32
1	A	396	ARG	CB-CG-CD	-5.67	98.25	111.30
1	A	400	ASN	OD1-CG-ND2	5.67	128.27	122.60
1	A	399	LYS	CD-CE-NZ	-5.67	93.75	111.90
1	A	213	PHE	CG-CD1-CE1	5.67	130.33	120.70
1	A	252	GLU	N-CA-CB	5.67	118.23	110.01
1	A	439	TYR	CA-CB-CG	-5.66	103.72	113.90
1	A	210	VAL	N-CA-C	-5.65	99.41	107.77
1	A	539	TYR	CZ-CE2-CD2	5.65	129.77	119.60
1	A	304	GLY	CA-C-N	5.64	132.31	121.54
1	A	304	GLY	C-N-CA	5.64	132.31	121.54
1	A	268	ASP	N-CA-C	5.64	117.88	111.11
1	A	422	SER	N-CA-C	5.64	117.78	109.50
1	A	386	HIS	CA-CB-CG	-5.63	108.17	113.80
1	A	304	GLY	O-C-N	5.63	129.22	122.98
1	A	192	GLU	O-C-N	-5.62	114.85	121.32
1	A	408	PHE	N-CA-CB	5.62	118.94	109.94
1	A	231	MET	CA-CB-CG	5.62	125.34	114.10
1	A	356	SER	O-C-N	5.62	130.06	122.59
1	A	517	LEU	CA-C-N	-5.62	111.77	120.31
1	A	517	LEU	C-N-CA	-5.62	111.77	120.31
1	A	212	ASN	CA-C-N	5.61	130.33	122.36
1	A	212	ASN	C-N-CA	5.61	130.33	122.36
1	A	460	ASP	O-C-N	5.61	130.78	122.81
1	A	612	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	422	SER	CA-C-N	5.61	124.81	118.97
1	A	422	SER	C-N-CA	5.61	124.81	118.97
1	A	478	ASP	O-C-N	5.61	130.05	122.59
1	A	333	GLU	O-C-N	-5.60	116.69	123.13
1	A	213	PHE	CA-C-O	5.59	128.33	121.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	GLU	CB-CG-CD	5.59	122.11	112.60
1	A	228	ILE	O-C-N	-5.59	116.43	121.91
1	A	490	GLN	O-C-N	5.59	128.04	122.12
1	A	166	TYR	CG-CD2-CE2	-5.58	112.83	121.20
1	A	224	GLN	CB-CA-C	5.58	119.63	110.88
1	A	134	VAL	CA-C-N	5.57	128.77	120.31
1	A	134	VAL	C-N-CA	5.57	128.77	120.31
1	A	77	GLU	CA-C-N	5.56	127.73	120.28
1	A	77	GLU	C-N-CA	5.56	127.73	120.28
1	A	221	LEU	N-CA-C	-5.56	105.22	112.23
1	A	497	GLN	CA-C-O	-5.56	114.65	120.55
1	A	479	HIS	CB-CA-C	5.55	121.47	110.42
1	A	321	VAL	CB-CA-C	5.54	117.67	110.96
1	A	81	LYS	N-CA-C	5.54	120.10	113.23
1	A	356	SER	CA-C-O	5.54	128.43	120.51
1	A	164	GLN	O-C-N	-5.53	115.47	122.27
1	A	410	ASN	CA-C-N	5.53	133.96	122.41
1	A	410	ASN	C-N-CA	5.53	133.96	122.41
1	A	265	THR	CA-C-O	-5.52	112.61	120.51
1	A	389	SER	O-C-N	5.52	128.44	122.15
1	A	609	ASP	CA-C-N	5.52	128.12	120.29
1	A	609	ASP	C-N-CA	5.52	128.12	120.29
1	A	271	ASP	CB-CG-OD1	5.51	131.08	118.40
1	A	430	ALA	CA-C-O	-5.51	114.71	120.55
1	A	479	HIS	CA-C-O	5.51	128.39	120.51
1	A	585	ILE	CA-C-N	5.51	131.46	122.81
1	A	585	ILE	C-N-CA	5.51	131.46	122.81
1	A	251	SER	CA-C-O	-5.51	113.29	119.79
1	A	368	GLU	N-CA-C	-5.50	99.09	110.80
1	A	440	GLN	CB-CG-CD	5.49	121.92	112.60
1	A	550	SER	O-C-N	-5.48	117.56	123.42
1	A	600	ALA	CA-C-N	-5.48	112.94	120.28
1	A	600	ALA	C-N-CA	-5.48	112.94	120.28
1	A	242	ILE	O-C-N	5.47	127.40	121.87
1	A	587	SER	N-CA-CB	5.47	119.89	111.46
1	A	388	ALA	O-C-N	5.47	127.92	122.12
1	A	152	LYS	CB-CA-C	5.46	123.49	111.09
1	A	213	PHE	CD1-CE1-CZ	-5.46	110.17	120.00
1	A	167	ARG	CB-CA-C	-5.46	100.94	110.17
1	A	491	LEU	N-CA-CB	5.46	118.14	110.12
1	A	404	ILE	CA-C-O	5.45	126.76	120.76
1	A	196	VAL	CA-C-O	5.45	129.09	121.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	GLN	CA-CB-CG	5.44	124.98	114.10
1	A	460	ASP	OD1-CG-OD2	-5.44	109.84	122.90
1	A	615	SER	CA-C-N	5.44	131.49	121.70
1	A	615	SER	C-N-CA	5.44	131.49	121.70
1	A	203	GLN	CG-CD-OE1	-5.43	109.93	120.80
1	A	466	THR	CB-CA-C	-5.43	100.96	109.11
1	A	453	ARG	CB-CA-C	5.43	121.78	110.32
1	A	301	HIS	ND1-CE1-NE2	5.42	113.83	108.40
1	A	468	GLU	O-C-N	-5.42	115.60	122.27
1	A	580	ALA	CB-CA-C	-5.42	100.54	110.62
1	A	160	LEU	CA-C-O	5.42	127.80	121.46
1	A	166	TYR	CA-C-O	5.41	126.21	119.12
1	A	242	ILE	CA-CB-CG2	5.41	119.70	110.50
1	A	324	ARG	CA-C-N	5.41	132.12	121.58
1	A	324	ARG	C-N-CA	5.41	132.12	121.58
1	A	149	ASP	CA-C-N	5.41	131.87	121.54
1	A	149	ASP	C-N-CA	5.41	131.87	121.54
1	A	218	GLU	N-CA-CB	5.41	118.59	109.78
1	A	220	ASP	CB-CA-C	-5.40	100.30	110.67
1	A	238	ARG	N-CA-C	-5.40	102.05	110.10
1	A	211	ILE	CA-C-N	-5.39	114.97	122.74
1	A	211	ILE	C-N-CA	-5.39	114.97	122.74
1	A	180	ASP	O-C-N	-5.39	116.02	122.65
1	A	378	LYS	N-CA-CB	-5.39	99.76	110.64
1	A	263	ASP	CB-CA-C	5.38	118.52	109.48
1	A	186	LYS	N-CA-CB	5.38	118.81	110.80
1	A	400	ASN	CB-CG-ND2	-5.37	108.34	116.40
1	A	400	ASN	CA-C-N	-5.37	114.62	122.19
1	A	400	ASN	C-N-CA	-5.37	114.62	122.19
1	A	222	PHE	CB-CG-CD2	5.37	129.83	120.70
1	A	208	ASP	O-C-N	5.37	129.53	122.93
1	A	337	PHE	CZ-CE2-CD2	-5.36	110.35	120.00
1	A	95	TYR	CA-C-N	-5.36	112.56	120.28
1	A	95	TYR	C-N-CA	-5.36	112.56	120.28
1	A	601	GLU	CA-CB-CG	-5.34	103.41	114.10
1	A	185	GLN	CB-CG-CD	5.34	121.68	112.60
1	A	530	PRO	N-CA-CB	5.34	108.26	103.08
1	A	107	SER	N-CA-C	5.33	117.31	109.42
1	A	441	ARG	N-CA-C	-5.33	100.82	108.60
1	A	366	VAL	CA-C-O	5.33	127.44	120.78
1	A	259	VAL	CA-C-O	5.33	126.49	120.95
1	A	471	ALA	O-C-N	5.33	127.63	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	PRO	CB-CA-C	-5.32	104.14	111.21
1	A	209	VAL	CA-C-N	-5.32	115.43	122.98
1	A	209	VAL	C-N-CA	-5.32	115.43	122.98
1	A	502	TYR	OH-CZ-CE2	-5.31	103.96	119.90
1	A	342	LEU	CA-C-O	-5.31	114.79	120.42
1	A	322	VAL	N-CA-CB	-5.31	107.34	112.65
1	A	216	LEU	O-C-N	5.31	129.00	123.06
1	A	521	GLU	O-C-N	5.30	128.79	122.27
1	A	294	HIS	CB-CA-C	5.29	119.58	110.79
1	A	488	LYS	CB-CA-C	5.29	119.67	110.68
1	A	194	GLU	CB-CG-CD	-5.27	103.64	112.60
1	A	570	TYR	CE1-CZ-CE2	5.27	130.83	120.30
1	A	483	MET	CG-SD-CE	-5.26	89.33	100.90
1	A	249	GLY	N-CA-C	5.26	117.98	111.93
1	A	284	GLY	O-C-N	-5.26	116.51	121.77
1	A	453	ARG	O-C-N	-5.26	115.56	122.39
1	A	357	ASN	CA-C-N	-5.25	113.51	122.11
1	A	357	ASN	C-N-CA	-5.25	113.51	122.11
1	A	279	LEU	CA-C-N	5.24	130.23	123.11
1	A	279	LEU	C-N-CA	5.24	130.23	123.11
1	A	580	ALA	O-C-N	-5.24	117.81	123.42
1	A	334	HIS	CA-CB-CG	-5.23	108.57	113.80
1	A	206	VAL	CB-CA-C	5.23	117.20	111.08
1	A	425	GLY	CA-C-O	5.22	126.13	120.75
1	A	202	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	A	315	ASP	CB-CG-OD1	5.22	130.41	118.40
1	A	587	SER	O-C-N	5.22	128.74	123.26
1	A	456	GLU	O-C-N	5.22	128.52	122.00
1	A	439	TYR	N-CA-CB	5.21	117.83	110.90
1	A	301	HIS	CE1-NE2-CD2	-5.21	103.79	109.00
1	A	265	THR	CA-C-N	-5.20	112.92	121.19
1	A	265	THR	C-N-CA	-5.20	112.92	121.19
1	A	151	ALA	CA-C-O	5.20	125.36	119.27
1	A	484	PRO	N-CA-C	5.20	119.74	111.26
1	A	466	THR	CA-C-O	5.20	125.99	120.64
1	A	523	ALA	CA-C-N	5.20	127.25	120.28
1	A	523	ALA	C-N-CA	5.20	127.25	120.28
1	A	212	ASN	O-C-N	-5.20	113.52	122.20
1	A	263	ASP	N-CA-CB	-5.19	101.95	110.52
1	A	382	GLU	CA-CB-CG	5.19	124.48	114.10
1	A	577	GLN	CB-CA-C	5.19	117.06	109.48
1	A	514	ASN	N-CA-CB	5.19	117.75	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	LEU	O-C-N	5.18	126.91	121.42
1	A	429	VAL	CA-C-N	5.18	127.22	120.28
1	A	429	VAL	C-N-CA	5.18	127.22	120.28
1	A	247	SER	O-C-N	5.18	129.37	122.43
1	A	49	GLU	CB-CG-CD	5.17	121.40	112.60
1	A	218	GLU	N-CA-C	5.17	119.90	111.37
1	A	555	THR	CB-CA-C	5.17	118.09	109.56
1	A	367	SER	O-C-N	5.15	128.10	123.26
1	A	504	VAL	N-CA-C	5.15	117.49	111.05
1	A	324	ARG	CA-C-O	-5.15	115.09	120.55
1	A	405	VAL	O-C-N	5.15	129.15	122.77
1	A	413	LYS	N-CA-CB	5.13	117.76	110.06
1	A	224	GLN	CG-CD-OE1	-5.13	110.54	120.80
1	A	280	VAL	CA-C-O	-5.13	114.66	120.66
1	A	346	THR	CA-C-N	-5.13	112.51	120.31
1	A	346	THR	C-N-CA	-5.13	112.51	120.31
1	A	485	ALA	O-C-N	-5.13	116.22	122.22
1	A	142	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	194	GLU	OE1-CD-OE2	5.11	135.17	122.90
1	A	229	VAL	CA-C-N	-5.11	113.79	120.44
1	A	229	VAL	C-N-CA	-5.11	113.79	120.44
1	A	403	PHE	N-CA-CB	-5.11	101.94	110.83
1	A	421	TYR	OH-CZ-CE2	5.11	135.22	119.90
1	A	374	ARG	N-CA-CB	5.10	118.58	110.16
1	A	226	ARG	CA-CB-CG	5.10	124.30	114.10
1	A	253	TRP	CD2-CE2-CZ2	-5.10	117.30	122.40
1	A	351	LYS	O-C-N	5.10	127.53	122.12
1	A	378	LYS	CA-CB-CG	5.10	124.30	114.10
1	A	474	GLN	CB-CG-CD	5.10	121.27	112.60
1	A	615	SER	CA-C-O	-5.10	111.36	121.35
1	A	257	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	A	396	ARG	CA-CB-CG	-5.10	103.91	114.10
1	A	410	ASN	CB-CA-C	-5.10	99.34	109.99
1	A	203	GLN	CB-CG-CD	5.09	121.25	112.60
1	A	184	ALA	O-C-N	5.09	129.29	123.29
1	A	250	ARG	CA-C-N	-5.09	112.03	120.68
1	A	250	ARG	C-N-CA	-5.09	112.03	120.68
1	A	411	TYR	CG-CD2-CE2	5.08	128.81	121.20
1	A	547	LEU	CA-C-N	-5.07	115.85	123.00
1	A	547	LEU	C-N-CA	-5.07	115.85	123.00
1	A	269	SER	N-CA-CB	5.07	117.42	110.07
1	A	274	GLU	CB-CG-CD	5.07	121.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	VAL	CG1-CB-CG2	-5.05	99.68	110.80
1	A	294	HIS	CB-CG-ND1	5.05	130.28	122.70
1	A	301	HIS	CG-ND1-CE1	-5.05	100.71	109.30
1	A	223	THR	N-CA-CB	5.05	117.47	109.94
1	A	239	LEU	N-CA-CB	5.05	118.48	110.10
1	A	436	TYR	CG-CD1-CE1	-5.05	113.63	121.20
1	A	333	GLU	N-CA-C	-5.05	100.93	108.96
1	A	521	GLU	CG-CD-OE2	-5.04	106.81	118.40
1	A	615	SER	CB-CA-C	5.04	119.25	111.85
1	A	533	MET	O-C-N	-5.04	116.78	122.12
1	A	221	LEU	CA-C-O	-5.02	113.86	119.79
1	A	545	PHE	CA-CB-CG	-5.02	108.78	113.80
1	A	240	PRO	N-CA-CB	5.02	107.95	103.08
1	A	454	PHE	N-CA-C	5.01	117.93	110.52
1	A	588	PHE	CD1-CE1-CZ	5.00	129.01	120.00
1	A	191	PRO	O-C-N	5.00	130.60	121.10
1	A	222	PHE	CA-C-N	5.00	127.29	120.54
1	A	222	PHE	C-N-CA	5.00	127.29	120.54

There are no chirality outliers.

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	TYR	Sidechain
1	A	167	ARG	Sidechain
1	A	185	GLN	Peptide
1	A	189	ILE	Mainchain
1	A	190	MET	Mainchain
1	A	196	VAL	Mainchain
1	A	205	PHE	Sidechain
1	A	208	ASP	Sidechain
1	A	213	PHE	Sidechain
1	A	220	ASP	Sidechain
1	A	224	GLN	Mainchain
1	A	239	LEU	Mainchain
1	A	249	GLY	Mainchain
1	A	257	ARG	Sidechain
1	A	265	THR	Mainchain
1	A	275	ARG	Mainchain
1	A	286	GLY	Mainchain
1	A	288	GLY	Peptide
1	A	289	GLU	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	A	290	LEU	Mainchain
1	A	294	HIS	Sidechain
1	A	341	VAL	Mainchain
1	A	344	GLN	Sidechain
1	A	348	HIS	Sidechain
1	A	352	HIS	Sidechain
1	A	368	GLU	Peptide
1	A	373	ARG	Mainchain
1	A	376	ARG	Sidechain
1	A	378	LYS	Mainchain
1	A	391	ALA	Mainchain
1	A	402	ASP	Mainchain
1	A	410	ASN	Mainchain
1	A	418	LYS	Mainchain
1	A	420	LYS	Mainchain
1	A	421	TYR	Sidechain
1	A	435	TYR	Sidechain
1	A	437	ARG	Mainchain
1	A	441	ARG	Sidechain
1	A	452	ARG	Sidechain
1	A	453	ARG	Sidechain
1	A	475	ALA	Mainchain
1	A	477	THR	Mainchain
1	A	482	ALA	Mainchain
1	A	487	GLU	Mainchain,Sidechain
1	A	555	THR	Mainchain
1	A	560	CYS	Mainchain
1	A	561	CYS	Mainchain
1	A	579	GLU	Sidechain
1	A	602	ALA	Mainchain
1	A	611	ARG	Sidechain
1	A	615	SER	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4711	0	4686	271	25

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	408	0	0	17	9
All	All	5119	0	4686	271	26

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 29.

All (271) 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:178:THR:CB	1:A:178:THR:CA	1.76	1.61
1:A:351:LYS:CE	1:A:351:LYS:CD	1.75	1.59
1:A:230:LYS:CE	1:A:230:LYS:CD	1.79	1.59
1:A:407:LYS:CD	1:A:407:LYS:CG	1.74	1.59
1:A:220:ASP:CG	1:A:220:ASP:CB	1.75	1.58
1:A:214:ARG:CZ	1:A:365:SER:HB3	1.10	1.56
1:A:350:LEU:CG	1:A:350:LEU:CD1	1.74	1.55
1:A:351:LYS:CD	1:A:351:LYS:CG	1.85	1.55
1:A:179:GLN:CD	1:A:179:GLN:CG	1.75	1.54
1:A:237:GLU:N	1:A:237:GLU:CA	1.67	1.54
1:A:453:ARG:NE	1:A:453:ARG:CD	1.70	1.53
1:A:418:LYS:CE	1:A:418:LYS:CD	1.85	1.53
1:A:396:ARG:CD	1:A:396:ARG:CG	1.80	1.52
1:A:418:LYS:CE	1:A:418:LYS:NZ	1.72	1.51
1:A:453:ARG:CB	1:A:453:ARG:CA	1.84	1.51
1:A:255:LYS:CE	1:A:255:LYS:NZ	1.75	1.50
1:A:373:ARG:CD	1:A:373:ARG:CG	1.89	1.50
1:A:475:ALA:N	1:A:475:ALA:CA	1.68	1.49
1:A:613:LEU:CD1	1:A:613:LEU:CG	1.91	1.49
1:A:530:PRO:CG	1:A:530:PRO:CB	1.74	1.48
1:A:255:LYS:CE	1:A:255:LYS:CD	1.87	1.47
1:A:262:LYS:CE	1:A:262:LYS:NZ	1.77	1.47
1:A:378:LYS:NZ	1:A:378:LYS:CE	1.81	1.43
1:A:365:SER:O	1:A:366:VAL:CG2	1.87	1.22
1:A:366:VAL:HG12	1:A:367:SER:N	1.52	1.17
1:A:154:GLN:O	1:A:155:LEU:CD1	1.91	1.17
1:A:214:ARG:NH2	1:A:365:SER:OG	1.75	1.15
1:A:362:ARG:O	1:A:364:ASP:N	1.78	1.15
1:A:361:VAL:HG12	1:A:362:ARG:H	1.09	1.14
1:A:111:ILE:HG13	1:A:299:LEU:HD12	1.31	1.12
1:A:154:GLN:O	1:A:155:LEU:HD12	1.42	1.11
1:A:391:ALA:O	1:A:395:GLN:HG3	1.47	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:THR:HG21	2:A:993:HOH:O	1.50	1.11
1:A:362:ARG:C	1:A:364:ASP:H	1.57	1.08
1:A:237:GLU:N	1:A:237:GLU:C	2.11	1.07
1:A:366:VAL:CG1	1:A:367:SER:H	1.65	1.07
1:A:365:SER:O	1:A:366:VAL:HG23	1.54	1.06
1:A:359:LYS:O	1:A:359:LYS:HG2	1.54	1.06
1:A:477:THR:O	1:A:477:THR:HG22	1.52	1.04
1:A:480:LYS:H	1:A:480:LYS:HD3	0.89	1.03
1:A:237:GLU:H	1:A:238:ARG:N	1.57	1.00
1:A:150:TRP:HA	1:A:154:GLN:HA	1.40	1.00
1:A:480:LYS:HD3	1:A:480:LYS:N	1.74	1.00
1:A:230:LYS:CE	1:A:230:LYS:CG	2.40	0.99
1:A:214:ARG:NH2	1:A:365:SER:CB	0.84	0.99
1:A:178:THR:CA	1:A:178:THR:CG2	2.40	0.98
1:A:237:GLU:N	1:A:238:ARG:N	2.09	0.98
1:A:153:GLY:O	1:A:154:GLN:HB3	1.63	0.96
1:A:342:LEU:C	1:A:342:LEU:HD23	1.91	0.96
1:A:97:ASN:O	1:A:99:ARG:HD3	1.65	0.95
1:A:480:LYS:H	1:A:480:LYS:CD	1.79	0.95
1:A:56:ALA:HB1	1:A:60:ARG:HH12	1.30	0.95
1:A:214:ARG:NH2	1:A:365:SER:CA	2.29	0.95
1:A:214:ARG:NE	1:A:365:SER:OG	2.01	0.93
1:A:365:SER:O	1:A:366:VAL:HG22	1.67	0.93
1:A:237:GLU:H	1:A:238:ARG:H	1.13	0.93
1:A:214:ARG:CZ	1:A:365:SER:CB	1.90	0.92
1:A:150:TRP:CA	1:A:154:GLN:HA	1.99	0.92
1:A:366:VAL:HG12	1:A:367:SER:H	1.07	0.91
1:A:361:VAL:HG12	1:A:362:ARG:N	1.83	0.90
1:A:97:ASN:O	1:A:99:ARG:CD	2.20	0.90
1:A:150:TRP:CB	1:A:154:GLN:HA	2.02	0.90
1:A:480:LYS:O	1:A:481:ALA:C	2.11	0.88
1:A:365:SER:C	1:A:366:VAL:HG23	1.98	0.87
1:A:396:ARG:CD	1:A:396:ARG:CB	2.53	0.86
1:A:453:ARG:CD	1:A:453:ARG:CZ	2.53	0.86
1:A:237:GLU:N	1:A:238:ARG:H	1.73	0.85
1:A:350:LEU:CD1	1:A:350:LEU:CB	2.55	0.85
1:A:98:ASN:C	1:A:99:ARG:HD2	2.02	0.84
1:A:361:VAL:CG1	1:A:362:ARG:H	1.89	0.84
1:A:56:ALA:HB1	1:A:60:ARG:NH1	1.93	0.83
1:A:214:ARG:NE	1:A:365:SER:CB	2.41	0.83
1:A:236:ASP:C	1:A:237:GLU:CA	2.51	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:SER:O	1:A:358:LYS:N	2.12	0.83
1:A:154:GLN:O	1:A:155:LEU:HD13	1.76	0.82
1:A:359:LYS:O	1:A:359:LYS:CG	2.26	0.82
1:A:150:TRP:HA	1:A:154:GLN:CA	2.08	0.82
1:A:362:ARG:O	1:A:364:ASP:HB2	1.80	0.82
1:A:407:LYS:CG	1:A:407:LYS:CE	2.55	0.81
1:A:351:LYS:HG3	1:A:556:MET:HE1	1.63	0.80
1:A:28:VAL:CG1	1:A:75:LEU:HD13	2.11	0.80
1:A:289:GLU:CD	1:A:290:LEU:HD23	2.07	0.80
1:A:351:LYS:CD	1:A:351:LYS:CB	2.59	0.80
1:A:152:LYS:O	1:A:153:GLY:O	2.00	0.79
1:A:184:ALA:O	1:A:185:GLN:HB2	1.79	0.79
1:A:356:SER:C	1:A:358:LYS:N	2.41	0.78
1:A:474:GLN:C	1:A:475:ALA:CA	2.56	0.78
1:A:350:LEU:CD1	1:A:350:LEU:CD2	2.59	0.78
1:A:366:VAL:HG12	1:A:367:SER:CA	2.14	0.78
1:A:150:TRP:N	1:A:152:LYS:O	2.17	0.77
1:A:477:THR:O	1:A:477:THR:CG2	2.27	0.77
1:A:555:THR:HG23	2:A:864:HOH:O	1.84	0.77
1:A:148:THR:O	1:A:151:ALA:HB3	1.85	0.77
1:A:52:ARG:HG2	2:A:1008:HOH:O	1.86	0.76
1:A:178:THR:CB	1:A:178:THR:C	2.58	0.76
1:A:289:GLU:O	1:A:290:LEU:HG	1.85	0.75
1:A:557:GLU:HG2	2:A:754:HOH:O	1.86	0.74
1:A:172:TYR:O	1:A:183:VAL:HG12	1.86	0.74
1:A:289:GLU:OE2	1:A:290:LEU:HD23	1.86	0.74
1:A:342:LEU:C	1:A:342:LEU:CD2	2.59	0.74
1:A:150:TRP:HA	1:A:153:GLY:O	1.88	0.74
1:A:186:LYS:HG3	1:A:193:PRO:HG3	1.69	0.74
1:A:110:VAL:C	1:A:111:ILE:HD12	2.11	0.73
1:A:179:GLN:CG	1:A:179:GLN:NE2	2.47	0.73
1:A:143:SER:OG	1:A:145:SER:HB2	1.88	0.73
1:A:111:ILE:CG1	1:A:299:LEU:HD12	2.16	0.73
1:A:148:THR:O	1:A:151:ALA:CB	2.37	0.73
1:A:214:ARG:NH2	1:A:365:SER:HB2	1.06	0.72
1:A:172:TYR:O	1:A:183:VAL:CG1	2.37	0.72
1:A:178:THR:CA	1:A:178:THR:OG1	2.38	0.72
1:A:111:ILE:HG13	1:A:299:LEU:CD1	2.16	0.72
1:A:366:VAL:CG1	1:A:367:SER:N	2.23	0.72
1:A:28:VAL:HG11	1:A:75:LEU:HD13	1.71	0.72
1:A:351:LYS:CD	1:A:351:LYS:NZ	2.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:SER:OG	1:A:357:ASN:N	2.21	0.72
1:A:351:LYS:HG3	1:A:556:MET:CE	2.20	0.71
1:A:613:LEU:CD1	1:A:613:LEU:CB	2.64	0.71
1:A:152:LYS:O	1:A:153:GLY:C	2.34	0.71
1:A:396:ARG:CG	1:A:396:ARG:NE	2.53	0.71
1:A:365:SER:C	1:A:366:VAL:CG2	2.58	0.71
1:A:111:ILE:HD12	1:A:299:LEU:HD13	1.73	0.70
1:A:490:GLN:HG3	1:A:491:LEU:N	2.07	0.70
1:A:179:GLN:CD	1:A:179:GLN:CB	2.65	0.69
1:A:230:LYS:CD	1:A:230:LYS:NZ	2.55	0.69
1:A:154:GLN:C	1:A:155:LEU:HD13	2.18	0.69
1:A:352:HIS:HD2	2:A:937:HOH:O	1.75	0.69
1:A:407:LYS:CD	1:A:407:LYS:CB	2.70	0.69
1:A:111:ILE:CD1	1:A:299:LEU:HD13	2.23	0.68
1:A:214:ARG:NH2	1:A:365:SER:HB3	0.69	0.68
1:A:214:ARG:NH2	1:A:365:SER:HG	1.88	0.67
1:A:151:ALA:O	1:A:152:LYS:HG2	1.93	0.67
1:A:294:HIS:ND1	1:A:297:LEU:HD12	2.11	0.66
1:A:362:ARG:O	1:A:364:ASP:CB	2.44	0.65
1:A:28:VAL:HG13	1:A:75:LEU:HD13	1.78	0.65
1:A:156:SER:OG	1:A:453:ARG:NH2	2.30	0.65
1:A:474:GLN:O	1:A:478:ASP:HB3	1.96	0.64
1:A:110:VAL:HG21	1:A:342:LEU:HD21	1.78	0.64
1:A:99:ARG:HD2	1:A:99:ARG:N	2.11	0.64
1:A:362:ARG:O	1:A:364:ASP:CA	2.45	0.64
1:A:342:LEU:HD23	1:A:342:LEU:O	1.99	0.63
1:A:366:VAL:O	1:A:367:SER:HB3	1.98	0.63
1:A:152:LYS:C	1:A:153:GLY:O	2.38	0.63
1:A:155:LEU:HD22	1:A:160:LEU:HD11	1.81	0.62
1:A:220:ASP:CB	1:A:220:ASP:OD1	2.46	0.62
1:A:20:GLU:N	2:A:934:HOH:O	2.33	0.62
1:A:184:ALA:O	1:A:185:GLN:CB	2.48	0.62
1:A:97:ASN:O	1:A:99:ARG:HD2	2.00	0.61
1:A:28:VAL:HG13	1:A:75:LEU:CD1	2.31	0.61
1:A:362:ARG:C	1:A:364:ASP:N	2.38	0.61
1:A:51:PHE:O	1:A:54:SER:N	2.34	0.61
1:A:103:PRO:HG3	1:A:314:TYR:CZ	2.37	0.59
1:A:289:GLU:C	1:A:290:LEU:HG	2.22	0.59
1:A:480:LYS:O	1:A:481:ALA:O	2.19	0.59
1:A:25:LYS:O	1:A:27:PRO:HD3	2.03	0.58
1:A:530:PRO:O	1:A:535:MET:HE2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:CG1	1:A:75:LEU:CD1	2.81	0.58
1:A:111:ILE:HD12	1:A:111:ILE:N	2.17	0.58
1:A:214:ARG:NH1	1:A:365:SER:HB3	1.97	0.58
1:A:153:GLY:O	1:A:154:GLN:CB	2.37	0.57
1:A:294:HIS:CG	2:A:925:HOH:O	2.58	0.57
1:A:111:ILE:CD1	1:A:299:LEU:CD1	2.83	0.57
1:A:149:ASP:O	1:A:150:TRP:CD1	2.58	0.56
1:A:158:GLN:CB	1:A:159:PRO:HD2	2.34	0.56
1:A:145:SER:O	1:A:147:PRO:HD3	2.06	0.56
1:A:56:ALA:O	1:A:60:ARG:CG	2.54	0.56
1:A:400:ASN:HD21	1:A:590:SER:H	1.54	0.56
1:A:192:GLU:O	1:A:194:GLU:N	2.39	0.55
1:A:56:ALA:O	1:A:60:ARG:HG2	2.06	0.55
1:A:361:VAL:CG1	1:A:362:ARG:N	2.55	0.55
1:A:220:ASP:CG	1:A:220:ASP:CA	2.75	0.55
1:A:111:ILE:CD1	1:A:111:ILE:N	2.70	0.54
1:A:224:GLN:HE22	1:A:227:LYS:NZ	2.04	0.54
1:A:214:ARG:CZ	1:A:365:SER:OG	2.29	0.54
1:A:56:ALA:CB	1:A:60:ARG:HH12	2.14	0.54
1:A:356:SER:O	1:A:359:LYS:N	2.40	0.54
1:A:475:ALA:N	1:A:475:ALA:CB	2.69	0.54
1:A:150:TRP:HB2	1:A:154:GLN:HA	1.90	0.54
1:A:234:ASN:ND2	2:A:909:HOH:O	2.37	0.54
1:A:418:LYS:CE	1:A:418:LYS:CG	2.83	0.53
1:A:407:LYS:CG	1:A:407:LYS:NZ	2.71	0.53
1:A:479:HIS:HA	1:A:480:LYS:HD3	1.90	0.53
1:A:108:PRO:HD2	1:A:332:CYS:O	2.09	0.52
1:A:150:TRP:CA	1:A:152:LYS:O	2.57	0.52
1:A:224:GLN:HE22	1:A:227:LYS:HZ2	1.58	0.52
1:A:84:ASN:OD1	1:A:86:VAL:HG12	2.11	0.51
1:A:356:SER:O	1:A:357:ASN:C	2.52	0.51
1:A:616:SER:C	2:A:928:HOH:O	2.54	0.51
1:A:299:LEU:HD11	1:A:329:GLY:HA3	1.93	0.51
1:A:238:ARG:NH1	2:A:1037:HOH:O	2.39	0.51
1:A:158:GLN:HB2	1:A:159:PRO:HD2	1.94	0.50
1:A:474:GLN:O	1:A:478:ASP:CB	2.59	0.50
1:A:407:LYS:NZ	1:A:407:LYS:HG2	2.27	0.49
1:A:136:SER:CB	1:A:352:HIS:HE1	2.25	0.49
1:A:172:TYR:O	1:A:183:VAL:HG13	2.11	0.49
1:A:138:LYS:HE2	1:A:142:ASP:OD2	2.11	0.49
1:A:178:THR:CB	1:A:178:THR:HA	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TRP:HA	1:A:154:GLN:CB	2.42	0.49
1:A:292:ASP:OD2	1:A:407:LYS:CE	2.61	0.48
1:A:363:ALA:C	1:A:365:SER:N	2.71	0.48
1:A:178:THR:CG2	1:A:178:THR:N	2.76	0.48
1:A:172:TYR:HB3	1:A:183:VAL:HG13	1.96	0.48
1:A:202:ASN:H	1:A:311:ASN:ND2	2.12	0.48
1:A:111:ILE:CG1	1:A:299:LEU:CD1	2.85	0.48
1:A:224:GLN:HA	1:A:224:GLN:NE2	2.28	0.48
1:A:236:ASP:O	1:A:237:GLU:CA	2.62	0.48
1:A:152:LYS:HB2	2:A:785:HOH:O	2.14	0.48
1:A:373:ARG:CG	1:A:373:ARG:NE	2.73	0.47
1:A:289:GLU:HB2	1:A:290:LEU:HA	1.95	0.47
1:A:117:PHE:O	1:A:118:GLN:C	2.57	0.47
1:A:69:GLU:O	1:A:73:GLU:OE1	2.32	0.47
1:A:151:ALA:C	1:A:152:LYS:HG2	2.39	0.47
1:A:155:LEU:HD12	1:A:155:LEU:HA	1.67	0.47
1:A:192:GLU:O	1:A:193:PRO:C	2.57	0.47
1:A:487:GLU:O	1:A:490:GLN:CG	2.64	0.46
1:A:490:GLN:HG3	1:A:491:LEU:H	1.79	0.46
1:A:479:HIS:CA	1:A:480:LYS:HD3	2.46	0.45
1:A:230:LYS:CE	1:A:230:LYS:HG2	2.42	0.45
1:A:238:ARG:NH1	2:A:1019:HOH:O	2.49	0.45
1:A:404:ILE:HD11	2:A:894:HOH:O	2.15	0.45
1:A:480:LYS:HA	1:A:488:LYS:NZ	2.31	0.45
1:A:136:SER:CB	1:A:352:HIS:CE1	2.99	0.45
1:A:158:GLN:HA	1:A:159:PRO:HD3	1.72	0.45
1:A:356:SER:C	1:A:358:LYS:H	2.23	0.45
1:A:453:ARG:CB	1:A:453:ARG:N	2.69	0.45
1:A:220:ASP:CB	1:A:220:ASP:OD2	2.46	0.45
1:A:103:PRO:O	1:A:105:ASN:N	2.45	0.45
1:A:150:TRP:HA	1:A:153:GLY:C	2.41	0.44
1:A:63:ALA:HB1	1:A:64:PRO:CD	2.47	0.44
1:A:111:ILE:HG12	1:A:296:ALA:HA	1.99	0.44
1:A:24:PRO:HB2	1:A:454:PHE:HD2	1.82	0.44
1:A:289:GLU:OE2	1:A:290:LEU:CD2	2.61	0.44
1:A:400:ASN:HD21	1:A:590:SER:HB3	1.83	0.44
1:A:449:ALA:HB2	1:A:462:ILE:HG13	1.99	0.44
1:A:482:ALA:O	1:A:483:MET:CB	2.58	0.44
1:A:229:VAL:O	1:A:233:SER:HB3	2.18	0.43
1:A:289:GLU:CG	1:A:290:LEU:HD23	2.48	0.43
1:A:525:ASP:C	1:A:525:ASP:OD1	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ASN:HD21	1:A:590:SER:CB	2.31	0.43
1:A:56:ALA:O	1:A:60:ARG:HG3	2.18	0.43
1:A:557:GLU:CD	2:A:754:HOH:O	2.59	0.43
1:A:578:PRO:HD2	2:A:1006:HOH:O	2.18	0.43
1:A:487:GLU:O	1:A:490:GLN:HG3	2.19	0.43
1:A:363:ALA:O	1:A:365:SER:N	2.52	0.43
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.84	0.43
1:A:186:LYS:HD2	1:A:186:LYS:O	2.19	0.43
1:A:86:VAL:HG22	1:A:86:VAL:O	2.18	0.42
1:A:172:TYR:HB3	1:A:183:VAL:CG1	2.49	0.42
1:A:137:TYR:HD1	1:A:348:HIS:CD2	2.38	0.42
1:A:186:LYS:NZ	1:A:190:MET:SD	2.92	0.42
1:A:368:GLU:O	1:A:369:LEU:O	2.38	0.42
1:A:405:VAL:HG12	1:A:407:LYS:HD2	2.01	0.42
1:A:453:ARG:CD	1:A:453:ARG:NH1	2.82	0.42
1:A:453:ARG:NH1	1:A:453:ARG:HD3	2.34	0.42
1:A:224:GLN:NE2	1:A:227:LYS:NZ	2.68	0.42
1:A:400:ASN:ND2	1:A:590:SER:H	2.17	0.42
1:A:476:MET:HE3	1:A:476:MET:HB3	1.90	0.42
1:A:441:ARG:NH2	2:A:890:HOH:O	2.37	0.41
1:A:20:GLU:HG3	1:A:163:LYS:NZ	2.35	0.41
1:A:478:ASP:O	1:A:479:HIS:C	2.62	0.41
1:A:79:GLN:O	1:A:79:GLN:HG2	2.13	0.41
1:A:294:HIS:CE1	1:A:297:LEU:HD12	2.56	0.41
1:A:186:LYS:HG3	1:A:193:PRO:CG	2.46	0.41
1:A:224:GLN:HA	1:A:224:GLN:HE21	1.86	0.41
1:A:521:GLU:O	1:A:524:ARG:HB2	2.21	0.41
1:A:154:GLN:O	1:A:154:GLN:HG3	2.21	0.40
1:A:574:TYR:HA	1:A:582:THR:O	2.21	0.40
1:A:186:LYS:O	1:A:193:PRO:HG2	2.22	0.40
1:A:149:ASP:O	1:A:150:TRP:HD1	2.03	0.40
1:A:613:LEU:CD1	1:A:613:LEU:CD2	2.82	0.40
1:A:247:SER:HB3	2:A:1025:HOH:O	2.20	0.40
1:A:351:LYS:CE	1:A:351:LYS:CG	2.95	0.40

All (26) 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)
2:A:773:HOH:O	2:A:898:HOH:O[2_544]	0.31	1.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLU:OE2	2:A:797:HOH:O[3_555]	0.70	1.50
1:A:192:GLU:C	2:A:687:HOH:O[2_544]	1.00	1.20
1:A:193:PRO:N	2:A:687:HOH:O[2_544]	1.33	0.87
1:A:392:GLU:CD	2:A:797:HOH:O[3_555]	1.47	0.73
1:A:192:GLU:OE2	1:A:354:MET:O[2_544]	1.49	0.71
1:A:214:ARG:CD	1:A:557:GLU:OE1[2_544]	1.55	0.65
1:A:192:GLU:CD	1:A:354:MET:O[2_544]	1.64	0.56
1:A:192:GLU:OE2	1:A:354:MET:CA[2_544]	1.66	0.54
1:A:192:GLU:OE2	1:A:354:MET:C[2_544]	1.70	0.50
1:A:192:GLU:CD	1:A:354:MET:C[2_544]	1.75	0.45
1:A:193:PRO:CD	2:A:687:HOH:O[2_544]	1.79	0.41
1:A:192:GLU:CA	2:A:687:HOH:O[2_544]	1.80	0.40
1:A:192:GLU:OE1	1:A:354:MET:C[2_544]	1.84	0.36
1:A:214:ARG:CG	1:A:557:GLU:OE1[2_544]	1.86	0.34
1:A:214:ARG:CD	1:A:557:GLU:OE2[2_544]	1.86	0.34
1:A:214:ARG:CD	1:A:557:GLU:CD[2_544]	1.87	0.33
1:A:592:LYS:NZ	1:A:615:SER:O[3_556]	1.87	0.33
1:A:214:ARG:CB	1:A:557:GLU:OE1[2_544]	1.89	0.31
1:A:192:GLU:OE2	1:A:354:MET:CB[2_544]	1.92	0.28
1:A:192:GLU:O	2:A:687:HOH:O[2_544]	1.92	0.28
1:A:275:ARG:NH2	1:A:357:ASN:ND2[2_544]	1.97	0.23
1:A:192:GLU:OE1	1:A:354:MET:CA[2_544]	1.98	0.22
1:A:192:GLU:CD	1:A:354:MET:CA[2_544]	2.05	0.15
1:A:592:LYS:NZ	1:A:615:SER:C[3_556]	2.14	0.06
1:A:392:GLU:CG	2:A:797:HOH:O[3_555]	2.15	0.05

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	595/639 (93%)	534 (90%)	35 (6%)	26 (4%)	2 0

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	GLY
1	A	156	SER
1	A	190	MET
1	A	192	GLU
1	A	237	GLU
1	A	287	THR
1	A	357	ASN
1	A	361	VAL
1	A	364	ASP
1	A	366	VAL
1	A	150	TRP
1	A	154	GLN
1	A	185	GLN
1	A	359	LYS
1	A	363	ALA
1	A	187	SER
1	A	368	GLU
1	A	157	GLY
1	A	290	LEU
1	A	525	ASP
1	A	104	VAL
1	A	193	PRO
1	A	356	SER
1	A	483	MET
1	A	191	PRO
1	A	477	THR

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	524/559 (94%)	476 (91%)	48 (9%)	80

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	PRO

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Mol	Chain	Res	Type
1	A	27	PRO
1	A	49	GLU
1	A	60	ARG
1	A	73	GLU
1	A	75	LEU
1	A	77	GLU
1	A	81	LYS
1	A	103	PRO
1	A	111	ILE
1	A	114	ARG
1	A	119	ASP
1	A	136	SER
1	A	145	SER
1	A	146	LEU
1	A	155	LEU
1	A	156	SER
1	A	158	GLN
1	A	183	VAL
1	A	185	GLN
1	A	186	LYS
1	A	191	PRO
1	A	192	GLU
1	A	193	PRO
1	A	233	SER
1	A	237	GLU
1	A	279	LEU
1	A	287	THR
1	A	289	GLU
1	A	290	LEU
1	A	294	HIS
1	A	331	VAL
1	A	342	LEU
1	A	358	LYS
1	A	359	LYS
1	A	362	ARG
1	A	365	SER
1	A	407	LYS
1	A	453	ARG
1	A	476	MET
1	A	480	LYS
1	A	490	GLN
1	A	524	ARG

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Mol	Chain	Res	Type
1	A	528	LYS
1	A	529	GLU
1	A	613	LEU
1	A	615	SER
1	A	616	SER

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	105	ASN
1	A	118	GLN
1	A	158	GLN
1	A	202	ASN
1	A	224	GLN
1	A	311	ASN
1	A	348	HIS
1	A	352	HIS
1	A	400	ASN
1	A	440	GLN
1	A	479	HIS
1	A	490	GLN
1	A	577	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	576:PRO	C	577:GLN	N	1.18
1	A	289:GLU	C	290:LEU	N	0.99
1	A	189:ILE	C	190:MET	N	0.95

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	597/639 (93%)	1.02	105 (17%) 4 5	12, 18, 54, 91	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	VAL	13.3
1	A	191	PRO	11.8
1	A	151	ALA	11.5
1	A	363	ALA	10.2
1	A	155	LEU	10.1
1	A	153	GLY	9.1
1	A	189	ILE	8.7
1	A	290	LEU	8.6
1	A	360	LEU	8.2
1	A	365	SER	7.9
1	A	367	SER	7.4
1	A	526	LEU	7.2
1	A	188	SER	7.2
1	A	150	TRP	7.0
1	A	481	ALA	7.0
1	A	361	VAL	6.9
1	A	288	GLY	6.7
1	A	156	SER	6.6
1	A	234	ASN	6.5
1	A	289	GLU	6.5
1	A	193	PRO	6.4
1	A	186	LYS	6.2
1	A	190	MET	6.1
1	A	478	ASP	6.1
1	A	477	THR	6.1
1	A	187	SER	6.0
1	A	515	HIS	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	237	GLU	5.6
1	A	154	GLN	5.4
1	A	479	HIS	5.4
1	A	287	THR	5.4
1	A	305	CYS	5.0
1	A	368	GLU	5.0
1	A	369	LEU	4.9
1	A	356	SER	4.7
1	A	357	ASN	4.5
1	A	527	CYS	4.3
1	A	157	GLY	4.3
1	A	482	ALA	4.2
1	A	236	ASP	4.2
1	A	529	GLU	4.2
1	A	364	ASP	4.0
1	A	525	ASP	4.0
1	A	177	HIS	3.9
1	A	355	THR	3.9
1	A	192	GLU	3.8
1	A	557	GLU	3.7
1	A	359	LYS	3.7
1	A	528	LYS	3.7
1	A	307	LEU	3.6
1	A	51	PHE	3.6
1	A	480	LYS	3.5
1	A	143	SER	3.5
1	A	152	LYS	3.5
1	A	395	GLN	3.4
1	A	76	LEU	3.4
1	A	354	MET	3.4
1	A	358	LYS	3.3
1	A	362	ARG	3.2
1	A	41	CYS	3.1
1	A	108	PRO	3.1
1	A	149	ASP	3.0
1	A	144	HIS	3.0
1	A	27	PRO	2.9
1	A	24	PRO	2.8
1	A	592	LYS	2.7
1	A	291	SER	2.7
1	A	616	SER	2.7
1	A	22	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	306	SER	2.7
1	A	535	MET	2.7
1	A	125	ARG	2.7
1	A	158	GLN	2.7
1	A	116	HIS	2.6
1	A	135	LEU	2.6
1	A	77	GLU	2.6
1	A	47	PRO	2.6
1	A	129	CYS	2.5
1	A	185	GLN	2.5
1	A	30	PRO	2.5
1	A	147	PRO	2.5
1	A	107	SER	2.5
1	A	117	PHE	2.4
1	A	65	GLY	2.4
1	A	20	GLU	2.4
1	A	46	VAL	2.3
1	A	476	MET	2.3
1	A	60	ARG	2.3
1	A	379	CYS	2.3
1	A	294	HIS	2.3
1	A	73	GLU	2.3
1	A	28	VAL	2.2
1	A	83	ALA	2.1
1	A	103	PRO	2.1
1	A	114	ARG	2.1
1	A	109	ALA	2.1
1	A	484	PRO	2.1
1	A	501	GLU	2.1
1	A	183	VAL	2.1
1	A	530	PRO	2.1
1	A	520	ARG	2.0
1	A	493	GLN	2.0
1	A	615	SER	2.0
1	A	510	MET	2.0
1	A	547	LEU	2.0

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

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.