Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 11:53 AM EDT

PDB ID	:	1K8Z
Title	:	CRYSTAL STRUCTURE OF THE TRYPTOPHAN SYNTHASE BETA-SER178PRO MUTANT COMPLEXED WITH N-[1H-INDOL-3-YL-ACETYL]GLYCINE ACID
Authors	:	Weyand, M.; Schlichting, I.; Marabotti, A.; Mozzarelli, A.
Deposited on	:	2001-10-26
Resolution	:	1.70 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 (i) 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 (i)) were used in the production of this report:

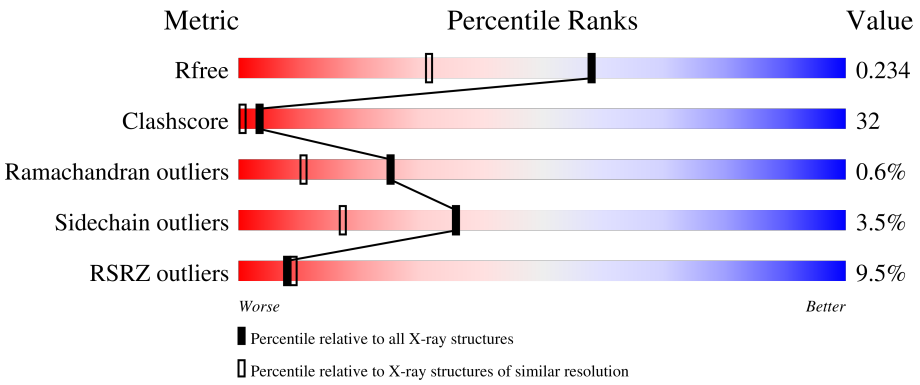
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	268	7%; 22%; 56%; 16%; • •
2	B	396	11%; 7%; 65%; 27%; ••

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5352 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 TRYPTOPHAN SYNTHASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	257	1955	1248	334	365	8	0	2	0

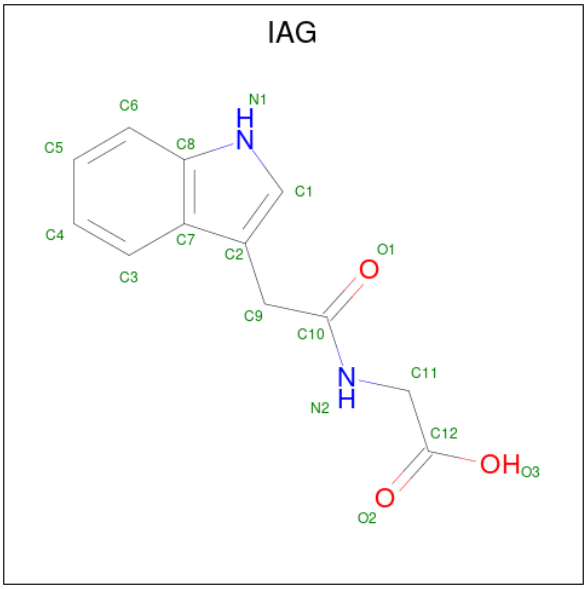
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	394	2987	1877	527	564	19	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	34	SER	ARG	cloning artifact	UNP P0A2K1
B	178	PRO	SER	engineered mutation	UNP P0A2K1

- Molecule 3 is N-[1H-INDOL-3-YL-ACETYL]GLYCINE ACID (three-letter code: IAG) (formula: $C_{12}H_{12}N_2O_3$).

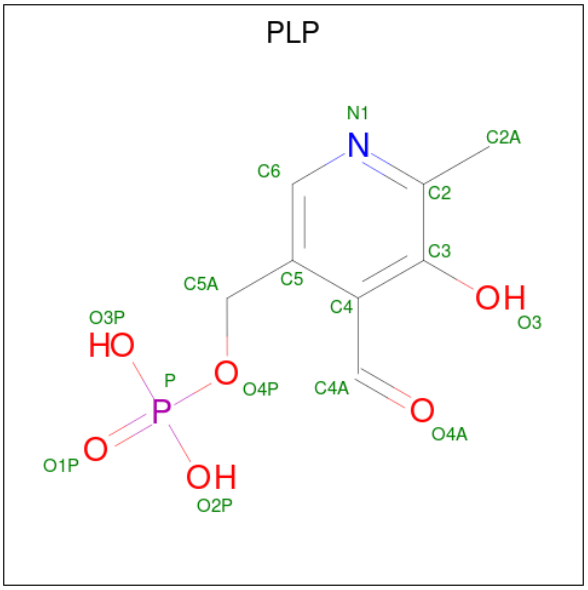


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	17	12	2	3	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	B	1	1	1	0	0

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	15	8	1	5	1	0	0

- Molecule 6 is water.

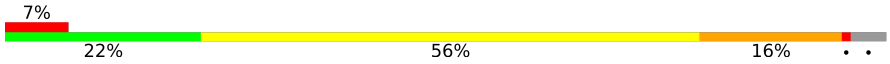
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	129	129	129	0	0
			Total	O		
6	B	248	248	248	0	0

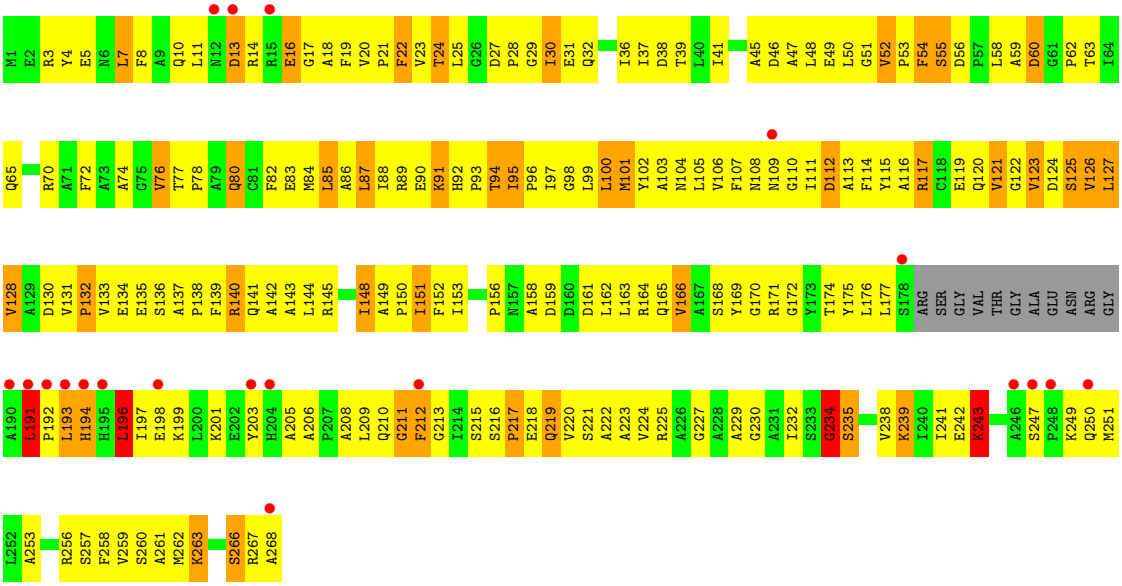
3 Residue-property plots (i)

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: TRYPTOPHAN SYNTHASE ALPHA CHAIN

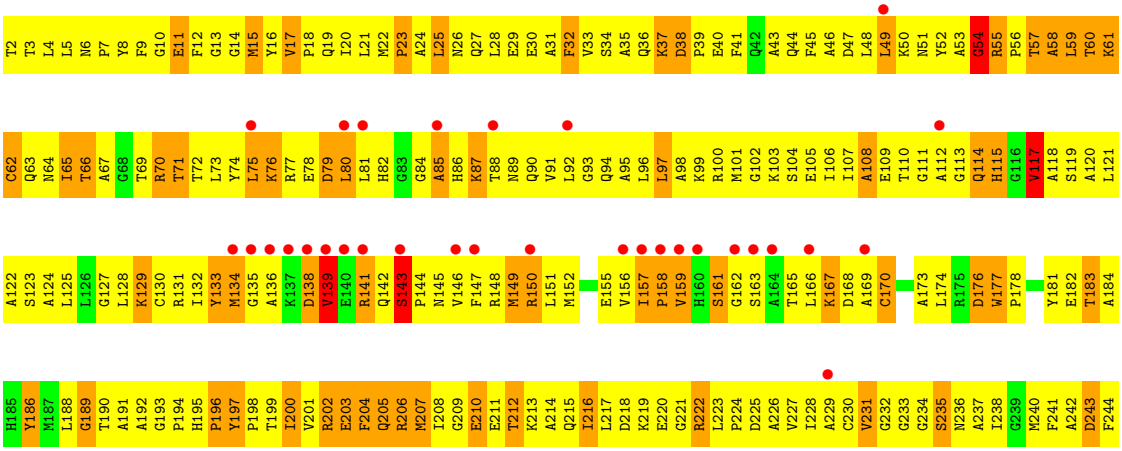
Chain A:

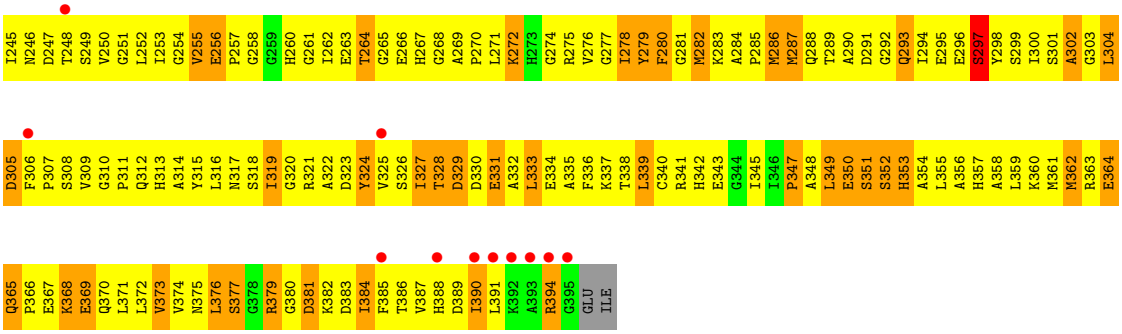




• Molecule 2: TRYPTOPHAN SYNTHASE BETA CHAIN

Chain B:




I245 N246 D247 T248 S249 V250 G251 L252 I253 G254 V255 E256 P257 G258 G259 H260 G261 I262 E263 T264 G265 E266 H267 G268 A269 P270 L271 K272 H273 G274 R275 V276 G277 I278 Y279 F280 G281 M282 K283 A284 P285 M286 M287 Q288 T289 A290 D291 G292 Q293 I294 E295 E296 S297 Y298 S299 I300 S301 A302 G303 L304
D305 F306 P307 S308 V309 G310 P311 Q312 H313 A314 Y315 L316 N317 S318 I319 G320 R321 A322 D323 Y324 V325 S326 I327 T328 D329 D330 E331 A332 L333 E334 A335 F336 K337 T338 L339 C340 R341 H342 E343 G344 I345 I346 P347 A348 L349 E350 S351 S352 H353 A354 L355 A356 H357 A358 L359 K360 M361 M362 R363 E364
Q365 P366 E367 K368 E369 Q370 L371 L372 V373 V374 N375 L376 S377 G378 R379 G380 D381 K382 D383 I384 F385 T386 V387 H388 D389 I390 L391 K392 A393 R394 G395 GLU ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	184.42Å 61.03Å 67.53Å 90.00° 94.69° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 43.36 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-1.70) 96.4 (43.36-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 1.70Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.209 , 0.265 0.188 , 0.234	Depositor DCC
R_{free} test set	4065 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 56.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5352	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: IAG, PLP, NA

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	3.32	245/2004 (12.2%)	2.86	199/2722 (7.3%)
2	B	4.35	703/3052 (23.0%)	4.01	646/4123 (15.7%)
All	All	3.97	948/5056 (18.8%)	3.60	845/6845 (12.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

All (948) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	TYR	CE2-CZ	24.33	1.70	1.38
2	B	30	GLU	CD-OE2	20.54	1.48	1.25
2	B	8	TYR	CE1-CZ	19.55	1.64	1.38
2	B	291	ASP	CB-CG	-17.49	1.15	1.51
2	B	16	TYR	CE2-CZ	16.98	1.60	1.38
2	B	286	MET	CB-CG	16.45	2.04	1.51
2	B	256	GLU	CG-CD	16.42	1.76	1.51
2	B	45	PHE	CE1-CZ	15.99	1.67	1.37
2	B	324	TYR	CE1-CZ	15.56	1.58	1.38
2	B	204	PHE	CD1-CE1	15.06	1.69	1.39
2	B	78	GLU	CD-OE1	14.48	1.41	1.25
2	B	202	ARG	NE-CZ	14.39	1.51	1.33
2	B	235	SER	CA-CB	14.39	1.74	1.52
2	B	280	PHE	CD2-CE2	14.14	1.67	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	373	VAL	CB-CG1	13.92	1.82	1.52
2	B	257	PRO	N-CD	13.83	1.67	1.47
2	B	295	GLU	CG-CD	13.72	1.72	1.51
2	B	123	SER	CB-OG	13.61	1.59	1.42
2	B	77	ARG	NE-CZ	13.47	1.50	1.33
2	B	78	GLU	CD-OE2	-13.36	1.10	1.25
2	B	12	PHE	CD1-CE1	13.36	1.66	1.39
1	A	212	PHE	CD1-CE1	13.31	1.65	1.39
1	A	101	MET	CG-SD	-13.23	1.46	1.81
2	B	72	THR	CA-CB	-13.22	1.19	1.53
2	B	352	SER	CB-OG	12.97	1.59	1.42
1	A	82	PHE	CD1-CE1	-12.94	1.13	1.39
2	B	6	ASN	C-O	12.86	1.47	1.23
1	A	212	PHE	CD2-CE2	12.84	1.65	1.39
2	B	61	LYS	N-CA	12.81	1.72	1.46
2	B	139	VAL	CB-CG2	12.70	1.79	1.52
2	B	11	GLU	CD-OE2	12.65	1.39	1.25
2	B	205	GLN	CG-CD	12.58	1.79	1.51
2	B	231	VAL	CB-CG1	12.47	1.79	1.52
2	B	32	PHE	CG-CD1	12.47	1.57	1.38
1	A	125	SER	CA-CB	12.46	1.71	1.52
2	B	233	GLY	C-N	12.46	1.55	1.33
2	B	108	ALA	CA-CB	12.42	1.78	1.52
2	B	29	GLU	CD-OE2	12.39	1.39	1.25
2	B	196	PRO	CA-C	12.38	1.77	1.52
2	B	254	GLY	C-O	12.37	1.43	1.23
2	B	231	VAL	C-N	12.36	1.55	1.33
2	B	59	LEU	N-CA	12.34	1.71	1.46
2	B	252	LEU	C-O	12.27	1.46	1.23
1	A	117	ARG	CG-CD	12.25	1.82	1.51
2	B	255	VAL	CA-CB	12.16	1.80	1.54
2	B	135	GLY	C-O	12.11	1.43	1.23
2	B	268	GLY	CA-C	-12.09	1.32	1.51
2	B	9	PHE	CD2-CE2	11.86	1.62	1.39
1	A	13	ASP	CB-CG	11.84	1.76	1.51
1	A	210	GLN	C-N	11.82	1.54	1.33
2	B	319	ILE	C-O	11.72	1.45	1.23
2	B	61	LYS	CB-CG	11.70	1.84	1.52
1	A	166	VAL	CB-CG2	11.54	1.77	1.52
2	B	205	GLN	C-O	11.52	1.45	1.23
2	B	211	GLU	CD-OE2	11.20	1.38	1.25
2	B	30	GLU	CG-CD	11.14	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	GLY	CA-C	11.05	1.69	1.51
2	B	55	ARG	CZ-NH2	11.05	1.47	1.33
2	B	58	ALA	CA-CB	11.02	1.75	1.52
2	B	314	ALA	C-O	11.01	1.44	1.23
2	B	243	ASP	N-CA	-10.99	1.24	1.46
2	B	16	TYR	CG-CD1	10.96	1.53	1.39
2	B	70	ARG	CA-C	10.93	1.81	1.52
1	A	219	GLN	CB-CG	10.91	1.82	1.52
2	B	12	PHE	CD2-CE2	10.81	1.60	1.39
2	B	394	ARG	CZ-NH1	10.80	1.47	1.33
1	A	126	VAL	CB-CG1	10.77	1.75	1.52
2	B	286	MET	CA-CB	10.76	1.77	1.53
2	B	296	GLU	CB-CG	10.76	1.72	1.52
1	A	97	ILE	C-N	10.73	1.52	1.33
2	B	353	HIS	CA-CB	10.73	1.77	1.53
2	B	51	ASN	CA-C	-10.72	1.25	1.52
1	A	151	ILE	CA-CB	-10.60	1.30	1.54
2	B	282	MET	CA-CB	10.58	1.77	1.53
1	A	52	VAL	CB-CG1	10.54	1.75	1.52
2	B	308	SER	C-O	10.54	1.43	1.23
1	A	169	TYR	CG-CD2	10.50	1.52	1.39
2	B	76	LYS	CD-CE	10.47	1.77	1.51
1	A	143	ALA	CA-CB	10.46	1.74	1.52
2	B	196	PRO	N-CD	10.44	1.62	1.47
2	B	40	GLU	CG-CD	10.40	1.67	1.51
2	B	343	GLU	CD-OE2	10.37	1.37	1.25
2	B	321	ARG	C-O	10.35	1.43	1.23
2	B	141	ARG	C-O	10.31	1.43	1.23
2	B	95	ALA	C-O	10.30	1.43	1.23
1	A	31	GLU	CD-OE2	10.29	1.36	1.25
2	B	373	VAL	C-O	10.27	1.42	1.23
2	B	120	ALA	CA-CB	-10.26	1.30	1.52
2	B	149	MET	CG-SD	10.26	2.07	1.81
2	B	367	GLU	C-O	10.25	1.42	1.23
1	A	145	ARG	CZ-NH2	10.16	1.46	1.33
1	A	123	VAL	CA-CB	10.16	1.76	1.54
1	A	65	GLN	CG-CD	10.14	1.74	1.51
2	B	138	ASP	C-O	10.14	1.42	1.23
2	B	324	TYR	CG-CD2	10.13	1.52	1.39
2	B	93	GLY	C-O	10.09	1.39	1.23
2	B	207	MET	C-O	10.09	1.42	1.23
2	B	17	VAL	CB-CG1	10.08	1.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	297	SER	CA-CB	-10.02	1.38	1.52
1	A	107	PHE	CE1-CZ	10.02	1.56	1.37
2	B	360	LYS	C-O	9.99	1.42	1.23
2	B	356	ALA	CA-CB	-9.97	1.31	1.52
2	B	36	GLN	CG-CD	9.96	1.74	1.51
2	B	95	ALA	CA-CB	9.89	1.73	1.52
1	A	140	ARG	CG-CD	9.85	1.76	1.51
2	B	31	ALA	N-CA	9.81	1.66	1.46
2	B	117	VAL	CA-CB	9.78	1.75	1.54
1	A	158	ALA	CA-CB	9.75	1.73	1.52
2	B	78	GLU	C-O	9.74	1.41	1.23
2	B	279	TYR	CE2-CZ	9.74	1.51	1.38
2	B	181	TYR	CD1-CE1	9.72	1.53	1.39
2	B	303	GLY	N-CA	-9.69	1.31	1.46
2	B	289	THR	CB-OG1	9.68	1.62	1.43
1	A	97	ILE	N-CA	9.67	1.65	1.46
2	B	85	ALA	N-CA	9.62	1.65	1.46
2	B	79	ASP	CG-OD2	9.60	1.47	1.25
2	B	59	LEU	CA-C	9.57	1.77	1.52
2	B	29	GLU	C-N	9.54	1.55	1.34
1	A	20	VAL	CB-CG1	9.53	1.72	1.52
2	B	260	HIS	CA-CB	-9.51	1.33	1.53
2	B	328	THR	CA-C	9.49	1.77	1.52
2	B	203	GLU	CA-C	9.44	1.77	1.52
2	B	204	PHE	CB-CG	9.41	1.67	1.51
2	B	182	GLU	CG-CD	9.38	1.66	1.51
2	B	208	ILE	CA-CB	-9.38	1.33	1.54
2	B	311	PRO	N-CD	9.36	1.60	1.47
2	B	194	PRO	CA-C	-9.35	1.34	1.52
2	B	52	TYR	CB-CG	-9.33	1.37	1.51
2	B	315	TYR	CB-CG	-9.32	1.37	1.51
2	B	305	ASP	CG-OD1	9.26	1.46	1.25
1	A	169	TYR	CE2-CZ	-9.25	1.26	1.38
2	B	30	GLU	CA-CB	9.25	1.74	1.53
2	B	232	GLY	CA-C	9.23	1.66	1.51
1	A	203	TYR	CE2-CZ	-9.22	1.26	1.38
2	B	361	MET	SD-CE	-9.22	1.26	1.77
2	B	117	VAL	CB-CG1	9.21	1.72	1.52
2	B	55	ARG	CG-CD	9.20	1.75	1.51
2	B	204	PHE	CD2-CE2	9.19	1.57	1.39
1	A	74	ALA	CA-CB	9.17	1.71	1.52
1	A	170	GLY	C-O	9.17	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	PRO	CA-C	9.16	1.71	1.52
2	B	195	HIS	N-CA	-9.13	1.28	1.46
2	B	22	MET	SD-CE	-9.12	1.26	1.77
2	B	52	TYR	CZ-OH	-9.11	1.22	1.37
2	B	6	ASN	CA-C	-9.09	1.29	1.52
2	B	351	SER	CA-C	9.05	1.76	1.52
2	B	340	CYS	CA-CB	-9.05	1.34	1.53
2	B	182	GLU	CD-OE2	9.00	1.35	1.25
2	B	360	LYS	CB-CG	-8.99	1.28	1.52
2	B	310	GLY	C-O	8.98	1.38	1.23
1	A	121	VAL	N-CA	-8.97	1.28	1.46
2	B	197	TYR	CA-CB	-8.96	1.34	1.53
2	B	367	GLU	CG-CD	-8.87	1.38	1.51
2	B	52	TYR	N-CA	-8.87	1.28	1.46
2	B	316	LEU	C-O	8.86	1.40	1.23
2	B	340	CYS	CB-SG	8.86	1.97	1.82
2	B	376	LEU	CG-CD2	8.86	1.84	1.51
2	B	252	LEU	CA-C	-8.84	1.29	1.52
2	B	276	VAL	CA-CB	-8.83	1.36	1.54
2	B	362	MET	SD-CE	-8.82	1.28	1.77
2	B	199	THR	N-CA	-8.80	1.28	1.46
2	B	167	LYS	CE-NZ	8.79	1.71	1.49
2	B	159	VAL	CB-CG1	8.76	1.71	1.52
1	A	229	ALA	CA-C	-8.76	1.30	1.52
2	B	296	GLU	CD-OE2	8.75	1.35	1.25
2	B	368	LYS	CA-C	8.75	1.75	1.52
2	B	227	VAL	C-O	8.73	1.40	1.23
1	A	140	ARG	NE-CZ	-8.71	1.21	1.33
2	B	212	THR	N-CA	8.70	1.63	1.46
2	B	151	LEU	C-O	8.69	1.39	1.23
1	A	54	PHE	CA-C	8.68	1.75	1.52
1	A	140	ARG	CB-CG	-8.67	1.29	1.52
2	B	245	ILE	C-O	8.66	1.39	1.23
2	B	362	MET	C-O	8.66	1.39	1.23
2	B	315	TYR	CE1-CZ	-8.65	1.27	1.38
2	B	214	ALA	CA-CB	8.64	1.70	1.52
2	B	215	GLN	N-CA	8.64	1.63	1.46
2	B	263	GLU	CG-CD	8.63	1.64	1.51
2	B	244	PHE	CB-CG	8.62	1.66	1.51
2	B	255	VAL	N-CA	-8.62	1.29	1.46
1	A	169	TYR	CG-CD1	-8.62	1.27	1.39
1	A	152	PHE	CA-CB	-8.61	1.35	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	GLY	CA-C	8.60	1.65	1.51
1	A	139	PHE	CB-CG	8.59	1.66	1.51
2	B	117	VAL	CA-C	-8.58	1.30	1.52
2	B	106	ILE	CA-C	-8.58	1.30	1.52
2	B	325	VAL	CA-CB	8.57	1.72	1.54
2	B	165	THR	C-O	8.56	1.39	1.23
1	A	136	SER	CA-CB	8.54	1.65	1.52
2	B	284	ALA	C-N	8.52	1.50	1.34
1	A	107	PHE	CG-CD1	-8.51	1.25	1.38
2	B	177	TRP	CD2-CE3	8.50	1.53	1.40
1	A	135	GLU	CD-OE2	8.48	1.34	1.25
2	B	82	HIS	CG-CD2	8.48	1.50	1.35
2	B	53	ALA	CA-CB	8.47	1.70	1.52
1	A	212	PHE	CE2-CZ	8.47	1.53	1.37
2	B	225	ASP	CG-OD2	8.45	1.44	1.25
2	B	374	VAL	CB-CG2	8.44	1.70	1.52
1	A	221	SER	CA-CB	8.44	1.65	1.52
2	B	304	LEU	CG-CD1	8.43	1.83	1.51
1	A	112	ASP	CB-CG	-8.43	1.34	1.51
1	A	120	GLN	CG-CD	8.43	1.70	1.51
2	B	280	PHE	C-N	8.43	1.48	1.33
2	B	203	GLU	N-CA	-8.41	1.29	1.46
1	A	102	TYR	CD2-CE2	8.40	1.51	1.39
2	B	19	GLN	CA-CB	8.38	1.72	1.53
1	A	94	THR	CA-CB	8.38	1.75	1.53
1	A	102	TYR	CA-CB	8.36	1.72	1.53
1	A	24	THR	CA-CB	8.35	1.75	1.53
2	B	341	ARG	CZ-NH1	8.35	1.44	1.33
2	B	189	GLY	N-CA	8.35	1.58	1.46
2	B	30	GLU	CD-OE1	8.34	1.34	1.25
2	B	324	TYR	C-O	8.33	1.39	1.23
2	B	221	GLY	CA-C	8.31	1.65	1.51
2	B	282	MET	CG-SD	8.31	2.02	1.81
2	B	223	LEU	C-O	8.30	1.39	1.23
2	B	8	TYR	CG-CD2	8.28	1.50	1.39
2	B	10	GLY	C-O	8.27	1.36	1.23
2	B	302	ALA	CA-CB	8.27	1.69	1.52
2	B	52	TYR	CG-CD2	8.26	1.49	1.39
2	B	211	GLU	CB-CG	8.24	1.67	1.52
2	B	27	GLN	CA-C	8.24	1.74	1.52
2	B	49	LEU	C-O	8.24	1.39	1.23
2	B	337	LYS	C-O	8.24	1.39	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ARG	C-O	8.21	1.39	1.23
2	B	10	GLY	CA-C	-8.20	1.38	1.51
2	B	285	PRO	CA-C	-8.20	1.36	1.52
2	B	119	SER	CA-CB	8.20	1.65	1.52
2	B	282	MET	SD-CE	-8.20	1.31	1.77
1	A	21	PRO	CA-CB	-8.19	1.37	1.53
2	B	230	CYS	CB-SG	8.19	1.96	1.82
1	A	83	GLU	CG-CD	8.18	1.64	1.51
1	A	116	ALA	CA-CB	8.16	1.69	1.52
2	B	241	PHE	CG-CD1	8.16	1.50	1.38
2	B	150	ARG	CB-CG	8.16	1.74	1.52
2	B	131	ARG	CZ-NH2	8.15	1.43	1.33
2	B	256	GLU	C-O	8.14	1.38	1.23
2	B	323	ASP	C-O	8.13	1.38	1.23
2	B	67	ALA	CA-CB	8.12	1.69	1.52
2	B	262	ILE	CA-CB	-8.12	1.36	1.54
1	A	134	GLU	CG-CD	8.11	1.64	1.51
2	B	367	GLU	CD-OE2	8.10	1.34	1.25
1	A	96	PRO	CA-CB	-8.10	1.37	1.53
2	B	77	ARG	CB-CG	8.07	1.74	1.52
2	B	40	GLU	CD-OE1	8.06	1.34	1.25
2	B	341	ARG	N-CA	8.06	1.62	1.46
2	B	123	SER	CA-CB	-8.05	1.40	1.52
2	B	118	ALA	N-CA	-8.04	1.30	1.46
2	B	13	GLY	CA-C	8.03	1.64	1.51
2	B	351	SER	CA-CB	8.03	1.65	1.52
2	B	109	GLU	CA-CB	8.02	1.71	1.53
2	B	21	LEU	CA-C	-8.00	1.32	1.52
2	B	245	ILE	N-CA	8.00	1.62	1.46
1	A	127	LEU	CA-C	8.00	1.73	1.52
1	A	137	ALA	CA-CB	-7.99	1.35	1.52
1	A	138	PRO	CA-CB	7.99	1.69	1.53
2	B	369	GLU	CA-CB	-7.98	1.36	1.53
2	B	227	VAL	N-CA	7.98	1.62	1.46
2	B	256	GLU	CD-OE2	7.98	1.34	1.25
1	A	169	TYR	CA-CB	7.97	1.71	1.53
2	B	306	PHE	CE1-CZ	7.97	1.52	1.37
2	B	287	MET	CB-CG	7.97	1.76	1.51
2	B	334	GLU	CD-OE2	7.96	1.34	1.25
1	A	115	TYR	CG-CD2	7.96	1.49	1.39
1	A	119	GLU	CB-CG	7.96	1.67	1.52
2	B	24	ALA	N-CA	7.96	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	269	ALA	CA-CB	7.95	1.69	1.52
1	A	84	MET	C-O	7.95	1.38	1.23
2	B	76	LYS	CA-CB	7.95	1.71	1.53
2	B	86	HIS	CA-C	7.95	1.73	1.52
2	B	335	ALA	CA-C	7.94	1.73	1.52
1	A	227	GLY	CA-C	7.93	1.64	1.51
2	B	9	PHE	CD1-CE1	7.92	1.55	1.39
1	A	51	GLY	N-CA	7.91	1.57	1.46
2	B	82	HIS	C-O	7.91	1.38	1.23
1	A	121	VAL	CA-CB	7.89	1.71	1.54
2	B	37	LYS	CD-CE	7.89	1.71	1.51
1	A	5	GLU	N-CA	7.87	1.62	1.46
2	B	238	ILE	CA-CB	7.87	1.73	1.54
1	A	145	ARG	CD-NE	7.86	1.59	1.46
2	B	362	MET	CG-SD	7.86	2.01	1.81
2	B	363	ARG	CB-CG	7.86	1.73	1.52
2	B	336	PHE	CD1-CE1	7.86	1.54	1.39
2	B	49	LEU	CG-CD2	7.86	1.80	1.51
2	B	380	GLY	N-CA	-7.86	1.34	1.46
2	B	374	VAL	N-CA	-7.85	1.30	1.46
2	B	52	TYR	CG-CD1	7.83	1.49	1.39
2	B	339	LEU	CG-CD2	7.83	1.80	1.51
2	B	128	LEU	CA-C	-7.81	1.32	1.52
2	B	63	GLN	CG-CD	7.81	1.69	1.51
2	B	152	MET	SD-CE	-7.80	1.34	1.77
1	A	206	ALA	CA-CB	7.79	1.68	1.52
2	B	50	LYS	CA-CB	-7.77	1.36	1.53
2	B	314	ALA	N-CA	7.76	1.61	1.46
2	B	228	ILE	CA-CB	7.75	1.72	1.54
2	B	194	PRO	C-O	7.75	1.38	1.23
2	B	317	ASN	CG-OD1	7.74	1.41	1.24
1	A	126	VAL	N-CA	7.74	1.61	1.46
2	B	59	LEU	CA-CB	-7.74	1.35	1.53
1	A	52	VAL	CA-C	7.73	1.73	1.52
2	B	12	PHE	CE2-CZ	-7.73	1.22	1.37
1	A	8	PHE	CD2-CE2	7.72	1.54	1.39
1	A	101	MET	CB-CG	7.72	1.76	1.51
2	B	353	HIS	C-O	7.71	1.38	1.23
2	B	385	PHE	CB-CG	-7.71	1.38	1.51
2	B	91	VAL	CB-CG1	7.70	1.69	1.52
2	B	26	ASN	CA-CB	7.69	1.73	1.53
2	B	263	GLU	CD-OE2	7.68	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	ARG	CG-CD	7.68	1.71	1.51
2	B	266	GLU	C-O	7.68	1.38	1.23
2	B	51	ASN	C-O	7.67	1.38	1.23
2	B	148	ARG	CB-CG	7.67	1.73	1.52
2	B	281	GLY	N-CA	-7.64	1.34	1.46
2	B	143	SER	CA-CB	-7.63	1.41	1.52
2	B	225	ASP	N-CA	7.60	1.61	1.46
2	B	369	GLU	CD-OE2	7.60	1.34	1.25
2	B	25	LEU	CA-C	-7.59	1.33	1.52
2	B	308	SER	CA-CB	7.59	1.64	1.52
2	B	349	LEU	CA-CB	-7.58	1.36	1.53
1	A	139	PHE	CD1-CE1	7.58	1.54	1.39
2	B	258	GLY	CA-C	-7.57	1.39	1.51
1	A	152	PHE	CD2-CE2	7.55	1.54	1.39
2	B	254	GLY	CA-C	-7.55	1.39	1.51
2	B	375	ASN	C-N	7.55	1.51	1.34
2	B	149	MET	CA-CB	7.54	1.70	1.53
1	A	16	GLU	CD-OE1	7.54	1.33	1.25
2	B	366	PRO	CA-C	-7.54	1.37	1.52
1	A	138	PRO	CA-C	-7.53	1.37	1.52
2	B	114	GLN	CB-CG	7.53	1.72	1.52
2	B	270	PRO	CA-CB	7.51	1.68	1.53
2	B	343	GLU	C-N	-7.51	1.19	1.33
2	B	241	PHE	CE2-CZ	7.51	1.51	1.37
2	B	212	THR	CB-CG2	7.50	1.77	1.52
2	B	71	THR	CB-CG2	7.49	1.77	1.52
2	B	257	PRO	N-CA	-7.49	1.34	1.47
2	B	32	PHE	N-CA	7.49	1.61	1.46
2	B	8	TYR	CD1-CE1	-7.49	1.28	1.39
2	B	80	LEU	N-CA	7.49	1.61	1.46
2	B	155	GLU	CD-OE1	7.48	1.33	1.25
2	B	260	HIS	CB-CG	7.48	1.63	1.50
2	B	323	ASP	CA-CB	7.46	1.70	1.53
2	B	12	PHE	CB-CG	7.45	1.64	1.51
2	B	19	GLN	CA-C	7.44	1.72	1.52
2	B	311	PRO	C-O	7.43	1.38	1.23
1	A	107	PHE	CG-CD2	7.42	1.49	1.38
1	A	175	TYR	CE1-CZ	-7.42	1.28	1.38
2	B	299	SER	CB-OG	7.40	1.51	1.42
2	B	373	VAL	CB-CG2	-7.40	1.37	1.52
2	B	74	TYR	CE2-CZ	7.40	1.48	1.38
2	B	280	PHE	CA-C	-7.38	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	ALA	CA-CB	-7.36	1.36	1.52
2	B	319	ILE	CB-CG2	7.36	1.75	1.52
2	B	120	ALA	C-O	7.35	1.37	1.23
2	B	104	SER	C-O	7.34	1.37	1.23
2	B	105	GLU	CA-C	7.34	1.72	1.52
2	B	201	VAL	CA-CB	-7.34	1.39	1.54
2	B	353	HIS	CA-C	-7.33	1.33	1.52
1	A	17	GLY	N-CA	7.32	1.57	1.46
1	A	95	ILE	C-O	7.32	1.37	1.23
2	B	207	MET	CA-CB	7.32	1.70	1.53
2	B	186	TYR	CE1-CZ	-7.32	1.29	1.38
2	B	63	GLN	C-O	7.32	1.37	1.23
2	B	242	ALA	CA-CB	7.30	1.67	1.52
2	B	219	LYS	CD-CE	7.29	1.69	1.51
2	B	281	GLY	CA-C	-7.29	1.40	1.51
2	B	237	ALA	CA-CB	7.29	1.67	1.52
2	B	20	ILE	N-CA	7.29	1.60	1.46
2	B	177	TRP	CZ3-CH2	-7.29	1.28	1.40
1	A	54	PHE	CA-CB	-7.28	1.38	1.53
2	B	369	GLU	C-O	7.27	1.37	1.23
1	A	257	SER	CB-OG	-7.24	1.32	1.42
2	B	106	ILE	C-N	7.23	1.50	1.34
2	B	76	LYS	C-N	7.22	1.50	1.34
2	B	190	THR	CB-OG1	7.22	1.57	1.43
1	A	7	LEU	CG-CD2	7.21	1.78	1.51
2	B	345	ILE	C-O	7.21	1.37	1.23
2	B	73	LEU	CA-CB	-7.21	1.37	1.53
1	A	222	ALA	CA-CB	7.21	1.67	1.52
2	B	6	ASN	C-N	-7.20	1.20	1.34
2	B	11	GLU	CG-CD	7.20	1.62	1.51
2	B	134	MET	C-O	7.20	1.37	1.23
2	B	335	ALA	N-CA	-7.19	1.31	1.46
2	B	219	LYS	CG-CD	-7.19	1.28	1.52
2	B	394	ARG	CZ-NH2	7.18	1.42	1.33
2	B	322	ALA	CA-CB	7.18	1.67	1.52
2	B	71	THR	CA-CB	-7.18	1.34	1.53
2	B	9	PHE	CA-C	7.17	1.71	1.52
2	B	241	PHE	C-N	7.17	1.50	1.34
1	A	104	ASN	N-CA	7.16	1.60	1.46
1	A	108	ASN	CG-OD1	-7.15	1.08	1.24
1	A	161	ASP	CG-OD1	7.15	1.41	1.25
1	A	211	GLY	CA-C	7.14	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	LYS	CE-NZ	7.14	1.67	1.49
2	B	44	GLN	CG-CD	7.14	1.67	1.51
1	A	149	ALA	C-N	-7.13	1.20	1.34
2	B	227	VAL	CB-CG2	7.13	1.67	1.52
1	A	140	ARG	C-O	7.12	1.36	1.23
1	A	82	PHE	CE1-CZ	7.12	1.50	1.37
1	A	16	GLU	C-N	7.12	1.45	1.33
2	B	3	THR	CA-C	-7.12	1.34	1.52
2	B	44	GLN	N-CA	-7.10	1.32	1.46
2	B	244	PHE	CD1-CE1	7.10	1.53	1.39
2	B	336	PHE	CA-C	7.10	1.71	1.52
1	A	5	GLU	CD-OE1	7.09	1.33	1.25
2	B	291	ASP	CA-CB	7.08	1.69	1.53
1	A	128	VAL	N-CA	7.07	1.60	1.46
2	B	253	ILE	CA-CB	7.07	1.71	1.54
2	B	247	ASP	N-CA	7.07	1.60	1.46
2	B	287	MET	SD-CE	-7.06	1.38	1.77
2	B	103	LYS	N-CA	-7.06	1.32	1.46
2	B	255	VAL	C-O	7.06	1.36	1.23
2	B	229	ALA	CA-C	-7.06	1.34	1.52
2	B	87	LYS	CA-CB	-7.04	1.38	1.53
2	B	315	TYR	CZ-OH	-7.04	1.25	1.37
2	B	311	PRO	CA-C	-7.04	1.38	1.52
2	B	198	PRO	C-O	7.03	1.37	1.23
2	B	203	GLU	CB-CG	7.03	1.65	1.52
2	B	90	GLN	CD-OE1	7.02	1.39	1.24
2	B	260	HIS	C-O	7.02	1.36	1.23
2	B	283	LYS	CE-NZ	7.01	1.66	1.49
2	B	66	THR	CB-CG2	7.01	1.75	1.52
2	B	285	PRO	C-O	7.00	1.37	1.23
1	A	38	ASP	N-CA	7.00	1.60	1.46
2	B	279	TYR	CD1-CE1	7.00	1.49	1.39
2	B	326	SER	CA-CB	-6.98	1.42	1.52
2	B	176	ASP	CA-CB	6.98	1.69	1.53
2	B	155	GLU	CG-CD	6.97	1.62	1.51
1	A	125	SER	CA-C	6.97	1.71	1.52
2	B	384	ILE	CA-CB	6.97	1.70	1.54
2	B	372	LEU	CA-CB	-6.97	1.37	1.53
1	A	205	ALA	CA-CB	6.96	1.67	1.52
2	B	258	GLY	C-N	6.96	1.45	1.33
2	B	313	HIS	N-CA	6.96	1.60	1.46
2	B	80	LEU	CB-CG	6.95	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	39	PRO	C-O	6.95	1.37	1.23
1	A	86	ALA	CA-CB	6.95	1.67	1.52
2	B	24	ALA	CA-CB	-6.95	1.37	1.52
2	B	32	PHE	CE1-CZ	6.93	1.50	1.37
2	B	211	GLU	CA-C	6.93	1.71	1.52
2	B	234	GLY	C-N	6.92	1.50	1.34
2	B	53	ALA	CA-C	6.92	1.71	1.52
2	B	117	VAL	CB-CG2	-6.91	1.38	1.52
2	B	177	TRP	CE3-CZ3	-6.90	1.26	1.38
2	B	339	LEU	CA-CB	6.90	1.69	1.53
2	B	264	THR	CB-CG2	6.90	1.75	1.52
2	B	37	LYS	CG-CD	6.88	1.75	1.52
2	B	364	GLU	CD-OE2	6.87	1.33	1.25
2	B	215	GLN	CB-CG	6.86	1.71	1.52
1	A	171	ARG	CA-C	-6.85	1.35	1.52
2	B	390	ILE	CA-C	-6.85	1.35	1.52
2	B	309	VAL	CA-CB	6.83	1.69	1.54
2	B	329	ASP	CA-CB	-6.83	1.39	1.53
2	B	338	THR	CA-CB	6.83	1.71	1.53
2	B	120	ALA	N-CA	6.83	1.60	1.46
1	A	70	ARG	NE-CZ	-6.83	1.24	1.33
2	B	100	ARG	CA-C	6.83	1.70	1.52
2	B	184	ALA	CA-CB	-6.82	1.38	1.52
2	B	317	ASN	CA-CB	-6.82	1.35	1.53
2	B	133	TYR	CD2-CE2	6.81	1.49	1.39
2	B	29	GLU	N-CA	-6.81	1.32	1.46
2	B	218	ASP	CB-CG	6.80	1.66	1.51
2	B	84	GLY	N-CA	6.79	1.56	1.46
2	B	183	THR	CB-CG2	6.78	1.74	1.52
1	A	136	SER	CB-OG	-6.78	1.33	1.42
2	B	203	GLU	CD-OE2	6.76	1.33	1.25
1	A	39	THR	C-O	6.76	1.36	1.23
2	B	278	ILE	CA-CB	6.75	1.70	1.54
1	A	212	PHE	CB-CG	6.74	1.62	1.51
2	B	281	GLY	C-N	6.74	1.49	1.34
2	B	8	TYR	CB-CG	-6.74	1.41	1.51
2	B	210	GLU	CD-OE1	6.74	1.33	1.25
1	A	165	GLN	CA-C	-6.74	1.35	1.52
2	B	56	PRO	C-O	6.73	1.36	1.23
2	B	261	GLY	CA-C	6.72	1.62	1.51
1	A	120	GLN	CA-C	-6.72	1.35	1.52
2	B	215	GLN	CA-CB	-6.71	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	285	PRO	CG-CD	6.71	1.72	1.50
2	B	231	VAL	N-CA	6.70	1.59	1.46
2	B	229	ALA	C-O	6.69	1.36	1.23
2	B	256	GLU	CA-CB	6.69	1.68	1.53
2	B	55	ARG	CA-C	-6.69	1.35	1.52
2	B	328	THR	CB-OG1	6.68	1.56	1.43
2	B	192	ALA	N-CA	6.68	1.59	1.46
2	B	29	GLU	CA-C	-6.67	1.35	1.52
1	A	213	GLY	CA-C	6.66	1.62	1.51
2	B	34	SER	CA-CB	6.66	1.62	1.52
2	B	129	LYS	CG-CD	6.66	1.75	1.52
2	B	131	ARG	CG-CD	6.65	1.68	1.51
1	A	116	ALA	CA-C	-6.65	1.35	1.52
2	B	41	PHE	CG-CD2	6.64	1.48	1.38
2	B	379	ARG	CA-C	-6.64	1.35	1.52
1	A	126	VAL	C-N	6.64	1.49	1.34
2	B	60	THR	CB-OG1	6.64	1.56	1.43
2	B	321	ARG	NE-CZ	6.63	1.41	1.33
2	B	367	GLU	N-CA	-6.63	1.33	1.46
2	B	20	ILE	CA-CB	-6.61	1.39	1.54
2	B	65	ILE	N-CA	6.61	1.59	1.46
1	A	139	PHE	CA-C	6.61	1.70	1.52
2	B	220	GLU	N-CA	6.61	1.59	1.46
2	B	369	GLU	CB-CG	6.61	1.64	1.52
2	B	333	LEU	CA-CB	-6.60	1.38	1.53
1	A	152	PHE	CE1-CZ	6.59	1.49	1.37
1	A	232	ILE	C-N	-6.59	1.18	1.34
2	B	380	GLY	C-O	-6.56	1.13	1.23
2	B	231	VAL	CB-CG2	-6.56	1.39	1.52
2	B	55	ARG	CD-NE	6.55	1.57	1.46
2	B	362	MET	C-N	-6.55	1.19	1.34
2	B	110	THR	CA-CB	6.55	1.70	1.53
2	B	283	LYS	CA-C	6.55	1.70	1.52
2	B	293	GLN	CA-CB	-6.54	1.39	1.53
1	A	139	PHE	N-CA	-6.54	1.33	1.46
1	A	55	SER	N-CA	6.54	1.59	1.46
1	A	142	ALA	CA-CB	6.54	1.66	1.52
2	B	157	ILE	C-N	-6.53	1.21	1.34
2	B	376	LEU	CA-CB	6.50	1.68	1.53
2	B	238	ILE	CB-CG2	6.50	1.73	1.52
2	B	23	PRO	CA-C	6.50	1.65	1.52
2	B	93	GLY	CA-C	6.49	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	94	GLN	CA-CB	-6.49	1.39	1.53
2	B	265	GLY	C-O	6.49	1.34	1.23
1	A	104	ASN	CB-CG	6.49	1.66	1.51
1	A	141	GLN	C-O	6.48	1.35	1.23
2	B	368	LYS	C-N	-6.48	1.19	1.34
1	A	136	SER	CA-C	6.48	1.69	1.52
2	B	218	ASP	C-O	6.48	1.35	1.23
1	A	120	GLN	CA-CB	6.47	1.68	1.53
1	A	203	TYR	CG-CD2	6.47	1.47	1.39
1	A	5	GLU	CD-OE2	6.46	1.32	1.25
2	B	198	PRO	CG-CD	6.46	1.72	1.50
2	B	133	TYR	CA-CB	6.46	1.68	1.53
1	A	220	VAL	CB-CG2	6.45	1.66	1.52
1	A	130	ASP	CA-C	-6.44	1.36	1.52
2	B	363	ARG	CZ-NH2	6.44	1.41	1.33
2	B	106	ILE	CB-CG2	6.44	1.72	1.52
2	B	347	PRO	CA-C	-6.44	1.40	1.52
1	A	217	PRO	CA-C	-6.43	1.40	1.52
2	B	327	ILE	N-CA	6.43	1.59	1.46
2	B	256	GLU	C-N	-6.42	1.22	1.34
2	B	94	GLN	CB-CG	6.41	1.69	1.52
2	B	105	GLU	CD-OE2	6.41	1.32	1.25
2	B	38	ASP	CB-CG	6.41	1.65	1.51
2	B	371	LEU	C-O	6.41	1.35	1.23
1	A	10	GLN	N-CA	-6.40	1.33	1.46
1	A	218	GLU	CD-OE1	6.40	1.32	1.25
2	B	360	LYS	CG-CD	6.40	1.74	1.52
1	A	259	VAL	CA-CB	6.40	1.68	1.54
1	A	223	ALA	CA-CB	6.39	1.65	1.52
2	B	121	LEU	CG-CD1	-6.39	1.28	1.51
1	A	105	LEU	CA-CB	-6.38	1.39	1.53
1	A	203	TYR	CE1-CZ	6.38	1.46	1.38
1	A	262	MET	SD-CE	-6.38	1.42	1.77
2	B	36	GLN	CA-CB	6.37	1.68	1.53
2	B	298	TYR	CD2-CE2	6.37	1.49	1.39
2	B	241	PHE	CB-CG	-6.37	1.40	1.51
2	B	295	GLU	CD-OE2	6.36	1.32	1.25
2	B	316	LEU	CA-CB	6.36	1.68	1.53
2	B	333	LEU	CG-CD2	6.33	1.75	1.51
2	B	59	LEU	CB-CG	6.33	1.71	1.52
2	B	130	CYS	CA-C	-6.33	1.36	1.52
2	B	385	PHE	CE2-CZ	6.33	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	ALA	CA-CB	6.32	1.65	1.52
2	B	58	ALA	CA-C	6.32	1.69	1.52
2	B	100	ARG	N-CA	-6.32	1.33	1.46
2	B	25	LEU	CG-CD2	6.31	1.75	1.51
2	B	70	ARG	N-CA	-6.31	1.33	1.46
1	A	72	PHE	CE1-CZ	6.31	1.49	1.37
1	A	113	ALA	CA-CB	6.31	1.65	1.52
2	B	82	HIS	CA-CB	6.31	1.67	1.53
1	A	110	GLY	CA-C	6.30	1.61	1.51
1	A	11	LEU	CA-CB	6.30	1.68	1.53
2	B	192	ALA	CA-C	6.30	1.69	1.52
2	B	372	LEU	CB-CG	6.29	1.70	1.52
1	A	162	LEU	N-CA	-6.29	1.33	1.46
1	A	53	PRO	CG-CD	6.28	1.71	1.50
2	B	352	SER	N-CA	6.28	1.58	1.46
2	B	48	LEU	CA-C	6.28	1.69	1.52
2	B	53	ALA	C-N	-6.27	1.21	1.33
2	B	234	GLY	CA-C	-6.27	1.41	1.51
2	B	279	TYR	CG-CD1	6.27	1.47	1.39
2	B	69	THR	CB-OG1	6.26	1.55	1.43
2	B	147	PHE	CE1-CZ	6.26	1.49	1.37
2	B	324	TYR	CD2-CE2	-6.26	1.29	1.39
2	B	157	ILE	CA-CB	6.26	1.69	1.54
2	B	199	THR	CB-OG1	6.26	1.55	1.43
1	A	18	ALA	CA-C	6.25	1.69	1.52
1	A	201	LYS	CE-NZ	6.24	1.64	1.49
2	B	209	GLY	CA-C	-6.24	1.41	1.51
1	A	235	SER	CB-OG	-6.24	1.34	1.42
1	A	37	ILE	CA-C	6.23	1.69	1.52
1	A	92	HIS	C-O	6.23	1.35	1.23
2	B	276	VAL	C-N	6.23	1.44	1.33
1	A	22	PHE	CD1-CE1	6.23	1.51	1.39
2	B	228	ILE	N-CA	-6.22	1.33	1.46
2	B	375	ASN	N-CA	6.22	1.58	1.46
2	B	192	ALA	CA-CB	-6.21	1.39	1.52
2	B	340	CYS	N-CA	6.21	1.58	1.46
1	A	87	LEU	CG-CD1	6.21	1.74	1.51
2	B	237	ALA	C-N	6.20	1.48	1.34
1	A	31	GLU	CG-CD	6.19	1.61	1.51
1	A	266	SER	CA-CB	6.19	1.62	1.52
2	B	60	THR	CA-CB	-6.19	1.37	1.53
1	A	62	PRO	N-CD	6.18	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	ALA	CA-C	-6.18	1.36	1.52
2	B	182	GLU	CA-C	6.18	1.69	1.52
2	B	157	ILE	N-CA	6.18	1.58	1.46
1	A	102	TYR	CD1-CE1	6.17	1.48	1.39
1	A	253	ALA	CA-CB	-6.17	1.39	1.52
2	B	315	TYR	CD2-CE2	6.17	1.48	1.39
2	B	359	LEU	N-CA	6.17	1.58	1.46
2	B	65	ILE	C-N	-6.17	1.19	1.34
2	B	243	ASP	CA-C	6.16	1.69	1.52
2	B	332	ALA	C-N	-6.16	1.19	1.34
2	B	368	LYS	CB-CG	6.16	1.69	1.52
2	B	220	GLU	CG-CD	6.16	1.61	1.51
2	B	321	ARG	C-N	-6.15	1.20	1.34
1	A	166	VAL	CA-C	6.14	1.69	1.52
2	B	40	GLU	CD-OE2	6.14	1.32	1.25
2	B	130	CYS	C-N	6.14	1.48	1.34
2	B	6	ASN	CA-CB	6.13	1.69	1.53
2	B	298	TYR	CE1-CZ	6.12	1.46	1.38
2	B	61	LYS	CA-C	-6.12	1.37	1.52
2	B	243	ASP	CG-OD1	6.12	1.39	1.25
2	B	35	ALA	N-CA	6.11	1.58	1.46
2	B	23	PRO	CB-CG	6.11	1.80	1.50
1	A	139	PHE	CD2-CE2	6.11	1.51	1.39
2	B	207	MET	CA-C	6.11	1.68	1.52
2	B	230	CYS	N-CA	-6.11	1.34	1.46
2	B	309	VAL	N-CA	-6.11	1.34	1.46
2	B	355	LEU	CB-CG	6.10	1.70	1.52
2	B	245	ILE	CB-CG2	6.10	1.71	1.52
2	B	201	VAL	CB-CG1	6.09	1.65	1.52
2	B	186	TYR	CZ-OH	6.09	1.48	1.37
1	A	104	ASN	CA-CB	6.08	1.69	1.53
2	B	323	ASP	CA-C	-6.08	1.37	1.52
1	A	261	ALA	C-O	6.08	1.34	1.23
1	A	249	LYS	CD-CE	6.07	1.66	1.51
2	B	47	ASP	C-O	6.07	1.34	1.23
2	B	373	VAL	N-CA	6.07	1.58	1.46
2	B	138	ASP	CA-CB	-6.06	1.40	1.53
2	B	242	ALA	CA-C	-6.06	1.37	1.52
1	A	135	GLU	CG-CD	6.06	1.61	1.51
2	B	100	ARG	CZ-NH2	-6.06	1.25	1.33
2	B	7	PRO	N-CA	-6.05	1.36	1.47
1	A	29	GLY	CA-C	6.05	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	ASN	CG-OD1	6.05	1.37	1.24
1	A	85	LEU	CA-CB	-6.05	1.39	1.53
2	B	56	PRO	CA-C	-6.05	1.40	1.52
2	B	206[A]	ARG	CA-C	6.05	1.68	1.52
2	B	206[B]	ARG	CA-C	6.05	1.68	1.52
2	B	85	ALA	C-O	6.05	1.34	1.23
1	A	107	PHE	CB-CG	-6.05	1.41	1.51
2	B	317	ASN	N-CA	6.05	1.58	1.46
2	B	97	LEU	CG-CD1	6.04	1.74	1.51
2	B	33	VAL	CA-CB	6.04	1.67	1.54
2	B	69	THR	CA-C	-6.04	1.37	1.52
1	A	268	ALA	C-O	6.04	1.34	1.23
2	B	119	SER	CA-C	6.04	1.68	1.52
2	B	262	ILE	N-CA	6.03	1.58	1.46
2	B	294	ILE	CB-CG1	6.03	1.71	1.54
2	B	371	LEU	N-CA	6.03	1.58	1.46
1	A	143	ALA	C-O	6.02	1.34	1.23
2	B	71	THR	N-CA	6.02	1.58	1.46
2	B	318	SER	N-CA	6.02	1.58	1.46
2	B	60	THR	N-CA	6.02	1.58	1.46
2	B	161	SER	CB-OG	6.01	1.50	1.42
2	B	17	VAL	CA-C	6.01	1.68	1.52
2	B	200	ILE	CB-CG2	6.01	1.71	1.52
2	B	235	SER	C-O	-6.01	1.11	1.23
2	B	100	ARG	CB-CG	-6.00	1.36	1.52
2	B	152	MET	CA-C	6.00	1.68	1.52
2	B	193	GLY	C-N	5.99	1.45	1.34
2	B	350	GLU	CA-CB	5.99	1.67	1.53
1	A	144	LEU	C-O	5.99	1.34	1.23
2	B	63	GLN	N-CA	5.99	1.58	1.46
1	A	77	THR	CA-C	5.99	1.68	1.52
2	B	86	HIS	CA-CB	5.98	1.67	1.53
1	A	224	VAL	CB-CG2	5.98	1.65	1.52
2	B	45	PHE	C-O	5.97	1.34	1.23
2	B	210	GLU	N-CA	-5.97	1.34	1.46
1	A	89	ARG	C-O	5.96	1.34	1.23
2	B	195	HIS	CB-CG	-5.96	1.39	1.50
1	A	171	ARG	CZ-NH2	-5.95	1.25	1.33
1	A	102	TYR	CG-CD2	-5.94	1.31	1.39
2	B	238	ILE	N-CA	-5.94	1.34	1.46
2	B	312	GLN	CD-NE2	-5.94	1.18	1.32
1	A	230	GLY	N-CA	-5.93	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	156	VAL	CB-CG1	-5.92	1.40	1.52
2	B	43	ALA	CA-CB	-5.91	1.40	1.52
2	B	365	GLN	CD-NE2	5.91	1.47	1.32
1	A	96	PRO	CA-C	5.90	1.64	1.52
2	B	208	ILE	C-O	5.90	1.34	1.23
2	B	55	ARG	C-O	5.89	1.34	1.23
2	B	202	ARG	CD-NE	-5.89	1.36	1.46
2	B	236	ASN	C-O	-5.89	1.12	1.23
2	B	336	PHE	CD2-CE2	5.89	1.51	1.39
2	B	368	LYS	CD-CE	5.88	1.66	1.51
2	B	188	LEU	CG-CD1	5.88	1.73	1.51
2	B	264	THR	C-N	-5.88	1.22	1.33
1	A	45	ALA	CA-CB	5.87	1.64	1.52
1	A	70	ARG	CG-CD	5.87	1.66	1.51
2	B	71	THR	CA-C	5.87	1.68	1.52
1	A	83	GLU	CA-CB	5.86	1.66	1.53
1	A	7	LEU	CA-CB	5.85	1.67	1.53
2	B	315	TYR	CG-CD1	5.85	1.46	1.39
2	B	356	ALA	N-CA	5.85	1.58	1.46
1	A	50	LEU	CA-C	5.84	1.68	1.52
1	A	90	GLU	CG-CD	5.84	1.60	1.51
2	B	201	VAL	N-CA	5.83	1.58	1.46
2	B	123	SER	N-CA	5.83	1.58	1.46
1	A	238	VAL	CB-CG1	5.82	1.65	1.52
2	B	146	VAL	CB-CG2	5.82	1.65	1.52
1	A	117	ARG	N-CA	-5.81	1.34	1.46
2	B	319	ILE	CB-CG1	5.81	1.70	1.54
2	B	388	HIS	C-O	-5.80	1.12	1.23
2	B	208	ILE	N-CA	5.79	1.57	1.46
2	B	331	GLU	N-CA	-5.79	1.34	1.46
2	B	99	LYS	CD-CE	5.78	1.65	1.51
2	B	121	LEU	C-N	5.78	1.47	1.34
1	A	250	GLN	CG-CD	5.77	1.64	1.51
2	B	106	ILE	N-CA	5.77	1.57	1.46
2	B	362	MET	CA-CB	5.77	1.66	1.53
2	B	55	ARG	CZ-NH1	-5.76	1.25	1.33
2	B	216	ILE	CA-C	-5.75	1.38	1.52
2	B	260	HIS	CA-C	-5.75	1.38	1.52
2	B	110	THR	CB-CG2	-5.74	1.33	1.52
2	B	57	THR	C-N	5.74	1.47	1.34
1	A	131	VAL	CB-CG2	5.73	1.64	1.52
2	B	146	VAL	C-O	5.73	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	287	MET	CG-SD	5.73	1.96	1.81
2	B	69	THR	CB-CG2	-5.73	1.33	1.52
2	B	271	LEU	C-O	5.73	1.34	1.23
1	A	145	ARG	NE-CZ	-5.72	1.25	1.33
2	B	222	ARG	N-CA	5.72	1.57	1.46
1	A	53	PRO	N-CA	5.72	1.56	1.47
2	B	374	VAL	CB-CG1	-5.72	1.40	1.52
2	B	139	VAL	CA-C	-5.72	1.38	1.52
2	B	298	TYR	CD1-CE1	5.72	1.48	1.39
1	A	168	SER	CA-CB	-5.71	1.44	1.52
2	B	274	GLY	N-CA	5.71	1.54	1.46
2	B	28	LEU	CB-CG	5.71	1.69	1.52
2	B	121	LEU	C-O	5.70	1.34	1.23
2	B	268	GLY	C-N	5.70	1.47	1.34
2	B	354	ALA	CA-C	5.70	1.67	1.52
2	B	215	GLN	CA-C	5.69	1.67	1.52
1	A	213	GLY	N-CA	5.69	1.54	1.46
2	B	188	LEU	CG-CD2	5.68	1.72	1.51
2	B	231	VAL	CA-C	-5.67	1.38	1.52
2	B	376	LEU	N-CA	-5.66	1.35	1.46
1	A	210	GLN	CA-C	-5.66	1.38	1.52
2	B	252	LEU	CB-CG	-5.66	1.36	1.52
2	B	165	THR	CA-CB	5.65	1.68	1.53
2	B	61	LYS	CE-NZ	5.64	1.63	1.49
2	B	270	PRO	CA-C	-5.64	1.41	1.52
2	B	312	GLN	N-CA	-5.64	1.35	1.46
1	A	131	VAL	CA-CB	5.63	1.66	1.54
1	A	152	PHE	CB-CG	5.63	1.60	1.51
2	B	190	THR	N-CA	5.63	1.57	1.46
2	B	18	PRO	C-N	5.62	1.47	1.34
2	B	13	GLY	N-CA	5.62	1.54	1.46
2	B	122	ALA	CA-C	5.62	1.67	1.52
1	A	142	ALA	N-CA	-5.62	1.35	1.46
2	B	279	TYR	CZ-OH	5.61	1.47	1.37
2	B	136	ALA	N-CA	5.61	1.57	1.46
1	A	171	ARG	NE-CZ	-5.61	1.25	1.33
2	B	32	PHE	CB-CG	5.60	1.60	1.51
2	B	297	SER	CA-C	5.60	1.67	1.52
2	B	197	TYR	CB-CG	5.60	1.60	1.51
2	B	78	GLU	CA-CB	5.60	1.66	1.53
2	B	170	CYS	CB-SG	5.59	1.91	1.82
2	B	206[A]	ARG	CB-CG	-5.59	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	206[B]	ARG	CB-CG	-5.59	1.37	1.52
2	B	55	ARG	C-N	5.59	1.44	1.34
2	B	46	ALA	CA-C	5.58	1.67	1.52
2	B	361	MET	CA-C	5.57	1.67	1.52
2	B	186	TYR	CE2-CZ	-5.57	1.31	1.38
2	B	322	ALA	C-O	5.57	1.33	1.23
2	B	297	SER	CB-OG	-5.56	1.35	1.42
1	A	259	VAL	CB-CG2	5.56	1.64	1.52
1	A	133	VAL	CA-CB	5.55	1.66	1.54
1	A	141	GLN	CA-C	-5.55	1.38	1.52
1	A	128	VAL	CB-CG2	5.53	1.64	1.52
1	A	119	GLU	CA-CB	-5.53	1.41	1.53
2	B	359	LEU	CB-CG	5.53	1.68	1.52
2	B	279	TYR	CA-C	5.52	1.67	1.52
2	B	363	ARG	CD-NE	5.52	1.55	1.46
2	B	121	LEU	CG-CD2	5.51	1.72	1.51
2	B	225	ASP	C-O	5.50	1.33	1.23
2	B	288	GLN	CG-CD	5.50	1.63	1.51
2	B	334	GLU	CA-CB	5.50	1.66	1.53
2	B	342	HIS	N-CA	-5.50	1.35	1.46
2	B	276	VAL	N-CA	5.48	1.57	1.46
2	B	91	VAL	N-CA	5.48	1.57	1.46
2	B	252	LEU	CG-CD1	5.48	1.72	1.51
2	B	85	ALA	CA-CB	-5.47	1.41	1.52
1	A	136	SER	C-N	-5.47	1.21	1.34
2	B	163	SER	CB-OG	5.46	1.49	1.42
2	B	363	ARG	CA-CB	-5.46	1.42	1.53
1	A	99	LEU	N-CA	5.46	1.57	1.46
1	A	106	VAL	CA-CB	5.46	1.66	1.54
2	B	216	ILE	CB-CG1	5.46	1.69	1.54
2	B	236	ASN	CB-CG	5.46	1.63	1.51
2	B	113	GLY	CA-C	-5.45	1.43	1.51
1	A	48	LEU	CG-CD2	5.45	1.72	1.51
2	B	366	PRO	C-O	5.44	1.34	1.23
1	A	45	ALA	C-O	5.44	1.33	1.23
1	A	174	THR	C-O	5.43	1.33	1.23
2	B	12	PHE	CG-CD1	-5.43	1.30	1.38
2	B	98	ALA	CA-CB	-5.43	1.41	1.52
1	A	5	GLU	CG-CD	5.42	1.60	1.51
1	A	54	PHE	CE1-CZ	-5.42	1.27	1.37
2	B	65	ILE	CA-CB	5.42	1.67	1.54
1	A	47	ALA	N-CA	5.42	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	360	LYS	CE-NZ	5.42	1.62	1.49
2	B	10	GLY	N-CA	5.42	1.54	1.46
2	B	371	LEU	CA-CB	-5.41	1.41	1.53
2	B	343	GLU	CA-C	5.41	1.67	1.52
2	B	63	GLN	CB-CG	-5.41	1.38	1.52
2	B	73	LEU	CA-C	5.40	1.67	1.52
1	A	199	LYS	C-O	5.40	1.33	1.23
2	B	213	LYS	CE-NZ	5.40	1.62	1.49
2	B	15	MET	C-O	5.40	1.33	1.23
2	B	86	HIS	CG-CD2	5.39	1.45	1.35
2	B	102	GLY	CA-C	-5.38	1.43	1.51
2	B	46	ALA	CA-CB	-5.37	1.41	1.52
2	B	272	LYS	N-CA	5.37	1.57	1.46
2	B	17	VAL	C-N	-5.37	1.24	1.34
2	B	12	PHE	CE1-CZ	-5.37	1.27	1.37
2	B	14	GLY	C-O	5.37	1.32	1.23
1	A	234	GLY	N-CA	5.37	1.54	1.46
2	B	115	HIS	C-N	-5.36	1.23	1.33
2	B	59	LEU	CG-CD2	-5.36	1.32	1.51
2	B	312	GLN	CA-C	5.36	1.66	1.52
2	B	81	LEU	CA-CB	5.35	1.66	1.53
2	B	125	LEU	N-CA	-5.35	1.35	1.46
2	B	310	GLY	CA-C	5.35	1.60	1.51
1	A	172	GLY	N-CA	-5.34	1.38	1.46
1	A	239	LYS	CG-CD	5.34	1.70	1.52
2	B	49	LEU	CA-C	5.34	1.66	1.52
2	B	360	LYS	CA-C	-5.34	1.39	1.52
1	A	134	GLU	CD-OE1	5.32	1.31	1.25
1	A	220	VAL	CA-C	5.32	1.66	1.52
2	B	251	GLY	C-O	5.32	1.32	1.23
1	A	99	LEU	C-N	5.32	1.46	1.34
2	B	311	PRO	CG-CD	5.32	1.68	1.50
2	B	389	ASP	CB-CG	5.32	1.62	1.51
2	B	16	TYR	CG-CD2	-5.31	1.32	1.39
2	B	79	ASP	CA-CB	5.31	1.65	1.53
1	A	20	VAL	CA-CB	-5.31	1.43	1.54
1	A	256	ARG	CZ-NH2	5.31	1.40	1.33
2	B	339	LEU	CA-C	5.31	1.66	1.52
2	B	166	LEU	CG-CD1	5.31	1.71	1.51
1	A	176	LEU	CG-CD2	5.29	1.71	1.51
2	B	231	VAL	CA-CB	5.29	1.65	1.54
1	A	95	ILE	N-CA	5.29	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	345	ILE	CB-CG2	5.29	1.69	1.52
1	A	111	ILE	C-O	5.26	1.33	1.23
2	B	330	ASP	CA-C	-5.26	1.39	1.52
2	B	232	GLY	N-CA	-5.25	1.38	1.46
1	A	20	VAL	C-N	-5.25	1.24	1.34
2	B	376	LEU	CG-CD1	5.24	1.71	1.51
1	A	14	ARG	C-O	-5.24	1.13	1.23
2	B	330	ASP	C-O	5.23	1.33	1.23
1	A	112	ASP	CA-C	-5.23	1.39	1.52
2	B	79	ASP	CA-C	5.23	1.66	1.52
2	B	347	PRO	N-CD	5.23	1.55	1.47
2	B	72	THR	C-O	5.23	1.33	1.23
1	A	130	ASP	CG-OD1	5.23	1.37	1.25
2	B	216	ILE	N-CA	5.22	1.56	1.46
2	B	244	PHE	CE1-CZ	5.22	1.47	1.37
2	B	214	ALA	C-N	-5.22	1.22	1.34
1	A	219	GLN	CA-CB	5.22	1.65	1.53
1	A	114	PHE	N-CA	-5.21	1.35	1.46
2	B	63	GLN	CD-OE1	5.21	1.35	1.24
1	A	3	ARG	CB-CG	5.21	1.66	1.52
2	B	38	ASP	C-N	-5.20	1.24	1.34
2	B	12	PHE	CA-C	5.20	1.66	1.52
2	B	348	ALA	C-O	5.20	1.33	1.23
2	B	132	ILE	CA-CB	-5.19	1.43	1.54
2	B	230	CYS	CA-C	5.19	1.66	1.52
2	B	277	GLY	CA-C	5.19	1.60	1.51
1	A	124	ASP	CG-OD2	-5.19	1.13	1.25
1	A	258	PHE	CB-CG	-5.19	1.42	1.51
2	B	347	PRO	C-N	5.18	1.46	1.34
2	B	379	ARG	CZ-NH2	-5.18	1.26	1.33
2	B	221	GLY	N-CA	-5.18	1.38	1.46
2	B	234	GLY	N-CA	-5.17	1.38	1.46
2	B	59	LEU	C-N	-5.17	1.22	1.34
1	A	60	ASP	CG-OD1	5.16	1.37	1.25
2	B	125	LEU	CA-C	5.16	1.66	1.52
1	A	25	LEU	CB-CG	5.16	1.67	1.52
1	A	261	ALA	CA-C	-5.15	1.39	1.52
2	B	41	PHE	CD2-CE2	5.15	1.49	1.39
2	B	319	ILE	C-N	-5.15	1.23	1.33
1	A	77	THR	C-N	-5.15	1.24	1.34
2	B	57	THR	CA-C	5.14	1.66	1.52
2	B	86	HIS	C-N	-5.14	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	320	GLY	C-N	5.14	1.45	1.34
2	B	333	LEU	N-CA	5.14	1.56	1.46
2	B	5	LEU	CA-CB	5.14	1.65	1.53
2	B	168	ASP	CA-CB	-5.14	1.42	1.53
2	B	188	LEU	CA-C	5.13	1.66	1.52
2	B	207	MET	N-CA	-5.13	1.36	1.46
2	B	215	GLN	CG-CD	-5.13	1.39	1.51
1	A	59	ALA	CA-CB	-5.13	1.41	1.52
2	B	236	ASN	CA-CB	5.13	1.66	1.53
2	B	360	LYS	N-CA	5.13	1.56	1.46
2	B	89	ASN	N-CA	-5.11	1.36	1.46
1	A	209	LEU	C-O	5.11	1.33	1.23
2	B	294	ILE	CA-CB	-5.11	1.43	1.54
2	B	60	THR	CA-C	5.10	1.66	1.52
2	B	253	ILE	N-CA	-5.10	1.36	1.46
2	B	381	ASP	CA-CB	5.10	1.65	1.53
2	B	148	ARG	CZ-NH2	5.09	1.39	1.33
1	A	249	LYS	CG-CD	5.09	1.69	1.52
1	A	132	PRO	C-O	5.09	1.33	1.23
2	B	353	HIS	CB-CG	-5.09	1.40	1.50
2	B	284	ALA	N-CA	5.08	1.56	1.46
1	A	169	TYR	CD1-CE1	5.08	1.47	1.39
2	B	348	ALA	C-N	-5.08	1.22	1.34
1	A	114	PHE	CG-CD2	5.07	1.46	1.38
2	B	287	MET	CA-CB	5.07	1.65	1.53
2	B	387	VAL	CA-CB	-5.07	1.44	1.54
2	B	59	LEU	C-O	5.07	1.32	1.23
2	B	138	ASP	CA-C	5.07	1.66	1.52
1	A	137	ALA	N-CA	5.06	1.56	1.46
1	A	170	GLY	N-CA	-5.06	1.38	1.46
2	B	152	MET	CB-CG	5.06	1.67	1.51
2	B	266	GLU	CD-OE1	-5.06	1.20	1.25
2	B	127	GLY	CA-C	5.06	1.59	1.51
1	A	263	LYS	CE-NZ	-5.05	1.36	1.49
2	B	145	ASN	C-O	5.05	1.32	1.23
2	B	357	HIS	CB-CG	5.05	1.59	1.50
2	B	37	LYS	CA-C	5.05	1.66	1.52
1	A	32	GLN	CB-CG	5.04	1.66	1.52
1	A	141	GLN	N-CA	5.04	1.56	1.46
2	B	100	ARG	CZ-NH1	-5.04	1.26	1.33
2	B	219	LYS	CE-NZ	5.04	1.61	1.49
2	B	87	LYS	N-CA	5.04	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	ARG	CA-CB	5.03	1.65	1.53
1	A	102	TYR	C-O	5.03	1.32	1.23
2	B	233	GLY	CA-C	-5.02	1.43	1.51
2	B	89	ASN	CG-ND2	5.02	1.45	1.32
1	A	218	GLU	CD-OE2	5.01	1.31	1.25
2	B	267	HIS	CB-CG	5.01	1.59	1.50
2	B	271	LEU	CG-CD2	5.01	1.70	1.51
2	B	78	GLU	N-CA	5.01	1.56	1.46
1	A	31	GLU	CD-OE1	5.00	1.31	1.25
2	B	213	LYS	C-N	5.00	1.45	1.34

All (845) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	55	ARG	NE-CZ-NH1	35.94	138.27	120.30
2	B	291	ASP	CB-CG-OD1	-34.65	87.12	118.30
2	B	55	ARG	NE-CZ-NH2	-29.76	105.42	120.30
1	A	140	ARG	NE-CZ-NH1	-28.07	106.26	120.30
2	B	222	ARG	NE-CZ-NH2	-26.74	106.93	120.30
2	B	222	ARG	NE-CZ-NH1	25.71	133.16	120.30
2	B	100	ARG	NE-CZ-NH1	25.32	132.96	120.30
1	A	225	ARG	NE-CZ-NH1	19.90	130.25	120.30
2	B	204	PHE	CB-CG-CD2	-19.72	107.00	120.80
2	B	9	PHE	CB-CG-CD2	-19.33	107.27	120.80
2	B	324	TYR	CZ-CE2-CD2	19.21	137.09	119.80
2	B	315	TYR	CB-CG-CD2	18.96	132.38	121.00
2	B	394	ARG	NE-CZ-NH1	-18.89	110.85	120.30
2	B	202	ARG	NE-CZ-NH1	-18.74	110.93	120.30
2	B	291	ASP	CB-CG-OD2	18.69	135.12	118.30
2	B	52	TYR	CB-CG-CD1	18.61	132.17	121.00
2	B	379	ARG	CD-NE-CZ	-18.61	97.55	123.60
1	A	107	PHE	CB-CG-CD1	18.13	133.49	120.80
2	B	79	ASP	CB-CG-OD1	17.58	134.12	118.30
2	B	315	TYR	CD1-CE1-CZ	17.57	135.61	119.80
2	B	286	MET	CA-CB-CG	17.38	142.85	113.30
2	B	330	ASP	CB-CG-OD1	17.04	133.64	118.30
2	B	204	PHE	CD1-CE1-CZ	-16.95	99.76	120.10
2	B	321	ARG	NE-CZ-NH2	-16.39	112.11	120.30
1	A	225	ARG	NE-CZ-NH2	-16.24	112.18	120.30
1	A	140	ARG	NE-CZ-NH2	16.11	128.35	120.30
2	B	368	LYS	O-C-N	16.03	148.35	122.70
2	B	339	LEU	CB-CG-CD1	15.71	137.70	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	97	LEU	CB-CG-CD2	15.60	137.51	111.00
2	B	323	ASP	CB-CG-OD2	15.37	132.13	118.30
2	B	324	TYR	CG-CD1-CE1	15.12	133.40	121.30
2	B	255	VAL	CG1-CB-CG2	14.96	134.84	110.90
2	B	70	ARG	O-C-N	14.54	145.97	122.70
2	B	334	GLU	OE1-CD-OE2	-14.51	105.89	123.30
2	B	353	HIS	O-C-N	-14.44	99.59	122.70
2	B	243	ASP	CB-CG-OD2	14.38	131.25	118.30
2	B	47	ASP	CB-CG-OD2	14.27	131.14	118.30
2	B	8	TYR	CG-CD1-CE1	14.16	132.62	121.30
2	B	328	THR	O-C-N	14.15	145.34	122.70
2	B	316	LEU	CB-CG-CD2	13.74	134.36	111.00
2	B	52	TYR	CD1-CG-CD2	-13.38	103.18	117.90
2	B	304	LEU	CB-CG-CD2	13.33	133.66	111.00
2	B	348	ALA	O-C-N	13.27	143.92	122.70
1	A	127	LEU	O-C-N	13.16	143.75	122.70
2	B	204	PHE	CE1-CZ-CE2	13.05	143.50	120.00
2	B	32	PHE	CB-CG-CD1	-13.03	111.68	120.80
1	A	107	PHE	CB-CG-CD2	-12.96	111.73	120.80
2	B	351	SER	O-C-N	12.92	143.37	122.70
2	B	23	PRO	O-C-N	12.73	143.07	122.70
2	B	297	SER	N-CA-CB	-12.68	91.48	110.50
2	B	196	PRO	O-C-N	12.57	142.81	122.70
2	B	47	ASP	CB-CG-OD1	-12.54	107.01	118.30
1	A	125	SER	O-C-N	12.52	142.73	122.70
2	B	54	GLY	O-C-N	-12.52	102.68	122.70
2	B	86	HIS	O-C-N	12.45	142.62	122.70
2	B	375	ASN	O-C-N	-12.40	102.85	122.70
1	A	107	PHE	CG-CD1-CE1	12.37	134.40	120.80
1	A	169	TYR	CB-CG-CD1	12.26	128.36	121.00
2	B	305	ASP	CB-CG-OD1	11.99	129.09	118.30
1	A	124	ASP	CB-CG-OD2	11.90	129.01	118.30
2	B	203	GLU	O-C-N	11.90	141.74	122.70
1	A	100	LEU	CB-CG-CD2	11.74	130.96	111.00
2	B	316	LEU	CB-CG-CD1	-11.71	91.09	111.00
2	B	204	PHE	CG-CD2-CE2	-11.65	107.98	120.80
1	A	56	ASP	CB-CG-OD2	11.63	128.77	118.30
2	B	8	TYR	CZ-CE2-CD2	11.61	130.25	119.80
2	B	59	LEU	O-C-N	11.55	141.18	122.70
2	B	252	LEU	O-C-N	-11.50	104.29	122.70
1	A	139	PHE	CB-CG-CD1	-11.44	112.80	120.80
2	B	12	PHE	CG-CD2-CE2	-11.42	108.24	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	29	GLU	O-C-N	-11.40	104.46	122.70
2	B	321	ARG	CA-C-O	-11.38	96.20	120.10
2	B	324	TYR	CD1-CE1-CZ	-11.38	109.56	119.80
2	B	243	ASP	O-C-N	11.36	140.88	122.70
2	B	204	PHE	CD1-CG-CD2	11.33	133.03	118.30
2	B	363	ARG	NE-CZ-NH1	11.26	125.93	120.30
2	B	183	THR	CA-CB-CG2	-11.19	96.73	112.40
2	B	339	LEU	O-C-N	11.18	140.58	122.70
2	B	18	PRO	O-C-N	-11.01	105.09	122.70
2	B	261	GLY	O-C-N	11.00	140.30	122.70
2	B	7	PRO	O-C-N	10.99	140.29	122.70
2	B	272	LYS	CB-CG-CD	10.98	140.16	111.60
2	B	375	ASN	CA-C-O	10.92	143.04	120.10
2	B	225	ASP	CB-CG-OD1	10.91	128.12	118.30
2	B	119	SER	N-CA-CB	-10.86	94.21	110.50
1	A	47	ALA	N-CA-CB	10.85	125.29	110.10
2	B	105	GLU	O-C-N	10.85	140.06	122.70
2	B	186	TYR	CZ-CE2-CD2	10.85	129.56	119.80
2	B	263	GLU	OE1-CD-OE2	10.85	136.31	123.30
2	B	60	THR	O-C-N	10.82	140.01	122.70
2	B	254	GLY	O-C-N	-10.79	105.43	122.70
1	A	139	PHE	CD1-CG-CD2	10.79	132.33	118.30
2	B	263	GLU	CG-CD-OE2	-10.76	96.79	118.30
2	B	354	ALA	N-CA-CB	10.75	125.15	110.10
2	B	211	GLU	OE1-CD-OE2	-10.71	110.45	123.30
1	A	11	LEU	CB-CG-CD2	10.68	129.16	111.00
2	B	152	MET	CG-SD-CE	-10.63	83.18	100.20
2	B	315	TYR	CE1-CZ-OH	10.61	148.74	120.10
1	A	171	ARG	NE-CZ-NH1	10.59	125.59	120.30
2	B	372	LEU	N-CA-CB	10.59	131.57	110.40
2	B	315	TYR	CG-CD2-CE2	10.56	129.75	121.30
2	B	19	GLN	O-C-N	10.52	139.53	122.70
2	B	12	PHE	CD1-CE1-CZ	-10.49	107.52	120.10
2	B	9	PHE	O-C-N	10.40	140.88	123.20
2	B	360	LYS	O-C-N	-10.38	106.09	122.70
2	B	341	ARG	NE-CZ-NH2	-10.30	115.15	120.30
2	B	379	ARG	NE-CZ-NH2	10.27	125.44	120.30
2	B	15	MET	CB-CG-SD	10.22	143.07	112.40
2	B	52	TYR	CG-CD1-CE1	10.21	129.47	121.30
2	B	333	LEU	CB-CG-CD2	-10.19	93.68	111.00
2	B	97	LEU	CA-CB-CG	-10.18	91.89	115.30
2	B	106	ILE	O-C-N	-10.17	106.43	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	12	PHE	CD1-CG-CD2	10.15	131.50	118.30
2	B	316	LEU	CA-C-O	-10.14	98.81	120.10
2	B	347	PRO	CA-C-O	10.12	144.48	120.20
2	B	58	ALA	N-CA-CB	-10.00	96.10	110.10
2	B	194	PRO	O-C-N	-10.00	106.70	122.70
2	B	74	TYR	CZ-CE2-CD2	9.98	128.78	119.80
2	B	341	ARG	O-C-N	-9.95	106.78	122.70
2	B	106	ILE	CA-C-O	9.93	140.94	120.10
2	B	30	GLU	O-C-N	9.87	138.49	122.70
2	B	122	ALA	O-C-N	9.86	138.48	122.70
2	B	29	GLU	CA-C-O	9.86	140.81	120.10
2	B	394	ARG	NH1-CZ-NH2	9.83	130.21	119.40
2	B	233	GLY	O-C-N	-9.83	106.50	123.20
1	A	7	LEU	CB-CG-CD2	-9.82	94.30	111.00
2	B	212	THR	CA-CB-OG1	9.80	129.58	109.00
2	B	6	ASN	CA-C-N	9.79	144.51	117.10
1	A	163	LEU	CB-CG-CD2	9.78	127.63	111.00
2	B	376	LEU	CB-CG-CD2	-9.78	94.37	111.00
2	B	370	GLN	CA-CB-CG	9.77	134.90	113.40
2	B	12	PHE	CB-CG-CD1	-9.76	113.97	120.80
2	B	49	LEU	CA-C-O	-9.72	99.68	120.10
2	B	226	ALA	N-CA-CB	9.65	123.61	110.10
2	B	336	PHE	O-C-N	9.65	138.14	122.70
2	B	3	THR	O-C-N	-9.64	107.27	122.70
2	B	77	ARG	NE-CZ-NH1	-9.62	115.49	120.30
2	B	17	VAL	CA-CB-CG2	9.62	125.33	110.90
2	B	91	VAL	CA-CB-CG1	9.62	125.33	110.90
2	B	98	ALA	N-CA-CB	9.59	123.53	110.10
2	B	9	PHE	CD1-CG-CD2	9.59	130.76	118.30
1	A	191	LEU	N-CA-C	9.53	136.72	111.00
2	B	213	LYS	CD-CE-NZ	-9.50	89.84	111.70
1	A	196	LEU	CB-CG-CD1	9.45	127.06	111.00
2	B	12	PHE	CB-CG-CD2	-9.43	114.20	120.80
2	B	368	LYS	CA-C-O	-9.42	100.31	120.10
2	B	93	GLY	CA-C-O	-9.42	103.64	120.60
2	B	319	ILE	CG1-CB-CG2	-9.36	90.82	111.40
2	B	258	GLY	CA-C-O	9.35	137.43	120.60
2	B	21	LEU	O-C-N	-9.33	107.77	122.70
2	B	244	PHE	CB-CG-CD2	-9.31	114.28	120.80
2	B	74	TYR	CG-CD1-CE1	9.27	128.72	121.30
2	B	128	LEU	O-C-N	-9.24	107.91	122.70
1	A	97	ILE	O-C-N	-9.21	107.53	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	6	ASN	CA-C-O	-9.20	100.78	120.10
2	B	78	GLU	O-C-N	-9.19	108.00	122.70
2	B	79	ASP	O-C-N	9.19	137.40	122.70
2	B	12	PHE	CE1-CZ-CE2	9.16	136.49	120.00
2	B	18	PRO	CA-C-O	9.14	142.14	120.20
2	B	230	CYS	O-C-N	9.13	137.32	122.70
2	B	215	GLN	CG-CD-OE1	9.13	139.86	121.60
2	B	314	ALA	O-C-N	-9.13	108.09	122.70
2	B	347	PRO	O-C-N	-9.12	108.10	122.70
1	A	13	ASP	CB-CG-OD1	9.12	126.51	118.30
2	B	373	VAL	CA-CB-CG2	9.12	124.58	110.90
2	B	284	ALA	CA-C-O	9.10	139.21	120.10
2	B	286	MET	CB-CG-SD	-9.08	85.15	112.40
2	B	374	VAL	CA-CB-CG1	9.07	124.51	110.90
2	B	202	ARG	NH1-CZ-NH2	9.07	129.38	119.40
1	A	145	ARG	NE-CZ-NH2	-9.07	115.77	120.30
2	B	69	THR	CA-CB-CG2	9.04	125.06	112.40
2	B	243	ASP	OD1-CG-OD2	-9.03	106.15	123.30
1	A	4	TYR	CB-CG-CD2	-9.01	115.59	121.00
2	B	281	GLY	CA-C-O	9.00	136.81	120.60
2	B	55	ARG	O-C-N	-9.00	104.00	121.10
1	A	145	ARG	NE-CZ-NH1	9.00	124.80	120.30
2	B	150	ARG	NE-CZ-NH2	-8.94	115.83	120.30
2	B	202	ARG	O-C-N	-8.95	108.39	122.70
2	B	206[A]	ARG	NE-CZ-NH2	-8.92	115.84	120.30
2	B	206[B]	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	148	ILE	CG1-CB-CG2	-8.92	91.78	111.40
2	B	9	PHE	CA-C-N	-8.91	98.38	116.20
1	A	139	PHE	CE1-CZ-CE2	8.88	135.99	120.00
2	B	336	PHE	CG-CD2-CE2	-8.88	111.03	120.80
2	B	308	SER	CA-C-N	8.85	136.66	117.20
2	B	298	TYR	CA-CB-CG	-8.84	96.61	113.40
1	A	46	ASP	CB-CG-OD2	8.83	126.25	118.30
2	B	33	VAL	CG1-CB-CG2	8.83	125.03	110.90
2	B	360	LYS	CA-C-N	8.82	136.61	117.20
2	B	32	PHE	CG-CD1-CE1	-8.82	111.10	120.80
2	B	133	TYR	CZ-CE2-CD2	-8.81	111.88	119.80
2	B	211	GLU	CG-CD-OE1	8.80	135.90	118.30
2	B	295	GLU	CG-CD-OE2	8.77	135.84	118.30
2	B	203	GLU	CA-C-O	-8.76	101.71	120.10
2	B	311	PRO	O-C-N	-8.75	108.71	122.70
2	B	117	VAL	O-C-N	-8.74	108.71	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	THR	CA-CB-CG2	-8.74	100.17	112.40
2	B	59	LEU	CA-C-O	-8.71	101.80	120.10
2	B	379	ARG	O-C-N	-8.71	108.39	123.20
2	B	380	GLY	N-CA-C	8.70	134.86	113.10
2	B	62	CYS	CA-CB-SG	-8.70	98.34	114.00
1	A	3	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	141	GLN	O-C-N	-8.66	108.85	122.70
2	B	241	PHE	CA-C-O	8.64	138.25	120.10
1	A	7	LEU	CB-CG-CD1	8.64	125.69	111.00
1	A	100	LEU	CB-CG-CD1	-8.63	96.33	111.00
2	B	99	LYS	CD-CE-NZ	-8.57	91.99	111.70
2	B	269	ALA	CB-CA-C	-8.56	97.25	110.10
2	B	105	GLU	N-CA-CB	8.56	126.00	110.60
2	B	66	THR	CA-CB-OG1	8.55	126.96	109.00
2	B	379	ARG	NE-CZ-NH1	-8.55	116.03	120.30
1	A	121	VAL	C-N-CA	-8.51	104.43	122.30
2	B	324	TYR	CG-CD2-CE2	-8.51	114.49	121.30
2	B	368	LYS	CD-CE-NZ	-8.49	92.17	111.70
1	A	139	PHE	CB-CG-CD2	-8.47	114.87	120.80
2	B	282	MET	O-C-N	8.46	136.23	122.70
2	B	231	VAL	O-C-N	-8.46	108.82	123.20
2	B	45	PHE	CD1-CE1-CZ	-8.45	109.96	120.10
1	A	163	LEU	CB-CG-CD1	-8.45	96.64	111.00
1	A	96	PRO	N-CA-CB	8.44	113.43	103.30
1	A	139	PHE	O-C-N	8.43	136.18	122.70
2	B	193	GLY	O-C-N	-8.42	105.10	121.10
1	A	176	LEU	CB-CG-CD2	-8.41	96.71	111.00
2	B	326	SER	N-CA-CB	8.39	123.08	110.50
2	B	12	PHE	O-C-N	8.38	137.46	123.20
2	B	350	GLU	O-C-N	-8.37	109.31	122.70
2	B	6	ASN	N-CA-C	8.37	133.59	111.00
2	B	193	GLY	CA-C-O	8.35	135.64	120.60
1	A	4	TYR	CD1-CE1-CZ	-8.33	112.30	119.80
2	B	103	LYS	CD-CE-NZ	-8.33	92.55	111.70
2	B	17	VAL	O-C-N	8.31	136.90	121.10
2	B	315	TYR	CZ-CE2-CD2	-8.30	112.33	119.80
2	B	264	THR	CA-CB-CG2	-8.30	100.78	112.40
2	B	373	VAL	CA-CB-CG1	-8.27	98.50	110.90
2	B	59	LEU	CB-CG-CD2	-8.26	96.95	111.00
2	B	331	GLU	N-CA-CB	8.26	125.47	110.60
2	B	61	LYS	N-CA-CB	-8.21	95.82	110.60
2	B	41	PHE	CB-CG-CD2	8.20	126.54	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	ASP	CB-CG-OD1	-8.15	110.96	118.30
2	B	76	LYS	CA-C-O	8.14	137.19	120.10
2	B	56	PRO	O-C-N	-8.13	109.69	122.70
1	A	175	TYR	CD1-CE1-CZ	8.13	127.11	119.80
2	B	275	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	A	153	ILE	CA-C-O	8.12	137.16	120.10
2	B	371	LEU	CB-CG-CD1	-8.13	97.19	111.00
2	B	345	ILE	CA-CB-CG1	8.12	126.43	111.00
2	B	73	LEU	CB-CG-CD1	-8.11	97.22	111.00
1	A	48	LEU	CA-C-O	8.10	137.12	120.10
2	B	8	TYR	CB-CG-CD1	8.09	125.85	121.00
2	B	315	TYR	CB-CG-CD1	-8.08	116.15	121.00
2	B	370	GLN	O-C-N	8.08	135.63	122.70
2	B	86	HIS	CA-C-O	-8.07	103.14	120.10
2	B	327	ILE	O-C-N	-8.06	109.80	122.70
2	B	242	ALA	O-C-N	-8.04	109.84	122.70
2	B	355	LEU	CB-CG-CD2	-8.02	97.37	111.00
2	B	271	LEU	N-CA-CB	8.01	126.42	110.40
2	B	280	PHE	O-C-N	-8.01	109.58	123.20
2	B	100	ARG	NH1-CZ-NH2	-8.00	110.60	119.40
2	B	372	LEU	CB-CG-CD2	-7.99	97.41	111.00
2	B	231	VAL	CA-CB-CG1	-7.99	98.92	110.90
1	A	41	ILE	CG1-CB-CG2	-7.97	93.86	111.40
2	B	67	ALA	O-C-N	7.97	136.75	123.20
2	B	9	PHE	CG-CD2-CE2	-7.96	112.04	120.80
2	B	305	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	A	139	PHE	CD1-CE1-CZ	-7.95	110.56	120.10
2	B	380	GLY	CA-C-O	7.93	134.87	120.60
2	B	59	LEU	CA-CB-CG	-7.91	97.12	115.30
2	B	376	LEU	CA-CB-CG	-7.90	97.14	115.30
2	B	56	PRO	C-N-CA	7.89	141.43	121.70
2	B	49	LEU	O-C-N	7.89	135.32	122.70
2	B	161	SER	CB-CA-C	-7.88	95.12	110.10
2	B	251	GLY	CA-C-O	-7.87	106.44	120.60
2	B	331	GLU	OE1-CD-OE2	-7.85	113.88	123.30
2	B	15	MET	CA-CB-CG	7.84	126.63	113.30
2	B	336	PHE	CB-CG-CD2	-7.84	115.31	120.80
2	B	119	SER	O-C-N	7.82	135.22	122.70
1	A	11	LEU	CA-CB-CG	-7.82	97.31	115.30
2	B	357	HIS	O-C-N	-7.79	110.24	122.70
2	B	181	TYR	CB-CG-CD1	-7.79	116.33	121.00
2	B	52	TYR	CZ-CE2-CD2	7.78	126.81	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	348	ALA	CA-C-O	-7.78	103.75	120.10
2	B	69	THR	O-C-N	-7.78	110.25	122.70
2	B	100	ARG	CD-NE-CZ	7.78	134.49	123.60
2	B	100	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	76	VAL	CA-CB-CG2	-7.74	99.29	110.90
2	B	330	ASP	OD1-CG-OD2	-7.73	108.61	123.30
2	B	343	GLU	OE1-CD-OE2	-7.72	114.03	123.30
2	B	6	ASN	N-CA-CB	-7.71	96.72	110.60
2	B	236	ASN	O-C-N	7.70	135.02	122.70
2	B	5	LEU	CA-C-O	7.70	136.26	120.10
2	B	70	ARG	CA-C-O	-7.70	103.94	120.10
2	B	332	ALA	O-C-N	7.69	135.01	122.70
2	B	91	VAL	CA-CB-CG2	-7.69	99.36	110.90
2	B	361	MET	CG-SD-CE	7.69	112.50	100.20
1	A	121	VAL	O-C-N	7.68	136.26	123.20
1	A	139	PHE	CG-CD2-CE2	-7.68	112.36	120.80
2	B	78	GLU	CG-CD-OE1	-7.67	102.95	118.30
2	B	328	THR	CA-C-O	-7.67	104.00	120.10
2	B	71	THR	O-C-N	7.66	134.95	122.70
2	B	275	ARG	O-C-N	7.66	134.95	122.70
1	A	136	SER	O-C-N	7.64	134.93	122.70
2	B	203	GLU	OE1-CD-OE2	-7.63	114.14	123.30
2	B	264	THR	O-C-N	7.63	136.18	123.20
2	B	57	THR	C-N-CA	-7.61	102.67	121.70
2	B	291	ASP	OD1-CG-OD2	7.61	137.75	123.30
2	B	373	VAL	O-C-N	-7.59	110.56	122.70
1	A	140	ARG	CD-NE-CZ	-7.58	112.98	123.60
1	A	134	GLU	CG-CD-OE1	7.57	133.43	118.30
2	B	228	ILE	CA-CB-CG1	-7.56	96.64	111.00
2	B	57	THR	N-CA-CB	7.56	124.66	110.30
2	B	323	ASP	OD1-CG-OD2	-7.55	108.94	123.30
2	B	194	PRO	CA-C-N	7.54	133.78	117.20
2	B	281	GLY	N-CA-C	7.54	131.94	113.10
2	B	343	GLU	CG-CD-OE1	7.52	133.34	118.30
2	B	58	ALA	O-C-N	7.50	134.70	122.70
2	B	295	GLU	OE1-CD-OE2	-7.50	114.30	123.30
2	B	32	PHE	O-C-N	-7.49	110.72	122.70
2	B	194	PRO	CA-N-CD	7.49	122.18	111.70
2	B	41	PHE	CG-CD2-CE2	7.48	129.03	120.80
2	B	367	GLU	N-CA-C	7.48	131.19	111.00
1	A	98	GLY	O-C-N	7.47	134.66	122.70
2	B	121	LEU	O-C-N	-7.45	110.77	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	GLN	CA-C-O	7.45	135.74	120.10
2	B	314	ALA	CA-C-N	7.45	133.58	117.20
2	B	339	LEU	CA-C-O	-7.44	104.47	120.10
2	B	343	GLU	O-C-N	7.44	135.85	123.20
1	A	114	PHE	CG-CD1-CE1	7.44	128.98	120.80
2	B	282	MET	CA-CB-CG	-7.43	100.67	113.30
2	B	362	MET	CA-CB-CG	-7.42	100.69	113.30
2	B	353	HIS	C-N-CA	7.42	140.24	121.70
1	A	131	VAL	CA-CB-CG2	-7.36	99.87	110.90
2	B	321	ARG	CA-C-N	7.34	133.34	117.20
1	A	100	LEU	O-C-N	7.33	134.43	122.70
1	A	197	ILE	CG1-CB-CG2	-7.33	95.28	111.40
1	A	142	ALA	CB-CA-C	-7.32	99.12	110.10
2	B	186	TYR	CG-CD2-CE2	-7.32	115.45	121.30
2	B	81	LEU	CB-CG-CD1	7.31	123.42	111.00
2	B	159	VAL	CA-CB-CG1	7.31	121.86	110.90
2	B	78	GLU	CG-CD-OE2	7.30	132.91	118.30
2	B	335	ALA	O-C-N	7.28	134.35	122.70
2	B	361	MET	CA-CB-CG	-7.28	100.92	113.30
2	B	207	MET	CB-CG-SD	7.28	134.24	112.40
2	B	221	GLY	O-C-N	7.28	134.34	122.70
2	B	207	MET	CG-SD-CE	-7.27	88.57	100.20
2	B	258	GLY	O-C-N	-7.24	110.89	123.20
2	B	353	HIS	CA-C-N	7.24	133.13	117.20
2	B	51	ASN	O-C-N	-7.24	111.12	122.70
2	B	188	LEU	C-N-CA	-7.24	107.11	122.30
2	B	207	MET	CA-C-O	-7.24	104.91	120.10
2	B	252	LEU	CA-C-N	7.23	133.10	117.20
1	A	259	VAL	CA-CB-CG2	-7.22	100.07	110.90
2	B	90	GLN	CG-CD-OE1	-7.22	107.16	121.60
2	B	200	ILE	O-C-N	7.19	134.21	122.70
2	B	358	ALA	O-C-N	7.17	134.17	122.70
2	B	287	MET	CG-SD-CE	7.17	111.67	100.20
2	B	45	PHE	CZ-CE2-CD2	7.16	128.69	120.10
2	B	71	THR	CA-C-O	-7.16	105.08	120.10
2	B	196	PRO	CA-CB-CG	-7.15	90.41	104.00
1	A	159	ASP	CB-CG-OD2	7.12	124.71	118.30
2	B	32	PHE	CB-CG-CD2	7.10	125.77	120.80
1	A	148	ILE	CB-CA-C	-7.09	97.41	111.60
2	B	158	PRO	CB-CA-C	-7.09	94.28	112.00
2	B	231	VAL	CA-C-O	7.09	134.99	120.10
2	B	360	LYS	C-N-CA	7.08	139.40	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	381	ASP	CB-CG-OD2	7.07	124.66	118.30
2	B	92	LEU	CB-CG-CD1	-7.06	98.99	111.00
2	B	52	TYR	CE1-CZ-CE2	-7.06	108.51	119.80
1	A	114	PHE	CB-CG-CD2	-7.06	115.86	120.80
1	A	131	VAL	CG1-CB-CG2	-7.05	99.61	110.90
2	B	52	TYR	CD1-CE1-CZ	7.05	126.14	119.80
2	B	373	VAL	CA-C-N	7.02	132.65	117.20
1	A	219	GLN	CG-CD-OE1	-7.02	107.57	121.60
2	B	271	LEU	CA-CB-CG	7.01	131.43	115.30
2	B	71	THR	CA-CB-CG2	-7.01	102.59	112.40
2	B	75	LEU	N-CA-CB	7.00	124.41	110.40
1	A	169	TYR	CZ-CE2-CD2	6.98	126.08	119.80
2	B	77	ARG	NH1-CZ-NH2	6.96	127.06	119.40
2	B	85	ALA	O-C-N	-6.96	111.56	122.70
2	B	337	LYS	O-C-N	-6.96	111.56	122.70
1	A	18	ALA	N-CA-CB	-6.92	100.41	110.10
2	B	28	LEU	CB-CG-CD1	-6.91	99.25	111.00
1	A	63	THR	CA-CB-CG2	-6.91	102.73	112.40
2	B	195	HIS	CG-ND1-CE1	6.91	117.87	108.20
1	A	37	ILE	CG1-CB-CG2	-6.89	96.23	111.40
1	A	93	PRO	N-CD-CG	-6.89	92.86	103.20
2	B	27	GLN	O-C-N	6.89	133.72	122.70
2	B	182	GLU	CG-CD-OE2	6.88	132.05	118.30
1	A	114	PHE	CB-CG-CD1	6.86	125.60	120.80
2	B	149	MET	CA-CB-CG	-6.86	101.64	113.30
1	A	143	ALA	CB-CA-C	-6.85	99.83	110.10
2	B	315	TYR	CE1-CZ-CE2	-6.84	108.86	119.80
2	B	205	GLN	CG-CD-OE1	-6.84	107.92	121.60
1	A	140	ARG	CG-CD-NE	-6.83	97.45	111.80
2	B	38	ASP	CB-CG-OD1	-6.83	112.16	118.30
2	B	222	ARG	CD-NE-CZ	6.81	133.13	123.60
2	B	248	THR	CA-CB-CG2	-6.79	102.89	112.40
1	A	229	ALA	N-CA-C	6.79	129.32	111.00
2	B	9	PHE	C-N-CA	-6.77	108.08	122.30
2	B	206[A]	ARG	CD-NE-CZ	6.77	133.07	123.60
2	B	206[B]	ARG	CD-NE-CZ	6.77	133.07	123.60
1	A	91	LYS	CD-CE-NZ	-6.74	96.21	111.70
2	B	316	LEU	CA-CB-CG	-6.71	99.86	115.30
1	A	63	THR	OG1-CB-CG2	-6.71	94.56	110.00
2	B	351	SER	CA-C-O	-6.71	106.01	120.10
2	B	45	PHE	CA-C-O	-6.70	106.02	120.10
2	B	285	PRO	CA-C-N	6.70	131.95	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	PRO	O-C-N	-6.70	111.98	122.70
2	B	198	PRO	O-C-N	-6.69	112.00	122.70
2	B	5	LEU	CB-CG-CD1	-6.68	99.64	111.00
2	B	45	PHE	O-C-N	6.68	133.39	122.70
1	A	175	TYR	CG-CD2-CE2	6.68	126.64	121.30
2	B	241	PHE	N-CA-C	6.66	128.98	111.00
2	B	270	PRO	O-C-N	-6.66	112.05	122.70
1	A	136	SER	CA-C-O	-6.65	106.13	120.10
1	A	52	VAL	CG1-CB-CG2	-6.63	100.29	110.90
2	B	85	ALA	CB-CA-C	6.63	120.04	110.10
1	A	116	ALA	O-C-N	-6.63	112.10	122.70
2	B	30	GLU	CG-CD-OE2	6.62	131.53	118.30
2	B	227	VAL	O-C-N	-6.59	112.15	122.70
2	B	214	ALA	O-C-N	6.59	133.25	122.70
2	B	361	MET	N-CA-CB	6.58	122.45	110.60
1	A	145	ARG	O-C-N	-6.58	112.17	122.70
2	B	324	TYR	CB-CG-CD1	6.58	124.94	121.00
1	A	4	TYR	CB-CA-C	-6.57	97.26	110.40
2	B	315	TYR	OH-CZ-CE2	-6.57	102.37	120.10
2	B	196	PRO	N-CD-CG	-6.55	93.37	103.20
2	B	324	TYR	OH-CZ-CE2	6.55	137.78	120.10
2	B	134	MET	C-N-CA	-6.53	108.59	122.30
2	B	196	PRO	CA-C-O	-6.53	104.53	120.20
2	B	371	LEU	CB-CG-CD2	6.53	122.10	111.00
2	B	114	GLN	N-CA-CB	6.53	122.35	110.60
2	B	77	ARG	CG-CD-NE	6.52	125.50	111.80
1	A	145	ARG	CA-C-N	6.52	131.54	117.20
1	A	107	PHE	CE1-CZ-CE2	-6.51	108.28	120.00
2	B	12	PHE	C-N-CA	-6.51	108.62	122.30
2	B	82	HIS	C-N-CA	6.51	135.98	122.30
2	B	90	GLN	OE1-CD-NE2	6.50	136.86	121.90
1	A	175	TYR	CG-CD1-CE1	-6.50	116.10	121.30
2	B	64	ASN	N-CA-CB	6.50	122.30	110.60
2	B	377	SER	N-CA-CB	-6.50	100.75	110.50
2	B	94	GLN	CA-CB-CG	-6.49	99.12	113.40
2	B	364	GLU	CA-CB-CG	6.49	127.67	113.40
2	B	357	HIS	CB-CG-ND1	-6.49	106.98	123.20
1	A	49[A]	GLU	C-N-CA	-6.47	105.52	121.70
1	A	49[B]	GLU	C-N-CA	-6.47	105.52	121.70
1	A	142	ALA	O-C-N	-6.47	112.35	122.70
2	B	362	MET	CA-C-O	-6.46	106.52	120.10
2	B	201	VAL	CG1-CB-CG2	-6.46	100.57	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	VAL	N-CA-CB	6.46	125.70	111.50
2	B	183	THR	CA-CB-OG1	6.45	122.55	109.00
2	B	242	ALA	N-CA-C	6.45	128.40	111.00
2	B	283	LYS	O-C-N	6.44	133.01	122.70
2	B	129	LYS	CD-CE-NZ	6.41	126.44	111.70
2	B	234	GLY	N-CA-C	6.41	129.11	113.10
2	B	325	VAL	O-C-N	-6.40	112.45	122.70
1	A	144	LEU	CB-CG-CD1	-6.40	100.11	111.00
1	A	219	GLN	O-C-N	6.39	132.93	122.70
2	B	256	GLU	CA-C-N	6.39	134.98	117.10
1	A	48	LEU	CA-C-N	-6.36	103.22	117.20
2	B	290	ALA	C-N-CA	6.36	137.59	121.70
2	B	284	ALA	O-C-N	-6.35	109.03	121.10
2	B	245	ILE	CA-C-N	6.35	131.16	117.20
2	B	7	PRO	CA-C-N	-6.33	103.26	117.20
1	A	126	VAL	CA-C-O	6.32	133.37	120.10
1	A	107	PHE	CZ-CE2-CD2	6.32	127.68	120.10
2	B	320	GLY	O-C-N	-6.31	112.60	122.70
2	B	283	LYS	CD-CE-NZ	-6.30	97.21	111.70
1	A	97	ILE	CA-C-O	6.29	133.32	120.10
2	B	236	ASN	CA-C-N	-6.29	103.35	117.20
2	B	370	GLN	CB-CG-CD	6.28	127.94	111.60
2	B	356	ALA	CB-CA-C	6.28	119.52	110.10
1	A	47	ALA	N-CA-C	-6.28	94.05	111.00
2	B	203	GLU	CB-CA-C	-6.28	97.85	110.40
2	B	296	GLU	CA-CB-CG	6.28	127.21	113.40
1	A	80	GLN	O-C-N	6.27	132.74	122.70
1	A	92	HIS	O-C-N	-6.27	109.18	121.10
2	B	306	PHE	CG-CD2-CE2	6.27	127.70	120.80
2	B	23	PRO	CA-C-O	-6.27	105.16	120.20
1	A	96	PRO	O-C-N	6.26	132.72	122.70
2	B	96	LEU	N-CA-CB	6.26	122.92	110.40
2	B	78	GLU	N-CA-CB	-6.25	99.34	110.60
2	B	53	ALA	O-C-N	6.25	133.83	123.20
2	B	206[A]	ARG	N-CA-CB	6.25	121.84	110.60
2	B	206[B]	ARG	N-CA-CB	6.25	121.84	110.60
2	B	205	GLN	O-C-N	-6.24	112.71	122.70
2	B	61	LYS	CB-CA-C	6.24	122.88	110.40
2	B	166	LEU	CB-CG-CD2	6.24	121.61	111.00
2	B	244	PHE	CD1-CG-CD2	6.24	126.41	118.30
2	B	228	ILE	CG1-CB-CG2	6.24	125.12	111.40
1	A	20	VAL	CG1-CB-CG2	-6.23	100.94	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	327	ILE	CA-CB-CG1	6.22	122.83	111.00
2	B	240	MET	C-N-CA	-6.22	106.14	121.70
2	B	206[A]	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	B	206[B]	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	B	30	GLU	OE1-CD-OE2	-6.21	115.85	123.30
2	B	97	LEU	CB-CG-CD1	-6.20	100.45	111.00
2	B	271	LEU	CB-CG-CD1	6.20	121.54	111.00
2	B	312	GLN	O-C-N	6.20	132.62	122.70
1	A	171	ARG	CD-NE-CZ	6.20	132.28	123.60
2	B	332	ALA	CA-C-O	-6.20	107.08	120.10
2	B	339	LEU	CA-CB-CG	-6.20	101.05	115.30
1	A	4	TYR	CB-CG-CD1	6.19	124.71	121.00
1	A	194	HIS	CB-CA-C	6.19	122.78	110.40
2	B	79	ASP	OD1-CG-OD2	-6.19	111.54	123.30
2	B	243	ASP	CA-C-N	-6.18	103.59	117.20
1	A	150	PRO	N-CD-CG	6.18	112.47	103.20
2	B	5	LEU	CB-CG-CD2	6.18	121.50	111.00
2	B	141	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	B	124	ALA	O-C-N	-6.17	112.83	122.70
2	B	197	TYR	CB-CG-CD2	-6.17	117.30	121.00
2	B	97	LEU	CB-CA-C	-6.16	98.49	110.20
2	B	200	ILE	CA-CB-CG1	-6.16	99.29	111.00
2	B	9	PHE	CD1-CE1-CZ	-6.16	112.71	120.10
2	B	9	PHE	CE1-CZ-CE2	6.16	131.09	120.00
2	B	316	LEU	N-CA-CB	-6.16	98.08	110.40
2	B	16	TYR	CB-CG-CD2	6.16	124.69	121.00
2	B	278	ILE	CA-C-O	6.15	133.02	120.10
2	B	67	ALA	N-CA-CB	-6.14	101.50	110.10
1	A	164	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	B	298	TYR	N-CA-C	-6.13	94.45	111.00
2	B	16	TYR	CD1-CE1-CZ	6.12	125.31	119.80
1	A	162	LEU	CB-CG-CD2	6.12	121.40	111.00
1	A	210	GLN	O-C-N	-6.12	112.80	123.20
2	B	375	ASN	CB-CA-C	-6.12	98.17	110.40
1	A	105	LEU	N-CA-CB	6.11	122.61	110.40
2	B	226	ALA	CB-CA-C	-6.11	100.94	110.10
1	A	96	PRO	CA-C-N	-6.11	103.77	117.20
2	B	280	PHE	N-CA-CB	-6.11	99.61	110.60
2	B	109	GLU	OE1-CD-OE2	-6.10	115.97	123.30
1	A	128	VAL	O-C-N	6.10	132.46	122.70
2	B	229	ALA	CA-C-N	6.09	130.60	117.20
1	A	139	PHE	CG-CD1-CE1	-6.08	114.11	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	45	PHE	CG-CD2-CE2	-6.08	114.11	120.80
1	A	230	GLY	O-C-N	6.08	132.42	122.70
2	B	207	MET	O-C-N	6.07	132.42	122.70
2	B	285	PRO	CA-N-CD	6.07	120.20	111.70
2	B	169	ALA	N-CA-C	6.05	127.34	111.00
2	B	28	LEU	CB-CA-C	6.04	121.69	110.20
2	B	159	VAL	CG1-CB-CG2	-6.03	101.25	110.90
2	B	306	PHE	N-CA-C	-6.03	94.72	111.00
2	B	250	VAL	CG1-CB-CG2	6.03	120.54	110.90
2	B	149	MET	O-C-N	6.02	132.34	122.70
2	B	8	TYR	CD1-CE1-CZ	-6.02	114.38	119.80
2	B	81	LEU	N-CA-CB	-6.02	98.36	110.40
2	B	245	ILE	O-C-N	-6.01	113.08	122.70
2	B	264	THR	CA-C-O	-6.01	107.47	120.10
2	B	41	PHE	CD1-CG-CD2	-6.00	110.51	118.30
2	B	223	LEU	CB-CG-CD2	-5.99	100.82	111.00
2	B	52	TYR	C-N-CA	-5.98	106.75	121.70
2	B	177	TRP	CE3-CZ3-CH2	5.98	127.78	121.20
2	B	30	GLU	CB-CG-CD	5.97	130.33	114.20
1	A	77	THR	CB-CA-C	-5.97	95.48	111.60
2	B	287	MET	CB-CA-C	-5.97	98.46	110.40
2	B	188	LEU	CA-CB-CG	-5.96	101.58	115.30
2	B	234	GLY	C-N-CA	-5.96	106.79	121.70
2	B	82	HIS	CA-C-O	-5.94	107.62	120.10
1	A	205	ALA	O-C-N	-5.94	113.20	122.70
2	B	241	PHE	CB-CG-CD1	5.94	124.95	120.80
1	A	161	ASP	CB-CG-OD1	5.93	123.64	118.30
2	B	337	LYS	CA-C-N	5.93	130.25	117.20
2	B	316	LEU	CA-C-N	5.93	130.25	117.20
1	A	120	GLN	N-CA-C	5.92	126.98	111.00
2	B	103	LYS	O-C-N	5.92	132.17	122.70
1	A	251	MET	CG-SD-CE	5.91	109.66	100.20
2	B	79	ASP	CA-C-O	-5.91	107.69	120.10
2	B	93	GLY	O-C-N	5.90	132.14	122.70
2	B	315	TYR	CD1-CG-CD2	-5.89	111.42	117.90
1	A	121	VAL	CG1-CB-CG2	5.89	120.33	110.90
1	A	256	ARG	NE-CZ-NH1	-5.89	117.35	120.30
2	B	262	ILE	O-C-N	-5.89	113.27	122.70
2	B	308	SER	O-C-N	-5.89	113.27	122.70
2	B	256	GLU	CB-CG-CD	-5.89	98.30	114.20
1	A	52	VAL	O-C-N	5.88	132.27	121.10
1	A	88	ILE	CA-CB-CG1	-5.87	99.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	262	ILE	CA-CB-CG1	5.86	122.14	111.00
2	B	65	ILE	CA-CB-CG1	-5.85	99.89	111.00
2	B	298	TYR	CD1-CE1-CZ	-5.83	114.55	119.80
2	B	26	ASN	O-C-N	5.83	132.03	122.70
2	B	181	TYR	CD1-CG-CD2	5.83	124.31	117.90
2	B	338	THR	CA-CB-OG1	-5.83	96.76	109.00
1	A	127	LEU	CB-CG-CD2	5.83	120.91	111.00
1	A	163	LEU	O-C-N	5.83	132.02	122.70
2	B	51	ASN	N-CA-CB	-5.83	100.12	110.60
2	B	77	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	B	194	PRO	C-N-CA	5.82	136.25	121.70
2	B	59	LEU	N-CA-CB	-5.81	98.79	110.40
2	B	308	SER	C-N-CA	5.81	136.22	121.70
2	B	278	ILE	CA-CB-CG2	-5.80	99.30	110.90
1	A	241	ILE	CG1-CB-CG2	-5.80	98.64	111.40
2	B	267	HIS	CA-C-O	-5.79	107.93	120.10
1	A	153	ILE	O-C-N	-5.79	113.43	122.70
2	B	133	TYR	CE1-CZ-CE2	5.79	129.07	119.80
2	B	13	GLY	O-C-N	5.79	133.04	123.20
2	B	341	ARG	CA-C-N	5.79	129.93	117.20
1	A	11	LEU	CB-CG-CD1	-5.77	101.20	111.00
2	B	19	GLN	CA-C-N	-5.77	104.52	117.20
2	B	257	PRO	N-CA-CB	5.77	110.22	103.30
1	A	7	LEU	CB-CA-C	-5.76	99.25	110.20
2	B	304	LEU	CA-CB-CG	-5.76	102.05	115.30
2	B	123	SER	CA-CB-OG	-5.76	95.65	111.20
1	A	19	PHE	CZ-CE2-CD2	-5.74	113.21	120.10
2	B	47	ASP	O-C-N	-5.73	113.53	122.70
2	B	17	VAL	CB-CA-C	-5.73	100.52	111.40
2	B	336	PHE	CD1-CG-CD2	5.73	125.75	118.30
1	A	171	ARG	O-C-N	-5.72	113.47	123.20
1	A	115	TYR	CB-CG-CD1	-5.72	117.57	121.00
2	B	202	ARG	CA-C-O	5.72	132.11	120.10
2	B	41	PHE	CZ-CE2-CD2	-5.71	113.24	120.10
2	B	374	VAL	CG1-CB-CG2	-5.71	101.76	110.90
1	A	112	ASP	O-C-N	-5.71	113.56	122.70
2	B	106	ILE	C-N-CA	5.71	135.98	121.70
2	B	328	THR	N-CA-CB	5.71	121.15	110.30
1	A	243	LYS	N-CA-C	5.71	126.41	111.00
2	B	255	VAL	O-C-N	-5.71	113.57	122.70
2	B	198	PRO	CA-C-N	5.71	129.75	117.20
2	B	51	ASN	N-CA-C	5.70	126.39	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	188	LEU	O-C-N	5.70	132.89	123.20
2	B	6	ASN	C-N-CD	-5.70	108.07	120.60
2	B	231	VAL	CA-CB-CG2	5.69	119.44	110.90
2	B	151	LEU	O-C-N	-5.69	113.60	122.70
2	B	52	TYR	CB-CG-CD2	5.68	124.41	121.00
2	B	224	PRO	N-CA-CB	5.68	110.12	103.30
1	A	121	VAL	CA-C-O	-5.68	108.17	120.10
2	B	212	THR	CA-CB-CG2	-5.68	104.45	112.40
1	A	262	MET	CG-SD-CE	5.67	109.27	100.20
2	B	233	GLY	CA-C-O	5.67	130.80	120.60
2	B	238	ILE	CB-CG1-CD1	-5.67	98.03	113.90
2	B	372	LEU	CD1-CG-CD2	5.67	127.49	110.50
1	A	126	VAL	CG1-CB-CG2	-5.66	101.84	110.90
2	B	336	PHE	CD1-CE1-CZ	-5.66	113.31	120.10
1	A	134	GLU	O-C-N	5.66	131.75	122.70
2	B	28	LEU	O-C-N	-5.66	113.65	122.70
2	B	45	PHE	CB-CG-CD2	-5.66	116.84	120.80
2	B	256	GLU	CA-C-O	-5.66	108.22	120.10
2	B	262	ILE	CG1-CB-CG2	-5.66	98.96	111.40
1	A	39	THR	CA-CB-CG2	-5.65	104.49	112.40
2	B	321	ARG	N-CA-C	-5.65	95.74	111.00
2	B	209	GLY	O-C-N	-5.65	113.67	122.70
2	B	4	LEU	CB-CG-CD2	-5.64	101.41	111.00
1	A	266	SER	CB-CA-C	-5.64	99.39	110.10
2	B	355	LEU	CA-C-O	-5.63	108.27	120.10
1	A	116	ALA	N-CA-C	5.62	126.19	111.00
2	B	322	ALA	N-CA-CB	-5.62	102.23	110.10
2	B	200	ILE	CB-CG1-CD1	-5.62	98.17	113.90
1	A	114	PHE	CG-CD2-CE2	-5.60	114.64	120.80
2	B	212	THR	O-C-N	-5.60	113.74	122.70
2	B	387	VAL	CA-CB-CG1	5.60	119.30	110.90
2	B	132	ILE	CA-CB-CG1	-5.60	100.37	111.00
2	B	365	GLN	CA-CB-CG	-5.59	101.09	113.40
2	B	89	ASN	O-C-N	5.58	131.63	122.70
2	B	70	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	123	VAL	CG1-CB-CG2	5.57	119.82	110.90
1	A	3	ARG	NH1-CZ-NH2	-5.57	113.28	119.40
1	A	48	LEU	CA-CB-CG	5.57	128.11	115.30
2	B	57	THR	CA-C-N	-5.57	104.95	117.20
2	B	334	GLU	O-C-N	-5.55	113.81	122.70
2	B	288	GLN	CG-CD-OE1	-5.55	110.50	121.60
2	B	70	ARG	CG-CD-NE	5.55	123.45	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	215	GLN	CA-CB-CG	-5.55	101.19	113.40
2	B	349	LEU	CB-CG-CD1	5.54	120.42	111.00
2	B	355	LEU	O-C-N	5.54	131.57	122.70
2	B	236	ASN	C-N-CA	-5.54	107.86	121.70
1	A	134	GLU	CG-CD-OE2	-5.53	107.23	118.30
1	A	56	ASP	CB-CG-OD1	-5.53	113.32	118.30
2	B	287	MET	CA-CB-CG	5.53	122.70	113.30
1	A	144	LEU	CB-CA-C	5.53	120.70	110.20
2	B	107	ILE	O-C-N	5.52	131.54	122.70
2	B	267	HIS	O-C-N	5.52	132.59	123.20
2	B	228	ILE	CA-CB-CG2	5.52	121.93	110.90
2	B	67	ALA	CA-C-N	-5.51	105.17	116.20
1	A	126	VAL	N-CA-CB	-5.51	99.38	111.50
2	B	3	THR	CA-CB-CG2	5.51	120.11	112.40
2	B	321	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	220	VAL	CA-CB-CG2	5.50	119.15	110.90
2	B	106	ILE	CB-CG1-CD1	5.50	129.29	113.90
2	B	122	ALA	CA-C-O	-5.50	108.56	120.10
1	A	60	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	169	TYR	CB-CG-CD2	-5.49	117.71	121.00
2	B	40	GLU	O-C-N	-5.49	113.92	122.70
2	B	43	ALA	CB-CA-C	5.49	118.33	110.10
2	B	256	GLU	N-CA-C	5.49	125.83	111.00
2	B	48	LEU	CB-CG-CD2	-5.48	101.68	111.00
2	B	321	ARG	CB-CA-C	-5.48	99.43	110.40
1	A	117	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	95	ILE	CB-CG1-CD1	-5.48	98.56	113.90
2	B	17	VAL	CA-CB-CG1	-5.48	102.68	110.90
2	B	217	LEU	N-CA-CB	5.47	121.35	110.40
2	B	281	GLY	CA-C-N	-5.47	105.16	117.20
1	A	140	ARG	CB-CA-C	5.47	121.34	110.40
2	B	55	ARG	CD-NE-CZ	-5.47	115.94	123.60
2	B	65	ILE	N-CA-CB	-5.47	98.22	110.80
2	B	117	VAL	N-CA-C	5.46	125.74	111.00
1	A	127	LEU	N-CA-CB	-5.45	99.50	110.40
2	B	59	LEU	CB-CA-C	5.45	120.55	110.20
1	A	140	ARG	NH1-CZ-NH2	5.44	125.38	119.40
1	A	107	PHE	O-C-N	5.43	131.39	122.70
2	B	232	GLY	N-CA-C	-5.43	99.52	113.10
2	B	22	MET	N-CA-CB	5.43	120.37	110.60
2	B	47	ASP	CA-C-N	5.42	129.12	117.20
1	A	260	SER	CA-CB-OG	-5.41	96.59	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	THR	OG1-CB-CG2	-5.41	97.57	110.00
2	B	317	ASN	CB-CG-OD1	-5.40	110.80	121.60
1	A	169	TYR	N-CA-C	5.39	125.56	111.00
1	A	117	ARG	NE-CZ-NH1	-5.39	117.60	120.30
2	B	15	MET	CG-SD-CE	-5.39	91.57	100.20
2	B	246	ASN	N-CA-CB	5.38	120.28	110.60
2	B	379	ARG	CA-C-O	5.37	131.38	120.10
2	B	104	SER	O-C-N	-5.37	114.12	122.70
2	B	52	TYR	CG-CD2-CE2	5.36	125.59	121.30
2	B	291	ASP	N-CA-CB	-5.36	100.95	110.60
2	B	275	ARG	N-CA-CB	-5.35	100.97	110.60
2	B	99	LYS	CB-CG-CD	-5.34	97.70	111.60
2	B	368	LYS	CG-CD-CE	-5.34	95.87	111.90
2	B	247	ASP	CA-C-N	-5.34	105.45	117.20
2	B	285	PRO	CA-C-O	-5.33	107.40	120.20
2	B	191	ALA	N-CA-CB	5.32	117.55	110.10
2	B	205	GLN	OE1-CD-NE2	5.32	134.14	121.90
2	B	168	ASP	C-N-CA	-5.32	108.40	121.70
2	B	199	THR	O-C-N	5.32	131.21	122.70
2	B	61	LYS	CA-CB-CG	-5.32	101.70	113.40
2	B	73	LEU	O-C-N	5.32	131.21	122.70
1	A	149	ALA	N-CA-CB	-5.31	102.66	110.10
2	B	360	LYS	CD-CE-NZ	5.31	123.92	111.70
2	B	236	ASN	CB-CG-OD1	-5.31	110.98	121.60
1	A	123	VAL	CA-C-O	5.31	131.24	120.10
2	B	391	LEU	CA-CB-CG	-5.31	103.10	115.30
2	B	76	LYS	C-N-CA	-5.30	108.46	121.70
2	B	211	GLU	CB-CA-C	-5.29	99.81	110.40
1	A	134	GLU	CA-C-O	-5.29	108.99	120.10
2	B	162	GLY	N-CA-C	-5.29	99.88	113.10
2	B	223	LEU	CB-CG-CD1	-5.28	102.02	111.00
1	A	127	LEU	CA-C-N	-5.28	105.58	117.20
1	A	176	LEU	N-CA-C	-5.28	96.74	111.00
1	A	27	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	232	ILE	CA-CB-CG2	-5.28	100.35	110.90
2	B	342	HIS	N-CA-C	5.27	125.24	111.00
1	A	150	PRO	O-C-N	5.27	131.13	122.70
2	B	101	MET	CA-CB-CG	-5.27	104.34	113.30
2	B	268	GLY	O-C-N	-5.27	114.27	122.70
1	A	101	MET	CA-CB-CG	-5.26	104.36	113.30
2	B	51	ASN	CA-C-N	5.26	128.77	117.20
2	B	183	THR	CB-CA-C	-5.26	97.40	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	94	THR	O-C-N	5.26	131.11	122.70
2	B	283	LYS	CG-CD-CE	-5.26	96.13	111.90
1	A	219	GLN	N-CA-C	5.25	125.19	111.00
1	A	171	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	B	43	ALA	O-C-N	-5.25	114.30	122.70
1	A	222	ALA	C-N-CA	-5.24	108.59	121.70
2	B	383	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	A	122	GLY	N-CA-C	5.24	126.19	113.10
2	B	13	GLY	CA-C-N	-5.23	105.73	116.20
2	B	250	VAL	C-N-CA	5.23	133.29	122.30
1	A	126	VAL	CB-CA-C	-5.23	101.47	111.40
2	B	366	PRO	O-C-N	-5.22	114.35	122.70
2	B	49	LEU	N-CA-CB	-5.21	99.97	110.40
2	B	21	LEU	CA-C-O	5.21	131.05	120.10
1	A	221	SER	O-C-N	-5.21	114.36	122.70
2	B	312	GLN	N-CA-CB	5.21	119.98	110.60
2	B	249	SER	N-CA-CB	-5.21	102.69	110.50
2	B	65	ILE	CG1-CB-CG2	-5.20	99.96	111.40
2	B	345	ILE	O-C-N	-5.20	114.38	122.70
2	B	335	ALA	CA-C-O	-5.19	109.20	120.10
2	B	25	LEU	O-C-N	-5.19	114.40	122.70
2	B	309	VAL	CA-CB-CG1	-5.18	103.12	110.90
2	B	334	GLU	CG-CD-OE2	5.18	128.66	118.30
2	B	222	ARG	O-C-N	-5.18	114.41	122.70
1	A	106	VAL	CG1-CB-CG2	5.18	119.19	110.90
2	B	292	GLY	CA-C-N	5.18	128.59	117.20
1	A	36	ILE	CA-CB-CG1	-5.17	101.17	111.00
2	B	244	PHE	C-N-CA	-5.17	108.77	121.70
2	B	152	MET	O-C-N	5.17	131.99	123.20
1	A	117	ARG	CD-NE-CZ	5.17	130.83	123.60
2	B	188	LEU	N-CA-CB	-5.17	100.07	110.40
1	A	149	ALA	O-C-N	5.16	130.91	121.10
1	A	257	SER	CB-CA-C	-5.16	100.30	110.10
2	B	241	PHE	CB-CA-C	-5.16	100.09	110.40
2	B	118	ALA	C-N-CA	-5.16	108.81	121.70
1	A	263	LYS	O-C-N	5.15	130.94	122.70
2	B	316	LEU	O-C-N	5.15	130.94	122.70
1	A	101	MET	CG-SD-CE	-5.15	91.97	100.20
1	A	218	GLU	C-N-CA	-5.14	108.85	121.70
2	B	7	PRO	N-CD-CG	-5.14	95.49	103.20
2	B	197	TYR	CG-CD1-CE1	-5.14	117.19	121.30
2	B	235	SER	C-N-CA	-5.14	108.86	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	324	TYR	CD1-CG-CD2	-5.13	112.25	117.90
2	B	212	THR	OG1-CB-CG2	-5.13	98.20	110.00
1	A	121	VAL	CB-CA-C	-5.13	101.66	111.40
2	B	110	THR	C-N-CA	-5.13	111.53	122.30
2	B	59	LEU	N-CA-C	-5.13	97.16	111.00
2	B	380	GLY	CA-C-N	-5.13	105.92	117.20
2	B	34	SER	O-C-N	5.12	130.90	122.70
2	B	74	TYR	CE1-CZ-CE2	-5.12	111.61	119.80
2	B	11	GLU	CG-CD-OE2	5.12	128.54	118.30
2	B	8	TYR	CE1-CZ-CE2	-5.12	111.61	119.80
1	A	127	LEU	CA-C-O	-5.12	109.36	120.10
1	A	196	LEU	CA-CB-CG	5.12	127.06	115.30
2	B	314	ALA	CB-CA-C	5.11	117.77	110.10
2	B	210	GLU	C-N-CA	-5.11	108.94	121.70
2	B	3	THR	CA-C-O	5.10	130.81	120.10
2	B	7	PRO	C-N-CA	-5.10	108.95	121.70
2	B	223	LEU	N-CA-C	5.10	124.77	111.00
2	B	254	GLY	CA-C-O	5.10	129.78	120.60
2	B	367	GLU	CG-CD-OE2	5.10	128.50	118.30
2	B	283	LYS	CA-CB-CG	-5.10	102.19	113.40
2	B	74	TYR	CB-CG-CD2	5.09	124.06	121.00
2	B	208	ILE	CA-CB-CG1	5.09	120.68	111.00
2	B	206[A]	ARG	CB-CA-C	-5.09	100.22	110.40
2	B	206[B]	ARG	CB-CA-C	-5.09	100.22	110.40
2	B	350	GLU	N-CA-CB	5.09	119.76	110.60
1	A	125	SER	CA-C-N	-5.09	106.01	117.20
2	B	252	LEU	C-N-CA	5.09	134.41	121.70
2	B	53	ALA	C-N-CA	-5.08	111.62	122.30
1	A	126	VAL	CA-CB-CG1	-5.08	103.28	110.90
2	B	39	PRO	N-CD-CG	-5.08	95.58	103.20
2	B	280	PHE	CZ-CE2-CD2	-5.08	114.01	120.10
2	B	330	ASP	N-CA-C	5.08	124.71	111.00
2	B	23	PRO	CA-CB-CG	-5.07	94.37	104.00
2	B	225	ASP	CA-C-N	5.07	128.35	117.20
1	A	89	ARG	CG-CD-NE	-5.07	101.16	111.80
1	A	175	TYR	CZ-CE2-CD2	-5.06	115.24	119.80
2	B	76	LYS	CA-C-N	-5.06	106.06	117.20
2	B	270	PRO	CA-C-N	5.06	128.33	117.20
2	B	220	GLU	CA-CB-CG	5.06	124.53	113.40
1	A	176	LEU	CA-C-N	-5.05	106.09	117.20
2	B	88	THR	O-C-N	-5.05	114.62	122.70
2	B	56	PRO	N-CD-CG	5.05	110.77	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	197	TYR	CD1-CG-CD2	5.05	123.45	117.90
2	B	248	THR	CA-C-O	-5.05	109.50	120.10
1	A	126	VAL	CA-CB-CG2	-5.04	103.33	110.90
2	B	102	GLY	N-CA-C	5.04	125.70	113.10
2	B	261	GLY	CA-C-O	-5.04	111.53	120.60
2	B	157	ILE	CG1-CB-CG2	-5.03	100.33	111.40
2	B	261	GLY	C-N-CA	-5.03	109.12	121.70
2	B	385	PHE	CB-CA-C	-5.03	100.34	110.40
1	A	151	ILE	CA-CB-CG1	5.03	120.56	111.00
1	A	130	ASP	O-C-N	-5.03	114.66	122.70
1	A	28	PRO	N-CD-CG	5.02	110.74	103.20
2	B	221	GLY	C-N-CA	-5.02	109.15	121.70
2	B	283	LYS	CA-C-N	-5.02	106.16	117.20
2	B	66	THR	OG1-CB-CG2	-5.02	98.46	110.00
2	B	382	LYS	CD-CE-NZ	-5.02	100.16	111.70
2	B	368	LYS	CA-CB-CG	-5.01	102.38	113.40
2	B	235	SER	O-C-N	5.01	130.71	122.70
2	B	61	LYS	CA-C-N	5.01	128.22	117.20
2	B	391	LEU	CB-CG-CD1	5.01	119.51	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	ARG	Peptide
2	B	54	GLY	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1955	0	1959	85	0
2	B	2987	0	2961	236	0
3	A	17	0	11	1	0
4	B	1	0	0	0	0
5	B	15	0	7	1	0
6	A	129	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	248	0	0	2	0
All	All	5352	0	4938	319	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (319) 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)
2:B:235:SER:CA	2:B:235:SER:CB	1.74	1.64
2:B:278:ILE:CG1	2:B:278:ILE:CD1	1.74	1.64
2:B:129:LYS:CD	2:B:129:LYS:CG	1.75	1.63
1:A:52:VAL:CB	1:A:52:VAL:CG1	1.75	1.63
1:A:126:VAL:CB	1:A:126:VAL:CG1	1.75	1.63
2:B:71:THR:CB	2:B:71:THR:CG2	1.77	1.63
2:B:37:LYS:CD	2:B:37:LYS:CG	1.75	1.62
1:A:87:LEU:CG	1:A:87:LEU:CD1	1.74	1.61
2:B:58:ALA:CA	2:B:58:ALA:CB	1.75	1.61
2:B:183:THR:CB	2:B:183:THR:CG2	1.74	1.61
1:A:140:ARG:CD	1:A:140:ARG:CG	1.76	1.60
2:B:231:VAL:CB	2:B:231:VAL:CG1	1.79	1.60
2:B:117:VAL:CA	2:B:117:VAL:CB	1.75	1.59
2:B:66:THR:CB	2:B:66:THR:CG2	1.75	1.58
2:B:212:THR:CB	2:B:212:THR:CG2	1.77	1.58
2:B:25:LEU:CD2	2:B:25:LEU:CG	1.75	1.58
2:B:319:ILE:CB	2:B:319:ILE:CG2	1.75	1.58
2:B:353:HIS:CB	2:B:353:HIS:CA	1.77	1.58
2:B:49:LEU:CD2	2:B:49:LEU:CG	1.80	1.57
2:B:286:MET:CA	2:B:286:MET:CB	1.77	1.57
2:B:55:ARG:CD	2:B:55:ARG:CG	1.75	1.57
2:B:333:LEU:CD2	2:B:333:LEU:CG	1.75	1.57
1:A:94:THR:CB	1:A:94:THR:CA	1.75	1.57
2:B:282:MET:CB	2:B:282:MET:CA	1.77	1.57
2:B:76:LYS:CE	2:B:76:LYS:CD	1.77	1.57
2:B:287:MET:CG	2:B:287:MET:CB	1.76	1.57
1:A:101:MET:CG	1:A:101:MET:CB	1.76	1.56
2:B:61:LYS:CG	2:B:61:LYS:CB	1.84	1.56
2:B:339:LEU:CD2	2:B:339:LEU:CG	1.80	1.56
2:B:150:ARG:CG	2:B:150:ARG:CB	1.74	1.56
2:B:264:THR:CB	2:B:264:THR:CG2	1.75	1.56
1:A:123:VAL:CB	1:A:123:VAL:CA	1.76	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:CG2	1:A:166:VAL:CB	1.77	1.55
2:B:139:VAL:CB	2:B:139:VAL:CG2	1.79	1.55
1:A:7:LEU:CD2	1:A:7:LEU:CG	1.78	1.54
1:A:54:PHE:C	1:A:54:PHE:CA	1.75	1.54
1:A:219:GLN:CG	1:A:219:GLN:CB	1.82	1.54
2:B:59:LEU:N	2:B:59:LEU:CA	1.71	1.54
2:B:108:ALA:CB	2:B:108:ALA:CA	1.78	1.54
2:B:373:VAL:CB	2:B:373:VAL:CG1	1.82	1.53
1:A:13:ASP:CG	1:A:13:ASP:CB	1.76	1.53
2:B:351:SER:CA	2:B:351:SER:C	1.76	1.53
2:B:23:PRO:CG	2:B:23:PRO:CB	1.80	1.53
1:A:117:ARG:CG	1:A:117:ARG:CD	1.82	1.52
1:A:24:THR:CB	1:A:24:THR:CA	1.75	1.52
2:B:304:LEU:CD1	2:B:304:LEU:CG	1.83	1.52
2:B:255:VAL:CA	2:B:255:VAL:CB	1.80	1.52
2:B:256:GLU:CG	2:B:256:GLU:CD	1.76	1.51
2:B:59:LEU:CA	2:B:59:LEU:C	1.77	1.50
2:B:203:GLU:CA	2:B:203:GLU:C	1.77	1.50
2:B:196:PRO:C	2:B:196:PRO:CA	1.77	1.50
2:B:205:GLN:CD	2:B:205:GLN:CG	1.80	1.50
2:B:61:LYS:N	2:B:61:LYS:CA	1.72	1.50
2:B:368:LYS:C	2:B:368:LYS:CA	1.75	1.50
2:B:167:LYS:CE	2:B:167:LYS:NZ	1.71	1.50
2:B:376:LEU:CG	2:B:376:LEU:CD2	1.84	1.49
2:B:362:MET:SD	2:B:362:MET:CG	2.01	1.49
2:B:328:THR:C	2:B:328:THR:CA	1.77	1.49
2:B:15:MET:CE	2:B:15:MET:SD	2.02	1.47
2:B:70:ARG:C	2:B:70:ARG:CA	1.81	1.47
2:B:282:MET:CG	2:B:282:MET:SD	2.02	1.45
2:B:149:MET:SD	2:B:149:MET:CG	2.07	1.40
2:B:286:MET:CB	2:B:286:MET:CG	2.04	1.35
1:A:191:LEU:HD12	1:A:192:PRO:CD	1.85	1.06
1:A:191:LEU:CD1	1:A:192:PRO:HD2	1.86	1.04
1:A:243:LYS:HD2	1:A:243:LYS:N	1.74	1.03
2:B:134:MET:CE	2:B:139:VAL:HG22	1.89	1.02
2:B:134:MET:HE3	2:B:139:VAL:HG22	1.40	1.02
1:A:194:HIS:O	1:A:198:GLU:HG2	1.63	0.98
2:B:376:LEU:CD2	2:B:376:LEU:CB	2.43	0.97
2:B:183:THR:CG2	2:B:183:THR:CA	2.41	0.97
2:B:71:THR:CG2	2:B:71:THR:CA	2.44	0.95
2:B:333:LEU:CD2	2:B:333:LEU:CB	2.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:CD2	1:A:7:LEU:CB	2.46	0.94
1:A:243:LYS:HD2	1:A:243:LYS:H	1.27	0.94
2:B:282:MET:CG	2:B:282:MET:CE	2.47	0.93
1:A:126:VAL:CG1	1:A:126:VAL:CG2	2.47	0.92
2:B:282:MET:CA	2:B:282:MET:CG	2.46	0.92
2:B:319:ILE:CG2	2:B:319:ILE:CG1	2.46	0.92
2:B:59:LEU:N	2:B:59:LEU:CB	2.33	0.90
2:B:333:LEU:CD2	2:B:333:LEU:CD1	2.50	0.89
1:A:24:THR:CA	1:A:24:THR:CG2	2.49	0.89
2:B:61:LYS:CB	2:B:61:LYS:N	2.36	0.88
2:B:25:LEU:CD2	2:B:25:LEU:CD1	2.52	0.87
1:A:215:SER:H	1:A:219:GLN:HE22	1.17	0.86
2:B:373:VAL:CG1	2:B:373:VAL:CG2	2.54	0.86
1:A:52:VAL:CG1	1:A:52:VAL:CG2	2.54	0.86
2:B:373:VAL:CG1	2:B:373:VAL:CA	2.53	0.86
1:A:140:ARG:CD	1:A:140:ARG:CB	2.54	0.84
1:A:54:PHE:C	1:A:54:PHE:CB	2.46	0.84
1:A:215:SER:H	1:A:219:GLN:NE2	1.74	0.84
2:B:297:SER:HB3	2:B:305:ASP:OD1	1.78	0.84
2:B:304:LEU:CD1	2:B:304:LEU:CD2	2.54	0.84
1:A:156:PRO:O	1:A:191:LEU:HB3	1.78	0.84
2:B:339:LEU:CD2	2:B:339:LEU:CD1	2.56	0.84
1:A:140:ARG:CG	1:A:140:ARG:NE	2.40	0.83
2:B:112:ALA:HB2	2:B:302:ALA:HB1	1.60	0.83
2:B:282:MET:CB	2:B:282:MET:SD	2.66	0.83
2:B:55:ARG:CD	2:B:55:ARG:CB	2.57	0.83
2:B:61:LYS:CG	2:B:61:LYS:CA	2.56	0.83
2:B:286:MET:CB	2:B:286:MET:SD	2.66	0.83
2:B:256:GLU:CD	2:B:256:GLU:CB	2.47	0.82
2:B:212:THR:CG2	2:B:212:THR:CA	2.57	0.82
2:B:255:VAL:CA	2:B:255:VAL:CG1	2.58	0.82
2:B:222:ARG:NH2	6:B:736:HOH:O	2.13	0.81
1:A:7:LEU:CD2	1:A:7:LEU:CD1	2.58	0.81
1:A:191:LEU:HD12	1:A:192:PRO:HD2	0.91	0.81
2:B:58:ALA:CB	2:B:58:ALA:N	2.45	0.80
2:B:368:LYS:CA	2:B:369:GLU:N	2.44	0.80
1:A:123:VAL:CA	1:A:123:VAL:CG1	2.59	0.80
2:B:362:MET:CG	2:B:362:MET:CE	2.59	0.79
2:B:264:THR:CG2	2:B:264:THR:CA	2.60	0.79
1:A:94:THR:CB	1:A:94:THR:C	2.51	0.79
1:A:87:LEU:CD1	1:A:87:LEU:CD2	2.61	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:LYS:CA	2:B:368:LYS:O	2.32	0.78
1:A:126:VAL:CG1	1:A:126:VAL:CA	2.62	0.78
2:B:362:MET:SD	2:B:362:MET:CB	2.71	0.78
1:A:52:VAL:CG1	1:A:52:VAL:CA	2.62	0.78
2:B:66:THR:CG2	2:B:66:THR:CA	2.62	0.78
2:B:353:HIS:CA	2:B:353:HIS:CG	2.66	0.78
2:B:231:VAL:CG1	2:B:231:VAL:CA	2.62	0.77
2:B:203:GLU:C	2:B:203:GLU:CB	2.53	0.77
2:B:339:LEU:CD2	2:B:339:LEU:CB	2.61	0.77
2:B:231:VAL:CG1	2:B:231:VAL:CG2	2.60	0.77
2:B:353:HIS:CB	2:B:353:HIS:C	2.53	0.77
1:A:239:LYS:O	1:A:243:LYS:HD3	1.85	0.77
2:B:287:MET:HG3	2:B:307:PRO:CB	2.16	0.75
2:B:60:THR:C	2:B:61:LYS:CA	2.53	0.74
2:B:351:SER:CA	2:B:352:SER:N	2.48	0.74
1:A:101:MET:CG	1:A:101:MET:CA	2.64	0.74
1:A:239:LYS:O	1:A:243:LYS:CD	2.36	0.74
2:B:70:ARG:CA	2:B:71:THR:N	2.49	0.74
2:B:76:LYS:CE	2:B:76:LYS:CG	2.64	0.74
1:A:94:THR:CA	1:A:94:THR:CG2	2.64	0.73
2:B:117:VAL:CA	2:B:117:VAL:CG2	2.64	0.73
2:B:255:VAL:CA	2:B:255:VAL:CG2	2.67	0.73
2:B:328:THR:C	2:B:328:THR:CB	2.57	0.73
2:B:15:MET:CE	2:B:15:MET:CG	2.66	0.73
2:B:49:LEU:CD2	2:B:49:LEU:CD1	2.66	0.73
2:B:203:GLU:C	2:B:203:GLU:N	2.39	0.73
1:A:123:VAL:CB	1:A:123:VAL:N	2.53	0.72
2:B:139:VAL:CG2	2:B:139:VAL:CG1	2.64	0.72
2:B:149:MET:SD	2:B:149:MET:CB	2.77	0.72
2:B:278:ILE:CD1	2:B:278:ILE:CB	2.66	0.72
2:B:37:LYS:CD	2:B:37:LYS:CB	2.68	0.72
2:B:54:GLY:O	6:B:735:HOH:O	2.06	0.72
2:B:61:LYS:CB	2:B:61:LYS:CD	2.68	0.72
1:A:166:VAL:CG2	1:A:166:VAL:CG1	2.66	0.72
2:B:376:LEU:CD2	2:B:376:LEU:CD1	2.68	0.72
2:B:297:SER:C	2:B:305:ASP:OD1	2.28	0.71
2:B:328:THR:CA	2:B:329:ASP:N	2.49	0.71
1:A:166:VAL:CG2	1:A:166:VAL:CA	2.68	0.71
1:A:54:PHE:C	1:A:54:PHE:N	2.44	0.70
2:B:235:SER:CB	2:B:235:SER:N	2.53	0.70
2:B:58:ALA:C	2:B:59:LEU:CA	2.59	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:THR:CG2	2:B:212:THR:OG1	2.39	0.70
2:B:150:ARG:CG	2:B:150:ARG:CA	2.69	0.69
2:B:255:VAL:CB	2:B:255:VAL:N	2.52	0.69
2:B:286:MET:CB	2:B:286:MET:N	2.55	0.69
2:B:304:LEU:CD1	2:B:304:LEU:CB	2.69	0.69
1:A:24:THR:CA	1:A:24:THR:OG1	2.41	0.69
2:B:134:MET:HE2	2:B:139:VAL:HG22	1.72	0.68
2:B:196:PRO:CA	2:B:197:TYR:N	2.52	0.68
2:B:203:GLU:CA	2:B:203:GLU:O	2.41	0.67
2:B:351:SER:CA	2:B:351:SER:O	2.38	0.67
2:B:287:MET:CG	2:B:307:PRO:CB	2.72	0.67
1:A:24:THR:CB	1:A:24:THR:C	2.62	0.67
2:B:70:ARG:CA	2:B:70:ARG:O	2.38	0.67
1:A:123:VAL:CA	1:A:123:VAL:CG2	2.70	0.67
2:B:59:LEU:CA	2:B:59:LEU:O	2.42	0.66
2:B:386:THR:O	2:B:390:ILE:HD12	1.95	0.66
2:B:206[B]:ARG:NH2	2:B:243:ASP:OD1	2.28	0.66
2:B:117:VAL:CB	2:B:117:VAL:N	2.57	0.66
2:B:235:SER:CB	2:B:235:SER:C	2.64	0.65
2:B:328:THR:CA	2:B:328:THR:O	2.40	0.65
2:B:11:GLU:HG2	2:B:11:GLU:O	1.94	0.65
1:A:60:ASP:OD1	3:A:501:IAG:N1	2.29	0.65
2:B:177:TRP:N	2:B:178:PRO:CD	2.59	0.65
2:B:353:HIS:CB	2:B:353:HIS:N	2.60	0.64
2:B:319:ILE:HD13	2:B:319:ILE:HG21	1.80	0.64
2:B:143:SER:N	2:B:144:PRO:CD	2.61	0.64
2:B:66:THR:CG2	2:B:66:THR:OG1	2.45	0.63
2:B:255:VAL:CB	2:B:255:VAL:C	2.62	0.63
2:B:327:ILE:HG23	2:B:331:GLU:HB2	1.80	0.63
2:B:282:MET:CB	2:B:282:MET:C	2.66	0.63
2:B:206[A]:ARG:HD2	2:B:210:GLU:OE2	1.99	0.63
2:B:55:ARG:CG	2:B:55:ARG:NE	2.63	0.62
2:B:196:PRO:CA	2:B:196:PRO:O	2.45	0.62
2:B:287:MET:CG	2:B:307:PRO:HA	2.30	0.61
1:A:24:THR:CB	1:A:24:THR:N	2.62	0.61
2:B:25:LEU:CD2	2:B:25:LEU:CB	2.69	0.60
2:B:76:LYS:CD	2:B:76:LYS:NZ	2.61	0.60
2:B:134:MET:O	2:B:158:PRO:HA	2.02	0.60
2:B:287:MET:CB	2:B:287:MET:SD	2.88	0.60
1:A:219:GLN:CB	1:A:219:GLN:CD	2.67	0.59
1:A:194:HIS:O	1:A:198:GLU:CG	2.47	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:C	1:A:58:LEU:HD12	2.23	0.59
2:B:287:MET:CG	2:B:307:PRO:CA	2.80	0.59
2:B:286:MET:CB	2:B:286:MET:C	2.69	0.59
2:B:264:THR:CG2	2:B:264:THR:OG1	2.46	0.58
1:A:177:LEU:HD11	1:A:212:PHE:CD2	2.38	0.58
2:B:70:ARG:C	2:B:70:ARG:CB	2.71	0.58
2:B:287:MET:HG3	2:B:307:PRO:HB3	1.86	0.58
1:A:87:LEU:CD1	1:A:87:LEU:CB	2.78	0.58
1:A:239:LYS:O	1:A:243:LYS:HD2	2.04	0.58
1:A:54:PHE:CA	1:A:55:SER:N	2.62	0.58
2:B:112:ALA:CB	2:B:302:ALA:HB1	2.32	0.57
2:B:362:MET:CG	2:B:362:MET:HE3	2.35	0.57
2:B:351:SER:C	2:B:351:SER:N	2.51	0.57
1:A:16:GLU:HG3	6:A:566:HOH:O	2.05	0.57
2:B:38:ASP:OD1	2:B:38:ASP:C	2.40	0.57
2:B:59:LEU:CA	2:B:60:THR:N	2.56	0.57
2:B:139:VAL:CG2	2:B:139:VAL:CA	2.78	0.57
1:A:117:ARG:CD	1:A:117:ARG:CB	2.74	0.56
1:A:211:GLY:O	1:A:212:PHE:HB2	2.04	0.56
2:B:87:LYS:HD2	2:B:114:GLN:HG3	1.87	0.56
2:B:287:MET:HG3	2:B:307:PRO:CA	2.36	0.56
2:B:117:VAL:CB	2:B:117:VAL:C	2.62	0.56
1:A:123:VAL:CB	1:A:123:VAL:C	2.68	0.55
2:B:333:LEU:CD2	2:B:333:LEU:HB3	2.36	0.55
2:B:287:MET:HB2	2:B:307:PRO:HB2	1.88	0.55
1:A:156:PRO:HA	1:A:196:LEU:HD21	1.89	0.55
2:B:319:ILE:CG2	2:B:319:ILE:CD1	2.84	0.55
2:B:203:GLU:CA	2:B:204:PHE:N	2.58	0.55
2:B:287:MET:HG3	2:B:307:PRO:HA	1.88	0.55
2:B:58:ALA:CB	2:B:58:ALA:C	2.73	0.54
1:A:16:GLU:CG	6:A:566:HOH:O	2.56	0.54
2:B:134:MET:O	2:B:159:VAL:N	2.41	0.53
2:B:297:SER:CB	2:B:305:ASP:OD1	2.53	0.53
2:B:205:GLN:CG	2:B:205:GLN:OE1	2.51	0.53
1:A:234:GLY:O	1:A:235:SER:C	2.42	0.53
2:B:129:LYS:CD	2:B:129:LYS:CB	2.77	0.52
2:B:59:LEU:N	2:B:59:LEU:C	2.61	0.52
2:B:32:PHE:CD1	2:B:200:ILE:HG12	2.44	0.52
2:B:287:MET:HG2	2:B:307:PRO:HA	1.91	0.52
2:B:255:VAL:CG1	2:B:255:VAL:C	2.78	0.51
2:B:287:MET:HG2	2:B:307:PRO:CA	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:MET:CA	2:B:286:MET:HB2	2.18	0.51
1:A:125:SER:HB2	1:A:151:ILE:HG12	1.91	0.51
2:B:111:GLY:O	2:B:138:ASP:HB3	2.10	0.51
2:B:117:VAL:HG23	2:B:117:VAL:H	1.76	0.51
2:B:319:ILE:CG2	2:B:319:ILE:CA	2.78	0.51
1:A:100:LEU:C	1:A:100:LEU:HD13	2.31	0.50
2:B:206[A]:ARG:CD	2:B:210:GLU:OE2	2.57	0.50
1:A:243:LYS:H	1:A:243:LYS:CD	2.11	0.50
2:B:143:SER:N	2:B:144:PRO:HD2	2.26	0.50
2:B:85:ALA:HA	2:B:377:SER:O	2.10	0.50
2:B:177:TRP:N	2:B:178:PRO:HD3	2.25	0.49
1:A:263:LYS:O	1:A:266:SER:OG	2.26	0.49
2:B:129:LYS:CG	2:B:129:LYS:CE	2.83	0.49
2:B:297:SER:O	2:B:305:ASP:OD1	2.31	0.49
2:B:150:ARG:CB	2:B:150:ARG:CD	2.81	0.49
2:B:142:GLN:C	2:B:144:PRO:HD2	2.33	0.48
2:B:328:THR:C	2:B:328:THR:N	2.59	0.48
2:B:319:ILE:CG2	2:B:319:ILE:HD13	2.40	0.48
1:A:125:SER:HB2	1:A:151:ILE:CG1	2.44	0.48
1:A:242:GLU:CD	1:A:243:LYS:HZ1	2.18	0.47
2:B:62:CYS:SG	2:B:75:LEU:HG	2.54	0.47
2:B:87:LYS:HD2	2:B:114:GLN:CG	2.44	0.47
2:B:286:MET:CA	2:B:286:MET:HB3	2.18	0.47
2:B:87:LYS:NZ	5:B:502:PLP:O3	2.47	0.47
2:B:373:VAL:CG1	2:B:373:VAL:C	2.82	0.47
1:A:148:ILE:HD12	1:A:148:ILE:HG23	1.54	0.47
2:B:59:LEU:HD12	2:B:59:LEU:HA	1.67	0.47
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.50	0.47
2:B:381:ASP:O	2:B:384:ILE:HG12	2.15	0.47
1:A:127:LEU:HD23	1:A:128:VAL:N	2.30	0.46
2:B:203:GLU:N	2:B:204:PHE:N	2.64	0.46
1:A:132:PRO:HD3	2:B:17:VAL:O	2.15	0.46
2:B:333:LEU:CD2	2:B:333:LEU:HD13	2.44	0.46
1:A:76:VAL:HA	1:A:80:GLN:OE1	2.16	0.45
1:A:216:SER:H	1:A:219:GLN:HE21	1.63	0.45
2:B:279:TYR:CG	2:B:280:PHE:N	2.83	0.45
2:B:117:VAL:CA	2:B:117:VAL:CG1	2.85	0.45
2:B:362:MET:CE	2:B:362:MET:CB	2.91	0.45
2:B:134:MET:HE2	2:B:134:MET:HB3	1.41	0.45
2:B:255:VAL:CG2	2:B:255:VAL:N	2.78	0.45
2:B:108:ALA:CB	2:B:108:ALA:C	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:ALA:HB2	2:B:302:ALA:CB	2.39	0.45
2:B:173:ALA:HB1	2:B:186:TYR:CE1	2.51	0.45
1:A:123:VAL:CG1	1:A:123:VAL:C	2.86	0.44
2:B:351:SER:N	2:B:352:SER:N	2.65	0.44
1:A:91:LYS:NZ	6:A:626:HOH:O	2.43	0.44
2:B:287:MET:CG	2:B:307:PRO:HB2	2.47	0.44
2:B:319:ILE:HG21	2:B:319:ILE:CD1	2.43	0.44
1:A:55:SER:HB3	2:B:293:GLN:HB3	1.99	0.44
2:B:70:ARG:C	2:B:70:ARG:N	2.57	0.44
2:B:264:THR:CG2	2:B:264:THR:N	2.81	0.43
2:B:272:LYS:HD3	2:B:324:TYR:HB2	2.00	0.43
2:B:287:MET:HG2	2:B:307:PRO:O	2.18	0.43
2:B:205:GLN:CG	2:B:205:GLN:NE2	2.68	0.43
2:B:279:TYR:CD1	2:B:280:PHE:N	2.84	0.43
1:A:95:ILE:HG21	1:A:95:ILE:HD13	1.64	0.43
2:B:157:ILE:HA	2:B:158:PRO:HD3	1.42	0.43
2:B:117:VAL:CG2	2:B:117:VAL:N	2.82	0.43
2:B:255:VAL:C	2:B:255:VAL:HG12	2.39	0.43
1:A:219:GLN:CG	1:A:219:GLN:CA	2.89	0.43
2:B:349:LEU:HD23	2:B:349:LEU:HA	1.90	0.43
1:A:193:LEU:HA	1:A:193:LEU:HD23	1.51	0.42
1:A:22:PHE:CD1	1:A:22:PHE:C	2.92	0.42
1:A:140:ARG:HH11	1:A:140:ARG:HD3	0.88	0.42
2:B:70:ARG:N	2:B:71:THR:N	2.67	0.42
2:B:301:SER:OG	2:B:350:GLU:HG3	2.19	0.42
2:B:80:LEU:HD23	2:B:80:LEU:HA	1.66	0.42
2:B:205:GLN:CD	2:B:205:GLN:CB	2.75	0.42
2:B:79:ASP:HB2	2:B:379:ARG:HB3	2.02	0.41
2:B:97:LEU:HD23	2:B:97:LEU:HA	2.00	0.41
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.95	0.41
2:B:57:THR:OG1	2:B:76:LYS:HE3	2.19	0.41
2:B:364:GLU:C	2:B:365:GLN:CG	2.88	0.41
1:A:216:SER:HA	1:A:217:PRO:HD3	1.91	0.41
2:B:174:LEU:HA	2:B:174:LEU:HD23	1.73	0.41
2:B:300:ILE:HB	2:B:329:ASP:CG	2.41	0.41
1:A:30:ILE:HD11	1:A:76:VAL:HG22	2.03	0.41
2:B:133:TYR:HA	2:B:157:ILE:O	2.21	0.41
2:B:167:LYS:O	2:B:170:CYS:HB2	2.21	0.41
2:B:71:THR:CG2	2:B:71:THR:OG1	2.61	0.40
2:B:202:ARG:HH11	2:B:202:ARG:HD3	1.48	0.40
2:B:66:THR:HA	2:B:362:MET:SD	2.61	0.40

There are no symmetry-related clashes.

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	255/268 (95%)	250 (98%)	3 (1%)	2 (1%)	19 6
2	B	393/396 (99%)	371 (94%)	20 (5%)	2 (0%)	29 13
All	All	648/664 (98%)	621 (96%)	23 (4%)	4 (1%)	25 11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	LEU
1	A	234	GLY
2	B	117	VAL
2	B	139	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	203/208 (98%)	195 (96%)	8 (4%)	32 13
2	B	309/310 (100%)	299 (97%)	10 (3%)	39 20
All	All	512/518 (99%)	494 (96%)	18 (4%)	36 17

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	78	PRO
1	A	112	ASP
1	A	121	VAL
1	A	193	LEU
1	A	196	LEU
1	A	243	LYS
1	A	247	SER
2	B	65	ILE
2	B	141	ARG
2	B	143	SER
2	B	161	SER
2	B	176	ASP
2	B	207	MET
2	B	216	ILE
2	B	297	SER
2	B	347	PRO
2	B	394	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	219	GLN
2	B	246	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	IAG	A	501	-	17,18,18	1.87	4 (23%)	18,24,24	2.92	10 (55%)
5	PLP	B	502	2	15,15,16	3.62	9 (60%)	20,22,23	2.94	5 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IAG	A	501	-	-	2/9/9/9	0/2/2/2
5	PLP	B	502	2	-	0/6/6/8	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	PLP	P-O4P	-6.76	1.38	1.60
5	B	502	PLP	C3-C2	-5.71	1.35	1.40
5	B	502	PLP	C2A-C2	5.64	1.59	1.50
5	B	502	PLP	P-O3P	-4.32	1.38	1.54
5	B	502	PLP	C5-C4	4.07	1.45	1.40
3	A	501	IAG	O1-C10	4.07	1.31	1.23
5	B	502	PLP	C5A-C5	3.94	1.61	1.50
3	A	501	IAG	O2-C12	3.66	1.34	1.22
3	A	501	IAG	C3-C7	-3.48	1.35	1.42
5	B	502	PLP	O4P-C5A	3.02	1.56	1.45
5	B	502	PLP	C2-N1	2.62	1.38	1.33
5	B	502	PLP	C3-C4	-2.20	1.35	1.40
3	A	501	IAG	C9-C2	-2.10	1.45	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	502	PLP	O4P-C5A-C5	8.30	125.17	109.35
5	B	502	PLP	O3P-P-O4P	6.90	125.09	106.73
3	A	501	IAG	C6-C8-N1	5.28	145.41	130.80
3	A	501	IAG	C11-N2-C10	-4.72	108.22	121.53
3	A	501	IAG	C7-C8-N1	-4.68	97.53	107.92
5	B	502	PLP	C4A-C4-C5	-4.30	116.50	120.94
3	A	501	IAG	C4-C5-C6	-3.98	114.86	120.44
3	A	501	IAG	O3-C12-O2	3.78	132.73	123.30
3	A	501	IAG	C9-C10-N2	-3.62	111.29	116.19
3	A	501	IAG	C12-C11-N2	-3.57	102.06	113.06
5	B	502	PLP	O4P-P-O1P	-3.52	96.60	106.47
3	A	501	IAG	C5-C6-C8	2.72	124.00	120.08
3	A	501	IAG	C5-C4-C3	2.52	123.97	120.44
5	B	502	PLP	C4A-C4-C3	2.44	124.64	120.50
3	A	501	IAG	C6-C8-C7	-2.11	116.91	120.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	IAG	O1-C10-C9-C2
3	A	501	IAG	N2-C10-C9-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	IAG	1	0
5	B	502	PLP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	6
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	65:ILE	C	66:THR	N	1.19
1	B	321:ARG	C	322:ALA	N	1.19
1	B	332:ALA	C	333:LEU	N	1.19
1	B	343:GLU	C	344:GLY	N	1.19
1	B	362:MET	C	363:ARG	N	1.19
1	B	368:LYS	C	369:GLU	N	1.19
1	A	232:ILE	C	233:SER	N	1.18

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	257/268 (95%)	0.51	20 (7%) 13 15	13, 26, 48, 78	0
2	B	394/396 (99%)	0.66	42 (10%) 6 7	11, 19, 42, 73	0
All	All	651/664 (98%)	0.60	62 (9%) 8 9	11, 22, 44, 78	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	ALA	7.2
2	B	159	VAL	6.9
1	A	190	ALA	6.4
2	B	385	PHE	6.3
1	A	191	LEU	5.8
1	A	194	HIS	5.2
2	B	164	ALA	5.0
2	B	393	ALA	4.5
2	B	160	HIS	4.5
2	B	395	GLY	4.3
2	B	135	GLY	4.1
2	B	158	PRO	3.9
2	B	394	ARG	3.8
2	B	143	SER	3.8
2	B	140	GLU	3.7
2	B	391	LEU	3.7
2	B	112	ALA	3.7
1	A	109	ASN	3.5
2	B	163	SER	3.4
1	A	195	HIS	3.3
2	B	138	ASP	3.3
2	B	134	MET	3.2
2	B	146	VAL	3.2
2	B	139	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	392	LYS	3.1
1	A	15	ARG	3.1
2	B	92	LEU	3.1
2	B	166	LEU	3.1
2	B	137	LYS	3.0
1	A	246	ALA	3.0
1	A	198	GLU	3.0
2	B	141	ARG	3.0
2	B	136	ALA	3.0
1	A	13	ASP	3.0
2	B	81	LEU	2.9
2	B	162	GLY	2.8
1	A	250	GLN	2.8
1	A	247	SER	2.7
2	B	390	ILE	2.7
2	B	80	LEU	2.7
1	A	248	PRO	2.7
2	B	147	PHE	2.7
1	A	204	HIS	2.6
2	B	248	THR	2.6
2	B	156	VAL	2.5
2	B	325	VAL	2.5
2	B	85	ALA	2.4
2	B	88	THR	2.4
2	B	157	ILE	2.4
2	B	150	ARG	2.3
1	A	203	TYR	2.3
2	B	49	LEU	2.3
1	A	193	LEU	2.2
2	B	388	HIS	2.2
2	B	169	ALA	2.2
2	B	306	PHE	2.1
2	B	75	LEU	2.1
1	A	12	ASN	2.1
1	A	212	PHE	2.1
1	A	178	SER	2.1
1	A	192	PRO	2.0
2	B	229	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IAG	A	501	17/17	0.84	0.15	22,35,50,52	0
5	PLP	B	502	15/16	0.98	0.12	15,18,28,30	0
4	NA	B	503	1/1	0.99	0.09	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.