



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:55 PM UTC

PDB ID : 1MZZ / pdb_00001mzz
Title : Crystal Structure of Mutant (M182T)of Nitrite Reductase
Authors : Guo, H.; Olesen, K.; Xue, Y.; Shapliegh, J.; Sjolín, L.
Deposited on : 2002-10-10
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

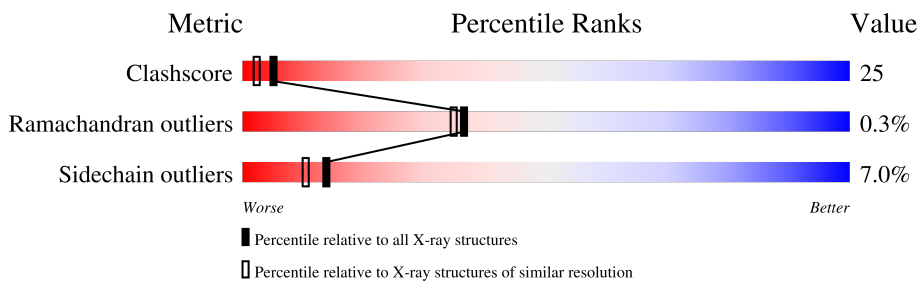
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	334	
1	B	334	
1	C	334	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8561 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 Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2567	1637	438	480	12			
1	B	334	Total	C	N	O	S	0	0	0
			2567	1637	438	480	12			
1	C	334	Total	C	N	O	S	0	0	0
			2567	1637	438	480	12			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	THR	MET	engineered mutation	UNP Q53239
A	230	ASP	THR	conflict	UNP Q53239
A	281	ASN	LYS	conflict	UNP Q53239
A	351	HIS	SER	conflict	UNP Q53239
A	367	VAL	TRP	conflict	UNP Q53239
A	368	ALA	PRO	conflict	UNP Q53239
A	372	LEU	-	cloning artifact	UNP Q53239
B	1182	THR	MET	engineered mutation	UNP Q53239
B	1230	ASP	THR	conflict	UNP Q53239
B	1281	ASN	LYS	conflict	UNP Q53239
B	1351	HIS	SER	conflict	UNP Q53239
B	1367	VAL	TRP	conflict	UNP Q53239
B	1368	ALA	PRO	conflict	UNP Q53239
B	1372	LEU	-	cloning artifact	UNP Q53239
C	2182	THR	MET	engineered mutation	UNP Q53239
C	2230	ASP	THR	conflict	UNP Q53239
C	2281	ASN	LYS	conflict	UNP Q53239
C	2351	HIS	SER	conflict	UNP Q53239
C	2367	VAL	TRP	conflict	UNP Q53239
C	2368	ALA	PRO	conflict	UNP Q53239
C	2372	LEU	-	cloning artifact	UNP Q53239

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Cu 2	0	0
2	B	2	Total 2	Cu 2	0	0
2	C	2	Total 2	Cu 2	0	0

- Molecule 3 is water.

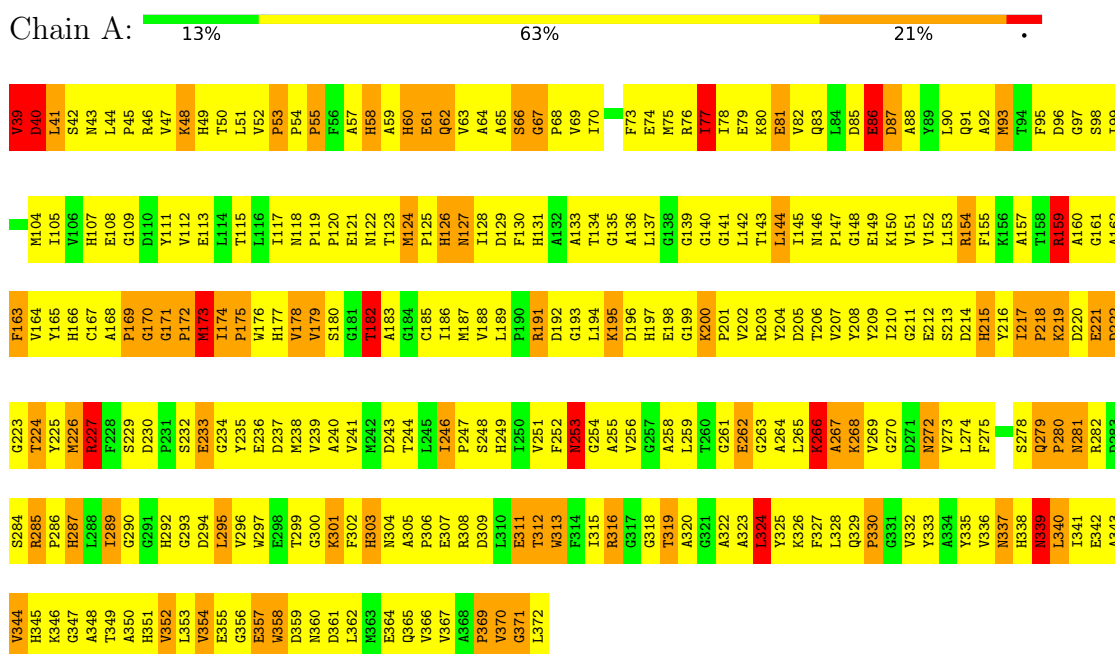
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	289	Total 289	O 289	0	0
3	B	276	Total 276	O 276	0	0
3	C	289	Total 289	O 289	0	0

3 Residue-property plots

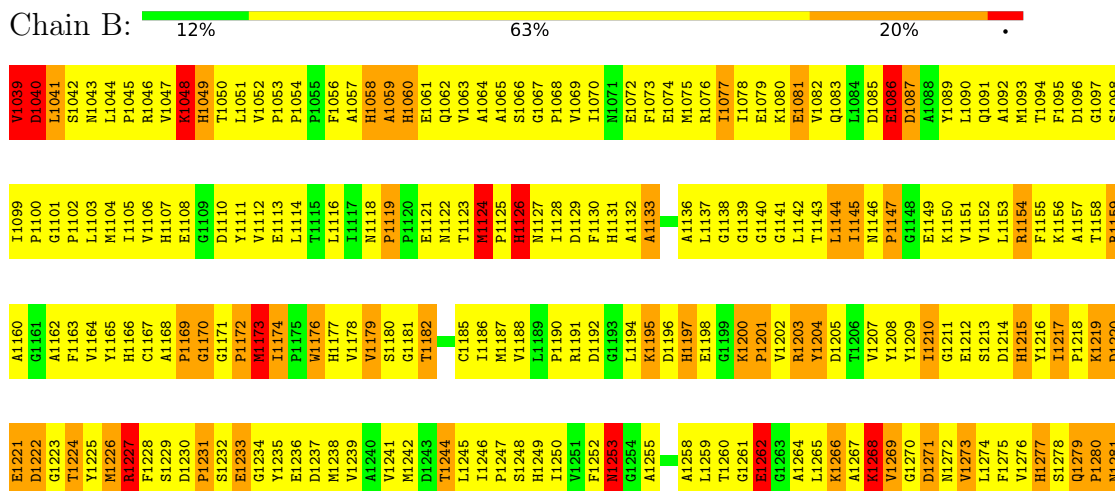
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: Copper-containing nitrite reductase



- Molecule 1: Copper-containing nitrite reductase



R1282 D1283 S1284 R1285 P1286 H1287 L1288 L1289 G1290 H1291 H1292 H1293 D1294 L1295 V1296 V1297 E1298 T1299 G1300 G1301 F1302 H1303 H1304 Q1305 A1306 E1307 R1308 D1309 L1310 E1311 T1312 W1313 F1314 I1315 R1316 G1317 G1318 T1319 A1320 G1321 A1322 A1323 L1324 Y1325 K1326 F1327 L1328 Q1329 P1330 G1331 V1332 Y1333 A1334 Y1335 V1336 N1337 H1338 N1339 L1340 I1341

E1342 A1343 V1344 S1345 K1346 G1347 A1348 T1349 A1350 H1351 L1352 L1353 V1354 E1355 G1356 E1357 W1358 D1359 G1360 N1361 D1362 M1363 E1364 Q1365 V1366 V1367 A1368 P1369 V1370 L1372

● Molecule 1: Copper-containing nitrite reductase

Chain C: 13% 60% 23% .

V2039 D2040 L2041 S2042 N2043 L2044 P2045 R2046 V2047 K2048 H2049 T2050 L2051 V2052 P2053 P2054 P2055 F2056 A2057 H2058 A2059 H2060 E2061 Q2062 V2063 A2064 A2065 S2066 G2067 P2068 V2069 I2070 N2071 F2072 F2073 E2074 N2075 R2076 I2077 I2078 E2079 K2080 E2081 V2082 Q2083 E2086 D2087 A2088 Y2089 L2090 Q2091 A2092 M2093 T2094 F2095 D2096 G2097 S2098 I2099

P2100 G2101 P2102 L2103 N2104 L2105 V2106 H2107 E2108 G2109 V2112 E2113 L2114 L2115 L2116 L2117 L2118 N2119 P2120 E2121 N2122 L2123 T2124 P2125 H2126 N2127 L2128 D2129 F2130 H2131 A2132 A2133 G2134 G2135 L2136 A2137 G2138 G2139 G2140 G2141 L2142 T2143 L2144 L2145 N2146 P2147 G2148 E2149 K2150 V2151 V2152 L2153 L2154 F2155 K2156 A2157 T2158 P2159 A2160

G2161 A2162 F2163 V2164 Y2165 H2166 C2167 A2168 P2169 G2170 G2171 P2172 H2173 I2174 P2175 W2176 H2177 V2178 N2179 S2180 G2181 T2182 G2184 C2185 I2186 N2187 L2188 L2189 P2190 R2191 D2192 G2193 L2194 K2195 D2196 H2197 E2198 G2199 R2200 P2201 V2202 R2203 Y2204 D2205 T2206 V2207 Y2208 I2209 I2210 G2211 E2212 S2213 D2214 H2215 Y2216 I2217 P2218 K2219 D2220

E2221 D2222 S2223 T2224 V2225 W2226 R2227 F2228 S2229 D2230 P2231 S2232 E2233 G2234 Y2235 E2236 D2237 N2238 V2239 A2240 M2241 D2242 D2243 T2244 L2245 L2246 F2247 S2248 H2249 L2250 V2251 F2252 N2253 G2254 A2255 V2256 G2257 A2258 L2259 T2260 G2261 E2262 L2265 K2266 A2267 K2268 V2269 G2270 G2271 V2272 V2273 L2274 F2275 V2276 H2277 S2278 Q2279 N2281

R2282 D2283 S2284 R2285 P2286 H2287 L2288 I2289 G2290 G2291 H2292 D2293 G2294 L2295 E2298 T2299 G2300 K2301 F2302 H2303 A2304 Q2305 P2306 E2307 R2308 D2309 L2310 E2311 T2312 W2313 F2314 L2315 R2316 G2317 G2318 T2319 A2320 G2321 A2322 A2323 L2324 Y2325 K2326 F2327 L2328 Q2329 P2330 G2331 V2332 Y2333 A2334 Y2335 V2336 N2337 H2338 N2339 L2340 I2341 E2342

A2343 V2344 H2345 K2346 G2347 A2348 T2349 A2350 H2351 L2352 L2353 V2354 E2355 G2356 E2357 W2358 D2359 N2360 D2361 L2362 M2363 E2364 Q2365 V2366 V2367 A2368 F2369 V2370 G2371 L2372

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.50Å 123.73Å 130.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	91.4 (30.00-2.00)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.170 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8561	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	4.08	478/2640 (18.1%)	2.77	226/3599 (6.3%)
1	B	4.00	509/2640 (19.3%)	2.69	242/3599 (6.7%)
1	C	4.01	462/2640 (17.5%)	2.74	242/3599 (6.7%)
All	All	4.03	1449/7920 (18.3%)	2.73	710/10797 (6.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	8
1	C	0	7
All	All	0	20

All (1449) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ARG	CZ-NH1	41.64	1.91	1.32
1	C	2226	MET	SD-CE	-27.78	1.10	1.79
1	C	2065	ALA	CA-CB	22.89	1.87	1.53
1	B	1040	ASP	C-O	19.77	1.48	1.24
1	A	226	MET	SD-CE	19.32	2.27	1.79
1	C	2173	MET	SD-CE	-19.14	1.31	1.79
1	C	2203	ARG	CZ-NH2	18.03	1.56	1.33
1	A	319	THR	CB-CG2	-17.81	0.93	1.52
1	C	2121	GLU	CD-OE2	17.80	1.59	1.25
1	C	2232	SER	CB-OG	17.65	1.77	1.42
1	A	40	ASP	C-O	17.62	1.46	1.24
1	A	191	ARG	NE-CZ	17.61	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2076	ARG	CZ-NH2	17.30	1.55	1.33
1	A	154	ARG	CD-NE	-17.15	1.22	1.46
1	C	2124	MET	SD-CE	-17.04	1.36	1.79
1	C	2262	GLU	CD-OE2	16.85	1.57	1.25
1	C	2154	ARG	NE-CZ	16.67	1.51	1.33
1	C	2262	GLU	CG-CD	16.46	1.93	1.52
1	A	86	GLU	CD-OE1	16.15	1.56	1.25
1	A	99	ILE	CA-CB	-16.06	1.40	1.54
1	C	2112	VAL	CA-CB	16.06	1.75	1.54
1	B	1173	MET	CA-CB	15.93	1.79	1.53
1	B	1170	GLY	C-O	15.50	1.44	1.23
1	B	1329	GLN	CA-C	-15.36	1.38	1.52
1	C	2266	LYS	CE-NZ	15.29	1.95	1.49
1	A	227	ARG	CD-NE	-15.28	1.24	1.46
1	B	1262	GLU	CD-OE2	15.18	1.54	1.25
1	A	86	GLU	CD-OE2	15.13	1.54	1.25
1	B	1226	MET	SD-CE	-15.04	1.42	1.79
1	C	2076	ARG	CZ-NH1	14.61	1.53	1.32
1	C	2203	ARG	CZ-NH1	14.55	1.53	1.32
1	C	2086	GLU	CD-OE1	14.50	1.52	1.25
1	C	2061	GLU	CD-OE2	14.34	1.52	1.25
1	A	269	VAL	CA-CB	14.27	1.70	1.54
1	C	2370	VAL	CA-C	14.14	1.69	1.52
1	B	1262	GLU	CG-CD	13.76	1.86	1.52
1	C	2061	GLU	CD-OE1	13.66	1.51	1.25
1	B	1086	GLU	CD-OE1	13.57	1.51	1.25
1	B	1087	ASP	CB-CG	13.36	1.85	1.52
1	A	200	LYS	CB-CG	-13.34	1.12	1.52
1	C	2355	GLU	CD-OE2	13.32	1.50	1.25
1	C	2151	VAL	C-O	13.29	1.39	1.23
1	C	2086	GLU	CG-CD	13.23	1.85	1.52
1	B	1367	VAL	CA-CB	13.21	1.71	1.54
1	A	339	ASN	C-O	13.08	1.39	1.24
1	B	1061	GLU	CD-OE1	12.97	1.50	1.25
1	C	2354	VAL	CA-C	12.96	1.68	1.52
1	C	2087	ASP	CG-OD2	12.79	1.49	1.25
1	B	1204	TYR	N-CA	-12.78	1.31	1.45
1	B	1272	ASN	N-CA	12.78	1.62	1.46
1	A	172	PRO	CA-C	-12.71	1.34	1.52
1	B	1121	GLU	CD-OE2	12.67	1.49	1.25
1	A	173	MET	CA-CB	12.66	1.74	1.53
1	B	1066	SER	C-O	12.65	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1052	VAL	C-O	-12.61	1.11	1.24
1	A	305	ALA	CA-CB	12.58	1.73	1.53
1	A	145	ILE	N-CA	12.56	1.61	1.46
1	C	2053	PRO	CA-C	12.43	1.63	1.52
1	B	1171	GLY	C-O	12.43	1.40	1.24
1	C	2154	ARG	CD-NE	-12.36	1.28	1.46
1	A	183	ALA	N-CA	12.34	1.60	1.46
1	A	48	LYS	CG-CD	12.34	1.89	1.52
1	B	1275	PHE	CA-CB	12.20	1.70	1.53
1	A	327	PHE	C-O	12.18	1.38	1.23
1	C	2048	LYS	CD-CE	12.18	1.89	1.52
1	A	76	ARG	CZ-NH2	12.15	1.49	1.33
1	C	2355	GLU	CD-OE1	12.14	1.48	1.25
1	C	2043	ASN	CG-OD1	12.07	1.46	1.23
1	B	1061	GLU	CD-OE2	11.99	1.48	1.25
1	B	1306	PRO	CA-C	11.95	1.67	1.52
1	B	1355	GLU	CD-OE1	11.94	1.48	1.25
1	A	255	ALA	CA-CB	11.89	1.73	1.53
1	C	2179	VAL	C-O	-11.87	1.09	1.24
1	B	1182	THR	CA-CB	11.80	1.68	1.52
1	B	1210	ILE	N-CA	-11.79	1.32	1.46
1	B	1220	ASP	CA-C	11.78	1.68	1.52
1	A	109	GLY	CA-C	11.70	1.67	1.51
1	A	127	ASN	C-O	11.70	1.32	1.24
1	A	81	GLU	N-CA	-11.67	1.31	1.46
1	A	215	HIS	CB-CG	-11.63	1.33	1.50
1	A	83	GLN	CA-C	11.62	1.67	1.52
1	A	279	GLN	CA-C	11.59	1.67	1.52
1	A	95	PHE	C-O	11.58	1.38	1.24
1	A	98	SER	CA-C	11.56	1.66	1.52
1	B	1086	GLU	CD-OE2	11.56	1.47	1.25
1	A	357	GLU	CD-OE2	11.55	1.47	1.25
1	A	174	ILE	CA-C	11.52	1.65	1.52
1	B	1191	ARG	CZ-NH2	11.51	1.48	1.33
1	B	1200	LYS	CD-CE	11.44	1.86	1.52
1	A	86	GLU	CG-CD	11.43	1.80	1.52
1	A	221	GLU	CD-OE1	11.40	1.47	1.25
1	B	1089	TYR	C-O	-11.40	1.09	1.23
1	C	2104	MET	SD-CE	-11.37	1.51	1.79
1	B	1087	ASP	CG-OD2	11.35	1.47	1.25
1	A	87	ASP	CB-CG	11.31	1.80	1.52
1	C	2355	GLU	CA-C	-11.30	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	MET	N-CA	11.30	1.58	1.45
1	B	1348	ALA	CA-CB	11.29	1.67	1.52
1	B	1308	ARG	NE-CZ	11.23	1.45	1.33
1	C	2154	ARG	CZ-NH1	11.23	1.48	1.32
1	C	2082	VAL	CA-CB	11.21	1.74	1.54
1	B	1266	LYS	CE-NZ	11.19	1.82	1.49
1	C	2227	ARG	CD-NE	-11.16	1.30	1.46
1	A	233	GLU	CG-CD	11.15	1.79	1.52
1	C	2327	PHE	CA-C	11.15	1.68	1.52
1	A	147	PRO	CA-CB	-11.12	1.38	1.53
1	B	1366	VAL	CA-C	11.04	1.66	1.52
1	C	2043	ASN	CG-ND2	11.04	1.56	1.33
1	B	1191	ARG	CZ-NH1	11.02	1.48	1.32
1	B	1172	PRO	C-O	-10.98	1.08	1.24
1	B	1196	ASP	N-CA	-10.97	1.34	1.46
1	B	1262	GLU	CD-OE1	10.95	1.46	1.25
1	A	258	ALA	CA-CB	10.93	1.70	1.53
1	A	195	LYS	CE-NZ	10.92	1.82	1.49
1	A	134	THR	CA-C	10.87	1.65	1.52
1	A	152	VAL	CA-CB	-10.86	1.40	1.54
1	B	1163	PHE	C-O	10.86	1.37	1.23
1	A	230	ASP	CA-C	10.85	1.62	1.52
1	A	343	ALA	CA-CB	10.84	1.70	1.53
1	B	1182	THR	C-O	10.84	1.38	1.23
1	B	1359	ASP	C-O	10.84	1.36	1.24
1	B	1361	ASP	CA-C	10.82	1.67	1.52
1	A	188	VAL	CA-C	10.81	1.64	1.52
1	A	48	LYS	CD-CE	10.79	1.84	1.52
1	A	40	ASP	CG-OD2	10.79	1.45	1.25
1	C	2040	ASP	CG-OD2	10.77	1.45	1.25
1	A	200	LYS	CE-NZ	10.77	1.81	1.49
1	B	1076	ARG	CZ-NH1	10.75	1.47	1.32
1	B	1259	LEU	CA-CB	10.74	1.67	1.53
1	A	76	ARG	CZ-NH1	10.72	1.47	1.32
1	B	1355	GLU	CD-OE2	10.69	1.45	1.25
1	C	2132	ALA	CA-C	10.63	1.67	1.52
1	C	2362	LEU	N-CA	10.63	1.59	1.46
1	B	1192	ASP	CG-OD2	10.63	1.45	1.25
1	B	1301	LYS	N-CA	10.62	1.58	1.46
1	A	357	GLU	CD-OE1	10.61	1.45	1.25
1	A	251	VAL	N-CA	-10.58	1.34	1.46
1	B	1275	PHE	C-O	10.58	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1216	TYR	CA-CB	10.57	1.67	1.53
1	A	164	VAL	N-CA	10.55	1.59	1.46
1	A	262	GLU	CD-OE2	10.53	1.45	1.25
1	B	1070	ILE	C-O	10.52	1.35	1.24
1	A	91	GLN	CA-C	10.51	1.66	1.52
1	A	222	ASP	CG-OD2	10.48	1.45	1.25
1	B	1173	MET	N-CA	-10.48	1.32	1.46
1	A	121	GLU	N-CA	-10.46	1.32	1.46
1	C	2319	THR	CB-CG2	-10.40	1.18	1.52
1	B	1274	LEU	CA-CB	10.38	1.66	1.53
1	C	2214	ASP	CA-C	10.35	1.65	1.52
1	C	2169	PRO	C-O	10.35	1.37	1.24
1	C	2190	PRO	CA-C	10.34	1.65	1.52
1	A	217	ILE	CA-CB	-10.31	1.40	1.54
1	C	2239	VAL	CA-CB	10.27	1.67	1.54
1	A	196	ASP	C-O	-10.24	1.12	1.23
1	B	1040	ASP	CA-C	10.24	1.66	1.52
1	C	2048	LYS	CG-CD	10.23	1.83	1.52
1	C	2143	THR	CA-C	-10.22	1.40	1.52
1	C	2167	CYS	CB-SG	-10.22	1.47	1.81
1	B	1076	ARG	CZ-NH2	10.19	1.46	1.33
1	B	1125	PRO	CA-C	10.18	1.65	1.52
1	B	1168	ALA	C-O	-10.18	1.11	1.24
1	B	1221	GLU	CD-OE2	10.18	1.44	1.25
1	C	2246	ILE	C-O	10.18	1.36	1.24
1	B	1039	VAL	CA-CB	10.17	1.81	1.54
1	C	2147	PRO	CA-CB	-10.17	1.40	1.53
1	C	2370	VAL	N-CA	-10.15	1.34	1.46
1	C	2121	GLU	CB-CG	-10.15	1.22	1.52
1	C	2039	VAL	N-CA	10.14	1.65	1.46
1	A	246	ILE	N-CA	10.14	1.54	1.46
1	A	327	PHE	CA-C	10.13	1.66	1.52
1	A	182	THR	CA-C	10.13	1.65	1.52
1	B	1116	LEU	CA-C	-10.12	1.40	1.52
1	A	152	VAL	C-O	10.12	1.35	1.24
1	A	360	ASN	CA-C	-10.11	1.38	1.52
1	A	91	GLN	CA-CB	10.07	1.65	1.52
1	A	151	VAL	C-O	10.01	1.35	1.23
1	C	2222	ASP	CG-OD2	9.98	1.44	1.25
1	B	1355	GLU	CA-C	-9.98	1.38	1.53
1	C	2156	LYS	CE-NZ	9.98	1.79	1.49
1	A	176	TRP	CZ3-CH2	9.96	1.65	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	ASN	CG-OD1	9.94	1.42	1.23
1	A	296	VAL	C-O	9.88	1.34	1.24
1	A	219	LYS	CA-C	9.86	1.64	1.52
1	B	1221	GLU	CG-CD	9.85	1.76	1.52
1	B	1217	ILE	C-O	9.84	1.36	1.24
1	B	1331	GLY	C-O	9.83	1.35	1.23
1	B	1363	MET	CA-C	9.81	1.64	1.52
1	B	1253	ASN	CG-OD1	9.80	1.42	1.23
1	C	2349	THR	CA-CB	9.79	1.72	1.53
1	B	1040	ASP	CG-OD2	9.76	1.43	1.25
1	C	2273	VAL	C-O	9.76	1.35	1.24
1	A	159	ARG	CB-CG	9.75	1.81	1.52
1	B	1319	THR	CB-CG2	-9.75	1.20	1.52
1	C	2361	ASP	CA-C	9.74	1.66	1.52
1	A	74	GLU	C-O	9.71	1.35	1.23
1	C	2156	LYS	C-O	9.70	1.35	1.23
1	A	191	ARG	CA-CB	9.66	1.69	1.53
1	A	337	ASN	CA-C	9.66	1.65	1.52
1	B	1181	GLY	C-O	9.66	1.34	1.24
1	A	262	GLU	CG-CD	9.66	1.76	1.52
1	B	1357	GLU	CG-CD	9.66	1.76	1.52
1	C	2173	MET	CG-SD	9.65	2.04	1.80
1	B	1227	ARG	CD-NE	-9.64	1.32	1.46
1	A	173	MET	CB-CG	9.62	1.81	1.52
1	A	215	HIS	C-O	9.63	1.35	1.23
1	B	1292	HIS	N-CA	9.63	1.57	1.46
1	A	210	ILE	C-O	9.62	1.34	1.24
1	B	1060	HIS	CA-C	-9.61	1.40	1.52
1	C	2295	LEU	C-O	9.61	1.34	1.24
1	C	2359	ASP	C-O	9.61	1.34	1.24
1	C	2200	LYS	CA-CB	-9.57	1.36	1.53
1	B	1126	HIS	C-O	9.56	1.36	1.23
1	A	187	MET	CA-CB	9.55	1.66	1.53
1	A	359	ASP	CA-C	9.55	1.65	1.52
1	C	2313	TRP	CA-C	9.55	1.65	1.52
1	B	1230	ASP	CG-OD1	9.55	1.43	1.25
1	B	1091	GLN	C-O	9.53	1.35	1.23
1	A	203	ARG	NE-CZ	-9.53	1.22	1.33
1	C	2308	ARG	NE-CZ	9.53	1.43	1.33
1	B	1268	LYS	CD-CE	9.53	1.81	1.52
1	A	159	ARG	CZ-NH1	9.52	1.46	1.32
1	A	144	LEU	CA-C	9.52	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1052	VAL	CA-CB	-9.49	1.46	1.55
1	B	1203	ARG	CZ-NH2	9.48	1.45	1.33
1	C	2119	PRO	C-O	-9.48	1.17	1.25
1	B	1237	ASP	C-O	-9.44	1.12	1.24
1	C	2371	GLY	CA-C	-9.44	1.43	1.52
1	A	338	HIS	CA-CB	9.43	1.69	1.53
1	A	361	ASP	CA-C	9.43	1.65	1.52
1	B	1124	MET	CA-CB	-9.42	1.42	1.54
1	C	2059	ALA	CA-CB	9.41	1.69	1.53
1	A	124	MET	C-O	-9.41	1.14	1.24
1	A	62	GLN	CG-CD	9.39	1.75	1.52
1	B	1295	LEU	N-CA	-9.39	1.34	1.46
1	A	274	LEU	C-O	9.37	1.35	1.24
1	B	1203	ARG	CZ-NH1	9.37	1.45	1.32
1	C	2098	SER	N-CA	9.35	1.57	1.45
1	C	2076	ARG	C-O	9.35	1.35	1.23
1	B	1203	ARG	NE-CZ	9.34	1.43	1.33
1	C	2233	GLU	CA-C	9.33	1.65	1.52
1	A	171	GLY	C-O	9.32	1.36	1.24
1	B	1192	ASP	C-O	9.28	1.36	1.24
1	C	2091	GLN	CD-OE1	9.28	1.41	1.23
1	A	135	GLY	C-O	9.26	1.34	1.23
1	B	1369	PRO	C-O	9.22	1.35	1.23
1	A	124	MET	CA-C	9.21	1.64	1.52
1	C	2372	LEU	C-O	9.21	1.42	1.23
1	B	1186	ILE	CA-CB	9.21	1.68	1.54
1	A	93	MET	SD-CE	-9.20	1.56	1.79
1	A	150	LYS	C-O	9.20	1.35	1.23
1	A	342	GLU	CA-C	9.20	1.64	1.52
1	A	371	GLY	CA-C	-9.19	1.41	1.52
1	C	2274	LEU	C-O	9.18	1.34	1.24
1	A	272	ASN	C-O	9.18	1.34	1.24
1	C	2336	VAL	C-O	9.16	1.34	1.23
1	A	285	ARG	N-CA	9.16	1.57	1.46
1	B	1269	VAL	CB-CG2	9.15	1.82	1.52
1	B	1059	ALA	CA-CB	9.13	1.68	1.53
1	C	2087	ASP	CB-CG	9.12	1.74	1.52
1	A	355	GLU	CD-OE1	9.12	1.42	1.25
1	B	1368	ALA	CA-C	9.12	1.65	1.53
1	C	2366	VAL	CA-C	9.12	1.64	1.52
1	A	364	GLU	CA-C	9.09	1.63	1.52
1	A	289	ILE	CA-C	9.08	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1124	MET	N-CA	9.07	1.55	1.45
1	B	1195	LYS	CD-CE	9.07	1.79	1.52
1	B	1058	HIS	CG-ND1	9.06	1.48	1.38
1	B	1046	ARG	CD-NE	9.05	1.58	1.46
1	B	1197	HIS	N-CA	9.03	1.58	1.46
1	C	2172	PRO	CA-C	-9.02	1.35	1.52
1	A	87	ASP	CA-C	9.01	1.64	1.53
1	A	193	GLY	CA-C	9.00	1.66	1.52
1	C	2236	GLU	CG-CD	9.00	1.74	1.52
1	B	1091	GLN	CA-CB	9.00	1.64	1.52
1	A	168	ALA	C-O	-8.98	1.12	1.24
1	B	1203	ARG	CB-CG	-8.97	1.25	1.52
1	A	370	VAL	N-CA	-8.96	1.36	1.46
1	B	1182	THR	CA-C	-8.95	1.41	1.52
1	C	2371	GLY	C-O	8.95	1.35	1.23
1	B	1235	TYR	N-CA	8.92	1.57	1.46
1	A	200	LYS	CA-CB	-8.92	1.40	1.53
1	C	2243	ASP	CA-C	8.90	1.65	1.52
1	B	1078	ILE	C-O	8.88	1.34	1.24
1	A	43	ASN	CG-ND2	8.87	1.51	1.33
1	A	335	TYR	N-CA	8.86	1.57	1.46
1	C	2066	SER	CB-OG	8.85	1.59	1.42
1	C	2338	HIS	CA-CB	8.85	1.65	1.53
1	A	229	SER	CB-OG	8.85	1.59	1.42
1	A	91	GLN	N-CA	8.83	1.57	1.46
1	A	266	LYS	CD-CE	8.83	1.78	1.52
1	A	209	TYR	C-O	8.83	1.34	1.24
1	B	1281	ASN	CA-C	8.82	1.62	1.52
1	A	159	ARG	N-CA	8.79	1.56	1.46
1	C	2191	ARG	CZ-NH1	8.78	1.45	1.32
1	C	2337	ASN	CA-C	8.78	1.63	1.52
1	A	308	ARG	CZ-NH1	8.77	1.45	1.32
1	B	1110	ASP	CA-CB	8.77	1.66	1.53
1	B	1149	GLU	C-O	8.76	1.35	1.23
1	A	165	TYR	C-O	8.75	1.34	1.23
1	C	2282	ARG	CZ-NH2	8.75	1.44	1.33
1	A	270	GLY	C-O	-8.74	1.11	1.24
1	C	2171	GLY	CA-C	-8.74	1.39	1.51
1	A	221	GLU	CD-OE2	8.74	1.42	1.25
1	A	162	ALA	C-O	8.73	1.34	1.23
1	C	2087	ASP	CA-CB	8.72	1.65	1.53
1	B	1123	THR	CA-CB	-8.72	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2163	PHE	CA-C	8.71	1.63	1.52
1	C	2305	ALA	CA-CB	8.71	1.66	1.53
1	C	2292	HIS	CA-C	8.69	1.63	1.52
1	C	2253	ASN	CA-CB	8.69	1.66	1.53
1	A	48	LYS	C-O	-8.68	1.13	1.24
1	A	203	ARG	C-O	8.68	1.34	1.23
1	A	237	ASP	CB-CG	8.67	1.73	1.52
1	C	2227	ARG	CZ-NH2	8.67	1.44	1.33
1	B	1143	THR	CA-CB	8.66	1.65	1.53
1	B	1242	MET	C-O	8.65	1.34	1.24
1	B	1339	ASN	CA-C	8.64	1.63	1.52
1	C	2142	LEU	CB-CG	8.64	1.70	1.53
1	C	2086	GLU	CD-OE2	8.61	1.41	1.25
1	B	1096	ASP	N-CA	8.60	1.57	1.46
1	B	1273	VAL	N-CA	-8.60	1.35	1.46
1	C	2182	THR	CA-CB	8.60	1.64	1.52
1	B	1281	ASN	CG-OD1	8.60	1.39	1.23
1	C	2242	MET	N-CA	8.60	1.56	1.46
1	B	1168	ALA	CA-C	8.58	1.63	1.52
1	C	2078	ILE	C-O	8.58	1.33	1.24
1	C	2192	ASP	CG-OD1	8.56	1.41	1.25
1	B	1056	PHE	C-O	8.55	1.35	1.23
1	A	263	GLY	CA-C	8.53	1.63	1.51
1	B	1311	GLU	N-CA	-8.53	1.35	1.46
1	B	1157	ALA	N-CA	8.51	1.57	1.46
1	C	2200	LYS	C-N	8.50	1.43	1.33
1	A	65	ALA	CA-C	8.49	1.64	1.52
1	C	2039	VAL	C-O	8.49	1.40	1.23
1	C	2109	GLY	C-N	8.49	1.44	1.33
1	B	1048	LYS	CD-CE	8.48	1.77	1.52
1	A	352	VAL	CA-C	8.48	1.63	1.52
1	C	2098	SER	CB-OG	8.47	1.59	1.42
1	A	88	ALA	CA-CB	8.47	1.68	1.53
1	A	303	HIS	CG-ND1	8.47	1.47	1.38
1	B	1330	PRO	CA-C	8.46	1.62	1.53
1	C	2121	GLU	CG-CD	8.46	1.73	1.52
1	B	1121	GLU	C-N	8.46	1.44	1.33
1	A	80	LYS	C-O	8.45	1.33	1.23
1	A	264	ALA	N-CA	-8.45	1.35	1.46
1	B	1176	TRP	CA-C	8.45	1.63	1.52
1	B	1249	HIS	CA-C	8.44	1.63	1.52
1	B	1165	TYR	C-O	8.44	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1113	GLU	CB-CG	-8.43	1.27	1.52
1	A	225	TYR	C-O	8.42	1.34	1.23
1	A	258	ALA	C-O	8.42	1.33	1.24
1	C	2174	ILE	CA-C	8.42	1.60	1.52
1	C	2213	SER	CB-OG	8.41	1.58	1.42
1	B	1083	GLN	CA-C	8.41	1.63	1.52
1	A	285	ARG	CD-NE	8.37	1.57	1.46
1	B	1297	TRP	CA-C	-8.37	1.42	1.53
1	B	1108	GLU	CA-C	8.36	1.63	1.52
1	C	2364	GLU	CA-CB	8.35	1.68	1.53
1	A	267	ALA	CA-CB	8.34	1.67	1.53
1	A	221	GLU	CA-C	-8.34	1.41	1.52
1	C	2039	VAL	CA-CB	8.32	1.76	1.54
1	C	2311	GLU	C-O	8.31	1.34	1.24
1	A	306	PRO	C-O	8.31	1.33	1.23
1	B	1260	THR	CA-C	8.30	1.63	1.52
1	C	2236	GLU	CD-OE2	8.30	1.41	1.25
1	B	1086	GLU	CG-CD	8.29	1.72	1.52
1	C	2247	PRO	CA-C	8.28	1.63	1.52
1	C	2099	ILE	CA-CB	-8.28	1.47	1.54
1	C	2289	ILE	C-O	8.27	1.32	1.24
1	A	163	PHE	C-O	8.26	1.33	1.23
1	B	1092	ALA	C-O	8.25	1.34	1.23
1	C	2353	LEU	N-CA	8.23	1.56	1.46
1	A	168	ALA	CA-CB	8.22	1.66	1.53
1	C	2198	GLU	CD-OE2	8.21	1.41	1.25
1	B	1212	GLU	C-O	8.20	1.33	1.23
1	A	66	SER	CA-C	-8.16	1.42	1.53
1	B	1209	TYR	CA-C	8.16	1.62	1.52
1	B	1320	ALA	CA-C	8.16	1.62	1.52
1	B	1182	THR	N-CA	8.16	1.57	1.46
1	C	2143	THR	C-O	8.14	1.36	1.24
1	C	2308	ARG	N-CA	8.14	1.55	1.45
1	C	2070	ILE	CA-C	8.13	1.62	1.52
1	A	130	PHE	CA-C	8.13	1.62	1.52
1	C	2169	PRO	C-N	-8.13	1.21	1.33
1	C	2246	ILE	CG1-CD1	8.12	1.83	1.51
1	B	1077	ILE	CG1-CD1	-8.12	1.20	1.51
1	A	126	HIS	C-N	8.11	1.41	1.33
1	C	2164	VAL	CA-CB	8.11	1.64	1.54
1	B	1226	MET	N-CA	-8.11	1.35	1.45
1	C	2127	ASN	C-O	8.10	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ILE	CB-CG1	8.10	1.69	1.53
1	B	1051	LEU	C-O	8.10	1.33	1.23
1	A	51	LEU	CA-C	8.10	1.63	1.52
1	A	154	ARG	CZ-NH1	8.10	1.44	1.32
1	A	136	ALA	CA-CB	8.09	1.67	1.53
1	B	1065	ALA	CA-CB	-8.09	1.39	1.53
1	C	2083	GLN	CA-C	8.08	1.63	1.52
1	B	1332	VAL	CA-CB	-8.06	1.44	1.54
1	B	1364	GLU	CA-CB	8.06	1.67	1.53
1	C	2334	ALA	CA-C	8.05	1.62	1.52
1	A	268	LYS	CE-NZ	8.04	1.73	1.49
1	A	280	PRO	CA-CB	8.04	1.65	1.53
1	A	279	GLN	C-O	-8.04	1.14	1.24
1	B	1327	PHE	CA-C	-8.04	1.41	1.52
1	A	170	GLY	C-O	8.04	1.34	1.23
1	B	1281	ASN	C-O	8.03	1.33	1.23
1	C	2191	ARG	CA-C	-8.02	1.41	1.52
1	A	212	GLU	C-O	8.01	1.33	1.24
1	B	1039	VAL	CA-C	8.00	1.69	1.52
1	A	76	ARG	CB-CG	-7.99	1.28	1.52
1	A	73	PHE	CA-C	7.99	1.62	1.52
1	B	1058	HIS	C-N	7.97	1.43	1.33
1	B	1283	ASP	CA-C	-7.97	1.42	1.53
1	B	1098	SER	CA-C	7.95	1.62	1.52
1	B	1333	TYR	N-CA	7.94	1.55	1.45
1	B	1255	ALA	CA-CB	7.94	1.67	1.53
1	C	2112	VAL	CA-C	-7.94	1.42	1.52
1	C	2349	THR	C-O	7.94	1.33	1.24
1	C	2344	VAL	CA-CB	7.93	1.64	1.54
1	C	2259	LEU	CG-CD1	7.92	1.78	1.52
1	B	1294	ASP	CG-OD2	7.92	1.40	1.25
1	B	1355	GLU	CG-CD	7.91	1.71	1.52
1	C	2324	LEU	CG-CD2	7.91	1.78	1.52
1	C	2166	HIS	CA-C	7.90	1.62	1.52
1	C	2127	ASN	CA-C	7.89	1.62	1.53
1	B	1048	LYS	CE-NZ	7.88	1.73	1.49
1	B	1114	LEU	CA-CB	7.87	1.67	1.53
1	C	2093	MET	CA-C	7.86	1.61	1.52
1	C	2221	GLU	CG-CD	7.86	1.71	1.52
1	B	1151	VAL	C-O	7.85	1.32	1.23
1	B	1192	ASP	CB-CG	-7.85	1.32	1.52
1	C	2149	GLU	C-O	7.84	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	ARG	CA-C	7.84	1.62	1.52
1	B	1221	GLU	N-CA	7.84	1.56	1.46
1	C	2365	GLN	C-O	7.81	1.34	1.23
1	A	320	ALA	CA-C	7.81	1.62	1.52
1	A	332	VAL	C-O	7.81	1.34	1.24
1	B	1073	PHE	CD2-CE2	7.80	1.62	1.38
1	A	287	HIS	CA-C	7.80	1.62	1.52
1	A	289	ILE	CB-CG1	7.79	1.69	1.53
1	B	1118	ASN	CA-C	7.79	1.62	1.52
1	A	203	ARG	CD-NE	-7.79	1.35	1.46
1	A	239	VAL	CA-CB	7.78	1.64	1.54
1	A	240	ALA	C-O	-7.78	1.14	1.24
1	A	372	LEU	CA-C	7.78	1.69	1.52
1	B	1292	HIS	CG-CD2	7.78	1.44	1.35
1	B	1344	VAL	CA-C	7.78	1.63	1.52
1	C	2049	HIS	ND1-CE1	7.75	1.40	1.32
1	C	2106	VAL	CA-C	-7.75	1.46	1.52
1	B	1209	TYR	CA-CB	7.74	1.64	1.53
1	C	2346	LYS	N-CA	7.74	1.56	1.46
1	C	2224	THR	CB-CG2	7.74	1.78	1.52
1	C	2331	GLY	C-O	7.74	1.30	1.23
1	B	1138	GLY	C-O	7.74	1.34	1.23
1	B	1267	ALA	C-O	7.73	1.33	1.23
1	A	344	VAL	C-O	-7.73	1.15	1.23
1	C	2112	VAL	C-O	7.72	1.32	1.24
1	B	1152	VAL	N-CA	7.71	1.55	1.46
1	A	339	ASN	CG-OD1	7.70	1.38	1.23
1	A	65	ALA	CA-CB	7.69	1.66	1.53
1	A	133	ALA	CA-CB	7.68	1.65	1.53
1	C	2108	GLU	C-O	7.67	1.32	1.23
1	A	322	ALA	CA-CB	7.67	1.66	1.53
1	A	366	VAL	CA-C	7.66	1.62	1.52
1	C	2208	TYR	CE2-CZ	7.66	1.56	1.38
1	B	1132	ALA	CA-C	7.64	1.63	1.52
1	B	1314	PHE	CA-C	-7.62	1.43	1.52
1	A	253	ASN	CA-CB	-7.62	1.42	1.53
1	B	1288	LEU	CA-CB	7.62	1.62	1.53
1	A	179	VAL	C-O	7.61	1.33	1.24
1	C	2176	TRP	C-O	7.61	1.33	1.24
1	C	2302	PHE	CE1-CZ	-7.61	1.15	1.38
1	C	2145	ILE	CB-CG1	7.60	1.68	1.53
1	B	1282	ARG	C-O	7.59	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	ASP	C-N	7.59	1.43	1.33
1	A	164	VAL	CA-C	7.58	1.61	1.52
1	B	1069	VAL	N-CA	-7.57	1.36	1.46
1	B	1210	ILE	CA-CB	7.56	1.62	1.53
1	A	240	ALA	CA-C	7.55	1.62	1.52
1	B	1086	GLU	CB-CG	7.54	1.75	1.52
1	C	2293	GLY	C-O	7.54	1.34	1.23
1	B	1174	ILE	CG1-CD1	7.53	1.81	1.51
1	A	226	MET	CA-C	-7.53	1.42	1.52
1	A	211	GLY	C-O	7.52	1.34	1.23
1	B	1345	HIS	CB-CG	7.52	1.60	1.50
1	A	209	TYR	CE2-CZ	7.51	1.56	1.38
1	A	174	ILE	CB-CG1	7.51	1.68	1.53
1	B	1221	GLU	CD-OE1	7.51	1.39	1.25
1	A	195	LYS	CD-CE	7.51	1.75	1.52
1	A	143	THR	CA-CB	7.50	1.64	1.53
1	C	2058	HIS	C-O	7.50	1.34	1.23
1	A	161	GLY	CA-C	7.49	1.59	1.51
1	A	210	ILE	CG1-CD1	-7.49	1.22	1.51
1	A	316	ARG	CD-NE	7.49	1.56	1.46
1	C	2191	ARG	NE-CZ	7.48	1.41	1.33
1	B	1048	LYS	CA-C	7.48	1.62	1.52
1	C	2042	SER	N-CA	7.47	1.55	1.46
1	B	1174	ILE	CA-C	7.47	1.60	1.52
1	C	2168	ALA	C-O	-7.46	1.14	1.24
1	A	98	SER	CB-OG	7.45	1.57	1.42
1	A	70	ILE	C-O	7.45	1.32	1.24
1	C	2262	GLU	CD-OE1	7.45	1.39	1.25
1	B	1239	VAL	N-CA	7.45	1.55	1.46
1	B	1326	LYS	N-CA	7.44	1.55	1.46
1	C	2045	PRO	CA-C	7.44	1.61	1.52
1	C	2217	ILE	CG1-CD1	7.44	1.80	1.51
1	C	2062	GLN	C-O	-7.43	1.15	1.24
1	B	1061	GLU	CG-CD	7.43	1.70	1.52
1	A	127	ASN	CA-CB	7.43	1.63	1.54
1	B	1242	MET	CA-CB	7.42	1.65	1.53
1	A	372	LEU	CG-CD1	-7.42	1.28	1.52
1	B	1208	TYR	CE2-CZ	7.41	1.56	1.38
1	A	343	ALA	CA-C	7.40	1.62	1.52
1	A	191	ARG	CZ-NH2	-7.40	1.23	1.33
1	C	2174	ILE	CA-CB	7.39	1.58	1.54
1	B	1234	GLY	C-O	-7.39	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1222	ASP	CG-OD2	7.39	1.39	1.25
1	A	330	PRO	N-CD	7.38	1.58	1.47
1	A	266	LYS	CG-CD	-7.38	1.30	1.52
1	A	337	ASN	CB-CG	7.38	1.70	1.52
1	C	2238	MET	CA-C	7.38	1.62	1.52
1	A	348	ALA	CA-C	7.37	1.61	1.53
1	C	2347	GLY	CA-C	-7.36	1.41	1.51
1	A	340	LEU	N-CA	7.35	1.55	1.46
1	A	92	ALA	C-O	7.35	1.33	1.23
1	C	2278	SER	N-CA	7.35	1.54	1.45
1	A	53	PRO	CA-CB	-7.34	1.44	1.54
1	B	1113	GLU	CG-CD	7.34	1.70	1.52
1	B	1232	SER	CA-CB	7.34	1.64	1.53
1	B	1236	GLU	CD-OE1	7.34	1.39	1.25
1	C	2092	ALA	CA-C	-7.33	1.42	1.53
1	C	2173	MET	CB-CG	7.33	1.74	1.52
1	C	2125	PRO	CA-C	7.33	1.62	1.52
1	A	77	ILE	C-O	7.33	1.32	1.24
1	A	76	ARG	C-O	7.32	1.32	1.23
1	C	2357	GLU	CD-OE1	7.32	1.39	1.25
1	B	1104	MET	SD-CE	-7.32	1.61	1.79
1	A	364	GLU	N-CA	7.31	1.54	1.46
1	C	2175	PRO	CA-C	7.31	1.62	1.52
1	B	1104	MET	CG-SD	7.31	1.99	1.80
1	A	62	GLN	C-O	-7.30	1.15	1.24
1	A	113	GLU	C-O	7.30	1.32	1.24
1	A	362	LEU	N-CA	7.29	1.55	1.46
1	C	2365	GLN	CA-CB	-7.28	1.42	1.52
1	C	2335	TYR	CA-C	7.28	1.61	1.52
1	C	2137	LEU	N-CA	-7.28	1.35	1.46
1	B	1287	HIS	CA-C	7.27	1.61	1.52
1	C	2154	ARG	CZ-NH2	7.27	1.42	1.33
1	A	43	ASN	CG-OD1	7.26	1.37	1.23
1	B	1047	VAL	CA-C	-7.26	1.43	1.52
1	B	1233	GLU	C-O	-7.26	1.15	1.24
1	C	2083	GLN	N-CA	-7.25	1.37	1.46
1	C	2058	HIS	CA-CB	-7.25	1.41	1.53
1	A	365	GLN	C-O	-7.24	1.13	1.23
1	B	1155	PHE	C-N	-7.23	1.23	1.33
1	C	2278	SER	CA-CB	7.23	1.65	1.53
1	C	2210	ILE	N-CA	7.23	1.54	1.46
1	C	2144	LEU	N-CA	7.21	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ARG	CZ-NH2	7.21	1.42	1.33
1	B	1198	GLU	CD-OE2	7.20	1.39	1.25
1	A	235	TYR	CD2-CE2	7.20	1.60	1.38
1	B	1149	GLU	CA-CB	-7.20	1.41	1.54
1	C	2046	ARG	N-CA	-7.19	1.37	1.46
1	C	2363	MET	CG-SD	7.19	1.98	1.80
1	C	2164	VAL	N-CA	7.19	1.54	1.46
1	A	338	HIS	ND1-CE1	7.19	1.39	1.32
1	C	2326	LYS	CE-NZ	7.19	1.71	1.49
1	A	304	ASN	C-N	-7.18	1.22	1.33
1	C	2064	ALA	C-O	-7.18	1.14	1.23
1	C	2246	ILE	CA-CB	7.18	1.61	1.53
1	B	1203	ARG	CG-CD	7.17	1.74	1.52
1	C	2305	ALA	CA-C	7.17	1.61	1.53
1	C	2330	PRO	CG-CD	7.17	1.75	1.50
1	B	1191	ARG	CG-CD	7.17	1.74	1.52
1	C	2343	ALA	C-O	7.16	1.32	1.24
1	C	2175	PRO	C-O	-7.16	1.15	1.24
1	B	1357	GLU	CA-C	7.15	1.61	1.52
1	B	1273	VAL	CA-C	7.15	1.61	1.52
1	A	312	THR	C-O	7.15	1.32	1.23
1	B	1324	LEU	N-CA	7.15	1.54	1.45
1	A	57	ALA	N-CA	7.15	1.55	1.45
1	B	1297	TRP	C-O	7.15	1.32	1.23
1	C	2330	PRO	C-O	7.13	1.33	1.24
1	C	2326	LYS	CD-CE	7.13	1.73	1.52
1	B	1334	ALA	C-O	7.13	1.33	1.24
1	B	1349	THR	CA-CB	7.13	1.68	1.53
1	B	1173	MET	CG-SD	7.12	1.98	1.80
1	A	179	VAL	CA-C	7.12	1.60	1.52
1	A	347	GLY	C-N	7.12	1.42	1.33
1	A	367	VAL	C-O	7.11	1.31	1.24
1	B	1052	VAL	CA-C	7.11	1.58	1.52
1	B	1312	THR	C-N	7.11	1.43	1.33
1	B	1165	TYR	CA-C	-7.11	1.44	1.52
1	C	2271	ASP	CA-C	7.11	1.62	1.52
1	C	2315	ILE	C-O	7.11	1.31	1.24
1	B	1075	MET	CG-SD	7.10	1.98	1.80
1	B	1121	GLU	CG-CD	7.10	1.69	1.52
1	B	1069	VAL	C-O	7.10	1.31	1.23
1	B	1187	MET	N-CA	-7.09	1.37	1.46
1	C	2256	VAL	CA-C	7.09	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1119	PRO	C-O	-7.09	1.19	1.25
1	A	48	LYS	CE-NZ	7.08	1.70	1.49
1	B	1094	THR	N-CA	-7.08	1.36	1.45
1	A	159	ARG	CG-CD	-7.07	1.31	1.52
1	C	2165	TYR	N-CA	7.07	1.54	1.45
1	C	2134	THR	CA-C	7.06	1.61	1.52
1	C	2126	HIS	C-N	7.06	1.42	1.33
1	B	1173	MET	CB-CG	7.06	1.73	1.52
1	A	295	LEU	C-O	7.05	1.32	1.23
1	B	1357	GLU	CD-OE1	7.05	1.38	1.25
1	C	2102	PRO	C-O	7.05	1.32	1.23
1	B	1217	ILE	CB-CG2	7.05	1.75	1.52
1	C	2159	ARG	N-CA	-7.04	1.37	1.46
1	B	1043	ASN	CG-OD1	7.03	1.36	1.23
1	C	2052	VAL	CA-C	7.03	1.60	1.52
1	B	1252	PHE	CE1-CZ	7.03	1.59	1.38
1	B	1058	HIS	CA-C	-7.03	1.43	1.53
1	C	2349	THR	CA-C	-7.03	1.44	1.52
1	B	1336	VAL	CA-CB	7.01	1.67	1.55
1	C	2096	ASP	CA-C	-7.01	1.43	1.52
1	B	1156	LYS	C-O	7.00	1.32	1.24
1	B	1244	THR	CB-CG2	7.00	1.75	1.52
1	A	214	ASP	N-CA	6.98	1.54	1.46
1	C	2063	VAL	C-O	6.98	1.31	1.24
1	C	2241	VAL	N-CA	6.98	1.54	1.46
1	A	268	LYS	CB-CG	-6.98	1.31	1.52
1	C	2274	LEU	CB-CG	6.97	1.67	1.53
1	B	1186	ILE	C-O	6.97	1.30	1.24
1	C	2305	ALA	C-N	-6.97	1.25	1.33
1	A	75	MET	C-O	6.96	1.32	1.23
1	C	2087	ASP	CA-C	6.96	1.61	1.52
1	B	1073	PHE	CG-CD1	6.96	1.53	1.38
1	B	1289	ILE	CA-C	6.96	1.60	1.52
1	A	173	MET	CG-SD	6.95	1.98	1.80
1	C	2333	TYR	N-CA	6.95	1.54	1.45
1	C	2065	ALA	C-O	6.95	1.35	1.24
1	B	1130	PHE	CD2-CE2	6.95	1.59	1.38
1	A	289	ILE	CB-CG2	6.95	1.75	1.52
1	C	2088	ALA	N-CA	-6.94	1.37	1.46
1	A	194	LEU	CA-C	6.94	1.62	1.53
1	C	2183	ALA	C-O	6.94	1.32	1.23
1	A	99	ILE	CA-C	6.94	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	PHE	C-N	6.93	1.43	1.33
1	B	1222	ASP	CG-OD1	6.93	1.38	1.25
1	C	2251	VAL	C-O	6.93	1.31	1.23
1	A	221	GLU	CG-CD	6.93	1.69	1.52
1	B	1113	GLU	CA-C	-6.93	1.44	1.52
1	C	2288	LEU	CA-C	6.93	1.61	1.52
1	A	372	LEU	C-O	6.93	1.37	1.23
1	B	1267	ALA	CA-CB	6.92	1.66	1.53
1	C	2233	GLU	CA-CB	6.92	1.64	1.53
1	B	1205	ASP	N-CA	6.92	1.55	1.46
1	A	79	GLU	CA-C	6.91	1.61	1.52
1	A	172	PRO	N-CA	-6.91	1.38	1.47
1	B	1244	THR	CA-C	6.91	1.62	1.52
1	C	2295	LEU	CG-CD1	6.91	1.75	1.52
1	A	97	GLY	C-N	6.91	1.43	1.33
1	B	1235	TYR	CA-C	-6.91	1.44	1.52
1	B	1131	HIS	C-N	6.90	1.43	1.33
1	C	2216	TYR	N-CA	6.90	1.56	1.46
1	C	2317	GLY	N-CA	6.90	1.55	1.45
1	A	75	MET	N-CA	6.90	1.54	1.46
1	C	2106	VAL	N-CA	-6.90	1.35	1.46
1	A	64	ALA	N-CA	6.90	1.54	1.46
1	C	2347	GLY	N-CA	6.90	1.55	1.45
1	B	1081	GLU	C-N	6.89	1.43	1.33
1	A	154	ARG	NE-CZ	6.89	1.40	1.33
1	C	2221	GLU	C-O	-6.89	1.15	1.24
1	B	1137	LEU	CB-CG	6.89	1.67	1.53
1	C	2225	TYR	CG-CD2	6.88	1.53	1.39
1	C	2287	HIS	C-O	6.88	1.32	1.23
1	C	2289	ILE	N-CA	6.88	1.54	1.46
1	C	2266	LYS	CD-CE	6.87	1.73	1.52
1	C	2104	MET	C-O	6.86	1.32	1.23
1	C	2369	PRO	N-CA	6.86	1.55	1.47
1	B	1299	THR	CA-CB	6.86	1.65	1.53
1	C	2197	HIS	C-O	-6.85	1.15	1.24
1	C	2240	ALA	CA-CB	6.85	1.64	1.53
1	B	1295	LEU	CA-C	6.85	1.60	1.52
1	A	229	SER	CA-CB	6.85	1.64	1.53
1	B	1043	ASN	CA-C	6.85	1.62	1.52
1	B	1277	HIS	C-O	6.84	1.31	1.24
1	C	2342	GLU	CA-C	6.84	1.61	1.52
1	C	2281	ASN	CA-C	6.83	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	GLY	CA-C	6.82	1.61	1.51
1	A	118	ASN	N-CA	-6.82	1.38	1.46
1	A	281	ASN	CG-OD1	6.82	1.36	1.23
1	A	178	VAL	CB-CG2	6.82	1.75	1.52
1	A	372	LEU	C-OXT	6.81	1.37	1.23
1	C	2357	GLU	CD-OE2	6.81	1.38	1.25
1	A	119	PRO	CA-CB	6.81	1.63	1.54
1	B	1098	SER	N-CA	6.80	1.54	1.45
1	B	1056	PHE	N-CA	6.80	1.54	1.45
1	B	1171	GLY	CA-C	-6.80	1.42	1.51
1	A	356	GLY	C-O	6.79	1.32	1.23
1	C	2066	SER	N-CA	6.79	1.54	1.46
1	B	1262	GLU	C-O	6.78	1.32	1.24
1	C	2237	ASP	N-CA	-6.78	1.38	1.46
1	B	1051	LEU	C-N	6.78	1.39	1.33
1	A	262	GLU	CB-CG	-6.77	1.32	1.52
1	A	333	TYR	CB-CG	-6.77	1.36	1.51
1	B	1186	ILE	CA-C	-6.77	1.44	1.52
1	A	92	ALA	CA-C	-6.77	1.43	1.53
1	A	191	ARG	CB-CG	6.76	1.72	1.52
1	C	2209	TYR	N-CA	-6.76	1.37	1.46
1	C	2230	ASP	N-CA	6.76	1.55	1.46
1	A	268	LYS	CD-CE	6.74	1.72	1.52
1	C	2141	GLY	C-N	6.74	1.44	1.33
1	B	1124	MET	SD-CE	6.73	1.96	1.79
1	B	1144	LEU	CG-CD2	6.73	1.74	1.52
1	C	2329	GLN	C-O	6.73	1.30	1.24
1	A	61	GLU	CD-OE1	6.72	1.38	1.25
1	B	1196	ASP	CA-C	6.72	1.61	1.53
1	C	2355	GLU	CA-CB	6.72	1.64	1.53
1	C	2078	ILE	CG1-CD1	-6.71	1.25	1.51
1	A	287	HIS	CA-CB	-6.71	1.42	1.53
1	B	1261	GLY	CA-C	-6.71	1.42	1.52
1	A	77	ILE	CB-CG1	6.71	1.66	1.53
1	C	2277	HIS	ND1-CE1	6.71	1.39	1.32
1	C	2360	ASN	N-CA	-6.70	1.37	1.46
1	C	2242	MET	CA-CB	6.70	1.63	1.53
1	A	256	VAL	CA-CB	6.69	1.61	1.54
1	B	1151	VAL	N-CA	6.69	1.54	1.46
1	C	2154	ARG	N-CA	-6.69	1.37	1.46
1	C	2282	ARG	CA-C	-6.69	1.44	1.52
1	A	62	GLN	CB-CG	-6.68	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	PHE	CD2-CE2	6.68	1.58	1.38
1	C	2063	VAL	CA-CB	6.67	1.61	1.54
1	B	1168	ALA	N-CA	6.67	1.55	1.46
1	B	1202	VAL	CA-CB	6.67	1.66	1.55
1	B	1099	ILE	CB-CG1	6.66	1.66	1.53
1	A	289	ILE	C-O	-6.66	1.17	1.24
1	B	1246	ILE	CA-CB	6.65	1.62	1.54
1	C	2182	THR	CA-C	-6.65	1.45	1.53
1	C	2326	LYS	N-CA	6.65	1.54	1.46
1	C	2178	VAL	CB-CG1	6.65	1.74	1.52
1	B	1233	GLU	CA-CB	6.64	1.63	1.53
1	B	1310	LEU	C-O	6.64	1.32	1.23
1	C	2053	PRO	C-N	-6.64	1.27	1.33
1	C	2186	ILE	C-O	-6.64	1.17	1.24
1	B	1102	PRO	C-O	6.64	1.31	1.23
1	B	1131	HIS	CA-C	-6.64	1.43	1.52
1	C	2331	GLY	CA-C	6.62	1.59	1.52
1	C	2065	ALA	C-N	6.62	1.43	1.33
1	A	67	GLY	CA-C	6.61	1.62	1.52
1	B	1372	LEU	C-O	6.61	1.36	1.23
1	A	90	LEU	CA-CB	6.61	1.64	1.53
1	B	1279	GLN	N-CA	-6.61	1.36	1.46
1	C	2367	VAL	CA-CB	6.61	1.62	1.54
1	B	1194	LEU	CA-CB	6.60	1.64	1.53
1	C	2187	MET	C-O	6.60	1.31	1.24
1	B	1355	GLU	N-CA	6.59	1.53	1.45
1	C	2077	ILE	CA-CB	6.59	1.63	1.54
1	A	49	HIS	N-CA	6.59	1.53	1.45
1	A	358	TRP	CA-C	6.59	1.61	1.52
1	C	2322	ALA	CA-C	6.58	1.60	1.52
1	C	2300	GLY	CA-C	6.58	1.60	1.51
1	A	287	HIS	CB-CG	6.58	1.59	1.50
1	A	61	GLU	CD-OE2	6.58	1.37	1.25
1	C	2236	GLU	CD-OE1	6.58	1.37	1.25
1	A	362	LEU	CA-CB	6.57	1.63	1.53
1	A	246	ILE	C-O	-6.57	1.16	1.24
1	A	285	ARG	CA-CB	6.57	1.62	1.53
1	B	1328	LEU	CA-C	6.57	1.60	1.52
1	B	1260	THR	N-CA	6.56	1.54	1.45
1	A	220	ASP	CA-CB	-6.56	1.43	1.53
1	C	2318	GLY	N-CA	-6.56	1.35	1.45
1	C	2357	GLU	CG-CD	6.56	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	ARG	CZ-NH2	6.55	1.42	1.33
1	A	217	ILE	CA-C	6.54	1.59	1.52
1	A	172	PRO	C-O	-6.54	1.15	1.24
1	A	42	SER	C-O	-6.54	1.15	1.24
1	B	1123	THR	C-O	-6.54	1.15	1.24
1	B	1126	HIS	CA-C	6.54	1.60	1.52
1	A	183	ALA	C-O	6.53	1.32	1.23
1	B	1262	GLU	CB-CG	-6.53	1.32	1.52
1	B	1228	PHE	C-O	-6.52	1.15	1.23
1	C	2075	MET	CG-SD	6.52	1.97	1.80
1	C	2200	LYS	N-CA	-6.51	1.36	1.46
1	A	86	GLU	CB-CG	6.51	1.72	1.52
1	A	246	ILE	CG1-CD1	6.51	1.77	1.51
1	C	2240	ALA	CA-C	6.51	1.61	1.52
1	C	2268	LYS	CG-CD	6.51	1.72	1.52
1	C	2184	GLY	C-O	6.51	1.32	1.23
1	C	2054	PRO	C-O	6.50	1.30	1.25
1	A	294	ASP	CA-CB	6.50	1.63	1.53
1	B	1266	LYS	N-CA	6.49	1.54	1.46
1	C	2198	GLU	CA-C	-6.48	1.43	1.52
1	B	1058	HIS	C-O	6.48	1.32	1.23
1	A	189	LEU	CA-C	6.48	1.60	1.53
1	B	1200	LYS	C-O	-6.48	1.14	1.23
1	B	1245	LEU	CA-CB	6.47	1.64	1.53
1	C	2147	PRO	CA-C	6.47	1.60	1.52
1	C	2233	GLU	CG-CD	6.46	1.68	1.52
1	A	52	VAL	CB-CG1	6.46	1.73	1.52
1	B	1082	VAL	CA-C	-6.46	1.44	1.52
1	B	1279	GLN	CA-CB	6.46	1.63	1.53
1	C	2217	ILE	CA-C	6.45	1.58	1.53
1	C	2269	VAL	C-O	6.45	1.31	1.24
1	B	1063	VAL	C-O	-6.45	1.17	1.24
1	B	1357	GLU	CD-OE2	6.45	1.37	1.25
1	B	1341	ILE	CA-CB	6.44	1.62	1.54
1	A	115	THR	CB-OG1	-6.44	1.33	1.43
1	C	2281	ASN	C-O	6.43	1.31	1.24
1	C	2139	GLY	C-O	6.43	1.33	1.24
1	A	225	TYR	N-CA	6.42	1.53	1.46
1	A	275	PHE	N-CA	6.42	1.54	1.46
1	B	1210	ILE	CG1-CD1	-6.42	1.26	1.51
1	C	2239	VAL	CB-CG1	6.41	1.73	1.52
1	C	2125	PRO	CB-CG	6.41	1.81	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	SER	CA-CB	6.40	1.63	1.53
1	C	2079	GLU	N-CA	-6.40	1.37	1.46
1	C	2202	VAL	CA-C	6.40	1.60	1.52
1	A	112	VAL	N-CA	-6.39	1.38	1.46
1	B	1289	ILE	C-N	-6.39	1.23	1.33
1	C	2081	GLU	CA-CB	6.39	1.62	1.53
1	C	2089	TYR	CA-CB	6.39	1.67	1.54
1	B	1335	TYR	C-O	6.37	1.31	1.24
1	B	1095	PHE	CD1-CE1	6.37	1.57	1.38
1	C	2285	ARG	C-N	6.36	1.42	1.33
1	A	55	PRO	N-CD	6.36	1.56	1.47
1	B	1162	ALA	C-O	6.36	1.31	1.23
1	C	2283	ASP	CA-C	-6.36	1.44	1.53
1	A	370	VAL	CA-C	6.36	1.60	1.52
1	C	2203	ARG	NE-CZ	6.35	1.40	1.33
1	C	2206	THR	C-O	6.35	1.31	1.23
1	C	2120	PRO	CA-CB	6.34	1.62	1.53
1	B	1076	ARG	N-CA	-6.34	1.38	1.45
1	C	2221	GLU	CD-OE2	6.34	1.37	1.25
1	A	166	HIS	ND1-CE1	6.33	1.38	1.32
1	A	129	ASP	N-CA	6.32	1.53	1.46
1	A	345	HIS	CD2-NE2	6.32	1.44	1.37
1	C	2362	LEU	CB-CG	-6.31	1.40	1.53
1	B	1126	HIS	CG-CD2	6.31	1.42	1.35
1	C	2182	THR	N-CA	6.31	1.55	1.46
1	B	1145	ILE	CB-CG1	6.30	1.66	1.53
1	C	2248	SER	C-O	6.30	1.32	1.24
1	A	344	VAL	CB-CG2	6.29	1.73	1.52
1	A	186	ILE	CB-CG1	6.28	1.66	1.53
1	A	350	ALA	CA-C	6.28	1.60	1.52
1	A	120	PRO	CA-CB	6.28	1.63	1.53
1	A	297	TRP	CA-C	-6.28	1.45	1.53
1	C	2327	PHE	C-O	-6.28	1.16	1.24
1	A	151	VAL	CA-C	6.27	1.60	1.52
1	A	256	VAL	C-O	6.27	1.31	1.24
1	B	1294	ASP	C-O	6.27	1.31	1.24
1	A	111	TYR	CD1-CE1	6.27	1.57	1.38
1	B	1064	ALA	CA-CB	6.27	1.63	1.53
1	B	1220	ASP	CG-OD1	6.26	1.37	1.25
1	C	2275	PHE	C-O	6.26	1.31	1.24
1	B	1238	MET	CB-CG	6.26	1.71	1.52
1	C	2355	GLU	C-O	6.26	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	GLY	CA-C	6.25	1.60	1.51
1	A	48	LYS	N-CA	-6.25	1.38	1.46
1	C	2265	LEU	CG-CD1	6.25	1.73	1.52
1	B	1200	LYS	CA-C	6.24	1.61	1.53
1	C	2237	ASP	C-O	6.24	1.31	1.24
1	B	1101	GLY	C-O	6.24	1.32	1.24
1	B	1156	LYS	CA-C	6.24	1.60	1.52
1	C	2103	LEU	N-CA	-6.24	1.38	1.46
1	C	2166	HIS	ND1-CE1	6.23	1.38	1.32
1	B	1265	LEU	N-CA	-6.23	1.37	1.45
1	A	93	MET	CG-SD	6.22	1.96	1.80
1	B	1219	LYS	C-O	6.22	1.31	1.24
1	C	2064	ALA	N-CA	6.22	1.54	1.46
1	B	1065	ALA	N-CA	6.22	1.54	1.46
1	B	1204	TYR	C-O	6.22	1.31	1.23
1	C	2234	GLY	CA-C	6.21	1.60	1.51
1	B	1306	PRO	C-O	-6.21	1.16	1.23
1	A	315	ILE	CA-C	6.21	1.60	1.52
1	C	2312	THR	C-N	6.21	1.42	1.33
1	A	336	VAL	CB-CG2	6.20	1.73	1.52
1	C	2182	THR	C-O	6.20	1.31	1.23
1	C	2346	LYS	CD-CE	6.20	1.71	1.52
1	B	1081	GLU	CA-CB	6.19	1.62	1.53
1	A	159	ARG	C-N	-6.18	1.25	1.33
1	A	278	SER	C-O	6.18	1.31	1.23
1	C	2251	VAL	CA-C	6.18	1.59	1.52
1	A	351	HIS	C-O	6.18	1.31	1.23
1	C	2113	GLU	N-CA	6.18	1.53	1.46
1	B	1166	HIS	N-CA	-6.18	1.38	1.46
1	C	2288	LEU	C-N	-6.17	1.26	1.33
1	B	1118	ASN	N-CA	6.17	1.53	1.46
1	C	2039	VAL	C-N	6.17	1.42	1.33
1	C	2208	TYR	CA-C	6.17	1.60	1.52
1	B	1232	SER	N-CA	6.17	1.53	1.46
1	A	104	MET	CA-CB	6.17	1.64	1.53
1	A	259	LEU	N-CA	6.17	1.52	1.46
1	B	1085	ASP	C-O	-6.17	1.16	1.23
1	C	2196	ASP	CA-CB	-6.17	1.44	1.53
1	B	1075	MET	N-CA	-6.16	1.38	1.45
1	A	238	MET	CA-C	6.16	1.60	1.52
1	B	1264	ALA	CA-C	-6.15	1.45	1.52
1	A	293	GLY	C-N	6.15	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1041	LEU	CA-C	-6.15	1.43	1.52
1	B	1225	TYR	CG-CD1	6.14	1.52	1.39
1	B	1348	ALA	CA-C	-6.14	1.46	1.53
1	C	2193	GLY	CA-C	6.14	1.61	1.52
1	B	1198	GLU	CD-OE1	6.14	1.37	1.25
1	B	1225	TYR	CE2-CZ	6.14	1.52	1.38
1	A	238	MET	SD-CE	6.13	1.94	1.79
1	B	1219	LYS	CE-NZ	6.13	1.67	1.49
1	C	2332	VAL	C-O	6.12	1.32	1.24
1	C	2326	LYS	CB-CG	6.12	1.70	1.52
1	A	289	ILE	N-CA	-6.11	1.39	1.46
1	A	338	HIS	CG-CD2	6.11	1.42	1.35
1	B	1141	GLY	C-N	6.11	1.43	1.33
1	C	2130	PHE	N-CA	-6.11	1.38	1.46
1	A	240	ALA	CA-CB	-6.11	1.43	1.53
1	A	355	GLU	CB-CG	-6.11	1.34	1.52
1	B	1366	VAL	CA-CB	6.10	1.62	1.54
1	A	194	LEU	CG-CD2	6.10	1.72	1.52
1	B	1093	MET	C-N	6.09	1.41	1.33
1	B	1201	PRO	CA-C	-6.09	1.45	1.52
1	B	1316	ARG	CA-CB	6.09	1.63	1.53
1	B	1078	ILE	CA-C	6.09	1.59	1.52
1	C	2076	ARG	CB-CG	-6.09	1.34	1.52
1	B	1124	MET	C-N	-6.08	1.25	1.33
1	B	1328	LEU	C-O	-6.08	1.16	1.23
1	C	2210	ILE	CB-CG1	6.08	1.65	1.53
1	C	2102	PRO	CA-CB	6.08	1.62	1.53
1	A	204	TYR	CA-C	6.08	1.59	1.52
1	C	2239	VAL	N-CA	-6.08	1.39	1.46
1	C	2275	PHE	CA-C	6.08	1.60	1.52
1	B	1354	VAL	C-O	6.07	1.30	1.24
1	B	1066	SER	CB-OG	6.07	1.54	1.42
1	B	1195	LYS	CG-CD	-6.07	1.34	1.52
1	B	1241	VAL	CA-CB	6.07	1.62	1.54
1	A	123	THR	CB-OG1	6.06	1.53	1.43
1	A	262	GLU	C-O	6.06	1.31	1.24
1	B	1159	ARG	C-O	-6.05	1.16	1.24
1	C	2080	LYS	CB-CG	6.05	1.70	1.52
1	B	1297	TRP	CD1-NE1	6.05	1.50	1.37
1	A	232	SER	CA-C	-6.05	1.45	1.52
1	A	366	VAL	C-O	-6.05	1.17	1.24
1	A	239	VAL	N-CA	-6.04	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	GLU	CD-OE2	6.04	1.36	1.25
1	B	1143	THR	C-N	6.04	1.42	1.33
1	B	1372	LEU	CG-CD1	-6.04	1.32	1.52
1	A	243	ASP	C-O	6.04	1.31	1.24
1	B	1077	ILE	CA-C	-6.02	1.45	1.52
1	A	176	TRP	N-CA	-6.02	1.39	1.46
1	B	1074	GLU	N-CA	-6.01	1.38	1.46
1	B	1221	GLU	CA-C	-6.01	1.44	1.52
1	B	1200	LYS	CB-CG	-6.01	1.34	1.52
1	B	1201	PRO	N-CA	-6.01	1.40	1.47
1	A	365	GLN	CA-C	6.01	1.60	1.52
1	B	1128	ILE	CB-CG2	6.01	1.72	1.52
1	A	326	LYS	N-CA	6.00	1.53	1.46
1	A	160	ALA	CA-C	6.00	1.60	1.52
1	C	2183	ALA	N-CA	6.00	1.53	1.46
1	B	1252	PHE	CG-CD2	6.00	1.51	1.38
1	A	302	PHE	N-CA	5.99	1.53	1.46
1	A	192	ASP	N-CA	5.99	1.52	1.46
1	B	1220	ASP	C-O	5.99	1.31	1.24
1	B	1370	VAL	CB-CG1	5.98	1.72	1.52
1	C	2154	ARG	CG-CD	5.98	1.70	1.52
1	B	1051	LEU	CA-C	5.98	1.60	1.52
1	B	1227	ARG	CA-C	-5.98	1.45	1.52
1	B	1277	HIS	N-CA	5.98	1.53	1.46
1	B	1266	LYS	CD-CE	5.97	1.70	1.52
1	A	168	ALA	N-CA	5.97	1.54	1.46
1	A	194	LEU	CB-CG	5.97	1.65	1.53
1	C	2040	ASP	CG-OD1	5.96	1.36	1.25
1	A	198	GLU	N-CA	5.95	1.53	1.46
1	B	1215	HIS	CG-ND1	5.95	1.44	1.38
1	C	2158	THR	C-O	5.95	1.31	1.24
1	A	241	VAL	C-O	5.94	1.31	1.24
1	A	90	LEU	N-CA	5.94	1.53	1.46
1	C	2150	LYS	C-O	5.94	1.31	1.23
1	A	299	THR	CA-C	5.94	1.61	1.52
1	C	2280	PRO	C-O	5.94	1.31	1.24
1	A	128	ILE	C-O	5.93	1.30	1.23
1	C	2176	TRP	N-CA	5.93	1.53	1.46
1	A	136	ALA	C-N	-5.92	1.25	1.33
1	B	1372	LEU	C-OXT	5.92	1.35	1.23
1	B	1368	ALA	CA-CB	5.92	1.62	1.53
1	B	1357	GLU	CB-CG	-5.92	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2046	ARG	C-N	5.92	1.40	1.33
1	B	1124	MET	CB-CG	-5.91	1.34	1.52
1	A	326	LYS	CE-NZ	5.91	1.67	1.49
1	C	2286	PRO	CA-CB	5.91	1.61	1.53
1	C	2206	THR	CA-C	5.91	1.59	1.52
1	A	49	HIS	CA-C	5.91	1.59	1.52
1	C	2195	LYS	CG-CD	-5.91	1.34	1.52
1	B	1089	TYR	N-CA	-5.90	1.38	1.45
1	A	234	GLY	CA-C	5.90	1.61	1.51
1	B	1287	HIS	ND1-CE1	5.90	1.38	1.32
1	B	1178	VAL	CA-CB	-5.90	1.47	1.54
1	B	1314	PHE	CD2-CE2	5.89	1.56	1.38
1	B	1325	TYR	CZ-OH	5.89	1.50	1.38
1	A	115	THR	C-O	5.89	1.30	1.24
1	B	1077	ILE	CB-CG1	5.89	1.65	1.53
1	B	1154	ARG	NE-CZ	5.89	1.39	1.33
1	A	154	ARG	C-O	5.88	1.31	1.23
1	B	1217	ILE	CA-CB	5.88	1.61	1.54
1	B	1078	ILE	N-CA	5.88	1.53	1.46
1	C	2112	VAL	N-CA	5.88	1.53	1.46
1	B	1049	HIS	CG-ND1	5.88	1.44	1.38
1	B	1316	ARG	CG-CD	5.87	1.70	1.52
1	C	2048	LYS	CA-C	5.87	1.60	1.52
1	A	68	PRO	CA-C	5.87	1.60	1.52
1	C	2357	GLU	CB-CG	-5.87	1.34	1.52
1	C	2172	PRO	C-O	-5.87	1.15	1.24
1	A	337	ASN	C-N	5.87	1.42	1.33
1	A	364	GLU	CG-CD	5.87	1.66	1.52
1	C	2091	GLN	CA-CB	5.87	1.60	1.52
1	C	2368	ALA	CA-CB	-5.87	1.44	1.53
1	C	2056	PHE	CE2-CZ	5.87	1.56	1.38
1	A	262	GLU	CD-OE1	5.87	1.36	1.25
1	A	282	ARG	NE-CZ	-5.87	1.26	1.33
1	B	1252	PHE	CA-C	-5.87	1.45	1.52
1	A	301	LYS	CE-NZ	5.86	1.67	1.49
1	B	1087	ASP	CA-C	5.86	1.61	1.52
1	C	2054	PRO	N-CA	5.86	1.53	1.46
1	A	236	GLU	CD-OE2	5.86	1.36	1.25
1	C	2320	ALA	CA-C	5.86	1.59	1.52
1	A	42	SER	C-N	-5.86	1.24	1.33
1	A	55	PRO	CB-CG	5.86	1.73	1.51
1	B	1177	HIS	CG-ND1	-5.86	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1300	GLY	CA-C	5.86	1.59	1.51
1	C	2176	TRP	CA-CB	5.85	1.62	1.53
1	B	1342	GLU	N-CA	-5.85	1.38	1.46
1	B	1043	ASN	CG-ND2	5.84	1.45	1.33
1	A	346	LYS	CA-C	5.84	1.60	1.52
1	B	1229	SER	CB-OG	5.84	1.53	1.42
1	A	253	ASN	CG-OD1	5.84	1.34	1.23
1	B	1238	MET	SD-CE	5.84	1.94	1.79
1	C	2132	ALA	C-O	5.83	1.31	1.24
1	B	1307	GLU	CA-CB	-5.83	1.43	1.53
1	C	2118	ASN	CG-OD1	5.83	1.34	1.23
1	B	1091	GLN	N-CA	5.83	1.54	1.46
1	B	1136	ALA	CA-C	-5.83	1.45	1.53
1	C	2146	ASN	CA-CB	5.83	1.62	1.53
1	B	1046	ARG	CB-CG	5.82	1.70	1.52
1	C	2130	PHE	CA-C	5.82	1.59	1.52
1	A	318	GLY	CA-C	5.82	1.59	1.51
1	A	159	ARG	CZ-NH2	5.82	1.41	1.33
1	A	180	SER	N-CA	5.82	1.53	1.46
1	A	370	VAL	C-O	-5.82	1.16	1.23
1	B	1167	CYS	CB-SG	-5.82	1.62	1.81
1	C	2086	GLU	CB-CG	5.82	1.70	1.52
1	A	130	PHE	CG-CD1	5.81	1.51	1.38
1	B	1155	PHE	CA-C	-5.81	1.45	1.52
1	A	355	GLU	CA-CB	5.80	1.62	1.53
1	C	2360	ASN	CA-C	-5.80	1.44	1.52
1	B	1334	ALA	CA-CB	5.80	1.67	1.53
1	B	1207	VAL	C-O	-5.79	1.18	1.24
1	C	2154	ARG	CA-CB	5.79	1.67	1.53
1	C	2255	ALA	CA-CB	5.79	1.63	1.53
1	C	2073	PHE	CD2-CE2	5.79	1.56	1.38
1	A	308	ARG	C-O	5.79	1.31	1.23
1	B	1278	SER	CA-C	5.79	1.59	1.52
1	A	244	THR	CA-CB	5.78	1.63	1.53
1	C	2287	HIS	CB-CG	-5.78	1.42	1.50
1	C	2369	PRO	CA-CB	-5.78	1.45	1.53
1	C	2173	MET	CA-CB	5.78	1.64	1.53
1	A	140	GLY	CA-C	5.77	1.59	1.51
1	B	1152	VAL	CA-C	5.77	1.59	1.52
1	B	1080	LYS	CD-CE	-5.76	1.35	1.52
1	B	1352	VAL	CA-C	5.76	1.59	1.52
1	C	2215	HIS	CA-C	5.76	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	PHE	C-N	5.76	1.42	1.33
1	B	1166	HIS	C-N	-5.76	1.25	1.33
1	A	87	ASP	CG-OD2	5.75	1.36	1.25
1	A	152	VAL	CA-C	5.75	1.60	1.52
1	B	1302	PHE	C-O	5.75	1.31	1.24
1	A	91	GLN	CD-NE2	5.74	1.45	1.33
1	C	2091	GLN	C-O	-5.74	1.15	1.23
1	B	1322	ALA	CA-CB	5.74	1.64	1.53
1	C	2059	ALA	CA-C	-5.74	1.45	1.52
1	B	1258	ALA	N-CA	5.73	1.53	1.46
1	B	1098	SER	CB-OG	5.73	1.53	1.42
1	A	142	LEU	CA-CB	5.73	1.62	1.53
1	C	2313	TRP	N-CA	-5.73	1.38	1.46
1	A	40	ASP	CA-C	5.73	1.60	1.52
1	C	2215	HIS	CD2-NE2	5.72	1.44	1.37
1	B	1312	THR	CA-CB	5.72	1.66	1.54
1	C	2291	GLY	C-N	5.72	1.41	1.33
1	C	2124	MET	C-N	5.71	1.41	1.33
1	A	324	LEU	CB-CG	-5.71	1.42	1.53
1	A	202	VAL	CA-CB	5.71	1.64	1.55
1	C	2050	THR	CB-CG2	5.71	1.71	1.52
1	C	2162	ALA	CA-C	-5.71	1.45	1.52
1	A	111	TYR	N-CA	5.71	1.52	1.45
1	A	124	MET	CB-CG	-5.71	1.35	1.52
1	B	1259	LEU	C-O	5.70	1.31	1.23
1	A	79	GLU	C-O	5.70	1.30	1.24
1	B	1095	PHE	N-CA	-5.70	1.39	1.46
1	C	2198	GLU	N-CA	5.70	1.53	1.46
1	A	224	THR	CB-OG1	-5.70	1.34	1.43
1	B	1049	HIS	N-CA	5.70	1.52	1.45
1	B	1204	TYR	C-N	-5.69	1.25	1.33
1	B	1283	ASP	C-N	5.69	1.40	1.33
1	C	2224	THR	CA-C	5.69	1.60	1.52
1	B	1078	ILE	C-N	-5.68	1.25	1.33
1	C	2289	ILE	CB-CG2	5.68	1.71	1.52
1	C	2181	GLY	N-CA	5.68	1.53	1.45
1	C	2152	VAL	C-N	5.67	1.41	1.33
1	A	301	LYS	N-CA	5.67	1.52	1.46
1	A	91	GLN	CG-CD	-5.67	1.37	1.52
1	A	210	ILE	CB-CG1	5.67	1.64	1.53
1	B	1158	THR	CB-CG2	5.67	1.71	1.52
1	A	163	PHE	C-N	-5.67	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	ASP	CG-OD1	5.67	1.36	1.25
1	C	2116	LEU	N-CA	5.66	1.52	1.46
1	B	1191	ARG	CB-CG	5.66	1.69	1.52
1	B	1231	PRO	C-O	5.66	1.31	1.24
1	C	2216	TYR	CB-CG	5.66	1.64	1.51
1	C	2368	ALA	C-O	-5.66	1.16	1.23
1	B	1112	VAL	N-CA	5.65	1.52	1.46
1	A	312	THR	CA-C	5.65	1.59	1.52
1	A	323	ALA	N-CA	-5.65	1.39	1.46
1	B	1345	HIS	ND1-CE1	5.65	1.38	1.32
1	B	1100	PRO	CA-C	5.65	1.64	1.52
1	C	2266	LYS	CA-C	5.65	1.59	1.52
1	B	1100	PRO	CA-CB	5.65	1.64	1.53
1	C	2064	ALA	CA-CB	-5.65	1.44	1.53
1	C	2040	ASP	C-O	5.64	1.31	1.24
1	B	1146	ASN	CG-ND2	-5.64	1.21	1.33
1	B	1214	ASP	C-O	5.63	1.30	1.24
1	C	2155	PHE	CD1-CE1	5.63	1.55	1.38
1	B	1274	LEU	C-O	5.63	1.30	1.24
1	B	1283	ASP	CA-CB	5.63	1.62	1.53
1	C	2056	PHE	CD2-CE2	-5.63	1.21	1.38
1	C	2366	VAL	C-O	-5.62	1.17	1.24
1	A	80	LYS	CA-C	5.62	1.59	1.52
1	C	2145	ILE	C-O	5.62	1.29	1.24
1	A	208	TYR	CA-C	5.62	1.59	1.52
1	A	325	TYR	CA-C	5.62	1.59	1.52
1	C	2150	LYS	N-CA	5.61	1.53	1.45
1	B	1174	ILE	CB-CG1	5.60	1.64	1.53
1	A	352	VAL	C-O	5.60	1.30	1.24
1	B	1069	VAL	CA-CB	-5.60	1.46	1.54
1	B	1154	ARG	C-O	5.59	1.31	1.24
1	B	1332	VAL	CA-C	5.59	1.59	1.52
1	A	198	GLU	CA-CB	5.59	1.62	1.53
1	B	1295	LEU	CG-CD1	5.59	1.71	1.52
1	C	2121	GLU	N-CA	-5.59	1.38	1.46
1	B	1097	GLY	N-CA	-5.58	1.36	1.45
1	B	1060	HIS	CD2-NE2	5.58	1.44	1.37
1	A	213	SER	N-CA	5.58	1.52	1.46
1	B	1249	HIS	N-CA	5.58	1.52	1.46
1	C	2122	ASN	CA-CB	-5.58	1.44	1.53
1	A	342	GLU	CA-CB	5.57	1.62	1.53
1	A	209	TYR	CZ-OH	-5.57	1.26	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1111	TYR	CG-CD1	-5.57	1.27	1.39
1	A	63	VAL	CA-C	5.56	1.59	1.52
1	B	1060	HIS	CA-CB	5.56	1.61	1.53
1	C	2133	ALA	C-N	5.56	1.41	1.33
1	A	129	ASP	C-O	5.56	1.30	1.24
1	C	2156	LYS	CA-C	5.56	1.59	1.52
1	A	313	TRP	CA-CB	5.55	1.61	1.53
1	B	1086	GLU	N-CA	5.55	1.53	1.46
1	A	76	ARG	CG-CD	5.55	1.69	1.52
1	A	282	ARG	CZ-NH2	5.55	1.40	1.33
1	B	1083	GLN	CG-CD	5.55	1.66	1.52
1	C	2336	VAL	CA-CB	5.55	1.63	1.54
1	C	2079	GLU	CA-CB	5.54	1.61	1.53
1	C	2324	LEU	CA-CB	-5.54	1.45	1.53
1	C	2205	ASP	CA-CB	5.54	1.62	1.53
1	B	1227	ARG	CZ-NH2	-5.54	1.26	1.33
1	B	1275	PHE	CA-C	5.54	1.59	1.52
1	C	2093	MET	C-O	5.54	1.30	1.24
1	B	1082	VAL	CA-CB	5.54	1.63	1.54
1	C	2158	THR	CB-OG1	5.53	1.52	1.43
1	C	2068	PRO	CA-C	5.53	1.59	1.52
1	C	2340	LEU	C-O	5.53	1.31	1.24
1	A	338	HIS	CD2-NE2	-5.53	1.31	1.37
1	C	2079	GLU	C-N	5.52	1.40	1.33
1	B	1138	GLY	C-N	5.52	1.40	1.33
1	A	330	PRO	C-O	-5.52	1.16	1.23
1	A	50	THR	CB-OG1	5.51	1.52	1.43
1	A	342	GLU	C-O	5.51	1.30	1.24
1	B	1241	VAL	CA-C	5.51	1.60	1.52
1	C	2190	PRO	CA-CB	5.51	1.61	1.53
1	C	2229	SER	CB-OG	5.51	1.53	1.42
1	B	1128	ILE	C-O	5.51	1.30	1.23
1	A	98	SER	CA-CB	-5.50	1.43	1.53
1	B	1216	TYR	CD2-CE2	5.50	1.55	1.38
1	A	261	GLY	C-N	-5.50	1.26	1.33
1	B	1215	HIS	N-CA	5.50	1.52	1.45
1	B	1050	THR	CA-CB	5.49	1.60	1.53
1	C	2228	PHE	CE2-CZ	5.49	1.55	1.38
1	A	284	SER	CA-C	5.49	1.59	1.52
1	B	1245	LEU	CB-CG	5.49	1.64	1.53
1	C	2308	ARG	C-O	5.49	1.30	1.23
1	A	159	ARG	C-O	5.48	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1342	GLU	CA-C	5.48	1.60	1.52
1	B	1057	ALA	CA-C	5.48	1.59	1.52
1	B	1075	MET	CA-CB	5.48	1.63	1.53
1	B	1179	VAL	CA-CB	5.48	1.62	1.54
1	B	1304	ASN	CG-ND2	-5.48	1.21	1.33
1	B	1215	HIS	CG-CD2	-5.47	1.29	1.35
1	B	1317	GLY	C-N	5.47	1.40	1.33
1	A	273	VAL	C-O	5.46	1.30	1.24
1	B	1140	GLY	C-O	5.46	1.30	1.23
1	C	2220	ASP	CG-OD1	5.46	1.35	1.25
1	B	1361	ASP	N-CA	-5.46	1.39	1.46
1	C	2150	LYS	CD-CE	5.46	1.68	1.52
1	B	1312	THR	C-O	5.46	1.30	1.23
1	C	2265	LEU	CA-C	5.45	1.60	1.53
1	C	2244	THR	C-O	5.45	1.31	1.24
1	A	311	GLU	CA-C	5.45	1.60	1.52
1	B	1345	HIS	CA-CB	5.45	1.62	1.53
1	A	347	GLY	N-CA	5.45	1.53	1.45
1	B	1156	LYS	CG-CD	5.44	1.68	1.52
1	C	2113	GLU	CG-CD	5.44	1.65	1.52
1	C	2220	ASP	CB-CG	-5.44	1.38	1.52
1	B	1164	VAL	C-O	5.44	1.31	1.24
1	A	169	PRO	CG-CD	5.44	1.69	1.50
1	B	1268	LYS	CB-CG	-5.43	1.36	1.52
1	B	1215	HIS	CE1-NE2	5.42	1.38	1.32
1	A	39	VAL	CA-C	5.42	1.64	1.52
1	A	157	ALA	N-CA	5.42	1.53	1.46
1	A	121	GLU	CD-OE2	5.42	1.35	1.25
1	A	303	HIS	CE1-NE2	5.42	1.38	1.32
1	B	1104	MET	CA-C	-5.42	1.46	1.52
1	C	2124	MET	C-O	-5.42	1.18	1.24
1	A	247	PRO	N-CD	5.41	1.55	1.47
1	B	1152	VAL	CA-CB	-5.41	1.47	1.54
1	B	1211	GLY	CA-C	5.41	1.59	1.51
1	A	208	TYR	CE2-CZ	5.40	1.51	1.38
1	C	2285	ARG	C-O	5.40	1.30	1.24
1	C	2144	LEU	C-O	5.40	1.30	1.24
1	A	39	VAL	CA-CB	5.40	1.69	1.54
1	B	1144	LEU	C-O	5.39	1.30	1.24
1	C	2337	ASN	CA-CB	5.39	1.60	1.53
1	A	265	LEU	CA-C	5.39	1.60	1.53
1	B	1190	PRO	CA-CB	5.38	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2250	ILE	C-O	5.38	1.29	1.24
1	A	206	THR	C-O	5.37	1.30	1.23
1	A	340	LEU	C-O	5.37	1.31	1.24
1	C	2191	ARG	CD-NE	5.37	1.53	1.46
1	A	155	PHE	C-N	-5.37	1.25	1.33
1	C	2352	VAL	CA-CB	5.37	1.61	1.54
1	A	301	LYS	CA-CB	-5.36	1.45	1.53
1	B	1330	PRO	C-N	-5.36	1.23	1.32
1	B	1296	VAL	CA-C	5.36	1.59	1.52
1	B	1165	TYR	N-CA	5.36	1.52	1.45
1	A	347	GLY	CA-C	-5.35	1.44	1.51
1	A	85	ASP	CA-C	5.35	1.59	1.52
1	C	2311	GLU	N-CA	-5.35	1.39	1.46
1	A	320	ALA	C-O	5.35	1.30	1.23
1	B	1104	MET	C-N	5.35	1.40	1.33
1	B	1352	VAL	C-O	5.34	1.29	1.24
1	B	1342	GLU	CA-CB	5.34	1.62	1.53
1	A	254	GLY	C-O	-5.34	1.16	1.24
1	C	2281	ASN	N-CA	5.33	1.53	1.46
1	B	1215	HIS	C-O	5.33	1.30	1.23
1	B	1062	GLN	CG-CD	5.32	1.65	1.52
1	C	2205	ASP	C-N	5.32	1.40	1.33
1	C	2302	PHE	N-CA	5.32	1.53	1.46
1	A	74	GLU	C-N	-5.32	1.26	1.33
1	A	369	PRO	N-CA	-5.31	1.40	1.47
1	A	353	LEU	N-CA	5.31	1.53	1.46
1	B	1225	TYR	C-N	-5.31	1.25	1.33
1	A	150	LYS	CA-C	-5.31	1.46	1.52
1	B	1236	GLU	CB-CG	5.31	1.68	1.52
1	C	2362	LEU	CA-C	-5.31	1.46	1.52
1	B	1124	MET	C-O	-5.31	1.18	1.24
1	B	1163	PHE	CG-CD2	5.30	1.50	1.38
1	B	1203	ARG	CD-NE	5.30	1.53	1.46
1	B	1221	GLU	C-O	5.30	1.30	1.24
1	B	1045	PRO	N-CA	5.30	1.53	1.47
1	A	307	GLU	CA-C	5.30	1.60	1.53
1	B	1087	ASP	CG-OD1	5.30	1.35	1.25
1	B	1250	ILE	CB-CG1	5.30	1.64	1.53
1	C	2299	THR	CA-C	5.30	1.60	1.52
1	A	128	ILE	CB-CG1	5.29	1.64	1.53
1	B	1264	ALA	C-O	-5.29	1.17	1.23
1	C	2267	ALA	CA-C	5.29	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	SER	N-CA	-5.29	1.39	1.46
1	A	308	ARG	CA-CB	5.29	1.64	1.53
1	B	1092	ALA	N-CA	5.29	1.52	1.45
1	B	1118	ASN	CG-ND2	5.29	1.44	1.33
1	B	1166	HIS	CB-CG	5.29	1.57	1.50
1	B	1288	LEU	CA-C	5.28	1.59	1.53
1	B	1360	ASN	N-CA	5.28	1.53	1.46
1	B	1364	GLU	CD-OE1	-5.28	1.15	1.25
1	B	1338	HIS	CD2-NE2	5.28	1.43	1.37
1	C	2281	ASN	CG-OD1	5.28	1.33	1.23
1	A	287	HIS	N-CA	5.28	1.52	1.46
1	A	41	LEU	CA-CB	-5.27	1.44	1.53
1	A	163	PHE	CE2-CZ	5.27	1.54	1.38
1	B	1291	GLY	N-CA	5.27	1.49	1.44
1	A	335	TYR	CD2-CE2	5.27	1.54	1.38
1	B	1176	TRP	CA-CB	5.27	1.61	1.53
1	B	1153	LEU	CG-CD2	5.27	1.70	1.52
1	B	1235	TYR	CD2-CE2	5.27	1.54	1.38
1	B	1103	LEU	C-O	5.26	1.30	1.23
1	C	2200	LYS	CE-NZ	5.26	1.65	1.49
1	B	1133	ALA	N-CA	-5.26	1.39	1.45
1	B	1278	SER	CB-OG	5.26	1.52	1.42
1	C	2082	VAL	CB-CG2	-5.26	1.35	1.52
1	A	186	ILE	C-O	5.26	1.29	1.24
1	A	216	TYR	CA-C	5.26	1.61	1.53
1	A	82	VAL	N-CA	5.25	1.52	1.46
1	B	1192	ASP	CA-CB	-5.25	1.45	1.53
1	A	309	ASP	N-CA	5.25	1.54	1.46
1	B	1086	GLU	CA-CB	5.25	1.61	1.53
1	A	357	GLU	CG-CD	5.25	1.65	1.52
1	B	1309	ASP	C-O	5.25	1.31	1.23
1	A	175	PRO	CA-CB	5.24	1.61	1.53
1	B	1324	LEU	CB-CG	-5.24	1.43	1.53
1	A	115	THR	CA-CB	5.24	1.59	1.53
1	A	131	HIS	ND1-CE1	5.24	1.37	1.32
1	A	244	THR	N-CA	5.24	1.52	1.46
1	B	1111	TYR	CG-CD2	5.23	1.50	1.39
1	C	2046	ARG	CZ-NH2	5.23	1.40	1.33
1	C	2143	THR	CA-CB	5.23	1.61	1.53
1	C	2312	THR	N-CA	5.23	1.52	1.45
1	A	357	GLU	C-N	-5.23	1.26	1.33
1	B	1046	ARG	CA-CB	5.23	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	ALA	CA-C	5.23	1.59	1.52
1	C	2062	GLN	CD-NE2	5.22	1.44	1.33
1	B	1316	ARG	C-O	5.22	1.30	1.23
1	C	2353	LEU	C-N	5.22	1.40	1.33
1	C	2049	HIS	CA-CB	5.22	1.62	1.53
1	B	1112	VAL	C-N	5.21	1.40	1.33
1	C	2250	ILE	CG1-CD1	5.21	1.72	1.51
1	B	1271	ASP	C-N	-5.21	1.26	1.33
1	A	111	TYR	CE1-CZ	-5.21	1.25	1.38
1	C	2197	HIS	CG-CD2	5.21	1.41	1.35
1	A	96	ASP	CG-OD1	5.21	1.35	1.25
1	A	176	TRP	C-O	5.21	1.30	1.24
1	C	2177	HIS	CA-C	5.21	1.59	1.52
1	C	2213	SER	CA-CB	5.20	1.64	1.53
1	B	1072	GLU	CA-CB	5.20	1.61	1.53
1	B	1224	THR	CA-CB	5.20	1.62	1.53
1	C	2301	LYS	CG-CD	5.20	1.68	1.52
1	B	1076	ARG	CG-CD	5.20	1.68	1.52
1	C	2233	GLU	CB-CG	-5.20	1.36	1.52
1	C	2060	HIS	CG-CD2	-5.19	1.30	1.35
1	B	1202	VAL	CB-CG1	-5.19	1.35	1.52
1	B	1258	ALA	CA-CB	-5.19	1.44	1.53
1	A	74	GLU	CD-OE2	5.19	1.35	1.25
1	A	367	VAL	CA-CB	-5.19	1.47	1.54
1	B	1314	PHE	CA-CB	5.19	1.62	1.53
1	A	178	VAL	CA-CB	5.18	1.61	1.54
1	B	1172	PRO	CA-C	-5.18	1.42	1.52
1	A	249	HIS	N-CA	5.18	1.52	1.45
1	C	2363	MET	CA-C	5.18	1.59	1.52
1	A	42	SER	N-CA	5.18	1.53	1.46
1	A	237	ASP	CA-CB	-5.18	1.45	1.53
1	C	2143	THR	CB-OG1	5.18	1.52	1.43
1	A	204	TYR	C-N	-5.18	1.26	1.33
1	A	313	TRP	CE3-CZ3	5.17	1.54	1.38
1	A	316	ARG	CA-C	5.17	1.59	1.52
1	C	2119	PRO	N-CD	-5.17	1.40	1.47
1	C	2119	PRO	CA-C	-5.17	1.49	1.51
1	C	2252	PHE	CG-CD1	5.17	1.49	1.38
1	C	2345	HIS	CG-CD2	5.17	1.41	1.35
1	C	2298	GLU	CB-CG	5.17	1.68	1.52
1	C	2151	VAL	CA-C	-5.17	1.46	1.52
1	B	1040	ASP	CG-OD1	5.17	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2088	ALA	CA-C	-5.16	1.46	1.52
1	C	2303	HIS	CE1-NE2	5.16	1.37	1.32
1	C	2361	ASP	N-CA	5.15	1.52	1.46
1	B	1142	LEU	CB-CG	5.15	1.63	1.53
1	A	290	GLY	C-O	5.15	1.31	1.24
1	C	2312	THR	C-O	5.15	1.30	1.23
1	C	2347	GLY	C-N	5.15	1.40	1.33
1	B	1308	ARG	CD-NE	5.15	1.53	1.46
1	A	78	ILE	CG1-CD1	-5.15	1.31	1.51
1	A	99	ILE	CG1-CD1	-5.14	1.31	1.51
1	C	2256	VAL	N-CA	5.14	1.52	1.46
1	C	2320	ALA	C-O	5.14	1.30	1.23
1	B	1262	GLU	N-CA	-5.14	1.39	1.46
1	B	1176	TRP	CE3-CZ3	5.14	1.54	1.38
1	B	1143	THR	N-CA	5.14	1.52	1.46
1	A	51	LEU	CB-CG	5.13	1.63	1.53
1	A	178	VAL	CB-CG1	5.13	1.69	1.52
1	B	1191	ARG	NE-CZ	5.13	1.38	1.33
1	A	199	GLY	C-O	-5.13	1.17	1.24
1	B	1081	GLU	CG-CD	5.13	1.64	1.52
1	B	1289	ILE	C-O	5.13	1.29	1.24
1	C	2319	THR	CB-OG1	5.13	1.51	1.43
1	A	251	VAL	C-N	5.13	1.40	1.33
1	A	70	ILE	N-CA	5.12	1.52	1.46
1	C	2361	ASP	C-O	-5.12	1.17	1.24
1	A	93	MET	CB-CG	5.12	1.67	1.52
1	A	218	PRO	CG-CD	5.12	1.68	1.50
1	B	1190	PRO	N-CD	5.12	1.54	1.47
1	C	2222	ASP	CG-OD1	5.12	1.35	1.25
1	C	2287	HIS	CA-CB	5.12	1.62	1.53
1	A	180	SER	C-O	-5.11	1.16	1.23
1	A	205	ASP	CG-OD1	5.11	1.35	1.25
1	A	338	HIS	CE1-NE2	5.11	1.37	1.32
1	C	2049	HIS	N-CA	5.11	1.51	1.45
1	A	125	PRO	N-CA	5.11	1.53	1.47
1	A	345	HIS	CG-CD2	5.11	1.41	1.35
1	B	1350	ALA	CA-C	-5.11	1.46	1.52
1	B	1225	TYR	CZ-OH	5.11	1.48	1.38
1	A	55	PRO	C-N	5.11	1.40	1.33
1	A	202	VAL	CB-CG2	-5.11	1.35	1.52
1	B	1159	ARG	CZ-NH1	5.11	1.39	1.32
1	B	1273	VAL	C-O	5.09	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1338	HIS	CG-CD2	5.09	1.41	1.35
1	A	148	GLY	C-O	5.09	1.31	1.24
1	B	1346	LYS	CD-CE	5.09	1.67	1.52
1	C	2166	HIS	CG-CD2	5.09	1.41	1.35
1	C	2079	GLU	C-O	5.08	1.30	1.23
1	C	2355	GLU	CG-CD	5.08	1.64	1.52
1	A	141	GLY	C-O	-5.08	1.18	1.23
1	B	1368	ALA	C-O	-5.08	1.17	1.23
1	C	2295	LEU	CA-CB	5.08	1.63	1.53
1	A	50	THR	CB-CG2	5.08	1.69	1.52
1	C	2118	ASN	CA-C	5.08	1.58	1.52
1	B	1198	GLU	N-CA	-5.08	1.39	1.46
1	B	1169	PRO	CG-CD	5.07	1.68	1.50
1	B	1246	ILE	C-O	5.07	1.29	1.24
1	C	2346	LYS	CB-CG	5.07	1.67	1.52
1	C	2145	ILE	CB-CG2	5.06	1.69	1.52
1	C	2336	VAL	N-CA	-5.06	1.40	1.46
1	C	2164	VAL	C-O	5.06	1.30	1.24
1	B	1042	SER	C-O	-5.05	1.17	1.24
1	B	1097	GLY	C-O	5.05	1.31	1.24
1	A	337	ASN	CA-CB	-5.05	1.46	1.53
1	A	220	ASP	CG-OD1	5.05	1.34	1.25
1	C	2120	PRO	C-O	-5.05	1.17	1.24
1	A	146	ASN	CG-OD1	-5.05	1.14	1.23
1	A	163	PHE	CD2-CE2	5.05	1.53	1.38
1	B	1040	ASP	C-N	5.05	1.40	1.33
1	B	1093	MET	CA-C	-5.05	1.46	1.52
1	A	324	LEU	CG-CD2	5.04	1.69	1.52
1	B	1113	GLU	C-O	5.04	1.29	1.24
1	C	2107	HIS	ND1-CE1	5.04	1.37	1.32
1	C	2350	ALA	N-CA	5.04	1.52	1.45
1	A	328	LEU	N-CA	5.04	1.52	1.45
1	B	1049	HIS	CA-CB	5.04	1.63	1.53
1	C	2221	GLU	CD-OE1	5.04	1.34	1.25
1	C	2284	SER	C-O	5.04	1.30	1.23
1	B	1272	ASN	CG-ND2	5.03	1.43	1.33
1	A	44	LEU	C-O	-5.03	1.17	1.23
1	A	123	THR	CA-CB	5.03	1.61	1.54
1	B	1358	TRP	N-CA	-5.03	1.39	1.45
1	C	2369	PRO	CA-C	5.03	1.58	1.52
1	A	272	ASN	N-CA	5.03	1.52	1.46
1	A	327	PHE	CG-CD1	-5.02	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2078	ILE	CB-CG2	5.02	1.69	1.52
1	C	2131	HIS	CD2-NE2	5.02	1.43	1.37
1	A	216	TYR	CD2-CE2	5.02	1.53	1.38
1	C	2292	HIS	ND1-CE1	5.02	1.37	1.32
1	C	2307	GLU	N-CA	5.02	1.51	1.45
1	A	244	THR	CA-C	5.01	1.59	1.52
1	C	2063	VAL	CA-C	5.01	1.59	1.52
1	A	69	VAL	N-CA	5.01	1.52	1.46
1	A	345	HIS	N-CA	-5.00	1.40	1.46

All (710) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ARG	NE-CZ-NH2	-22.35	99.08	119.20
1	A	124	MET	CG-SD-CE	-21.90	52.72	100.90
1	B	1124	MET	CG-SD-CE	-18.11	61.06	100.90
1	C	2227	ARG	NE-CZ-NH2	-17.71	103.26	119.20
1	A	203	ARG	NE-CZ-NH2	-17.46	103.48	119.20
1	A	227	ARG	NE-CZ-NH1	14.14	135.64	121.50
1	A	48	LYS	CD-CE-NZ	-14.06	66.90	111.90
1	B	1227	ARG	NE-CZ-NH2	-13.73	106.85	119.20
1	C	2227	ARG	NE-CZ-NH1	13.60	135.09	121.50
1	C	2076	ARG	NE-CZ-NH1	-13.49	108.01	121.50
1	A	227	ARG	NE-CZ-NH2	-12.67	107.80	119.20
1	A	191	ARG	NE-CZ-NH1	12.48	133.98	121.50
1	B	1227	ARG	NE-CZ-NH1	12.47	133.97	121.50
1	C	2048	LYS	CD-CE-NZ	-12.40	72.23	111.90
1	C	2339	ASN	N-CA-C	-11.92	89.22	108.41
1	A	205	ASP	N-CA-C	-11.57	99.26	113.50
1	A	226	MET	CG-SD-CE	11.46	126.11	100.90
1	B	1139	GLY	N-CA-C	-11.31	99.58	114.85
1	C	2154	ARG	CG-CD-NE	-11.31	87.12	112.00
1	A	203	ARG	NH1-CZ-NH2	11.08	133.70	119.30
1	C	2065	ALA	N-CA-C	-11.00	100.56	113.21
1	B	1339	ASN	N-CA-C	-10.94	90.80	108.41
1	C	2076	ARG	NH1-CZ-NH2	10.74	133.26	119.30
1	B	1048	LYS	CD-CE-NZ	-10.64	77.84	111.90
1	C	2171	GLY	CA-C-N	-10.50	109.53	119.82
1	C	2171	GLY	C-N-CA	-10.50	109.53	119.82
1	A	200	LYS	CB-CG-CD	-10.39	87.40	111.30
1	A	268	LYS	CG-CD-CE	-10.34	87.51	111.30
1	B	1226	MET	CG-SD-CE	10.28	123.51	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1200	LYS	CD-CE-NZ	-10.01	79.87	111.90
1	A	76	ARG	NE-CZ-NH1	-10.00	111.50	121.50
1	A	154	ARG	NE-CZ-NH1	-9.96	111.54	121.50
1	A	203	ARG	CA-C-O	-9.87	109.57	121.11
1	B	1319	THR	CA-CB-CG2	-9.81	93.83	110.50
1	B	1192	ASP	CB-CA-C	-9.73	93.97	110.81
1	B	1319	THR	CB-CA-C	-9.64	92.27	111.17
1	C	2262	GLU	CA-CB-CG	9.60	133.30	114.10
1	A	256	VAL	CA-C-O	-9.59	110.97	121.23
1	B	1124	MET	CB-CA-C	-9.50	94.54	109.08
1	A	171	GLY	CA-C-O	9.40	134.96	121.52
1	B	1233	GLU	OE1-CD-OE2	-9.39	100.35	122.90
1	A	326	LYS	CB-CG-CD	-9.29	89.93	111.30
1	C	2139	GLY	N-CA-C	-9.23	101.72	114.64
1	C	2244	THR	N-CA-C	-9.22	102.03	113.18
1	C	2316	ARG	NE-CZ-NH1	-9.15	112.35	121.50
1	A	77	ILE	CB-CG1-CD1	-9.08	94.72	113.80
1	A	233	GLU	CG-CD-OE2	9.07	139.26	118.40
1	C	2210	ILE	CB-CG1-CD1	-9.04	94.82	113.80
1	B	1125	PRO	CB-CA-C	-9.03	97.72	110.63
1	C	2332	VAL	CB-CA-C	-9.01	98.87	111.21
1	A	171	GLY	CA-C-N	-8.98	108.62	119.84
1	A	171	GLY	C-N-CA	-8.98	108.62	119.84
1	B	1186	ILE	CA-C-O	8.94	130.68	120.67
1	B	1200	LYS	N-CA-CB	-8.93	98.23	110.29
1	A	180	SER	N-CA-C	-8.84	102.03	113.17
1	C	2290	GLY	N-CA-C	-8.84	103.42	114.92
1	B	1335	TYR	N-CA-C	-8.83	94.51	108.90
1	C	2054	PRO	N-CA-C	-8.70	102.12	110.47
1	C	2319	THR	CA-CB-OG1	8.61	122.52	109.60
1	A	61	GLU	CA-CB-CG	-8.58	96.94	114.10
1	B	1316	ARG	CA-CB-CG	-8.57	96.95	114.10
1	A	339	ASN	N-CA-C	-8.57	96.14	109.25
1	B	1268	LYS	CA-CB-CG	-8.57	96.96	114.10
1	A	366	VAL	N-CA-C	-8.54	102.50	110.53
1	C	2357	GLU	CB-CG-CD	-8.51	98.14	112.60
1	C	2087	ASP	N-CA-CB	-8.50	99.22	111.54
1	A	290	GLY	N-CA-C	-8.45	104.23	115.21
1	B	1181	GLY	CA-C-N	-8.44	108.83	122.34
1	B	1181	GLY	C-N-CA	-8.44	108.83	122.34
1	A	241	VAL	CB-CA-C	-8.43	100.59	112.22
1	B	1361	ASP	N-CA-C	-8.40	102.08	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	MET	CB-CA-C	-8.33	96.34	109.08
1	C	2299	THR	N-CA-C	-8.31	102.86	113.16
1	B	1219	LYS	CA-C-N	-8.26	105.76	121.54
1	B	1219	LYS	C-N-CA	-8.26	105.76	121.54
1	B	1059	ALA	CA-C-O	-8.26	112.56	121.56
1	C	2241	VAL	N-CA-C	-8.26	102.00	111.00
1	C	2121	GLU	N-CA-C	8.25	123.16	113.18
1	C	2050	THR	CA-CB-OG1	-8.23	97.25	109.60
1	B	1319	THR	OG1-CB-CG2	-8.22	92.85	109.30
1	A	96	ASP	N-CA-C	8.21	122.98	113.38
1	C	2131	HIS	N-CA-C	-8.20	103.17	113.01
1	A	67	GLY	CA-C-N	8.17	130.06	119.84
1	A	67	GLY	C-N-CA	8.17	130.06	119.84
1	A	151	VAL	CA-C-O	-8.17	112.78	121.19
1	C	2158	THR	CA-C-O	-8.15	108.68	119.11
1	C	2127	ASN	N-CA-C	-8.13	97.51	108.24
1	C	2063	VAL	N-CA-C	-8.12	96.14	107.99
1	A	319	THR	N-CA-C	8.08	121.00	108.96
1	C	2331	GLY	CA-C-O	-8.07	114.94	122.13
1	A	147	PRO	CA-C-O	-8.07	112.53	121.32
1	A	171	GLY	N-CA-C	8.05	128.77	112.34
1	B	1048	LYS	CG-CD-CE	8.05	129.83	111.30
1	C	2215	HIS	CA-CB-CG	-8.05	105.75	113.80
1	C	2355	GLU	CA-CB-CG	-8.04	98.02	114.10
1	B	1077	ILE	CB-CG1-CD1	-8.03	96.93	113.80
1	A	227	ARG	CB-CG-CD	-8.00	92.90	111.30
1	C	2182	THR	OG1-CB-CG2	-7.96	93.38	109.30
1	A	326	LYS	CD-CE-NZ	-7.92	86.55	111.90
1	C	2203	ARG	CB-CA-C	-7.92	91.99	109.56
1	C	2319	THR	CB-CA-C	-7.90	95.63	111.91
1	B	1210	ILE	CB-CG1-CD1	-7.90	97.21	113.80
1	B	1233	GLU	CG-CD-OE2	7.89	136.56	118.40
1	A	149	GLU	CA-C-O	-7.84	112.26	121.44
1	C	2203	ARG	CB-CG-CD	-7.80	93.35	111.30
1	C	2355	GLU	OE1-CD-OE2	7.80	141.62	122.90
1	A	173	MET	CB-CA-C	-7.79	93.71	109.99
1	C	2226	MET	CG-SD-CE	7.79	118.03	100.90
1	B	1250	ILE	N-CA-C	-7.76	96.29	107.77
1	A	191	ARG	CG-CD-NE	-7.74	94.97	112.00
1	C	2138	GLY	N-CA-C	-7.71	105.37	115.47
1	B	1180	SER	N-CA-C	-7.71	103.46	113.17
1	C	2292	HIS	CA-C-O	-7.69	113.20	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ILE	N-CA-C	-7.69	96.76	107.99
1	C	2370	VAL	CA-C-N	7.68	127.63	120.34
1	C	2370	VAL	C-N-CA	7.68	127.63	120.34
1	C	2340	LEU	CD1-CG-CD2	-7.66	93.95	110.80
1	C	2334	ALA	N-CA-C	-7.65	97.27	109.59
1	C	2135	GLY	O-C-N	7.62	130.80	122.87
1	C	2262	GLU	N-CA-CB	-7.62	97.36	110.32
1	A	154	ARG	NE-CZ-NH2	7.62	126.05	119.20
1	C	2355	GLU	CA-C-O	-7.62	112.71	121.47
1	A	76	ARG	NH1-CZ-NH2	7.61	129.19	119.30
1	B	1295	LEU	N-CA-C	-7.60	95.65	108.26
1	B	1338	HIS	CA-C-N	-7.58	112.33	122.42
1	B	1338	HIS	C-N-CA	-7.58	112.33	122.42
1	A	218	PRO	O-C-N	7.57	132.23	123.00
1	A	112	VAL	CA-C-N	-7.55	112.14	122.86
1	A	112	VAL	C-N-CA	-7.55	112.14	122.86
1	A	327	PHE	CA-CB-CG	-7.54	106.26	113.80
1	B	1087	ASP	N-CA-CB	-7.53	100.28	111.43
1	B	1173	MET	CB-CA-C	-7.52	94.29	109.55
1	C	2326	LYS	CD-CE-NZ	-7.51	87.87	111.90
1	A	239	VAL	CA-CB-CG2	-7.50	97.65	110.40
1	A	246	ILE	CA-C-N	-7.49	112.29	119.85
1	A	246	ILE	C-N-CA	-7.49	112.29	119.85
1	C	2046	ARG	O-C-N	-7.48	114.59	123.27
1	B	1127	ASN	CA-C-O	-7.46	113.32	120.56
1	B	1286	PRO	CB-CA-C	-7.46	101.20	110.98
1	B	1119	PRO	N-CA-CB	7.44	107.36	103.19
1	A	235	TYR	N-CA-C	7.43	120.09	111.02
1	B	1344	VAL	CA-C-N	-7.40	108.10	120.68
1	B	1344	VAL	C-N-CA	-7.40	108.10	120.68
1	B	1332	VAL	CG1-CB-CG2	-7.37	94.60	110.80
1	C	2115	THR	CA-C-N	-7.34	112.28	122.93
1	C	2115	THR	C-N-CA	-7.34	112.28	122.93
1	A	162	ALA	N-CA-C	-7.32	98.68	110.32
1	C	2137	LEU	N-CA-C	7.32	121.25	111.30
1	C	2167	CYS	CA-CB-SG	-7.32	97.58	114.40
1	C	2352	VAL	CA-C-O	-7.28	112.65	120.36
1	C	2067	GLY	CA-C-N	7.27	127.71	119.93
1	C	2067	GLY	C-N-CA	7.27	127.71	119.93
1	C	2353	LEU	CA-C-N	-7.27	113.62	123.14
1	C	2353	LEU	C-N-CA	-7.27	113.62	123.14
1	B	1048	LYS	CB-CG-CD	7.26	128.01	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2119	PRO	O-C-N	7.25	124.64	121.31
1	C	2305	ALA	CB-CA-C	-7.23	97.63	109.27
1	A	280	PRO	CA-C-N	-7.23	110.92	121.98
1	A	280	PRO	C-N-CA	-7.23	110.92	121.98
1	B	1227	ARG	CB-CG-CD	-7.21	94.72	111.30
1	B	1043	ASN	N-CA-C	7.20	121.91	113.20
1	C	2180	SER	N-CA-C	-7.16	104.15	113.17
1	B	1149	GLU	CG-CD-OE1	7.16	134.87	118.40
1	A	191	ARG	CD-NE-CZ	-7.15	114.39	124.40
1	A	189	LEU	CB-CA-C	-7.14	98.76	109.26
1	A	45	PRO	CB-CA-C	-7.14	102.09	111.23
1	A	169	PRO	O-C-N	-7.13	112.68	122.24
1	B	1246	ILE	N-CA-CB	-7.13	103.98	111.61
1	B	1058	HIS	CA-C-N	-7.13	109.75	120.94
1	B	1058	HIS	C-N-CA	-7.13	109.75	120.94
1	A	232	SER	N-CA-C	7.12	119.05	111.28
1	B	1357	GLU	N-CA-CB	-7.11	99.04	110.63
1	A	180	SER	CA-CB-OG	-7.10	96.91	111.10
1	B	1192	ASP	CA-C-N	-7.09	113.05	121.85
1	B	1192	ASP	C-N-CA	-7.09	113.05	121.85
1	C	2233	GLU	CG-CD-OE2	7.08	134.68	118.40
1	C	2338	HIS	CA-C-N	-7.06	113.03	122.42
1	C	2338	HIS	C-N-CA	-7.06	113.03	122.42
1	C	2232	SER	CA-CB-OG	-7.04	97.01	111.10
1	B	1126	HIS	N-CA-C	-7.04	98.65	109.14
1	C	2200	LYS	N-CA-CB	-7.04	100.79	110.29
1	C	2357	GLU	CA-C-O	-7.02	113.00	120.80
1	A	337	ASN	N-CA-C	-7.01	97.12	108.41
1	A	93	MET	N-CA-C	-7.01	96.28	108.69
1	B	1281	ASN	CB-CA-C	-7.01	99.58	110.37
1	A	157	ALA	O-C-N	7.00	130.79	122.46
1	B	1108	GLU	CA-C-N	-7.00	112.64	122.86
1	B	1108	GLU	C-N-CA	-7.00	112.64	122.86
1	B	1092	ALA	N-CA-C	6.99	119.99	110.55
1	A	305	ALA	CB-CA-C	-6.98	98.03	109.27
1	B	1319	THR	CA-CB-OG1	6.97	120.05	109.60
1	B	1319	THR	O-C-N	6.97	130.58	123.26
1	B	1198	GLU	CA-CB-CG	-6.93	100.23	114.10
1	B	1232	SER	CA-CB-OG	-6.92	97.27	111.10
1	A	319	THR	CA-C-N	-6.90	111.98	122.81
1	A	319	THR	C-N-CA	-6.90	111.98	122.81
1	A	365	GLN	CA-C-N	6.88	129.36	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	GLN	C-N-CA	6.88	129.36	120.56
1	C	2303	HIS	CA-CB-CG	-6.87	106.93	113.80
1	B	1131	HIS	N-CA-C	-6.87	104.16	112.54
1	A	66	SER	N-CA-C	6.86	117.33	108.34
1	C	2246	ILE	CB-CA-C	-6.86	103.30	111.18
1	A	76	ARG	CA-C-O	-6.85	113.42	121.16
1	C	2109	GLY	CA-C-O	-6.84	112.15	119.27
1	C	2109	GLY	N-CA-C	-6.83	106.95	115.08
1	C	2205	ASP	N-CA-C	-6.83	103.95	112.90
1	A	292	HIS	CA-C-O	-6.82	114.15	121.38
1	C	2096	ASP	CA-C-N	-6.82	111.80	122.51
1	C	2096	ASP	C-N-CA	-6.82	111.80	122.51
1	A	316	ARG	CD-NE-CZ	-6.80	114.87	124.40
1	A	182	THR	OG1-CB-CG2	-6.80	95.70	109.30
1	A	150	LYS	CA-C-O	-6.79	113.67	121.68
1	B	1067	GLY	CA-C-N	6.78	126.81	119.90
1	B	1067	GLY	C-N-CA	6.78	126.81	119.90
1	C	2252	PHE	N-CA-C	-6.76	98.70	109.59
1	C	2043	ASN	N-CA-C	6.76	121.53	113.28
1	A	50	THR	CA-CB-OG1	-6.75	99.47	109.60
1	B	1200	LYS	CA-CB-CG	-6.75	100.60	114.10
1	A	216	TYR	N-CA-CB	-6.73	101.34	111.64
1	A	161	GLY	N-CA-C	-6.73	100.92	110.88
1	C	2199	GLY	N-CA-C	-6.72	105.95	115.43
1	C	2336	VAL	CB-CA-C	-6.72	99.97	110.52
1	A	160	ALA	CA-C-N	-6.72	111.55	121.22
1	A	160	ALA	C-N-CA	-6.72	111.55	121.22
1	A	182	THR	CB-CA-C	-6.72	100.40	111.68
1	C	2101	GLY	O-C-N	-6.72	115.05	121.77
1	C	2156	LYS	CD-CE-NZ	-6.71	90.41	111.90
1	B	1326	LYS	CB-CG-CD	-6.70	95.88	111.30
1	C	2364	GLU	CA-CB-CG	-6.70	100.70	114.10
1	C	2303	HIS	N-CA-C	-6.69	105.11	113.20
1	A	60	HIS	O-C-N	-6.67	116.85	123.46
1	B	1171	GLY	CA-C-N	-6.67	113.28	119.82
1	B	1171	GLY	C-N-CA	-6.67	113.28	119.82
1	B	1077	ILE	CA-C-N	-6.66	114.93	123.19
1	B	1077	ILE	C-N-CA	-6.66	114.93	123.19
1	C	2220	ASP	CB-CG-OD2	-6.66	103.09	118.40
1	B	1076	ARG	NE-CZ-NH2	-6.64	113.22	119.20
1	B	1236	GLU	OE1-CD-OE2	-6.64	106.96	122.90
1	A	246	ILE	N-CA-C	6.63	114.12	107.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	LYS	CA-C-N	-6.63	109.49	122.02
1	A	219	LYS	C-N-CA	-6.63	109.49	122.02
1	B	1241	VAL	CB-CA-C	-6.62	103.38	112.24
1	C	2211	GLY	O-C-N	-6.61	119.19	123.35
1	C	2290	GLY	CA-C-O	-6.61	111.67	119.07
1	C	2113	GLU	CA-C-N	-6.61	113.35	122.93
1	C	2113	GLU	C-N-CA	-6.61	113.35	122.93
1	C	2061	GLU	CA-CB-CG	-6.60	100.90	114.10
1	C	2074	GLU	CB-CG-CD	-6.60	101.38	112.60
1	C	2185	CYS	CA-C-O	-6.60	112.68	120.60
1	C	2114	LEU	CB-CA-C	-6.59	97.52	109.38
1	B	1244	THR	N-CA-C	-6.59	105.24	113.28
1	B	1324	LEU	N-CA-CB	-6.56	100.35	110.85
1	B	1101	GLY	O-C-N	-6.56	115.21	121.77
1	B	1336	VAL	CB-CA-C	-6.56	99.22	110.30
1	B	1332	VAL	CB-CA-C	-6.55	102.23	111.21
1	B	1147	PRO	CA-C-O	-6.55	113.96	121.36
1	B	1227	ARG	CD-NE-CZ	6.54	133.56	124.40
1	B	1129	ASP	N-CA-C	-6.52	97.65	108.34
1	A	42	SER	O-C-N	-6.51	113.70	122.43
1	B	1044	LEU	CA-C-O	6.50	126.86	120.23
1	C	2202	VAL	N-CA-C	-6.48	98.25	108.95
1	C	2169	PRO	CA-C-N	-6.48	108.71	121.41
1	C	2169	PRO	C-N-CA	-6.48	108.71	121.41
1	B	1276	VAL	CA-C-N	-6.47	113.64	122.77
1	B	1276	VAL	C-N-CA	-6.47	113.64	122.77
1	A	142	LEU	CA-C-O	-6.47	111.54	119.18
1	A	217	ILE	CA-C-N	6.47	126.44	120.03
1	A	217	ILE	C-N-CA	6.47	126.44	120.03
1	A	169	PRO	CA-C-N	-6.46	108.74	121.41
1	A	169	PRO	C-N-CA	-6.46	108.74	121.41
1	A	65	ALA	N-CA-C	-6.45	105.23	113.23
1	C	2293	GLY	N-CA-C	-6.45	97.88	113.18
1	A	170	GLY	N-CA-C	-6.45	97.91	113.18
1	B	1078	ILE	CB-CA-C	-6.44	101.23	110.83
1	B	1191	ARG	NE-CZ-NH1	6.44	127.94	121.50
1	C	2152	VAL	CB-CA-C	-6.44	101.73	110.42
1	A	39	VAL	N-CA-C	-6.43	93.00	111.00
1	B	1192	ASP	CA-C-O	-6.42	111.70	119.59
1	C	2250	ILE	N-CA-C	-6.42	98.22	107.78
1	C	2223	GLY	O-C-N	-6.41	114.25	122.39
1	B	1172	PRO	CA-C-N	6.41	132.94	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1172	PRO	C-N-CA	6.41	132.94	121.66
1	A	210	ILE	CB-CA-C	-6.40	102.29	111.19
1	A	370	VAL	CA-C-N	6.40	126.84	120.31
1	A	370	VAL	C-N-CA	6.40	126.84	120.31
1	A	61	GLU	CG-CD-OE1	-6.40	103.69	118.40
1	A	315	ILE	N-CA-C	-6.40	98.53	107.80
1	A	327	PHE	O-C-N	6.39	130.69	122.89
1	C	2198	GLU	CA-CB-CG	-6.39	101.32	114.10
1	B	1132	ALA	CA-C-O	-6.39	111.53	119.38
1	A	154	ARG	CD-NE-CZ	6.38	133.34	124.40
1	B	1086	GLU	CA-C-O	-6.38	113.74	120.63
1	A	155	PHE	N-CA-C	-6.36	99.41	109.07
1	A	262	GLU	N-CA-CB	-6.36	99.84	110.39
1	A	43	ASN	CA-CB-CG	-6.35	106.25	112.60
1	A	332	VAL	CB-CA-C	-6.35	102.51	111.21
1	A	48	LYS	O-C-N	-6.34	116.00	123.22
1	A	172	PRO	CA-C-N	6.33	132.22	121.14
1	A	172	PRO	C-N-CA	6.33	132.22	121.14
1	A	355	GLU	CB-CA-C	-6.33	98.69	109.51
1	B	1269	VAL	N-CA-C	-6.32	101.40	109.30
1	C	2338	HIS	N-CA-C	6.31	119.66	112.97
1	A	200	LYS	N-CA-CB	-6.31	99.62	110.10
1	C	2333	TYR	N-CA-C	-6.30	99.89	109.85
1	B	1200	LYS	CB-CG-CD	6.28	125.75	111.30
1	C	2190	PRO	CB-CA-C	-6.28	103.19	111.23
1	A	188	VAL	CB-CA-C	-6.28	103.37	111.53
1	B	1167	CYS	CA-CB-SG	-6.27	99.97	114.40
1	B	1326	LYS	CD-CE-NZ	-6.27	91.82	111.90
1	B	1348	ALA	N-CA-C	6.27	119.03	109.62
1	B	1329	GLN	CB-CG-CD	-6.25	101.97	112.60
1	B	1040	ASP	O-C-N	6.24	130.89	122.59
1	A	43	ASN	N-CA-C	6.24	120.89	113.28
1	C	2355	GLU	O-C-N	6.23	130.00	122.96
1	C	2109	GLY	CA-C-N	-6.23	110.46	121.29
1	C	2109	GLY	C-N-CA	-6.23	110.46	121.29
1	B	1108	GLU	CA-C-O	-6.21	114.19	120.96
1	C	2281	ASN	CB-CA-C	-6.21	101.15	109.16
1	B	1223	GLY	CA-C-N	-6.20	112.01	122.92
1	B	1223	GLY	C-N-CA	-6.20	112.01	122.92
1	C	2316	ARG	NH1-CZ-NH2	6.19	127.35	119.30
1	B	1344	VAL	N-CA-C	-6.18	105.79	111.67
1	C	2113	GLU	CG-CD-OE1	-6.18	104.17	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2071	ASN	CA-CB-CG	-6.18	106.42	112.60
1	A	81	GLU	N-CA-CB	6.16	119.50	109.95
1	C	2261	GLY	CA-C-O	6.16	129.64	121.51
1	B	1160	ALA	CA-C-O	-6.15	113.68	120.69
1	C	2367	VAL	O-C-N	-6.13	117.08	123.03
1	B	1302	PHE	CA-C-N	-6.13	111.29	122.38
1	B	1302	PHE	C-N-CA	-6.13	111.29	122.38
1	A	285	ARG	NE-CZ-NH1	-6.12	115.38	121.50
1	B	1337	ASN	N-CA-C	-6.12	99.88	109.25
1	B	1171	GLY	CA-C-O	6.12	130.27	121.52
1	C	2319	THR	OG1-CB-CG2	-6.11	97.08	109.30
1	C	2197	HIS	N-CA-C	-6.11	105.09	112.54
1	B	1248	SER	N-CA-C	-6.10	104.54	112.23
1	B	1192	ASP	CB-CG-OD2	6.10	132.43	118.40
1	B	1327	PHE	N-CA-C	6.10	119.05	109.96
1	B	1262	GLU	CB-CA-C	6.09	122.59	110.17
1	A	46	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	B	1312	THR	CA-C-O	-6.07	114.02	121.06
1	C	2254	GLY	CA-C-O	-6.07	112.27	119.06
1	B	1046	ARG	CA-CB-CG	-6.06	101.98	114.10
1	C	2039	VAL	CG1-CB-CG2	-6.05	97.48	110.80
1	C	2355	GLU	CG-CD-OE2	-6.04	104.51	118.40
1	A	139	GLY	N-CA-C	-6.03	106.19	114.64
1	A	299	THR	N-CA-C	-6.03	105.68	113.16
1	A	302	PHE	CA-C-N	-6.03	109.88	121.94
1	A	302	PHE	C-N-CA	-6.03	109.88	121.94
1	C	2128	ILE	CB-CG1-CD1	-6.03	101.15	113.80
1	A	58	HIS	N-CA-C	-6.02	102.76	110.53
1	A	303	HIS	CA-CB-CG	-6.01	107.79	113.80
1	C	2118	ASN	CA-C-N	6.01	124.05	119.66
1	C	2118	ASN	C-N-CA	6.01	124.05	119.66
1	C	2227	ARG	CB-CG-CD	-6.00	97.50	111.30
1	B	1076	ARG	NH1-CZ-NH2	5.99	127.09	119.30
1	B	1062	GLN	CA-CB-CG	-5.99	102.12	114.10
1	B	1224	THR	CA-CB-OG1	-5.99	100.62	109.60
1	B	1259	LEU	CA-C-O	5.98	127.79	120.55
1	C	2053	PRO	CB-CA-C	-5.98	103.63	110.92
1	B	1172	PRO	CA-C-O	-5.97	109.87	118.89
1	B	1107	HIS	CA-C-O	5.96	127.85	121.11
1	B	1154	ARG	CA-C-O	-5.96	114.26	120.70
1	C	2295	LEU	CA-C-N	-5.95	114.71	122.99
1	C	2295	LEU	C-N-CA	-5.95	114.71	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1081	GLU	CA-CB-CG	-5.95	102.20	114.10
1	A	370	VAL	CA-CB-CG2	-5.94	100.30	110.40
1	B	1201	PRO	CA-CB-CG	-5.94	93.22	104.50
1	C	2077	ILE	CB-CG1-CD1	-5.94	101.33	113.80
1	B	1224	THR	OG1-CB-CG2	-5.93	97.44	109.30
1	B	1259	LEU	CA-C-N	-5.92	112.87	122.82
1	B	1259	LEU	C-N-CA	-5.92	112.87	122.82
1	A	286	PRO	CB-CA-C	-5.91	103.20	110.95
1	B	1043	ASN	CA-CB-CG	-5.91	106.69	112.60
1	B	1133	ALA	N-CA-C	5.91	119.26	110.52
1	A	332	VAL	CG1-CB-CG2	-5.90	97.82	110.80
1	C	2058	HIS	ND1-CE1-NE2	-5.90	102.50	108.40
1	A	109	GLY	N-CA-C	-5.89	108.07	115.08
1	B	1308	ARG	CA-CB-CG	-5.89	102.32	114.10
1	C	2236	GLU	CG-CD-OE2	5.89	131.95	118.40
1	C	2094	THR	OG1-CB-CG2	-5.89	97.52	109.30
1	A	199	GLY	N-CA-C	-5.88	106.62	115.32
1	C	2366	VAL	CA-CB-CG2	-5.88	100.40	110.40
1	A	191	ARG	NH1-CZ-NH2	5.87	126.93	119.30
1	A	119	PRO	CB-CA-C	5.87	118.08	110.92
1	B	1364	GLU	CA-CB-CG	-5.87	102.36	114.10
1	A	239	VAL	CB-CA-C	-5.87	104.36	112.04
1	C	2087	ASP	CB-CA-C	-5.86	102.04	111.18
1	A	86	GLU	CA-C-O	-5.86	114.30	120.63
1	A	62	GLN	CA-CB-CG	-5.85	102.39	114.10
1	B	1039	VAL	N-CA-C	-5.85	94.63	111.00
1	A	249	HIS	CA-CB-CG	-5.84	107.96	113.80
1	B	1123	THR	CB-CA-C	-5.84	99.75	109.55
1	B	1191	ARG	NH1-CZ-NH2	-5.84	111.71	119.30
1	B	1040	ASP	CB-CG-OD1	-5.83	104.98	118.40
1	A	125	PRO	N-CD-CG	-5.83	94.46	103.20
1	C	2092	ALA	N-CA-C	5.82	119.14	110.52
1	C	2324	LEU	CA-C-N	-5.82	113.30	122.73
1	C	2324	LEU	C-N-CA	-5.82	113.30	122.73
1	C	2122	ASN	O-C-N	5.82	129.75	122.65
1	B	1093	MET	O-C-N	-5.82	116.46	123.27
1	B	1333	TYR	N-CA-C	-5.82	100.31	109.50
1	C	2114	LEU	CA-C-N	-5.81	115.04	122.77
1	C	2114	LEU	C-N-CA	-5.81	115.04	122.77
1	B	1215	HIS	CA-CB-CG	-5.81	107.99	113.80
1	C	2233	GLU	N-CA-C	-5.81	105.08	111.82
1	A	319	THR	CB-CA-C	-5.80	97.92	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1040	ASP	OD1-CG-OD2	5.80	136.82	122.90
1	A	113	GLU	CA-C-N	-5.80	114.53	122.93
1	A	113	GLU	C-N-CA	-5.80	114.53	122.93
1	B	1106	VAL	CA-C-N	-5.79	113.71	122.81
1	B	1106	VAL	C-N-CA	-5.79	113.71	122.81
1	B	1052	VAL	O-C-N	-5.79	116.59	121.40
1	A	51	LEU	CA-C-O	-5.79	115.42	121.55
1	A	210	ILE	N-CA-C	-5.79	98.81	107.37
1	C	2192	ASP	OD1-CG-OD2	-5.79	109.01	122.90
1	C	2174	ILE	CA-C-O	5.78	122.56	118.69
1	B	1284	SER	CA-C-O	-5.78	115.09	121.33
1	A	118	ASN	N-CA-C	-5.77	96.82	109.11
1	B	1337	ASN	CA-C-O	5.77	127.18	120.49
1	B	1324	LEU	N-CA-C	-5.76	100.79	109.95
1	B	1185	CYS	CA-C-N	-5.76	114.94	122.94
1	B	1185	CYS	C-N-CA	-5.76	114.94	122.94
1	B	1090	LEU	CA-C-N	-5.75	112.85	122.17
1	B	1090	LEU	C-N-CA	-5.75	112.85	122.17
1	B	1102	PRO	CA-C-O	-5.75	114.66	121.67
1	B	1191	ARG	CG-CD-NE	-5.75	99.36	112.00
1	C	2344	VAL	O-C-N	-5.75	116.09	122.07
1	C	2189	LEU	CA-C-N	-5.74	113.86	119.78
1	C	2189	LEU	C-N-CA	-5.74	113.86	119.78
1	C	2116	LEU	O-C-N	5.74	130.50	123.21
1	C	2253	ASN	N-CA-C	5.74	119.47	111.90
1	C	2258	ALA	CA-C-N	-5.74	114.62	123.17
1	C	2258	ALA	C-N-CA	-5.74	114.62	123.17
1	B	1160	ALA	CA-C-N	-5.73	112.27	121.32
1	B	1160	ALA	C-N-CA	-5.73	112.27	121.32
1	C	2252	PHE	CA-C-O	5.73	126.78	120.71
1	B	1087	ASP	CA-C-O	-5.73	114.58	121.34
1	A	306	PRO	CA-C-O	-5.72	114.76	122.08
1	A	174	ILE	CA-CB-CG1	-5.72	100.68	110.40
1	A	149	GLU	N-CA-C	5.71	118.37	109.52
1	C	2065	ALA	CA-C-O	-5.71	109.03	119.36
1	B	1341	ILE	CB-CA-C	-5.68	104.37	112.22
1	A	282	ARG	CA-C-O	-5.68	114.98	121.40
1	B	1186	ILE	O-C-N	-5.67	117.03	123.10
1	B	1174	ILE	CA-CB-CG1	-5.67	100.76	110.40
1	C	2309	ASP	N-CA-CB	-5.66	103.69	112.30
1	C	2178	VAL	O-C-N	-5.66	116.36	121.91
1	A	289	ILE	CB-CA-C	-5.66	103.74	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1370	VAL	CA-CB-CG1	5.66	120.02	110.40
1	C	2206	THR	CA-C-O	-5.66	114.50	121.06
1	A	332	VAL	CA-CB-CG2	-5.65	100.79	110.40
1	B	1113	GLU	N-CA-C	-5.65	99.20	108.41
1	C	2078	ILE	O-C-N	-5.65	117.30	123.18
1	B	1334	ALA	CA-C-N	-5.65	115.02	122.99
1	B	1334	ALA	C-N-CA	-5.65	115.02	122.99
1	A	115	THR	CA-C-N	-5.65	114.74	122.93
1	A	115	THR	C-N-CA	-5.65	114.74	122.93
1	B	1275	PHE	CA-CB-CG	-5.65	108.15	113.80
1	C	2165	TYR	CA-C-N	-5.65	112.14	121.80
1	C	2165	TYR	C-N-CA	-5.65	112.14	121.80
1	C	2198	GLU	CG-CD-OE1	-5.64	105.42	118.40
1	C	2343	ALA	O-C-N	5.64	128.10	122.12
1	A	130	PHE	CB-CA-C	-5.64	101.06	110.19
1	C	2266	LYS	CA-CB-CG	5.64	125.37	114.10
1	B	1160	ALA	O-C-N	5.63	129.63	123.04
1	C	2224	THR	OG1-CB-CG2	-5.63	98.03	109.30
1	B	1144	LEU	CD1-CG-CD2	-5.63	98.42	110.80
1	B	1330	PRO	CA-C-O	-5.61	113.65	121.90
1	B	1296	VAL	CA-CB-CG2	-5.60	100.87	110.40
1	C	2283	ASP	CB-CG-OD1	5.60	131.29	118.40
1	A	198	GLU	N-CA-C	-5.60	105.65	112.88
1	A	163	PHE	CZ-CE2-CD2	-5.60	109.92	120.00
1	C	2343	ALA	CA-C-N	-5.60	117.23	122.66
1	C	2343	ALA	C-N-CA	-5.60	117.23	122.66
1	A	79	GLU	CA-C-O	-5.59	114.33	120.43
1	B	1182	THR	OG1-CB-CG2	-5.59	98.11	109.30
1	B	1357	GLU	CB-CG-CD	-5.59	103.10	112.60
1	C	2076	ARG	CB-CA-C	-5.59	99.15	109.37
1	B	1222	ASP	N-CA-C	-5.58	106.51	113.15
1	C	2289	ILE	CB-CA-C	-5.58	103.85	111.33
1	C	2152	VAL	CA-C-O	5.58	125.90	120.27
1	C	2159	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	A	194	LEU	CA-C-O	-5.57	115.15	121.72
1	A	268	LYS	CB-CA-C	-5.56	98.39	109.79
1	C	2043	ASN	CA-CB-CG	-5.56	107.04	112.60
1	C	2284	SER	CA-C-N	-5.56	116.84	122.74
1	C	2284	SER	C-N-CA	-5.56	116.84	122.74
1	B	1247	PRO	CB-CA-C	-5.56	102.68	110.63
1	C	2302	PHE	CA-C-N	-5.56	110.82	121.94
1	C	2302	PHE	C-N-CA	-5.56	110.82	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	HIS	CA-C-N	-5.56	113.66	121.72
1	A	338	HIS	C-N-CA	-5.56	113.66	121.72
1	B	1048	LYS	CA-C-N	-5.56	113.47	122.81
1	B	1048	LYS	C-N-CA	-5.56	113.47	122.81
1	C	2105	ILE	CB-CA-C	-5.55	102.93	110.42
1	A	203	ARG	CB-CG-CD	-5.55	98.54	111.30
1	A	354	VAL	N-CA-CB	-5.54	104.48	111.46
1	C	2183	ALA	N-CA-C	-5.54	100.00	108.76
1	B	1340	LEU	CB-CG-CD1	-5.54	94.08	110.70
1	B	1102	PRO	N-CA-C	5.54	120.18	111.38
1	B	1293	GLY	N-CA-C	-5.54	100.06	113.18
1	B	1178	VAL	CA-C-O	-5.53	115.19	120.95
1	C	2185	CYS	CA-C-N	-5.53	115.30	122.99
1	C	2185	CYS	C-N-CA	-5.53	115.30	122.99
1	A	81	GLU	N-CA-C	-5.52	100.99	109.76
1	B	1079	GLU	O-C-N	-5.52	117.03	123.27
1	B	1264	ALA	N-CA-C	5.52	118.02	110.24
1	A	47	VAL	N-CA-C	-5.50	100.19	108.12
1	C	2059	ALA	N-CA-C	5.50	118.46	110.42
1	B	1308	ARG	O-C-N	5.50	130.01	123.24
1	A	366	VAL	O-C-N	-5.50	116.18	121.90
1	C	2342	GLU	CA-CB-CG	-5.50	103.11	114.10
1	A	327	PHE	CA-C-O	-5.49	115.02	121.16
1	C	2256	VAL	CA-CB-CG2	-5.48	101.09	110.40
1	B	1076	ARG	CA-C-N	-5.47	115.53	122.37
1	B	1076	ARG	C-N-CA	-5.47	115.53	122.37
1	B	1104	MET	CA-CB-CG	-5.47	103.16	114.10
1	A	292	HIS	CB-CA-C	-5.47	100.45	111.17
1	A	199	GLY	O-C-N	-5.47	115.88	122.38
1	B	1275	PHE	O-C-N	5.46	129.72	123.27
1	B	1092	ALA	N-CA-CB	-5.46	102.15	110.45
1	A	153	LEU	CA-C-N	-5.46	114.24	122.81
1	A	153	LEU	C-N-CA	-5.46	114.24	122.81
1	A	164	VAL	CB-CA-C	-5.45	102.97	111.26
1	A	281	ASN	CA-C-N	-5.45	113.38	122.21
1	A	281	ASN	C-N-CA	-5.45	113.38	122.21
1	C	2135	GLY	CA-C-O	-5.45	118.68	122.22
1	A	258	ALA	N-CA-CB	5.44	118.11	110.12
1	B	1093	MET	CG-SD-CE	5.44	112.86	100.90
1	B	1049	HIS	CA-C-N	-5.43	115.39	123.11
1	B	1049	HIS	C-N-CA	-5.43	115.39	123.11
1	B	1366	VAL	O-C-N	5.43	127.14	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2228	PHE	CA-C-O	-5.42	115.29	121.58
1	B	1355	GLU	CA-CB-CG	-5.42	103.26	114.10
1	A	320	ALA	N-CA-C	-5.41	101.06	109.72
1	C	2302	PHE	CA-C-O	-5.40	112.73	119.38
1	C	2095	PHE	CE1-CZ-CE2	-5.40	110.28	120.00
1	C	2141	GLY	N-CA-C	-5.40	108.73	114.67
1	B	1173	MET	CA-CB-CG	5.39	124.88	114.10
1	B	1070	ILE	CA-C-O	-5.39	114.72	120.59
1	A	329	GLN	CA-C-N	-5.39	115.03	120.85
1	A	329	GLN	C-N-CA	-5.39	115.03	120.85
1	A	173	MET	CB-CG-SD	5.38	128.85	112.70
1	C	2057	ALA	CA-C-O	-5.38	115.03	121.11
1	A	355	GLU	CG-CD-OE2	-5.38	106.02	118.40
1	A	371	GLY	N-CA-C	-5.38	104.22	111.54
1	A	328	LEU	N-CA-C	-5.38	107.38	114.31
1	A	307	GLU	CB-CG-CD	-5.38	103.46	112.60
1	A	61	GLU	CG-CD-OE2	5.37	130.76	118.40
1	B	1337	ASN	N-CA-CB	-5.37	101.11	109.87
1	B	1355	GLU	OE1-CD-OE2	5.37	135.78	122.90
1	C	2076	ARG	CA-C-O	-5.36	115.10	121.16
1	C	2103	LEU	O-C-N	-5.36	117.11	123.22
1	A	40	ASP	OD1-CG-OD2	5.36	135.77	122.90
1	A	297	TRP	CE3-CZ3-CH2	-5.36	114.13	121.10
1	C	2150	LYS	CD-CE-NZ	-5.36	94.76	111.90
1	C	2346	LYS	CA-C-O	-5.36	113.00	119.27
1	C	2238	MET	CG-SD-CE	-5.35	89.12	100.90
1	A	195	LYS	CG-CD-CE	5.35	123.61	111.30
1	B	1249	HIS	CA-C-O	-5.35	113.96	120.54
1	C	2361	ASP	N-CA-C	-5.35	105.49	112.23
1	C	2143	THR	O-C-N	-5.35	114.93	122.26
1	A	93	MET	CB-CG-SD	-5.34	96.67	112.70
1	A	309	ASP	CA-CB-CG	-5.34	107.26	112.60
1	B	1195	LYS	CB-CA-C	-5.34	98.83	109.79
1	C	2306	PRO	CA-C-O	-5.34	115.56	122.13
1	A	336	VAL	CB-CA-C	-5.34	102.92	110.82
1	C	2173	MET	CB-CA-C	-5.34	99.46	109.72
1	B	1270	GLY	CA-C-O	-5.34	113.56	119.27
1	A	223	GLY	CA-C-N	-5.33	113.57	122.64
1	A	223	GLY	C-N-CA	-5.33	113.57	122.64
1	A	189	LEU	CA-C-N	-5.33	114.22	119.92
1	A	189	LEU	C-N-CA	-5.33	114.22	119.92
1	B	1280	PRO	CA-C-N	-5.33	112.01	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1280	PRO	C-N-CA	-5.33	112.01	120.70
1	B	1340	LEU	CA-CB-CG	-5.33	97.66	116.30
1	C	2308	ARG	CA-CB-CG	-5.33	103.45	114.10
1	A	364	GLU	CA-CB-CG	-5.32	103.45	114.10
1	A	365	GLN	CB-CG-CD	-5.32	103.55	112.60
1	B	1311	GLU	N-CA-C	-5.32	105.06	112.45
1	B	1163	PHE	N-CA-CB	-5.31	101.65	111.53
1	A	76	ARG	CD-NE-CZ	-5.31	116.96	124.40
1	A	318	GLY	O-C-N	-5.31	116.23	122.45
1	C	2176	TRP	CA-C-O	-5.31	114.92	120.55
1	B	1352	VAL	CG1-CB-CG2	-5.31	99.13	110.80
1	C	2200	LYS	CD-CE-NZ	-5.30	94.93	111.90
1	B	1222	ASP	CB-CG-OD2	5.30	130.59	118.40
1	B	1142	LEU	N-CA-C	-5.30	105.66	113.61
1	A	293	GLY	N-CA-C	-5.29	100.65	113.18
1	B	1047	VAL	N-CA-CB	-5.29	104.77	111.64
1	B	1310	LEU	CA-C-O	-5.29	115.39	121.47
1	A	204	TYR	N-CA-C	-5.28	101.55	109.95
1	C	2370	VAL	CA-CB-CG2	-5.28	101.43	110.40
1	B	1152	VAL	N-CA-C	-5.27	100.74	108.11
1	B	1068	PRO	CA-C-O	-5.26	115.41	121.36
1	B	1236	GLU	CB-CG-CD	-5.26	103.66	112.60
1	C	2314	PHE	CA-CB-CG	-5.26	108.54	113.80
1	A	144	LEU	CB-CG-CD2	-5.26	94.92	110.70
1	A	222	ASP	CB-CG-OD2	5.26	130.49	118.40
1	B	1308	ARG	CA-C-O	-5.26	114.96	121.11
1	C	2285	ARG	N-CA-CB	-5.25	104.58	111.09
1	C	2205	ASP	CA-CB-CG	-5.25	107.35	112.60
1	C	2213	SER	CA-CB-OG	-5.25	100.60	111.10
1	B	1367	VAL	CA-CB-CG1	-5.24	101.50	110.40
1	C	2068	PRO	CA-CB-CG	-5.24	94.55	104.50
1	A	125	PRO	N-CA-C	-5.23	103.07	111.38
1	A	95	PHE	CA-CB-CG	-5.22	108.58	113.80
1	B	1076	ARG	CB-CA-C	-5.22	99.54	109.66
1	B	1097	GLY	CA-C-N	-5.21	114.41	122.59
1	B	1097	GLY	C-N-CA	-5.21	114.41	122.59
1	B	1229	SER	O-C-N	-5.21	115.32	122.46
1	C	2275	PHE	N-CA-C	-5.20	99.30	108.20
1	A	335	TYR	CA-C-N	-5.20	115.43	122.92
1	A	335	TYR	C-N-CA	-5.20	115.43	122.92
1	C	2048	LYS	CG-CD-CE	5.20	123.26	111.30
1	B	1268	LYS	CD-CE-NZ	-5.19	95.28	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2046	ARG	CB-CG-CD	-5.19	99.36	111.30
1	A	113	GLU	CG-CD-OE2	5.18	130.32	118.40
1	C	2243	ASP	CA-CB-CG	-5.18	107.42	112.60
1	B	1203	ARG	CB-CA-C	-5.18	98.56	109.38
1	C	2303	HIS	CA-C-O	-5.18	112.34	119.12
1	A	196	ASP	N-CA-C	5.17	117.86	109.79
1	B	1308	ARG	CG-CD-NE	-5.17	100.62	112.00
1	A	221	GLU	CA-C-O	-5.17	115.05	120.63
1	C	2328	LEU	CB-CG-CD1	5.17	126.20	110.70
1	A	86	GLU	CA-CB-CG	-5.16	103.77	114.10
1	C	2256	VAL	CA-C-O	-5.16	114.33	120.78
1	B	1076	ARG	CG-CD-NE	-5.16	100.66	112.00
1	C	2101	GLY	CA-C-N	5.16	125.14	120.03
1	C	2101	GLY	C-N-CA	5.16	125.14	120.03
1	C	2233	GLU	CG-CD-OE1	-5.16	106.54	118.40
1	B	1074	GLU	CA-C-O	-5.14	114.43	120.60
1	C	2076	ARG	CA-CB-CG	-5.14	103.82	114.10
1	A	112	VAL	CG1-CB-CG2	-5.14	99.50	110.80
1	A	87	ASP	CB-CA-C	-5.13	103.17	111.28
1	A	238	MET	CA-C-N	5.13	127.77	120.53
1	A	238	MET	C-N-CA	5.13	127.77	120.53
1	C	2076	ARG	CG-CD-NE	-5.13	100.71	112.00
1	A	107	HIS	CA-C-O	5.13	127.46	121.46
1	B	1108	GLU	O-C-N	5.13	129.21	123.06
1	B	1101	GLY	CA-C-O	5.12	128.84	121.52
1	B	1350	ALA	N-CA-C	-5.12	101.58	109.52
1	C	2074	GLU	CA-CB-CG	-5.12	103.86	114.10
1	A	86	GLU	CA-C-N	-5.12	114.45	122.79
1	A	86	GLU	C-N-CA	-5.12	114.45	122.79
1	B	1200	LYS	CB-CA-C	5.12	116.09	108.87
1	C	2210	ILE	CA-C-N	-5.12	117.73	122.29
1	C	2210	ILE	C-N-CA	-5.12	117.73	122.29
1	C	2188	VAL	N-CA-C	-5.12	99.80	107.37
1	C	2217	ILE	CB-CA-C	-5.12	106.18	110.94
1	C	2279	GLN	N-CA-C	-5.11	98.52	109.81
1	B	1315	ILE	CA-C-O	-5.10	114.69	120.66
1	C	2153	LEU	CD1-CG-CD2	-5.10	99.58	110.80
1	A	232	SER	CA-CB-OG	-5.10	100.90	111.10
1	B	1159	ARG	O-C-N	5.10	129.37	123.30
1	C	2220	ASP	OD1-CG-OD2	5.10	135.13	122.90
1	C	2268	LYS	CG-CD-CE	-5.10	99.58	111.30
1	A	319	THR	CA-CB-OG1	5.10	117.24	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	GLN	CA-C-O	-5.09	115.70	121.66
1	B	1205	ASP	CB-CG-OD2	5.09	130.10	118.40
1	A	149	GLU	O-C-N	5.09	129.76	123.15
1	C	2189	LEU	CB-CA-C	-5.09	101.70	108.87
1	B	1279	GLN	N-CA-C	-5.08	98.58	109.81
1	C	2165	TYR	N-CA-C	-5.08	101.58	109.72
1	A	324	LEU	CA-CB-CG	5.08	134.09	116.30
1	B	1275	PHE	CD1-CE1-CZ	-5.08	110.85	120.00
1	B	1277	HIS	CE1-NE2-CD2	-5.08	103.92	109.00
1	A	349	THR	CA-C-O	-5.08	114.69	120.32
1	C	2325	TYR	CA-C-N	-5.08	116.24	122.84
1	C	2325	TYR	C-N-CA	-5.08	116.24	122.84
1	A	117	ILE	O-C-N	-5.07	117.67	123.10
1	C	2069	VAL	CA-CB-CG2	5.07	119.02	110.40
1	C	2319	THR	CA-C-O	-5.07	115.88	121.31
1	C	2363	MET	CB-CA-C	-5.07	100.73	109.86
1	B	1244	THR	O-C-N	5.07	129.61	122.41
1	B	1159	ARG	N-CA-CB	-5.06	102.18	110.68
1	A	258	ALA	N-CA-C	-5.06	105.77	111.28
1	B	1113	GLU	CA-C-N	-5.05	115.60	122.93
1	B	1113	GLU	C-N-CA	-5.05	115.60	122.93
1	C	2250	ILE	CA-C-O	5.05	125.25	120.25
1	A	42	SER	CA-CB-OG	-5.05	101.00	111.10
1	C	2265	LEU	CD1-CG-CD2	-5.05	99.70	110.80
1	B	1283	ASP	N-CA-C	5.04	117.04	110.43
1	C	2086	GLU	CB-CG-CD	5.04	121.18	112.60
1	C	2318	GLY	CA-C-N	-5.04	113.73	122.10
1	C	2318	GLY	C-N-CA	-5.04	113.73	122.10
1	B	1173	MET	CB-CG-SD	5.04	127.82	112.70
1	C	2125	PRO	CB-CG-CD	-5.04	89.98	106.10
1	C	2332	VAL	O-C-N	-5.04	116.99	122.83
1	C	2339	ASN	O-C-N	-5.04	116.89	122.93
1	C	2216	TYR	N-CA-CB	-5.03	101.55	110.60
1	B	1158	THR	CA-CB-CG2	-5.03	101.95	110.50
1	A	122	ASN	O-C-N	-5.03	116.52	122.65
1	B	1174	ILE	CA-C-N	-5.03	113.37	118.85
1	B	1174	ILE	C-N-CA	-5.03	113.37	118.85
1	B	1191	ARG	N-CA-C	5.02	116.76	111.28
1	C	2068	PRO	N-CA-CB	5.02	107.71	103.19
1	A	174	ILE	N-CA-CB	-5.02	104.18	111.21
1	A	137	LEU	CA-C-O	-5.02	115.78	121.65
1	B	1188	VAL	CA-CB-CG2	-5.02	101.87	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	VAL	CA-C-N	5.01	125.54	120.38
1	A	52	VAL	C-N-CA	5.01	125.54	120.38
1	C	2049	HIS	N-CA-CB	-5.01	103.13	110.85
1	A	129	ASP	N-CA-C	-5.01	100.13	108.34
1	B	1294	ASP	CA-CB-CG	5.00	117.61	112.60
1	C	2203	ARG	CA-CB-CG	-5.00	104.09	114.10
1	C	2240	ALA	CA-C-N	-5.00	112.55	120.55
1	C	2240	ALA	C-N-CA	-5.00	112.55	120.55
1	B	1229	SER	CA-CB-OG	-5.00	101.10	111.10

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	GLU	Mainchain
1	A	159	ARG	Sidechain
1	A	173	MET	Mainchain
1	A	272	ASN	Mainchain
1	A	352	VAL	Mainchain
1	B	1126	HIS	Mainchain
1	B	1159	ARG	Sidechain
1	B	1169	PRO	Mainchain
1	B	1170	GLY	Mainchain
1	B	1173	MET	Mainchain
1	B	1233	GLU	Sidechain
1	B	1268	LYS	Mainchain
1	B	1317	GLY	Mainchain
1	C	2046	ARG	Mainchain
1	C	2159	ARG	Sidechain
1	C	2169	PRO	Mainchain
1	C	2209	TYR	Sidechain
1	C	2225	TYR	Sidechain
1	C	2278	SER	Mainchain
1	C	2302	PHE	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2567	0	2477	139	0
1	B	2567	0	2477	118	0
1	C	2567	0	2477	143	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	289	0	0	11	0
3	B	276	0	0	7	0
3	C	289	0	0	10	0
All	All	8561	0	7431	375	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 25.

All (375) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2178:VAL:CB	1:C:2178:VAL:CG1	1.74	1.65
1:A:173:MET:CB	1:A:173:MET:CA	1.74	1.64
1:B:1086:GLU:CB	1:B:1086:GLU:CG	1.75	1.63
1:C:2295:LEU:CG	1:C:2295:LEU:CD1	1.75	1.62
1:A:289:ILE:CB	1:A:289:ILE:CG2	1.75	1.62
1:B:1217:ILE:CG2	1:B:1217:ILE:CB	1.75	1.61
1:C:2039:VAL:CA	1:C:2039:VAL:CB	1.76	1.61
1:B:1244:THR:CG2	1:B:1244:THR:CB	1.75	1.60
1:A:246:ILE:CD1	1:A:246:ILE:CG1	1.77	1.60
1:B:1144:LEU:CD2	1:B:1144:LEU:CG	1.74	1.60
1:B:1048:LYS:CD	1:B:1048:LYS:CE	1.77	1.60
1:C:2324:LEU:CD2	1:C:2324:LEU:CG	1.78	1.60
1:C:2259:LEU:CG	1:C:2259:LEU:CD1	1.78	1.59
1:B:1173:MET:CB	1:B:1173:MET:CA	1.79	1.59
1:C:2112:VAL:CA	1:C:2112:VAL:CB	1.75	1.59
1:A:62:GLN:CD	1:A:62:GLN:CG	1.75	1.58
1:C:2224:THR:CB	1:C:2224:THR:CG2	1.78	1.58
1:B:1221:GLU:CD	1:B:1221:GLU:CG	1.76	1.58
1:A:173:MET:CB	1:A:173:MET:CG	1.81	1.58
1:B:1174:ILE:CD1	1:B:1174:ILE:CG1	1.81	1.57
1:B:1269:VAL:CG2	1:B:1269:VAL:CB	1.82	1.57
1:C:2087:ASP:CG	1:C:2087:ASP:CB	1.74	1.57
1:A:262:GLU:CD	1:A:262:GLU:CG	1.76	1.57
1:C:2236:GLU:CD	1:C:2236:GLU:CG	1.74	1.57
1:C:2048:LYS:CD	1:C:2048:LYS:CG	1.83	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:VAL:CG2	1:A:178:VAL:CB	1.75	1.56
1:A:266:LYS:CE	1:A:266:LYS:CD	1.78	1.56
1:A:195:LYS:CE	1:A:195:LYS:CD	1.75	1.56
1:B:1357:GLU:CD	1:B:1357:GLU:CG	1.76	1.56
1:C:2246:ILE:CG1	1:C:2246:ILE:CD1	1.83	1.56
1:B:1195:LYS:CE	1:B:1195:LYS:CD	1.79	1.55
1:A:87:ASP:CG	1:A:87:ASP:CB	1.80	1.55
1:A:233:GLU:CD	1:A:233:GLU:CG	1.79	1.55
1:B:1039:VAL:CA	1:B:1039:VAL:CB	1.81	1.55
1:A:159:ARG:CG	1:A:159:ARG:CB	1.81	1.55
1:C:2217:ILE:CG1	1:C:2217:ILE:CD1	1.80	1.55
1:B:1219:LYS:CE	1:B:1219:LYS:NZ	1.67	1.54
1:B:1268:LYS:CD	1:B:1268:LYS:CE	1.81	1.53
1:A:48:LYS:CE	1:A:48:LYS:NZ	1.70	1.53
1:C:2326:LYS:CE	1:C:2326:LYS:NZ	1.70	1.53
1:A:86:GLU:CD	1:A:86:GLU:CG	1.80	1.52
1:A:48:LYS:CE	1:A:48:LYS:CD	1.84	1.51
1:B:1200:LYS:CE	1:B:1200:LYS:CD	1.86	1.51
1:C:2125:PRO:CG	1:C:2125:PRO:CB	1.81	1.50
1:C:2065:ALA:CB	1:C:2065:ALA:CA	1.87	1.50
1:B:1048:LYS:CE	1:B:1048:LYS:NZ	1.73	1.50
1:C:2330:PRO:CD	1:C:2330:PRO:CG	1.75	1.49
1:A:268:LYS:CE	1:A:268:LYS:NZ	1.73	1.49
1:B:1262:GLU:CD	1:B:1262:GLU:CG	1.86	1.48
1:C:2048:LYS:CD	1:C:2048:LYS:CE	1.89	1.48
1:A:48:LYS:CD	1:A:48:LYS:CG	1.89	1.48
1:B:1087:ASP:CG	1:B:1087:ASP:CB	1.85	1.47
1:C:2086:GLU:CG	1:C:2086:GLU:CD	1.85	1.46
1:C:2173:MET:CG	1:C:2173:MET:SD	2.04	1.45
1:C:2156:LYS:CE	1:C:2156:LYS:NZ	1.79	1.45
1:A:195:LYS:CE	1:A:195:LYS:NZ	1.82	1.43
1:A:200:LYS:NZ	1:A:200:LYS:CE	1.81	1.42
1:C:2262:GLU:CD	1:C:2262:GLU:CG	1.93	1.42
1:B:1266:LYS:NZ	1:B:1266:LYS:CE	1.82	1.41
1:A:191:ARG:CZ	1:A:191:ARG:NH1	1.91	1.34
1:A:319:THR:CG2	1:A:319:THR:CA	2.06	1.33
1:C:2232:SER:CB	1:C:2232:SER:OG	1.77	1.31
1:C:2266:LYS:NZ	1:C:2266:LYS:CE	1.95	1.30
1:A:48:LYS:NZ	1:A:48:LYS:CD	1.96	1.27
1:A:226:MET:SD	1:A:226:MET:CE	2.27	1.21
1:C:2226:MET:CE	1:C:2226:MET:SD	1.10	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:THR:CG2	1:A:319:THR:OG1	1.94	1.15
1:C:2048:LYS:CD	1:C:2048:LYS:NZ	2.08	1.14
1:A:319:THR:CG2	1:A:319:THR:HB	1.59	1.10
1:A:39:VAL:O	1:A:40:ASP:HB3	1.48	1.09
1:C:2226:MET:SD	1:C:2226:MET:HE2	1.69	1.08
1:A:173:MET:HG2	3:A:3773:HOH:O	1.54	1.07
1:C:2226:MET:SD	1:C:2226:MET:HE1	1.69	1.07
1:A:319:THR:CB	1:A:319:THR:HG21	1.55	1.06
1:A:319:THR:CB	1:A:319:THR:HG23	1.55	1.05
1:B:1048:LYS:CD	1:B:1048:LYS:NZ	2.20	1.05
1:B:1173:MET:HG3	3:B:3638:HOH:O	1.54	1.04
1:C:2226:MET:SD	1:C:2226:MET:HE3	1.69	1.03
1:A:319:THR:CB	1:A:319:THR:HG22	1.55	1.02
1:B:1200:LYS:CD	1:B:1200:LYS:NZ	2.22	1.02
1:B:1039:VAL:O	1:B:1040:ASP:HB3	1.59	1.01
1:B:1218:PRO:HB2	1:B:1226:MET:HE3	1.43	1.00
1:A:48:LYS:CD	1:A:48:LYS:HZ2	1.63	0.98
1:A:173:MET:CB	1:A:173:MET:C	2.37	0.97
1:B:1222:ASP:OD1	1:B:1224:THR:HG23	1.64	0.96
1:C:2039:VAL:O	1:C:2040:ASP:HB3	1.62	0.95
1:B:1040:ASP:OD1	1:B:1041:LEU:N	2.00	0.94
1:B:1173:MET:CB	1:B:1173:MET:C	2.39	0.94
1:A:319:THR:CG2	1:A:319:THR:CB	0.93	0.93
1:B:1058:HIS:HE1	1:B:1105:ILE:H	1.16	0.92
1:B:1357:GLU:CD	1:B:1357:GLU:CB	2.44	0.91
1:B:1144:LEU:CD2	1:B:1144:LEU:CB	2.51	0.89
1:A:173:MET:HE2	1:A:173:MET:HA	1.54	0.89
3:A:3467:HOH:O	1:C:2039:VAL:HG11	1.72	0.88
1:A:40:ASP:OD1	1:A:41:LEU:N	2.06	0.88
1:C:2295:LEU:CD1	1:C:2295:LEU:CB	2.52	0.88
1:A:48:LYS:HZ2	1:A:48:LYS:HD2	1.39	0.87
1:A:218:PRO:HB2	1:A:226:MET:HE3	1.55	0.87
1:B:1040:ASP:CG	1:B:1041:LEU:N	2.32	0.86
1:C:2121:GLU:OE1	3:C:3785:HOH:O	1.92	0.86
1:A:62:GLN:CD	1:A:62:GLN:CB	2.47	0.85
1:B:1173:MET:HE2	1:B:1173:MET:HA	1.57	0.85
1:C:2324:LEU:CD2	1:C:2324:LEU:CB	2.55	0.85
1:C:2326:LYS:NZ	1:C:2326:LYS:CD	2.39	0.85
1:B:1144:LEU:CD2	1:B:1144:LEU:CD1	2.54	0.84
1:C:2178:VAL:CG1	1:C:2178:VAL:CG2	2.55	0.84
1:C:2040:ASP:CG	1:C:2041:LEU:H	1.81	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2295:LEU:CD1	1:C:2295:LEU:CD2	2.55	0.84
1:A:340:LEU:H	1:C:2281:ASN:ND2	1.74	0.84
1:A:40:ASP:CG	1:A:41:LEU:H	1.81	0.84
1:C:2040:ASP:CG	1:C:2041:LEU:N	2.34	0.82
1:A:262:GLU:CD	1:A:262:GLU:CB	2.53	0.82
1:A:48:LYS:NZ	1:A:48:LYS:HD3	1.94	0.81
1:B:1039:VAL:N	3:B:3809:HOH:O	2.14	0.81
1:C:2226:MET:CE	1:C:2226:MET:CG	2.59	0.81
1:B:1058:HIS:CE1	1:B:1105:ILE:H	1.98	0.80
1:C:2156:LYS:NZ	1:C:2156:LYS:CD	2.43	0.80
1:A:40:ASP:CG	1:A:41:LEU:N	2.34	0.80
1:A:39:VAL:O	1:A:40:ASP:CB	2.27	0.79
1:C:2173:MET:CA	1:C:2173:MET:HE2	2.12	0.79
1:C:2112:VAL:CA	1:C:2112:VAL:CG2	2.59	0.79
1:A:222:ASP:OD1	1:A:224:THR:HG23	1.83	0.78
1:C:2112:VAL:CB	1:C:2112:VAL:C	2.56	0.78
1:A:262:GLU:OE2	3:A:3715:HOH:O	2.00	0.78
1:B:1195:LYS:CE	1:B:1195:LYS:CG	2.60	0.78
1:C:2048:LYS:NZ	1:C:2048:LYS:HD3	1.98	0.78
1:A:266:LYS:CE	1:A:266:LYS:CG	2.59	0.78
1:C:2048:LYS:HD3	1:C:2048:LYS:HZ3	1.49	0.78
1:C:2259:LEU:CD1	1:C:2259:LEU:CB	2.62	0.78
1:B:1053:PRO:HD2	3:B:3442:HOH:O	1.83	0.77
1:B:1040:ASP:CG	1:B:1041:LEU:H	1.82	0.77
1:B:1077:ILE:N	1:B:1077:ILE:HD12	1.98	0.77
1:C:2039:VAL:CA	1:C:2039:VAL:CG1	2.63	0.77
1:C:2112:VAL:CA	1:C:2112:VAL:CG1	2.62	0.76
1:B:1269:VAL:CG2	1:B:1269:VAL:CG1	2.65	0.75
1:C:2222:ASP:OD1	1:C:2224:THR:HG23	1.86	0.74
1:C:2324:LEU:CD2	1:C:2324:LEU:CD1	2.64	0.74
1:B:1048:LYS:NZ	1:B:1048:LYS:HD3	2.03	0.74
1:C:2218:PRO:HB2	1:C:2226:MET:HE3	1.68	0.74
1:C:2058:HIS:HE1	1:C:2105:ILE:H	1.36	0.74
1:B:1200:LYS:HE3	3:B:3789:HOH:O	1.87	0.73
1:A:40:ASP:OD2	3:A:3685:HOH:O	2.06	0.72
1:A:191:ARG:NE	3:A:3798:HOH:O	1.77	0.72
1:C:2178:VAL:CG1	1:C:2178:VAL:CA	2.67	0.72
1:C:2236:GLU:HG3	3:C:3679:HOH:O	1.90	0.71
1:B:1268:LYS:CD	1:B:1268:LYS:NZ	2.55	0.70
1:A:178:VAL:CG2	1:A:178:VAL:CA	2.69	0.70
1:B:1289:ILE:HD12	1:B:1334:ALA:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2224:THR:CG2	1:C:2224:THR:OG1	2.38	0.70
1:C:2040:ASP:OD1	1:C:2041:LEU:N	2.20	0.70
1:B:1217:ILE:CG2	1:B:1217:ILE:CG1	2.69	0.69
1:B:1173:MET:CA	1:B:1173:MET:HE2	2.22	0.69
1:A:58:HIS:HE1	1:A:105:ILE:H	1.39	0.69
1:A:246:ILE:CD1	1:A:246:ILE:CB	2.68	0.69
1:A:58:HIS:CE1	1:A:105:ILE:H	2.11	0.68
1:C:2266:LYS:NZ	1:C:2266:LYS:HG3	2.08	0.68
1:C:2039:VAL:O	1:C:2040:ASP:CB	2.40	0.68
1:C:2167:CYS:HB2	1:C:2182:THR:HB	1.74	0.68
1:A:289:ILE:CG2	1:A:289:ILE:CA	2.71	0.68
1:A:344:VAL:HG11	1:C:2172:PRO:HA	1.75	0.68
1:B:1339:ASN:C	1:B:1339:ASN:HD22	2.02	0.67
1:C:2217:ILE:CD1	1:C:2217:ILE:CB	2.71	0.67
1:A:312:THR:HB	1:C:2319:THR:CG2	2.25	0.67
1:B:1281:ASN:O	1:C:2339:ASN:HA	1.94	0.67
1:A:159:ARG:CG	1:A:159:ARG:CA	2.72	0.66
1:B:1200:LYS:CD	1:B:1200:LYS:HZ2	2.06	0.66
1:C:2266:LYS:NZ	1:C:2266:LYS:CG	2.58	0.66
1:C:2197:HIS:CE1	1:C:2308:ARG:HD3	2.30	0.66
1:C:2173:MET:CG	1:C:2173:MET:CE	2.68	0.66
1:B:1219:LYS:NZ	1:B:1219:LYS:CD	2.57	0.66
1:B:1269:VAL:CG2	1:B:1269:VAL:CA	2.73	0.66
1:A:173:MET:HA	1:A:173:MET:CE	2.25	0.66
1:B:1173:MET:CB	1:B:1173:MET:N	2.56	0.65
1:C:2058:HIS:O	1:C:2060:HIS:HD2	1.77	0.65
1:B:1048:LYS:HD3	1:B:1048:LYS:HZ3	1.60	0.65
1:B:1203:ARG:NE	3:B:3401:HOH:O	2.03	0.65
1:B:1174:ILE:CD1	1:B:1174:ILE:CB	2.73	0.65
1:A:281:ASN:ND2	1:B:1340:LEU:H	1.95	0.65
1:C:2200:LYS:HE3	3:C:3589:HOH:O	1.94	0.65
1:B:1200:LYS:NZ	1:B:1200:LYS:HD3	2.10	0.64
1:B:1281:ASN:ND2	1:C:2340:LEU:H	1.96	0.64
1:C:2339:ASN:C	1:C:2339:ASN:HD22	2.06	0.64
1:A:159:ARG:CB	1:A:159:ARG:CD	2.68	0.63
1:A:289:ILE:CG2	1:A:289:ILE:CG1	2.76	0.63
1:B:1244:THR:CG2	1:B:1244:THR:CA	2.74	0.63
1:C:2173:MET:HE2	1:C:2173:MET:N	2.12	0.63
1:A:340:LEU:H	1:C:2281:ASN:HD21	1.47	0.63
1:C:2173:MET:HE2	1:C:2173:MET:HA	1.79	0.63
1:B:1268:LYS:CE	1:B:1268:LYS:CG	2.75	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2039:VAL:CA	1:C:2039:VAL:CG2	2.75	0.62
1:A:179:VAL:O	1:A:215:HIS:HD2	1.82	0.62
1:C:2058:HIS:CE1	1:C:2105:ILE:H	2.17	0.62
1:A:266:LYS:HG3	1:A:266:LYS:NZ	2.14	0.62
1:A:319:THR:CG2	1:A:319:THR:N	2.61	0.62
1:A:127:ASN:HB3	1:A:144:LEU:HA	1.80	0.61
1:A:339:ASN:C	1:A:339:ASN:HD22	2.09	0.61
1:C:2093:MET:HE2	1:C:2124:MET:HE1	1.81	0.61
1:A:319:THR:HG23	1:A:319:THR:N	2.15	0.61
1:B:1319:THR:CG2	1:C:2312:THR:HB	2.31	0.60
1:B:1060:HIS:HE1	1:B:1204:TYR:OH	1.84	0.60
1:B:1039:VAL:HG21	3:C:3695:HOH:O	2.01	0.60
1:B:1213:SER:OG	1:B:1215:HIS:HE1	1.84	0.60
1:A:233:GLU:CD	1:A:233:GLU:CB	2.68	0.59
1:A:339:ASN:HD22	1:A:341:ILE:H	1.49	0.59
1:A:58:HIS:HD2	1:A:59:ALA:O	1.85	0.59
1:C:2324:LEU:CD2	1:C:2324:LEU:HB2	2.32	0.59
1:A:266:LYS:CD	1:A:266:LYS:NZ	2.65	0.59
1:C:2040:ASP:OD2	3:C:3269:HOH:O	2.17	0.58
1:B:1039:VAL:CA	1:B:1039:VAL:CG2	2.77	0.58
1:A:173:MET:C	1:A:173:MET:HB3	2.25	0.58
1:B:1086:GLU:CG	1:B:1086:GLU:CA	2.77	0.57
1:A:87:ASP:CG	1:A:87:ASP:CA	2.75	0.57
1:A:178:VAL:CG2	1:A:178:VAL:CG1	2.78	0.57
1:A:266:LYS:CG	1:A:266:LYS:NZ	2.68	0.57
1:A:370:VAL:HG22	1:A:371:GLY:N	2.20	0.57
1:B:1058:HIS:HE1	1:B:1105:ILE:N	1.97	0.57
1:B:1217:ILE:CG2	1:B:1217:ILE:CA	2.78	0.56
1:A:154:ARG:HD2	3:A:3611:HOH:O	2.05	0.56
1:B:1213:SER:OG	1:B:1215:HIS:CE1	2.58	0.56
1:A:281:ASN:O	1:B:1339:ASN:HA	2.06	0.56
1:C:2326:LYS:NZ	1:C:2326:LYS:HG3	2.21	0.56
1:B:1154:ARG:NH1	3:B:3808:HOH:O	2.39	0.56
1:B:1039:VAL:O	1:B:1040:ASP:CB	2.37	0.55
1:C:2266:LYS:HG3	1:C:2266:LYS:HZ3	1.71	0.55
1:A:287:HIS:HD2	1:A:289:ILE:HG12	1.70	0.55
1:B:1060:HIS:CE1	1:B:1204:TYR:OH	2.60	0.55
1:B:1173:MET:C	1:B:1173:MET:HB3	2.29	0.55
1:A:173:MET:CA	1:A:173:MET:CE	2.85	0.55
1:A:167:CYS:HB2	1:A:182:THR:HB	1.88	0.54
1:C:2171:GLY:O	1:C:2172:PRO:C	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASN:ND2	1:A:341:ILE:H	2.05	0.54
1:B:1297:TRP:CE2	1:B:1306:PRO:HB3	2.42	0.54
1:C:2197:HIS:HA	1:C:2306:PRO:HD2	1.89	0.54
1:A:173:MET:CG	3:A:3773:HOH:O	2.31	0.54
1:A:319:THR:CG2	1:A:319:THR:HG1	2.17	0.54
1:A:319:THR:HG22	1:B:1311:GLU:CG	2.37	0.54
1:C:2326:LYS:NZ	1:C:2326:LYS:CG	2.70	0.54
1:B:1262:GLU:CD	1:B:1262:GLU:CB	2.69	0.54
1:C:2048:LYS:CD	1:C:2048:LYS:HZ2	2.12	0.54
1:B:1222:ASP:OD1	1:B:1222:ASP:C	2.51	0.53
1:A:66:SER:O	1:A:191:ARG:NH2	2.42	0.53
1:C:2167:CYS:HB2	1:C:2182:THR:CB	2.39	0.53
1:C:2171:GLY:O	1:C:2173:MET:N	2.41	0.53
1:C:2246:ILE:CD1	1:C:2246:ILE:CB	2.81	0.52
1:B:1172:PRO:HA	1:C:2344:VAL:HG11	1.92	0.52
1:C:2061:GLU:OE1	1:C:2065:ALA:HB2	2.10	0.52
1:A:268:LYS:NZ	1:A:268:LYS:CD	2.70	0.52
1:A:339:ASN:HA	1:C:2281:ASN:O	2.10	0.52
1:C:2179:VAL:O	1:C:2215:HIS:HD2	1.92	0.52
1:A:267:ALA:O	1:A:354:VAL:HA	2.10	0.51
1:A:62:GLN:CG	1:A:62:GLN:NE2	2.58	0.51
1:A:287:HIS:CD2	1:A:289:ILE:HG12	2.46	0.51
1:C:2232:SER:OG	1:C:2232:SER:CA	2.53	0.51
1:C:2262:GLU:CD	1:C:2262:GLU:CB	2.77	0.51
1:C:2039:VAL:CB	1:C:2039:VAL:C	2.77	0.51
1:A:54:PRO:HB2	1:A:253:ASN:HD21	1.76	0.51
1:A:319:THR:HG22	1:B:1311:GLU:HG3	1.91	0.50
1:C:2224:THR:CG2	1:C:2224:THR:CA	2.82	0.50
1:C:2213:SER:OG	1:C:2215:HIS:CE1	2.64	0.50
1:A:93:MET:HE2	1:A:124:MET:HE1	1.94	0.50
1:B:1179:VAL:O	1:B:1215:HIS:HD2	1.94	0.50
1:C:2127:ASN:HB3	1:C:2144:LEU:HA	1.94	0.50
1:B:1119:PRO:HD2	1:B:1122:ASN:ND2	2.27	0.49
1:C:2224:THR:CG2	1:C:2224:THR:HG1	2.23	0.49
1:C:2112:VAL:CB	1:C:2112:VAL:N	2.68	0.49
1:B:1048:LYS:HD2	1:B:1049:HIS:N	2.27	0.49
1:B:1357:GLU:CD	1:B:1357:GLU:HB2	2.36	0.49
1:C:2370:VAL:HG22	1:C:2371:GLY:N	2.27	0.49
1:A:344:VAL:CG1	1:C:2172:PRO:HA	2.42	0.49
1:B:1087:ASP:CG	1:B:1087:ASP:CA	2.80	0.49
1:A:163:PHE:O	1:A:185:CYS:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:HA	1:A:313:TRP:O	2.13	0.49
1:B:1319:THR:HG21	1:C:2312:THR:HB	1.94	0.49
1:C:2060:HIS:HE1	1:C:2204:TYR:OH	1.95	0.49
1:A:340:LEU:N	1:C:2281:ASN:HD21	2.11	0.48
1:C:2287:HIS:CD2	1:C:2289:ILE:HG12	2.47	0.48
1:C:2154:ARG:HD2	3:C:3248:HOH:O	2.14	0.48
1:B:1195:LYS:CD	1:B:1195:LYS:NZ	2.66	0.48
1:C:2326:LYS:CD	1:C:2326:LYS:HZ3	2.24	0.48
1:A:173:MET:CB	1:A:173:MET:N	2.62	0.48
1:A:339:ASN:HD22	1:A:341:ILE:N	2.10	0.48
1:C:2210:ILE:HD12	1:C:2210:ILE:HG23	1.65	0.48
1:B:1197:HIS:CE1	1:B:1308:ARG:HD3	2.49	0.47
1:C:2195:LYS:HE2	1:C:2201:PRO:HG3	1.96	0.47
1:A:174:ILE:N	1:A:175:PRO:HD2	2.29	0.47
1:C:2259:LEU:CD1	1:C:2259:LEU:CD2	2.83	0.47
1:B:1287:HIS:CD2	1:B:1338:HIS:HD2	2.33	0.47
1:A:170:GLY:H	1:A:174:ILE:HG13	1.79	0.47
1:A:174:ILE:HB	1:A:175:PRO:HD3	1.96	0.47
1:B:1319:THR:HG22	1:C:2311:GLU:HG3	1.97	0.47
1:A:172:PRO:HA	1:B:1344:VAL:HG11	1.96	0.47
1:C:2217:ILE:CD1	1:C:2217:ILE:CA	2.94	0.47
1:A:262:GLU:CG	1:A:262:GLU:OE1	2.54	0.46
1:A:311:GLU:HG3	1:C:2319:THR:HG22	1.98	0.46
1:C:2287:HIS:HD2	1:C:2289:ILE:HG12	1.80	0.46
1:B:1222:ASP:OD1	1:B:1224:THR:CG2	2.52	0.46
1:A:312:THR:HB	1:C:2319:THR:HG22	1.98	0.46
1:A:319:THR:CA	1:A:319:THR:HG22	2.18	0.46
1:A:58:HIS:O	1:A:60:HIS:HD2	1.99	0.45
1:A:197:HIS:ND1	1:A:197:HIS:N	2.64	0.45
1:A:319:THR:CG2	1:B:1312:THR:HB	2.47	0.45
1:A:330:PRO:HD2	1:A:358:TRP:HA	1.98	0.45
1:A:222:ASP:OD1	1:A:222:ASP:C	2.60	0.45
1:A:53:PRO:HD2	3:A:3632:HOH:O	2.17	0.45
1:C:2161:GLY:HA2	1:C:2302:PHE:CD2	2.52	0.45
1:A:233:GLU:O	1:A:233:GLU:HG2	2.16	0.44
1:C:2326:LYS:HG3	1:C:2326:LYS:HZ2	1.82	0.44
1:A:169:PRO:HG2	1:A:177:HIS:CE1	2.52	0.44
1:B:1220:ASP:C	1:B:1220:ASP:OD1	2.61	0.44
1:B:1058:HIS:HD2	1:B:1059:ALA:O	2.00	0.44
1:C:2213:SER:OG	1:C:2215:HIS:HE1	2.00	0.44
1:A:295:LEU:HD12	1:A:324:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1361:ASP:HA	3:B:3287:HOH:O	2.17	0.43
1:A:233:GLU:CG	1:A:233:GLU:OE1	2.46	0.43
1:B:1150:LYS:O	1:C:2369:PRO:HA	2.17	0.43
1:A:175:PRO:HG3	1:B:1344:VAL:HB	2.01	0.43
1:A:300:GLY:O	1:A:301:LYS:HD3	2.19	0.43
1:C:2044:LEU:HA	1:C:2045:PRO:HD3	1.84	0.43
1:A:163:PHE:CE2	1:A:301:LYS:HE3	2.54	0.43
1:A:173:MET:CA	1:A:173:MET:HE2	2.34	0.43
1:B:1271:ASP:O	1:B:1326:LYS:HA	2.18	0.43
1:B:1285:ARG:HA	1:B:1313:TRP:O	2.18	0.43
1:C:2112:VAL:C	1:C:2112:VAL:CG1	2.88	0.43
1:A:195:LYS:HG2	3:A:3554:HOH:O	2.19	0.43
1:C:2216:TYR:O	1:C:2238:MET:HG3	2.19	0.43
1:A:54:PRO:HB2	1:A:253:ASN:ND2	2.34	0.43
1:A:66:SER:HB2	1:A:67:GLY:H	1.70	0.43
1:A:81:GLU:OE2	1:A:227:ARG:HD3	2.19	0.42
1:C:2236:GLU:CB	3:C:3679:HOH:O	2.67	0.42
1:B:1081:GLU:OE2	1:B:1227:ARG:HD3	2.18	0.42
1:B:1210:ILE:O	1:B:1277:HIS:HA	2.19	0.42
1:C:2081:GLU:OE2	1:C:2227:ARG:HD3	2.18	0.42
1:A:370:VAL:HG22	1:A:371:GLY:H	1.85	0.42
1:A:303:HIS:HD2	3:A:3377:HOH:O	2.01	0.42
1:C:2039:VAL:CB	1:C:2039:VAL:HA	2.19	0.42
1:A:39:VAL:O	3:A:3511:HOH:O	2.22	0.42
1:A:316:ARG:HG2	1:B:1314:PHE:HB2	2.01	0.42
1:B:1048:LYS:HD2	1:B:1049:HIS:H	1.85	0.42
1:B:1124:MET:HE1	1:B:1176:TRP:CH2	2.55	0.42
1:B:1218:PRO:CB	1:B:1226:MET:HE3	2.32	0.42
1:C:2166:HIS:HA	1:C:2183:ALA:HA	2.01	0.41
1:B:1273:VAL:O	1:B:1324:LEU:HA	2.20	0.41
1:B:1316:ARG:O	1:B:1317:GLY:C	2.63	0.41
1:C:2048:LYS:CD	1:C:2048:LYS:HZ3	1.99	0.41
1:A:77:ILE:HD12	1:A:77:ILE:N	2.35	0.41
1:B:1058:HIS:O	1:B:1060:HIS:HD2	2.03	0.41
1:B:1200:LYS:HA	1:B:1201:PRO:HD3	1.81	0.41
1:C:2076:ARG:HH11	1:C:2076:ARG:HD2	1.56	0.41
1:C:2200:LYS:HA	1:C:2201:PRO:HD3	2.00	0.41
1:C:2238:MET:HE3	3:C:3694:HOH:O	2.20	0.41
1:B:1058:HIS:CE1	1:B:1105:ILE:N	2.77	0.41
1:B:1133:ALA:HB1	1:C:2363:MET:CE	2.51	0.41
1:C:2203:ARG:HH11	1:C:2203:ARG:HD2	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2216:TYR:CD1	1:C:2216:TYR:N	2.88	0.41
1:C:2339:ASN:C	1:C:2339:ASN:ND2	2.74	0.41
1:C:2339:ASN:ND2	1:C:2341:ILE:H	2.18	0.41
1:A:262:GLU:CD	1:A:262:GLU:HB3	2.41	0.41
1:B:1333:TYR:HB2	1:B:1352:VAL:HB	2.03	0.41
1:B:1039:VAL:HA	3:C:3512:HOH:O	2.21	0.41
1:A:174:ILE:HB	1:A:175:PRO:CD	2.50	0.41
1:A:217:ILE:N	1:A:217:ILE:HD13	2.36	0.41
1:B:1077:ILE:HG21	1:B:1126:HIS:CD2	2.56	0.41
1:B:1287:HIS:CD2	1:B:1289:ILE:HG12	2.56	0.41
1:C:2173:MET:SD	1:C:2173:MET:CB	3.04	0.41
1:C:2196:ASP:OD1	1:C:2198:GLU:N	2.50	0.41
1:B:1054:PRO:HB2	1:B:1253:ASN:ND2	2.36	0.41
1:C:2058:HIS:HD2	1:C:2059:ALA:O	2.04	0.40
1:C:2266:LYS:NZ	1:C:2266:LYS:CD	2.82	0.40
1:A:77:ILE:HG21	1:A:126:HIS:CD2	2.56	0.40
1:A:171:GLY:O	1:A:172:PRO:C	2.58	0.40
1:A:219:LYS:O	1:A:226:MET:HE2	2.22	0.40
1:B:1173:MET:CA	1:B:1173:MET:CE	2.96	0.40
1:C:2203:ARG:NE	3:C:3331:HOH:O	2.30	0.40
1:A:200:LYS:HA	1:A:201:PRO:HD3	1.98	0.40
1:C:2100:PRO:HG3	1:C:2211:GLY:HA3	2.02	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	332/334 (99%)	321 (97%)	10 (3%)	1 (0%)	36	35
1	B	332/334 (99%)	319 (96%)	12 (4%)	1 (0%)	36	35
1	C	332/334 (99%)	316 (95%)	15 (4%)	1 (0%)	36	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	996/1002 (99%)	956 (96%)	37 (4%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	B	1040	ASP
1	C	2040	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/270 (100%)	250 (93%)	20 (7%)	13	9
1	B	270/270 (100%)	251 (93%)	19 (7%)	14	10
1	C	270/270 (100%)	252 (93%)	18 (7%)	15	11
All	All	810/810 (100%)	753 (93%)	57 (7%)	14	10

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	VAL
1	A	40	ASP
1	A	55	PRO
1	A	61	GLU
1	A	77	ILE
1	A	86	GLU
1	A	173	MET
1	A	182	THR
1	A	207	VAL
1	A	221	GLU
1	A	227	ARG
1	A	253	ASN
1	A	266	LYS

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Mol	Chain	Res	Type
1	A	279	GLN
1	A	280	PRO
1	A	324	LEU
1	A	337	ASN
1	A	339	ASN
1	A	357	GLU
1	A	369	PRO
1	B	1039	VAL
1	B	1040	ASP
1	B	1048	LYS
1	B	1086	GLU
1	B	1124	MET
1	B	1145	ILE
1	B	1147	PRO
1	B	1173	MET
1	B	1182	THR
1	B	1227	ARG
1	B	1231	PRO
1	B	1253	ASN
1	B	1262	GLU
1	B	1279	GLN
1	B	1280	PRO
1	B	1313	TRP
1	B	1324	LEU
1	B	1339	ASN
1	B	1357	GLU
1	C	2039	VAL
1	C	2048	LYS
1	C	2086	GLU
1	C	2147	PRO
1	C	2173	MET
1	C	2182	THR
1	C	2200	LYS
1	C	2214	ASP
1	C	2227	ARG
1	C	2230	ASP
1	C	2253	ASN
1	C	2279	GLN
1	C	2313	TRP
1	C	2324	LEU
1	C	2337	ASN
1	C	2339	ASN

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Mol	Chain	Res	Type
1	C	2357	GLU
1	C	2369	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	58	HIS
1	A	60	HIS
1	A	215	HIS
1	A	253	ASN
1	A	281	ASN
1	A	339	ASN
1	B	1058	HIS
1	B	1060	HIS
1	B	1215	HIS
1	B	1253	ASN
1	B	1281	ASN
1	B	1339	ASN
1	B	1360	ASN
1	C	2058	HIS
1	C	2060	HIS
1	C	2146	ASN
1	C	2215	HIS
1	C	2253	ASN
1	C	2281	ASN
1	C	2339	ASN
1	C	2365	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.