Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:28 AM UTC

PDB ID	:	5NZT / pdb_00005nzt
EMDB ID	:	EMD-3722
Title	:	The structure of the COPI coat linkage I
Authors	:	Dodonova, S.O.; Aderhold, P.; Kopp, J.; Ganeva, I.; Roehling, S.; Hagen, W.J.H.; Sinning, I.; Wieland, F.; Briggs, J.A.G.
Deposited on	:	2017-05-15
Resolution	:	17.00 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

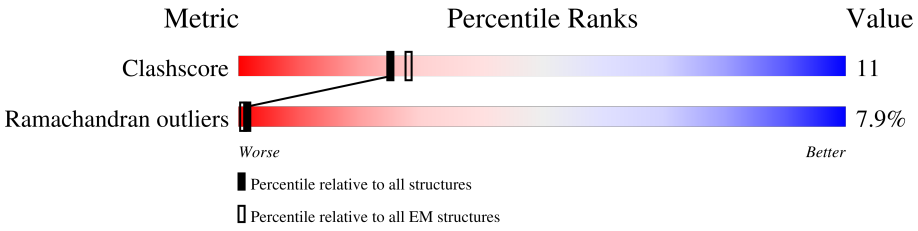
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

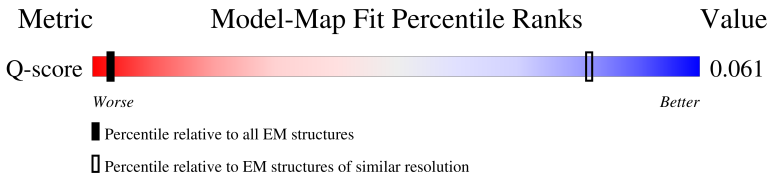
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 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.





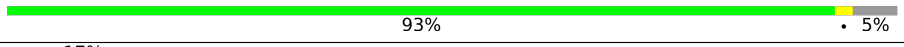
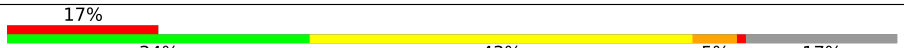
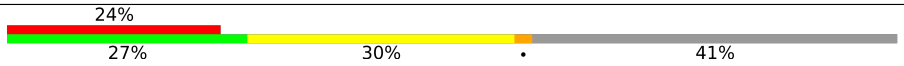
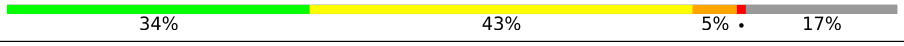
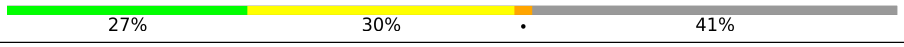
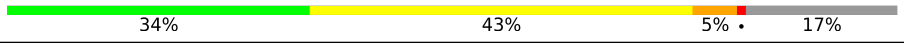
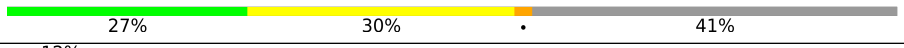
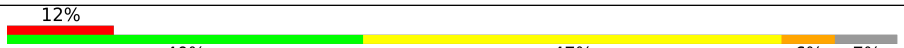
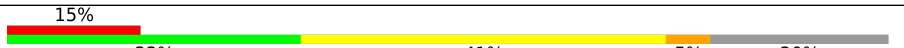
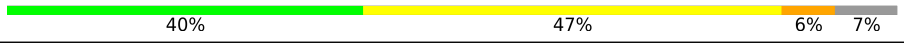
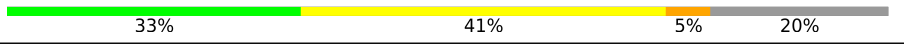
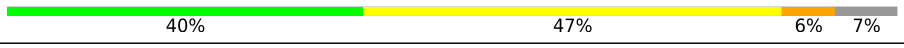
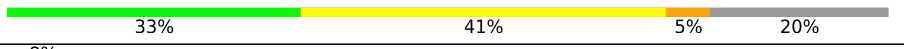
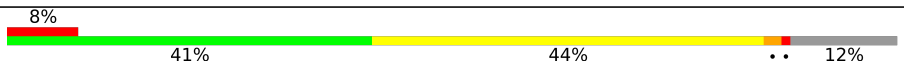
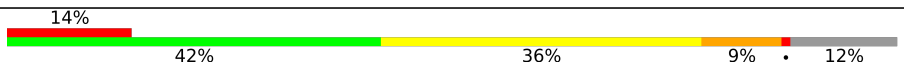
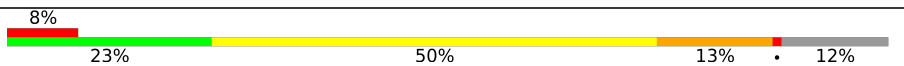
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	38 (16.50 - 17.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	1262	9% 50% 34% • • 11%
1	2-A	1262	50% 34% • • 11%
1	3-A	1262	50% 34% • • 11%
2	1-E	308	19% 93% • 5%
2	2-E	308	93% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	3-E	308	
3	1-B	968	
3	1-N	968	
3	2-B	968	
3	2-N	968	
3	3-B	968	
3	3-N	968	
4	1-C	905	
4	1-H	905	
4	2-C	905	
4	2-H	905	
4	3-C	905	
4	3-H	905	
5	1-D	511	
5	1-I	511	
5	2-D	511	
5	2-I	511	
5	3-D	511	
5	3-I	511	
6	1-F	181	
6	1-J	181	
6	1-M	181	
6	1-R	181	
6	2-F	181	
6	2-J	181	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	2-M	181	42% 36% 9% 12%
6	2-R	181	23% 50% 13% 12%
6	3-F	181	41% 43% 12%
6	3-J	181	41% 44% 12%
6	3-M	181	42% 37% 8% 12%
6	3-R	181	23% 50% 13% 12%
7	1-G	874	6% 39% 46% 6% 9%
7	1-K	874	28% 23% 36% 5% 36%
7	2-G	874	39% 45% 6% 9%
7	2-K	874	23% 36% 5% 36%
7	3-G	874	39% 46% 6% 9%
7	3-K	874	23% 36% 5% 36%
8	1-L	177	36% 22% 53% 21%
8	1-Z	177	12% 29% 48% 21%
8	2-L	177	22% 51% 5% 21%
8	2-Z	177	29% 48% 21%
8	3-L	177	22% 53% 21%
8	3-Z	177	29% 48% 21%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 83685 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Coatomer subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1-A	1126	Total 4503	C 2252	N 1126	O 1125	0	0
1	2-A	1126	Total 4503	C 2252	N 1126	O 1125	0	0
1	3-A	1126	Total 4503	C 2252	N 1126	O 1125	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1225	LEU	-	expression tag	UNP Q8CIE6
A	1226	GLU	-	expression tag	UNP Q8CIE6
A	1227	VAL	-	expression tag	UNP Q8CIE6
A	1228	LEU	-	expression tag	UNP Q8CIE6
A	1229	PHE	-	expression tag	UNP Q8CIE6
A	1230	GLN	-	expression tag	UNP Q8CIE6
A	1231	GLY	-	expression tag	UNP Q8CIE6
A	1232	PRO	-	expression tag	UNP Q8CIE6
A	1233	SER	-	expression tag	UNP Q8CIE6
A	1234	ALA	-	expression tag	UNP Q8CIE6
A	1235	TRP	-	expression tag	UNP Q8CIE6
A	1236	SER	-	expression tag	UNP Q8CIE6
A	1237	HIS	-	expression tag	UNP Q8CIE6
A	1238	PRO	-	expression tag	UNP Q8CIE6
A	1239	GLN	-	expression tag	UNP Q8CIE6
A	1240	PHE	-	expression tag	UNP Q8CIE6
A	1241	GLU	-	expression tag	UNP Q8CIE6
A	1242	LYS	-	expression tag	UNP Q8CIE6
A	1243	GLY	-	expression tag	UNP Q8CIE6
A	1244	GLY	-	expression tag	UNP Q8CIE6
A	1245	GLY	-	expression tag	UNP Q8CIE6
A	1246	SER	-	expression tag	UNP Q8CIE6
A	1247	GLY	-	expression tag	UNP Q8CIE6
A	1248	GLY	-	expression tag	UNP Q8CIE6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1249	GLY	-	expression tag	UNP Q8CIE6
A	1250	SER	-	expression tag	UNP Q8CIE6
A	1251	GLY	-	expression tag	UNP Q8CIE6
A	1252	GLY	-	expression tag	UNP Q8CIE6
A	1253	SER	-	expression tag	UNP Q8CIE6
A	1254	ALA	-	expression tag	UNP Q8CIE6
A	1255	TRP	-	expression tag	UNP Q8CIE6
A	1256	SER	-	expression tag	UNP Q8CIE6
A	1257	HIS	-	expression tag	UNP Q8CIE6
A	1258	PRO	-	expression tag	UNP Q8CIE6
A	1259	GLN	-	expression tag	UNP Q8CIE6
A	1260	PHE	-	expression tag	UNP Q8CIE6
A	1261	GLU	-	expression tag	UNP Q8CIE6
A	1262	LYS	-	expression tag	UNP Q8CIE6

- Molecule 2 is a protein called Coatomer subunit epsilon.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1-E	292	Total 1169	C 584	N 292	O 293	0	0
2	2-E	292	Total 1169	C 584	N 292	O 293	0	0
2	3-E	292	Total 1169	C 584	N 292	O 293	0	0

- Molecule 3 is a protein called Coatomer subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	1-B	800	Total 3198	C 1600	N 800	O 798	0	0
3	2-B	800	Total 3198	C 1600	N 800	O 798	0	0
3	3-B	800	Total 3198	C 1600	N 800	O 798	0	0
3	1-N	570	Total 2279	C 1140	N 570	O 569	0	0
3	2-N	570	Total 2279	C 1140	N 570	O 569	0	0
3	3-N	570	Total 2279	C 1140	N 570	O 569	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q9JIF7
B	2	HIS	-	expression tag	UNP Q9JIF7
B	3	HIS	-	expression tag	UNP Q9JIF7
B	4	HIS	-	expression tag	UNP Q9JIF7
B	5	HIS	-	expression tag	UNP Q9JIF7
B	6	HIS	-	expression tag	UNP Q9JIF7
B	7	HIS	-	expression tag	UNP Q9JIF7
B	8	GLU	-	expression tag	UNP Q9JIF7
B	9	ASN	-	expression tag	UNP Q9JIF7
B	10	LEU	-	expression tag	UNP Q9JIF7
B	11	TYR	-	expression tag	UNP Q9JIF7
B	12	PHE	-	expression tag	UNP Q9JIF7
B	13	GLN	-	expression tag	UNP Q9JIF7
B	14	GLY	-	expression tag	UNP Q9JIF7
B	15	HIS	-	expression tag	UNP Q9JIF7
N	1	MET	-	initiating methionine	UNP Q9JIF7
N	2	HIS	-	expression tag	UNP Q9JIF7
N	3	HIS	-	expression tag	UNP Q9JIF7
N	4	HIS	-	expression tag	UNP Q9JIF7
N	5	HIS	-	expression tag	UNP Q9JIF7
N	6	HIS	-	expression tag	UNP Q9JIF7
N	7	HIS	-	expression tag	UNP Q9JIF7
N	8	GLU	-	expression tag	UNP Q9JIF7
N	9	ASN	-	expression tag	UNP Q9JIF7
N	10	LEU	-	expression tag	UNP Q9JIF7
N	11	TYR	-	expression tag	UNP Q9JIF7
N	12	PHE	-	expression tag	UNP Q9JIF7
N	13	GLN	-	expression tag	UNP Q9JIF7
N	14	GLY	-	expression tag	UNP Q9JIF7
N	15	HIS	-	expression tag	UNP Q9JIF7

- Molecule 4 is a protein called Coatomer subunit beta'.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	1-C	843	Total	C	N	O	0	0
			3371	1686	843	842		
4	2-C	843	Total	C	N	O	0	0
			3371	1686	843	842		
4	3-C	843	Total	C	N	O	0	0
			3371	1686	843	842		
4	1-H	721	Total	C	N	O	0	0
			2884	1442	721	721		
4	2-H	721	Total	C	N	O	0	0
			2884	1442	721	721		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3-H	721	Total 2884	C 1442	N 721	O 721	0	0

- Molecule 5 is a protein called Coatomer subunit delta.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	1-D	177	Total 706	C 354	N 177	O 175	0	0
5	2-D	177	Total 706	C 354	N 177	O 175	0	0
5	3-D	177	Total 706	C 354	N 177	O 175	0	0
5	1-I	177	Total 706	C 354	N 177	O 175	0	0
5	2-I	177	Total 706	C 354	N 177	O 175	0	0
5	3-I	177	Total 706	C 354	N 177	O 175	0	0

- Molecule 6 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	1-F	159	Total 635	C 318	N 159	O 158	0	0
6	2-F	159	Total 635	C 318	N 159	O 158	0	0
6	3-F	159	Total 635	C 318	N 159	O 158	0	0
6	1-R	159	Total 635	C 318	N 159	O 158	0	0
6	2-R	159	Total 635	C 318	N 159	O 158	0	0
6	3-R	159	Total 635	C 318	N 159	O 158	0	0
6	1-M	159	Total 635	C 318	N 159	O 158	0	0
6	2-M	159	Total 635	C 318	N 159	O 158	0	0
6	3-M	159	Total 635	C 318	N 159	O 158	0	0
6	1-J	159	Total 635	C 318	N 159	O 158	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
6	2-J	159	Total 635	C 318	N 159	O 158	0	0
6	3-J	159	Total 635	C 318	N 159	O 158	0	0

- Molecule 7 is a protein called Coatomer subunit gamma-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	1-G	798	Total 3190	C 1596	N 798	O 796	0	0
7	2-G	798	Total 3190	C 1596	N 798	O 796	0	0
7	3-G	798	Total 3190	C 1596	N 798	O 796	0	0
7	1-K	560	Total 2239	C 1120	N 560	O 559	0	0
7	2-K	560	Total 2239	C 1120	N 560	O 559	0	0
7	3-K	560	Total 2239	C 1120	N 560	O 559	0	0

- Molecule 8 is a protein called Coatomer subunit zeta-1.

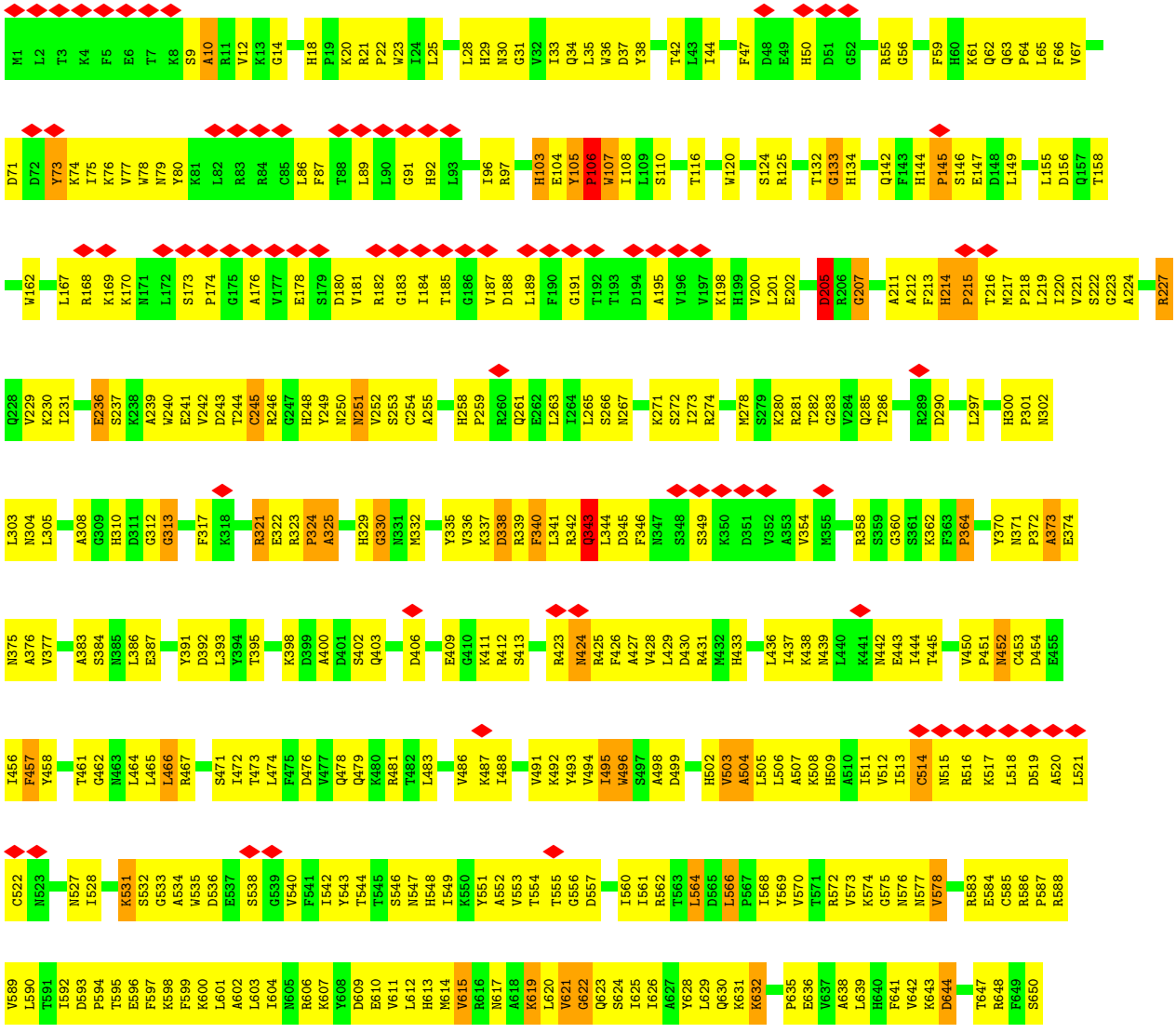
Mol	Chain	Residues	Atoms				AltConf	Trace
8	1-Z	139	Total 555	C 278	N 139	O 138	0	0
8	2-Z	139	Total 555	C 278	N 139	O 138	0	0
8	3-Z	139	Total 555	C 278	N 139	O 138	0	0
8	1-L	139	Total 555	C 278	N 139	O 138	0	0
8	2-L	139	Total 555	C 278	N 139	O 138	0	0
8	3-L	139	Total 555	C 278	N 139	O 138	0	0

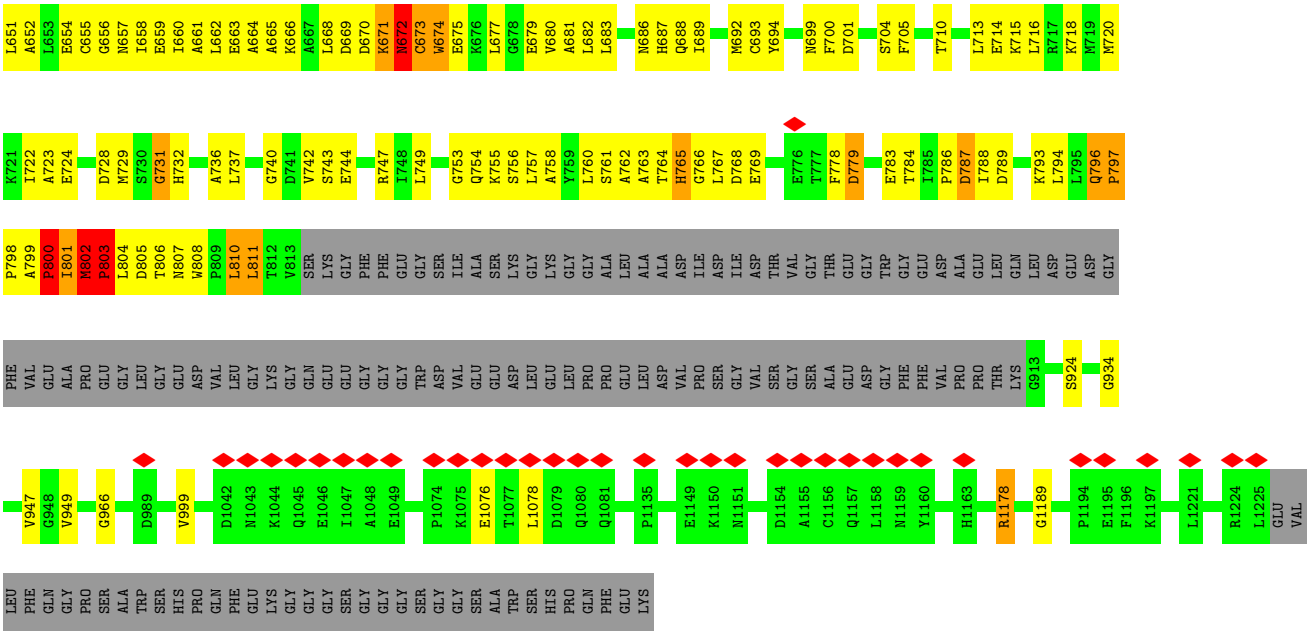
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Coatomer subunit alpha

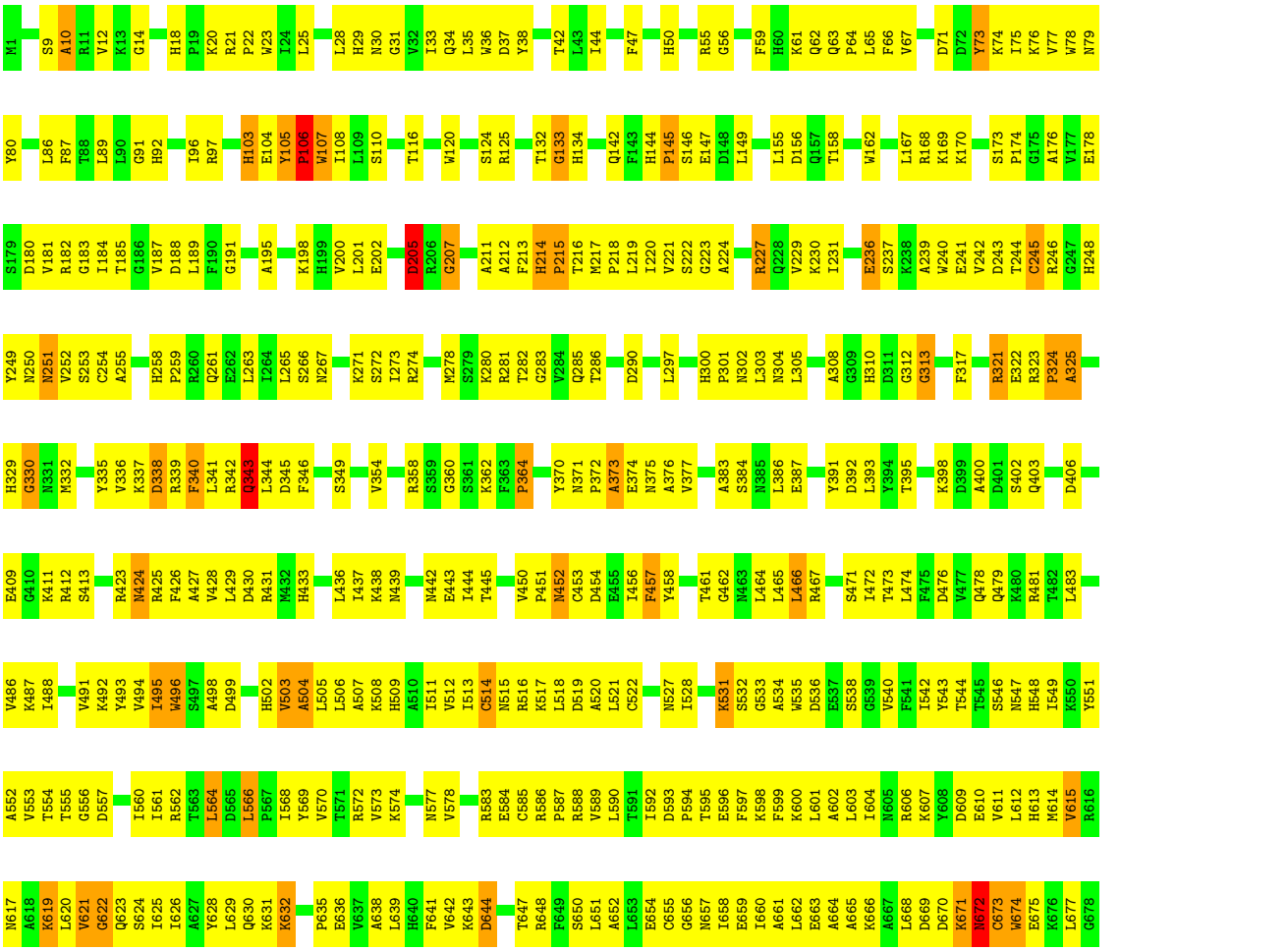
Chain 1-A:

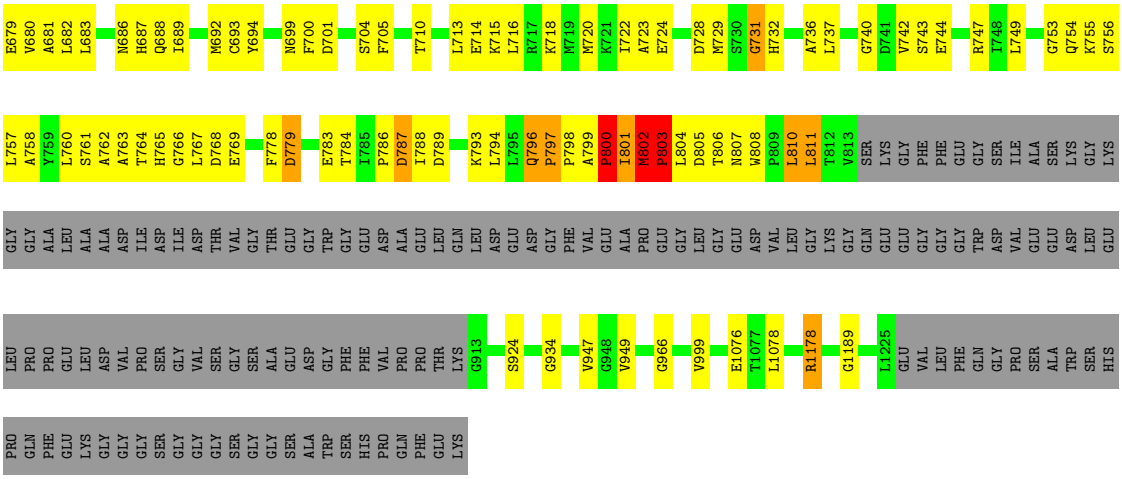




• Molecule 1: Coatomer subunit alpha

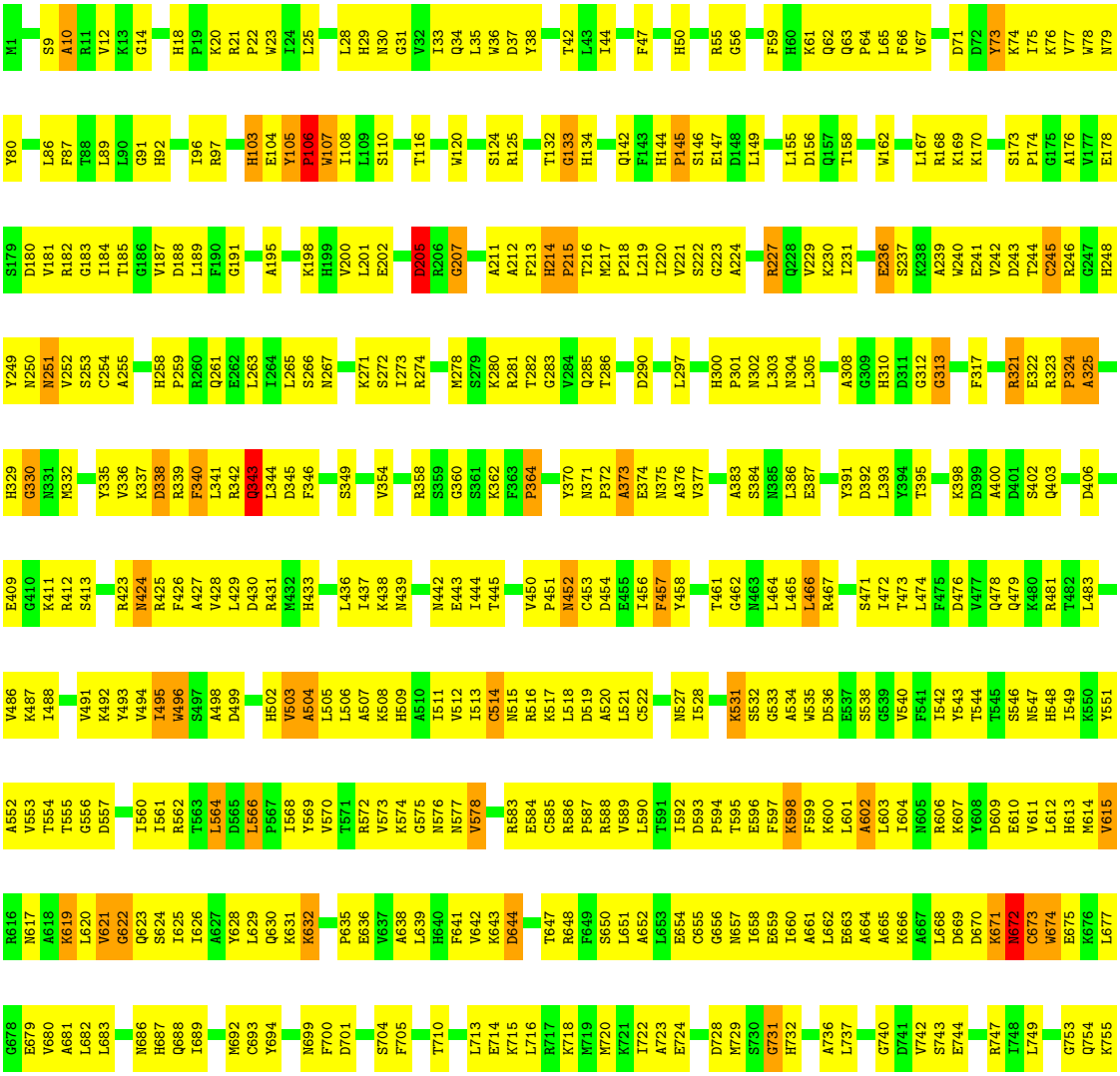
Chain 2-A:

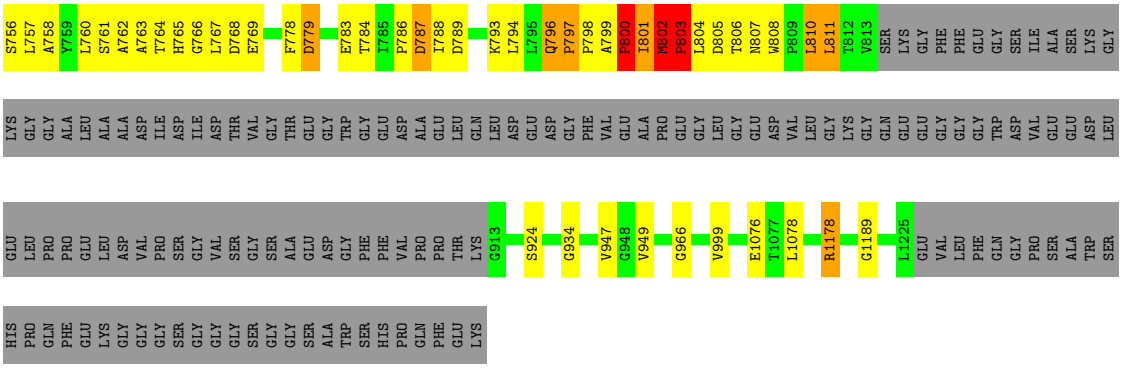




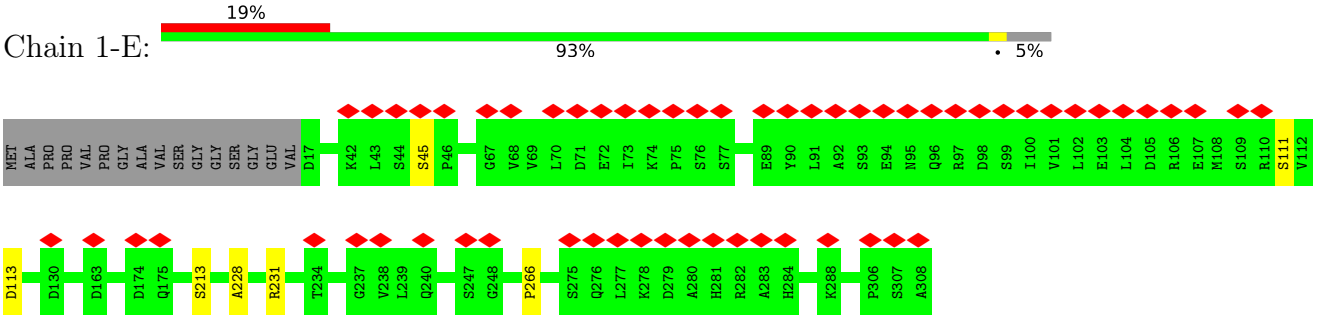
• Molecule 1: Coatomer subunit alpha

Chain 3-A:

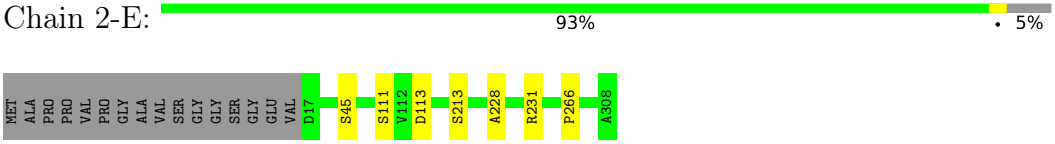




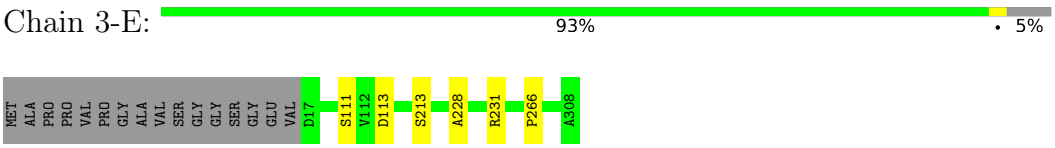
• Molecule 2: Coatomer subunit epsilon



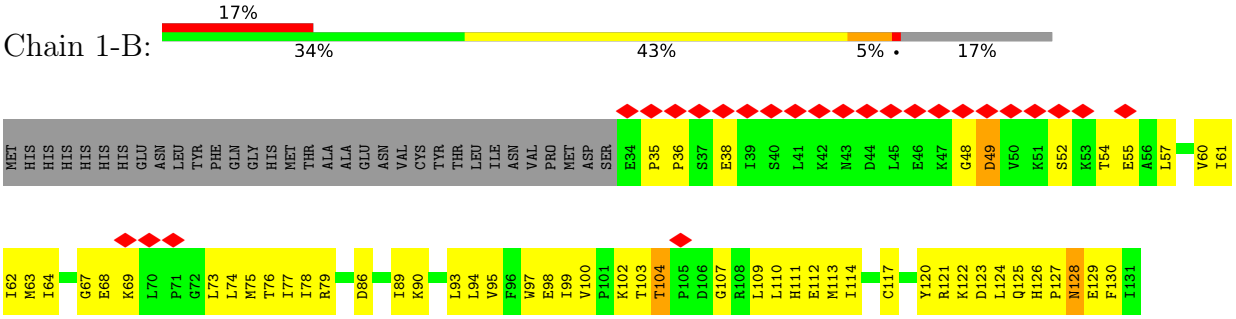
• Molecule 2: Coatomer subunit epsilon

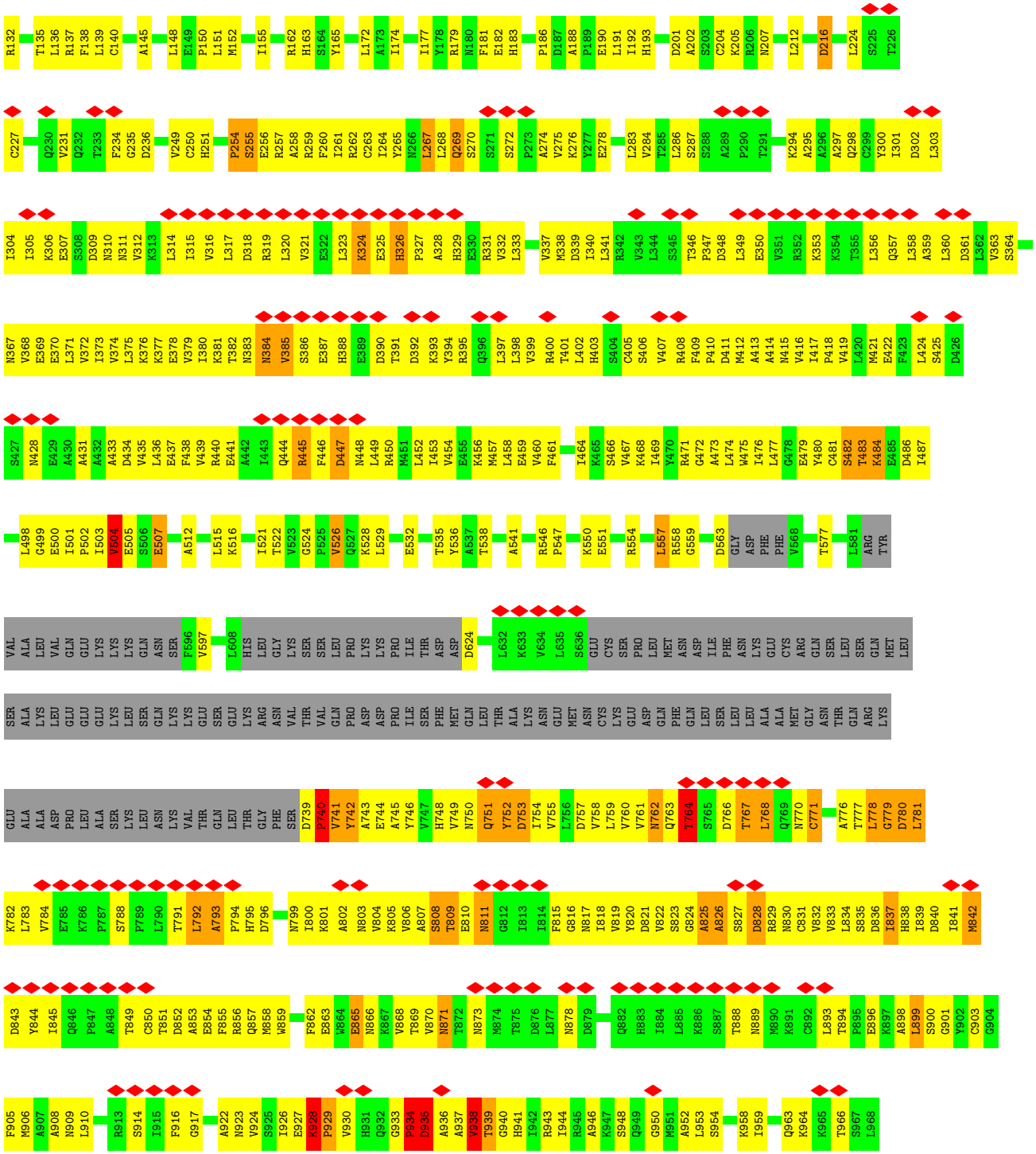


• Molecule 2: Coatomer subunit epsilon

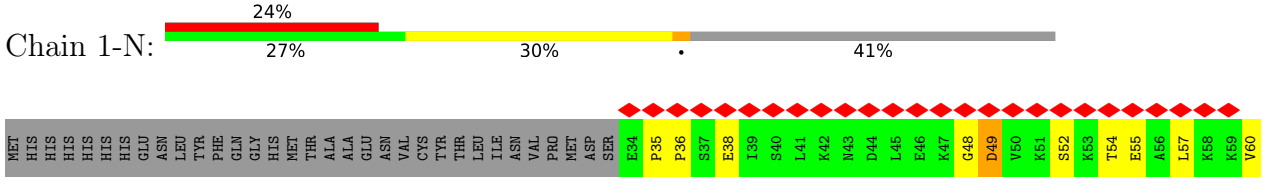


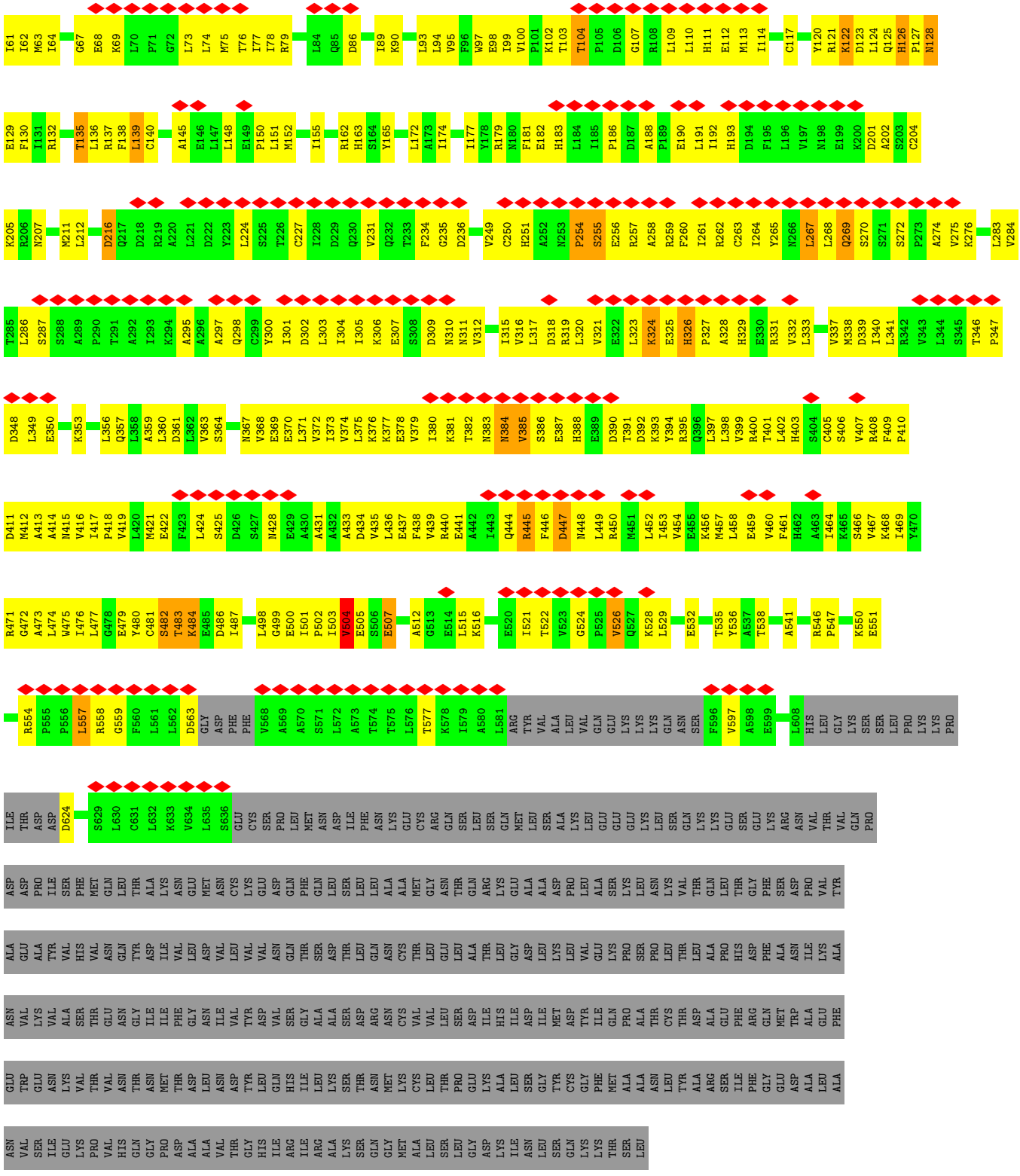
• Molecule 3: Coatomer subunit beta





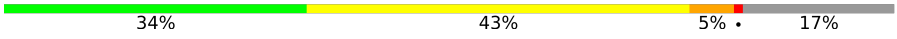
• Molecule 3: Coatomer subunit beta

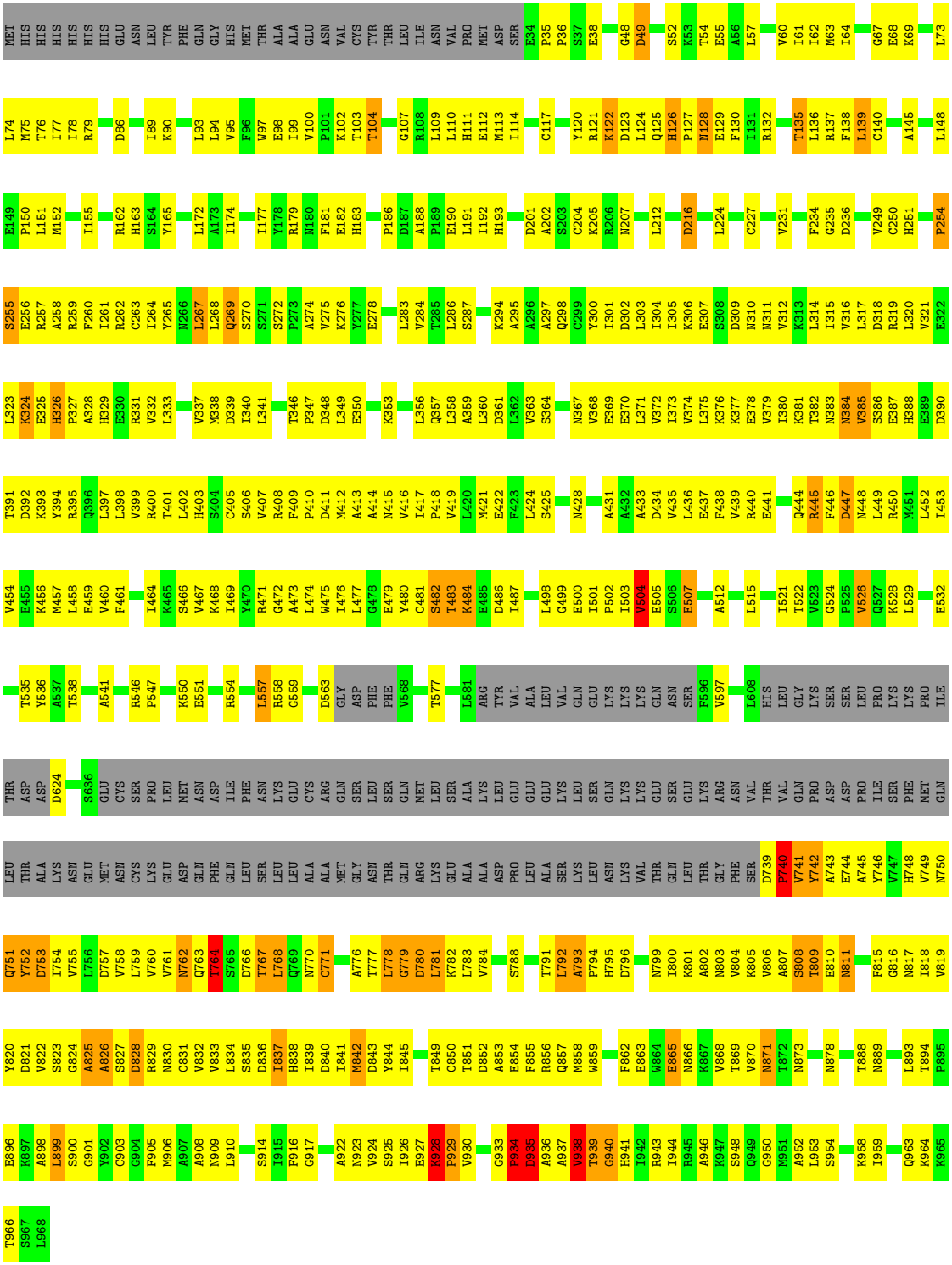




• Molecule 3: Coatomer subunit beta

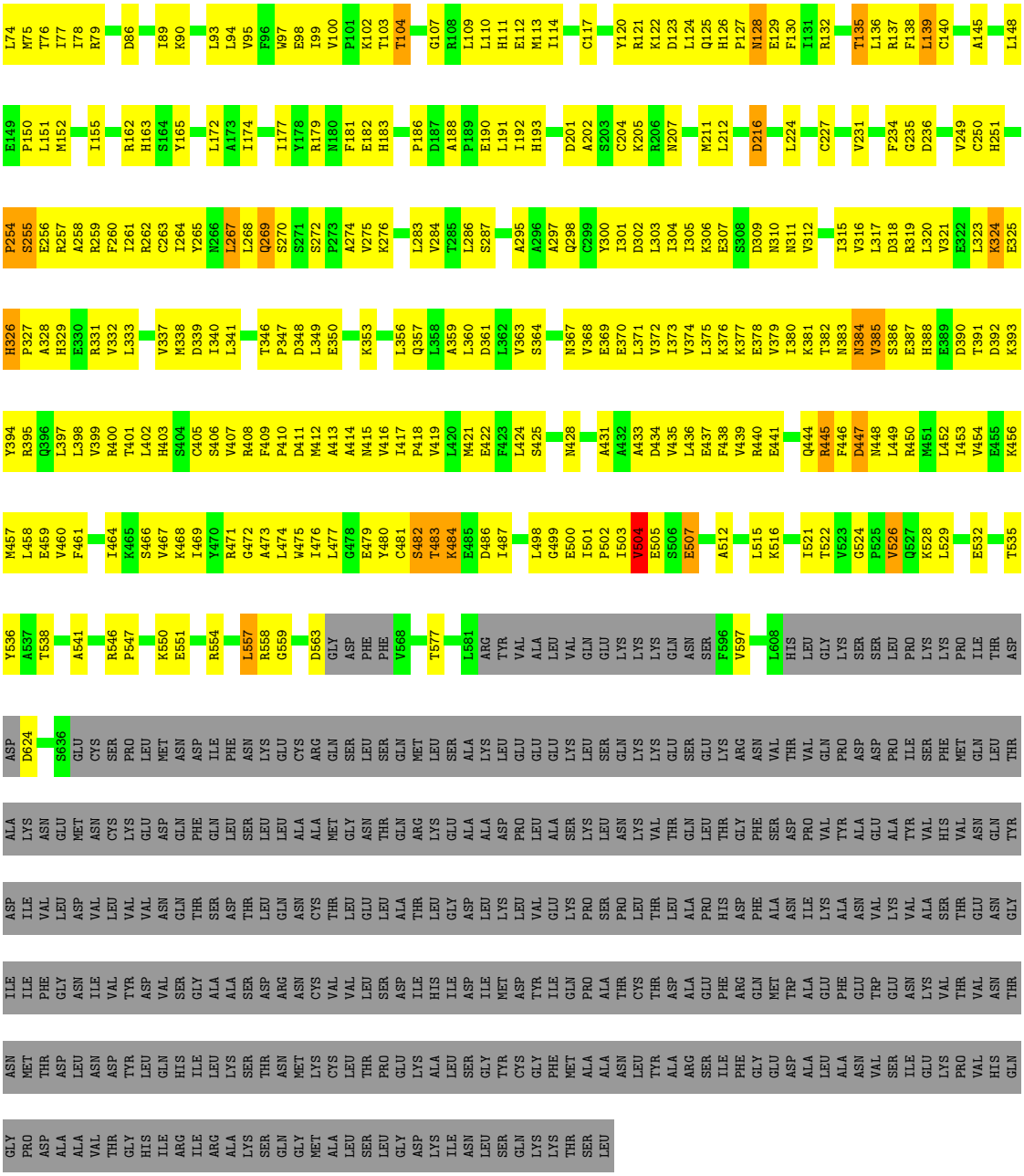
Chain 2-B:





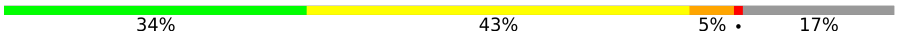
• Molecule 3: Coatomer subunit beta

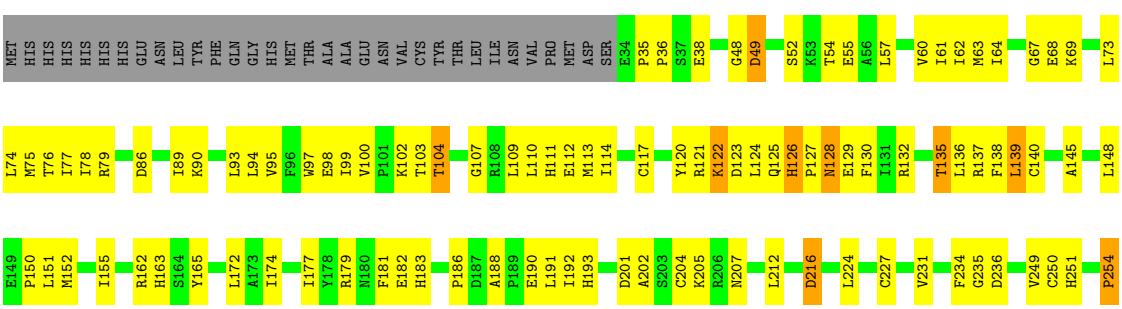
Chain 2-N:

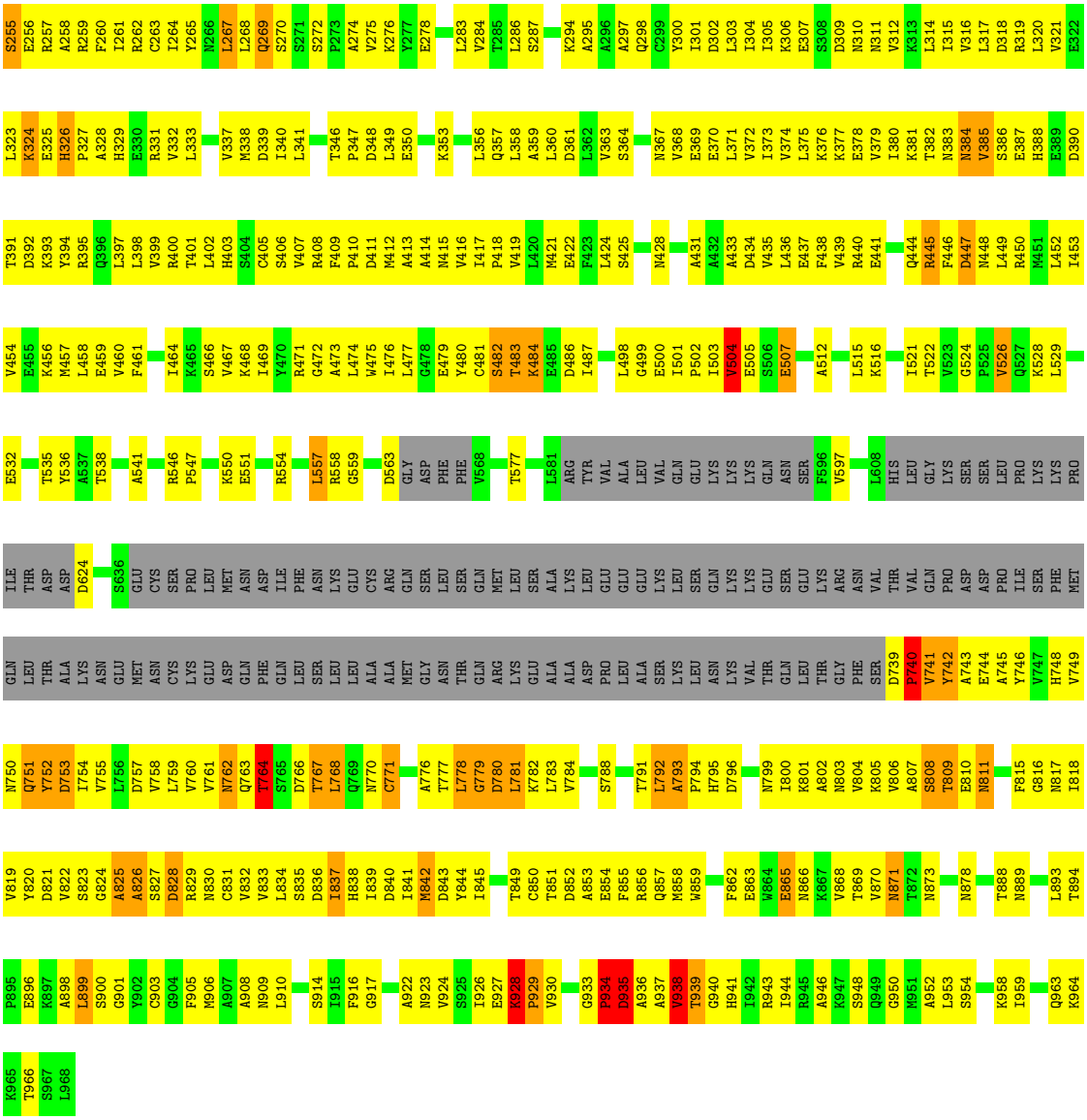


• Molecule 3: Coatomer subunit beta

Chain 3-B:

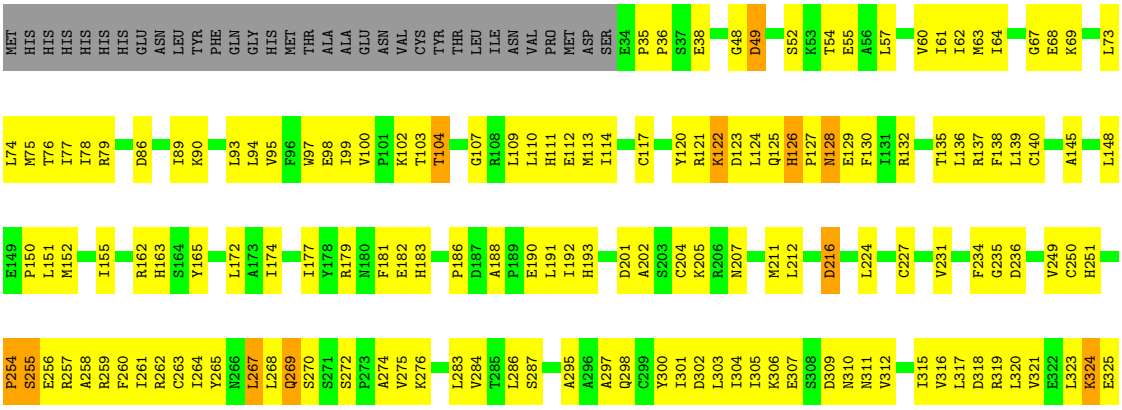


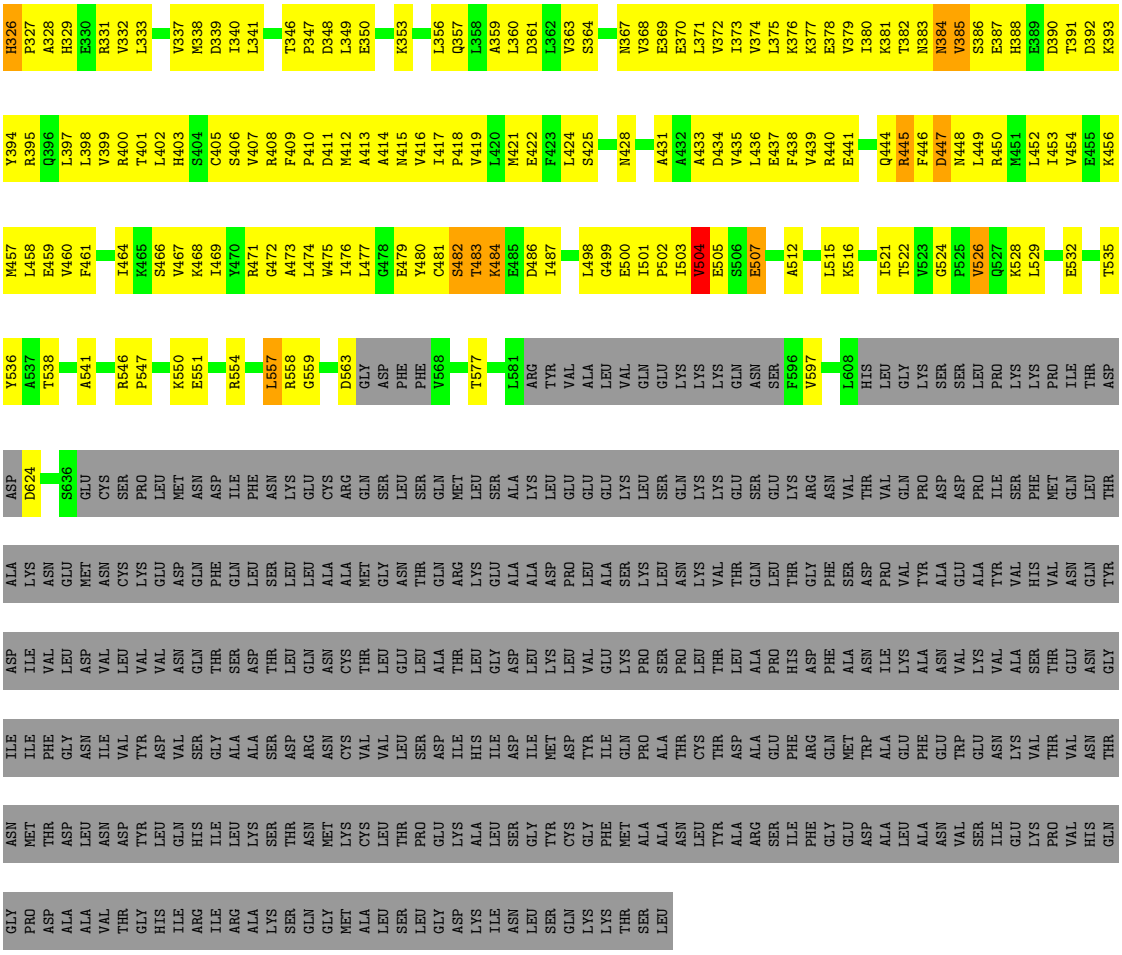




• Molecule 3: Coatomer subunit beta

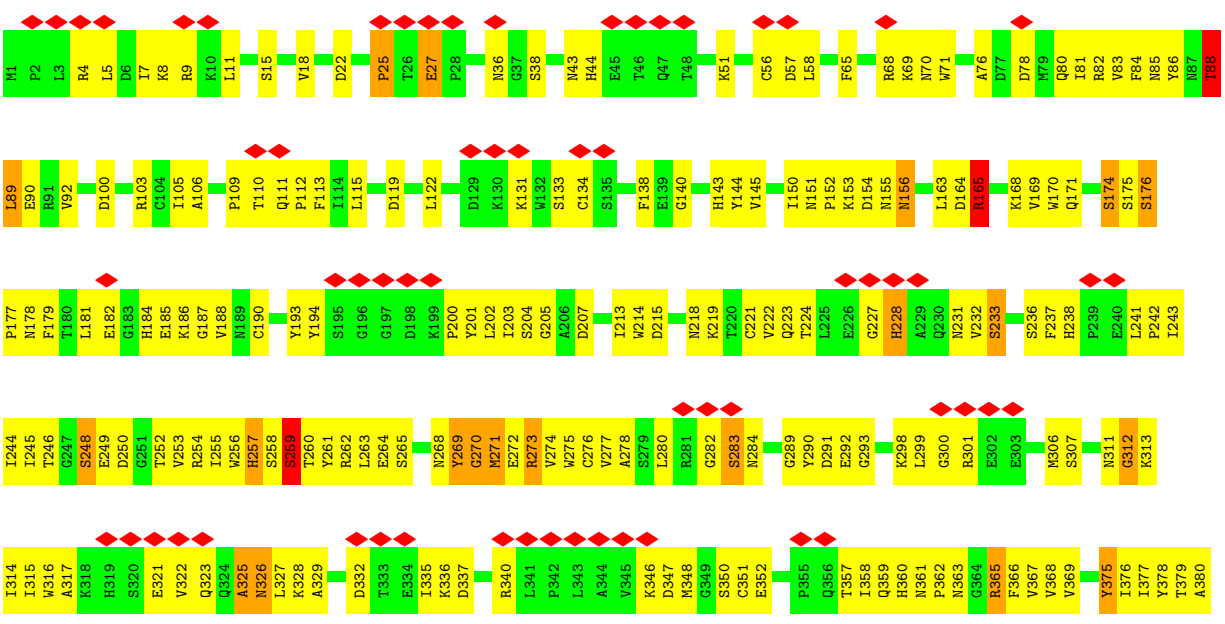
Chain 3-N:

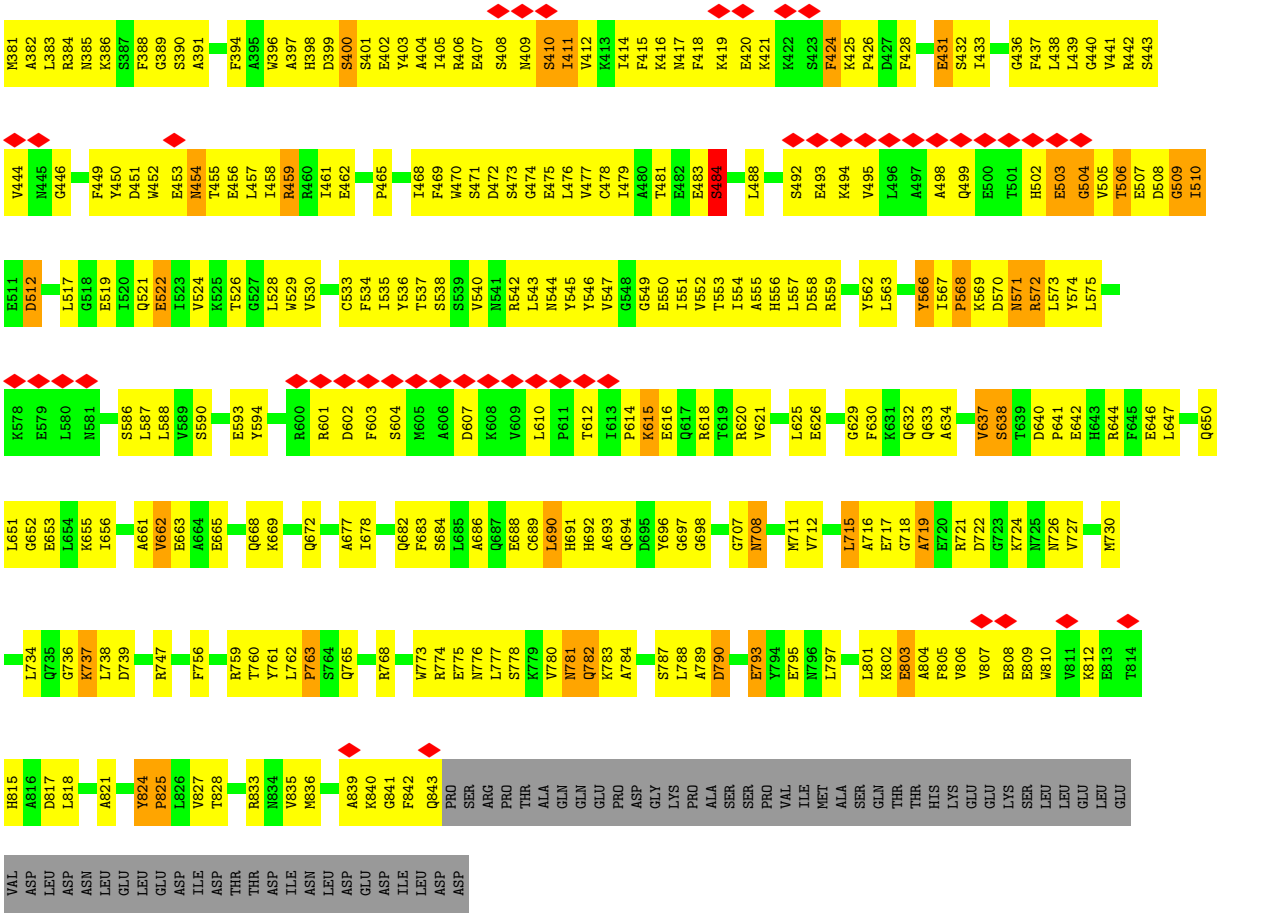




• Molecule 4: Coatomer subunit beta'

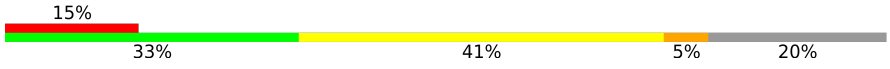
Chain 1-C:

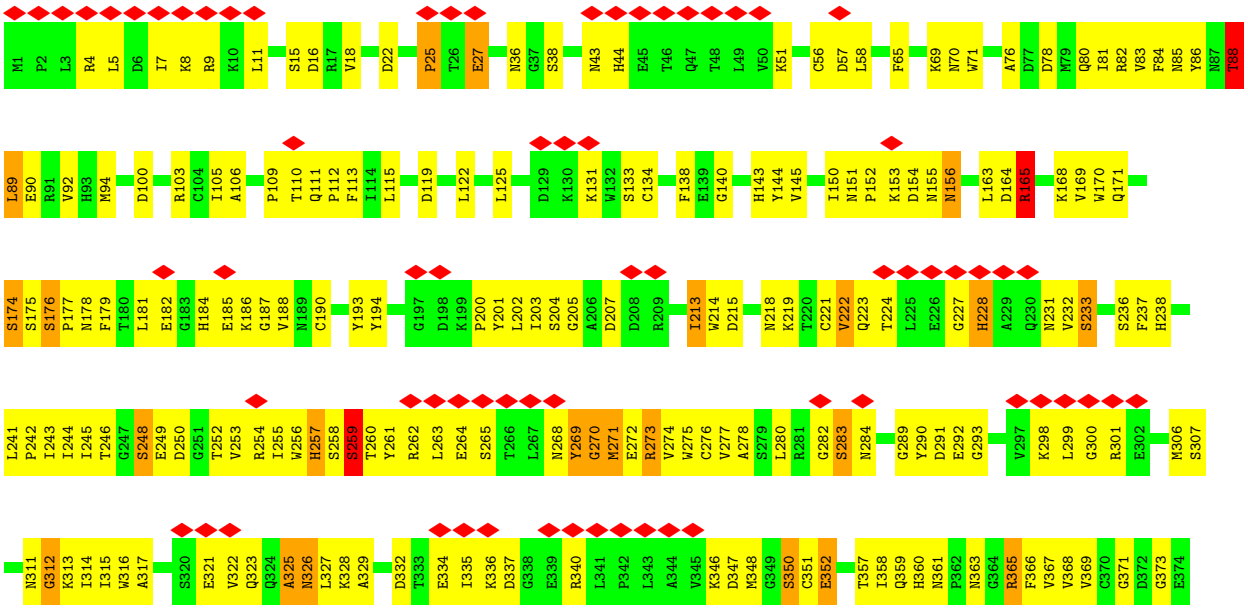


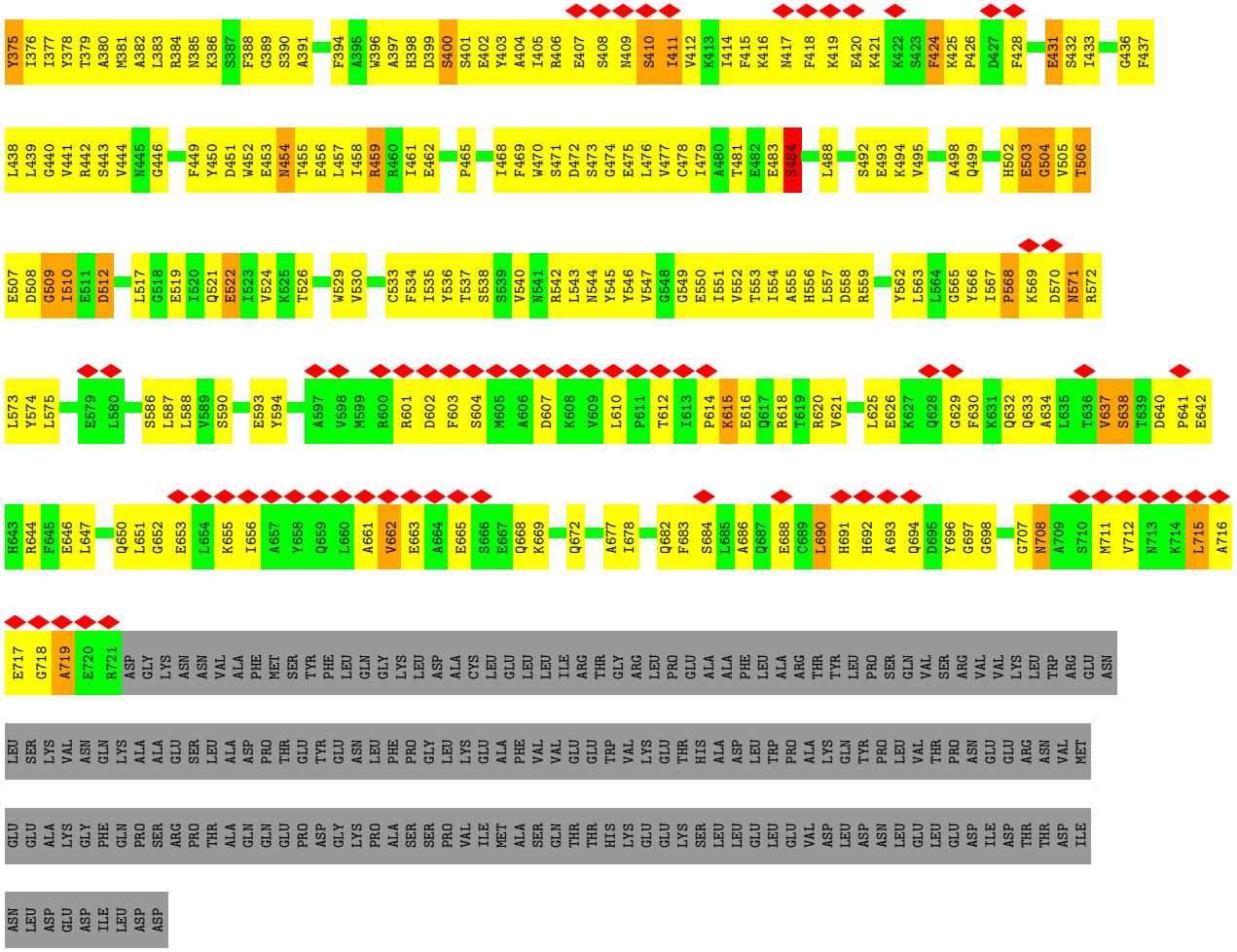


• Molecule 4: Coatomer subunit beta'

Chain 1-H:

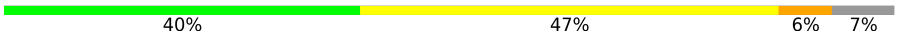


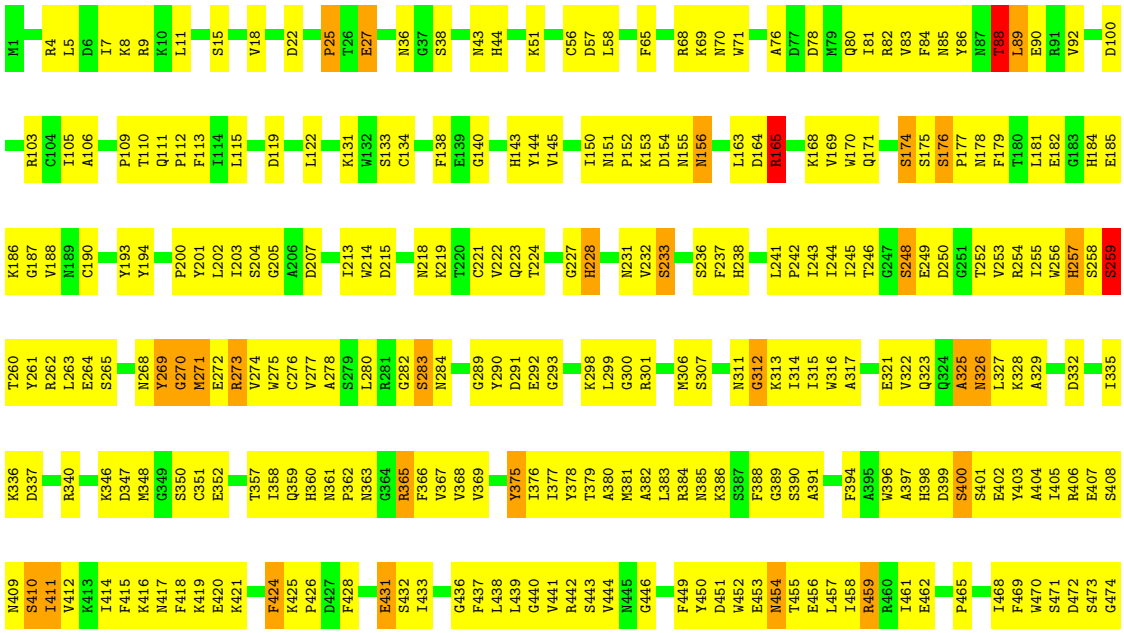


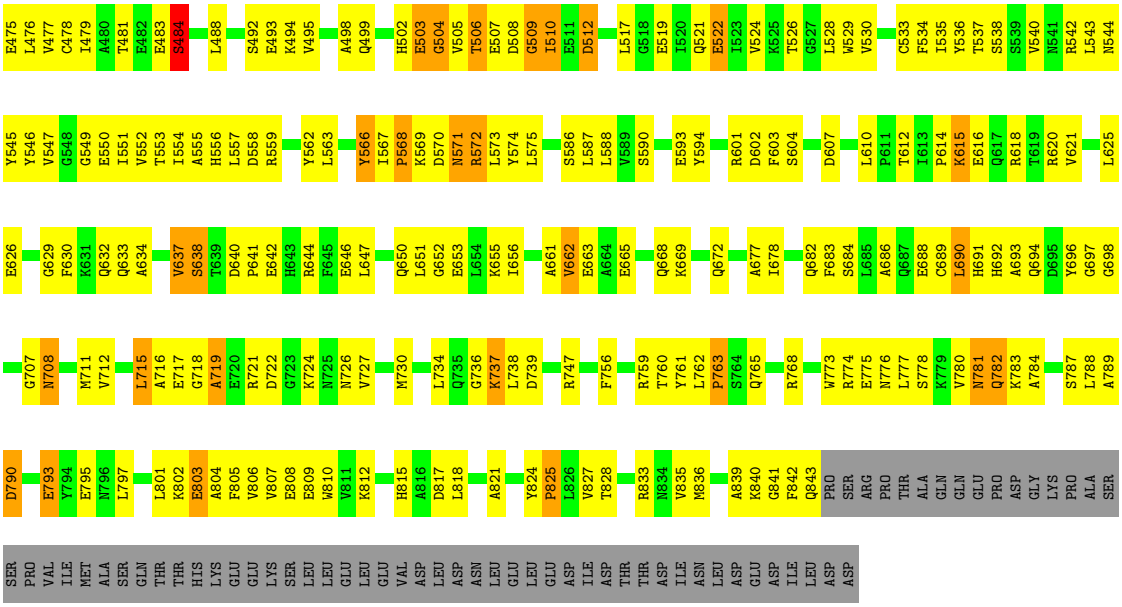


• Molecule 4: Coatomer subunit beta'

Chain 2-C:

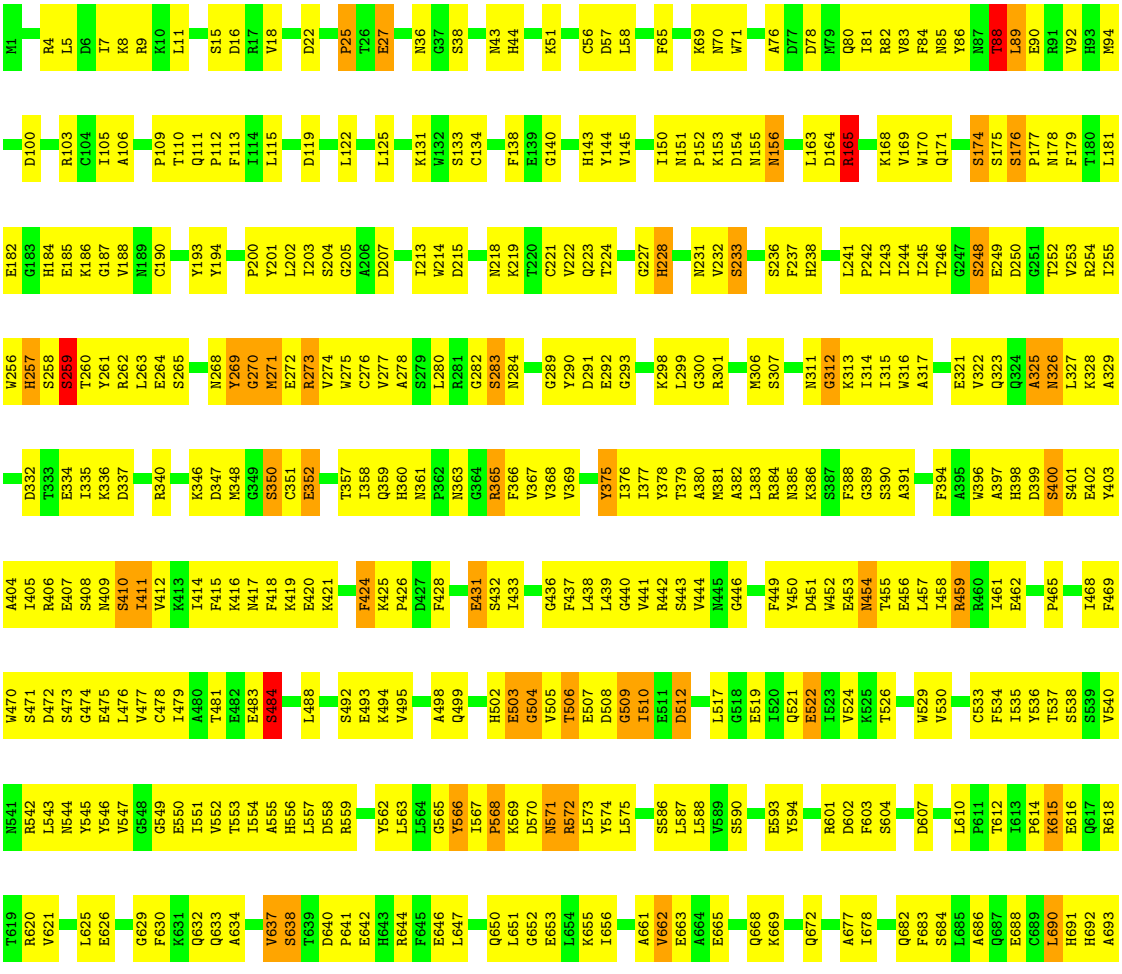


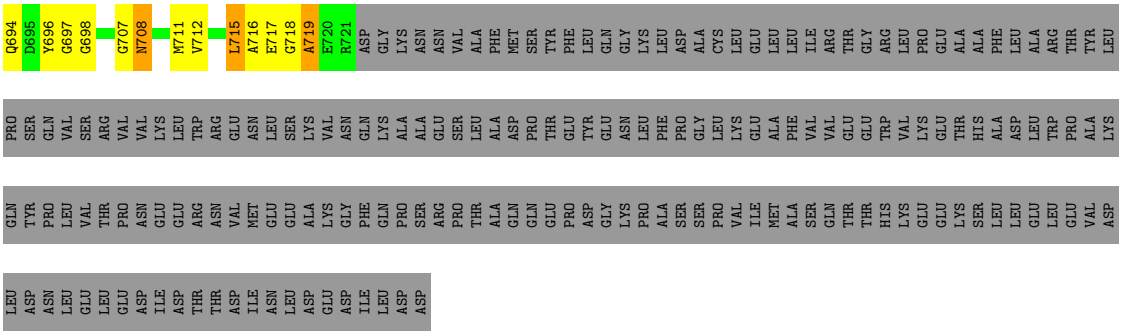




• Molecule 4: Coatomer subunit beta'

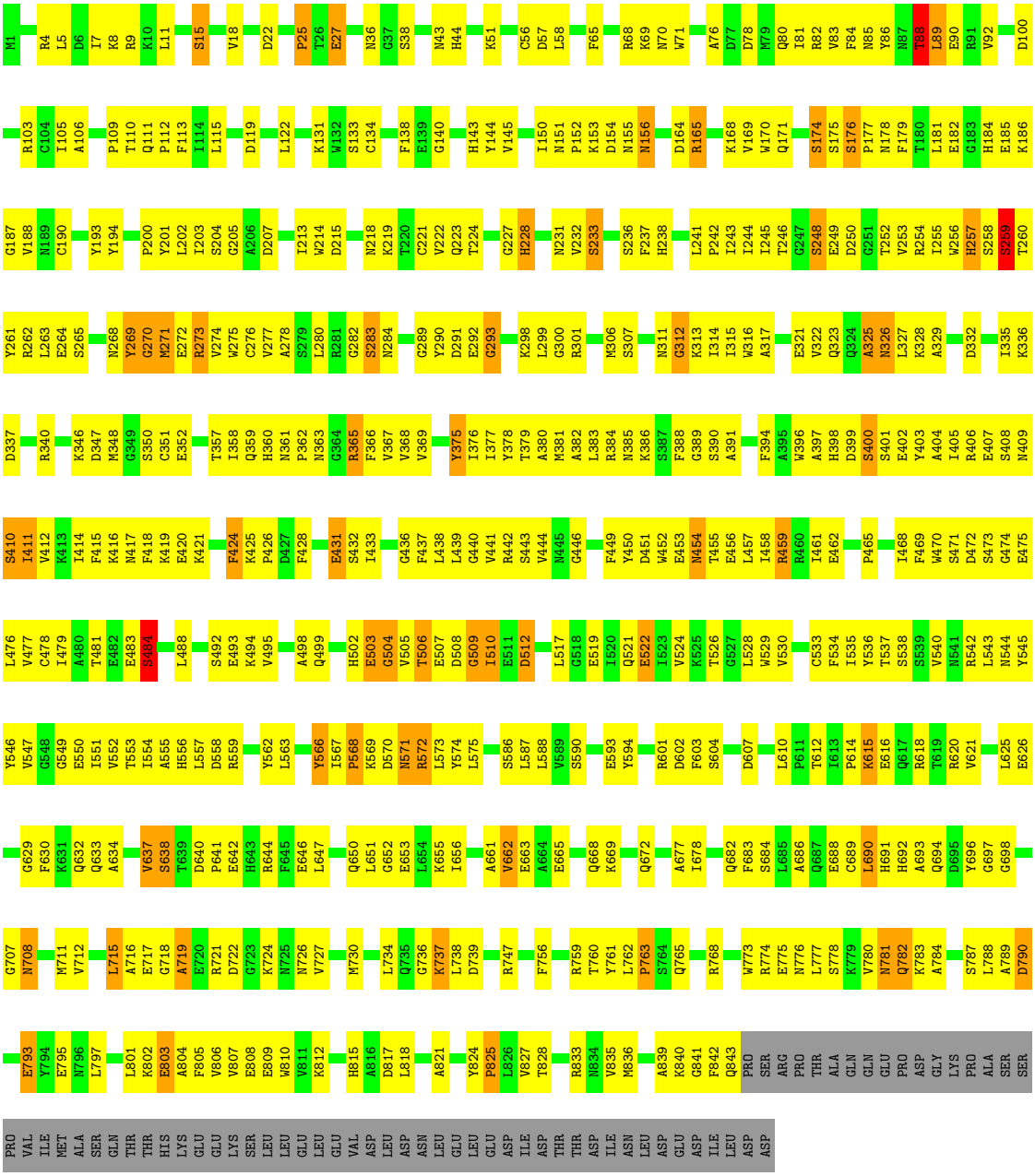
Chain 2-H:





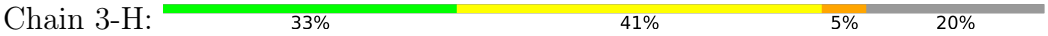
• Molecule 4: Coatomer subunit beta'

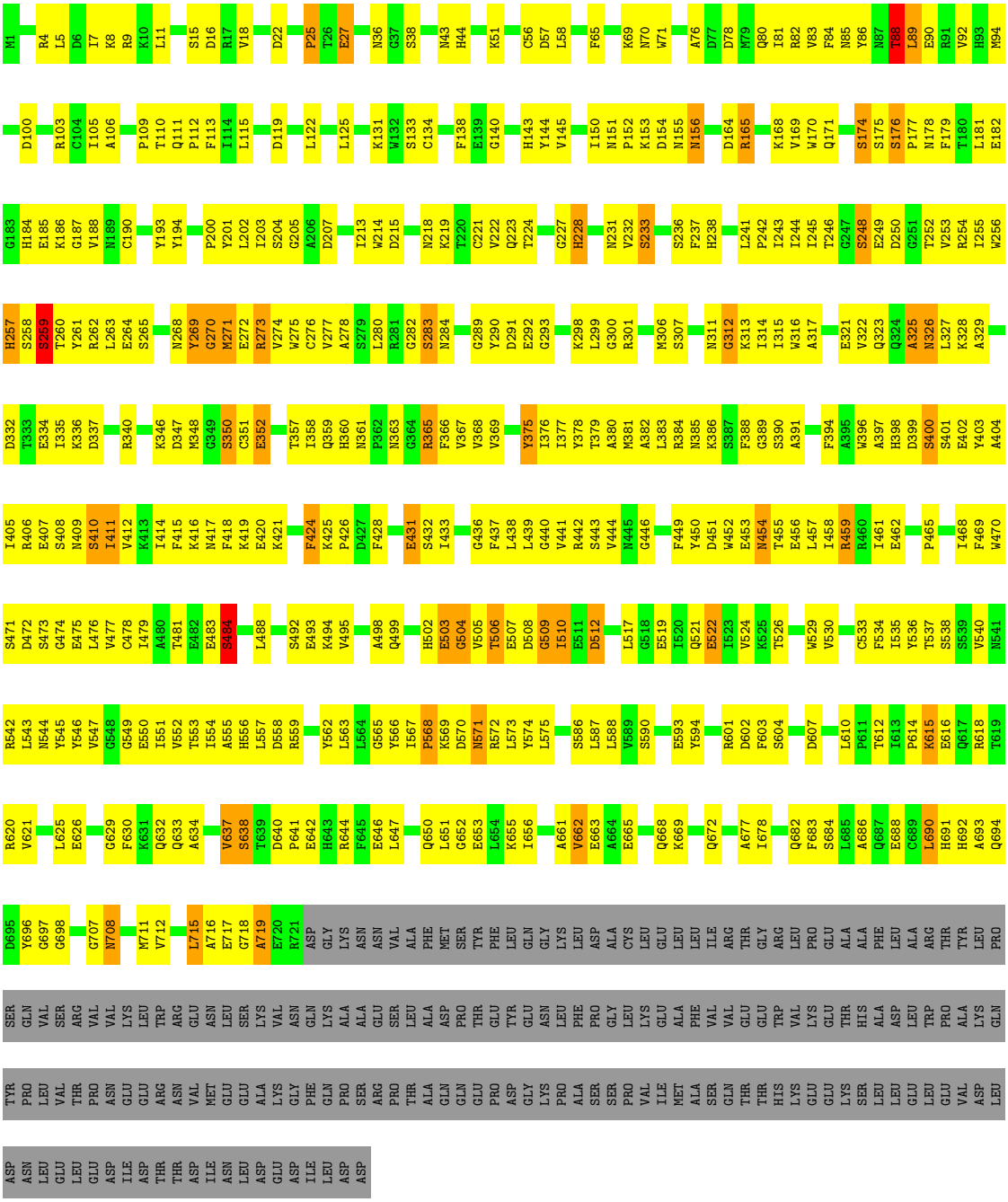
Chain 3-C:



• Molecule 4: Coatomer subunit beta'

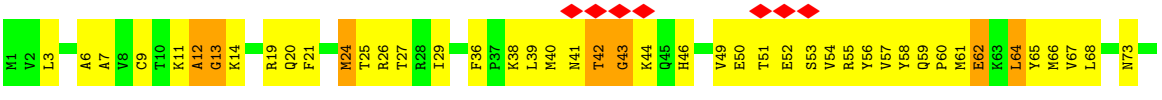
Chain 3-H:

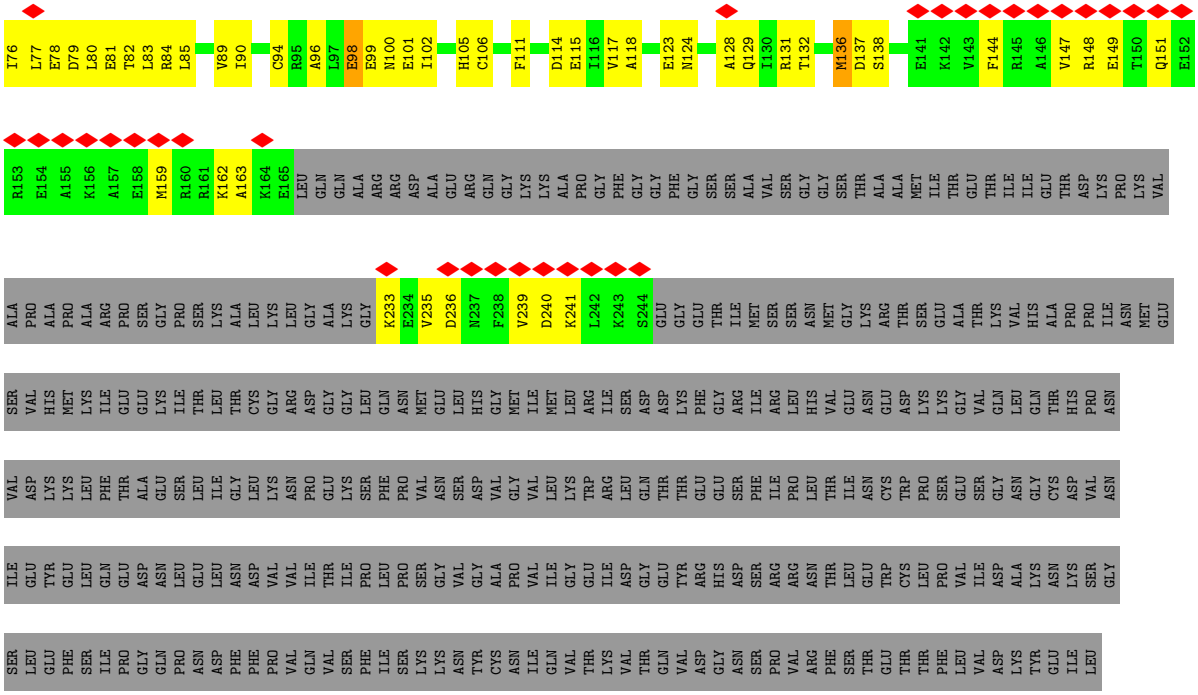




• Molecule 5: Coatomer subunit delta

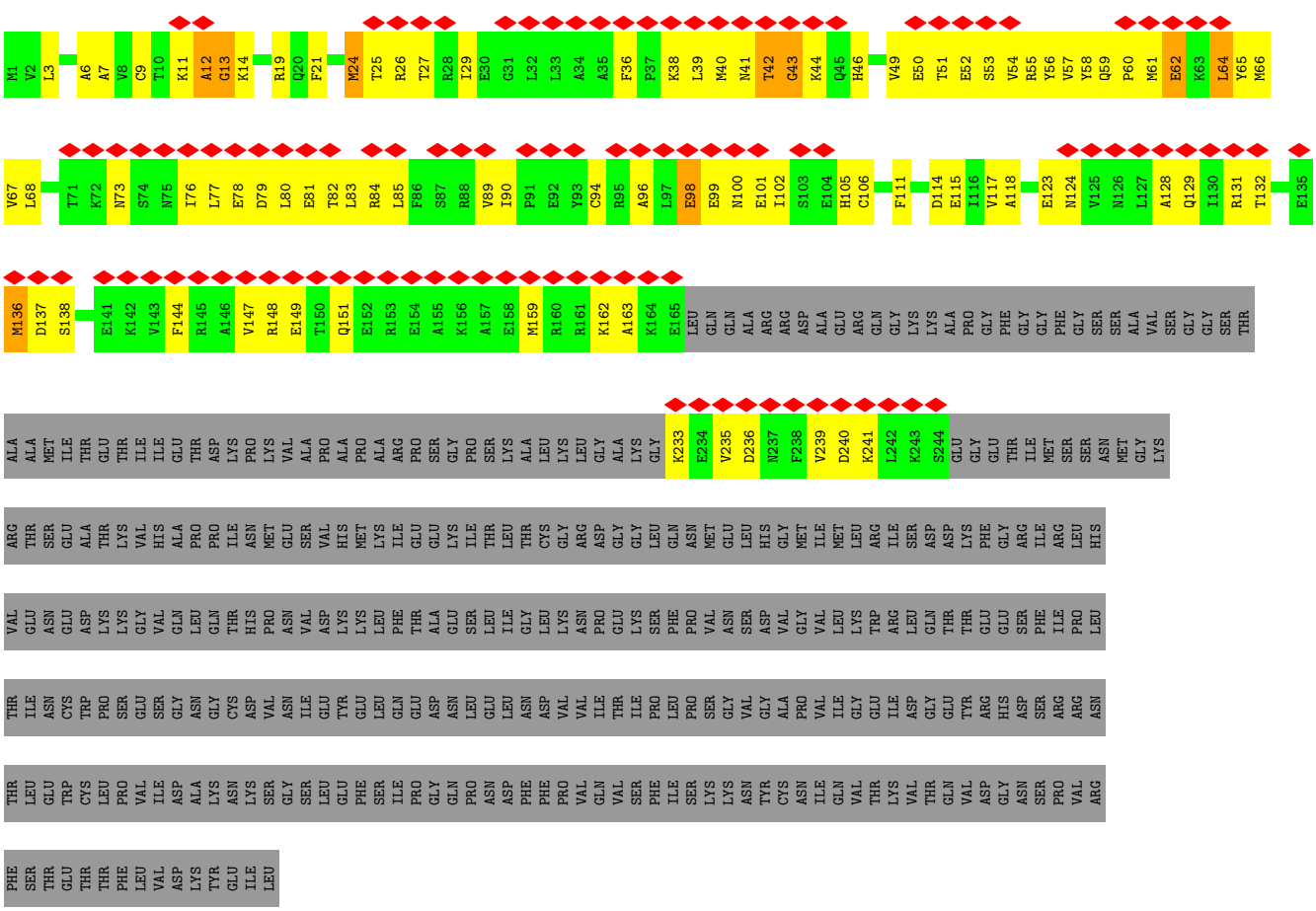
Chain 1-D:





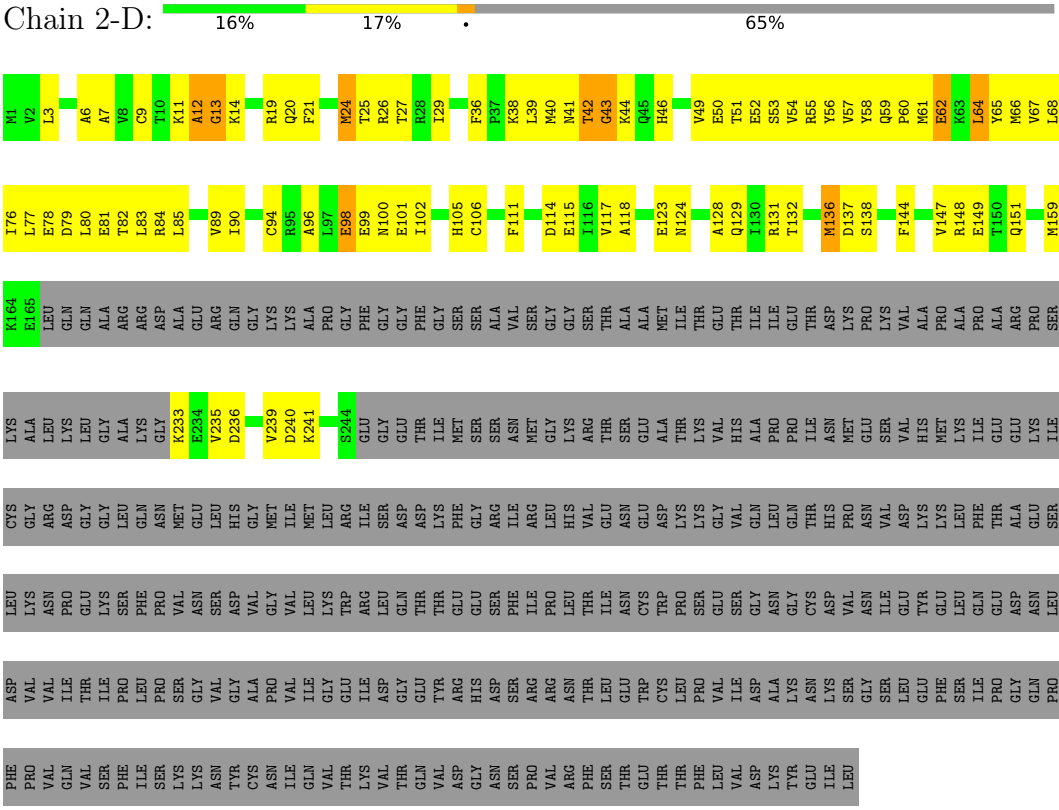
• Molecule 5: Coatomer subunit delta

Chain 1-I:



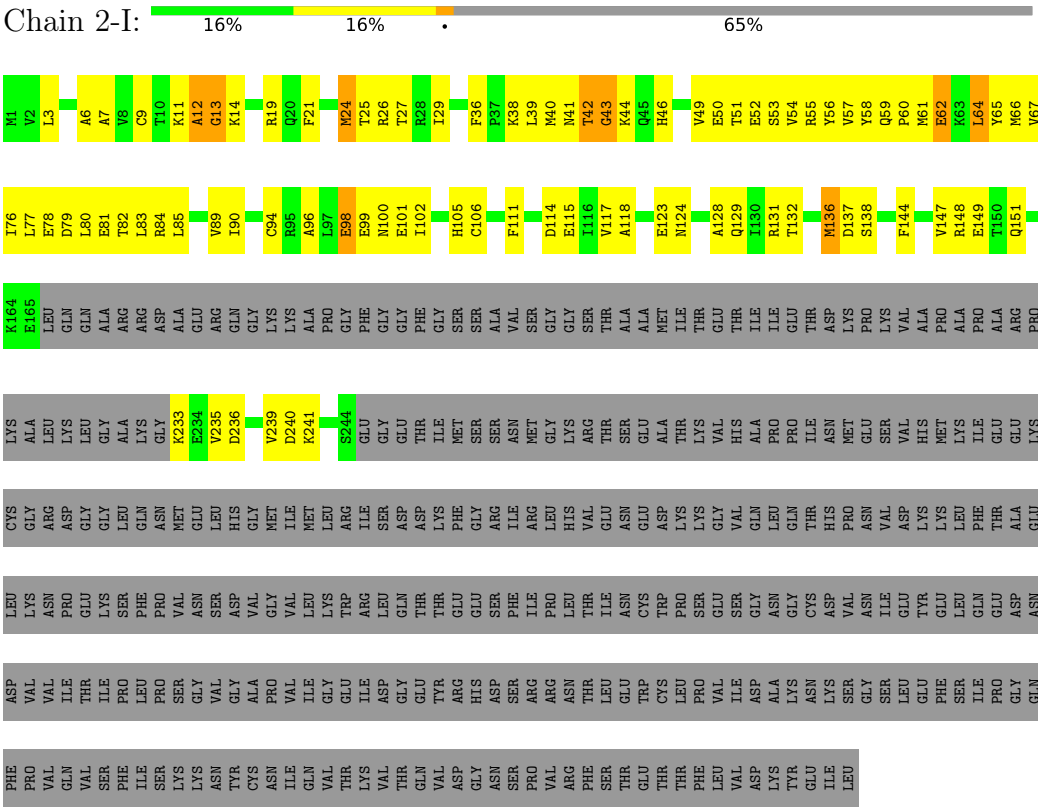
• Molecule 5: Coatomer subunit delta

Chain 2-D:



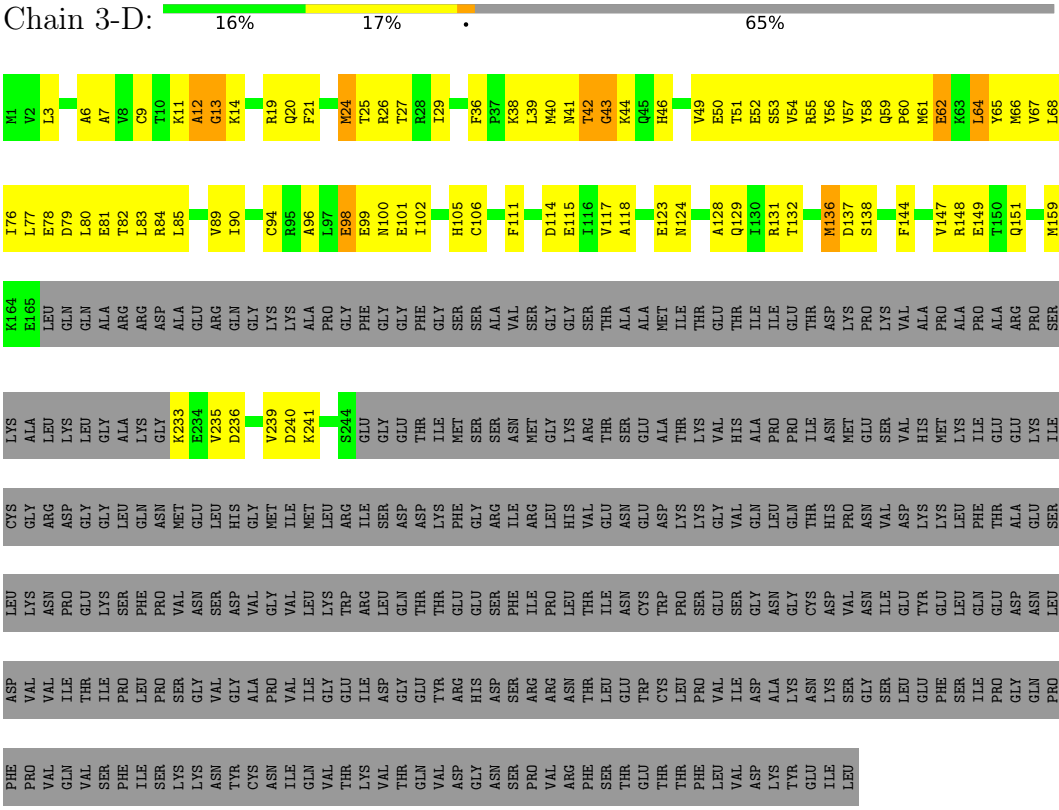
• Molecule 5: Coatomer subunit delta

Chain 2-I:



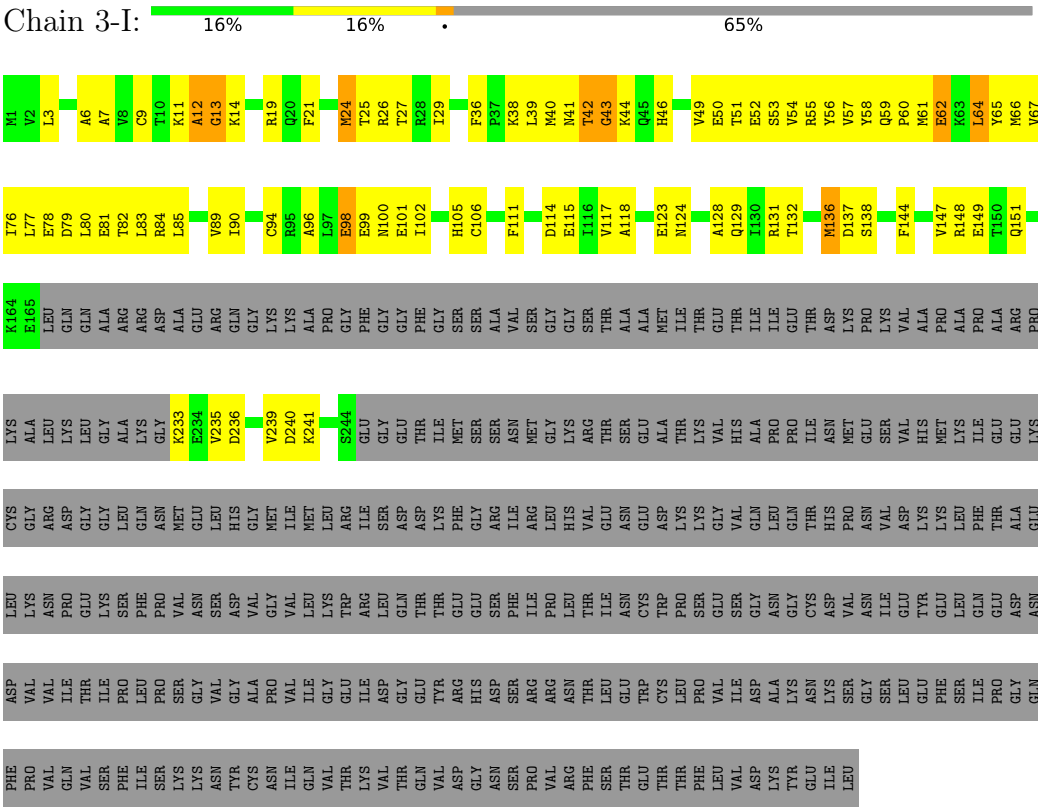
• Molecule 5: Coatomer subunit delta

Chain 3-D:



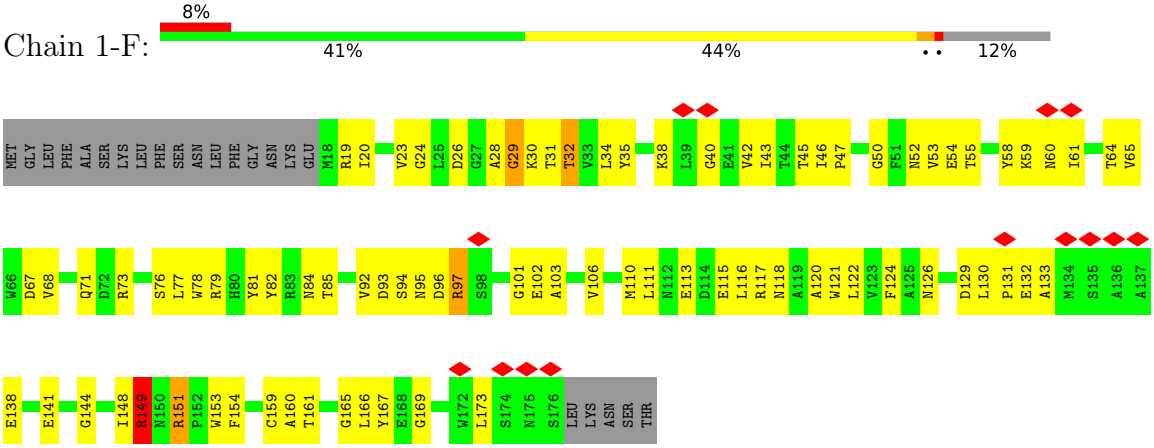
• Molecule 5: Coatomer subunit delta

Chain 3-I:



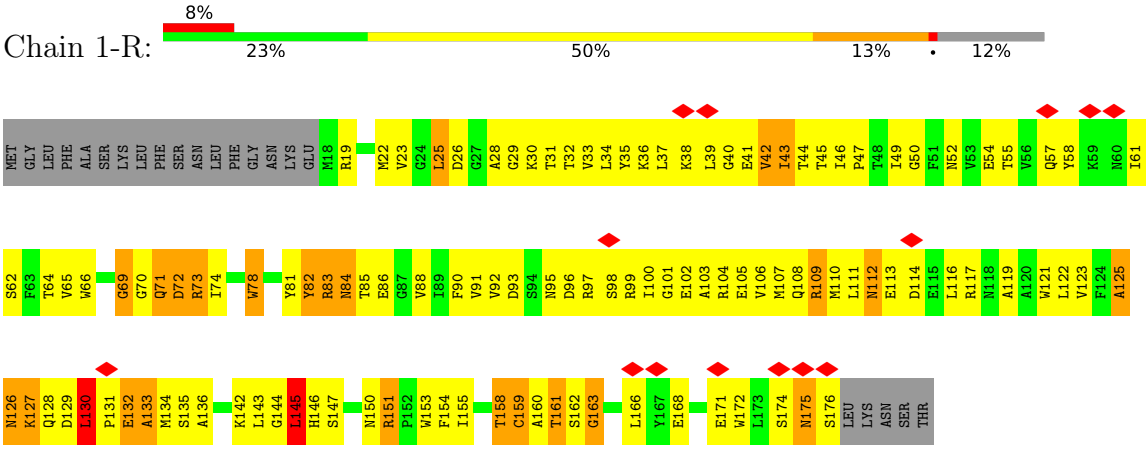
• Molecule 6: ADP-ribosylation factor 1

Chain 1-F:



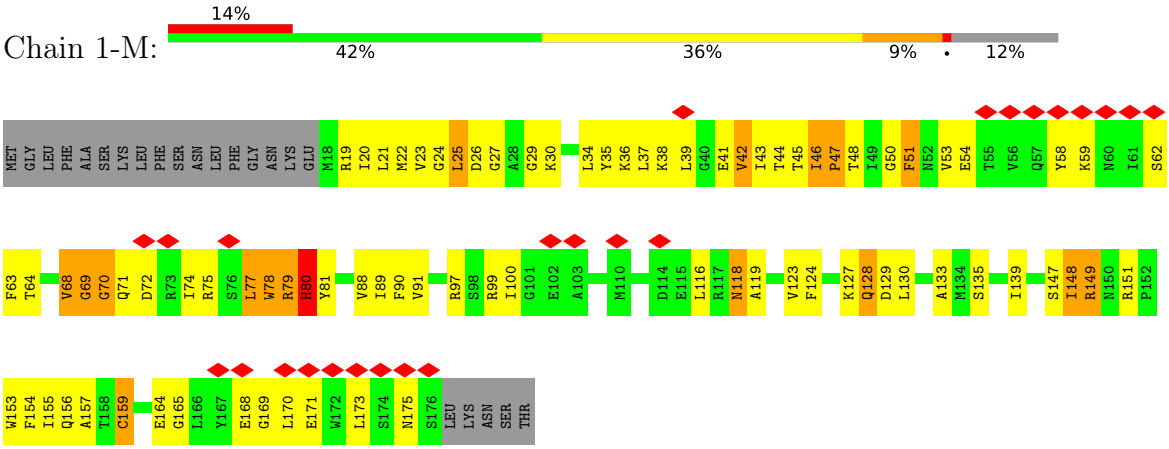
• Molecule 6: ADP-ribosylation factor 1

Chain 1-R:



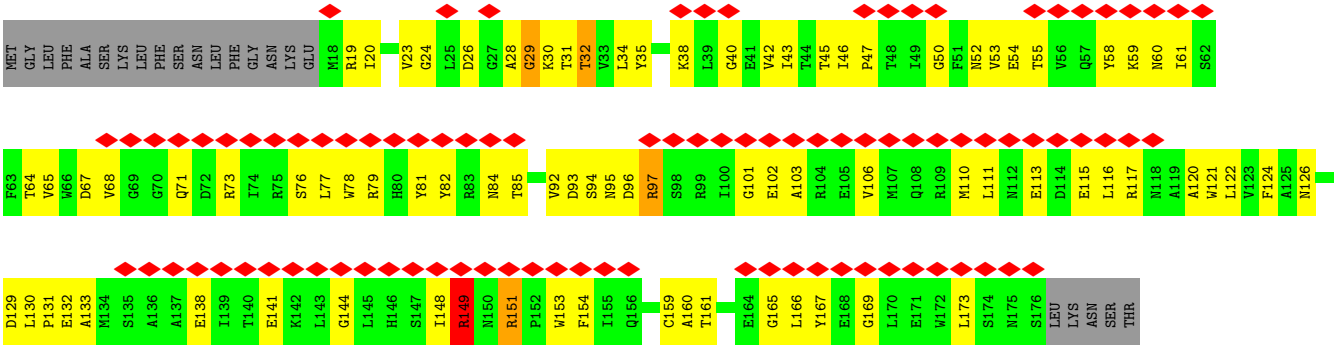
• Molecule 6: ADP-ribosylation factor 1

Chain 1-M:



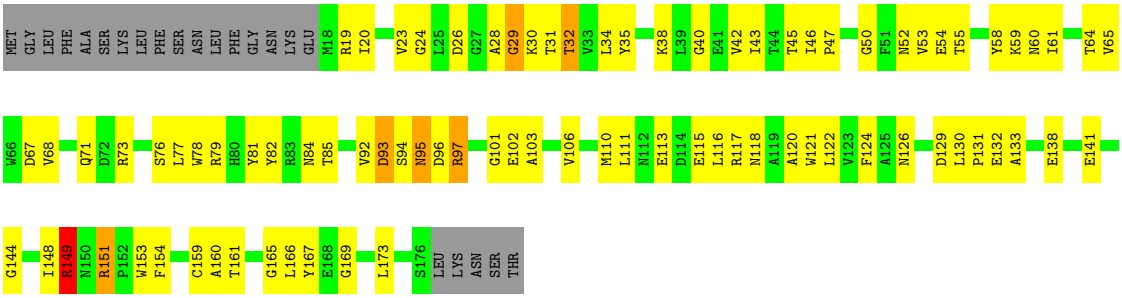
• Molecule 6: ADP-ribosylation factor 1

Chain 1-J:



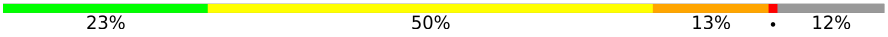
• Molecule 6: ADP-ribosylation factor 1

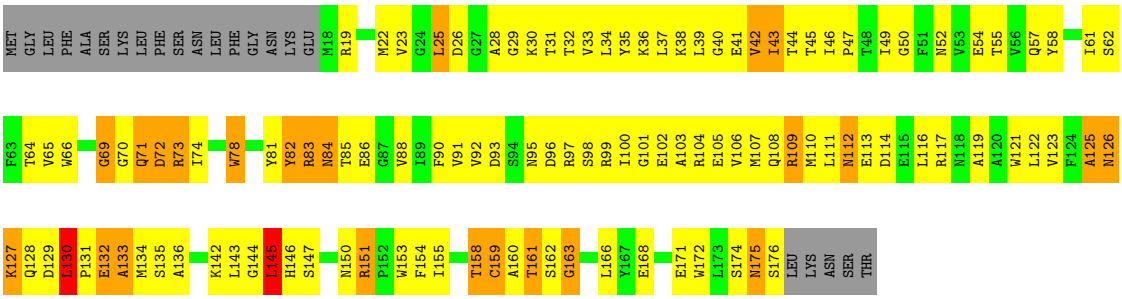
Chain 2-F:



• Molecule 6: ADP-ribosylation factor 1

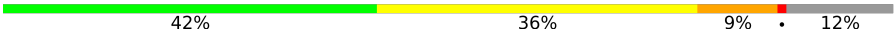
Chain 2-R:

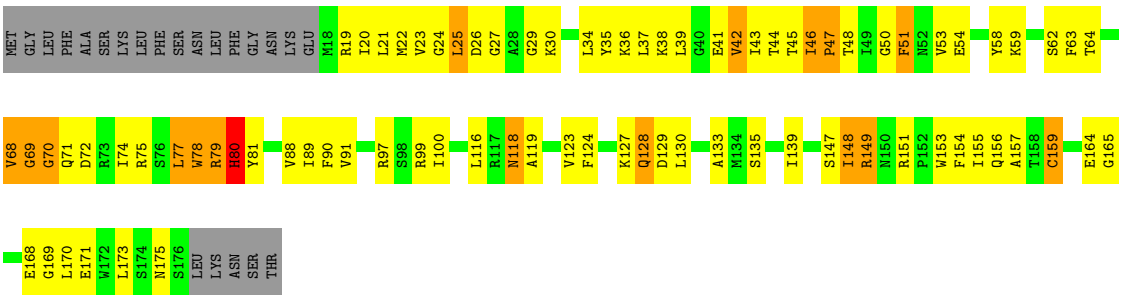




• Molecule 6: ADP-ribosylation factor 1

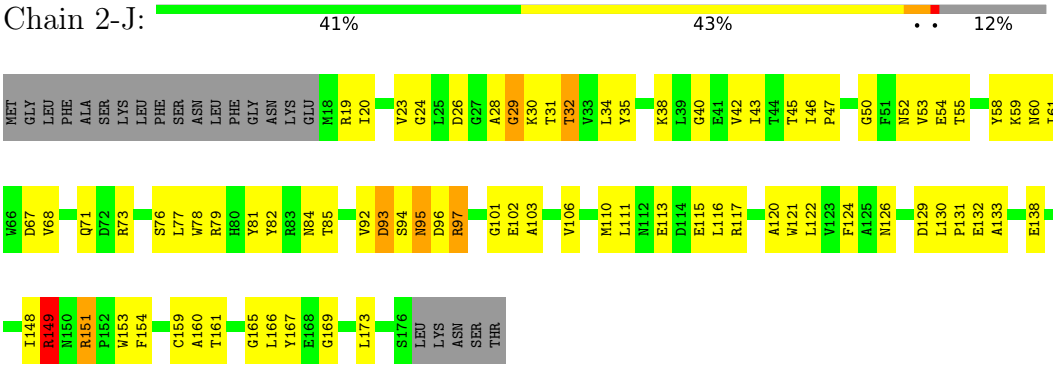
Chain 2-M:





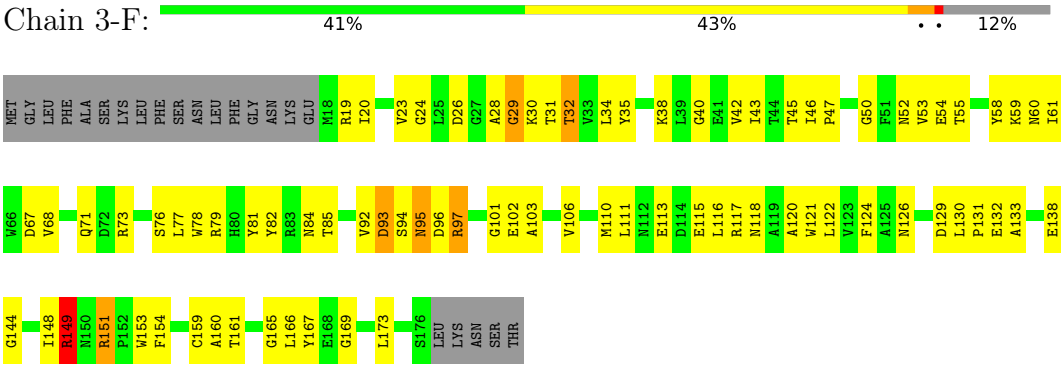
• Molecule 6: ADP-ribosylation factor 1

Chain 2-J:



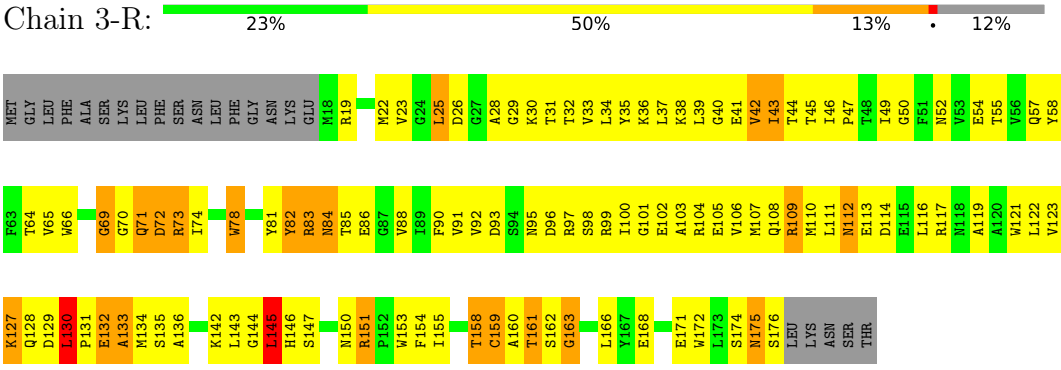
• Molecule 6: ADP-ribosylation factor 1

Chain 3-F:



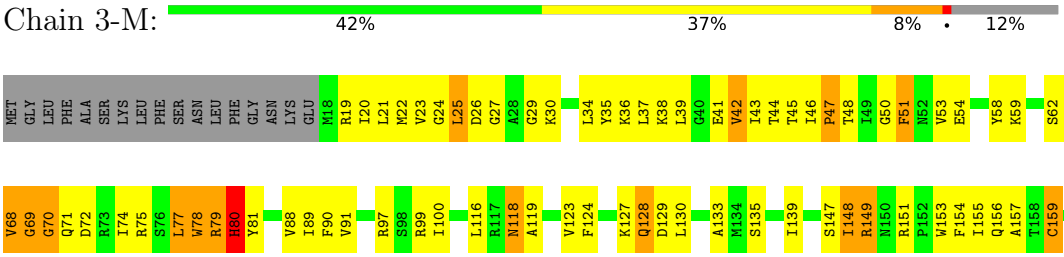
• Molecule 6: ADP-ribosylation factor 1

Chain 3-R:



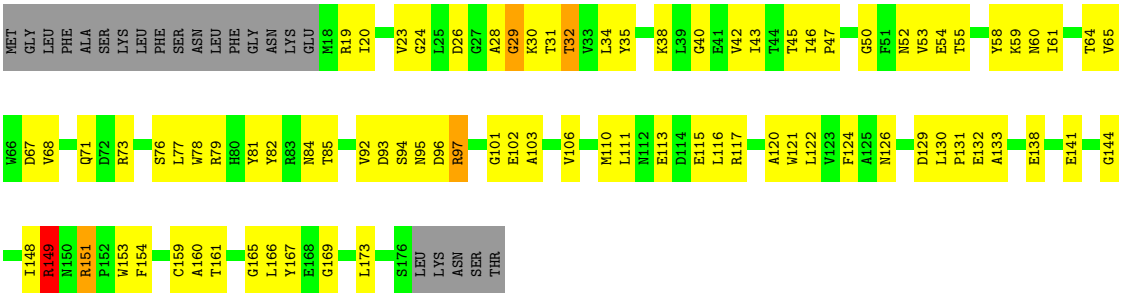
• Molecule 6: ADP-ribosylation factor 1

Chain 3-M:



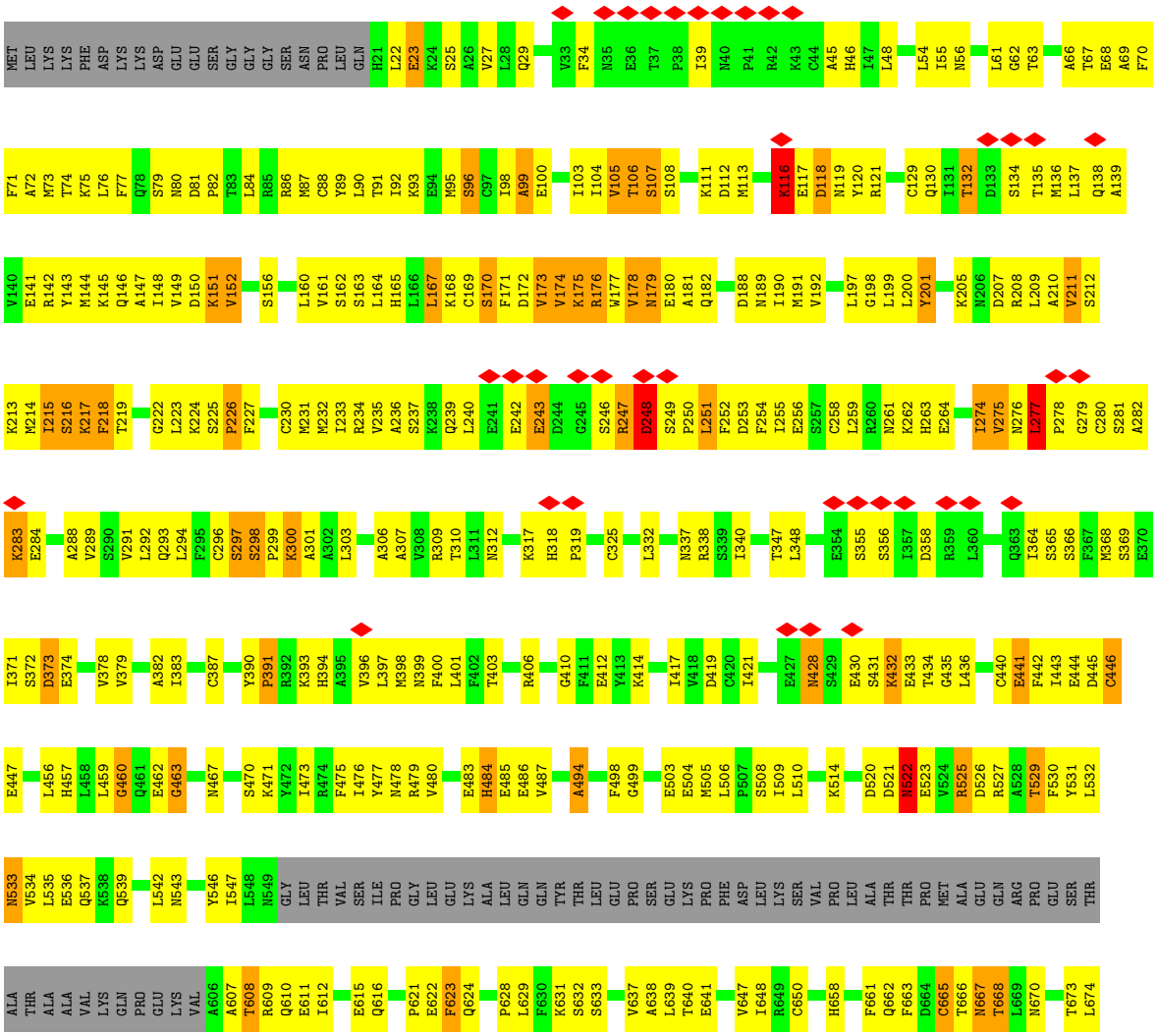
• Molecule 6: ADP-ribosylation factor 1

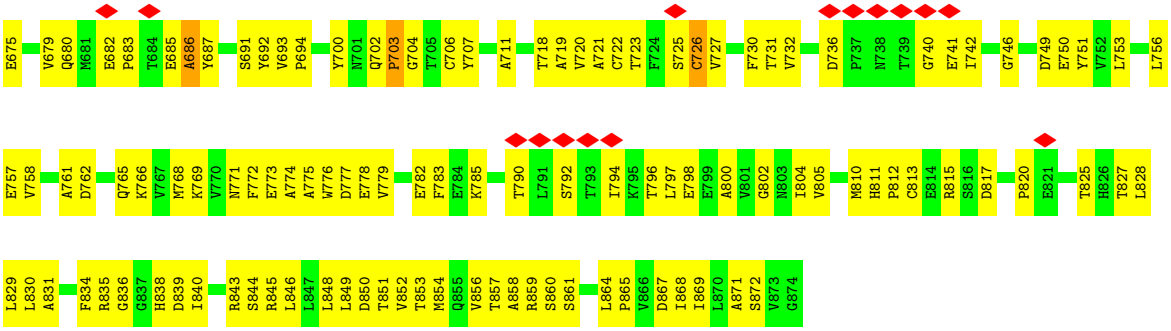
Chain 3-J:



• Molecule 7: Coatomer subunit gamma-1

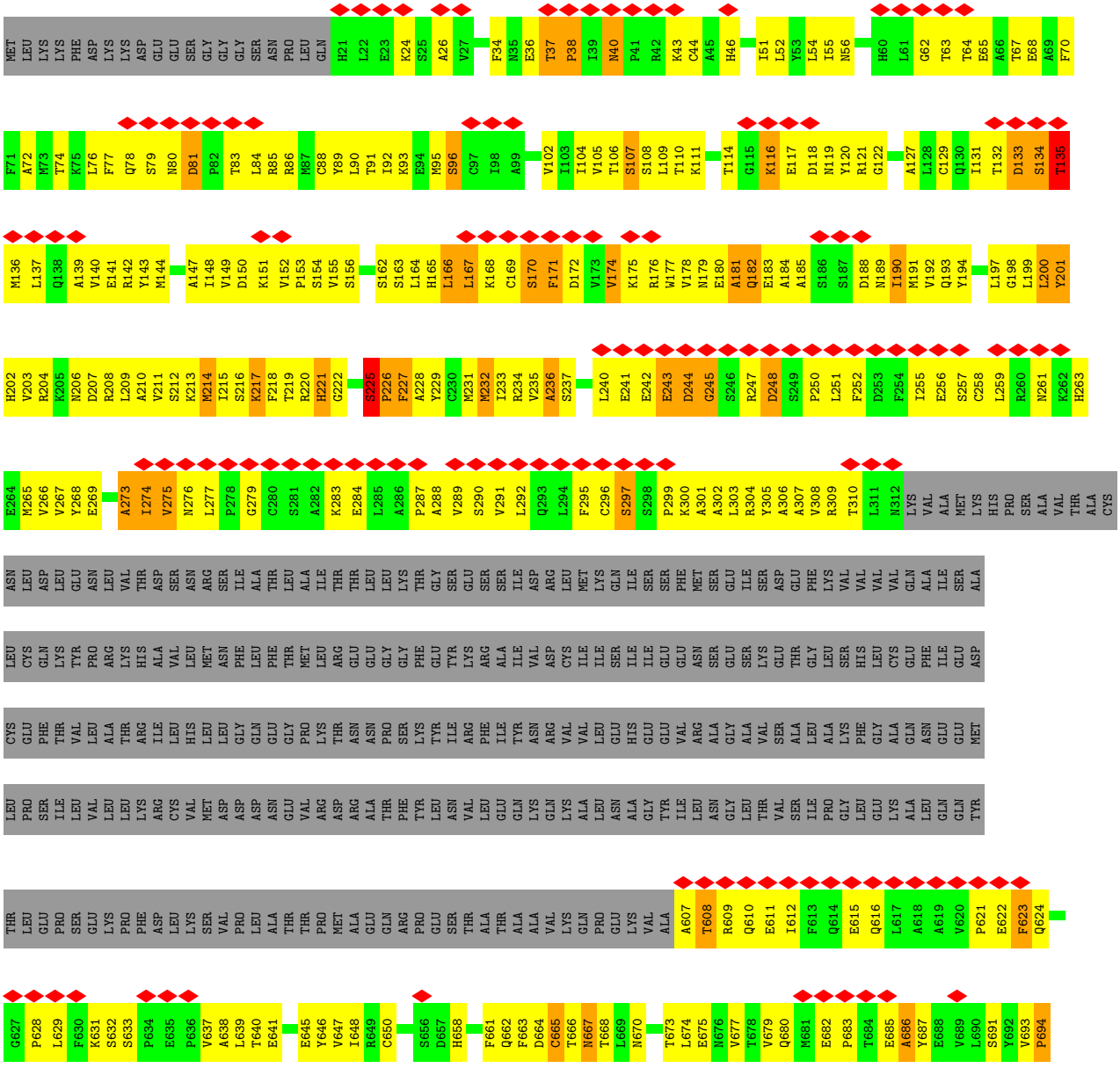
Chain 1-G:

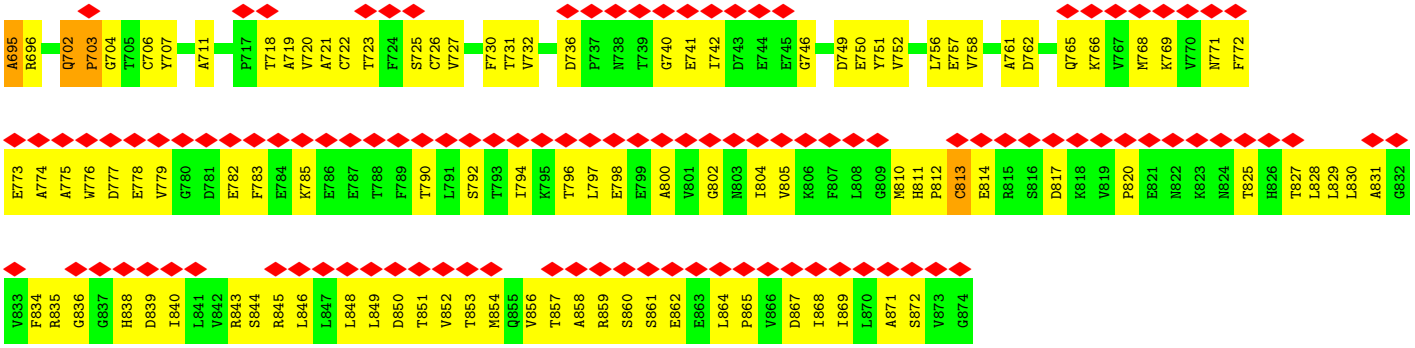




• Molecule 7: Coatomer subunit gamma-1

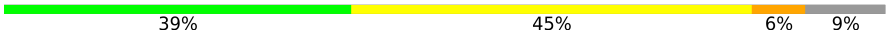
Chain 1-K:

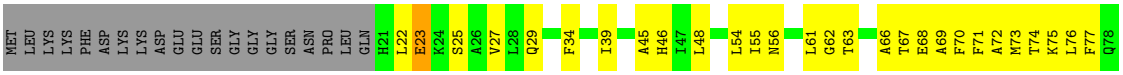


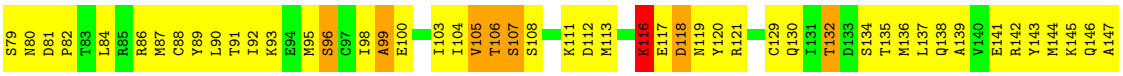


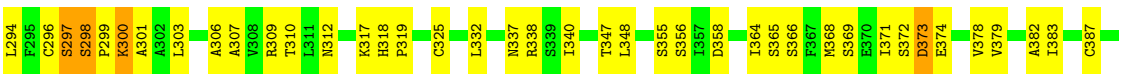
• Molecule 7: Coatomer subunit gamma-1

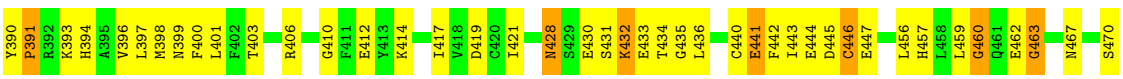
Chain 2-G:

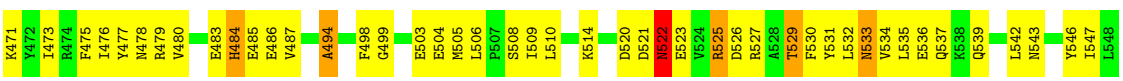


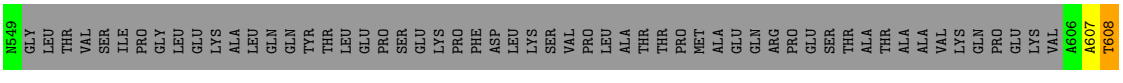


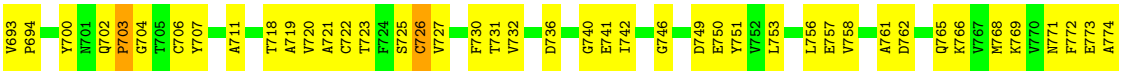


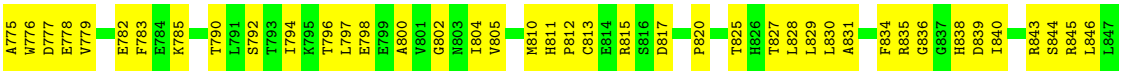






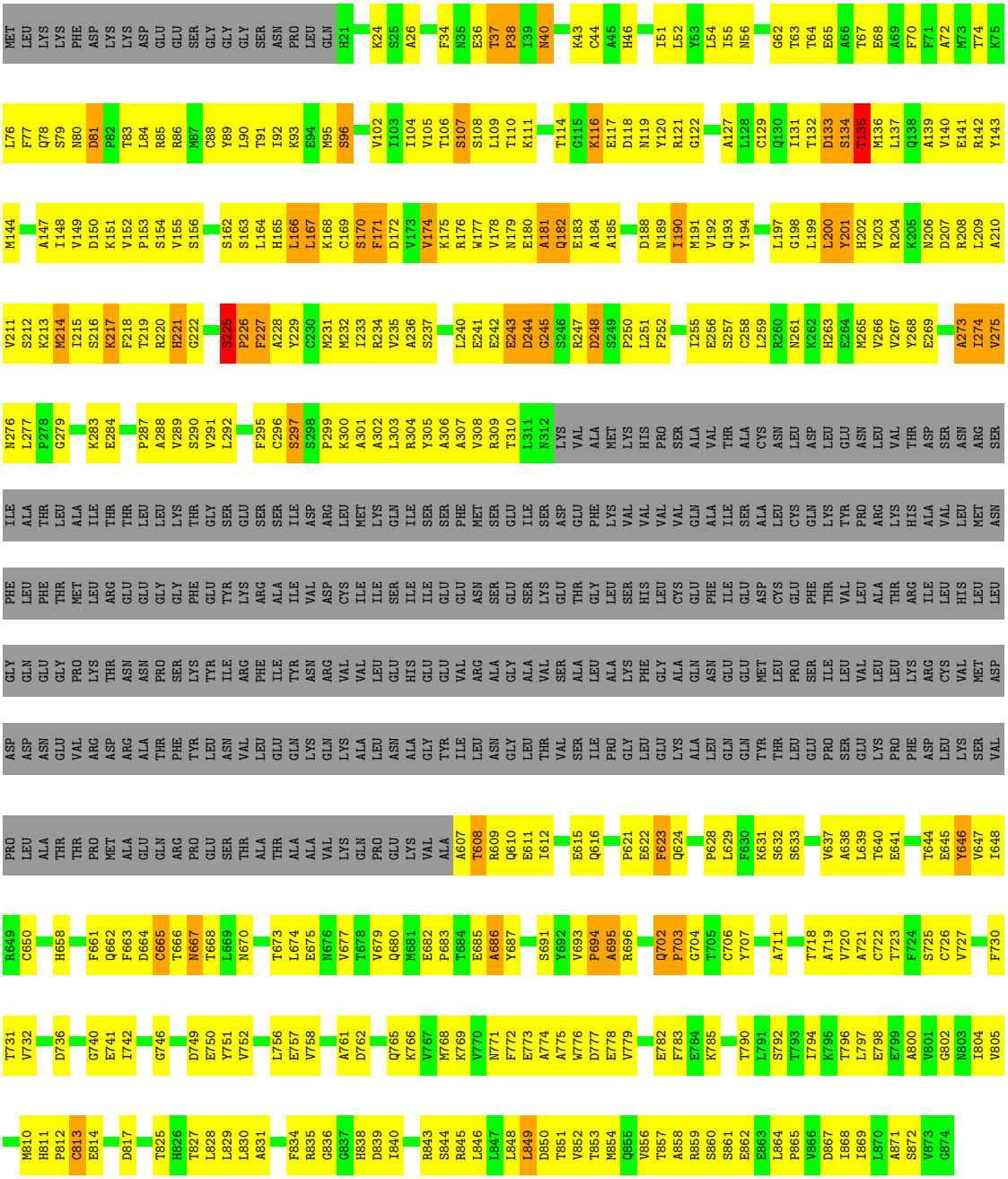






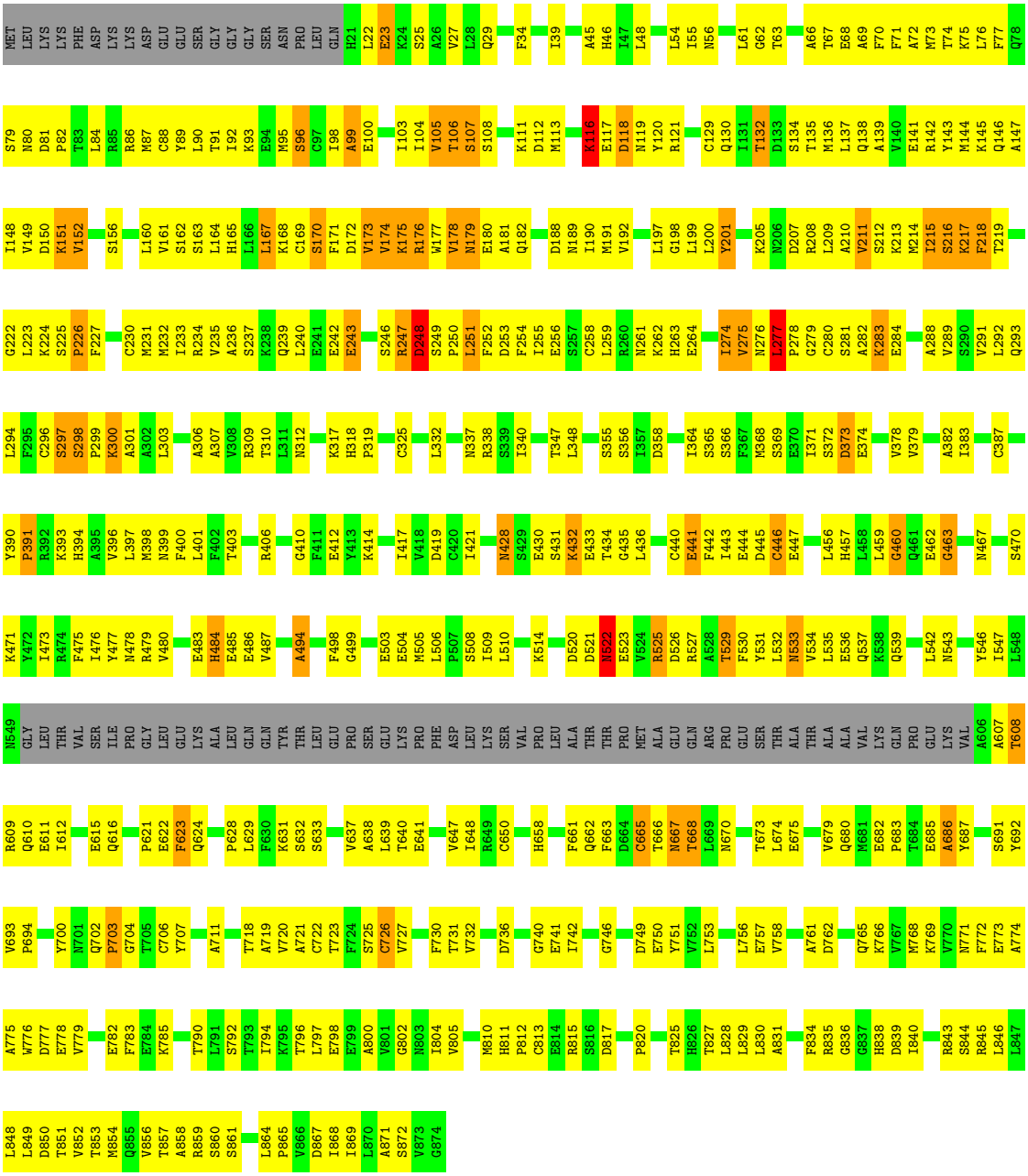
• Molecule 7: Coatomer subunit gamma-1

Chain 2-K:



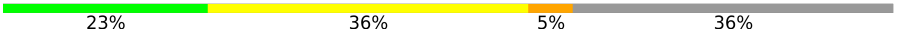
• Molecule 7: Coatomer subunit gamma-1

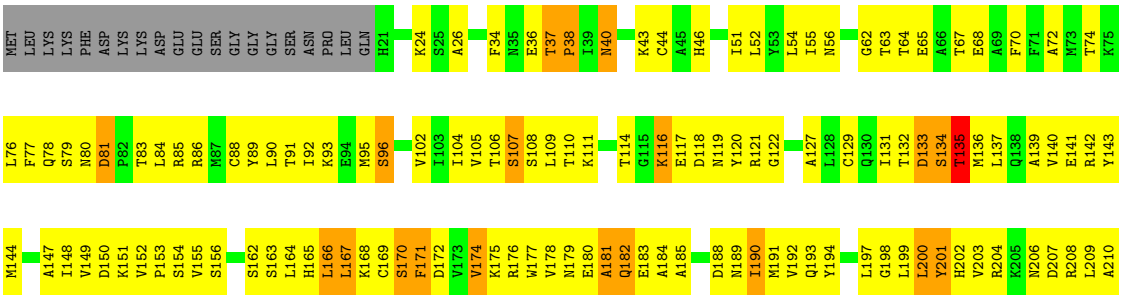
Chain 3-G:

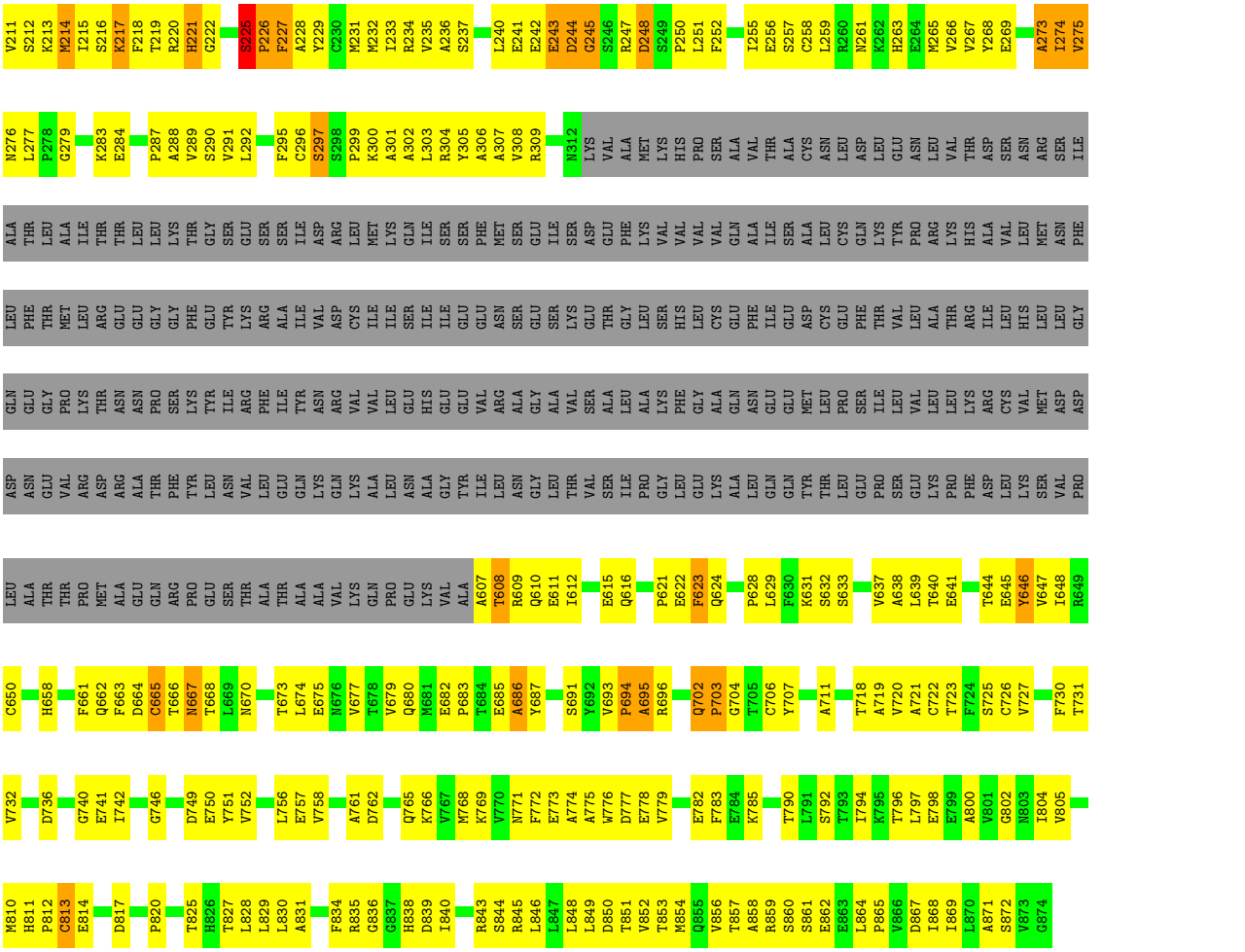


• Molecule 7: Coatomer subunit gamma-1

Chain 3-K:

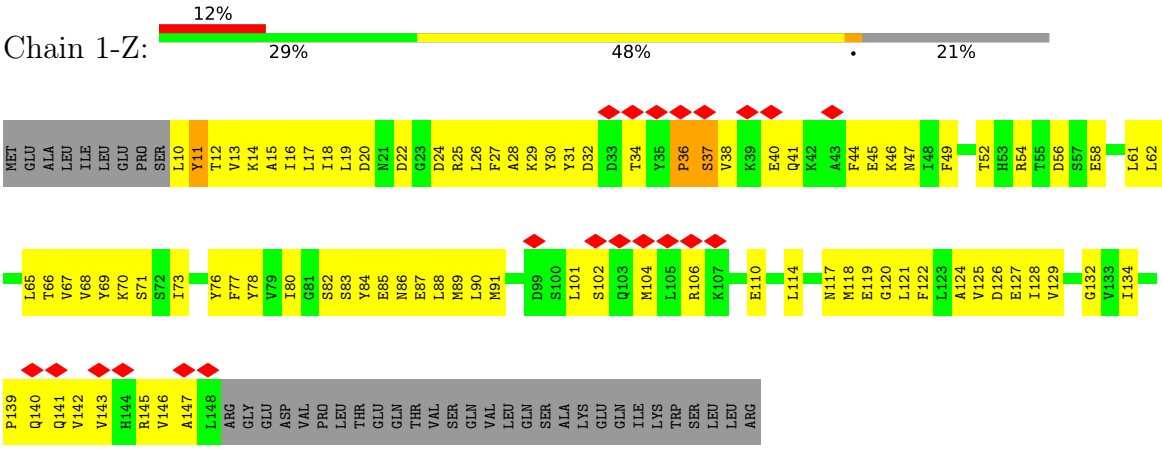






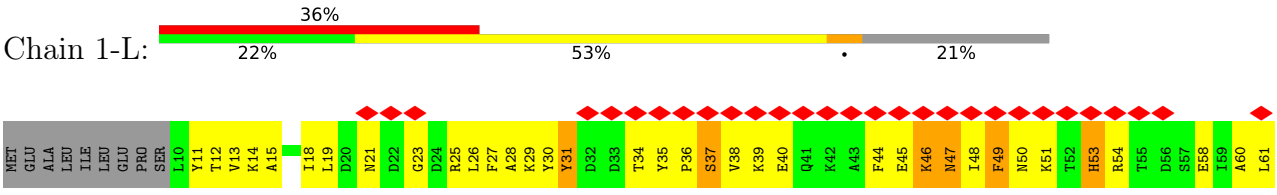
• Molecule 8: Coatomer subunit zeta-1

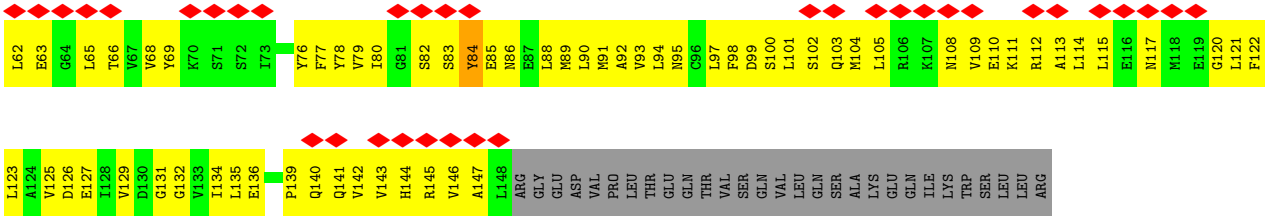
Chain 1-Z:



• Molecule 8: Coatomer subunit zeta-1

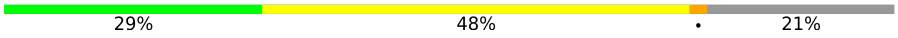
Chain 1-L:

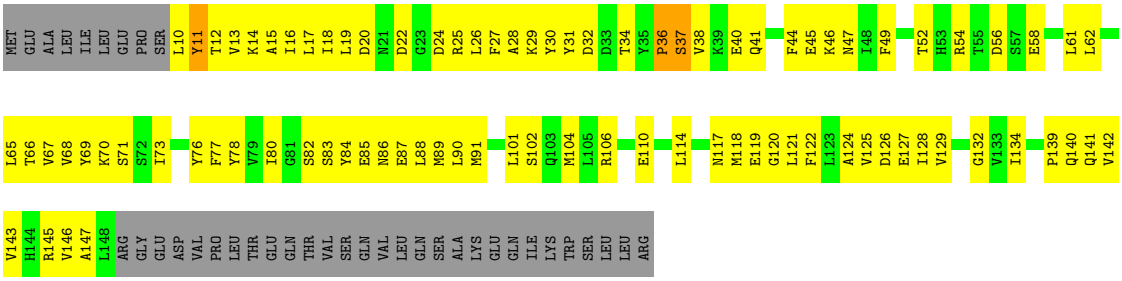




• Molecule 8: Coatomer subunit zeta-1

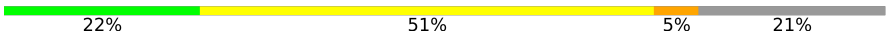
Chain 2-Z:

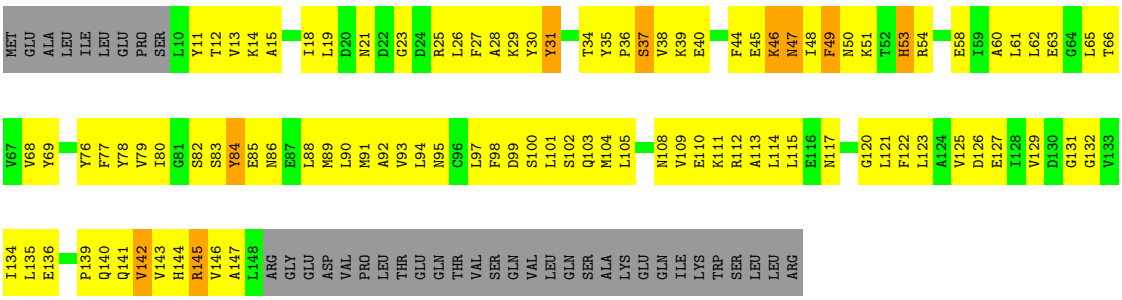




• Molecule 8: Coatomer subunit zeta-1

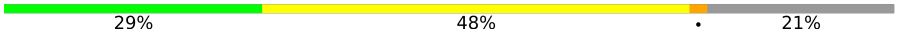
Chain 2-L:

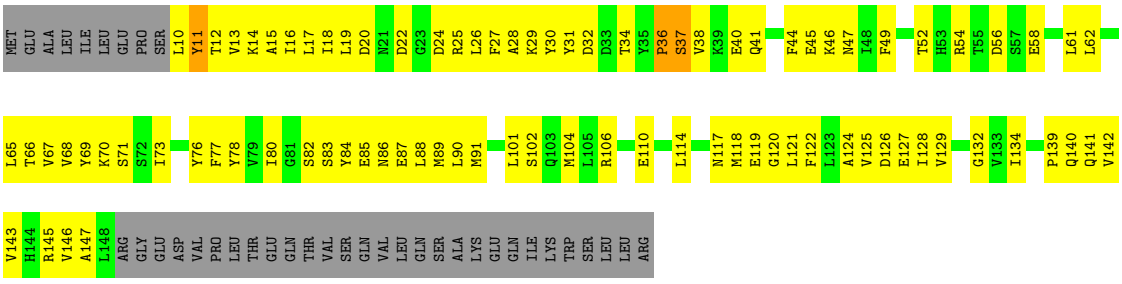




• Molecule 8: Coatomer subunit zeta-1

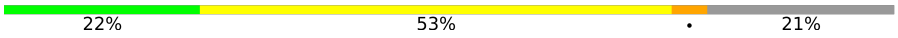
Chain 3-Z:

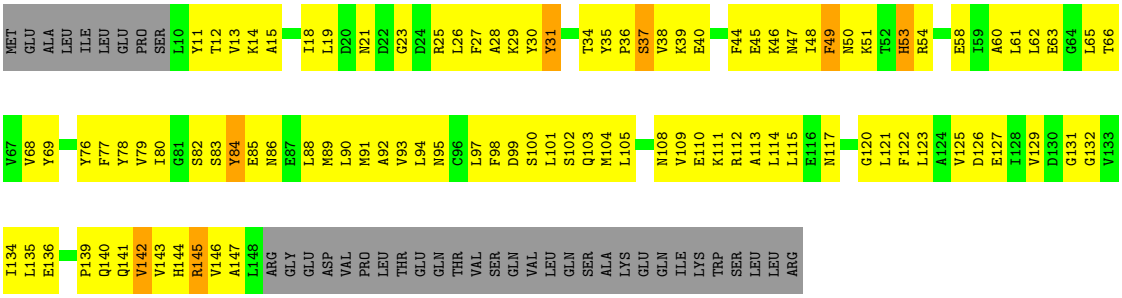




• Molecule 8: Coatomer subunit zeta-1

Chain 3-L:




MET GLU ALA LEU ILE LEU GLU PRO SER L10 Y11 T12 V13 K14 A15 I18 L19 D20 N21 D22 G23 D24 R25 L26 F27 A28 K29 Y30 Y31 T34 Y35 P36 S37 V38 K39 E40 F44 E45 K46 N47 I48 F49 N50 K51 T52 H53 R54 E58 I59 A60 L61 L62 E63 G64 L65 T66
V67 V68 Y69 Y76 F77 Y78 V79 I80 G81 S82 S83 Y84 E85 N86 E87 L88 M89 L90 M91 A92 V93 L94 N95 C96 L97 F98 D99 S100 L101 S102 Q103 M104 L105 N108 V109 E110 K111 R112 A113 L114 L115 E116 N117 G120 L121 F122 L123 A124 V125 D126 E127 I128 V129 D130 G131 G132 V133
I134 L135 E136 P139 Q140 Q141 V142 V143 H144 R145 V146 A147 L148 ARG GLY GLU ASP VAL PRO LEU THR GLU GLN THR VAL SER GLN VAL LEU GLN SER ALA LYS GLU GLN ILE LYS TRP SER LEU LEU ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	2547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; CTF-determination for each individual tilt image was performed using CTFFIND4. Strip-based CTF-correction and tomogram reconstruction was performed in Imod.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.153	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	377.36, 377.36, 377.36	wwPDB
Map dimensions	212, 212, 212	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.78, 1.78, 1.78	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	1-A	2.46	257/4501 (5.7%)	2.74	418/5623 (7.4%)
1	2-A	2.46	257/4501 (5.7%)	2.74	418/5623 (7.4%)
1	3-A	2.46	257/4501 (5.7%)	2.74	418/5623 (7.4%)
2	1-E	1.55	0/1168	1.36	2/1457 (0.1%)
2	2-E	1.55	0/1168	1.36	2/1457 (0.1%)
2	3-E	1.55	0/1168	1.36	2/1457 (0.1%)
3	1-B	3.07	370/3193 (11.6%)	2.83	293/3983 (7.4%)
3	1-N	3.02	250/2275 (11.0%)	2.62	173/2837 (6.1%)
3	2-B	3.07	370/3193 (11.6%)	2.83	293/3983 (7.4%)
3	2-N	3.02	250/2275 (11.0%)	2.62	173/2837 (6.1%)
3	3-B	3.07	370/3193 (11.6%)	2.83	293/3983 (7.4%)
3	3-N	3.02	250/2275 (11.0%)	2.62	173/2837 (6.1%)
4	1-C	3.10	357/3370 (10.6%)	2.83	368/4211 (8.7%)
4	1-H	3.18	328/2883 (11.4%)	2.84	321/3602 (8.9%)
4	2-C	3.10	357/3370 (10.6%)	2.83	368/4211 (8.7%)
4	2-H	3.18	328/2883 (11.4%)	2.84	321/3602 (8.9%)
4	3-C	3.10	357/3370 (10.6%)	2.83	368/4211 (8.7%)
4	3-H	3.18	328/2883 (11.4%)	2.84	321/3602 (8.9%)
5	1-D	3.02	75/704 (10.7%)	2.96	74/877 (8.4%)
5	1-I	3.02	74/704 (10.5%)	2.96	74/877 (8.4%)
5	2-D	3.02	75/704 (10.7%)	2.96	74/877 (8.4%)
5	2-I	3.02	74/704 (10.5%)	2.96	74/877 (8.4%)
5	3-D	3.02	75/704 (10.7%)	2.96	74/877 (8.4%)
5	3-I	3.02	74/704 (10.5%)	2.96	74/877 (8.4%)
6	1-F	2.68	40/634 (6.3%)	2.99	72/791 (9.1%)
6	1-J	2.68	39/634 (6.2%)	3.02	72/791 (9.1%)
6	1-M	2.72	49/634 (7.7%)	2.79	57/791 (7.2%)
6	1-R	3.25	87/634 (13.7%)	2.99	72/791 (9.1%)
6	2-F	2.68	40/634 (6.3%)	2.99	72/791 (9.1%)
6	2-J	2.68	39/634 (6.2%)	3.02	72/791 (9.1%)
6	2-M	2.72	49/634 (7.7%)	2.79	57/791 (7.2%)
6	2-R	3.25	87/634 (13.7%)	2.99	72/791 (9.1%)
6	3-F	2.68	40/634 (6.3%)	2.99	72/791 (9.1%)
6	3-J	2.68	39/634 (6.2%)	3.02	72/791 (9.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	3-M	2.72	49/634 (7.7%)	2.79	57/791 (7.2%)
6	3-R	3.25	87/634 (13.7%)	2.99	72/791 (9.1%)
7	1-G	2.91	307/3188 (9.6%)	2.97	350/3982 (8.8%)
7	1-K	3.07	248/2237 (11.1%)	3.03	269/2793 (9.6%)
7	2-G	2.91	307/3188 (9.6%)	2.97	350/3982 (8.8%)
7	2-K	3.07	248/2237 (11.1%)	3.03	269/2793 (9.6%)
7	3-G	2.91	307/3188 (9.6%)	2.97	350/3982 (8.8%)
7	3-K	3.07	248/2237 (11.1%)	3.03	269/2793 (9.6%)
8	1-L	3.63	106/554 (19.1%)	2.94	62/691 (9.0%)
8	1-Z	3.32	84/554 (15.2%)	2.78	59/691 (8.5%)
8	2-L	3.63	106/554 (19.1%)	2.94	62/691 (9.0%)
8	2-Z	3.32	84/554 (15.2%)	2.78	59/691 (8.5%)
8	3-L	3.63	106/554 (19.1%)	2.94	62/691 (9.0%)
8	3-Z	3.32	84/554 (15.2%)	2.78	59/691 (8.5%)
All	All	2.92	8013/83601 (9.6%)	2.81	8208/104364 (7.9%)

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
3	1-B	0	3
3	2-B	0	3
3	3-B	0	3
7	2-G	0	1
7	2-K	0	1
All	All	0	11

All (8013) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-G	215	ILE	CA-C	-13.79	1.35	1.52
7	2-G	215	ILE	CA-C	-13.79	1.35	1.52
7	3-G	215	ILE	CA-C	-13.79	1.35	1.52
1	1-A	595	THR	CA-C	-13.67	1.43	1.52
1	2-A	595	THR	CA-C	-13.67	1.43	1.52
1	3-A	595	THR	CA-C	-13.67	1.43	1.52
4	1-H	572	ARG	CA-C	-13.52	1.35	1.52
4	2-H	572	ARG	CA-C	-13.52	1.35	1.52
4	3-H	572	ARG	CA-C	-13.52	1.35	1.52
4	1-C	572	ARG	CA-C	-13.50	1.35	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-C	572	ARG	CA-C	-13.50	1.35	1.52
4	3-C	572	ARG	CA-C	-13.50	1.35	1.52
6	1-R	35	TYR	CA-C	-13.48	1.33	1.52
6	2-R	35	TYR	CA-C	-13.48	1.33	1.52
6	3-R	35	TYR	CA-C	-13.48	1.33	1.52
4	1-H	416	LYS	CA-C	-13.07	1.37	1.52
4	2-H	416	LYS	CA-C	-13.07	1.37	1.52
4	3-H	416	LYS	CA-C	-13.07	1.37	1.52
4	1-C	416	LYS	CA-C	-13.05	1.37	1.52
4	2-C	416	LYS	CA-C	-13.05	1.37	1.52
4	3-C	416	LYS	CA-C	-13.05	1.37	1.52
4	1-H	378	TYR	CA-C	-12.99	1.37	1.52
4	2-H	378	TYR	CA-C	-12.99	1.37	1.52
4	3-H	378	TYR	CA-C	-12.99	1.37	1.52
4	1-C	378	TYR	CA-C	-12.98	1.37	1.52
4	2-C	378	TYR	CA-C	-12.98	1.37	1.52
4	3-C	378	TYR	CA-C	-12.98	1.37	1.52
7	1-K	211	VAL	CA-C	-12.80	1.36	1.52
7	2-K	211	VAL	CA-C	-12.80	1.36	1.52
7	3-K	211	VAL	CA-C	-12.80	1.36	1.52
4	1-H	384	ARG	CA-C	-12.80	1.37	1.52
4	2-H	384	ARG	CA-C	-12.80	1.37	1.52
4	3-H	384	ARG	CA-C	-12.80	1.37	1.52
4	1-C	384	ARG	CA-C	-12.80	1.37	1.52
4	2-C	384	ARG	CA-C	-12.80	1.37	1.52
4	3-C	384	ARG	CA-C	-12.80	1.37	1.52
5	1-D	55	ARG	CA-C	-12.67	1.36	1.52
5	2-D	55	ARG	CA-C	-12.67	1.36	1.52
5	3-D	55	ARG	CA-C	-12.67	1.36	1.52
5	1-I	55	ARG	CA-C	-12.63	1.36	1.52
5	2-I	55	ARG	CA-C	-12.63	1.36	1.52
5	3-I	55	ARG	CA-C	-12.63	1.36	1.52
7	1-G	839	ASP	CA-C	-12.46	1.36	1.52
7	2-G	839	ASP	CA-C	-12.46	1.36	1.52
7	3-G	839	ASP	CA-C	-12.46	1.36	1.52
7	1-K	839	ASP	CA-C	-12.35	1.36	1.52
7	2-K	839	ASP	CA-C	-12.35	1.36	1.52
7	3-K	839	ASP	CA-C	-12.35	1.36	1.52
4	1-H	377	ILE	CA-C	-12.27	1.38	1.52
4	2-H	377	ILE	CA-C	-12.27	1.38	1.52
4	3-H	377	ILE	CA-C	-12.27	1.38	1.52
7	1-K	214	MET	CA-C	-12.26	1.36	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-K	214	MET	CA-C	-12.26	1.36	1.52
7	3-K	214	MET	CA-C	-12.26	1.36	1.52
4	1-C	377	ILE	CA-C	-12.23	1.38	1.52
4	2-C	377	ILE	CA-C	-12.23	1.38	1.52
4	3-C	377	ILE	CA-C	-12.23	1.38	1.52
3	1-B	762	ASN	CA-C	-12.04	1.37	1.53
3	2-B	762	ASN	CA-C	-12.04	1.37	1.53
3	3-B	762	ASN	CA-C	-12.04	1.37	1.53
3	1-B	126	HIS	CA-C	-11.77	1.38	1.52
3	2-B	126	HIS	CA-C	-11.77	1.38	1.52
3	3-B	126	HIS	CA-C	-11.77	1.38	1.52
3	1-N	126	HIS	CA-C	-11.76	1.38	1.52
3	2-N	126	HIS	CA-C	-11.76	1.38	1.52
3	3-N	126	HIS	CA-C	-11.76	1.38	1.52
4	1-H	449	PHE	CA-C	-11.66	1.38	1.52
4	2-H	449	PHE	CA-C	-11.66	1.38	1.52
4	3-H	449	PHE	CA-C	-11.66	1.38	1.52
4	1-C	449	PHE	CA-C	-11.58	1.39	1.52
4	2-C	449	PHE	CA-C	-11.58	1.39	1.52
4	3-C	449	PHE	CA-C	-11.58	1.39	1.52
6	1-R	109	ARG	CA-C	-11.58	1.36	1.52
6	2-R	109	ARG	CA-C	-11.58	1.36	1.52
6	3-R	109	ARG	CA-C	-11.58	1.36	1.52
7	1-K	235	VAL	N-CA	-11.32	1.33	1.46
7	2-K	235	VAL	N-CA	-11.32	1.33	1.46
7	3-K	235	VAL	N-CA	-11.32	1.33	1.46
1	1-A	679	GLU	CA-C	-11.32	1.38	1.52
1	2-A	679	GLU	CA-C	-11.32	1.38	1.52
1	3-A	679	GLU	CA-C	-11.32	1.38	1.52
4	1-H	223	GLN	CA-C	-11.19	1.39	1.52
4	2-H	223	GLN	CA-C	-11.19	1.39	1.52
4	3-H	223	GLN	CA-C	-11.19	1.39	1.52
7	1-G	442	PHE	CA-C	-11.18	1.38	1.52
7	2-G	442	PHE	CA-C	-11.18	1.38	1.52
7	3-G	442	PHE	CA-C	-11.18	1.38	1.52
8	1-Z	19	LEU	CA-C	-11.18	1.39	1.52
8	2-Z	19	LEU	CA-C	-11.18	1.39	1.52
8	3-Z	19	LEU	CA-C	-11.18	1.39	1.52
5	1-D	56	TYR	CA-C	-11.16	1.39	1.52
5	2-D	56	TYR	CA-C	-11.16	1.39	1.52
5	3-D	56	TYR	CA-C	-11.16	1.39	1.52
4	1-C	223	GLN	CA-C	-11.14	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-C	223	GLN	CA-C	-11.14	1.39	1.52
4	3-C	223	GLN	CA-C	-11.14	1.39	1.52
4	1-C	8	LYS	CA-C	-11.14	1.39	1.52
4	2-C	8	LYS	CA-C	-11.14	1.39	1.52
4	3-C	8	LYS	CA-C	-11.14	1.39	1.52
4	1-H	8	LYS	CA-C	-11.13	1.39	1.52
5	1-I	56	TYR	CA-C	-11.13	1.39	1.52
4	2-H	8	LYS	CA-C	-11.13	1.39	1.52
5	2-I	56	TYR	CA-C	-11.13	1.39	1.52
4	3-H	8	LYS	CA-C	-11.13	1.39	1.52
5	3-I	56	TYR	CA-C	-11.13	1.39	1.52
4	1-H	573	LEU	CA-C	-10.95	1.39	1.52
4	2-H	573	LEU	CA-C	-10.95	1.39	1.52
4	3-H	573	LEU	CA-C	-10.95	1.39	1.52
3	1-N	378	GLU	CA-C	-10.92	1.38	1.52
3	2-N	378	GLU	CA-C	-10.92	1.38	1.52
3	3-N	378	GLU	CA-C	-10.92	1.38	1.52
3	1-B	378	GLU	CA-C	-10.92	1.38	1.52
3	2-B	378	GLU	CA-C	-10.92	1.38	1.52
3	3-B	378	GLU	CA-C	-10.92	1.38	1.52
7	1-K	165	HIS	CA-C	-10.90	1.38	1.52
7	2-K	165	HIS	CA-C	-10.90	1.38	1.52
7	3-K	165	HIS	CA-C	-10.90	1.38	1.52
4	1-C	573	LEU	CA-C	-10.89	1.39	1.52
4	2-C	573	LEU	CA-C	-10.89	1.39	1.52
4	3-C	573	LEU	CA-C	-10.89	1.39	1.52
3	1-B	938	VAL	CA-C	-10.82	1.39	1.52
3	2-B	938	VAL	CA-C	-10.82	1.39	1.52
3	3-B	938	VAL	CA-C	-10.82	1.39	1.52
7	1-K	771	ASN	CA-C	-10.76	1.42	1.53
7	2-K	771	ASN	CA-C	-10.76	1.42	1.53
7	3-K	771	ASN	CA-C	-10.76	1.42	1.53
7	1-G	771	ASN	CA-C	-10.71	1.42	1.53
7	2-G	771	ASN	CA-C	-10.71	1.42	1.53
7	3-G	771	ASN	CA-C	-10.71	1.42	1.53
6	1-J	148	ILE	CA-C	-10.69	1.43	1.52
6	2-J	148	ILE	CA-C	-10.69	1.43	1.52
6	3-J	148	ILE	CA-C	-10.69	1.43	1.52
4	1-C	415	PHE	CA-C	-10.69	1.39	1.52
4	2-C	415	PHE	CA-C	-10.69	1.39	1.52
4	3-C	415	PHE	CA-C	-10.69	1.39	1.52
8	1-L	49	PHE	CA-C	-10.66	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2-L	49	PHE	CA-C	-10.66	1.39	1.52
8	3-L	49	PHE	CA-C	-10.66	1.39	1.52
1	1-A	612	LEU	N-CA	-10.63	1.33	1.46
7	1-G	112	ASP	CA-C	-10.63	1.39	1.52
1	2-A	612	LEU	N-CA	-10.63	1.33	1.46
7	2-G	112	ASP	CA-C	-10.63	1.39	1.52
1	3-A	612	LEU	N-CA	-10.63	1.33	1.46
7	3-G	112	ASP	CA-C	-10.63	1.39	1.52
6	1-F	148	ILE	CA-C	-10.62	1.43	1.52
6	2-F	148	ILE	CA-C	-10.62	1.43	1.52
6	3-F	148	ILE	CA-C	-10.62	1.43	1.52
3	1-B	440	ARG	CA-C	-10.58	1.39	1.52
3	2-B	440	ARG	CA-C	-10.58	1.39	1.52
3	3-B	440	ARG	CA-C	-10.58	1.39	1.52
6	1-R	105	GLU	CA-C	-10.58	1.39	1.52
6	2-R	105	GLU	CA-C	-10.58	1.39	1.52
6	3-R	105	GLU	CA-C	-10.58	1.39	1.52
1	1-A	612	LEU	CA-C	-10.58	1.39	1.52
1	2-A	612	LEU	CA-C	-10.58	1.39	1.52
1	3-A	612	LEU	CA-C	-10.58	1.39	1.52
6	1-R	96	ASP	CA-C	-10.55	1.39	1.52
6	2-R	96	ASP	CA-C	-10.55	1.39	1.52
6	3-R	96	ASP	CA-C	-10.55	1.39	1.52
3	1-N	440	ARG	CA-C	-10.55	1.39	1.52
3	2-N	440	ARG	CA-C	-10.55	1.39	1.52
3	3-N	440	ARG	CA-C	-10.55	1.39	1.52
4	1-H	415	PHE	CA-C	-10.55	1.39	1.52
4	2-H	415	PHE	CA-C	-10.55	1.39	1.52
4	3-H	415	PHE	CA-C	-10.55	1.39	1.52
3	1-B	940	GLY	CA-C	-10.54	1.42	1.51
3	2-B	940	GLY	CA-C	-10.54	1.42	1.51
3	3-B	940	GLY	CA-C	-10.54	1.42	1.51
3	1-B	749	VAL	CA-C	-10.51	1.39	1.52
5	1-I	81	GLU	CA-C	-10.51	1.39	1.52
3	2-B	749	VAL	CA-C	-10.51	1.39	1.52
5	2-I	81	GLU	CA-C	-10.51	1.39	1.52
3	3-B	749	VAL	CA-C	-10.51	1.39	1.52
5	3-I	81	GLU	CA-C	-10.51	1.39	1.52
5	1-D	81	GLU	CA-C	-10.50	1.39	1.52
5	2-D	81	GLU	CA-C	-10.50	1.39	1.52
5	3-D	81	GLU	CA-C	-10.50	1.39	1.52
3	1-B	940	GLY	N-CA	-10.48	1.34	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	940	GLY	N-CA	-10.48	1.34	1.45
3	3-B	940	GLY	N-CA	-10.48	1.34	1.45
3	1-B	783	LEU	CA-C	-10.46	1.39	1.52
3	2-B	783	LEU	CA-C	-10.46	1.39	1.52
3	3-B	783	LEU	CA-C	-10.46	1.39	1.52
3	1-B	799	ASN	CA-C	-10.42	1.40	1.52
3	2-B	799	ASN	CA-C	-10.42	1.40	1.52
3	3-B	799	ASN	CA-C	-10.42	1.40	1.52
4	1-H	470	TRP	CA-C	-10.40	1.40	1.52
4	2-H	470	TRP	CA-C	-10.40	1.40	1.52
4	3-H	470	TRP	CA-C	-10.40	1.40	1.52
4	1-C	470	TRP	CA-C	-10.37	1.40	1.52
4	2-C	470	TRP	CA-C	-10.37	1.40	1.52
4	3-C	470	TRP	CA-C	-10.37	1.40	1.52
1	1-A	242	VAL	CA-C	-10.34	1.44	1.52
1	2-A	242	VAL	CA-C	-10.34	1.44	1.52
1	3-A	242	VAL	CA-C	-10.34	1.44	1.52
6	1-R	90	PHE	CA-C	-10.30	1.40	1.52
6	2-R	90	PHE	CA-C	-10.30	1.40	1.52
6	3-R	90	PHE	CA-C	-10.30	1.40	1.52
4	1-H	213	ILE	CA-C	-10.29	1.40	1.52
4	2-H	213	ILE	CA-C	-10.29	1.40	1.52
4	3-H	213	ILE	CA-C	-10.29	1.40	1.52
4	1-C	213	ILE	CA-C	-10.26	1.40	1.52
4	2-C	213	ILE	CA-C	-10.26	1.40	1.52
4	3-C	213	ILE	CA-C	-10.26	1.40	1.52
4	1-H	314	ILE	CA-C	-10.24	1.39	1.52
4	2-H	314	ILE	CA-C	-10.24	1.39	1.52
4	3-H	314	ILE	CA-C	-10.24	1.39	1.52
6	1-R	110	MET	CA-C	-10.21	1.39	1.52
6	2-R	110	MET	CA-C	-10.21	1.39	1.52
6	3-R	110	MET	CA-C	-10.21	1.39	1.52
4	1-C	314	ILE	CA-C	-10.21	1.39	1.52
8	1-Z	15	ALA	CA-C	-10.21	1.40	1.52
4	1-H	367	VAL	CA-C	-10.21	1.39	1.52
4	2-C	314	ILE	CA-C	-10.21	1.39	1.52
8	2-Z	15	ALA	CA-C	-10.21	1.40	1.52
4	2-H	367	VAL	CA-C	-10.21	1.39	1.52
4	3-C	314	ILE	CA-C	-10.21	1.39	1.52
8	3-Z	15	ALA	CA-C	-10.21	1.40	1.52
4	3-H	367	VAL	CA-C	-10.21	1.39	1.52
4	1-C	367	VAL	CA-C	-10.19	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-C	367	VAL	CA-C	-10.19	1.39	1.52
4	3-C	367	VAL	CA-C	-10.19	1.39	1.52
7	1-G	174	VAL	CA-C	-10.18	1.39	1.52
7	2-G	174	VAL	CA-C	-10.18	1.39	1.52
7	3-G	174	VAL	CA-C	-10.18	1.39	1.52
4	1-C	529	TRP	CA-C	-10.16	1.40	1.52
4	2-C	529	TRP	CA-C	-10.16	1.40	1.52
4	3-C	529	TRP	CA-C	-10.16	1.40	1.52
1	1-A	243	ASP	CA-C	-10.16	1.40	1.52
1	2-A	243	ASP	CA-C	-10.16	1.40	1.52
1	3-A	243	ASP	CA-C	-10.16	1.40	1.52
3	1-N	300	TYR	CA-C	-10.14	1.40	1.52
3	2-N	300	TYR	CA-C	-10.14	1.40	1.52
3	3-N	300	TYR	CA-C	-10.14	1.40	1.52
4	1-C	553	THR	CA-C	-10.12	1.40	1.52
4	2-C	553	THR	CA-C	-10.12	1.40	1.52
4	3-C	553	THR	CA-C	-10.12	1.40	1.52
4	1-H	553	THR	CA-C	-10.12	1.40	1.52
4	2-H	553	THR	CA-C	-10.12	1.40	1.52
4	3-H	553	THR	CA-C	-10.12	1.40	1.52
4	1-H	529	TRP	CA-C	-10.10	1.40	1.52
4	2-H	529	TRP	CA-C	-10.10	1.40	1.52
4	3-H	529	TRP	CA-C	-10.10	1.40	1.52
6	1-R	107	MET	CA-C	-10.09	1.39	1.52
6	2-R	107	MET	CA-C	-10.09	1.39	1.52
6	3-R	107	MET	CA-C	-10.09	1.39	1.52
4	1-H	545	TYR	CA-C	-10.08	1.40	1.52
4	2-H	545	TYR	CA-C	-10.08	1.40	1.52
4	3-H	545	TYR	CA-C	-10.08	1.40	1.52
3	1-B	941	HIS	CA-C	-10.07	1.40	1.52
3	2-B	941	HIS	CA-C	-10.07	1.40	1.52
3	3-B	941	HIS	CA-C	-10.07	1.40	1.52
3	1-N	317	LEU	CA-C	-10.07	1.39	1.52
3	2-N	317	LEU	CA-C	-10.07	1.39	1.52
3	3-N	317	LEU	CA-C	-10.07	1.39	1.52
7	1-G	774	ALA	N-CA	-10.06	1.34	1.46
7	2-G	774	ALA	N-CA	-10.06	1.34	1.46
7	3-G	774	ALA	N-CA	-10.06	1.34	1.46
3	1-N	375	LEU	CA-C	-10.05	1.39	1.52
3	2-N	375	LEU	CA-C	-10.05	1.39	1.52
3	3-N	375	LEU	CA-C	-10.05	1.39	1.52
1	1-A	600	LYS	CA-C	-10.04	1.38	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	375	LEU	CA-C	-10.04	1.39	1.52
1	2-A	600	LYS	CA-C	-10.04	1.38	1.52
3	2-B	375	LEU	CA-C	-10.04	1.39	1.52
1	3-A	600	LYS	CA-C	-10.04	1.38	1.52
3	3-B	375	LEU	CA-C	-10.04	1.39	1.52
4	1-C	545	TYR	CA-C	-10.03	1.40	1.52
8	1-L	65	LEU	CA-C	-10.03	1.40	1.52
4	2-C	545	TYR	CA-C	-10.03	1.40	1.52
8	2-L	65	LEU	CA-C	-10.03	1.40	1.52
4	3-C	545	TYR	CA-C	-10.03	1.40	1.52
8	3-L	65	LEU	CA-C	-10.03	1.40	1.52
3	1-B	300	TYR	CA-C	-10.03	1.40	1.52
3	2-B	300	TYR	CA-C	-10.03	1.40	1.52
3	3-B	300	TYR	CA-C	-10.03	1.40	1.52
3	1-B	317	LEU	CA-C	-10.02	1.39	1.52
8	1-Z	61	LEU	CA-C	-10.02	1.40	1.52
3	2-B	317	LEU	CA-C	-10.02	1.39	1.52
8	2-Z	61	LEU	CA-C	-10.02	1.40	1.52
3	3-B	317	LEU	CA-C	-10.02	1.39	1.52
8	3-Z	61	LEU	CA-C	-10.02	1.40	1.52
8	1-L	142	VAL	CA-C	-10.01	1.40	1.52
8	2-L	142	VAL	CA-C	-10.01	1.40	1.52
8	3-L	142	VAL	CA-C	-10.01	1.40	1.52
7	1-G	693	VAL	CA-C	-9.99	1.42	1.52
7	2-G	693	VAL	CA-C	-9.99	1.42	1.52
7	3-G	693	VAL	CA-C	-9.99	1.42	1.52
7	1-K	774	ALA	N-CA	-9.95	1.34	1.46
7	2-K	774	ALA	N-CA	-9.95	1.34	1.46
7	3-K	774	ALA	N-CA	-9.95	1.34	1.46
8	1-Z	65	LEU	CA-C	-9.94	1.40	1.52
8	2-Z	65	LEU	CA-C	-9.94	1.40	1.52
8	3-Z	65	LEU	CA-C	-9.94	1.40	1.52
3	1-B	753	ASP	CA-C	-9.94	1.40	1.52
3	2-B	753	ASP	CA-C	-9.94	1.40	1.52
3	3-B	753	ASP	CA-C	-9.94	1.40	1.52
7	1-K	234	ARG	CA-C	-9.93	1.39	1.52
7	2-K	234	ARG	CA-C	-9.93	1.39	1.52
7	3-K	234	ARG	CA-C	-9.93	1.39	1.52
3	1-B	379	VAL	CA-C	-9.93	1.40	1.52
3	2-B	379	VAL	CA-C	-9.93	1.40	1.52
3	3-B	379	VAL	CA-C	-9.93	1.40	1.52
4	1-H	201	TYR	CA-C	-9.87	1.40	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-H	201	TYR	CA-C	-9.87	1.40	1.52
4	3-H	201	TYR	CA-C	-9.87	1.40	1.52
4	1-C	535	ILE	CA-C	-9.86	1.40	1.52
4	2-C	535	ILE	CA-C	-9.86	1.40	1.52
4	3-C	535	ILE	CA-C	-9.86	1.40	1.52
4	1-C	414	ILE	CA-C	-9.85	1.40	1.52
4	2-C	414	ILE	CA-C	-9.85	1.40	1.52
4	3-C	414	ILE	CA-C	-9.85	1.40	1.52
7	1-G	225	SER	CA-C	-9.85	1.41	1.52
7	2-G	225	SER	CA-C	-9.85	1.41	1.52
7	3-G	225	SER	CA-C	-9.85	1.41	1.52
4	1-C	201	TYR	CA-C	-9.84	1.40	1.52
4	2-C	201	TYR	CA-C	-9.84	1.40	1.52
4	3-C	201	TYR	CA-C	-9.84	1.40	1.52
3	1-N	349	LEU	CA-C	-9.84	1.40	1.52
4	1-H	414	ILE	CA-C	-9.84	1.40	1.52
3	2-N	349	LEU	CA-C	-9.84	1.40	1.52
4	2-H	414	ILE	CA-C	-9.84	1.40	1.52
3	3-N	349	LEU	CA-C	-9.84	1.40	1.52
4	3-H	414	ILE	CA-C	-9.84	1.40	1.52
4	1-H	535	ILE	CA-C	-9.84	1.40	1.52
4	2-H	535	ILE	CA-C	-9.84	1.40	1.52
4	3-H	535	ILE	CA-C	-9.84	1.40	1.52
3	1-B	349	LEU	CA-C	-9.81	1.40	1.52
3	2-B	349	LEU	CA-C	-9.81	1.40	1.52
3	3-B	349	LEU	CA-C	-9.81	1.40	1.52
4	1-H	221	CYS	CA-C	-9.80	1.40	1.52
4	2-H	221	CYS	CA-C	-9.80	1.40	1.52
4	3-H	221	CYS	CA-C	-9.80	1.40	1.52
4	1-C	571	ASN	CA-C	-9.80	1.40	1.53
4	2-C	571	ASN	CA-C	-9.80	1.40	1.53
4	3-C	571	ASN	CA-C	-9.80	1.40	1.53
7	1-K	217	LYS	CA-C	-9.78	1.40	1.52
7	2-K	217	LYS	CA-C	-9.78	1.40	1.52
7	3-K	217	LYS	CA-C	-9.78	1.40	1.52
1	1-A	660	ILE	CA-C	-9.77	1.38	1.52
1	2-A	660	ILE	CA-C	-9.77	1.38	1.52
1	3-A	660	ILE	CA-C	-9.77	1.38	1.52
3	1-B	909	ASN	CA-C	-9.76	1.41	1.52
3	2-B	909	ASN	CA-C	-9.76	1.41	1.52
3	3-B	909	ASN	CA-C	-9.76	1.41	1.52
4	1-C	221	CYS	CA-C	-9.76	1.40	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-C	221	CYS	CA-C	-9.76	1.40	1.52
4	3-C	221	CYS	CA-C	-9.76	1.40	1.52
8	1-L	26	LEU	CA-C	-9.74	1.40	1.52
8	2-L	26	LEU	CA-C	-9.74	1.40	1.52
8	3-L	26	LEU	CA-C	-9.74	1.40	1.52
3	1-B	792	LEU	CA-C	-9.74	1.41	1.53
3	2-B	792	LEU	CA-C	-9.74	1.41	1.53
3	3-B	792	LEU	CA-C	-9.74	1.41	1.53
8	1-Z	30	TYR	CA-C	-9.73	1.40	1.52
4	1-H	571	ASN	CA-C	-9.73	1.40	1.53
8	2-Z	30	TYR	CA-C	-9.73	1.40	1.52
4	2-H	571	ASN	CA-C	-9.73	1.40	1.53
8	3-Z	30	TYR	CA-C	-9.73	1.40	1.52
4	3-H	571	ASN	CA-C	-9.73	1.40	1.53
7	1-K	190	ILE	CA-C	-9.72	1.41	1.52
7	2-K	190	ILE	CA-C	-9.72	1.41	1.52
7	3-K	190	ILE	CA-C	-9.72	1.41	1.52
7	1-K	200	LEU	CA-C	-9.71	1.40	1.52
7	2-K	200	LEU	CA-C	-9.71	1.40	1.52
7	3-K	200	LEU	CA-C	-9.71	1.40	1.52
4	1-H	244	ILE	CA-C	-9.66	1.40	1.52
4	2-H	244	ILE	CA-C	-9.66	1.40	1.52
4	3-H	244	ILE	CA-C	-9.66	1.40	1.52
4	1-C	521	GLN	CA-C	-9.65	1.40	1.52
8	1-Z	19	LEU	N-CA	-9.65	1.33	1.45
7	1-K	773	GLU	CA-C	-9.65	1.40	1.52
4	2-C	521	GLN	CA-C	-9.65	1.40	1.52
8	2-Z	19	LEU	N-CA	-9.65	1.33	1.45
7	2-K	773	GLU	CA-C	-9.65	1.40	1.52
4	3-C	521	GLN	CA-C	-9.65	1.40	1.52
8	3-Z	19	LEU	N-CA	-9.65	1.33	1.45
7	3-K	773	GLU	CA-C	-9.65	1.40	1.52
7	1-G	773	GLU	CA-C	-9.64	1.40	1.52
7	2-G	773	GLU	CA-C	-9.64	1.40	1.52
7	3-G	773	GLU	CA-C	-9.64	1.40	1.52
4	1-C	244	ILE	CA-C	-9.64	1.40	1.52
7	1-G	235	VAL	N-CA	-9.64	1.35	1.46
4	2-C	244	ILE	CA-C	-9.64	1.40	1.52
7	2-G	235	VAL	N-CA	-9.64	1.35	1.46
4	3-C	244	ILE	CA-C	-9.64	1.40	1.52
7	3-G	235	VAL	N-CA	-9.64	1.35	1.46
1	1-A	596	GLU	N-CA	-9.63	1.34	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	596	GLU	N-CA	-9.63	1.34	1.46
1	3-A	596	GLU	N-CA	-9.63	1.34	1.46
4	1-C	283	SER	CA-C	-9.63	1.44	1.53
4	2-C	283	SER	CA-C	-9.63	1.44	1.53
4	3-C	283	SER	CA-C	-9.63	1.44	1.53
4	1-H	521	GLN	CA-C	-9.61	1.40	1.52
4	2-H	521	GLN	CA-C	-9.61	1.40	1.52
4	3-H	521	GLN	CA-C	-9.61	1.40	1.52
4	1-C	313	LYS	CA-C	-9.58	1.41	1.52
4	2-C	313	LYS	CA-C	-9.58	1.41	1.52
4	3-C	313	LYS	CA-C	-9.58	1.41	1.52
7	1-G	135	THR	CA-C	-9.58	1.40	1.52
7	2-G	135	THR	CA-C	-9.58	1.40	1.52
7	3-G	135	THR	CA-C	-9.58	1.40	1.52
1	1-A	631	LYS	CA-C	-9.55	1.40	1.52
1	2-A	631	LYS	CA-C	-9.55	1.40	1.52
1	3-A	631	LYS	CA-C	-9.55	1.40	1.52
4	1-H	313	LYS	CA-C	-9.54	1.41	1.52
4	2-H	313	LYS	CA-C	-9.54	1.41	1.52
4	3-H	313	LYS	CA-C	-9.54	1.41	1.52
4	1-H	245	ILE	N-CA	-9.53	1.35	1.46
4	2-H	245	ILE	N-CA	-9.53	1.35	1.46
4	3-H	245	ILE	N-CA	-9.53	1.35	1.46
4	1-C	245	ILE	N-CA	-9.53	1.35	1.46
4	2-C	245	ILE	N-CA	-9.53	1.35	1.46
4	3-C	245	ILE	N-CA	-9.53	1.35	1.46
5	1-I	59	GLN	CA-C	-9.52	1.41	1.52
5	2-I	59	GLN	CA-C	-9.52	1.41	1.52
5	3-I	59	GLN	CA-C	-9.52	1.41	1.52
4	1-H	283	SER	CA-C	-9.48	1.44	1.53
4	2-H	283	SER	CA-C	-9.48	1.44	1.53
4	3-H	283	SER	CA-C	-9.48	1.44	1.53
3	1-N	434	ASP	CA-C	-9.47	1.40	1.52
3	2-N	434	ASP	CA-C	-9.47	1.40	1.52
3	3-N	434	ASP	CA-C	-9.47	1.40	1.52
4	1-C	262	ARG	CA-C	-9.46	1.41	1.52
4	2-C	262	ARG	CA-C	-9.46	1.41	1.52
4	3-C	262	ARG	CA-C	-9.46	1.41	1.52
7	1-K	210	ALA	CA-C	-9.46	1.40	1.52
7	2-K	210	ALA	CA-C	-9.46	1.40	1.52
7	3-K	210	ALA	CA-C	-9.46	1.40	1.52
7	1-K	731	THR	CA-C	-9.44	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-K	731	THR	CA-C	-9.44	1.41	1.52
7	3-K	731	THR	CA-C	-9.44	1.41	1.52
5	1-D	59	GLN	CA-C	-9.43	1.41	1.52
8	1-L	27	PHE	CA-C	-9.43	1.40	1.52
5	2-D	59	GLN	CA-C	-9.43	1.41	1.52
8	2-L	27	PHE	CA-C	-9.43	1.40	1.52
5	3-D	59	GLN	CA-C	-9.43	1.41	1.52
8	3-L	27	PHE	CA-C	-9.43	1.40	1.52
4	1-H	574	TYR	CA-C	-9.43	1.41	1.52
4	2-H	574	TYR	CA-C	-9.43	1.41	1.52
4	3-H	574	TYR	CA-C	-9.43	1.41	1.52
3	1-B	434	ASP	CA-C	-9.42	1.40	1.52
3	2-B	434	ASP	CA-C	-9.42	1.40	1.52
3	3-B	434	ASP	CA-C	-9.42	1.40	1.52
4	1-H	262	ARG	CA-C	-9.42	1.41	1.52
4	2-H	262	ARG	CA-C	-9.42	1.41	1.52
4	3-H	262	ARG	CA-C	-9.42	1.41	1.52
3	1-N	379	VAL	CA-C	-9.41	1.40	1.52
3	2-N	379	VAL	CA-C	-9.41	1.40	1.52
3	3-N	379	VAL	CA-C	-9.41	1.40	1.52
7	1-K	872	SER	CA-C	-9.41	1.40	1.52
7	2-K	872	SER	CA-C	-9.41	1.40	1.52
7	3-K	872	SER	CA-C	-9.41	1.40	1.52
6	1-M	35	TYR	CA-C	-9.39	1.39	1.52
6	2-M	35	TYR	CA-C	-9.39	1.39	1.52
6	3-M	35	TYR	CA-C	-9.39	1.39	1.52
7	1-G	731	THR	CA-C	-9.39	1.41	1.52
7	2-G	731	THR	CA-C	-9.39	1.41	1.52
7	3-G	731	THR	CA-C	-9.39	1.41	1.52
4	1-C	151	ASN	CA-C	-9.38	1.42	1.52
4	2-C	151	ASN	CA-C	-9.38	1.42	1.52
4	3-C	151	ASN	CA-C	-9.38	1.42	1.52
3	1-B	183	HIS	CA-C	-9.36	1.40	1.52
3	2-B	183	HIS	CA-C	-9.36	1.40	1.52
3	3-B	183	HIS	CA-C	-9.36	1.40	1.52
6	1-M	47	PRO	CA-C	-9.36	1.40	1.52
6	2-M	47	PRO	CA-C	-9.36	1.40	1.52
6	3-M	47	PRO	CA-C	-9.36	1.40	1.52
3	1-N	183	HIS	CA-C	-9.35	1.40	1.52
3	2-N	183	HIS	CA-C	-9.35	1.40	1.52
3	3-N	183	HIS	CA-C	-9.35	1.40	1.52
6	1-R	58	TYR	CA-C	-9.34	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-H	151	ASN	CA-C	-9.34	1.42	1.52
6	2-R	58	TYR	CA-C	-9.34	1.41	1.52
4	2-H	151	ASN	CA-C	-9.34	1.42	1.52
6	3-R	58	TYR	CA-C	-9.34	1.41	1.52
4	3-H	151	ASN	CA-C	-9.34	1.42	1.52
8	1-L	45	GLU	CA-C	-9.33	1.40	1.52
8	2-L	45	GLU	CA-C	-9.33	1.40	1.52
8	3-L	45	GLU	CA-C	-9.33	1.40	1.52
4	1-C	574	TYR	CA-C	-9.33	1.41	1.52
4	2-C	574	TYR	CA-C	-9.33	1.41	1.52
4	3-C	574	TYR	CA-C	-9.33	1.41	1.52
5	1-D	117	VAL	CA-C	-9.33	1.40	1.52
5	2-D	117	VAL	CA-C	-9.33	1.40	1.52
5	3-D	117	VAL	CA-C	-9.33	1.40	1.52
7	1-G	872	SER	CA-C	-9.32	1.40	1.52
7	2-G	872	SER	CA-C	-9.32	1.40	1.52
7	3-G	872	SER	CA-C	-9.32	1.40	1.52
4	1-C	661	ALA	CA-C	-9.30	1.41	1.52
4	2-C	661	ALA	CA-C	-9.30	1.41	1.52
4	3-C	661	ALA	CA-C	-9.30	1.41	1.52
4	1-C	361	ASN	CA-C	-9.30	1.40	1.52
4	2-C	361	ASN	CA-C	-9.30	1.40	1.52
4	3-C	361	ASN	CA-C	-9.30	1.40	1.52
7	1-K	203	VAL	N-CA	-9.29	1.35	1.46
7	2-K	203	VAL	N-CA	-9.29	1.35	1.46
7	3-K	203	VAL	N-CA	-9.29	1.35	1.46
4	1-H	361	ASN	CA-C	-9.28	1.40	1.52
4	2-H	361	ASN	CA-C	-9.28	1.40	1.52
4	3-H	361	ASN	CA-C	-9.28	1.40	1.52
4	1-H	256	TRP	CA-C	-9.28	1.41	1.52
4	2-H	256	TRP	CA-C	-9.28	1.41	1.52
4	3-H	256	TRP	CA-C	-9.28	1.41	1.52
3	1-N	372	VAL	CA-C	-9.28	1.41	1.52
3	2-N	372	VAL	CA-C	-9.28	1.41	1.52
3	3-N	372	VAL	CA-C	-9.28	1.41	1.52
3	1-B	869	THR	CA-C	-9.27	1.41	1.52
3	2-B	869	THR	CA-C	-9.27	1.41	1.52
3	3-B	869	THR	CA-C	-9.27	1.41	1.52
3	1-B	372	VAL	CA-C	-9.27	1.41	1.52
3	2-B	372	VAL	CA-C	-9.27	1.41	1.52
3	3-B	372	VAL	CA-C	-9.27	1.41	1.52
4	1-H	661	ALA	CA-C	-9.26	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-H	661	ALA	CA-C	-9.26	1.41	1.52
4	3-H	661	ALA	CA-C	-9.26	1.41	1.52
8	1-L	89	MET	CA-C	-9.25	1.40	1.52
8	2-L	89	MET	CA-C	-9.25	1.40	1.52
8	3-L	89	MET	CA-C	-9.25	1.40	1.52
4	1-C	256	TRP	CA-C	-9.24	1.41	1.52
4	2-C	256	TRP	CA-C	-9.24	1.41	1.52
4	3-C	256	TRP	CA-C	-9.24	1.41	1.52
5	1-I	117	VAL	CA-C	-9.21	1.40	1.52
5	2-I	117	VAL	CA-C	-9.21	1.40	1.52
5	3-I	117	VAL	CA-C	-9.21	1.40	1.52
1	1-A	663	GLU	CA-C	-9.19	1.41	1.52
1	2-A	663	GLU	CA-C	-9.19	1.41	1.52
1	3-A	663	GLU	CA-C	-9.19	1.41	1.52
1	1-A	599	PHE	N-CA	-9.19	1.35	1.46
1	1-A	808	TRP	CA-C	-9.19	1.45	1.52
4	1-H	253	VAL	CA-C	-9.19	1.41	1.52
1	2-A	599	PHE	N-CA	-9.19	1.35	1.46
1	2-A	808	TRP	CA-C	-9.19	1.45	1.52
4	2-H	253	VAL	CA-C	-9.19	1.41	1.52
1	3-A	599	PHE	N-CA	-9.19	1.35	1.46
1	3-A	808	TRP	CA-C	-9.19	1.45	1.52
4	3-H	253	VAL	CA-C	-9.19	1.41	1.52
3	1-B	374	VAL	CA-C	-9.18	1.40	1.52
6	1-R	84	ASN	CA-C	-9.18	1.40	1.52
3	2-B	374	VAL	CA-C	-9.18	1.40	1.52
6	2-R	84	ASN	CA-C	-9.18	1.40	1.52
3	3-B	374	VAL	CA-C	-9.18	1.40	1.52
6	3-R	84	ASN	CA-C	-9.18	1.40	1.52
4	1-C	602	ASP	CA-C	-9.17	1.42	1.53
4	2-C	602	ASP	CA-C	-9.17	1.42	1.53
4	3-C	602	ASP	CA-C	-9.17	1.42	1.53
4	1-C	555	ALA	CA-C	-9.17	1.41	1.52
4	2-C	555	ALA	CA-C	-9.17	1.41	1.52
4	3-C	555	ALA	CA-C	-9.17	1.41	1.52
4	1-C	253	VAL	CA-C	-9.17	1.41	1.52
4	2-C	253	VAL	CA-C	-9.17	1.41	1.52
4	3-C	253	VAL	CA-C	-9.17	1.41	1.52
3	1-N	374	VAL	CA-C	-9.16	1.41	1.52
3	2-N	374	VAL	CA-C	-9.16	1.41	1.52
3	3-N	374	VAL	CA-C	-9.16	1.41	1.52
4	1-H	602	ASP	CA-C	-9.15	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-H	602	ASP	CA-C	-9.15	1.42	1.53
4	3-H	602	ASP	CA-C	-9.15	1.42	1.53
5	1-I	50	GLU	CA-C	-9.15	1.41	1.52
5	2-I	50	GLU	CA-C	-9.15	1.41	1.52
5	3-I	50	GLU	CA-C	-9.15	1.41	1.52
7	1-G	70	PHE	CA-C	-9.14	1.41	1.52
7	2-G	70	PHE	CA-C	-9.14	1.41	1.52
7	3-G	70	PHE	CA-C	-9.14	1.41	1.52
7	1-K	202	HIS	CA-C	-9.13	1.41	1.52
7	2-K	202	HIS	CA-C	-9.13	1.41	1.52
7	3-K	202	HIS	CA-C	-9.13	1.41	1.52
1	1-A	230	LYS	CA-C	-9.12	1.41	1.52
1	2-A	230	LYS	CA-C	-9.12	1.41	1.52
1	3-A	230	LYS	CA-C	-9.12	1.41	1.52
3	1-B	849	THR	C-N	9.11	1.44	1.33
3	2-B	849	THR	C-N	9.11	1.44	1.33
3	3-B	849	THR	C-N	9.11	1.44	1.33
5	1-D	50	GLU	CA-C	-9.10	1.41	1.52
5	2-D	50	GLU	CA-C	-9.10	1.41	1.52
5	3-D	50	GLU	CA-C	-9.10	1.41	1.52
1	1-A	14	GLY	CA-C	-9.08	1.44	1.51
1	2-A	14	GLY	CA-C	-9.08	1.44	1.51
1	3-A	14	GLY	CA-C	-9.08	1.44	1.51
7	1-G	827	THR	CA-C	-9.07	1.41	1.52
4	1-H	555	ALA	CA-C	-9.07	1.41	1.52
7	2-G	827	THR	CA-C	-9.07	1.41	1.52
4	2-H	555	ALA	CA-C	-9.07	1.41	1.52
7	3-G	827	THR	CA-C	-9.07	1.41	1.52
4	3-H	555	ALA	CA-C	-9.07	1.41	1.52
6	1-M	90	PHE	CA-C	-9.06	1.41	1.52
6	2-M	90	PHE	CA-C	-9.06	1.41	1.52
6	3-M	90	PHE	CA-C	-9.06	1.41	1.52
5	1-I	52	GLU	CA-C	-9.05	1.41	1.53
5	2-I	52	GLU	CA-C	-9.05	1.41	1.53
5	3-I	52	GLU	CA-C	-9.05	1.41	1.53
7	1-G	190	ILE	CA-C	-9.05	1.41	1.52
7	2-G	190	ILE	CA-C	-9.05	1.41	1.52
7	3-G	190	ILE	CA-C	-9.05	1.41	1.52
1	1-A	74	LYS	CA-C	-9.03	1.40	1.52
3	1-B	398	LEU	CA-C	-9.04	1.41	1.52
1	2-A	74	LYS	CA-C	-9.03	1.40	1.52
3	2-B	398	LEU	CA-C	-9.04	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-A	74	LYS	CA-C	-9.03	1.40	1.52
3	3-B	398	LEU	CA-C	-9.04	1.41	1.52
1	1-A	519	ASP	CA-C	-9.01	1.42	1.52
7	1-K	142	ARG	CA-C	-9.01	1.41	1.52
7	1-K	827	THR	CA-C	-9.01	1.41	1.52
1	2-A	519	ASP	CA-C	-9.01	1.42	1.52
1	3-A	519	ASP	CA-C	-9.01	1.42	1.52
7	2-K	142	ARG	CA-C	-9.01	1.41	1.52
7	2-K	827	THR	CA-C	-9.01	1.41	1.52
7	3-K	142	ARG	CA-C	-9.01	1.41	1.52
7	3-K	827	THR	CA-C	-9.01	1.41	1.52
3	1-B	373	ILE	CA-C	-9.00	1.41	1.52
3	2-B	373	ILE	CA-C	-9.00	1.41	1.52
3	3-B	373	ILE	CA-C	-9.00	1.41	1.52
4	1-H	245	ILE	CA-C	-8.98	1.41	1.52
4	2-H	245	ILE	CA-C	-8.98	1.41	1.52
4	3-H	245	ILE	CA-C	-8.98	1.41	1.52
3	1-B	870	VAL	CA-C	-8.98	1.42	1.52
3	2-B	870	VAL	CA-C	-8.98	1.42	1.52
3	3-B	870	VAL	CA-C	-8.98	1.42	1.52
5	1-D	52	GLU	CA-C	-8.98	1.41	1.53
5	2-D	52	GLU	CA-C	-8.98	1.41	1.53
5	3-D	52	GLU	CA-C	-8.98	1.41	1.53
7	1-K	109	LEU	CA-C	-8.97	1.41	1.52
7	2-K	109	LEU	CA-C	-8.97	1.41	1.52
7	3-K	109	LEU	CA-C	-8.97	1.41	1.52
6	1-J	54	GLU	CA-C	-8.96	1.41	1.52
6	2-J	54	GLU	CA-C	-8.96	1.41	1.52
6	3-J	54	GLU	CA-C	-8.96	1.41	1.52
7	1-K	201	TYR	CA-C	-8.95	1.41	1.52
7	2-K	201	TYR	CA-C	-8.95	1.41	1.52
7	3-K	201	TYR	CA-C	-8.95	1.41	1.52
6	1-F	54	GLU	CA-C	-8.94	1.41	1.52
7	1-G	232	MET	CA-C	-8.94	1.40	1.52
6	2-F	54	GLU	CA-C	-8.94	1.41	1.52
7	2-G	232	MET	CA-C	-8.94	1.40	1.52
6	3-F	54	GLU	CA-C	-8.94	1.41	1.52
7	3-G	232	MET	CA-C	-8.94	1.40	1.52
3	1-N	373	ILE	CA-C	-8.94	1.41	1.52
3	2-N	373	ILE	CA-C	-8.94	1.41	1.52
3	3-N	373	ILE	CA-C	-8.94	1.41	1.52
1	1-A	285	GLN	CA-C	-8.93	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1-I	54	VAL	CA-C	-8.93	1.41	1.52
1	2-A	285	GLN	CA-C	-8.93	1.41	1.52
5	2-I	54	VAL	CA-C	-8.93	1.41	1.52
1	3-A	285	GLN	CA-C	-8.93	1.41	1.52
5	3-I	54	VAL	CA-C	-8.93	1.41	1.52
3	1-N	398	LEU	CA-C	-8.92	1.41	1.52
3	2-N	398	LEU	CA-C	-8.92	1.41	1.52
3	3-N	398	LEU	CA-C	-8.92	1.41	1.52
5	1-D	54	VAL	CA-C	-8.92	1.41	1.52
5	2-D	54	VAL	CA-C	-8.92	1.41	1.52
5	3-D	54	VAL	CA-C	-8.92	1.41	1.52
4	1-H	459	ARG	CA-C	-8.91	1.41	1.52
4	2-H	459	ARG	CA-C	-8.91	1.41	1.52
4	3-H	459	ARG	CA-C	-8.91	1.41	1.52
4	1-C	245	ILE	CA-C	-8.91	1.41	1.52
4	1-H	567	ILE	N-CA	-8.91	1.39	1.46
4	2-C	245	ILE	CA-C	-8.91	1.41	1.52
4	2-H	567	ILE	N-CA	-8.91	1.39	1.46
4	3-C	245	ILE	CA-C	-8.91	1.41	1.52
4	3-H	567	ILE	N-CA	-8.91	1.39	1.46
1	1-A	594	PRO	CA-C	-8.90	1.39	1.52
1	2-A	594	PRO	CA-C	-8.90	1.39	1.52
1	3-A	594	PRO	CA-C	-8.90	1.39	1.52
6	1-R	112	ASN	CA-C	-8.89	1.40	1.52
6	2-R	112	ASN	CA-C	-8.89	1.40	1.52
6	3-R	112	ASN	CA-C	-8.89	1.40	1.52
4	1-C	459	ARG	CA-C	-8.89	1.41	1.52
8	1-Z	69	TYR	CA-C	-8.89	1.41	1.52
3	1-N	368	VAL	N-CA	-8.89	1.35	1.46
4	2-C	459	ARG	CA-C	-8.89	1.41	1.52
8	2-Z	69	TYR	CA-C	-8.89	1.41	1.52
3	2-N	368	VAL	N-CA	-8.89	1.35	1.46
4	3-C	459	ARG	CA-C	-8.89	1.41	1.52
8	3-Z	69	TYR	CA-C	-8.89	1.41	1.52
3	3-N	368	VAL	N-CA	-8.89	1.35	1.46
1	1-A	674	TRP	CA-C	-8.87	1.41	1.52
1	2-A	674	TRP	CA-C	-8.87	1.41	1.52
1	3-A	674	TRP	CA-C	-8.87	1.41	1.52
7	1-G	180	GLU	N-CA	-8.87	1.35	1.46
7	1-K	251	LEU	CA-C	-8.87	1.41	1.52
7	2-G	180	GLU	N-CA	-8.87	1.35	1.46
7	2-K	251	LEU	CA-C	-8.87	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3-G	180	GLU	N-CA	-8.87	1.35	1.46
7	3-K	251	LEU	CA-C	-8.87	1.41	1.52
3	1-B	368	VAL	N-CA	-8.87	1.35	1.46
3	2-B	368	VAL	N-CA	-8.87	1.35	1.46
3	3-B	368	VAL	N-CA	-8.87	1.35	1.46
4	1-H	453	GLU	CA-C	-8.86	1.41	1.52
4	2-H	453	GLU	CA-C	-8.86	1.41	1.52
4	3-H	453	GLU	CA-C	-8.86	1.41	1.52
4	1-H	315	ILE	N-CA	-8.82	1.35	1.46
4	2-H	315	ILE	N-CA	-8.82	1.35	1.46
4	3-H	315	ILE	N-CA	-8.82	1.35	1.46
7	1-G	90	LEU	CA-C	-8.81	1.41	1.52
7	2-G	90	LEU	CA-C	-8.81	1.41	1.52
7	3-G	90	LEU	CA-C	-8.81	1.41	1.52
3	1-B	760	VAL	CA-C	-8.80	1.41	1.52
3	2-B	760	VAL	CA-C	-8.80	1.41	1.52
3	3-B	760	VAL	CA-C	-8.80	1.41	1.52
4	1-C	453	GLU	CA-C	-8.80	1.41	1.52
4	2-C	453	GLU	CA-C	-8.80	1.41	1.52
4	3-C	453	GLU	CA-C	-8.80	1.41	1.52
6	1-R	33	VAL	N-CA	-8.79	1.36	1.46
6	2-R	33	VAL	N-CA	-8.79	1.36	1.46
6	3-R	33	VAL	N-CA	-8.79	1.36	1.46
7	1-K	722	CYS	CA-C	-8.79	1.42	1.52
4	1-H	630	PHE	CA-C	-8.79	1.44	1.53
7	2-K	722	CYS	CA-C	-8.79	1.42	1.52
4	2-H	630	PHE	CA-C	-8.79	1.44	1.53
7	3-K	722	CYS	CA-C	-8.79	1.42	1.52
4	3-H	630	PHE	CA-C	-8.79	1.44	1.53
6	1-M	38	LYS	CA-C	-8.78	1.41	1.52
6	2-M	38	LYS	CA-C	-8.78	1.41	1.52
6	3-M	38	LYS	CA-C	-8.78	1.41	1.52
7	1-G	89	TYR	CA-C	-8.78	1.41	1.52
7	2-G	89	TYR	CA-C	-8.78	1.41	1.52
7	3-G	89	TYR	CA-C	-8.78	1.41	1.52
4	1-C	315	ILE	N-CA	-8.77	1.35	1.46
4	1-C	567	ILE	N-CA	-8.77	1.39	1.46
4	2-C	315	ILE	N-CA	-8.77	1.35	1.46
4	2-C	567	ILE	N-CA	-8.77	1.39	1.46
4	3-C	315	ILE	N-CA	-8.77	1.35	1.46
4	3-C	567	ILE	N-CA	-8.77	1.39	1.46
1	1-A	506	LEU	CA-C	-8.77	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	506	LEU	CA-C	-8.77	1.41	1.52
1	3-A	506	LEU	CA-C	-8.77	1.41	1.52
7	1-K	291	VAL	N-CA	-8.77	1.36	1.46
7	2-K	291	VAL	N-CA	-8.77	1.36	1.46
7	3-K	291	VAL	N-CA	-8.77	1.36	1.46
1	1-A	610	GLU	N-CA	-8.76	1.35	1.46
6	1-R	106	VAL	N-CA	-8.76	1.36	1.46
1	2-A	610	GLU	N-CA	-8.76	1.35	1.46
6	2-R	106	VAL	N-CA	-8.76	1.36	1.46
1	3-A	610	GLU	N-CA	-8.76	1.35	1.46
6	3-R	106	VAL	N-CA	-8.76	1.36	1.46
4	1-C	630	PHE	CA-C	-8.76	1.44	1.53
4	2-C	630	PHE	CA-C	-8.76	1.44	1.53
4	3-C	630	PHE	CA-C	-8.76	1.44	1.53
8	1-L	30	TYR	CA-C	-8.74	1.41	1.52
8	2-L	30	TYR	CA-C	-8.74	1.41	1.52
8	3-L	30	TYR	CA-C	-8.74	1.41	1.52
8	1-L	140	GLN	CA-C	-8.73	1.41	1.52
8	2-L	140	GLN	CA-C	-8.73	1.41	1.52
8	3-L	140	GLN	CA-C	-8.73	1.41	1.52
4	1-C	289	GLY	CA-C	-8.71	1.46	1.52
4	2-C	289	GLY	CA-C	-8.71	1.46	1.52
4	3-C	289	GLY	CA-C	-8.71	1.46	1.52
1	1-A	611	VAL	CA-C	-8.71	1.41	1.52
1	2-A	611	VAL	CA-C	-8.71	1.41	1.52
1	3-A	611	VAL	CA-C	-8.71	1.41	1.52
7	1-K	204	ARG	CA-C	-8.69	1.40	1.52
7	2-K	204	ARG	CA-C	-8.69	1.40	1.52
7	3-K	204	ARG	CA-C	-8.69	1.40	1.52
6	1-R	90	PHE	N-CA	-8.68	1.35	1.46
6	2-R	90	PHE	N-CA	-8.68	1.35	1.46
6	3-R	90	PHE	N-CA	-8.68	1.35	1.46
8	1-L	100	SER	CA-C	-8.68	1.41	1.52
8	2-L	100	SER	CA-C	-8.68	1.41	1.52
8	3-L	100	SER	CA-C	-8.68	1.41	1.52
7	1-K	810	MET	CA-C	-8.68	1.41	1.52
7	2-K	810	MET	CA-C	-8.68	1.41	1.52
7	3-K	810	MET	CA-C	-8.68	1.41	1.52
6	1-M	58	TYR	CA-C	-8.66	1.42	1.52
6	2-M	58	TYR	CA-C	-8.66	1.42	1.52
6	3-M	58	TYR	CA-C	-8.66	1.42	1.52
8	1-L	141	GLN	CA-C	-8.65	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2-L	141	GLN	CA-C	-8.65	1.41	1.52
8	3-L	141	GLN	CA-C	-8.65	1.41	1.52
8	1-L	50	ASN	CA-C	-8.65	1.41	1.52
8	2-L	50	ASN	CA-C	-8.65	1.41	1.52
8	3-L	50	ASN	CA-C	-8.65	1.41	1.52
1	1-A	505	LEU	CA-C	-8.64	1.42	1.52
1	2-A	505	LEU	CA-C	-8.64	1.42	1.52
1	3-A	505	LEU	CA-C	-8.64	1.42	1.52
7	1-G	722	CYS	CA-C	-8.63	1.42	1.52
7	2-G	722	CYS	CA-C	-8.63	1.42	1.52
7	3-G	722	CYS	CA-C	-8.63	1.42	1.52
7	1-G	163	SER	CA-C	-8.63	1.41	1.52
7	2-G	163	SER	CA-C	-8.63	1.41	1.52
7	3-G	163	SER	CA-C	-8.63	1.41	1.52
7	1-G	810	MET	CA-C	-8.62	1.41	1.52
7	2-G	810	MET	CA-C	-8.62	1.41	1.52
7	3-G	810	MET	CA-C	-8.62	1.41	1.52
3	1-B	750	ASN	N-CA	-8.61	1.36	1.46
6	1-R	29	GLY	CA-C	-8.61	1.39	1.51
3	2-B	750	ASN	N-CA	-8.61	1.36	1.46
6	2-R	29	GLY	CA-C	-8.61	1.39	1.51
3	3-B	750	ASN	N-CA	-8.61	1.36	1.46
6	3-R	29	GLY	CA-C	-8.61	1.39	1.51
3	1-B	753	ASP	N-CA	-8.61	1.35	1.46
3	2-B	753	ASP	N-CA	-8.61	1.35	1.46
3	3-B	753	ASP	N-CA	-8.61	1.35	1.46
8	1-Z	62	LEU	CA-C	-8.59	1.42	1.52
8	2-Z	62	LEU	CA-C	-8.59	1.42	1.52
8	3-Z	62	LEU	CA-C	-8.59	1.42	1.52
7	1-G	234	ARG	CA-C	-8.59	1.41	1.52
7	2-G	234	ARG	CA-C	-8.59	1.41	1.52
7	3-G	234	ARG	CA-C	-8.59	1.41	1.52
1	1-A	534	ALA	CA-C	-8.57	1.42	1.52
4	1-C	534	PHE	CA-C	-8.57	1.42	1.52
1	2-A	534	ALA	CA-C	-8.57	1.42	1.52
4	2-C	534	PHE	CA-C	-8.57	1.42	1.52
1	3-A	534	ALA	CA-C	-8.57	1.42	1.52
4	3-C	534	PHE	CA-C	-8.57	1.42	1.52
4	1-H	546	TYR	CA-C	-8.57	1.42	1.52
4	2-H	546	TYR	CA-C	-8.57	1.42	1.52
4	3-H	546	TYR	CA-C	-8.57	1.42	1.52
3	1-N	468	LYS	CA-C	-8.57	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-N	468	LYS	CA-C	-8.57	1.42	1.52
3	3-N	468	LYS	CA-C	-8.57	1.42	1.52
7	1-K	232	MET	CA-C	-8.56	1.41	1.52
7	2-K	232	MET	CA-C	-8.56	1.41	1.52
7	3-K	232	MET	CA-C	-8.56	1.41	1.52
3	1-B	468	LYS	CA-C	-8.56	1.42	1.52
3	2-B	468	LYS	CA-C	-8.56	1.42	1.52
3	3-B	468	LYS	CA-C	-8.56	1.42	1.52
3	1-B	923	ASN	CA-C	-8.55	1.42	1.52
3	2-B	923	ASN	CA-C	-8.55	1.42	1.52
3	3-B	923	ASN	CA-C	-8.55	1.42	1.52
7	1-G	726	CYS	CA-C	-8.55	1.42	1.52
7	2-G	726	CYS	CA-C	-8.55	1.42	1.52
7	3-G	726	CYS	CA-C	-8.55	1.42	1.52
4	1-C	546	TYR	CA-C	-8.54	1.42	1.52
4	2-C	546	TYR	CA-C	-8.54	1.42	1.52
4	3-C	546	TYR	CA-C	-8.54	1.42	1.52
3	1-B	742	TYR	CA-C	-8.53	1.42	1.52
3	2-B	742	TYR	CA-C	-8.53	1.42	1.52
3	3-B	742	TYR	CA-C	-8.53	1.42	1.52
4	1-C	778	SER	CA-C	-8.53	1.41	1.52
8	1-L	13	VAL	CA-C	-8.53	1.42	1.52
4	2-C	778	SER	CA-C	-8.53	1.41	1.52
8	2-L	13	VAL	CA-C	-8.53	1.42	1.52
4	3-C	778	SER	CA-C	-8.53	1.41	1.52
8	3-L	13	VAL	CA-C	-8.53	1.42	1.52
7	1-G	214	MET	CA-C	-8.53	1.41	1.52
7	2-G	214	MET	CA-C	-8.53	1.41	1.52
7	3-G	214	MET	CA-C	-8.53	1.41	1.52
7	1-G	92	ILE	CA-C	-8.52	1.42	1.52
7	2-G	92	ILE	CA-C	-8.52	1.42	1.52
7	3-G	92	ILE	CA-C	-8.52	1.42	1.52
8	1-Z	65	LEU	N-CA	-8.51	1.35	1.45
4	1-H	534	PHE	CA-C	-8.51	1.42	1.52
8	2-Z	65	LEU	N-CA	-8.51	1.35	1.45
4	2-H	534	PHE	CA-C	-8.51	1.42	1.52
8	3-Z	65	LEU	N-CA	-8.51	1.35	1.45
4	3-H	534	PHE	CA-C	-8.51	1.42	1.52
3	1-B	60	VAL	CA-C	-8.51	1.42	1.52
3	2-B	60	VAL	CA-C	-8.51	1.42	1.52
3	3-B	60	VAL	CA-C	-8.51	1.42	1.52
4	1-H	530	VAL	CA-C	-8.51	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-H	530	VAL	CA-C	-8.51	1.43	1.52
4	3-H	530	VAL	CA-C	-8.51	1.43	1.52
7	1-G	441	GLU	CA-C	-8.50	1.42	1.52
7	2-G	441	GLU	CA-C	-8.50	1.42	1.52
7	3-G	441	GLU	CA-C	-8.50	1.42	1.52
3	1-B	836	ASP	CA-C	-8.49	1.41	1.53
3	2-B	836	ASP	CA-C	-8.49	1.41	1.53
3	3-B	836	ASP	CA-C	-8.49	1.41	1.53
4	1-H	289	GLY	CA-C	-8.49	1.46	1.52
4	2-H	289	GLY	CA-C	-8.49	1.46	1.52
4	3-H	289	GLY	CA-C	-8.49	1.46	1.52
4	1-C	84	PHE	CA-C	-8.48	1.42	1.52
4	1-H	550	GLU	CA-C	-8.48	1.42	1.52
4	2-C	84	PHE	CA-C	-8.48	1.42	1.52
4	2-H	550	GLU	CA-C	-8.48	1.42	1.52
4	3-C	84	PHE	CA-C	-8.48	1.42	1.52
4	3-H	550	GLU	CA-C	-8.48	1.42	1.52
4	1-C	550	GLU	CA-C	-8.47	1.42	1.52
4	2-C	550	GLU	CA-C	-8.47	1.42	1.52
4	3-C	550	GLU	CA-C	-8.47	1.42	1.52
3	1-N	60	VAL	CA-C	-8.47	1.42	1.52
3	2-N	60	VAL	CA-C	-8.47	1.42	1.52
3	3-N	60	VAL	CA-C	-8.47	1.42	1.52
3	1-B	332	VAL	CA-C	-8.46	1.41	1.52
3	1-B	801	LYS	CA-C	-8.46	1.42	1.52
3	2-B	332	VAL	CA-C	-8.46	1.41	1.52
3	2-B	801	LYS	CA-C	-8.46	1.42	1.52
3	3-B	332	VAL	CA-C	-8.46	1.41	1.52
3	3-B	801	LYS	CA-C	-8.46	1.42	1.52
4	1-C	71	TRP	CA-C	-8.45	1.42	1.52
4	2-C	71	TRP	CA-C	-8.45	1.42	1.52
4	3-C	71	TRP	CA-C	-8.45	1.42	1.52
3	1-N	332	VAL	CA-C	-8.45	1.42	1.52
3	1-N	369	GLU	CA-C	-8.45	1.41	1.52
3	2-N	332	VAL	CA-C	-8.45	1.42	1.52
3	2-N	369	GLU	CA-C	-8.45	1.41	1.52
3	3-N	332	VAL	CA-C	-8.45	1.42	1.52
3	3-N	369	GLU	CA-C	-8.45	1.41	1.52
7	1-K	163	SER	CA-C	-8.45	1.41	1.52
7	2-K	163	SER	CA-C	-8.45	1.41	1.52
7	3-K	163	SER	CA-C	-8.45	1.41	1.52
1	1-A	514	CYS	CA-C	-8.44	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	514	CYS	CA-C	-8.44	1.42	1.52
1	3-A	514	CYS	CA-C	-8.44	1.42	1.52
4	1-H	71	TRP	CA-C	-8.44	1.42	1.52
4	2-H	71	TRP	CA-C	-8.44	1.42	1.52
4	3-H	71	TRP	CA-C	-8.44	1.42	1.52
8	1-L	103	GLN	CA-C	-8.42	1.41	1.52
8	2-L	103	GLN	CA-C	-8.42	1.41	1.52
8	3-L	103	GLN	CA-C	-8.42	1.41	1.52
3	1-B	759	LEU	N-CA	-8.41	1.35	1.46
7	1-K	168	LYS	CA-C	-8.41	1.42	1.52
3	2-B	759	LEU	N-CA	-8.41	1.35	1.46
7	2-K	168	LYS	CA-C	-8.41	1.42	1.52
3	3-B	759	LEU	N-CA	-8.41	1.35	1.46
7	3-K	168	LYS	CA-C	-8.41	1.42	1.52
4	1-H	84	PHE	CA-C	-8.40	1.42	1.52
4	2-H	84	PHE	CA-C	-8.40	1.42	1.52
4	3-H	84	PHE	CA-C	-8.40	1.42	1.52
1	1-A	413	SER	CA-C	-8.40	1.42	1.52
1	2-A	413	SER	CA-C	-8.40	1.42	1.52
1	3-A	413	SER	CA-C	-8.40	1.42	1.52
3	1-B	754	ILE	N-CA	-8.40	1.35	1.46
3	2-B	754	ILE	N-CA	-8.40	1.35	1.46
3	3-B	754	ILE	N-CA	-8.40	1.35	1.46
4	1-C	530	VAL	CA-C	-8.40	1.43	1.52
4	2-C	530	VAL	CA-C	-8.40	1.43	1.52
4	3-C	530	VAL	CA-C	-8.40	1.43	1.52
4	1-C	150	ILE	CA-C	-8.39	1.42	1.52
4	2-C	150	ILE	CA-C	-8.39	1.42	1.52
4	3-C	150	ILE	CA-C	-8.39	1.42	1.52
3	1-B	374	VAL	N-CA	-8.38	1.36	1.46
3	2-B	374	VAL	N-CA	-8.38	1.36	1.46
3	3-B	374	VAL	N-CA	-8.38	1.36	1.46
1	1-A	596	GLU	CA-C	-8.38	1.41	1.52
3	1-B	418	PRO	CA-C	-8.38	1.39	1.52
1	2-A	596	GLU	CA-C	-8.38	1.41	1.52
3	2-B	418	PRO	CA-C	-8.38	1.39	1.52
1	3-A	596	GLU	CA-C	-8.38	1.41	1.52
3	3-B	418	PRO	CA-C	-8.38	1.39	1.52
7	1-K	726	CYS	CA-C	-8.36	1.42	1.52
7	2-K	726	CYS	CA-C	-8.36	1.42	1.52
7	3-K	726	CYS	CA-C	-8.36	1.42	1.52
3	1-B	369	GLU	CA-C	-8.36	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	369	GLU	CA-C	-8.36	1.42	1.52
3	3-B	369	GLU	CA-C	-8.36	1.42	1.52
3	1-B	380	ILE	CA-C	-8.35	1.42	1.52
3	2-B	380	ILE	CA-C	-8.35	1.42	1.52
3	3-B	380	ILE	CA-C	-8.35	1.42	1.52
7	1-G	211	VAL	CA-C	-8.34	1.42	1.52
8	1-L	129	VAL	CA-C	-8.34	1.42	1.52
7	2-G	211	VAL	CA-C	-8.34	1.42	1.52
8	2-L	129	VAL	CA-C	-8.34	1.42	1.52
7	3-G	211	VAL	CA-C	-8.34	1.42	1.52
8	3-L	129	VAL	CA-C	-8.34	1.42	1.52
1	1-A	613	HIS	CA-C	-8.33	1.42	1.52
8	1-L	48	ILE	N-CA	-8.33	1.36	1.46
1	2-A	613	HIS	CA-C	-8.33	1.42	1.52
8	2-L	48	ILE	N-CA	-8.33	1.36	1.46
1	3-A	613	HIS	CA-C	-8.33	1.42	1.52
8	3-L	48	ILE	N-CA	-8.33	1.36	1.46
4	1-H	379	THR	N-CA	-8.31	1.35	1.46
4	2-H	379	THR	N-CA	-8.31	1.35	1.46
4	3-H	379	THR	N-CA	-8.31	1.35	1.46
3	1-N	374	VAL	N-CA	-8.31	1.36	1.46
3	2-N	374	VAL	N-CA	-8.31	1.36	1.46
3	3-N	374	VAL	N-CA	-8.31	1.36	1.46
4	1-C	80	GLN	CA-C	-8.31	1.42	1.52
7	1-G	91	THR	N-CA	-8.31	1.36	1.46
4	2-C	80	GLN	CA-C	-8.31	1.42	1.52
7	2-G	91	THR	N-CA	-8.31	1.36	1.46
4	3-C	80	GLN	CA-C	-8.31	1.42	1.52
7	3-G	91	THR	N-CA	-8.31	1.36	1.46
4	1-C	494	LYS	CA-C	-8.30	1.42	1.52
8	1-Z	142	VAL	CA-C	-8.30	1.42	1.52
4	2-C	494	LYS	CA-C	-8.30	1.42	1.52
8	2-Z	142	VAL	CA-C	-8.30	1.42	1.52
4	3-C	494	LYS	CA-C	-8.30	1.42	1.52
8	3-Z	142	VAL	CA-C	-8.30	1.42	1.52
3	1-B	908	ALA	CA-C	-8.30	1.42	1.52
3	2-B	908	ALA	CA-C	-8.30	1.42	1.52
3	3-B	908	ALA	CA-C	-8.30	1.42	1.52
4	1-H	150	ILE	CA-C	-8.30	1.42	1.52
4	2-H	150	ILE	CA-C	-8.30	1.42	1.52
4	3-H	150	ILE	CA-C	-8.30	1.42	1.52
3	1-N	76	THR	CA-C	-8.29	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-N	76	THR	CA-C	-8.29	1.42	1.52
3	3-N	76	THR	CA-C	-8.29	1.42	1.52
3	1-N	371	LEU	N-CA	-8.28	1.36	1.46
4	1-H	494	LYS	CA-C	-8.28	1.42	1.52
3	2-N	371	LEU	N-CA	-8.28	1.36	1.46
4	2-H	494	LYS	CA-C	-8.28	1.42	1.52
3	3-N	371	LEU	N-CA	-8.28	1.36	1.46
4	3-H	494	LYS	CA-C	-8.28	1.42	1.52
7	1-G	74	THR	CA-C	-8.28	1.41	1.52
7	2-G	74	THR	CA-C	-8.28	1.41	1.52
7	3-G	74	THR	CA-C	-8.28	1.41	1.52
3	1-N	380	ILE	CA-C	-8.27	1.42	1.52
3	2-N	380	ILE	CA-C	-8.27	1.42	1.52
3	3-N	380	ILE	CA-C	-8.27	1.42	1.52
4	1-C	760	THR	CA-C	-8.27	1.42	1.52
4	2-C	760	THR	CA-C	-8.27	1.42	1.52
4	3-C	760	THR	CA-C	-8.27	1.42	1.52
3	1-N	477	LEU	CA-C	-8.26	1.42	1.52
3	2-N	477	LEU	CA-C	-8.26	1.42	1.52
3	3-N	477	LEU	CA-C	-8.26	1.42	1.52
7	1-G	476	ILE	CA-C	-8.26	1.42	1.52
7	2-G	476	ILE	CA-C	-8.26	1.42	1.52
7	3-G	476	ILE	CA-C	-8.26	1.42	1.52
7	1-G	72	ALA	N-CA	-8.25	1.36	1.46
3	1-N	418	PRO	CA-C	-8.25	1.39	1.52
7	2-G	72	ALA	N-CA	-8.25	1.36	1.46
3	2-N	418	PRO	CA-C	-8.25	1.39	1.52
7	3-G	72	ALA	N-CA	-8.25	1.36	1.46
3	3-N	418	PRO	CA-C	-8.25	1.39	1.52
1	1-A	391	TYR	CA-C	-8.25	1.42	1.52
4	1-C	379	THR	N-CA	-8.25	1.36	1.46
4	1-H	80	GLN	CA-C	-8.25	1.42	1.52
1	2-A	391	TYR	CA-C	-8.25	1.42	1.52
4	2-C	379	THR	N-CA	-8.25	1.36	1.46
4	2-H	80	GLN	CA-C	-8.25	1.42	1.52
1	3-A	391	TYR	CA-C	-8.25	1.42	1.52
4	3-C	379	THR	N-CA	-8.25	1.36	1.46
4	3-H	80	GLN	CA-C	-8.25	1.42	1.52
6	1-R	103	ALA	CA-C	-8.24	1.42	1.52
6	2-R	103	ALA	CA-C	-8.24	1.42	1.52
6	3-R	103	ALA	CA-C	-8.24	1.42	1.52
1	1-A	588	ARG	CA-C	8.23	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	76	THR	CA-C	-8.23	1.42	1.52
3	1-N	456	LYS	CA-C	-8.23	1.42	1.52
1	2-A	588	ARG	CA-C	8.23	1.62	1.52
3	2-B	76	THR	CA-C	-8.23	1.42	1.52
3	2-N	456	LYS	CA-C	-8.23	1.42	1.52
1	3-A	588	ARG	CA-C	8.23	1.62	1.52
3	3-B	76	THR	CA-C	-8.23	1.42	1.52
3	3-N	456	LYS	CA-C	-8.23	1.42	1.52
3	1-B	371	LEU	N-CA	-8.22	1.36	1.46
5	1-I	51	THR	CA-C	-8.22	1.42	1.52
3	2-B	371	LEU	N-CA	-8.22	1.36	1.46
5	2-I	51	THR	CA-C	-8.22	1.42	1.52
3	3-B	371	LEU	N-CA	-8.22	1.36	1.46
5	3-I	51	THR	CA-C	-8.22	1.42	1.52
3	1-B	456	LYS	CA-C	-8.21	1.42	1.52
7	1-K	211	VAL	N-CA	-8.21	1.36	1.46
3	2-B	456	LYS	CA-C	-8.21	1.42	1.52
7	2-K	211	VAL	N-CA	-8.21	1.36	1.46
3	3-B	456	LYS	CA-C	-8.21	1.42	1.52
7	3-K	211	VAL	N-CA	-8.21	1.36	1.46
7	1-K	203	VAL	CA-C	-8.21	1.42	1.52
7	2-K	203	VAL	CA-C	-8.21	1.42	1.52
7	3-K	203	VAL	CA-C	-8.21	1.42	1.52
3	1-N	61	ILE	CA-C	-8.20	1.42	1.52
5	1-I	61	MET	CA-C	-8.20	1.43	1.52
3	2-N	61	ILE	CA-C	-8.20	1.42	1.52
5	2-I	61	MET	CA-C	-8.20	1.43	1.52
3	3-N	61	ILE	CA-C	-8.20	1.42	1.52
5	3-I	61	MET	CA-C	-8.20	1.43	1.52
4	1-H	552	VAL	CA-C	-8.19	1.42	1.52
4	2-H	552	VAL	CA-C	-8.19	1.42	1.52
4	3-H	552	VAL	CA-C	-8.19	1.42	1.52
5	1-D	51	THR	CA-C	-8.19	1.42	1.52
5	2-D	51	THR	CA-C	-8.19	1.42	1.52
5	3-D	51	THR	CA-C	-8.19	1.42	1.52
8	1-L	48	ILE	CA-C	-8.18	1.42	1.52
4	1-H	154	ASP	CA-C	-8.18	1.42	1.53
8	2-L	48	ILE	CA-C	-8.18	1.42	1.52
4	2-H	154	ASP	CA-C	-8.18	1.42	1.53
8	3-L	48	ILE	CA-C	-8.18	1.42	1.52
4	3-H	154	ASP	CA-C	-8.18	1.42	1.53
5	1-D	61	MET	CA-C	-8.18	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2-D	61	MET	CA-C	-8.18	1.43	1.52
5	3-D	61	MET	CA-C	-8.18	1.43	1.52
1	1-A	602	ALA	CA-C	-8.18	1.42	1.52
3	1-B	61	ILE	CA-C	-8.18	1.42	1.52
8	1-Z	129	VAL	CA-C	-8.18	1.43	1.52
1	2-A	602	ALA	CA-C	-8.18	1.42	1.52
3	2-B	61	ILE	CA-C	-8.18	1.42	1.52
8	2-Z	129	VAL	CA-C	-8.18	1.43	1.52
1	3-A	602	ALA	CA-C	-8.18	1.42	1.52
3	3-B	61	ILE	CA-C	-8.18	1.42	1.52
8	3-Z	129	VAL	CA-C	-8.18	1.43	1.52
6	1-M	171	GLU	CA-C	-8.18	1.42	1.52
6	2-M	171	GLU	CA-C	-8.18	1.42	1.52
6	3-M	171	GLU	CA-C	-8.18	1.42	1.52
3	1-B	373	ILE	N-CA	-8.17	1.36	1.46
3	2-B	373	ILE	N-CA	-8.17	1.36	1.46
3	3-B	373	ILE	N-CA	-8.17	1.36	1.46
3	1-N	275	VAL	CA-C	-8.16	1.42	1.52
3	2-N	275	VAL	CA-C	-8.16	1.42	1.52
3	3-N	275	VAL	CA-C	-8.16	1.42	1.52
4	1-C	154	ASP	CA-C	-8.16	1.42	1.53
4	2-C	154	ASP	CA-C	-8.16	1.42	1.53
4	3-C	154	ASP	CA-C	-8.16	1.42	1.53
3	1-B	477	LEU	CA-C	-8.16	1.42	1.52
3	2-B	477	LEU	CA-C	-8.16	1.42	1.52
3	3-B	477	LEU	CA-C	-8.16	1.42	1.52
1	1-A	56	GLY	CA-C	-8.15	1.44	1.51
3	1-B	417	ILE	CA-C	-8.15	1.45	1.52
1	2-A	56	GLY	CA-C	-8.15	1.44	1.51
3	2-B	417	ILE	CA-C	-8.15	1.45	1.52
1	3-A	56	GLY	CA-C	-8.15	1.44	1.51
3	3-B	417	ILE	CA-C	-8.15	1.45	1.52
8	1-L	18	ILE	CA-C	-8.14	1.42	1.52
3	1-N	417	ILE	CA-C	-8.14	1.45	1.52
8	2-L	18	ILE	CA-C	-8.14	1.42	1.52
3	2-N	417	ILE	CA-C	-8.14	1.45	1.52
8	3-L	18	ILE	CA-C	-8.14	1.42	1.52
3	3-N	417	ILE	CA-C	-8.14	1.45	1.52
4	1-H	383	LEU	CA-C	-8.13	1.42	1.53
4	2-H	383	LEU	CA-C	-8.13	1.42	1.53
4	3-H	383	LEU	CA-C	-8.13	1.42	1.53
7	1-G	233	ILE	CA-C	-8.12	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	233	ILE	CA-C	-8.12	1.42	1.52
7	3-G	233	ILE	CA-C	-8.12	1.42	1.52
3	1-B	275	VAL	CA-C	-8.11	1.43	1.52
3	2-B	275	VAL	CA-C	-8.11	1.43	1.52
3	3-B	275	VAL	CA-C	-8.11	1.43	1.52
1	1-A	21	ARG	CA-C	-8.11	1.43	1.52
1	1-A	598	LYS	CA-C	-8.11	1.42	1.52
1	2-A	21	ARG	CA-C	-8.11	1.43	1.52
1	2-A	598	LYS	CA-C	-8.11	1.42	1.52
1	3-A	21	ARG	CA-C	-8.11	1.43	1.52
1	3-A	598	LYS	CA-C	-8.11	1.42	1.52
4	1-C	552	VAL	CA-C	-8.10	1.43	1.52
4	2-C	552	VAL	CA-C	-8.10	1.43	1.52
4	3-C	552	VAL	CA-C	-8.10	1.43	1.52
4	1-C	383	LEU	CA-C	-8.10	1.42	1.53
4	2-C	383	LEU	CA-C	-8.10	1.42	1.53
4	3-C	383	LEU	CA-C	-8.10	1.42	1.53
6	1-M	34	LEU	CA-C	-8.09	1.42	1.52
6	2-M	34	LEU	CA-C	-8.09	1.42	1.52
6	3-M	34	LEU	CA-C	-8.09	1.42	1.52
3	1-B	457	MET	N-CA	-8.08	1.36	1.46
3	1-N	373	ILE	N-CA	-8.08	1.36	1.46
3	2-B	457	MET	N-CA	-8.08	1.36	1.46
3	2-N	373	ILE	N-CA	-8.08	1.36	1.46
3	3-B	457	MET	N-CA	-8.08	1.36	1.46
3	3-N	373	ILE	N-CA	-8.08	1.36	1.46
6	1-R	38	LYS	CA-C	-8.07	1.42	1.52
3	1-N	440	ARG	N-CA	-8.07	1.36	1.46
6	2-R	38	LYS	CA-C	-8.07	1.42	1.52
3	2-N	440	ARG	N-CA	-8.07	1.36	1.46
6	3-R	38	LYS	CA-C	-8.07	1.42	1.52
3	3-N	440	ARG	N-CA	-8.07	1.36	1.46
7	1-K	105	VAL	N-CA	-8.06	1.34	1.46
4	1-H	169	VAL	CA-C	-8.06	1.43	1.52
7	2-K	105	VAL	N-CA	-8.06	1.34	1.46
4	2-H	169	VAL	CA-C	-8.06	1.43	1.52
7	3-K	105	VAL	N-CA	-8.06	1.34	1.46
4	3-H	169	VAL	CA-C	-8.06	1.43	1.52
1	1-A	715	LYS	CA-C	-8.06	1.42	1.52
1	2-A	715	LYS	CA-C	-8.06	1.42	1.52
1	3-A	715	LYS	CA-C	-8.06	1.42	1.52
7	1-G	173	VAL	CA-C	-8.05	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	173	VAL	CA-C	-8.05	1.42	1.52
7	3-G	173	VAL	CA-C	-8.05	1.42	1.52
3	1-B	440	ARG	N-CA	-8.05	1.36	1.46
3	2-B	440	ARG	N-CA	-8.05	1.36	1.46
3	3-B	440	ARG	N-CA	-8.05	1.36	1.46
7	1-G	143	TYR	CA-C	-8.04	1.42	1.52
7	2-G	143	TYR	CA-C	-8.04	1.42	1.52
7	3-G	143	TYR	CA-C	-8.04	1.42	1.52
7	1-G	869	ILE	CA-C	-8.04	1.42	1.52
7	2-G	869	ILE	CA-C	-8.04	1.42	1.52
7	3-G	869	ILE	CA-C	-8.04	1.42	1.52
7	1-G	254	PHE	CA-C	-8.04	1.42	1.52
7	2-G	254	PHE	CA-C	-8.04	1.42	1.52
7	3-G	254	PHE	CA-C	-8.04	1.42	1.52
3	1-N	339	ASP	CA-C	-8.04	1.42	1.52
3	2-N	339	ASP	CA-C	-8.04	1.42	1.52
3	3-N	339	ASP	CA-C	-8.04	1.42	1.52
7	1-K	869	ILE	CA-C	-8.03	1.42	1.52
7	2-K	869	ILE	CA-C	-8.03	1.42	1.52
7	3-K	869	ILE	CA-C	-8.03	1.42	1.52
1	1-A	673	CYS	N-CA	-8.02	1.36	1.46
1	2-A	673	CYS	N-CA	-8.02	1.36	1.46
1	3-A	673	CYS	N-CA	-8.02	1.36	1.46
3	1-B	810	GLU	CA-C	-8.02	1.42	1.52
7	1-K	843	ARG	CA-C	-8.02	1.42	1.52
3	2-B	810	GLU	CA-C	-8.02	1.42	1.52
7	2-K	843	ARG	CA-C	-8.02	1.42	1.52
3	3-B	810	GLU	CA-C	-8.02	1.42	1.52
7	3-K	843	ARG	CA-C	-8.02	1.42	1.52
1	1-A	659	GLU	CA-C	-8.02	1.42	1.52
7	1-G	173	VAL	N-CA	-8.02	1.37	1.46
1	2-A	659	GLU	CA-C	-8.02	1.42	1.52
7	2-G	173	VAL	N-CA	-8.02	1.37	1.46
1	3-A	659	GLU	CA-C	-8.02	1.42	1.52
7	3-G	173	VAL	N-CA	-8.02	1.37	1.46
3	1-N	460	VAL	CA-C	-8.01	1.43	1.52
3	2-N	460	VAL	CA-C	-8.01	1.43	1.52
3	3-N	460	VAL	CA-C	-8.01	1.43	1.52
6	1-R	23	VAL	CA-C	-8.01	1.43	1.52
6	2-R	23	VAL	CA-C	-8.01	1.43	1.52
6	3-R	23	VAL	CA-C	-8.01	1.43	1.52
7	1-G	730	PHE	CA-C	-8.00	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	730	PHE	CA-C	-8.00	1.43	1.52
7	3-G	730	PHE	CA-C	-8.00	1.43	1.52
3	1-N	457	MET	N-CA	-8.00	1.36	1.46
3	2-N	457	MET	N-CA	-8.00	1.36	1.46
3	3-N	457	MET	N-CA	-8.00	1.36	1.46
1	1-A	191	GLY	CA-C	-7.99	1.40	1.51
7	1-G	843	ARG	CA-C	-7.99	1.42	1.52
1	2-A	191	GLY	CA-C	-7.99	1.40	1.51
7	2-G	843	ARG	CA-C	-7.99	1.42	1.52
1	3-A	191	GLY	CA-C	-7.99	1.40	1.51
7	3-G	843	ARG	CA-C	-7.99	1.42	1.52
7	1-K	730	PHE	CA-C	-7.99	1.43	1.52
7	2-K	730	PHE	CA-C	-7.99	1.43	1.52
7	3-K	730	PHE	CA-C	-7.99	1.43	1.52
1	1-A	675	GLU	CA-C	-7.99	1.42	1.52
4	1-C	601	ARG	CA-C	-7.99	1.42	1.52
1	2-A	675	GLU	CA-C	-7.99	1.42	1.52
4	2-C	601	ARG	CA-C	-7.99	1.42	1.52
1	3-A	675	GLU	CA-C	-7.99	1.42	1.52
4	3-C	601	ARG	CA-C	-7.99	1.42	1.52
3	1-B	460	VAL	CA-C	-7.98	1.43	1.52
8	1-Z	134	ILE	CA-C	-7.98	1.43	1.52
3	2-B	460	VAL	CA-C	-7.98	1.43	1.52
8	2-Z	134	ILE	CA-C	-7.98	1.43	1.52
3	3-B	460	VAL	CA-C	-7.98	1.43	1.52
8	3-Z	134	ILE	CA-C	-7.98	1.43	1.52
4	1-C	419	LYS	CA-C	-7.96	1.42	1.52
4	2-C	419	LYS	CA-C	-7.96	1.42	1.52
4	3-C	419	LYS	CA-C	-7.96	1.42	1.52
3	1-B	339	ASP	CA-C	-7.96	1.42	1.52
3	2-B	339	ASP	CA-C	-7.96	1.42	1.52
3	3-B	339	ASP	CA-C	-7.96	1.42	1.52
4	1-C	169	VAL	CA-C	-7.95	1.43	1.52
4	2-C	169	VAL	CA-C	-7.95	1.43	1.52
4	3-C	169	VAL	CA-C	-7.95	1.43	1.52
1	1-A	213	PHE	CA-C	-7.95	1.43	1.52
3	1-B	379	VAL	N-CA	-7.95	1.37	1.46
6	1-R	154	PHE	CA-C	-7.95	1.42	1.52
1	2-A	213	PHE	CA-C	-7.95	1.43	1.52
3	2-B	379	VAL	N-CA	-7.95	1.37	1.46
6	2-R	154	PHE	CA-C	-7.95	1.42	1.52
1	3-A	213	PHE	CA-C	-7.95	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	379	VAL	N-CA	-7.95	1.37	1.46
6	3-R	154	PHE	CA-C	-7.95	1.42	1.52
4	1-H	601	ARG	CA-C	-7.94	1.42	1.52
4	2-H	601	ARG	CA-C	-7.94	1.42	1.52
4	3-H	601	ARG	CA-C	-7.94	1.42	1.52
4	1-H	419	LYS	CA-C	-7.94	1.42	1.52
4	2-H	419	LYS	CA-C	-7.94	1.42	1.52
4	3-H	419	LYS	CA-C	-7.94	1.42	1.52
7	1-K	191	MET	CA-C	-7.94	1.42	1.52
7	2-K	191	MET	CA-C	-7.94	1.42	1.52
7	3-K	191	MET	CA-C	-7.94	1.42	1.52
3	1-B	453	ILE	N-CA	-7.93	1.37	1.46
7	1-K	84	LEU	CA-C	-7.93	1.42	1.52
3	2-B	453	ILE	N-CA	-7.93	1.37	1.46
7	2-K	84	LEU	CA-C	-7.93	1.42	1.52
3	3-B	453	ILE	N-CA	-7.93	1.37	1.46
7	3-K	84	LEU	CA-C	-7.93	1.42	1.52
4	1-C	85	ASN	N-CA	-7.93	1.35	1.46
4	2-C	85	ASN	N-CA	-7.93	1.35	1.46
4	3-C	85	ASN	N-CA	-7.93	1.35	1.46
3	1-N	453	ILE	N-CA	-7.93	1.37	1.46
3	2-N	453	ILE	N-CA	-7.93	1.37	1.46
3	3-N	453	ILE	N-CA	-7.93	1.37	1.46
8	1-L	143	VAL	CA-C	-7.92	1.43	1.52
8	2-L	143	VAL	CA-C	-7.92	1.43	1.52
8	3-L	143	VAL	CA-C	-7.92	1.43	1.52
7	1-G	530	PHE	CA-C	-7.92	1.42	1.52
7	2-G	530	PHE	CA-C	-7.92	1.42	1.52
7	3-G	530	PHE	CA-C	-7.92	1.42	1.52
4	1-C	544	ASN	CA-C	-7.92	1.42	1.52
4	2-C	544	ASN	CA-C	-7.92	1.42	1.52
4	3-C	544	ASN	CA-C	-7.92	1.42	1.52
4	1-H	544	ASN	CA-C	-7.92	1.42	1.52
4	2-H	544	ASN	CA-C	-7.92	1.42	1.52
4	3-H	544	ASN	CA-C	-7.92	1.42	1.52
4	1-C	379	THR	CA-C	-7.91	1.43	1.52
4	1-H	359	GLN	CA-C	-7.91	1.42	1.52
4	2-C	379	THR	CA-C	-7.91	1.43	1.52
4	2-H	359	GLN	CA-C	-7.91	1.42	1.52
4	3-C	379	THR	CA-C	-7.91	1.43	1.52
4	3-H	359	GLN	CA-C	-7.91	1.42	1.52
3	1-B	758	VAL	CA-C	-7.90	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	758	VAL	CA-C	-7.90	1.43	1.52
3	3-B	758	VAL	CA-C	-7.90	1.43	1.52
7	1-G	499	GLY	CA-C	-7.89	1.43	1.52
7	2-G	499	GLY	CA-C	-7.89	1.43	1.52
7	3-G	499	GLY	CA-C	-7.89	1.43	1.52
4	1-C	359	GLN	CA-C	-7.88	1.42	1.52
4	2-C	359	GLN	CA-C	-7.88	1.42	1.52
4	3-C	359	GLN	CA-C	-7.88	1.42	1.52
6	1-M	90	PHE	N-CA	-7.88	1.36	1.46
6	2-M	90	PHE	N-CA	-7.88	1.36	1.46
6	3-M	90	PHE	N-CA	-7.88	1.36	1.46
4	1-C	360	HIS	CA-C	-7.88	1.42	1.53
4	2-C	360	HIS	CA-C	-7.88	1.42	1.53
4	3-C	360	HIS	CA-C	-7.88	1.42	1.53
6	1-M	159	CYS	CA-C	-7.87	1.43	1.52
6	2-M	159	CYS	CA-C	-7.87	1.43	1.52
6	3-M	159	CYS	CA-C	-7.87	1.43	1.52
4	1-H	360	HIS	CA-C	-7.87	1.42	1.53
4	2-H	360	HIS	CA-C	-7.87	1.42	1.53
4	3-H	360	HIS	CA-C	-7.87	1.42	1.53
3	1-B	820	TYR	CA-C	-7.87	1.42	1.52
4	1-C	535	ILE	N-CA	-7.87	1.36	1.46
7	1-G	484	HIS	CA-C	-7.87	1.42	1.52
3	2-B	820	TYR	CA-C	-7.87	1.42	1.52
4	2-C	535	ILE	N-CA	-7.87	1.36	1.46
7	2-G	484	HIS	CA-C	-7.87	1.42	1.52
3	3-B	820	TYR	CA-C	-7.87	1.42	1.52
4	3-C	535	ILE	N-CA	-7.87	1.36	1.46
7	3-G	484	HIS	CA-C	-7.87	1.42	1.52
8	1-L	113	ALA	CA-C	-7.85	1.42	1.52
8	2-L	113	ALA	CA-C	-7.85	1.42	1.52
8	3-L	113	ALA	CA-C	-7.85	1.42	1.52
3	1-B	770	ASN	CA-C	-7.85	1.43	1.52
3	2-B	770	ASN	CA-C	-7.85	1.43	1.52
3	3-B	770	ASN	CA-C	-7.85	1.43	1.52
1	1-A	659	GLU	N-CA	-7.85	1.36	1.46
4	1-H	379	THR	CA-C	-7.85	1.43	1.52
1	2-A	659	GLU	N-CA	-7.85	1.36	1.46
4	2-H	379	THR	CA-C	-7.85	1.43	1.52
1	3-A	659	GLU	N-CA	-7.85	1.36	1.46
4	3-H	379	THR	CA-C	-7.85	1.43	1.52
8	1-L	44	PHE	CA-C	-7.84	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2-L	44	PHE	CA-C	-7.84	1.42	1.52
8	3-L	44	PHE	CA-C	-7.84	1.42	1.52
4	1-C	442	ARG	CA-C	-7.84	1.43	1.52
4	2-C	442	ARG	CA-C	-7.84	1.43	1.52
4	3-C	442	ARG	CA-C	-7.84	1.43	1.52
4	1-H	85	ASN	N-CA	-7.83	1.35	1.46
4	2-H	85	ASN	N-CA	-7.83	1.35	1.46
4	3-H	85	ASN	N-CA	-7.83	1.35	1.46
4	1-C	385	ASN	CA-C	-7.83	1.42	1.52
4	1-H	385	ASN	CA-C	-7.83	1.42	1.52
4	2-C	385	ASN	CA-C	-7.83	1.42	1.52
4	2-H	385	ASN	CA-C	-7.83	1.42	1.52
4	3-C	385	ASN	CA-C	-7.83	1.42	1.52
4	3-H	385	ASN	CA-C	-7.83	1.42	1.52
7	1-K	166	LEU	CA-C	-7.82	1.42	1.52
4	1-H	535	ILE	N-CA	-7.82	1.36	1.46
7	2-K	166	LEU	CA-C	-7.82	1.42	1.52
4	2-H	535	ILE	N-CA	-7.82	1.36	1.46
7	3-K	166	LEU	CA-C	-7.82	1.42	1.52
4	3-H	535	ILE	N-CA	-7.82	1.36	1.46
3	1-N	318	ASP	CA-C	-7.82	1.42	1.52
3	2-N	318	ASP	CA-C	-7.82	1.42	1.52
3	3-N	318	ASP	CA-C	-7.82	1.42	1.52
3	1-B	318	ASP	CA-C	-7.81	1.42	1.52
3	2-B	318	ASP	CA-C	-7.81	1.42	1.52
3	3-B	318	ASP	CA-C	-7.81	1.42	1.52
6	1-R	31	THR	CA-C	-7.81	1.42	1.52
6	2-R	31	THR	CA-C	-7.81	1.42	1.52
6	3-R	31	THR	CA-C	-7.81	1.42	1.52
7	1-G	141	GLU	N-CA	-7.80	1.36	1.46
7	2-G	141	GLU	N-CA	-7.80	1.36	1.46
7	3-G	141	GLU	N-CA	-7.80	1.36	1.46
1	1-A	631	LYS	N-CA	-7.80	1.36	1.46
1	1-A	681	ALA	CA-C	-7.80	1.43	1.52
1	2-A	631	LYS	N-CA	-7.80	1.36	1.46
1	2-A	681	ALA	CA-C	-7.80	1.43	1.52
1	3-A	631	LYS	N-CA	-7.80	1.36	1.46
1	3-A	681	ALA	CA-C	-7.80	1.43	1.52
7	1-K	306	ALA	CA-C	-7.79	1.42	1.52
7	2-K	306	ALA	CA-C	-7.79	1.42	1.52
7	3-K	306	ALA	CA-C	-7.79	1.42	1.52
8	1-L	101	LEU	CA-C	-7.78	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2-L	101	LEU	CA-C	-7.78	1.42	1.52
8	3-L	101	LEU	CA-C	-7.78	1.42	1.52
1	1-A	321	ARG	CA-C	-7.78	1.42	1.53
1	2-A	321	ARG	CA-C	-7.78	1.42	1.53
1	3-A	321	ARG	CA-C	-7.78	1.42	1.53
4	1-C	730	MET	CA-C	-7.77	1.42	1.52
4	2-C	730	MET	CA-C	-7.77	1.42	1.52
4	3-C	730	MET	CA-C	-7.77	1.42	1.52
1	1-A	428	VAL	N-CA	-7.77	1.37	1.46
3	1-N	447	ASP	CA-C	-7.77	1.42	1.52
1	2-A	428	VAL	N-CA	-7.77	1.37	1.46
3	2-N	447	ASP	CA-C	-7.77	1.42	1.52
1	3-A	428	VAL	N-CA	-7.77	1.37	1.46
3	3-N	447	ASP	CA-C	-7.77	1.42	1.52
7	1-K	182	GLN	CA-C	-7.76	1.42	1.52
7	2-K	182	GLN	CA-C	-7.76	1.42	1.52
7	3-K	182	GLN	CA-C	-7.76	1.42	1.52
3	1-N	177	ILE	CA-C	-7.75	1.42	1.52
3	2-N	177	ILE	CA-C	-7.75	1.42	1.52
3	3-N	177	ILE	CA-C	-7.75	1.42	1.52
7	1-G	258	CYS	CA-C	-7.75	1.42	1.52
7	2-G	258	CYS	CA-C	-7.75	1.42	1.52
7	3-G	258	CYS	CA-C	-7.75	1.42	1.52
7	1-K	775	ALA	CA-C	-7.75	1.42	1.52
4	1-H	484	SER	CA-C	-7.75	1.42	1.52
7	2-K	775	ALA	CA-C	-7.75	1.42	1.52
4	2-H	484	SER	CA-C	-7.75	1.42	1.52
7	3-K	775	ALA	CA-C	-7.75	1.42	1.52
4	3-H	484	SER	CA-C	-7.75	1.42	1.52
3	1-B	833	VAL	CA-C	-7.74	1.43	1.52
3	2-B	833	VAL	CA-C	-7.74	1.43	1.52
3	3-B	833	VAL	CA-C	-7.74	1.43	1.52
7	1-G	165	HIS	CA-C	-7.74	1.42	1.52
4	1-H	566	TYR	CA-C	-7.74	1.43	1.52
7	2-G	165	HIS	CA-C	-7.74	1.42	1.52
4	2-H	566	TYR	CA-C	-7.74	1.43	1.52
7	3-G	165	HIS	CA-C	-7.74	1.42	1.52
4	3-H	566	TYR	CA-C	-7.74	1.43	1.52
4	1-H	442	ARG	CA-C	-7.73	1.43	1.52
4	2-H	442	ARG	CA-C	-7.73	1.43	1.52
4	3-H	442	ARG	CA-C	-7.73	1.43	1.52
3	1-B	777	THR	CA-C	-7.73	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	777	THR	CA-C	-7.73	1.43	1.52
3	3-B	777	THR	CA-C	-7.73	1.43	1.52
3	1-N	77	ILE	CA-C	-7.73	1.43	1.52
3	2-N	77	ILE	CA-C	-7.73	1.43	1.52
3	3-N	77	ILE	CA-C	-7.73	1.43	1.52
3	1-N	379	VAL	N-CA	-7.73	1.37	1.46
3	2-N	379	VAL	N-CA	-7.73	1.37	1.46
3	3-N	379	VAL	N-CA	-7.73	1.37	1.46
1	1-A	520	ALA	CA-C	-7.73	1.43	1.52
3	1-B	77	ILE	CA-C	-7.73	1.43	1.52
1	2-A	520	ALA	CA-C	-7.73	1.43	1.52
3	2-B	77	ILE	CA-C	-7.73	1.43	1.52
1	3-A	520	ALA	CA-C	-7.73	1.43	1.52
3	3-B	77	ILE	CA-C	-7.73	1.43	1.52
3	1-B	457	MET	CA-C	-7.72	1.42	1.52
4	1-H	573	LEU	N-CA	-7.72	1.36	1.46
3	2-B	457	MET	CA-C	-7.72	1.42	1.52
4	2-H	573	LEU	N-CA	-7.72	1.36	1.46
3	3-B	457	MET	CA-C	-7.72	1.42	1.52
4	3-H	573	LEU	N-CA	-7.72	1.36	1.46
6	1-R	121	TRP	CA-C	-7.72	1.43	1.52
6	2-R	121	TRP	CA-C	-7.72	1.43	1.52
6	3-R	121	TRP	CA-C	-7.72	1.43	1.52
4	1-C	573	LEU	N-CA	-7.72	1.36	1.46
4	2-C	573	LEU	N-CA	-7.72	1.36	1.46
4	3-C	573	LEU	N-CA	-7.72	1.36	1.46
6	1-R	106	VAL	CA-C	-7.71	1.43	1.52
6	2-R	106	VAL	CA-C	-7.71	1.43	1.52
6	3-R	106	VAL	CA-C	-7.71	1.43	1.52
3	1-B	177	ILE	CA-C	-7.71	1.42	1.52
3	2-B	177	ILE	CA-C	-7.71	1.42	1.52
3	3-B	177	ILE	CA-C	-7.71	1.42	1.52
6	1-R	100	ILE	N-CA	-7.71	1.37	1.46
6	2-R	100	ILE	N-CA	-7.71	1.37	1.46
6	3-R	100	ILE	N-CA	-7.71	1.37	1.46
4	1-C	380	ALA	CA-C	-7.70	1.43	1.52
4	2-C	380	ALA	CA-C	-7.70	1.43	1.52
4	3-C	380	ALA	CA-C	-7.70	1.43	1.52
3	1-B	94	LEU	CA-C	-7.70	1.42	1.52
3	2-B	94	LEU	CA-C	-7.70	1.42	1.52
3	3-B	94	LEU	CA-C	-7.70	1.42	1.52
3	1-N	457	MET	CA-C	-7.70	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-H	380	ALA	CA-C	-7.70	1.43	1.52
3	2-N	457	MET	CA-C	-7.70	1.42	1.52
4	2-H	380	ALA	CA-C	-7.70	1.43	1.52
3	3-N	457	MET	CA-C	-7.70	1.42	1.52
4	3-H	380	ALA	CA-C	-7.70	1.43	1.52
3	1-B	761	VAL	N-CA	-7.69	1.37	1.46
3	2-B	761	VAL	N-CA	-7.69	1.37	1.46
3	3-B	761	VAL	N-CA	-7.69	1.37	1.46
7	1-G	178	VAL	N-CA	-7.69	1.37	1.46
7	2-G	178	VAL	N-CA	-7.69	1.37	1.46
7	3-G	178	VAL	N-CA	-7.69	1.37	1.46
3	1-B	447	ASP	CA-C	-7.69	1.42	1.52
4	1-C	566	TYR	CA-C	-7.69	1.43	1.52
3	2-B	447	ASP	CA-C	-7.69	1.42	1.52
4	2-C	566	TYR	CA-C	-7.69	1.43	1.52
3	3-B	447	ASP	CA-C	-7.69	1.42	1.52
4	3-C	566	TYR	CA-C	-7.69	1.43	1.52
8	1-L	105	LEU	CA-C	-7.68	1.42	1.52
8	2-L	105	LEU	CA-C	-7.68	1.42	1.52
8	3-L	105	LEU	CA-C	-7.68	1.42	1.52
4	1-C	774	ARG	CA-C	-7.68	1.42	1.52
8	1-Z	16	ILE	N-CA	-7.68	1.37	1.46
4	2-C	774	ARG	CA-C	-7.68	1.42	1.52
8	2-Z	16	ILE	N-CA	-7.68	1.37	1.46
4	3-C	774	ARG	CA-C	-7.68	1.42	1.52
8	3-Z	16	ILE	N-CA	-7.68	1.37	1.46
1	1-A	675	GLU	N-CA	-7.67	1.37	1.46
4	1-C	588	LEU	N-CA	-7.67	1.36	1.46
1	2-A	675	GLU	N-CA	-7.67	1.37	1.46
4	2-C	588	LEU	N-CA	-7.67	1.36	1.46
1	3-A	675	GLU	N-CA	-7.67	1.37	1.46
4	3-C	588	LEU	N-CA	-7.67	1.36	1.46
4	1-H	326	ASN	CA-C	-7.66	1.42	1.52
4	2-H	326	ASN	CA-C	-7.66	1.42	1.52
4	3-H	326	ASN	CA-C	-7.66	1.42	1.52
4	1-H	588	LEU	N-CA	-7.66	1.36	1.46
4	2-H	588	LEU	N-CA	-7.66	1.36	1.46
4	3-H	588	LEU	N-CA	-7.66	1.36	1.46
3	1-N	94	LEU	CA-C	-7.65	1.43	1.52
3	2-N	94	LEU	CA-C	-7.65	1.43	1.52
3	3-N	94	LEU	CA-C	-7.65	1.43	1.52
4	1-C	484	SER	CA-C	-7.65	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-C	484	SER	CA-C	-7.65	1.42	1.52
4	3-C	484	SER	CA-C	-7.65	1.42	1.52
4	1-H	690	LEU	CA-C	-7.64	1.43	1.52
4	2-H	690	LEU	CA-C	-7.64	1.43	1.52
4	3-H	690	LEU	CA-C	-7.64	1.43	1.52
7	1-G	775	ALA	CA-C	-7.64	1.42	1.52
7	2-G	775	ALA	CA-C	-7.64	1.42	1.52
7	3-G	775	ALA	CA-C	-7.64	1.42	1.52
3	1-B	393	LYS	CA-C	-7.63	1.42	1.52
7	1-G	475	PHE	CA-C	-7.63	1.43	1.52
7	1-K	220	ARG	CA-C	-7.63	1.43	1.52
3	2-B	393	LYS	CA-C	-7.63	1.42	1.52
7	2-G	475	PHE	CA-C	-7.63	1.43	1.52
7	2-K	220	ARG	CA-C	-7.63	1.43	1.52
3	3-B	393	LYS	CA-C	-7.63	1.42	1.52
7	3-G	475	PHE	CA-C	-7.63	1.43	1.52
7	3-K	220	ARG	CA-C	-7.63	1.43	1.52
8	1-Z	68	VAL	CA-C	-7.62	1.43	1.52
8	2-Z	68	VAL	CA-C	-7.62	1.43	1.52
8	3-Z	68	VAL	CA-C	-7.62	1.43	1.52
4	1-C	326	ASN	CA-C	-7.62	1.42	1.52
4	2-C	326	ASN	CA-C	-7.62	1.42	1.52
4	3-C	326	ASN	CA-C	-7.62	1.42	1.52
5	1-I	235	VAL	CA-C	-7.62	1.43	1.52
5	2-I	235	VAL	CA-C	-7.62	1.43	1.52
5	3-I	235	VAL	CA-C	-7.62	1.43	1.52
7	1-G	237	SER	CA-C	-7.62	1.43	1.52
7	2-G	237	SER	CA-C	-7.62	1.43	1.52
7	3-G	237	SER	CA-C	-7.62	1.43	1.52
5	1-D	84	ARG	CA-C	-7.61	1.42	1.52
5	2-D	84	ARG	CA-C	-7.61	1.42	1.52
5	3-D	84	ARG	CA-C	-7.61	1.42	1.52
3	1-B	406	SER	CA-C	-7.61	1.42	1.52
3	2-B	406	SER	CA-C	-7.61	1.42	1.52
3	3-B	406	SER	CA-C	-7.61	1.42	1.52
7	1-G	168	LYS	CA-C	-7.61	1.43	1.52
7	2-G	168	LYS	CA-C	-7.61	1.43	1.52
7	3-G	168	LYS	CA-C	-7.61	1.43	1.52
3	1-B	272	SER	CA-C	-7.61	1.42	1.52
3	2-B	272	SER	CA-C	-7.61	1.42	1.52
3	3-B	272	SER	CA-C	-7.61	1.42	1.52
1	1-A	486	VAL	CA-C	-7.61	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	870	VAL	N-CA	-7.61	1.37	1.46
5	1-D	235	VAL	CA-C	-7.61	1.43	1.52
1	2-A	486	VAL	CA-C	-7.61	1.43	1.52
3	2-B	870	VAL	N-CA	-7.61	1.37	1.46
5	2-D	235	VAL	CA-C	-7.61	1.43	1.52
1	3-A	486	VAL	CA-C	-7.61	1.43	1.52
3	3-B	870	VAL	N-CA	-7.61	1.37	1.46
5	3-D	235	VAL	CA-C	-7.61	1.43	1.52
4	1-H	691	HIS	CA-C	-7.61	1.42	1.52
4	2-H	691	HIS	CA-C	-7.61	1.42	1.52
4	3-H	691	HIS	CA-C	-7.61	1.42	1.52
7	1-K	215	ILE	CA-C	-7.60	1.43	1.52
7	2-K	215	ILE	CA-C	-7.60	1.43	1.52
7	3-K	215	ILE	CA-C	-7.60	1.43	1.52
7	1-K	105	VAL	CA-C	-7.60	1.41	1.52
7	2-K	105	VAL	CA-C	-7.60	1.41	1.52
7	3-K	105	VAL	CA-C	-7.60	1.41	1.52
4	1-C	690	LEU	CA-C	-7.60	1.43	1.52
4	2-C	690	LEU	CA-C	-7.60	1.43	1.52
4	3-C	690	LEU	CA-C	-7.60	1.43	1.52
6	1-M	89	ILE	CA-C	-7.60	1.43	1.52
6	2-M	89	ILE	CA-C	-7.60	1.43	1.52
6	3-M	89	ILE	CA-C	-7.60	1.43	1.52
7	1-K	164	LEU	CA-C	-7.59	1.43	1.52
7	2-K	164	LEU	CA-C	-7.59	1.43	1.52
7	3-K	164	LEU	CA-C	-7.59	1.43	1.52
3	1-N	450	ARG	CA-C	-7.59	1.42	1.52
3	2-N	450	ARG	CA-C	-7.59	1.42	1.52
3	3-N	450	ARG	CA-C	-7.59	1.42	1.52
4	1-C	691	HIS	CA-C	-7.58	1.43	1.52
6	1-F	73	ARG	CA-C	-7.58	1.43	1.52
4	2-C	691	HIS	CA-C	-7.58	1.43	1.52
6	2-F	73	ARG	CA-C	-7.58	1.43	1.52
4	3-C	691	HIS	CA-C	-7.58	1.43	1.52
6	3-F	73	ARG	CA-C	-7.58	1.43	1.52
7	1-G	69	ALA	CA-C	-7.57	1.43	1.52
7	1-K	55	ILE	N-CA	-7.57	1.37	1.46
7	2-G	69	ALA	CA-C	-7.57	1.43	1.52
7	2-K	55	ILE	N-CA	-7.57	1.37	1.46
7	3-G	69	ALA	CA-C	-7.57	1.43	1.52
7	3-K	55	ILE	N-CA	-7.57	1.37	1.46
3	1-B	450	ARG	CA-C	-7.57	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	450	ARG	CA-C	-7.57	1.42	1.52
3	3-B	450	ARG	CA-C	-7.57	1.42	1.52
5	1-I	64	LEU	CA-C	-7.57	1.43	1.52
5	2-I	64	LEU	CA-C	-7.57	1.43	1.52
5	3-I	64	LEU	CA-C	-7.57	1.43	1.52
8	1-L	83	SER	CA-C	-7.56	1.43	1.53
8	2-L	83	SER	CA-C	-7.56	1.43	1.53
8	3-L	83	SER	CA-C	-7.56	1.43	1.53
1	1-A	23	TRP	CA-C	-7.56	1.43	1.52
1	2-A	23	TRP	CA-C	-7.56	1.43	1.52
1	3-A	23	TRP	CA-C	-7.56	1.43	1.52
8	1-L	51	LYS	CA-C	-7.55	1.43	1.52
8	2-L	51	LYS	CA-C	-7.55	1.43	1.52
8	3-L	51	LYS	CA-C	-7.55	1.43	1.52
6	1-R	108	GLN	CA-C	-7.54	1.43	1.52
6	2-R	108	GLN	CA-C	-7.54	1.43	1.52
6	3-R	108	GLN	CA-C	-7.54	1.43	1.52
3	1-N	393	LYS	CA-C	-7.54	1.43	1.52
3	2-N	393	LYS	CA-C	-7.54	1.43	1.52
3	3-N	393	LYS	CA-C	-7.54	1.43	1.52
7	1-G	144	MET	CA-C	-7.54	1.43	1.52
8	1-Z	29	LYS	CA-C	-7.54	1.43	1.52
7	2-G	144	MET	CA-C	-7.54	1.43	1.52
8	2-Z	29	LYS	CA-C	-7.54	1.43	1.52
7	3-G	144	MET	CA-C	-7.54	1.43	1.52
8	3-Z	29	LYS	CA-C	-7.54	1.43	1.52
3	1-N	272	SER	CA-C	-7.54	1.42	1.52
3	2-N	272	SER	CA-C	-7.54	1.42	1.52
3	3-N	272	SER	CA-C	-7.54	1.42	1.52
6	1-R	153	TRP	CA-C	-7.54	1.43	1.52
5	1-I	84	ARG	CA-C	-7.54	1.43	1.52
6	2-R	153	TRP	CA-C	-7.54	1.43	1.52
5	2-I	84	ARG	CA-C	-7.54	1.43	1.52
6	3-R	153	TRP	CA-C	-7.54	1.43	1.52
5	3-I	84	ARG	CA-C	-7.54	1.43	1.52
7	1-G	108	SER	N-CA	-7.53	1.37	1.46
7	2-G	108	SER	N-CA	-7.53	1.37	1.46
7	3-G	108	SER	N-CA	-7.53	1.37	1.46
6	1-R	31	THR	N-CA	-7.52	1.37	1.46
6	1-R	37	LEU	N-CA	-7.52	1.37	1.46
6	1-J	73	ARG	CA-C	-7.52	1.43	1.52
6	2-R	31	THR	N-CA	-7.52	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2-R	37	LEU	N-CA	-7.52	1.37	1.46
6	2-J	73	ARG	CA-C	-7.52	1.43	1.52
6	3-R	31	THR	N-CA	-7.52	1.37	1.46
6	3-R	37	LEU	N-CA	-7.52	1.37	1.46
6	3-J	73	ARG	CA-C	-7.52	1.43	1.52
4	1-C	495	VAL	N-CA	-7.51	1.37	1.46
4	2-C	495	VAL	N-CA	-7.51	1.37	1.46
4	3-C	495	VAL	N-CA	-7.51	1.37	1.46
3	1-B	507	GLU	CA-C	-7.50	1.43	1.52
3	2-B	507	GLU	CA-C	-7.50	1.43	1.52
3	3-B	507	GLU	CA-C	-7.50	1.43	1.52
4	1-H	222	VAL	N-CA	-7.50	1.37	1.46
4	2-H	222	VAL	N-CA	-7.50	1.37	1.46
4	3-H	222	VAL	N-CA	-7.50	1.37	1.46
8	1-L	46	LYS	CA-C	-7.50	1.43	1.52
8	2-L	46	LYS	CA-C	-7.50	1.43	1.52
8	3-L	46	LYS	CA-C	-7.50	1.43	1.52
7	1-K	77	PHE	CA-C	-7.50	1.44	1.53
7	2-K	77	PHE	CA-C	-7.50	1.44	1.53
7	3-K	77	PHE	CA-C	-7.50	1.44	1.53
1	1-A	595	THR	N-CA	-7.50	1.35	1.45
1	2-A	595	THR	N-CA	-7.50	1.35	1.45
1	3-A	595	THR	N-CA	-7.50	1.35	1.45
5	1-D	236	ASP	CA-C	-7.49	1.43	1.52
5	1-I	236	ASP	CA-C	-7.49	1.43	1.52
5	2-D	236	ASP	CA-C	-7.49	1.43	1.52
5	2-I	236	ASP	CA-C	-7.49	1.43	1.52
5	3-D	236	ASP	CA-C	-7.49	1.43	1.52
5	3-I	236	ASP	CA-C	-7.49	1.43	1.52
4	1-C	222	VAL	N-CA	-7.49	1.37	1.46
4	2-C	222	VAL	N-CA	-7.49	1.37	1.46
4	3-C	222	VAL	N-CA	-7.49	1.37	1.46
8	1-L	101	LEU	N-CA	-7.48	1.37	1.46
4	1-H	495	VAL	N-CA	-7.48	1.37	1.46
8	2-L	101	LEU	N-CA	-7.48	1.37	1.46
4	2-H	495	VAL	N-CA	-7.48	1.37	1.46
8	3-L	101	LEU	N-CA	-7.48	1.37	1.46
4	3-H	495	VAL	N-CA	-7.48	1.37	1.46
3	1-B	761	VAL	CA-C	-7.48	1.43	1.52
4	1-H	205	GLY	CA-C	-7.48	1.45	1.52
3	2-B	761	VAL	CA-C	-7.48	1.43	1.52
4	2-H	205	GLY	CA-C	-7.48	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	761	VAL	CA-C	-7.48	1.43	1.52
4	3-H	205	GLY	CA-C	-7.48	1.45	1.52
8	1-Z	25	ARG	CA-C	-7.47	1.43	1.52
8	2-Z	25	ARG	CA-C	-7.47	1.43	1.52
8	3-Z	25	ARG	CA-C	-7.47	1.43	1.52
7	1-G	525	ARG	CA-C	-7.47	1.43	1.52
8	1-L	112	ARG	CA-C	-7.47	1.43	1.52
7	2-G	525	ARG	CA-C	-7.47	1.43	1.52
8	2-L	112	ARG	CA-C	-7.47	1.43	1.52
7	3-G	525	ARG	CA-C	-7.47	1.43	1.52
8	3-L	112	ARG	CA-C	-7.47	1.43	1.52
3	1-B	341	LEU	CA-C	-7.46	1.42	1.52
3	2-B	341	LEU	CA-C	-7.46	1.42	1.52
3	3-B	341	LEU	CA-C	-7.46	1.42	1.52
5	1-D	64	LEU	CA-C	-7.46	1.43	1.52
5	2-D	64	LEU	CA-C	-7.46	1.43	1.52
5	3-D	64	LEU	CA-C	-7.46	1.43	1.52
3	1-N	303	LEU	CA-C	-7.45	1.43	1.52
3	2-N	303	LEU	CA-C	-7.45	1.43	1.52
3	3-N	303	LEU	CA-C	-7.45	1.43	1.52
7	1-K	121	ARG	N-CA	-7.45	1.37	1.46
7	2-K	121	ARG	N-CA	-7.45	1.37	1.46
7	3-K	121	ARG	N-CA	-7.45	1.37	1.46
4	1-H	69	LYS	CA-C	-7.44	1.42	1.52
4	2-H	69	LYS	CA-C	-7.44	1.42	1.52
4	3-H	69	LYS	CA-C	-7.44	1.42	1.52
7	1-G	255	ILE	CA-C	-7.44	1.43	1.52
3	1-N	507	GLU	CA-C	-7.44	1.43	1.52
7	2-G	255	ILE	CA-C	-7.44	1.43	1.52
3	2-N	507	GLU	CA-C	-7.44	1.43	1.52
7	3-G	255	ILE	CA-C	-7.44	1.43	1.52
3	3-N	507	GLU	CA-C	-7.44	1.43	1.52
6	1-R	42	VAL	C-N	7.44	1.43	1.33
6	2-R	42	VAL	C-N	7.44	1.43	1.33
6	3-R	42	VAL	C-N	7.44	1.43	1.33
3	1-B	759	LEU	CA-C	-7.44	1.43	1.52
3	2-B	759	LEU	CA-C	-7.44	1.43	1.52
3	3-B	759	LEU	CA-C	-7.44	1.43	1.52
7	1-G	251	LEU	CA-C	-7.43	1.43	1.52
6	1-M	169	GLY	CA-C	-7.43	1.44	1.52
7	2-G	251	LEU	CA-C	-7.43	1.43	1.52
6	2-M	169	GLY	CA-C	-7.43	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3-G	251	LEU	CA-C	-7.43	1.43	1.52
6	3-M	169	GLY	CA-C	-7.43	1.44	1.52
4	1-C	181	LEU	CA-C	-7.43	1.43	1.52
4	2-C	181	LEU	CA-C	-7.43	1.43	1.52
4	3-C	181	LEU	CA-C	-7.43	1.43	1.52
3	1-N	341	LEU	CA-C	-7.42	1.42	1.52
3	2-N	341	LEU	CA-C	-7.42	1.42	1.52
3	3-N	341	LEU	CA-C	-7.42	1.42	1.52
4	1-C	69	LYS	CA-C	-7.42	1.42	1.52
4	2-C	69	LYS	CA-C	-7.42	1.42	1.52
4	3-C	69	LYS	CA-C	-7.42	1.42	1.52
7	1-G	366	SER	CA-C	-7.42	1.43	1.52
6	1-R	98	SER	CA-C	-7.42	1.42	1.52
7	2-G	366	SER	CA-C	-7.42	1.43	1.52
6	2-R	98	SER	CA-C	-7.42	1.42	1.52
7	3-G	366	SER	CA-C	-7.42	1.43	1.52
6	3-R	98	SER	CA-C	-7.42	1.42	1.52
6	1-R	26	ASP	N-CA	-7.41	1.37	1.46
6	2-R	26	ASP	N-CA	-7.41	1.37	1.46
6	3-R	26	ASP	N-CA	-7.41	1.37	1.46
4	1-C	81	ILE	CA-C	-7.41	1.43	1.52
6	1-R	69	GLY	CA-C	-7.41	1.45	1.52
4	1-H	181	LEU	CA-C	-7.41	1.43	1.52
4	2-C	81	ILE	CA-C	-7.41	1.43	1.52
6	2-R	69	GLY	CA-C	-7.41	1.45	1.52
4	2-H	181	LEU	CA-C	-7.41	1.43	1.52
4	3-C	81	ILE	CA-C	-7.41	1.43	1.52
6	3-R	69	GLY	CA-C	-7.41	1.45	1.52
4	3-H	181	LEU	CA-C	-7.41	1.43	1.52
1	1-A	322	GLU	CA-C	-7.41	1.42	1.52
1	2-A	322	GLU	CA-C	-7.41	1.42	1.52
1	3-A	322	GLU	CA-C	-7.41	1.42	1.52
1	1-A	538	SER	CA-C	-7.40	1.42	1.52
7	1-K	774	ALA	CA-C	-7.40	1.43	1.52
1	2-A	538	SER	CA-C	-7.40	1.42	1.52
7	2-K	774	ALA	CA-C	-7.40	1.43	1.52
1	3-A	538	SER	CA-C	-7.40	1.42	1.52
7	3-K	774	ALA	CA-C	-7.40	1.43	1.52
4	1-C	205	GLY	CA-C	-7.39	1.45	1.52
4	2-C	205	GLY	CA-C	-7.39	1.45	1.52
4	3-C	205	GLY	CA-C	-7.39	1.45	1.52
7	1-K	215	ILE	N-CA	-7.39	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-K	215	ILE	N-CA	-7.39	1.37	1.46
7	3-K	215	ILE	N-CA	-7.39	1.37	1.46
7	1-K	36	GLU	CA-C	-7.38	1.43	1.52
4	1-H	717	GLU	N-CA	-7.38	1.37	1.46
7	2-K	36	GLU	CA-C	-7.38	1.43	1.52
4	2-H	717	GLU	N-CA	-7.38	1.37	1.46
7	3-K	36	GLU	CA-C	-7.38	1.43	1.52
4	3-H	717	GLU	N-CA	-7.38	1.37	1.46
3	1-B	452	LEU	CA-C	-7.38	1.43	1.52
3	2-B	452	LEU	CA-C	-7.38	1.43	1.52
3	3-B	452	LEU	CA-C	-7.38	1.43	1.52
7	1-G	177	TRP	CA-C	-7.38	1.42	1.52
7	2-G	177	TRP	CA-C	-7.38	1.42	1.52
7	3-G	177	TRP	CA-C	-7.38	1.42	1.52
4	1-H	202	LEU	CA-C	-7.38	1.43	1.52
4	2-H	202	LEU	CA-C	-7.38	1.43	1.52
4	3-H	202	LEU	CA-C	-7.38	1.43	1.52
4	1-C	202	LEU	CA-C	-7.37	1.43	1.52
7	1-G	80	ASN	CA-C	-7.37	1.43	1.52
4	2-C	202	LEU	CA-C	-7.37	1.43	1.52
7	2-G	80	ASN	CA-C	-7.37	1.43	1.52
4	3-C	202	LEU	CA-C	-7.37	1.43	1.52
7	3-G	80	ASN	CA-C	-7.37	1.43	1.52
7	1-K	675	GLU	CA-C	-7.37	1.43	1.52
4	1-H	575	LEU	CA-C	-7.37	1.43	1.52
7	2-K	675	GLU	CA-C	-7.37	1.43	1.52
4	2-H	575	LEU	CA-C	-7.37	1.43	1.52
7	3-K	675	GLU	CA-C	-7.37	1.43	1.52
4	3-H	575	LEU	CA-C	-7.37	1.43	1.52
3	1-B	303	LEU	CA-C	-7.37	1.43	1.52
3	2-B	303	LEU	CA-C	-7.37	1.43	1.52
3	3-B	303	LEU	CA-C	-7.37	1.43	1.52
7	1-K	707	TYR	CA-C	-7.36	1.43	1.52
7	2-K	707	TYR	CA-C	-7.36	1.43	1.52
7	3-K	707	TYR	CA-C	-7.36	1.43	1.52
1	1-A	543	TYR	N-CA	-7.36	1.36	1.45
1	2-A	543	TYR	N-CA	-7.36	1.36	1.45
1	3-A	543	TYR	N-CA	-7.36	1.36	1.45
7	1-K	219	THR	CA-C	-7.34	1.43	1.52
7	2-K	219	THR	CA-C	-7.34	1.43	1.52
7	3-K	219	THR	CA-C	-7.34	1.43	1.52
3	1-B	745	ALA	CA-C	-7.34	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	745	ALA	CA-C	-7.34	1.43	1.52
3	3-B	745	ALA	CA-C	-7.34	1.43	1.52
7	1-K	106	THR	CA-C	-7.34	1.43	1.52
7	1-K	107	SER	N-CA	-7.34	1.37	1.46
4	1-H	81	ILE	CA-C	-7.34	1.44	1.52
7	2-K	106	THR	CA-C	-7.34	1.43	1.52
7	2-K	107	SER	N-CA	-7.34	1.37	1.46
4	2-H	81	ILE	CA-C	-7.34	1.44	1.52
7	3-K	106	THR	CA-C	-7.34	1.43	1.52
7	3-K	107	SER	N-CA	-7.34	1.37	1.46
4	3-H	81	ILE	CA-C	-7.34	1.44	1.52
3	1-N	452	LEU	CA-C	-7.34	1.43	1.52
3	2-N	452	LEU	CA-C	-7.34	1.43	1.52
3	3-N	452	LEU	CA-C	-7.34	1.43	1.52
7	1-G	182	GLN	CA-C	-7.33	1.43	1.52
7	2-G	182	GLN	CA-C	-7.33	1.43	1.52
7	3-G	182	GLN	CA-C	-7.33	1.43	1.52
1	1-A	683	LEU	N-CA	-7.33	1.37	1.46
4	1-C	563	LEU	CA-C	-7.33	1.43	1.52
7	1-G	774	ALA	CA-C	-7.33	1.43	1.52
1	2-A	683	LEU	N-CA	-7.33	1.37	1.46
4	2-C	563	LEU	CA-C	-7.33	1.43	1.52
7	2-G	774	ALA	CA-C	-7.33	1.43	1.52
1	3-A	683	LEU	N-CA	-7.33	1.37	1.46
4	3-C	563	LEU	CA-C	-7.33	1.43	1.52
7	3-G	774	ALA	CA-C	-7.33	1.43	1.52
4	1-C	575	LEU	CA-C	-7.33	1.43	1.52
7	1-G	675	GLU	CA-C	-7.33	1.43	1.52
8	1-Z	91	MET	CA-C	-7.33	1.43	1.52
4	2-C	575	LEU	CA-C	-7.33	1.43	1.52
7	2-G	675	GLU	CA-C	-7.33	1.43	1.52
8	2-Z	91	MET	CA-C	-7.33	1.43	1.52
4	3-C	575	LEU	CA-C	-7.33	1.43	1.52
7	3-G	675	GLU	CA-C	-7.33	1.43	1.52
8	3-Z	91	MET	CA-C	-7.33	1.43	1.52
4	1-C	717	GLU	N-CA	-7.33	1.37	1.46
4	2-C	717	GLU	N-CA	-7.33	1.37	1.46
4	3-C	717	GLU	N-CA	-7.33	1.37	1.46
1	1-A	673	CYS	CA-C	-7.32	1.43	1.52
1	2-A	673	CYS	CA-C	-7.32	1.43	1.52
1	3-A	673	CYS	CA-C	-7.32	1.43	1.52
3	1-N	125	GLN	CA-C	-7.32	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-N	125	GLN	CA-C	-7.32	1.42	1.52
3	3-N	125	GLN	CA-C	-7.32	1.42	1.52
8	1-Z	46	LYS	CA-C	-7.32	1.43	1.52
8	2-Z	46	LYS	CA-C	-7.32	1.43	1.52
8	3-Z	46	LYS	CA-C	-7.32	1.43	1.52
7	1-G	93	LYS	CA-C	-7.31	1.42	1.52
7	2-G	93	LYS	CA-C	-7.31	1.42	1.52
7	3-G	93	LYS	CA-C	-7.31	1.42	1.52
7	1-K	89	TYR	CA-C	-7.31	1.43	1.52
7	2-K	89	TYR	CA-C	-7.31	1.43	1.52
7	3-K	89	TYR	CA-C	-7.31	1.43	1.52
3	1-B	461	PHE	N-CA	-7.31	1.37	1.46
4	1-H	450	TYR	CA-C	-7.31	1.43	1.52
3	2-B	461	PHE	N-CA	-7.31	1.37	1.46
4	2-H	450	TYR	CA-C	-7.31	1.43	1.52
3	3-B	461	PHE	N-CA	-7.31	1.37	1.46
4	3-H	450	TYR	CA-C	-7.31	1.43	1.52
6	1-J	149	ARG	CA-C	-7.31	1.43	1.52
6	2-J	149	ARG	CA-C	-7.31	1.43	1.52
6	3-J	149	ARG	CA-C	-7.31	1.43	1.52
4	1-C	450	TYR	CA-C	-7.30	1.43	1.52
4	2-C	450	TYR	CA-C	-7.30	1.43	1.52
4	3-C	450	TYR	CA-C	-7.30	1.43	1.52
3	1-B	125	GLN	CA-C	-7.30	1.42	1.52
6	1-M	74	ILE	CA-C	-7.30	1.43	1.52
6	1-J	77	LEU	CA-C	-7.30	1.44	1.52
3	2-B	125	GLN	CA-C	-7.30	1.42	1.52
6	2-M	74	ILE	CA-C	-7.30	1.43	1.52
6	2-J	77	LEU	CA-C	-7.30	1.44	1.52
3	3-B	125	GLN	CA-C	-7.30	1.42	1.52
6	3-M	74	ILE	CA-C	-7.30	1.43	1.52
6	3-J	77	LEU	CA-C	-7.30	1.44	1.52
7	1-K	611	GLU	CA-C	-7.30	1.43	1.52
7	2-K	611	GLU	CA-C	-7.30	1.43	1.52
7	3-K	611	GLU	CA-C	-7.30	1.43	1.52
7	1-G	611	GLU	CA-C	-7.29	1.43	1.52
4	1-H	563	LEU	CA-C	-7.29	1.43	1.52
5	1-I	100	ASN	CA-C	-7.29	1.43	1.52
7	2-G	611	GLU	CA-C	-7.29	1.43	1.52
4	2-H	563	LEU	CA-C	-7.29	1.43	1.52
5	2-I	100	ASN	CA-C	-7.29	1.43	1.52
7	3-G	611	GLU	CA-C	-7.29	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-H	563	LEU	CA-C	-7.29	1.43	1.52
5	3-I	100	ASN	CA-C	-7.29	1.43	1.52
1	1-A	603	LEU	CA-C	-7.29	1.43	1.52
1	2-A	603	LEU	CA-C	-7.29	1.43	1.52
1	3-A	603	LEU	CA-C	-7.29	1.43	1.52
3	1-N	406	SER	CA-C	-7.29	1.42	1.52
3	2-N	406	SER	CA-C	-7.29	1.42	1.52
3	3-N	406	SER	CA-C	-7.29	1.42	1.52
8	1-L	93	VAL	N-CA	-7.28	1.37	1.46
8	2-L	93	VAL	N-CA	-7.28	1.37	1.46
8	3-L	93	VAL	N-CA	-7.28	1.37	1.46
8	1-L	121	LEU	CA-C	-7.28	1.43	1.52
8	2-L	121	LEU	CA-C	-7.28	1.43	1.52
8	3-L	121	LEU	CA-C	-7.28	1.43	1.52
6	1-F	149	ARG	CA-C	-7.28	1.43	1.52
6	2-F	149	ARG	CA-C	-7.28	1.43	1.52
6	3-F	149	ARG	CA-C	-7.28	1.43	1.52
3	1-N	461	PHE	N-CA	-7.27	1.37	1.46
4	1-H	155	ASN	CA-C	-7.27	1.43	1.52
3	2-N	461	PHE	N-CA	-7.27	1.37	1.46
4	2-H	155	ASN	CA-C	-7.27	1.43	1.52
3	3-N	461	PHE	N-CA	-7.27	1.37	1.46
4	3-H	155	ASN	CA-C	-7.27	1.43	1.52
4	1-C	276	CYS	CA-C	-7.27	1.43	1.52
6	1-M	128	GLN	CA-C	-7.27	1.42	1.52
4	2-C	276	CYS	CA-C	-7.27	1.43	1.52
6	2-M	128	GLN	CA-C	-7.27	1.42	1.52
4	3-C	276	CYS	CA-C	-7.27	1.43	1.52
6	3-M	128	GLN	CA-C	-7.27	1.42	1.52
6	1-R	64	THR	CA-C	-7.26	1.43	1.52
6	1-M	36	LYS	CA-C	-7.26	1.43	1.52
6	2-R	64	THR	CA-C	-7.26	1.43	1.52
6	2-M	36	LYS	CA-C	-7.26	1.43	1.52
6	3-R	64	THR	CA-C	-7.26	1.43	1.52
6	3-M	36	LYS	CA-C	-7.26	1.43	1.52
6	1-R	171	GLU	N-CA	-7.26	1.37	1.46
6	2-R	171	GLU	N-CA	-7.26	1.37	1.46
6	3-R	171	GLU	N-CA	-7.26	1.37	1.46
5	1-I	94	CYS	CA-C	-7.26	1.43	1.52
5	2-I	94	CYS	CA-C	-7.26	1.43	1.52
5	3-I	94	CYS	CA-C	-7.26	1.43	1.52
7	1-G	471	LYS	CA-C	-7.26	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	471	LYS	CA-C	-7.26	1.43	1.52
7	3-G	471	LYS	CA-C	-7.26	1.43	1.52
4	1-H	276	CYS	CA-C	-7.26	1.43	1.52
4	2-H	276	CYS	CA-C	-7.26	1.43	1.52
4	3-H	276	CYS	CA-C	-7.26	1.43	1.52
1	1-A	427	ALA	CA-C	-7.25	1.44	1.52
1	2-A	427	ALA	CA-C	-7.25	1.44	1.52
1	3-A	427	ALA	CA-C	-7.25	1.44	1.52
7	1-G	306	ALA	CA-C	-7.25	1.43	1.52
7	2-G	306	ALA	CA-C	-7.25	1.43	1.52
7	3-G	306	ALA	CA-C	-7.25	1.43	1.52
7	1-G	707	TYR	CA-C	-7.25	1.43	1.52
7	2-G	707	TYR	CA-C	-7.25	1.43	1.52
7	3-G	707	TYR	CA-C	-7.25	1.43	1.52
4	1-C	260	THR	CA-C	-7.24	1.43	1.53
4	2-C	260	THR	CA-C	-7.24	1.43	1.53
4	3-C	260	THR	CA-C	-7.24	1.43	1.53
3	1-N	182	GLU	CA-C	-7.24	1.43	1.52
3	2-N	182	GLU	CA-C	-7.24	1.43	1.52
3	3-N	182	GLU	CA-C	-7.24	1.43	1.52
7	1-G	845	ARG	CA-C	-7.24	1.43	1.52
8	1-L	95	ASN	N-CA	-7.24	1.37	1.46
7	2-G	845	ARG	CA-C	-7.24	1.43	1.52
8	2-L	95	ASN	N-CA	-7.24	1.37	1.46
7	3-G	845	ARG	CA-C	-7.24	1.43	1.52
8	3-L	95	ASN	N-CA	-7.24	1.37	1.46
7	1-G	179	ASN	CA-C	-7.24	1.43	1.52
7	2-G	179	ASN	CA-C	-7.24	1.43	1.52
7	3-G	179	ASN	CA-C	-7.24	1.43	1.52
4	1-C	316	TRP	CA-C	-7.24	1.43	1.52
4	2-C	316	TRP	CA-C	-7.24	1.43	1.52
4	3-C	316	TRP	CA-C	-7.24	1.43	1.52
8	1-L	91	MET	CA-C	-7.23	1.43	1.52
8	2-L	91	MET	CA-C	-7.23	1.43	1.52
8	3-L	91	MET	CA-C	-7.23	1.43	1.52
1	1-A	472	ILE	CA-C	-7.23	1.43	1.52
3	1-B	771	CYS	N-CA	-7.23	1.36	1.46
6	1-R	36	LYS	N-CA	-7.23	1.37	1.46
1	2-A	472	ILE	CA-C	-7.23	1.43	1.52
3	2-B	771	CYS	N-CA	-7.23	1.36	1.46
6	2-R	36	LYS	N-CA	-7.23	1.37	1.46
1	3-A	472	ILE	CA-C	-7.23	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	771	CYS	N-CA	-7.23	1.36	1.46
6	3-R	36	LYS	N-CA	-7.23	1.37	1.46
5	1-D	100	ASN	CA-C	-7.23	1.43	1.52
5	2-D	100	ASN	CA-C	-7.23	1.43	1.52
5	3-D	100	ASN	CA-C	-7.23	1.43	1.52
3	1-B	182	GLU	CA-C	-7.22	1.43	1.52
3	2-B	182	GLU	CA-C	-7.22	1.43	1.52
3	3-B	182	GLU	CA-C	-7.22	1.43	1.52
6	1-F	77	LEU	CA-C	-7.21	1.44	1.52
6	2-F	77	LEU	CA-C	-7.21	1.44	1.52
6	3-F	77	LEU	CA-C	-7.21	1.44	1.52
4	1-C	641	PRO	CA-C	-7.21	1.41	1.52
5	1-D	94	CYS	CA-C	-7.21	1.43	1.52
4	1-H	316	TRP	CA-C	-7.21	1.43	1.52
4	2-C	641	PRO	CA-C	-7.21	1.41	1.52
5	2-D	94	CYS	CA-C	-7.21	1.43	1.52
4	2-H	316	TRP	CA-C	-7.21	1.43	1.52
4	3-C	641	PRO	CA-C	-7.21	1.41	1.52
5	3-D	94	CYS	CA-C	-7.21	1.43	1.52
4	3-H	316	TRP	CA-C	-7.21	1.43	1.52
7	1-K	845	ARG	CA-C	-7.21	1.43	1.52
7	2-K	845	ARG	CA-C	-7.21	1.43	1.52
7	3-K	845	ARG	CA-C	-7.21	1.43	1.52
1	1-A	551	TYR	CA-C	-7.20	1.43	1.52
7	1-K	143	TYR	CA-C	-7.20	1.43	1.52
7	1-K	309	ARG	CA-C	-7.20	1.44	1.52
1	2-A	551	TYR	CA-C	-7.20	1.43	1.52
7	2-K	143	TYR	CA-C	-7.20	1.43	1.52
7	2-K	309	ARG	CA-C	-7.20	1.44	1.52
1	3-A	551	TYR	CA-C	-7.20	1.43	1.52
7	3-K	143	TYR	CA-C	-7.20	1.43	1.52
7	3-K	309	ARG	CA-C	-7.20	1.44	1.52
1	1-A	35	LEU	CA-C	-7.20	1.44	1.52
1	2-A	35	LEU	CA-C	-7.20	1.44	1.52
1	3-A	35	LEU	CA-C	-7.20	1.44	1.52
7	1-K	70	PHE	CA-C	-7.20	1.43	1.52
4	1-H	641	PRO	CA-C	-7.20	1.41	1.52
7	2-K	70	PHE	CA-C	-7.20	1.43	1.52
4	2-H	641	PRO	CA-C	-7.20	1.41	1.52
7	3-K	70	PHE	CA-C	-7.20	1.43	1.52
4	3-H	641	PRO	CA-C	-7.20	1.41	1.52
7	1-G	174	VAL	N-CA	-7.20	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	174	VAL	N-CA	-7.20	1.37	1.46
7	3-G	174	VAL	N-CA	-7.20	1.37	1.46
1	1-A	766	GLY	CA-C	-7.19	1.41	1.51
1	2-A	766	GLY	CA-C	-7.19	1.41	1.51
1	3-A	766	GLY	CA-C	-7.19	1.41	1.51
5	1-D	80	LEU	CA-C	-7.19	1.43	1.52
8	1-Z	45	GLU	CA-C	-7.19	1.43	1.52
5	2-D	80	LEU	CA-C	-7.19	1.43	1.52
8	2-Z	45	GLU	CA-C	-7.19	1.43	1.52
5	3-D	80	LEU	CA-C	-7.19	1.43	1.52
8	3-Z	45	GLU	CA-C	-7.19	1.43	1.52
3	1-N	227	CYS	CA-C	-7.19	1.42	1.52
3	2-N	227	CYS	CA-C	-7.19	1.42	1.52
3	3-N	227	CYS	CA-C	-7.19	1.42	1.52
3	1-B	227	CYS	CA-C	-7.18	1.42	1.52
3	2-B	227	CYS	CA-C	-7.18	1.42	1.52
3	3-B	227	CYS	CA-C	-7.18	1.42	1.52
6	1-R	155	ILE	N-CA	-7.18	1.37	1.46
6	2-R	155	ILE	N-CA	-7.18	1.37	1.46
6	3-R	155	ILE	N-CA	-7.18	1.37	1.46
8	1-Z	77	PHE	CA-C	-7.18	1.44	1.52
5	1-I	80	LEU	CA-C	-7.18	1.43	1.52
8	2-Z	77	PHE	CA-C	-7.18	1.44	1.52
5	2-I	80	LEU	CA-C	-7.18	1.43	1.52
8	3-Z	77	PHE	CA-C	-7.18	1.44	1.52
5	3-I	80	LEU	CA-C	-7.18	1.43	1.52
3	1-B	370	GLU	CA-C	-7.18	1.43	1.52
3	1-B	948	SER	CA-C	-7.18	1.43	1.52
7	1-G	88	CYS	CA-C	-7.18	1.43	1.52
3	2-B	370	GLU	CA-C	-7.18	1.43	1.52
3	2-B	948	SER	CA-C	-7.18	1.43	1.52
7	2-G	88	CYS	CA-C	-7.18	1.43	1.52
3	3-B	370	GLU	CA-C	-7.18	1.43	1.52
3	3-B	948	SER	CA-C	-7.18	1.43	1.52
7	3-G	88	CYS	CA-C	-7.18	1.43	1.52
6	1-J	60	ASN	CA-C	-7.18	1.43	1.53
6	2-J	60	ASN	CA-C	-7.18	1.43	1.53
6	3-J	60	ASN	CA-C	-7.18	1.43	1.53
3	1-N	310	ASN	CA-C	-7.17	1.43	1.52
3	2-N	310	ASN	CA-C	-7.17	1.43	1.52
3	3-N	310	ASN	CA-C	-7.17	1.43	1.52
4	1-C	155	ASN	CA-C	-7.17	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-C	155	ASN	CA-C	-7.17	1.43	1.52
4	3-C	155	ASN	CA-C	-7.17	1.43	1.52
1	1-A	244	THR	N-CA	-7.17	1.37	1.46
7	1-K	218	PHE	CA-C	-7.17	1.42	1.52
1	2-A	244	THR	N-CA	-7.17	1.37	1.46
7	2-K	218	PHE	CA-C	-7.17	1.42	1.52
1	3-A	244	THR	N-CA	-7.17	1.37	1.46
7	3-K	218	PHE	CA-C	-7.17	1.42	1.52
7	1-G	148	ILE	CA-C	-7.17	1.43	1.52
7	2-G	148	ILE	CA-C	-7.17	1.43	1.52
7	3-G	148	ILE	CA-C	-7.17	1.43	1.52
8	1-Z	87	GLU	CA-C	-7.16	1.43	1.52
8	2-Z	87	GLU	CA-C	-7.16	1.43	1.52
8	3-Z	87	GLU	CA-C	-7.16	1.43	1.52
7	1-G	750	GLU	CA-C	-7.16	1.44	1.52
7	2-G	750	GLU	CA-C	-7.16	1.44	1.52
7	3-G	750	GLU	CA-C	-7.16	1.44	1.52
4	1-H	260	THR	CA-C	-7.16	1.43	1.53
4	2-H	260	THR	CA-C	-7.16	1.43	1.53
4	3-H	260	THR	CA-C	-7.16	1.43	1.53
3	1-N	370	GLU	CA-C	-7.15	1.43	1.52
3	2-N	370	GLU	CA-C	-7.15	1.43	1.52
3	3-N	370	GLU	CA-C	-7.15	1.43	1.52
3	1-B	800	ILE	CA-C	-7.15	1.44	1.52
3	2-B	800	ILE	CA-C	-7.15	1.44	1.52
3	3-B	800	ILE	CA-C	-7.15	1.44	1.52
3	1-B	817	ASN	CA-C	-7.15	1.43	1.52
3	2-B	817	ASN	CA-C	-7.15	1.43	1.52
3	3-B	817	ASN	CA-C	-7.15	1.43	1.52
4	1-H	471	SER	CA-C	-7.15	1.43	1.53
4	2-H	471	SER	CA-C	-7.15	1.43	1.53
4	3-H	471	SER	CA-C	-7.15	1.43	1.53
4	1-C	315	ILE	CA-C	-7.14	1.44	1.52
4	1-C	776	ASN	CA-C	-7.14	1.43	1.52
4	1-H	367	VAL	N-CA	-7.14	1.37	1.46
4	2-C	315	ILE	CA-C	-7.14	1.44	1.52
4	2-C	776	ASN	CA-C	-7.14	1.43	1.52
4	2-H	367	VAL	N-CA	-7.14	1.37	1.46
4	3-C	315	ILE	CA-C	-7.14	1.44	1.52
4	3-C	776	ASN	CA-C	-7.14	1.43	1.52
4	3-H	367	VAL	N-CA	-7.14	1.37	1.46
4	1-H	215	ASP	CA-C	-7.14	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-H	315	ILE	CA-C	-7.14	1.44	1.52
4	2-H	215	ASP	CA-C	-7.14	1.44	1.52
4	2-H	315	ILE	CA-C	-7.14	1.44	1.52
4	3-H	215	ASP	CA-C	-7.14	1.44	1.52
4	3-H	315	ILE	CA-C	-7.14	1.44	1.52
3	1-B	400	ARG	CA-C	-7.13	1.43	1.52
3	2-B	400	ARG	CA-C	-7.13	1.43	1.52
3	3-B	400	ARG	CA-C	-7.13	1.43	1.52
3	1-B	310	ASN	CA-C	-7.13	1.43	1.52
3	1-B	363	VAL	N-CA	-7.13	1.38	1.46
3	2-B	310	ASN	CA-C	-7.13	1.43	1.52
3	2-B	363	VAL	N-CA	-7.13	1.38	1.46
3	3-B	310	ASN	CA-C	-7.13	1.43	1.52
3	3-B	363	VAL	N-CA	-7.13	1.38	1.46
1	1-A	578	VAL	CA-C	-7.12	1.44	1.52
1	2-A	578	VAL	CA-C	-7.12	1.44	1.52
1	3-A	578	VAL	CA-C	-7.12	1.44	1.52
3	1-B	435	VAL	CA-C	-7.12	1.44	1.52
4	1-C	471	SER	CA-C	-7.12	1.43	1.53
3	2-B	435	VAL	CA-C	-7.12	1.44	1.52
4	2-C	471	SER	CA-C	-7.12	1.43	1.53
3	3-B	435	VAL	CA-C	-7.12	1.44	1.52
4	3-C	471	SER	CA-C	-7.12	1.43	1.53
3	1-B	804	VAL	N-CA	-7.12	1.37	1.46
6	1-M	153	TRP	CA-C	-7.12	1.44	1.52
3	2-B	804	VAL	N-CA	-7.12	1.37	1.46
6	2-M	153	TRP	CA-C	-7.12	1.44	1.52
3	3-B	804	VAL	N-CA	-7.12	1.37	1.46
6	3-M	153	TRP	CA-C	-7.12	1.44	1.52
6	1-R	85	THR	CA-C	-7.11	1.43	1.52
6	2-R	85	THR	CA-C	-7.11	1.43	1.52
6	3-R	85	THR	CA-C	-7.11	1.43	1.52
3	1-B	837	ILE	N-CA	-7.11	1.37	1.46
4	1-C	840	LYS	CA-C	-7.11	1.43	1.52
4	1-H	327	LEU	CA-C	-7.11	1.43	1.52
3	2-B	837	ILE	N-CA	-7.11	1.37	1.46
4	2-C	840	LYS	CA-C	-7.11	1.43	1.52
4	2-H	327	LEU	CA-C	-7.11	1.43	1.52
3	3-B	837	ILE	N-CA	-7.11	1.37	1.46
4	3-C	840	LYS	CA-C	-7.11	1.43	1.52
4	3-H	327	LEU	CA-C	-7.11	1.43	1.52
1	1-A	243	ASP	N-CA	-7.11	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	243	ASP	N-CA	-7.11	1.37	1.46
1	3-A	243	ASP	N-CA	-7.11	1.37	1.46
6	1-R	36	LYS	CA-C	-7.10	1.43	1.52
6	2-R	36	LYS	CA-C	-7.10	1.43	1.52
6	3-R	36	LYS	CA-C	-7.10	1.43	1.52
4	1-C	215	ASP	CA-C	-7.10	1.44	1.52
4	2-C	215	ASP	CA-C	-7.10	1.44	1.52
4	3-C	215	ASP	CA-C	-7.10	1.44	1.52
4	1-C	188	VAL	CA-C	-7.09	1.43	1.52
4	2-C	188	VAL	CA-C	-7.09	1.43	1.52
4	3-C	188	VAL	CA-C	-7.09	1.43	1.52
7	1-K	263	HIS	CA-C	-7.09	1.45	1.53
7	2-K	263	HIS	CA-C	-7.09	1.45	1.53
7	3-K	263	HIS	CA-C	-7.09	1.45	1.53
7	1-G	460	GLY	CA-C	-7.08	1.43	1.51
7	2-G	460	GLY	CA-C	-7.08	1.43	1.51
7	3-G	460	GLY	CA-C	-7.08	1.43	1.51
6	1-M	29	GLY	CA-C	-7.08	1.42	1.51
6	2-M	29	GLY	CA-C	-7.08	1.42	1.51
6	3-M	29	GLY	CA-C	-7.08	1.42	1.51
4	1-C	567	ILE	CA-C	-7.08	1.47	1.53
4	1-H	567	ILE	CA-C	-7.08	1.47	1.53
4	2-C	567	ILE	CA-C	-7.08	1.47	1.53
4	2-H	567	ILE	CA-C	-7.08	1.47	1.53
4	3-C	567	ILE	CA-C	-7.08	1.47	1.53
4	3-H	567	ILE	CA-C	-7.08	1.47	1.53
5	1-D	57	VAL	CA-C	-7.07	1.44	1.52
5	2-D	57	VAL	CA-C	-7.07	1.44	1.52
5	3-D	57	VAL	CA-C	-7.07	1.44	1.52
3	1-N	400	ARG	CA-C	-7.07	1.43	1.52
5	1-I	57	VAL	CA-C	-7.07	1.44	1.52
3	2-N	400	ARG	CA-C	-7.07	1.43	1.52
5	2-I	57	VAL	CA-C	-7.07	1.44	1.52
3	3-N	400	ARG	CA-C	-7.07	1.43	1.52
5	3-I	57	VAL	CA-C	-7.07	1.44	1.52
6	1-M	46	ILE	CA-C	-7.07	1.47	1.53
6	2-M	46	ILE	CA-C	-7.07	1.47	1.53
6	3-M	46	ILE	CA-C	-7.07	1.47	1.53
3	1-N	181	PHE	CA-C	-7.06	1.43	1.52
3	2-N	181	PHE	CA-C	-7.06	1.43	1.52
3	3-N	181	PHE	CA-C	-7.06	1.43	1.52
7	1-G	397	LEU	CA-C	-7.06	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	397	LEU	CA-C	-7.06	1.43	1.52
7	3-G	397	LEU	CA-C	-7.06	1.43	1.52
6	1-J	53	VAL	CA-C	-7.05	1.44	1.52
6	2-J	53	VAL	CA-C	-7.05	1.44	1.52
6	3-J	53	VAL	CA-C	-7.05	1.44	1.52
3	1-B	181	PHE	CA-C	-7.05	1.43	1.52
3	2-B	181	PHE	CA-C	-7.05	1.43	1.52
3	3-B	181	PHE	CA-C	-7.05	1.43	1.52
4	1-C	367	VAL	N-CA	-7.05	1.37	1.46
8	1-Z	27	PHE	CA-C	-7.05	1.43	1.52
7	1-K	268	TYR	CA-C	-7.05	1.43	1.52
4	2-C	367	VAL	N-CA	-7.05	1.37	1.46
8	2-Z	27	PHE	CA-C	-7.05	1.43	1.52
7	2-K	268	TYR	CA-C	-7.05	1.43	1.52
4	3-C	367	VAL	N-CA	-7.05	1.37	1.46
8	3-Z	27	PHE	CA-C	-7.05	1.43	1.52
7	3-K	268	TYR	CA-C	-7.05	1.43	1.52
1	1-A	66	PHE	CA-C	-7.05	1.44	1.52
1	2-A	66	PHE	CA-C	-7.05	1.44	1.52
1	3-A	66	PHE	CA-C	-7.05	1.44	1.52
6	1-R	43	ILE	CA-C	7.04	1.61	1.52
6	2-R	43	ILE	CA-C	7.04	1.61	1.52
6	3-R	43	ILE	CA-C	7.04	1.61	1.52
4	1-C	177	PRO	CA-C	-7.04	1.45	1.52
6	1-F	60	ASN	N-CA	-7.04	1.37	1.46
7	1-G	522	ASN	CA-C	-7.04	1.43	1.52
4	1-H	534	PHE	N-CA	-7.04	1.37	1.46
4	2-C	177	PRO	CA-C	-7.04	1.45	1.52
6	2-F	60	ASN	N-CA	-7.04	1.37	1.46
7	2-G	522	ASN	CA-C	-7.04	1.43	1.52
4	2-H	534	PHE	N-CA	-7.04	1.37	1.46
4	3-C	177	PRO	CA-C	-7.04	1.45	1.52
6	3-F	60	ASN	N-CA	-7.04	1.37	1.46
7	3-G	522	ASN	CA-C	-7.04	1.43	1.52
4	3-H	534	PHE	N-CA	-7.04	1.37	1.46
4	1-H	543	LEU	CA-C	-7.04	1.44	1.52
4	2-H	543	LEU	CA-C	-7.04	1.44	1.52
4	3-H	543	LEU	CA-C	-7.04	1.44	1.52
4	1-C	15	SER	CA-C	-7.04	1.47	1.53
4	2-C	15	SER	CA-C	-7.04	1.47	1.53
4	3-C	15	SER	CA-C	-7.04	1.47	1.53
6	1-F	60	ASN	CA-C	-7.03	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1-Z	102	SER	N-CA	-7.03	1.38	1.46
6	2-F	60	ASN	CA-C	-7.03	1.43	1.52
8	2-Z	102	SER	N-CA	-7.03	1.38	1.46
6	3-F	60	ASN	CA-C	-7.03	1.43	1.52
8	3-Z	102	SER	N-CA	-7.03	1.38	1.46
4	1-C	327	LEU	CA-C	-7.03	1.43	1.52
5	1-D	61	MET	N-CA	-7.03	1.38	1.46
4	2-C	327	LEU	CA-C	-7.03	1.43	1.52
5	2-D	61	MET	N-CA	-7.03	1.38	1.46
4	3-C	327	LEU	CA-C	-7.03	1.43	1.52
5	3-D	61	MET	N-CA	-7.03	1.38	1.46
4	1-H	15	SER	CA-C	-7.02	1.47	1.53
4	2-H	15	SER	CA-C	-7.02	1.47	1.53
4	3-H	15	SER	CA-C	-7.02	1.47	1.53
1	1-A	672	ASN	CA-C	-7.02	1.43	1.52
7	1-G	284	GLU	CA-C	-7.02	1.43	1.52
1	2-A	672	ASN	CA-C	-7.02	1.43	1.52
7	2-G	284	GLU	CA-C	-7.02	1.43	1.52
1	3-A	672	ASN	CA-C	-7.02	1.43	1.52
7	3-G	284	GLU	CA-C	-7.02	1.43	1.52
8	1-Z	18	ILE	CA-C	-7.02	1.43	1.52
8	2-Z	18	ILE	CA-C	-7.02	1.43	1.52
8	3-Z	18	ILE	CA-C	-7.02	1.43	1.52
1	1-A	21	ARG	N-CA	-7.02	1.41	1.46
3	1-B	381	LYS	N-CA	-7.02	1.37	1.46
3	1-B	850	CYS	CA-C	7.02	1.61	1.52
3	1-B	943	ARG	CA-C	-7.02	1.44	1.52
4	1-C	257	HIS	N-CA	-7.02	1.37	1.46
6	1-F	166	LEU	CA-C	-7.02	1.44	1.52
1	2-A	21	ARG	N-CA	-7.02	1.41	1.46
3	2-B	381	LYS	N-CA	-7.02	1.37	1.46
3	2-B	850	CYS	CA-C	7.02	1.61	1.52
3	2-B	943	ARG	CA-C	-7.02	1.44	1.52
4	2-C	257	HIS	N-CA	-7.02	1.37	1.46
6	2-F	166	LEU	CA-C	-7.02	1.44	1.52
1	3-A	21	ARG	N-CA	-7.02	1.41	1.46
3	3-B	381	LYS	N-CA	-7.02	1.37	1.46
3	3-B	850	CYS	CA-C	7.02	1.61	1.52
3	3-B	943	ARG	CA-C	-7.02	1.44	1.52
4	3-C	257	HIS	N-CA	-7.02	1.37	1.46
6	3-F	166	LEU	CA-C	-7.02	1.44	1.52
4	1-C	165	ARG	CA-C	-7.02	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1-F	167	TYR	N-CA	-7.02	1.37	1.46
3	1-N	435	VAL	CA-C	-7.02	1.44	1.52
4	2-C	165	ARG	CA-C	-7.02	1.43	1.52
6	2-F	167	TYR	N-CA	-7.02	1.37	1.46
3	2-N	435	VAL	CA-C	-7.02	1.44	1.52
4	3-C	165	ARG	CA-C	-7.02	1.43	1.52
6	3-F	167	TYR	N-CA	-7.02	1.37	1.46
3	3-N	435	VAL	CA-C	-7.02	1.44	1.52
7	1-G	347	THR	CA-C	-7.01	1.43	1.52
7	2-G	347	THR	CA-C	-7.01	1.43	1.52
7	3-G	347	THR	CA-C	-7.01	1.43	1.52
4	1-C	543	LEU	CA-C	-7.01	1.44	1.52
6	1-F	53	VAL	CA-C	-7.01	1.44	1.52
4	2-C	543	LEU	CA-C	-7.01	1.44	1.52
6	2-F	53	VAL	CA-C	-7.01	1.44	1.52
4	3-C	543	LEU	CA-C	-7.01	1.44	1.52
6	3-F	53	VAL	CA-C	-7.01	1.44	1.52
7	1-G	390	TYR	N-CA	-7.00	1.40	1.46
5	1-I	61	MET	N-CA	-7.00	1.38	1.46
6	1-J	167	TYR	N-CA	-7.00	1.37	1.46
7	2-G	390	TYR	N-CA	-7.00	1.40	1.46
5	2-I	61	MET	N-CA	-7.00	1.38	1.46
6	2-J	167	TYR	N-CA	-7.00	1.37	1.46
7	3-G	390	TYR	N-CA	-7.00	1.40	1.46
5	3-I	61	MET	N-CA	-7.00	1.38	1.46
6	3-J	167	TYR	N-CA	-7.00	1.37	1.46
3	1-B	340	ILE	N-CA	-7.00	1.38	1.46
3	2-B	340	ILE	N-CA	-7.00	1.38	1.46
3	3-B	340	ILE	N-CA	-7.00	1.38	1.46
3	1-N	363	VAL	N-CA	-7.00	1.39	1.46
3	2-N	363	VAL	N-CA	-7.00	1.39	1.46
3	3-N	363	VAL	N-CA	-7.00	1.39	1.46
4	1-C	534	PHE	N-CA	-6.99	1.37	1.46
4	2-C	534	PHE	N-CA	-6.99	1.37	1.46
4	3-C	534	PHE	N-CA	-6.99	1.37	1.46
8	1-Z	104	MET	CA-C	-6.99	1.44	1.52
4	1-H	190	CYS	CA-C	-6.99	1.43	1.52
8	2-Z	104	MET	CA-C	-6.99	1.44	1.52
4	2-H	190	CYS	CA-C	-6.99	1.43	1.52
8	3-Z	104	MET	CA-C	-6.99	1.44	1.52
4	3-H	190	CYS	CA-C	-6.99	1.43	1.52
7	1-K	750	GLU	CA-C	-6.99	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-N	340	ILE	N-CA	-6.99	1.38	1.46
7	2-K	750	GLU	CA-C	-6.99	1.44	1.52
3	2-N	340	ILE	N-CA	-6.99	1.38	1.46
7	3-K	750	GLU	CA-C	-6.99	1.44	1.52
3	3-N	340	ILE	N-CA	-6.99	1.38	1.46
7	1-K	290	SER	CA-C	-6.98	1.44	1.52
4	1-H	165	ARG	CA-C	-6.98	1.43	1.52
7	2-K	290	SER	CA-C	-6.98	1.44	1.52
4	2-H	165	ARG	CA-C	-6.98	1.43	1.52
7	3-K	290	SER	CA-C	-6.98	1.44	1.52
4	3-H	165	ARG	CA-C	-6.98	1.43	1.52
3	1-B	437	GLU	CA-C	-6.98	1.43	1.52
6	1-M	77	LEU	CA-C	-6.98	1.43	1.52
3	2-B	437	GLU	CA-C	-6.98	1.43	1.52
6	2-M	77	LEU	CA-C	-6.98	1.43	1.52
3	3-B	437	GLU	CA-C	-6.98	1.43	1.52
6	3-M	77	LEU	CA-C	-6.98	1.43	1.52
7	1-G	72	ALA	CA-C	-6.98	1.44	1.52
8	1-L	123	LEU	CA-C	-6.98	1.43	1.52
7	2-G	72	ALA	CA-C	-6.98	1.44	1.52
8	2-L	123	LEU	CA-C	-6.98	1.43	1.52
7	3-G	72	ALA	CA-C	-6.98	1.44	1.52
8	3-L	123	LEU	CA-C	-6.98	1.43	1.52
3	1-N	437	GLU	CA-C	-6.98	1.43	1.52
3	2-N	437	GLU	CA-C	-6.98	1.43	1.52
3	3-N	437	GLU	CA-C	-6.98	1.43	1.52
6	1-J	166	LEU	CA-C	-6.97	1.44	1.52
6	2-J	166	LEU	CA-C	-6.97	1.44	1.52
6	3-J	166	LEU	CA-C	-6.97	1.44	1.52
3	1-B	371	LEU	CA-C	-6.97	1.44	1.52
4	1-H	188	VAL	CA-C	-6.97	1.43	1.52
3	2-B	371	LEU	CA-C	-6.97	1.44	1.52
4	2-H	188	VAL	CA-C	-6.97	1.43	1.52
3	3-B	371	LEU	CA-C	-6.97	1.44	1.52
4	3-H	188	VAL	CA-C	-6.97	1.43	1.52
3	1-N	371	LEU	CA-C	-6.96	1.44	1.52
3	2-N	371	LEU	CA-C	-6.96	1.44	1.52
3	3-N	371	LEU	CA-C	-6.96	1.44	1.52
4	1-H	386	LYS	N-CA	-6.96	1.38	1.46
4	2-H	386	LYS	N-CA	-6.96	1.38	1.46
4	3-H	386	LYS	N-CA	-6.96	1.38	1.46
8	1-L	122	PHE	CA-C	-6.96	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2-L	122	PHE	CA-C	-6.96	1.44	1.52
8	3-L	122	PHE	CA-C	-6.96	1.44	1.52
4	1-H	407	GLU	CA-C	-6.96	1.43	1.52
4	2-H	407	GLU	CA-C	-6.96	1.43	1.52
4	3-H	407	GLU	CA-C	-6.96	1.43	1.52
3	1-B	261	ILE	CA-C	-6.96	1.44	1.52
7	1-K	79	SER	CA-C	-6.96	1.44	1.52
4	1-H	439	LEU	CA-C	-6.96	1.43	1.52
3	2-B	261	ILE	CA-C	-6.96	1.44	1.52
7	2-K	79	SER	CA-C	-6.96	1.44	1.52
4	2-H	439	LEU	CA-C	-6.96	1.43	1.52
3	3-B	261	ILE	CA-C	-6.96	1.44	1.52
7	3-K	79	SER	CA-C	-6.96	1.44	1.52
4	3-H	439	LEU	CA-C	-6.96	1.43	1.52
7	1-G	526	ASP	CA-C	-6.96	1.43	1.52
7	2-G	526	ASP	CA-C	-6.96	1.43	1.52
7	3-G	526	ASP	CA-C	-6.96	1.43	1.52
1	1-A	757	LEU	CA-C	-6.95	1.43	1.52
7	1-G	248	ASP	N-CA	-6.95	1.37	1.46
1	2-A	757	LEU	CA-C	-6.95	1.43	1.52
7	2-G	248	ASP	N-CA	-6.95	1.37	1.46
1	3-A	757	LEU	CA-C	-6.95	1.43	1.52
7	3-G	248	ASP	N-CA	-6.95	1.37	1.46
4	1-C	493	GLU	CA-C	-6.95	1.43	1.52
4	2-C	493	GLU	CA-C	-6.95	1.43	1.52
4	3-C	493	GLU	CA-C	-6.95	1.43	1.52
3	1-N	261	ILE	CA-C	-6.95	1.44	1.52
3	1-N	409	PHE	CA-C	-6.95	1.44	1.52
3	2-N	261	ILE	CA-C	-6.95	1.44	1.52
3	2-N	409	PHE	CA-C	-6.95	1.44	1.52
3	3-N	261	ILE	CA-C	-6.95	1.44	1.52
3	3-N	409	PHE	CA-C	-6.95	1.44	1.52
4	1-C	407	GLU	CA-C	-6.94	1.43	1.52
4	2-C	407	GLU	CA-C	-6.94	1.43	1.52
4	3-C	407	GLU	CA-C	-6.94	1.43	1.52
4	1-H	493	GLU	CA-C	-6.94	1.43	1.52
4	2-H	493	GLU	CA-C	-6.94	1.43	1.52
4	3-H	493	GLU	CA-C	-6.94	1.43	1.52
8	1-Z	27	PHE	N-CA	-6.94	1.37	1.46
8	1-Z	78	TYR	N-CA	-6.94	1.37	1.46
7	1-K	54	LEU	CA-C	-6.94	1.43	1.52
8	2-Z	27	PHE	N-CA	-6.94	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2-Z	78	TYR	N-CA	-6.94	1.37	1.46
7	2-K	54	LEU	CA-C	-6.94	1.43	1.52
8	3-Z	27	PHE	N-CA	-6.94	1.37	1.46
8	3-Z	78	TYR	N-CA	-6.94	1.37	1.46
7	3-K	54	LEU	CA-C	-6.94	1.43	1.52
4	1-H	257	HIS	N-CA	-6.93	1.37	1.46
4	2-H	257	HIS	N-CA	-6.93	1.37	1.46
4	3-H	257	HIS	N-CA	-6.93	1.37	1.46
4	1-C	593	GLU	CA-C	-6.93	1.43	1.52
4	2-C	593	GLU	CA-C	-6.93	1.43	1.52
4	3-C	593	GLU	CA-C	-6.93	1.43	1.52
3	1-N	381	LYS	N-CA	-6.93	1.38	1.46
3	2-N	381	LYS	N-CA	-6.93	1.38	1.46
3	3-N	381	LYS	N-CA	-6.93	1.38	1.46
4	1-C	190	CYS	CA-C	-6.93	1.44	1.52
4	2-C	190	CYS	CA-C	-6.93	1.44	1.52
4	3-C	190	CYS	CA-C	-6.93	1.44	1.52
4	1-H	177	PRO	CA-C	-6.92	1.45	1.52
4	1-H	382	ALA	N-CA	-6.92	1.37	1.46
4	2-H	177	PRO	CA-C	-6.92	1.45	1.52
4	2-H	382	ALA	N-CA	-6.92	1.37	1.46
4	3-H	177	PRO	CA-C	-6.92	1.45	1.52
4	3-H	382	ALA	N-CA	-6.92	1.37	1.46
3	1-B	409	PHE	CA-C	-6.92	1.44	1.52
3	1-N	399	VAL	N-CA	-6.92	1.38	1.46
3	2-B	409	PHE	CA-C	-6.92	1.44	1.52
3	2-N	399	VAL	N-CA	-6.92	1.38	1.46
3	3-B	409	PHE	CA-C	-6.92	1.44	1.52
3	3-N	399	VAL	N-CA	-6.92	1.38	1.46
3	1-B	399	VAL	N-CA	-6.91	1.38	1.46
3	2-B	399	VAL	N-CA	-6.91	1.38	1.46
3	3-B	399	VAL	N-CA	-6.91	1.38	1.46
7	1-G	255	ILE	N-CA	-6.91	1.38	1.46
7	1-K	200	LEU	N-CA	-6.91	1.38	1.46
7	2-G	255	ILE	N-CA	-6.91	1.38	1.46
7	2-K	200	LEU	N-CA	-6.91	1.38	1.46
7	3-G	255	ILE	N-CA	-6.91	1.38	1.46
7	3-K	200	LEU	N-CA	-6.91	1.38	1.46
4	1-C	119	ASP	CA-C	-6.91	1.42	1.52
8	1-L	134	ILE	CA-C	-6.91	1.44	1.52
4	2-C	119	ASP	CA-C	-6.91	1.42	1.52
8	2-L	134	ILE	CA-C	-6.91	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-C	119	ASP	CA-C	-6.91	1.42	1.52
8	3-L	134	ILE	CA-C	-6.91	1.44	1.52
7	1-G	210	ALA	CA-C	-6.90	1.43	1.52
7	2-G	210	ALA	CA-C	-6.90	1.43	1.52
7	3-G	210	ALA	CA-C	-6.90	1.43	1.52
3	1-B	763	GLN	CA-C	-6.90	1.42	1.52
4	1-C	533	CYS	CA-C	-6.90	1.43	1.52
4	1-H	533	CYS	CA-C	-6.90	1.43	1.52
3	2-B	763	GLN	CA-C	-6.90	1.42	1.52
4	2-C	533	CYS	CA-C	-6.90	1.43	1.52
4	2-H	533	CYS	CA-C	-6.90	1.43	1.52
3	3-B	763	GLN	CA-C	-6.90	1.42	1.52
4	3-C	533	CYS	CA-C	-6.90	1.43	1.52
4	3-H	533	CYS	CA-C	-6.90	1.43	1.52
1	1-A	554	THR	CA-C	6.90	1.60	1.52
1	2-A	554	THR	CA-C	6.90	1.60	1.52
1	3-A	554	THR	CA-C	6.90	1.60	1.52
4	1-C	477	VAL	CA-C	-6.90	1.44	1.52
4	1-H	384	ARG	N-CA	-6.90	1.37	1.45
4	2-C	477	VAL	CA-C	-6.90	1.44	1.52
4	2-H	384	ARG	N-CA	-6.90	1.37	1.45
4	3-C	477	VAL	CA-C	-6.90	1.44	1.52
4	3-H	384	ARG	N-CA	-6.90	1.37	1.45
8	1-L	143	VAL	N-CA	-6.90	1.38	1.46
4	1-H	593	GLU	CA-C	-6.90	1.44	1.52
8	2-L	143	VAL	N-CA	-6.90	1.38	1.46
4	2-H	593	GLU	CA-C	-6.90	1.44	1.52
8	3-L	143	VAL	N-CA	-6.90	1.38	1.46
4	3-H	593	GLU	CA-C	-6.90	1.44	1.52
4	1-C	382	ALA	N-CA	-6.89	1.37	1.46
4	2-C	382	ALA	N-CA	-6.89	1.37	1.46
4	3-C	382	ALA	N-CA	-6.89	1.37	1.46
4	1-C	439	LEU	CA-C	-6.89	1.43	1.52
4	2-C	439	LEU	CA-C	-6.89	1.43	1.52
4	3-C	439	LEU	CA-C	-6.89	1.43	1.52
5	1-D	100	ASN	N-CA	-6.89	1.38	1.46
5	2-D	100	ASN	N-CA	-6.89	1.38	1.46
5	3-D	100	ASN	N-CA	-6.89	1.38	1.46
4	1-C	384	ARG	N-CA	-6.89	1.37	1.45
7	1-K	825	THR	C-N	6.89	1.42	1.33
4	2-C	384	ARG	N-CA	-6.89	1.37	1.45
7	2-K	825	THR	C-N	6.89	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-C	384	ARG	N-CA	-6.89	1.37	1.45
7	3-K	825	THR	C-N	6.89	1.42	1.33
7	1-G	680	GLN	CA-C	-6.89	1.43	1.52
7	2-G	680	GLN	CA-C	-6.89	1.43	1.52
7	3-G	680	GLN	CA-C	-6.89	1.43	1.52
4	1-C	386	LYS	N-CA	-6.88	1.38	1.46
3	1-N	435	VAL	N-CA	-6.88	1.38	1.46
4	2-C	386	LYS	N-CA	-6.88	1.38	1.46
3	2-N	435	VAL	N-CA	-6.88	1.38	1.46
4	3-C	386	LYS	N-CA	-6.88	1.38	1.46
3	3-N	435	VAL	N-CA	-6.88	1.38	1.46
4	1-C	347	ASP	CA-C	-6.88	1.43	1.53
4	2-C	347	ASP	CA-C	-6.88	1.43	1.53
4	3-C	347	ASP	CA-C	-6.88	1.43	1.53
1	1-A	569	TYR	N-CA	-6.87	1.37	1.46
4	1-H	138	PHE	CA-C	-6.87	1.44	1.52
1	2-A	569	TYR	N-CA	-6.87	1.37	1.46
4	2-H	138	PHE	CA-C	-6.87	1.44	1.52
1	3-A	569	TYR	N-CA	-6.87	1.37	1.46
4	3-H	138	PHE	CA-C	-6.87	1.44	1.52
4	1-H	154	ASP	N-CA	-6.87	1.37	1.46
4	2-H	154	ASP	N-CA	-6.87	1.37	1.46
4	3-H	154	ASP	N-CA	-6.87	1.37	1.46
6	1-M	70	GLY	CA-C	-6.86	1.42	1.51
6	2-M	70	GLY	CA-C	-6.86	1.42	1.51
6	3-M	70	GLY	CA-C	-6.86	1.42	1.51
6	1-R	111	LEU	N-CA	-6.86	1.37	1.46
6	1-J	68	VAL	CA-C	-6.86	1.44	1.52
6	2-R	111	LEU	N-CA	-6.86	1.37	1.46
6	2-J	68	VAL	CA-C	-6.86	1.44	1.52
6	3-R	111	LEU	N-CA	-6.86	1.37	1.46
6	3-J	68	VAL	CA-C	-6.86	1.44	1.52
4	1-C	263	LEU	CA-C	-6.86	1.44	1.52
4	2-C	263	LEU	CA-C	-6.86	1.44	1.52
4	3-C	263	LEU	CA-C	-6.86	1.44	1.52
5	1-I	100	ASN	N-CA	-6.86	1.38	1.46
5	2-I	100	ASN	N-CA	-6.86	1.38	1.46
5	3-I	100	ASN	N-CA	-6.86	1.38	1.46
6	1-F	68	VAL	CA-C	-6.85	1.44	1.52
6	2-F	68	VAL	CA-C	-6.85	1.44	1.52
6	3-F	68	VAL	CA-C	-6.85	1.44	1.52
7	1-K	706	CYS	CA-C	-6.85	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-K	706	CYS	CA-C	-6.85	1.44	1.52
7	3-K	706	CYS	CA-C	-6.85	1.44	1.52
3	1-B	435	VAL	N-CA	-6.85	1.38	1.46
3	2-B	435	VAL	N-CA	-6.85	1.38	1.46
3	3-B	435	VAL	N-CA	-6.85	1.38	1.46
7	1-G	379	VAL	N-CA	-6.84	1.38	1.46
7	2-G	379	VAL	N-CA	-6.84	1.38	1.46
7	3-G	379	VAL	N-CA	-6.84	1.38	1.46
4	1-C	138	PHE	CA-C	-6.84	1.44	1.52
4	2-C	138	PHE	CA-C	-6.84	1.44	1.52
4	3-C	138	PHE	CA-C	-6.84	1.44	1.52
1	1-A	630	GLN	CA-C	-6.84	1.42	1.52
7	1-G	45	ALA	CA-C	-6.84	1.43	1.52
1	2-A	630	GLN	CA-C	-6.84	1.42	1.52
7	2-G	45	ALA	CA-C	-6.84	1.43	1.52
1	3-A	630	GLN	CA-C	-6.84	1.42	1.52
7	3-G	45	ALA	CA-C	-6.84	1.43	1.52
4	1-C	154	ASP	N-CA	-6.84	1.37	1.46
4	1-H	477	VAL	CA-C	-6.84	1.44	1.52
4	2-C	154	ASP	N-CA	-6.84	1.37	1.46
4	2-H	477	VAL	CA-C	-6.84	1.44	1.52
4	3-C	154	ASP	N-CA	-6.84	1.37	1.46
4	3-H	477	VAL	CA-C	-6.84	1.44	1.52
4	1-H	119	ASP	CA-C	-6.84	1.42	1.52
4	2-H	119	ASP	CA-C	-6.84	1.42	1.52
4	3-H	119	ASP	CA-C	-6.84	1.42	1.52
4	1-H	347	ASP	CA-C	-6.84	1.43	1.53
4	2-H	347	ASP	CA-C	-6.84	1.43	1.53
4	3-H	347	ASP	CA-C	-6.84	1.43	1.53
5	1-I	236	ASP	N-CA	-6.83	1.38	1.46
5	2-I	236	ASP	N-CA	-6.83	1.38	1.46
5	3-I	236	ASP	N-CA	-6.83	1.38	1.46
4	1-C	716	ALA	CA-C	-6.83	1.44	1.52
7	1-G	825	THR	C-N	6.83	1.42	1.33
4	1-H	716	ALA	CA-C	-6.83	1.44	1.52
4	2-C	716	ALA	CA-C	-6.83	1.44	1.52
7	2-G	825	THR	C-N	6.83	1.42	1.33
4	2-H	716	ALA	CA-C	-6.83	1.44	1.52
4	3-C	716	ALA	CA-C	-6.83	1.44	1.52
7	3-G	825	THR	C-N	6.83	1.42	1.33
4	3-H	716	ALA	CA-C	-6.83	1.44	1.52
8	1-L	53	HIS	N-CA	-6.83	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2-L	53	HIS	N-CA	-6.83	1.37	1.46
8	3-L	53	HIS	N-CA	-6.83	1.37	1.46
1	1-A	568	ILE	CA-C	-6.83	1.44	1.52
1	2-A	568	ILE	CA-C	-6.83	1.44	1.52
1	3-A	568	ILE	CA-C	-6.83	1.44	1.52
5	1-D	236	ASP	N-CA	-6.82	1.38	1.46
5	2-D	236	ASP	N-CA	-6.82	1.38	1.46
5	3-D	236	ASP	N-CA	-6.82	1.38	1.46
8	1-L	104	MET	CA-C	-6.82	1.44	1.52
8	2-L	104	MET	CA-C	-6.82	1.44	1.52
8	3-L	104	MET	CA-C	-6.82	1.44	1.52
5	1-D	27	THR	CA-C	-6.82	1.43	1.52
5	2-D	27	THR	CA-C	-6.82	1.43	1.52
5	3-D	27	THR	CA-C	-6.82	1.43	1.52
7	1-K	680	GLN	CA-C	-6.82	1.43	1.52
7	2-K	680	GLN	CA-C	-6.82	1.43	1.52
7	3-K	680	GLN	CA-C	-6.82	1.43	1.52
3	1-B	958	LYS	CA-C	-6.81	1.44	1.52
3	2-B	958	LYS	CA-C	-6.81	1.44	1.52
3	3-B	958	LYS	CA-C	-6.81	1.44	1.52
8	1-L	141	GLN	N-CA	-6.80	1.38	1.46
8	2-L	141	GLN	N-CA	-6.80	1.38	1.46
8	3-L	141	GLN	N-CA	-6.80	1.38	1.46
4	1-C	368	VAL	CA-C	-6.80	1.44	1.52
6	1-M	88	VAL	CA-C	-6.80	1.43	1.52
6	1-J	151	ARG	CA-C	-6.80	1.44	1.52
4	2-C	368	VAL	CA-C	-6.80	1.44	1.52
6	2-M	88	VAL	CA-C	-6.80	1.43	1.52
6	2-J	151	ARG	CA-C	-6.80	1.44	1.52
4	3-C	368	VAL	CA-C	-6.80	1.44	1.52
6	3-M	88	VAL	CA-C	-6.80	1.43	1.52
6	3-J	151	ARG	CA-C	-6.80	1.44	1.52
8	1-L	99	ASP	CA-C	-6.80	1.44	1.52
3	1-N	163	HIS	CA-C	-6.80	1.44	1.52
4	1-H	202	LEU	N-CA	-6.80	1.37	1.45
8	2-L	99	ASP	CA-C	-6.80	1.44	1.52
3	2-N	163	HIS	CA-C	-6.80	1.44	1.52
4	2-H	202	LEU	N-CA	-6.80	1.37	1.45
8	3-L	99	ASP	CA-C	-6.80	1.44	1.52
3	3-N	163	HIS	CA-C	-6.80	1.44	1.52
4	3-H	202	LEU	N-CA	-6.80	1.37	1.45
4	1-C	202	LEU	N-CA	-6.80	1.37	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-C	202	LEU	N-CA	-6.80	1.37	1.45
4	3-C	202	LEU	N-CA	-6.80	1.37	1.45
4	1-C	478	CYS	CA-C	-6.80	1.44	1.52
4	1-H	390	SER	CA-C	-6.80	1.44	1.52
4	2-C	478	CYS	CA-C	-6.80	1.44	1.52
4	2-H	390	SER	CA-C	-6.80	1.44	1.52
4	3-C	478	CYS	CA-C	-6.80	1.44	1.52
4	3-H	390	SER	CA-C	-6.80	1.44	1.52
1	1-A	336	VAL	CA-C	-6.80	1.44	1.52
3	1-B	782	LYS	CA-C	-6.80	1.44	1.52
1	2-A	336	VAL	CA-C	-6.80	1.44	1.52
3	2-B	782	LYS	CA-C	-6.80	1.44	1.52
1	3-A	336	VAL	CA-C	-6.80	1.44	1.52
3	3-B	782	LYS	CA-C	-6.80	1.44	1.52
3	1-B	378	GLU	N-CA	-6.79	1.38	1.46
3	2-B	378	GLU	N-CA	-6.79	1.38	1.46
3	3-B	378	GLU	N-CA	-6.79	1.38	1.46
1	1-A	590	LEU	CA-C	-6.79	1.44	1.52
5	1-I	85	LEU	CA-C	-6.79	1.44	1.52
1	2-A	590	LEU	CA-C	-6.79	1.44	1.52
5	2-I	85	LEU	CA-C	-6.79	1.44	1.52
1	3-A	590	LEU	CA-C	-6.79	1.44	1.52
5	3-I	85	LEU	CA-C	-6.79	1.44	1.52
5	1-D	85	LEU	CA-C	-6.79	1.44	1.52
7	1-G	239	GLN	N-CA	-6.79	1.38	1.46
3	1-N	416	VAL	CA-C	-6.79	1.44	1.52
6	1-J	64	THR	CA-C	-6.79	1.44	1.52
5	2-D	85	LEU	CA-C	-6.79	1.44	1.52
7	2-G	239	GLN	N-CA	-6.79	1.38	1.46
3	2-N	416	VAL	CA-C	-6.79	1.44	1.52
6	2-J	64	THR	CA-C	-6.79	1.44	1.52
5	3-D	85	LEU	CA-C	-6.79	1.44	1.52
7	3-G	239	GLN	N-CA	-6.79	1.38	1.46
3	3-N	416	VAL	CA-C	-6.79	1.44	1.52
6	3-J	64	THR	CA-C	-6.79	1.44	1.52
1	1-A	615	VAL	N-CA	-6.79	1.37	1.46
3	1-B	151	LEU	CA-C	-6.79	1.43	1.52
4	1-C	390	SER	CA-C	-6.79	1.44	1.52
6	1-F	151	ARG	CA-C	-6.79	1.44	1.52
7	1-G	706	CYS	CA-C	-6.79	1.44	1.52
1	2-A	615	VAL	N-CA	-6.79	1.37	1.46
3	2-B	151	LEU	CA-C	-6.79	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-C	390	SER	CA-C	-6.79	1.44	1.52
6	2-F	151	ARG	CA-C	-6.79	1.44	1.52
7	2-G	706	CYS	CA-C	-6.79	1.44	1.52
1	3-A	615	VAL	N-CA	-6.79	1.37	1.46
3	3-B	151	LEU	CA-C	-6.79	1.43	1.52
4	3-C	390	SER	CA-C	-6.79	1.44	1.52
6	3-F	151	ARG	CA-C	-6.79	1.44	1.52
7	3-G	706	CYS	CA-C	-6.79	1.44	1.52
8	1-L	23	GLY	CA-C	-6.79	1.42	1.51
8	1-L	54	ARG	CA-C	-6.79	1.44	1.52
8	2-L	23	GLY	CA-C	-6.79	1.42	1.51
8	2-L	54	ARG	CA-C	-6.79	1.44	1.52
8	3-L	23	GLY	CA-C	-6.79	1.42	1.51
8	3-L	54	ARG	CA-C	-6.79	1.44	1.52
3	1-N	378	GLU	N-CA	-6.78	1.38	1.46
3	2-N	378	GLU	N-CA	-6.78	1.38	1.46
3	3-N	378	GLU	N-CA	-6.78	1.38	1.46
7	1-K	80	ASN	N-CA	-6.78	1.37	1.46
4	1-H	554	ILE	CA-C	-6.78	1.44	1.52
7	2-K	80	ASN	N-CA	-6.78	1.37	1.46
4	2-H	554	ILE	CA-C	-6.78	1.44	1.52
7	3-K	80	ASN	N-CA	-6.78	1.37	1.46
4	3-H	554	ILE	CA-C	-6.78	1.44	1.52
7	1-K	234	ARG	C-N	-6.78	1.25	1.33
7	2-K	234	ARG	C-N	-6.78	1.25	1.33
7	3-K	234	ARG	C-N	-6.78	1.25	1.33
6	1-F	64	THR	CA-C	-6.78	1.44	1.52
6	2-F	64	THR	CA-C	-6.78	1.44	1.52
6	3-F	64	THR	CA-C	-6.78	1.44	1.52
8	1-L	31	TYR	N-CA	-6.78	1.38	1.46
8	1-L	108	ASN	CA-C	-6.78	1.44	1.52
8	2-L	31	TYR	N-CA	-6.78	1.38	1.46
8	2-L	108	ASN	CA-C	-6.78	1.44	1.52
8	3-L	31	TYR	N-CA	-6.78	1.38	1.46
8	3-L	108	ASN	CA-C	-6.78	1.44	1.52
4	1-H	368	VAL	CA-C	-6.77	1.44	1.52
4	2-H	368	VAL	CA-C	-6.77	1.44	1.52
4	3-H	368	VAL	CA-C	-6.77	1.44	1.52
1	1-A	665	ALA	CA-C	-6.77	1.44	1.52
3	1-B	319	ARG	CA-C	-6.77	1.44	1.52
5	1-I	53	SER	CA-C	-6.77	1.43	1.53
1	2-A	665	ALA	CA-C	-6.77	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	319	ARG	CA-C	-6.77	1.44	1.52
5	2-I	53	SER	CA-C	-6.77	1.43	1.53
1	3-A	665	ALA	CA-C	-6.77	1.44	1.52
3	3-B	319	ARG	CA-C	-6.77	1.44	1.52
5	3-I	53	SER	CA-C	-6.77	1.43	1.53
4	1-H	438	LEU	CA-C	-6.76	1.44	1.52
4	2-H	438	LEU	CA-C	-6.76	1.44	1.52
4	3-H	438	LEU	CA-C	-6.76	1.44	1.52
1	1-A	629	LEU	CA-C	-6.76	1.43	1.52
1	1-A	672	ASN	N-CA	-6.76	1.37	1.46
6	1-M	168	GLU	CA-C	-6.76	1.43	1.52
1	2-A	629	LEU	CA-C	-6.76	1.43	1.52
1	2-A	672	ASN	N-CA	-6.76	1.37	1.46
6	2-M	168	GLU	CA-C	-6.76	1.43	1.52
1	3-A	629	LEU	CA-C	-6.76	1.43	1.52
1	3-A	672	ASN	N-CA	-6.76	1.37	1.46
6	3-M	168	GLU	CA-C	-6.76	1.43	1.52
5	1-I	27	THR	CA-C	-6.76	1.43	1.52
5	2-I	27	THR	CA-C	-6.76	1.43	1.52
5	3-I	27	THR	CA-C	-6.76	1.43	1.52
1	1-A	628	TYR	CA-C	-6.76	1.43	1.52
8	1-Z	77	PHE	N-CA	-6.76	1.37	1.46
1	2-A	628	TYR	CA-C	-6.76	1.43	1.52
8	2-Z	77	PHE	N-CA	-6.76	1.37	1.46
1	3-A	628	TYR	CA-C	-6.76	1.43	1.52
8	3-Z	77	PHE	N-CA	-6.76	1.37	1.46
3	1-B	190	GLU	CA-C	-6.75	1.44	1.52
7	1-K	860	SER	CA-C	-6.75	1.44	1.52
3	2-B	190	GLU	CA-C	-6.75	1.44	1.52
7	2-K	860	SER	CA-C	-6.75	1.44	1.52
3	3-B	190	GLU	CA-C	-6.75	1.44	1.52
7	3-K	860	SER	CA-C	-6.75	1.44	1.52
5	1-I	60	PRO	CA-C	-6.75	1.44	1.52
5	2-I	60	PRO	CA-C	-6.75	1.44	1.52
5	3-I	60	PRO	CA-C	-6.75	1.44	1.52
3	1-B	407	VAL	CA-C	-6.75	1.44	1.52
4	1-C	554	ILE	CA-C	-6.75	1.44	1.52
3	2-B	407	VAL	CA-C	-6.75	1.44	1.52
4	2-C	554	ILE	CA-C	-6.75	1.44	1.52
3	3-B	407	VAL	CA-C	-6.75	1.44	1.52
4	3-C	554	ILE	CA-C	-6.75	1.44	1.52
1	1-A	632	LYS	CA-C	-6.75	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-C	438	LEU	CA-C	-6.75	1.44	1.52
8	1-L	27	PHE	N-CA	-6.75	1.37	1.46
4	1-H	263	LEU	CA-C	-6.75	1.44	1.52
1	2-A	632	LYS	CA-C	-6.75	1.43	1.52
4	2-C	438	LEU	CA-C	-6.75	1.44	1.52
8	2-L	27	PHE	N-CA	-6.75	1.37	1.46
4	2-H	263	LEU	CA-C	-6.75	1.44	1.52
1	3-A	632	LYS	CA-C	-6.75	1.43	1.52
4	3-C	438	LEU	CA-C	-6.75	1.44	1.52
8	3-L	27	PHE	N-CA	-6.75	1.37	1.46
4	3-H	263	LEU	CA-C	-6.75	1.44	1.52
3	1-N	151	LEU	CA-C	-6.74	1.43	1.52
3	2-N	151	LEU	CA-C	-6.74	1.43	1.52
3	3-N	151	LEU	CA-C	-6.74	1.43	1.52
1	1-A	620	LEU	N-CA	-6.74	1.37	1.46
3	1-N	407	VAL	CA-C	-6.74	1.44	1.52
4	1-H	293	GLY	N-CA	-6.74	1.38	1.45
1	2-A	620	LEU	N-CA	-6.74	1.37	1.46
3	2-N	407	VAL	CA-C	-6.74	1.44	1.52
4	2-H	293	GLY	N-CA	-6.74	1.38	1.45
1	3-A	620	LEU	N-CA	-6.74	1.37	1.46
3	3-N	407	VAL	CA-C	-6.74	1.44	1.52
4	3-H	293	GLY	N-CA	-6.74	1.38	1.45
8	1-Z	69	TYR	N-CA	-6.74	1.37	1.45
4	1-H	455	THR	CA-C	-6.74	1.43	1.52
8	2-Z	69	TYR	N-CA	-6.74	1.37	1.45
4	2-H	455	THR	CA-C	-6.74	1.43	1.52
8	3-Z	69	TYR	N-CA	-6.74	1.37	1.45
4	3-H	455	THR	CA-C	-6.74	1.43	1.52
3	1-B	416	VAL	CA-C	-6.73	1.44	1.52
3	2-B	416	VAL	CA-C	-6.73	1.44	1.52
3	3-B	416	VAL	CA-C	-6.73	1.44	1.52
4	1-H	244	ILE	N-CA	-6.73	1.38	1.46
4	2-H	244	ILE	N-CA	-6.73	1.38	1.46
4	3-H	244	ILE	N-CA	-6.73	1.38	1.46
3	1-B	163	HIS	CA-C	-6.73	1.44	1.52
3	2-B	163	HIS	CA-C	-6.73	1.44	1.52
3	3-B	163	HIS	CA-C	-6.73	1.44	1.52
4	1-C	439	LEU	N-CA	-6.73	1.37	1.46
7	1-G	860	SER	CA-C	-6.73	1.44	1.52
3	1-N	363	VAL	CA-C	-6.73	1.45	1.53
4	2-C	439	LEU	N-CA	-6.73	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	860	SER	CA-C	-6.73	1.44	1.52
3	2-N	363	VAL	CA-C	-6.73	1.45	1.53
4	3-C	439	LEU	N-CA	-6.73	1.37	1.46
7	3-G	860	SER	CA-C	-6.73	1.44	1.52
3	3-N	363	VAL	CA-C	-6.73	1.45	1.53
1	1-A	202	GLU	CA-C	-6.73	1.44	1.52
1	2-A	202	GLU	CA-C	-6.73	1.44	1.52
1	3-A	202	GLU	CA-C	-6.73	1.44	1.52
4	1-C	293	GLY	N-CA	-6.72	1.38	1.45
7	1-K	304	ARG	N-CA	-6.72	1.38	1.46
6	1-M	39	LEU	CA-C	-6.72	1.43	1.52
4	2-C	293	GLY	N-CA	-6.72	1.38	1.45
7	2-K	304	ARG	N-CA	-6.72	1.38	1.46
6	2-M	39	LEU	CA-C	-6.72	1.43	1.52
4	3-C	293	GLY	N-CA	-6.72	1.38	1.45
7	3-K	304	ARG	N-CA	-6.72	1.38	1.46
6	3-M	39	LEU	CA-C	-6.72	1.43	1.52
4	1-H	403	TYR	N-CA	-6.72	1.37	1.45
4	2-H	403	TYR	N-CA	-6.72	1.37	1.45
4	3-H	403	TYR	N-CA	-6.72	1.37	1.45
7	1-G	236	ALA	CA-C	-6.72	1.43	1.52
7	2-G	236	ALA	CA-C	-6.72	1.43	1.52
7	3-G	236	ALA	CA-C	-6.72	1.43	1.52
4	1-C	293	GLY	CA-C	-6.72	1.42	1.51
4	2-C	293	GLY	CA-C	-6.72	1.42	1.51
4	3-C	293	GLY	CA-C	-6.72	1.42	1.51
7	1-G	356	SER	CA-C	-6.71	1.44	1.52
3	1-N	190	GLU	CA-C	-6.71	1.44	1.52
4	1-H	293	GLY	CA-C	-6.71	1.42	1.51
7	2-G	356	SER	CA-C	-6.71	1.44	1.52
3	2-N	190	GLU	CA-C	-6.71	1.44	1.52
4	2-H	293	GLY	CA-C	-6.71	1.42	1.51
7	3-G	356	SER	CA-C	-6.71	1.44	1.52
3	3-N	190	GLU	CA-C	-6.71	1.44	1.52
4	3-H	293	GLY	CA-C	-6.71	1.42	1.51
4	1-C	403	TYR	N-CA	-6.71	1.37	1.45
4	1-H	478	CYS	CA-C	-6.71	1.44	1.52
4	2-C	403	TYR	N-CA	-6.71	1.37	1.45
4	2-H	478	CYS	CA-C	-6.71	1.44	1.52
4	3-C	403	TYR	N-CA	-6.71	1.37	1.45
4	3-H	478	CYS	CA-C	-6.71	1.44	1.52
1	1-A	342	ARG	CA-C	-6.71	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-N	319	ARG	CA-C	-6.71	1.44	1.52
1	2-A	342	ARG	CA-C	-6.71	1.43	1.52
3	2-N	319	ARG	CA-C	-6.71	1.44	1.52
1	3-A	342	ARG	CA-C	-6.71	1.43	1.52
3	3-N	319	ARG	CA-C	-6.71	1.44	1.52
4	1-H	439	LEU	N-CA	-6.71	1.37	1.46
4	2-H	439	LEU	N-CA	-6.71	1.37	1.46
4	3-H	439	LEU	N-CA	-6.71	1.37	1.46
3	1-B	964	LYS	CA-C	-6.70	1.43	1.53
4	1-C	244	ILE	N-CA	-6.70	1.38	1.46
3	2-B	964	LYS	CA-C	-6.70	1.43	1.53
4	2-C	244	ILE	N-CA	-6.70	1.38	1.46
3	3-B	964	LYS	CA-C	-6.70	1.43	1.53
4	3-C	244	ILE	N-CA	-6.70	1.38	1.46
1	1-A	687	HIS	CA-C	-6.70	1.44	1.52
1	2-A	687	HIS	CA-C	-6.70	1.44	1.52
1	3-A	687	HIS	CA-C	-6.70	1.44	1.52
3	1-B	755	VAL	N-CA	-6.70	1.38	1.46
3	2-B	755	VAL	N-CA	-6.70	1.38	1.46
3	3-B	755	VAL	N-CA	-6.70	1.38	1.46
6	1-R	65	VAL	N-CA	-6.70	1.38	1.46
6	2-R	65	VAL	N-CA	-6.70	1.38	1.46
6	3-R	65	VAL	N-CA	-6.70	1.38	1.46
1	1-A	77	VAL	CA-C	-6.70	1.44	1.52
8	1-L	109	VAL	N-CA	-6.70	1.38	1.46
1	2-A	77	VAL	CA-C	-6.70	1.44	1.52
8	2-L	109	VAL	N-CA	-6.70	1.38	1.46
1	3-A	77	VAL	CA-C	-6.70	1.44	1.52
8	3-L	109	VAL	N-CA	-6.70	1.38	1.46
8	1-L	90	LEU	N-CA	-6.69	1.38	1.46
8	2-L	90	LEU	N-CA	-6.69	1.38	1.46
8	3-L	90	LEU	N-CA	-6.69	1.38	1.46
7	1-G	436	LEU	CA-C	-6.69	1.44	1.52
7	2-G	436	LEU	CA-C	-6.69	1.44	1.52
7	3-G	436	LEU	CA-C	-6.69	1.44	1.52
1	1-A	305	LEU	CA-C	-6.68	1.44	1.52
3	1-B	752	TYR	CA-C	-6.68	1.43	1.52
1	2-A	305	LEU	CA-C	-6.68	1.44	1.52
3	2-B	752	TYR	CA-C	-6.68	1.43	1.52
1	3-A	305	LEU	CA-C	-6.68	1.44	1.52
3	3-B	752	TYR	CA-C	-6.68	1.43	1.52
7	1-G	176	ARG	CA-C	-6.68	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	176	ARG	CA-C	-6.68	1.43	1.52
7	3-G	176	ARG	CA-C	-6.68	1.43	1.52
3	1-B	437	GLU	N-CA	-6.67	1.38	1.46
8	1-Z	134	ILE	N-CA	-6.67	1.38	1.46
3	2-B	437	GLU	N-CA	-6.67	1.38	1.46
8	2-Z	134	ILE	N-CA	-6.67	1.38	1.46
3	3-B	437	GLU	N-CA	-6.67	1.38	1.46
8	3-Z	134	ILE	N-CA	-6.67	1.38	1.46
8	1-L	134	ILE	N-CA	-6.67	1.38	1.46
8	2-L	134	ILE	N-CA	-6.67	1.38	1.46
8	3-L	134	ILE	N-CA	-6.67	1.38	1.46
4	1-H	257	HIS	CA-C	-6.67	1.44	1.52
4	2-H	257	HIS	CA-C	-6.67	1.44	1.52
4	3-H	257	HIS	CA-C	-6.67	1.44	1.52
8	1-L	104	MET	N-CA	-6.66	1.38	1.46
8	2-L	104	MET	N-CA	-6.66	1.38	1.46
8	3-L	104	MET	N-CA	-6.66	1.38	1.46
1	1-A	569	TYR	CA-C	-6.66	1.44	1.52
5	1-D	53	SER	CA-C	-6.66	1.43	1.53
7	1-G	22	LEU	CA-C	-6.66	1.44	1.52
7	1-K	731	THR	N-CA	-6.66	1.38	1.46
1	2-A	569	TYR	CA-C	-6.66	1.44	1.52
5	2-D	53	SER	CA-C	-6.66	1.43	1.53
7	2-G	22	LEU	CA-C	-6.66	1.44	1.52
7	2-K	731	THR	N-CA	-6.66	1.38	1.46
1	3-A	569	TYR	CA-C	-6.66	1.44	1.52
5	3-D	53	SER	CA-C	-6.66	1.43	1.53
7	3-G	22	LEU	CA-C	-6.66	1.44	1.52
7	3-K	731	THR	N-CA	-6.66	1.38	1.46
4	1-C	476	LEU	CA-C	-6.66	1.44	1.52
3	1-N	437	GLU	N-CA	-6.66	1.38	1.46
4	2-C	476	LEU	CA-C	-6.66	1.44	1.52
3	2-N	437	GLU	N-CA	-6.66	1.38	1.46
4	3-C	476	LEU	CA-C	-6.66	1.44	1.52
3	3-N	437	GLU	N-CA	-6.66	1.38	1.46
4	1-C	455	THR	CA-C	-6.65	1.43	1.52
4	2-C	455	THR	CA-C	-6.65	1.43	1.52
4	3-C	455	THR	CA-C	-6.65	1.43	1.52
1	1-A	465	LEU	N-CA	-6.65	1.37	1.46
5	1-D	65	TYR	CA-C	-6.65	1.44	1.52
7	1-G	145	LYS	CA-C	-6.65	1.44	1.52
7	1-G	623	PHE	CA-C	-6.65	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-K	110	THR	CA-C	-6.65	1.44	1.52
3	1-N	89	ILE	CA-C	-6.65	1.44	1.52
1	2-A	465	LEU	N-CA	-6.65	1.37	1.46
5	2-D	65	TYR	CA-C	-6.65	1.44	1.52
7	2-G	145	LYS	CA-C	-6.65	1.44	1.52
7	2-G	623	PHE	CA-C	-6.65	1.43	1.52
7	2-K	110	THR	CA-C	-6.65	1.44	1.52
3	2-N	89	ILE	CA-C	-6.65	1.44	1.52
1	3-A	465	LEU	N-CA	-6.65	1.37	1.46
5	3-D	65	TYR	CA-C	-6.65	1.44	1.52
7	3-G	145	LYS	CA-C	-6.65	1.44	1.52
7	3-G	623	PHE	CA-C	-6.65	1.43	1.52
7	3-K	110	THR	CA-C	-6.65	1.44	1.52
3	3-N	89	ILE	CA-C	-6.65	1.44	1.52
7	1-G	783	PHE	CA-C	-6.65	1.44	1.52
7	2-G	783	PHE	CA-C	-6.65	1.44	1.52
7	3-G	783	PHE	CA-C	-6.65	1.44	1.52
5	1-D	60	PRO	CA-C	-6.65	1.44	1.52
5	1-I	148	ARG	CA-C	-6.65	1.44	1.52
5	2-D	60	PRO	CA-C	-6.65	1.44	1.52
5	2-I	148	ARG	CA-C	-6.65	1.44	1.52
5	3-D	60	PRO	CA-C	-6.65	1.44	1.52
5	3-I	148	ARG	CA-C	-6.65	1.44	1.52
7	1-G	731	THR	N-CA	-6.64	1.38	1.46
7	2-G	731	THR	N-CA	-6.64	1.38	1.46
7	3-G	731	THR	N-CA	-6.64	1.38	1.46
4	1-C	418	PHE	CA-C	-6.63	1.44	1.53
7	1-G	175	LYS	N-CA	-6.63	1.38	1.46
4	2-C	418	PHE	CA-C	-6.63	1.44	1.53
7	2-G	175	LYS	N-CA	-6.63	1.38	1.46
4	3-C	418	PHE	CA-C	-6.63	1.44	1.53
7	3-G	175	LYS	N-CA	-6.63	1.38	1.46
7	1-G	107	SER	N-CA	-6.63	1.38	1.46
3	1-N	475	TRP	CA-C	-6.63	1.44	1.52
7	2-G	107	SER	N-CA	-6.63	1.38	1.46
3	2-N	475	TRP	CA-C	-6.63	1.44	1.52
7	3-G	107	SER	N-CA	-6.63	1.38	1.46
3	3-N	475	TRP	CA-C	-6.63	1.44	1.52
7	1-G	259	LEU	N-CA	-6.62	1.38	1.46
7	1-K	255	ILE	CA-C	-6.62	1.44	1.52
7	2-G	259	LEU	N-CA	-6.62	1.38	1.46
7	2-K	255	ILE	CA-C	-6.62	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3-G	259	LEU	N-CA	-6.62	1.38	1.46
7	3-K	255	ILE	CA-C	-6.62	1.44	1.52
7	1-K	623	PHE	CA-C	-6.62	1.43	1.52
7	2-K	623	PHE	CA-C	-6.62	1.43	1.52
7	3-K	623	PHE	CA-C	-6.62	1.43	1.52
7	1-G	233	ILE	N-CA	-6.62	1.38	1.46
7	2-G	233	ILE	N-CA	-6.62	1.38	1.46
7	3-G	233	ILE	N-CA	-6.62	1.38	1.46
4	1-C	243	ILE	CA-C	-6.62	1.44	1.52
4	1-H	232	VAL	CA-C	-6.62	1.44	1.52
4	2-C	243	ILE	CA-C	-6.62	1.44	1.52
4	2-H	232	VAL	CA-C	-6.62	1.44	1.52
4	3-C	243	ILE	CA-C	-6.62	1.44	1.52
4	3-H	232	VAL	CA-C	-6.62	1.44	1.52
3	1-N	402	LEU	CA-C	-6.61	1.44	1.52
3	2-N	402	LEU	CA-C	-6.61	1.44	1.52
3	3-N	402	LEU	CA-C	-6.61	1.44	1.52
4	1-C	232	VAL	CA-C	-6.61	1.44	1.52
4	2-C	232	VAL	CA-C	-6.61	1.44	1.52
4	3-C	232	VAL	CA-C	-6.61	1.44	1.52
3	1-N	338	MET	CA-C	-6.61	1.44	1.52
4	1-H	243	ILE	CA-C	-6.61	1.44	1.52
3	2-N	338	MET	CA-C	-6.61	1.44	1.52
4	2-H	243	ILE	CA-C	-6.61	1.44	1.52
3	3-N	338	MET	CA-C	-6.61	1.44	1.52
4	3-H	243	ILE	CA-C	-6.61	1.44	1.52
3	1-B	363	VAL	CA-C	-6.60	1.45	1.53
3	2-B	363	VAL	CA-C	-6.60	1.45	1.53
3	3-B	363	VAL	CA-C	-6.60	1.45	1.53
1	1-A	699	ASN	CA-C	-6.60	1.44	1.52
1	2-A	699	ASN	CA-C	-6.60	1.44	1.52
1	3-A	699	ASN	CA-C	-6.60	1.44	1.52
3	1-B	475	TRP	CA-C	-6.60	1.44	1.52
3	2-B	475	TRP	CA-C	-6.60	1.44	1.52
3	3-B	475	TRP	CA-C	-6.60	1.44	1.52
4	1-C	272	GLU	N-CA	-6.60	1.37	1.46
4	2-C	272	GLU	N-CA	-6.60	1.37	1.46
4	3-C	272	GLU	N-CA	-6.60	1.37	1.46
3	1-B	469	ILE	CA-C	-6.60	1.44	1.52
4	1-H	476	LEU	CA-C	-6.60	1.44	1.52
3	2-B	469	ILE	CA-C	-6.60	1.44	1.52
4	2-H	476	LEU	CA-C	-6.60	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	469	ILE	CA-C	-6.60	1.44	1.52
4	3-H	476	LEU	CA-C	-6.60	1.44	1.52
4	1-C	257	HIS	CA-C	-6.59	1.44	1.52
5	1-I	84	ARG	N-CA	-6.59	1.38	1.46
4	2-C	257	HIS	CA-C	-6.59	1.44	1.52
5	2-I	84	ARG	N-CA	-6.59	1.38	1.46
4	3-C	257	HIS	CA-C	-6.59	1.44	1.52
5	3-I	84	ARG	N-CA	-6.59	1.38	1.46
3	1-B	89	ILE	CA-C	-6.59	1.44	1.52
3	1-B	338	MET	CA-C	-6.59	1.44	1.52
7	1-K	63	THR	CA-C	-6.59	1.44	1.52
3	1-N	469	ILE	CA-C	-6.59	1.44	1.52
3	2-B	89	ILE	CA-C	-6.59	1.44	1.52
3	2-B	338	MET	CA-C	-6.59	1.44	1.52
7	2-K	63	THR	CA-C	-6.59	1.44	1.52
3	2-N	469	ILE	CA-C	-6.59	1.44	1.52
3	3-B	89	ILE	CA-C	-6.59	1.44	1.52
3	3-B	338	MET	CA-C	-6.59	1.44	1.52
7	3-K	63	THR	CA-C	-6.59	1.44	1.52
3	3-N	469	ILE	CA-C	-6.59	1.44	1.52
3	1-N	392	ASP	CA-C	-6.59	1.44	1.52
3	2-N	392	ASP	CA-C	-6.59	1.44	1.52
3	3-N	392	ASP	CA-C	-6.59	1.44	1.52
8	1-Z	140	GLN	CA-C	-6.59	1.44	1.52
8	2-Z	140	GLN	CA-C	-6.59	1.44	1.52
8	3-Z	140	GLN	CA-C	-6.59	1.44	1.52
4	1-H	432	SER	CA-C	-6.59	1.44	1.52
4	2-H	432	SER	CA-C	-6.59	1.44	1.52
4	3-H	432	SER	CA-C	-6.59	1.44	1.52
4	1-H	272	GLU	N-CA	-6.58	1.37	1.46
4	2-H	272	GLU	N-CA	-6.58	1.37	1.46
4	3-H	272	GLU	N-CA	-6.58	1.37	1.46
1	1-A	661	ALA	N-CA	-6.58	1.38	1.46
1	2-A	661	ALA	N-CA	-6.58	1.38	1.46
1	3-A	661	ALA	N-CA	-6.58	1.38	1.46
4	1-C	495	VAL	CA-C	-6.58	1.44	1.52
4	2-C	495	VAL	CA-C	-6.58	1.44	1.52
4	3-C	495	VAL	CA-C	-6.58	1.44	1.52
4	1-H	376	ILE	N-CA	-6.58	1.38	1.46
4	2-H	376	ILE	N-CA	-6.58	1.38	1.46
4	3-H	376	ILE	N-CA	-6.58	1.38	1.46
1	1-A	286	THR	CA-C	-6.58	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	286	THR	CA-C	-6.58	1.44	1.52
1	3-A	286	THR	CA-C	-6.58	1.44	1.52
4	1-C	432	SER	CA-C	-6.58	1.44	1.52
5	1-D	148	ARG	CA-C	-6.58	1.44	1.52
8	1-L	62	LEU	CA-C	-6.58	1.44	1.52
4	2-C	432	SER	CA-C	-6.58	1.44	1.52
5	2-D	148	ARG	CA-C	-6.58	1.44	1.52
8	2-L	62	LEU	CA-C	-6.58	1.44	1.52
4	3-C	432	SER	CA-C	-6.58	1.44	1.52
5	3-D	148	ARG	CA-C	-6.58	1.44	1.52
8	3-L	62	LEU	CA-C	-6.58	1.44	1.52
3	1-B	376	LYS	N-CA	-6.57	1.38	1.46
3	1-B	859	TRP	CA-C	-6.57	1.44	1.52
5	1-I	65	TYR	CA-C	-6.57	1.44	1.52
3	2-B	376	LYS	N-CA	-6.57	1.38	1.46
3	2-B	859	TRP	CA-C	-6.57	1.44	1.52
5	2-I	65	TYR	CA-C	-6.57	1.44	1.52
3	3-B	376	LYS	N-CA	-6.57	1.38	1.46
3	3-B	859	TRP	CA-C	-6.57	1.44	1.52
5	3-I	65	TYR	CA-C	-6.57	1.44	1.52
1	1-A	688	GLN	CA-C	-6.57	1.44	1.52
4	1-H	495	VAL	CA-C	-6.57	1.44	1.52
1	2-A	688	GLN	CA-C	-6.57	1.44	1.52
4	2-H	495	VAL	CA-C	-6.57	1.44	1.52
1	3-A	688	GLN	CA-C	-6.57	1.44	1.52
4	3-H	495	VAL	CA-C	-6.57	1.44	1.52
3	1-B	894	THR	C-N	6.57	1.41	1.33
7	1-G	358	ASP	CA-C	-6.57	1.44	1.52
6	1-M	22	MET	CA-C	-6.57	1.44	1.52
3	2-B	894	THR	C-N	6.57	1.41	1.33
7	2-G	358	ASP	CA-C	-6.57	1.44	1.52
6	2-M	22	MET	CA-C	-6.57	1.44	1.52
3	3-B	894	THR	C-N	6.57	1.41	1.33
7	3-G	358	ASP	CA-C	-6.57	1.44	1.52
6	3-M	22	MET	CA-C	-6.57	1.44	1.52
7	1-K	266	VAL	CA-C	-6.56	1.44	1.52
7	2-K	266	VAL	CA-C	-6.56	1.44	1.52
7	3-K	266	VAL	CA-C	-6.56	1.44	1.52
4	1-H	418	PHE	CA-C	-6.56	1.44	1.53
4	2-H	418	PHE	CA-C	-6.56	1.44	1.53
4	3-H	418	PHE	CA-C	-6.56	1.44	1.53
3	1-B	850	CYS	N-CA	6.55	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-C	187	GLY	CA-C	-6.55	1.44	1.51
3	2-B	850	CYS	N-CA	6.55	1.54	1.46
4	2-C	187	GLY	CA-C	-6.55	1.44	1.51
3	3-B	850	CYS	N-CA	6.55	1.54	1.46
4	3-C	187	GLY	CA-C	-6.55	1.44	1.51
3	1-B	744	GLU	CA-C	-6.55	1.44	1.52
7	1-K	783	PHE	CA-C	-6.55	1.44	1.52
3	2-B	744	GLU	CA-C	-6.55	1.44	1.52
7	2-K	783	PHE	CA-C	-6.55	1.44	1.52
3	3-B	744	GLU	CA-C	-6.55	1.44	1.52
7	3-K	783	PHE	CA-C	-6.55	1.44	1.52
1	1-A	597	PHE	CA-C	-6.54	1.44	1.52
1	2-A	597	PHE	CA-C	-6.54	1.44	1.52
1	3-A	597	PHE	CA-C	-6.54	1.44	1.52
3	1-B	402	LEU	CA-C	-6.54	1.44	1.52
3	2-B	402	LEU	CA-C	-6.54	1.44	1.52
3	3-B	402	LEU	CA-C	-6.54	1.44	1.52
8	1-L	47	ASN	CA-C	-6.54	1.44	1.52
8	2-L	47	ASN	CA-C	-6.54	1.44	1.52
8	3-L	47	ASN	CA-C	-6.54	1.44	1.52
7	1-K	181	ALA	CA-C	-6.54	1.44	1.52
7	2-K	181	ALA	CA-C	-6.54	1.44	1.52
7	3-K	181	ALA	CA-C	-6.54	1.44	1.52
7	1-K	201	TYR	N-CA	-6.54	1.38	1.46
6	1-M	41	GLU	CA-C	-6.54	1.44	1.52
7	2-K	201	TYR	N-CA	-6.54	1.38	1.46
6	2-M	41	GLU	CA-C	-6.54	1.44	1.52
7	3-K	201	TYR	N-CA	-6.54	1.38	1.46
6	3-M	41	GLU	CA-C	-6.54	1.44	1.52
7	1-G	119	ASN	N-CA	-6.53	1.38	1.46
6	1-M	54	GLU	CA-C	-6.53	1.44	1.52
7	2-G	119	ASN	N-CA	-6.53	1.38	1.46
6	2-M	54	GLU	CA-C	-6.53	1.44	1.52
7	3-G	119	ASN	N-CA	-6.53	1.38	1.46
6	3-M	54	GLU	CA-C	-6.53	1.44	1.52
4	1-C	261	TYR	CA-C	-6.53	1.43	1.53
7	1-G	54	LEU	CA-C	-6.53	1.44	1.52
5	1-I	105	HIS	CA-C	-6.53	1.44	1.52
6	1-J	124	PHE	CA-C	-6.53	1.44	1.52
4	2-C	261	TYR	CA-C	-6.53	1.43	1.53
7	2-G	54	LEU	CA-C	-6.53	1.44	1.52
5	2-I	105	HIS	CA-C	-6.53	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2-J	124	PHE	CA-C	-6.53	1.44	1.52
4	3-C	261	TYR	CA-C	-6.53	1.43	1.53
7	3-G	54	LEU	CA-C	-6.53	1.44	1.52
5	3-I	105	HIS	CA-C	-6.53	1.44	1.52
6	3-J	124	PHE	CA-C	-6.53	1.44	1.52
4	1-C	69	LYS	N-CA	-6.53	1.37	1.46
4	2-C	69	LYS	N-CA	-6.53	1.37	1.46
4	3-C	69	LYS	N-CA	-6.53	1.37	1.46
4	1-H	458	ILE	CA-C	-6.52	1.43	1.52
4	2-H	458	ILE	CA-C	-6.52	1.43	1.52
4	3-H	458	ILE	CA-C	-6.52	1.43	1.52
1	1-A	610	GLU	CA-C	-6.52	1.44	1.52
1	2-A	610	GLU	CA-C	-6.52	1.44	1.52
1	3-A	610	GLU	CA-C	-6.52	1.44	1.52
4	1-C	571	ASN	N-CA	-6.52	1.37	1.46
6	1-R	54	GLU	CA-C	-6.52	1.44	1.52
4	2-C	571	ASN	N-CA	-6.52	1.37	1.46
6	2-R	54	GLU	CA-C	-6.52	1.44	1.52
4	3-C	571	ASN	N-CA	-6.52	1.37	1.46
6	3-R	54	GLU	CA-C	-6.52	1.44	1.52
3	1-N	376	LYS	N-CA	-6.51	1.38	1.46
3	2-N	376	LYS	N-CA	-6.51	1.38	1.46
3	3-N	376	LYS	N-CA	-6.51	1.38	1.46
4	1-H	261	TYR	CA-C	-6.51	1.43	1.53
4	2-H	261	TYR	CA-C	-6.51	1.43	1.53
4	3-H	261	TYR	CA-C	-6.51	1.43	1.53
3	1-B	415	ASN	CA-C	-6.50	1.44	1.52
4	1-H	441	VAL	CA-C	-6.50	1.44	1.52
3	2-B	415	ASN	CA-C	-6.50	1.44	1.52
4	2-H	441	VAL	CA-C	-6.50	1.44	1.52
3	3-B	415	ASN	CA-C	-6.50	1.44	1.52
4	3-H	441	VAL	CA-C	-6.50	1.44	1.52
7	1-K	139	ALA	CA-C	-6.50	1.44	1.52
7	2-K	139	ALA	CA-C	-6.50	1.44	1.52
7	3-K	139	ALA	CA-C	-6.50	1.44	1.52
4	1-C	778	SER	N-CA	-6.50	1.38	1.46
7	1-G	249	SER	CA-C	-6.50	1.45	1.52
4	2-C	778	SER	N-CA	-6.50	1.38	1.46
7	2-G	249	SER	CA-C	-6.50	1.45	1.52
4	3-C	778	SER	N-CA	-6.50	1.38	1.46
7	3-G	249	SER	CA-C	-6.50	1.45	1.52
7	1-K	307	ALA	N-CA	-6.50	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-K	307	ALA	N-CA	-6.50	1.38	1.46
7	3-K	307	ALA	N-CA	-6.50	1.38	1.46
6	1-F	124	PHE	CA-C	-6.49	1.44	1.52
6	2-F	124	PHE	CA-C	-6.49	1.44	1.52
6	3-F	124	PHE	CA-C	-6.49	1.44	1.52
1	1-A	266	SER	CA-C	-6.49	1.45	1.52
8	1-Z	25	ARG	N-CA	-6.49	1.38	1.46
1	2-A	266	SER	CA-C	-6.49	1.45	1.52
8	2-Z	25	ARG	N-CA	-6.49	1.38	1.46
1	3-A	266	SER	CA-C	-6.49	1.45	1.52
8	3-Z	25	ARG	N-CA	-6.49	1.38	1.46
3	1-B	392	ASP	CA-C	-6.49	1.44	1.52
4	1-C	546	TYR	N-CA	-6.49	1.38	1.46
3	2-B	392	ASP	CA-C	-6.49	1.44	1.52
4	2-C	546	TYR	N-CA	-6.49	1.38	1.46
3	3-B	392	ASP	CA-C	-6.49	1.44	1.52
4	3-C	546	TYR	N-CA	-6.49	1.38	1.46
1	1-A	518	LEU	CA-C	-6.49	1.44	1.52
4	1-C	547	VAL	N-CA	-6.49	1.38	1.46
1	2-A	518	LEU	CA-C	-6.49	1.44	1.52
4	2-C	547	VAL	N-CA	-6.49	1.38	1.46
1	3-A	518	LEU	CA-C	-6.49	1.44	1.52
4	3-C	547	VAL	N-CA	-6.49	1.38	1.46
3	1-B	844	TYR	CA-C	-6.49	1.44	1.52
3	2-B	844	TYR	CA-C	-6.49	1.44	1.52
3	3-B	844	TYR	CA-C	-6.49	1.44	1.52
4	1-C	441	VAL	CA-C	-6.48	1.44	1.52
4	2-C	441	VAL	CA-C	-6.48	1.44	1.52
4	3-C	441	VAL	CA-C	-6.48	1.44	1.52
3	1-N	415	ASN	CA-C	-6.48	1.44	1.52
3	2-N	415	ASN	CA-C	-6.48	1.44	1.52
3	3-N	415	ASN	CA-C	-6.48	1.44	1.52
4	1-C	376	ILE	N-CA	-6.48	1.38	1.46
5	1-D	84	ARG	N-CA	-6.48	1.38	1.46
4	2-C	376	ILE	N-CA	-6.48	1.38	1.46
5	2-D	84	ARG	N-CA	-6.48	1.38	1.46
4	3-C	376	ILE	N-CA	-6.48	1.38	1.46
5	3-D	84	ARG	N-CA	-6.48	1.38	1.46
7	1-G	648	ILE	CA-C	-6.48	1.44	1.52
7	2-G	648	ILE	CA-C	-6.48	1.44	1.52
7	3-G	648	ILE	CA-C	-6.48	1.44	1.52
4	1-H	69	LYS	N-CA	-6.47	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-H	69	LYS	N-CA	-6.47	1.37	1.46
4	3-H	69	LYS	N-CA	-6.47	1.37	1.46
4	1-C	458	ILE	CA-C	-6.47	1.43	1.52
8	1-L	11	TYR	CA-C	-6.47	1.44	1.52
4	1-H	571	ASN	N-CA	-6.47	1.37	1.46
4	2-C	458	ILE	CA-C	-6.47	1.43	1.52
8	2-L	11	TYR	CA-C	-6.47	1.44	1.52
4	2-H	571	ASN	N-CA	-6.47	1.37	1.46
4	3-C	458	ILE	CA-C	-6.47	1.43	1.52
8	3-L	11	TYR	CA-C	-6.47	1.44	1.52
4	3-H	571	ASN	N-CA	-6.47	1.37	1.46
4	1-H	187	GLY	CA-C	-6.47	1.44	1.51
4	2-H	187	GLY	CA-C	-6.47	1.44	1.51
4	3-H	187	GLY	CA-C	-6.47	1.44	1.51
3	1-B	823	SER	CA-C	-6.46	1.44	1.52
4	1-H	574	TYR	N-CA	-6.46	1.38	1.46
3	2-B	823	SER	CA-C	-6.46	1.44	1.52
4	2-H	574	TYR	N-CA	-6.46	1.38	1.46
3	3-B	823	SER	CA-C	-6.46	1.44	1.52
4	3-H	574	TYR	N-CA	-6.46	1.38	1.46
1	1-A	573	VAL	CA-C	-6.46	1.44	1.52
3	1-N	152	MET	N-CA	-6.46	1.40	1.46
1	2-A	573	VAL	CA-C	-6.46	1.44	1.52
3	2-N	152	MET	N-CA	-6.46	1.40	1.46
1	3-A	573	VAL	CA-C	-6.46	1.44	1.52
3	3-N	152	MET	N-CA	-6.46	1.40	1.46
4	1-H	231	ASN	CA-C	-6.46	1.44	1.52
4	2-H	231	ASN	CA-C	-6.46	1.44	1.52
4	3-H	231	ASN	CA-C	-6.46	1.44	1.52
4	1-C	765	GLN	CA-C	-6.46	1.43	1.52
8	1-Z	121	LEU	CA-C	-6.46	1.44	1.52
4	1-H	669	LYS	CA-C	-6.46	1.44	1.52
5	1-I	102	ILE	N-CA	-6.46	1.38	1.46
4	2-C	765	GLN	CA-C	-6.46	1.43	1.52
8	2-Z	121	LEU	CA-C	-6.46	1.44	1.52
4	2-H	669	LYS	CA-C	-6.46	1.44	1.52
5	2-I	102	ILE	N-CA	-6.46	1.38	1.46
4	3-C	765	GLN	CA-C	-6.46	1.43	1.52
8	3-Z	121	LEU	CA-C	-6.46	1.44	1.52
4	3-H	669	LYS	CA-C	-6.46	1.44	1.52
5	3-I	102	ILE	N-CA	-6.46	1.38	1.46
3	1-B	750	ASN	CA-C	-6.46	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-C	574	TYR	N-CA	-6.46	1.38	1.46
3	2-B	750	ASN	CA-C	-6.46	1.45	1.52
4	2-C	574	TYR	N-CA	-6.46	1.38	1.46
3	3-B	750	ASN	CA-C	-6.46	1.45	1.52
4	3-C	574	TYR	N-CA	-6.46	1.38	1.46
1	1-A	619	LYS	CA-C	-6.45	1.44	1.52
1	2-A	619	LYS	CA-C	-6.45	1.44	1.52
1	3-A	619	LYS	CA-C	-6.45	1.44	1.52
8	1-Z	46	LYS	N-CA	-6.45	1.38	1.46
4	1-H	378	TYR	N-CA	-6.45	1.38	1.45
4	1-H	546	TYR	N-CA	-6.45	1.38	1.46
4	1-H	642	GLU	CA-C	-6.45	1.44	1.52
8	2-Z	46	LYS	N-CA	-6.45	1.38	1.46
4	2-H	378	TYR	N-CA	-6.45	1.38	1.45
4	2-H	546	TYR	N-CA	-6.45	1.38	1.46
4	2-H	642	GLU	CA-C	-6.45	1.44	1.52
8	3-Z	46	LYS	N-CA	-6.45	1.38	1.46
4	3-H	378	TYR	N-CA	-6.45	1.38	1.45
4	3-H	546	TYR	N-CA	-6.45	1.38	1.46
4	3-H	642	GLU	CA-C	-6.45	1.44	1.52
7	1-G	84	LEU	N-CA	-6.45	1.38	1.46
7	2-G	84	LEU	N-CA	-6.45	1.38	1.46
7	3-G	84	LEU	N-CA	-6.45	1.38	1.46
3	1-B	754	ILE	CA-C	-6.45	1.44	1.52
3	1-B	818	ILE	N-CA	-6.45	1.38	1.46
3	2-B	754	ILE	CA-C	-6.45	1.44	1.52
3	2-B	818	ILE	N-CA	-6.45	1.38	1.46
3	3-B	754	ILE	CA-C	-6.45	1.44	1.52
3	3-B	818	ILE	N-CA	-6.45	1.38	1.46
7	1-G	487	VAL	CA-C	-6.44	1.44	1.52
7	1-K	177	TRP	CA-C	-6.44	1.41	1.52
7	2-G	487	VAL	CA-C	-6.44	1.44	1.52
7	2-K	177	TRP	CA-C	-6.44	1.41	1.52
7	3-G	487	VAL	CA-C	-6.44	1.44	1.52
7	3-K	177	TRP	CA-C	-6.44	1.41	1.52
4	1-H	115	LEU	CA-C	-6.44	1.45	1.52
4	2-H	115	LEU	CA-C	-6.44	1.45	1.52
4	3-H	115	LEU	CA-C	-6.44	1.45	1.52
5	1-D	102	ILE	N-CA	-6.44	1.38	1.46
7	1-K	648	ILE	CA-C	-6.44	1.44	1.52
6	1-J	19	ARG	CA-C	-6.44	1.45	1.52
5	2-D	102	ILE	N-CA	-6.44	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-K	648	ILE	CA-C	-6.44	1.44	1.52
6	2-J	19	ARG	CA-C	-6.44	1.45	1.52
5	3-D	102	ILE	N-CA	-6.44	1.38	1.46
7	3-K	648	ILE	CA-C	-6.44	1.44	1.52
6	3-J	19	ARG	CA-C	-6.44	1.45	1.52
5	1-D	105	HIS	CA-C	-6.43	1.44	1.52
8	1-L	145	ARG	CA-C	-6.43	1.44	1.52
6	1-M	154	PHE	N-CA	-6.43	1.38	1.46
4	1-H	519	GLU	CA-C	-6.43	1.44	1.52
5	2-D	105	HIS	CA-C	-6.43	1.44	1.52
8	2-L	145	ARG	CA-C	-6.43	1.44	1.52
6	2-M	154	PHE	N-CA	-6.43	1.38	1.46
4	2-H	519	GLU	CA-C	-6.43	1.44	1.52
5	3-D	105	HIS	CA-C	-6.43	1.44	1.52
8	3-L	145	ARG	CA-C	-6.43	1.44	1.52
6	3-M	154	PHE	N-CA	-6.43	1.38	1.46
4	3-H	519	GLU	CA-C	-6.43	1.44	1.52
4	1-C	642	GLU	CA-C	-6.43	1.44	1.52
4	2-C	642	GLU	CA-C	-6.43	1.44	1.52
4	3-C	642	GLU	CA-C	-6.43	1.44	1.52
3	1-B	760	VAL	N-CA	-6.43	1.38	1.46
3	2-B	760	VAL	N-CA	-6.43	1.38	1.46
3	3-B	760	VAL	N-CA	-6.43	1.38	1.46
1	1-A	245	CYS	CA-C	-6.42	1.44	1.52
8	1-Z	28	ALA	CA-C	-6.42	1.44	1.52
4	1-H	76	ALA	CA-C	-6.42	1.44	1.52
1	2-A	245	CYS	CA-C	-6.42	1.44	1.52
8	2-Z	28	ALA	CA-C	-6.42	1.44	1.52
4	2-H	76	ALA	CA-C	-6.42	1.44	1.52
1	3-A	245	CYS	CA-C	-6.42	1.44	1.52
8	3-Z	28	ALA	CA-C	-6.42	1.44	1.52
4	3-H	76	ALA	CA-C	-6.42	1.44	1.52
7	1-G	237	SER	N-CA	-6.42	1.38	1.46
7	2-G	237	SER	N-CA	-6.42	1.38	1.46
7	3-G	237	SER	N-CA	-6.42	1.38	1.46
6	1-M	23	VAL	CA-C	-6.42	1.45	1.52
6	2-M	23	VAL	CA-C	-6.42	1.45	1.52
6	3-M	23	VAL	CA-C	-6.42	1.45	1.52
3	1-B	414	ALA	CA-C	-6.42	1.44	1.52
4	1-C	519	GLU	CA-C	-6.42	1.44	1.52
3	2-B	414	ALA	CA-C	-6.42	1.44	1.52
4	2-C	519	GLU	CA-C	-6.42	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	414	ALA	CA-C	-6.42	1.44	1.52
4	3-C	519	GLU	CA-C	-6.42	1.44	1.52
7	1-G	167	LEU	CA-C	-6.42	1.44	1.52
7	2-G	167	LEU	CA-C	-6.42	1.44	1.52
7	3-G	167	LEU	CA-C	-6.42	1.44	1.52
4	1-H	547	VAL	N-CA	-6.42	1.38	1.46
4	2-H	547	VAL	N-CA	-6.42	1.38	1.46
4	3-H	547	VAL	N-CA	-6.42	1.38	1.46
1	1-A	613	HIS	N-CA	-6.41	1.38	1.46
4	1-C	306	MET	CA-C	-6.41	1.44	1.52
1	2-A	613	HIS	N-CA	-6.41	1.38	1.46
4	2-C	306	MET	CA-C	-6.41	1.44	1.52
1	3-A	613	HIS	N-CA	-6.41	1.38	1.46
4	3-C	306	MET	CA-C	-6.41	1.44	1.52
1	1-A	807	ASN	CA-C	-6.41	1.44	1.52
4	1-C	378	TYR	N-CA	-6.41	1.38	1.45
1	2-A	807	ASN	CA-C	-6.41	1.44	1.52
4	2-C	378	TYR	N-CA	-6.41	1.38	1.45
1	3-A	807	ASN	CA-C	-6.41	1.44	1.52
4	3-C	378	TYR	N-CA	-6.41	1.38	1.45
4	1-C	231	ASN	CA-C	-6.41	1.44	1.52
7	1-G	175	LYS	CA-C	-6.41	1.44	1.52
4	2-C	231	ASN	CA-C	-6.41	1.44	1.52
7	2-G	175	LYS	CA-C	-6.41	1.44	1.52
4	3-C	231	ASN	CA-C	-6.41	1.44	1.52
7	3-G	175	LYS	CA-C	-6.41	1.44	1.52
4	1-C	669	LYS	CA-C	-6.41	1.44	1.52
4	2-C	669	LYS	CA-C	-6.41	1.44	1.52
4	3-C	669	LYS	CA-C	-6.41	1.44	1.52
5	1-D	68	LEU	CA-C	-6.41	1.44	1.52
8	1-Z	120	GLY	CA-C	-6.41	1.45	1.52
5	1-I	68	LEU	CA-C	-6.41	1.44	1.52
5	2-D	68	LEU	CA-C	-6.41	1.44	1.52
8	2-Z	120	GLY	CA-C	-6.41	1.45	1.52
5	2-I	68	LEU	CA-C	-6.41	1.44	1.52
5	3-D	68	LEU	CA-C	-6.41	1.44	1.52
8	3-Z	120	GLY	CA-C	-6.41	1.45	1.52
5	3-I	68	LEU	CA-C	-6.41	1.44	1.52
4	1-C	568	PRO	CA-C	-6.40	1.41	1.52
4	2-C	568	PRO	CA-C	-6.40	1.41	1.52
4	3-C	568	PRO	CA-C	-6.40	1.41	1.52
4	1-H	9	ARG	N-CA	-6.40	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-H	9	ARG	N-CA	-6.40	1.38	1.46
4	3-H	9	ARG	N-CA	-6.40	1.38	1.46
5	1-D	118	ALA	N-CA	-6.40	1.38	1.46
3	1-N	394	TYR	CA-C	-6.40	1.44	1.52
5	2-D	118	ALA	N-CA	-6.40	1.38	1.46
3	2-N	394	TYR	CA-C	-6.40	1.44	1.52
5	3-D	118	ALA	N-CA	-6.40	1.38	1.46
3	3-N	394	TYR	CA-C	-6.40	1.44	1.52
3	1-B	854	GLU	CA-C	-6.39	1.44	1.52
7	1-G	91	THR	CA-C	-6.39	1.44	1.52
3	2-B	854	GLU	CA-C	-6.39	1.44	1.52
7	2-G	91	THR	CA-C	-6.39	1.44	1.52
3	3-B	854	GLU	CA-C	-6.39	1.44	1.52
7	3-G	91	THR	CA-C	-6.39	1.44	1.52
7	1-K	828	LEU	CA-C	-6.39	1.45	1.52
7	2-K	828	LEU	CA-C	-6.39	1.45	1.52
7	3-K	828	LEU	CA-C	-6.39	1.45	1.52
3	1-B	472	GLY	CA-C	-6.39	1.45	1.52
3	2-B	472	GLY	CA-C	-6.39	1.45	1.52
3	3-B	472	GLY	CA-C	-6.39	1.45	1.52
3	1-B	122	LYS	CA-C	-6.39	1.44	1.52
6	1-F	19	ARG	CA-C	-6.39	1.45	1.52
3	2-B	122	LYS	CA-C	-6.39	1.44	1.52
6	2-F	19	ARG	CA-C	-6.39	1.45	1.52
3	3-B	122	LYS	CA-C	-6.39	1.44	1.52
6	3-F	19	ARG	CA-C	-6.39	1.45	1.52
3	1-B	152	MET	N-CA	-6.39	1.40	1.46
4	1-C	115	LEU	CA-C	-6.39	1.45	1.52
3	1-N	438	PHE	CA-C	-6.39	1.44	1.52
3	2-B	152	MET	N-CA	-6.39	1.40	1.46
4	2-C	115	LEU	CA-C	-6.39	1.45	1.52
3	2-N	438	PHE	CA-C	-6.39	1.44	1.52
3	3-B	152	MET	N-CA	-6.39	1.40	1.46
4	3-C	115	LEU	CA-C	-6.39	1.45	1.52
3	3-N	438	PHE	CA-C	-6.39	1.44	1.52
4	1-C	9	ARG	N-CA	-6.38	1.38	1.46
7	1-G	176	ARG	N-CA	-6.38	1.38	1.46
7	1-K	242	GLU	CA-C	-6.38	1.44	1.52
4	2-C	9	ARG	N-CA	-6.38	1.38	1.46
7	2-G	176	ARG	N-CA	-6.38	1.38	1.46
7	2-K	242	GLU	CA-C	-6.38	1.44	1.52
4	3-C	9	ARG	N-CA	-6.38	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3-G	176	ARG	N-CA	-6.38	1.38	1.46
7	3-K	242	GLU	CA-C	-6.38	1.44	1.52
1	1-A	36	TRP	CA-C	-6.38	1.44	1.52
6	1-F	61	ILE	N-CA	-6.38	1.38	1.46
7	1-K	840	ILE	N-CA	-6.38	1.38	1.46
1	2-A	36	TRP	CA-C	-6.38	1.44	1.52
6	2-F	61	ILE	N-CA	-6.38	1.38	1.46
7	2-K	840	ILE	N-CA	-6.38	1.38	1.46
1	3-A	36	TRP	CA-C	-6.38	1.44	1.52
6	3-F	61	ILE	N-CA	-6.38	1.38	1.46
7	3-K	840	ILE	N-CA	-6.38	1.38	1.46
1	1-A	274	ARG	CA-C	-6.38	1.45	1.52
1	1-A	664	ALA	CA-C	-6.38	1.44	1.52
3	1-B	763	GLN	N-CA	-6.38	1.38	1.46
3	1-N	122	LYS	CA-C	-6.38	1.44	1.52
4	1-H	306	MET	CA-C	-6.38	1.44	1.52
4	1-H	668	GLN	CA-C	-6.38	1.44	1.52
1	2-A	274	ARG	CA-C	-6.38	1.45	1.52
1	2-A	664	ALA	CA-C	-6.38	1.44	1.52
3	2-B	763	GLN	N-CA	-6.38	1.38	1.46
3	2-N	122	LYS	CA-C	-6.38	1.44	1.52
4	2-H	306	MET	CA-C	-6.38	1.44	1.52
4	2-H	668	GLN	CA-C	-6.38	1.44	1.52
1	3-A	274	ARG	CA-C	-6.38	1.45	1.52
1	3-A	664	ALA	CA-C	-6.38	1.44	1.52
3	3-B	763	GLN	N-CA	-6.38	1.38	1.46
3	3-N	122	LYS	CA-C	-6.38	1.44	1.52
4	3-H	306	MET	CA-C	-6.38	1.44	1.52
4	3-H	668	GLN	CA-C	-6.38	1.44	1.52
3	1-B	394	TYR	CA-C	-6.38	1.44	1.52
3	2-B	394	TYR	CA-C	-6.38	1.44	1.52
3	3-B	394	TYR	CA-C	-6.38	1.44	1.52
1	1-A	134	HIS	N-CA	-6.37	1.38	1.46
7	1-K	209	LEU	CA-C	-6.37	1.44	1.52
3	1-N	472	GLY	CA-C	-6.37	1.45	1.52
4	1-H	568	PRO	CA-C	-6.37	1.41	1.52
6	1-J	103	ALA	CA-C	-6.37	1.44	1.52
1	2-A	134	HIS	N-CA	-6.37	1.38	1.46
7	2-K	209	LEU	CA-C	-6.37	1.44	1.52
3	2-N	472	GLY	CA-C	-6.37	1.45	1.52
4	2-H	568	PRO	CA-C	-6.37	1.41	1.52
6	2-J	103	ALA	CA-C	-6.37	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-A	134	HIS	N-CA	-6.37	1.38	1.46
7	3-K	209	LEU	CA-C	-6.37	1.44	1.52
3	3-N	472	GLY	CA-C	-6.37	1.45	1.52
4	3-H	568	PRO	CA-C	-6.37	1.41	1.52
6	3-J	103	ALA	CA-C	-6.37	1.44	1.52
7	1-K	252	PHE	N-CA	-6.37	1.38	1.46
7	2-K	252	PHE	N-CA	-6.37	1.38	1.46
7	3-K	252	PHE	N-CA	-6.37	1.38	1.46
5	1-D	151	GLN	CA-C	-6.37	1.44	1.52
5	2-D	151	GLN	CA-C	-6.37	1.44	1.52
5	3-D	151	GLN	CA-C	-6.37	1.44	1.52
8	1-Z	15	ALA	N-CA	-6.37	1.38	1.46
8	2-Z	15	ALA	N-CA	-6.37	1.38	1.46
8	3-Z	15	ALA	N-CA	-6.37	1.38	1.46
1	1-A	654	GLU	CA-C	-6.37	1.44	1.52
7	1-G	840	ILE	N-CA	-6.37	1.38	1.46
1	2-A	654	GLU	CA-C	-6.37	1.44	1.52
7	2-G	840	ILE	N-CA	-6.37	1.38	1.46
1	3-A	654	GLU	CA-C	-6.37	1.44	1.52
7	3-G	840	ILE	N-CA	-6.37	1.38	1.46
4	1-H	391	ALA	CA-C	-6.36	1.44	1.53
4	2-H	391	ALA	CA-C	-6.36	1.44	1.53
4	3-H	391	ALA	CA-C	-6.36	1.44	1.53
3	1-B	370	GLU	N-CA	-6.36	1.38	1.46
3	2-B	370	GLU	N-CA	-6.36	1.38	1.46
3	3-B	370	GLU	N-CA	-6.36	1.38	1.46
3	1-B	778	LEU	N-CA	-6.36	1.38	1.46
7	1-K	612	ILE	CA-C	-6.36	1.44	1.52
3	2-B	778	LEU	N-CA	-6.36	1.38	1.46
7	2-K	612	ILE	CA-C	-6.36	1.44	1.52
3	3-B	778	LEU	N-CA	-6.36	1.38	1.46
7	3-K	612	ILE	CA-C	-6.36	1.44	1.52
4	1-C	76	ALA	CA-C	-6.36	1.44	1.52
4	1-H	446	GLY	CA-C	-6.36	1.46	1.52
4	2-C	76	ALA	CA-C	-6.36	1.44	1.52
4	2-H	446	GLY	CA-C	-6.36	1.46	1.52
4	3-C	76	ALA	CA-C	-6.36	1.44	1.52
4	3-H	446	GLY	CA-C	-6.36	1.46	1.52
1	1-A	574	LYS	N-CA	-6.35	1.38	1.46
1	2-A	574	LYS	N-CA	-6.35	1.38	1.46
1	3-A	574	LYS	N-CA	-6.35	1.38	1.46
3	1-N	370	GLU	N-CA	-6.35	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-N	370	GLU	N-CA	-6.35	1.38	1.46
3	3-N	370	GLU	N-CA	-6.35	1.38	1.46
4	1-C	446	GLY	CA-C	-6.35	1.46	1.52
4	2-C	446	GLY	CA-C	-6.35	1.46	1.52
4	3-C	446	GLY	CA-C	-6.35	1.46	1.52
3	1-N	297	ALA	CA-C	-6.34	1.44	1.52
3	2-N	297	ALA	CA-C	-6.34	1.44	1.52
3	3-N	297	ALA	CA-C	-6.34	1.44	1.52
3	1-B	207	ASN	CA-C	-6.34	1.44	1.52
3	2-B	207	ASN	CA-C	-6.34	1.44	1.52
3	3-B	207	ASN	CA-C	-6.34	1.44	1.52
8	1-Z	142	VAL	N-CA	-6.34	1.39	1.46
3	1-N	207	ASN	CA-C	-6.34	1.44	1.52
3	1-N	439	VAL	CA-C	-6.34	1.45	1.52
8	2-Z	142	VAL	N-CA	-6.34	1.39	1.46
3	2-N	207	ASN	CA-C	-6.34	1.44	1.52
3	2-N	439	VAL	CA-C	-6.34	1.45	1.52
8	3-Z	142	VAL	N-CA	-6.34	1.39	1.46
3	3-N	207	ASN	CA-C	-6.34	1.44	1.52
3	3-N	439	VAL	CA-C	-6.34	1.45	1.52
5	1-I	99	GLU	CA-C	-6.34	1.44	1.52
5	1-I	239	VAL	CA-C	-6.34	1.45	1.52
5	2-I	99	GLU	CA-C	-6.34	1.44	1.52
5	2-I	239	VAL	CA-C	-6.34	1.45	1.52
5	3-I	99	GLU	CA-C	-6.34	1.44	1.52
5	3-I	239	VAL	CA-C	-6.34	1.45	1.52
4	1-C	668	GLN	CA-C	-6.34	1.44	1.52
6	1-R	32	THR	CA-C	-6.34	1.44	1.52
4	2-C	668	GLN	CA-C	-6.34	1.44	1.52
6	2-R	32	THR	CA-C	-6.34	1.44	1.52
4	3-C	668	GLN	CA-C	-6.34	1.44	1.52
6	3-R	32	THR	CA-C	-6.34	1.44	1.52
3	1-B	297	ALA	CA-C	-6.33	1.44	1.52
7	1-G	144	MET	N-CA	-6.33	1.38	1.46
3	2-B	297	ALA	CA-C	-6.33	1.44	1.52
7	2-G	144	MET	N-CA	-6.33	1.38	1.46
3	3-B	297	ALA	CA-C	-6.33	1.44	1.52
7	3-G	144	MET	N-CA	-6.33	1.38	1.46
1	1-A	473	THR	N-CA	-6.33	1.38	1.46
6	1-R	55	THR	CA-C	-6.33	1.45	1.52
5	1-I	118	ALA	N-CA	-6.33	1.38	1.46
1	2-A	473	THR	N-CA	-6.33	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2-R	55	THR	CA-C	-6.33	1.45	1.52
5	2-I	118	ALA	N-CA	-6.33	1.38	1.46
1	3-A	473	THR	N-CA	-6.33	1.38	1.46
6	3-R	55	THR	CA-C	-6.33	1.45	1.52
5	3-I	118	ALA	N-CA	-6.33	1.38	1.46
6	1-F	103	ALA	CA-C	-6.33	1.44	1.52
6	2-F	103	ALA	CA-C	-6.33	1.44	1.52
6	3-F	103	ALA	CA-C	-6.33	1.44	1.52
4	1-C	391	ALA	CA-C	-6.33	1.44	1.53
4	1-C	761	TYR	CA-C	-6.33	1.45	1.53
5	1-D	14	LYS	N-CA	-6.33	1.38	1.46
4	2-C	391	ALA	CA-C	-6.33	1.44	1.53
4	2-C	761	TYR	CA-C	-6.33	1.45	1.53
5	2-D	14	LYS	N-CA	-6.33	1.38	1.46
4	3-C	391	ALA	CA-C	-6.33	1.44	1.53
4	3-C	761	TYR	CA-C	-6.33	1.45	1.53
5	3-D	14	LYS	N-CA	-6.33	1.38	1.46
8	1-L	99	ASP	N-CA	-6.32	1.38	1.46
4	1-H	255	ILE	CA-C	-6.32	1.44	1.52
8	2-L	99	ASP	N-CA	-6.32	1.38	1.46
4	2-H	255	ILE	CA-C	-6.32	1.44	1.52
8	3-L	99	ASP	N-CA	-6.32	1.38	1.46
4	3-H	255	ILE	CA-C	-6.32	1.44	1.52
6	1-R	168	GLU	CA-C	-6.32	1.44	1.52
7	1-K	65	GLU	N-CA	-6.32	1.38	1.46
6	2-R	168	GLU	CA-C	-6.32	1.44	1.52
7	2-K	65	GLU	N-CA	-6.32	1.38	1.46
6	3-R	168	GLU	CA-C	-6.32	1.44	1.52
7	3-K	65	GLU	N-CA	-6.32	1.38	1.46
6	1-J	61	ILE	N-CA	-6.31	1.38	1.46
6	2-J	61	ILE	N-CA	-6.31	1.38	1.46
6	3-J	61	ILE	N-CA	-6.31	1.38	1.46
1	1-A	329	HIS	CA-C	-6.31	1.45	1.52
7	1-G	612	ILE	CA-C	-6.31	1.44	1.52
1	2-A	329	HIS	CA-C	-6.31	1.45	1.52
7	2-G	612	ILE	CA-C	-6.31	1.44	1.52
1	3-A	329	HIS	CA-C	-6.31	1.45	1.52
7	3-G	612	ILE	CA-C	-6.31	1.44	1.52
6	1-F	116	LEU	N-CA	-6.31	1.38	1.46
7	1-G	610	GLN	N-CA	-6.31	1.38	1.46
6	2-F	116	LEU	N-CA	-6.31	1.38	1.46
7	2-G	610	GLN	N-CA	-6.31	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	3-F	116	LEU	N-CA	-6.31	1.38	1.46
7	3-G	610	GLN	N-CA	-6.31	1.38	1.46
7	1-G	76	LEU	N-CA	-6.31	1.38	1.46
8	1-L	46	LYS	N-CA	-6.31	1.38	1.46
7	2-G	76	LEU	N-CA	-6.31	1.38	1.46
8	2-L	46	LYS	N-CA	-6.31	1.38	1.46
7	3-G	76	LEU	N-CA	-6.31	1.38	1.46
8	3-L	46	LYS	N-CA	-6.31	1.38	1.46
6	1-R	39	LEU	CA-C	-6.31	1.43	1.52
6	2-R	39	LEU	CA-C	-6.31	1.43	1.52
6	3-R	39	LEU	CA-C	-6.31	1.43	1.52
1	1-A	644	ASP	CA-C	-6.30	1.44	1.52
3	1-B	307	GLU	CA-C	-6.30	1.45	1.52
1	2-A	644	ASP	CA-C	-6.30	1.44	1.52
3	2-B	307	GLU	CA-C	-6.30	1.45	1.52
1	3-A	644	ASP	CA-C	-6.30	1.44	1.52
3	3-B	307	GLU	CA-C	-6.30	1.45	1.52
5	1-I	117	VAL	N-CA	-6.30	1.38	1.46
5	2-I	117	VAL	N-CA	-6.30	1.38	1.46
5	3-I	117	VAL	N-CA	-6.30	1.38	1.46
8	1-L	51	LYS	N-CA	-6.30	1.38	1.46
8	2-L	51	LYS	N-CA	-6.30	1.38	1.46
8	3-L	51	LYS	N-CA	-6.30	1.38	1.46
5	1-I	151	GLN	CA-C	-6.30	1.44	1.52
5	2-I	151	GLN	CA-C	-6.30	1.44	1.52
5	3-I	151	GLN	CA-C	-6.30	1.44	1.52
7	1-G	401	LEU	CA-C	-6.29	1.44	1.52
7	2-G	401	LEU	CA-C	-6.29	1.44	1.52
7	3-G	401	LEU	CA-C	-6.29	1.44	1.52
7	1-K	83	THR	CA-C	-6.29	1.44	1.52
7	2-K	83	THR	CA-C	-6.29	1.44	1.52
7	3-K	83	THR	CA-C	-6.29	1.44	1.52
5	1-D	115	GLU	CA-C	-6.29	1.45	1.52
5	2-D	115	GLU	CA-C	-6.29	1.45	1.52
5	3-D	115	GLU	CA-C	-6.29	1.45	1.52
8	1-Z	17	LEU	CA-C	-6.29	1.45	1.52
7	1-K	844	SER	CA-C	-6.29	1.45	1.52
8	2-Z	17	LEU	CA-C	-6.29	1.45	1.52
7	2-K	844	SER	CA-C	-6.29	1.45	1.52
8	3-Z	17	LEU	CA-C	-6.29	1.45	1.52
7	3-K	844	SER	CA-C	-6.29	1.45	1.52
1	1-A	535	TRP	CA-C	-6.29	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	411	ASP	CA-C	-6.29	1.47	1.53
1	2-A	535	TRP	CA-C	-6.29	1.45	1.52
3	2-B	411	ASP	CA-C	-6.29	1.47	1.53
1	3-A	535	TRP	CA-C	-6.29	1.45	1.52
3	3-B	411	ASP	CA-C	-6.29	1.47	1.53
3	1-N	174	ILE	CA-C	-6.29	1.44	1.52
3	2-N	174	ILE	CA-C	-6.29	1.44	1.52
3	3-N	174	ILE	CA-C	-6.29	1.44	1.52
3	1-B	438	PHE	CA-C	-6.29	1.44	1.52
4	1-H	588	LEU	CA-C	-6.29	1.44	1.52
3	2-B	438	PHE	CA-C	-6.29	1.44	1.52
4	2-H	588	LEU	CA-C	-6.29	1.44	1.52
3	3-B	438	PHE	CA-C	-6.29	1.44	1.52
4	3-H	588	LEU	CA-C	-6.29	1.44	1.52
5	1-D	99	GLU	CA-C	-6.28	1.44	1.52
5	2-D	99	GLU	CA-C	-6.28	1.44	1.52
5	3-D	99	GLU	CA-C	-6.28	1.44	1.52
7	1-K	292	LEU	CA-C	-6.28	1.44	1.52
7	2-K	292	LEU	CA-C	-6.28	1.44	1.52
7	3-K	292	LEU	CA-C	-6.28	1.44	1.52
3	1-N	397	LEU	CA-C	-6.28	1.44	1.52
6	1-J	116	LEU	N-CA	-6.28	1.38	1.46
3	2-N	397	LEU	CA-C	-6.28	1.44	1.52
6	2-J	116	LEU	N-CA	-6.28	1.38	1.46
3	3-N	397	LEU	CA-C	-6.28	1.44	1.52
6	3-J	116	LEU	N-CA	-6.28	1.38	1.46
3	1-N	453	ILE	CA-C	-6.27	1.44	1.52
3	2-N	453	ILE	CA-C	-6.27	1.44	1.52
3	3-N	453	ILE	CA-C	-6.27	1.44	1.52
7	1-G	828	LEU	N-CA	-6.27	1.38	1.46
7	2-G	828	LEU	N-CA	-6.27	1.38	1.46
7	3-G	828	LEU	N-CA	-6.27	1.38	1.46
4	1-C	588	LEU	CA-C	-6.27	1.44	1.52
4	2-C	588	LEU	CA-C	-6.27	1.44	1.52
4	3-C	588	LEU	CA-C	-6.27	1.44	1.52
3	1-B	174	ILE	CA-C	-6.27	1.44	1.52
3	2-B	174	ILE	CA-C	-6.27	1.44	1.52
3	3-B	174	ILE	CA-C	-6.27	1.44	1.52
5	1-D	239	VAL	CA-C	-6.27	1.45	1.52
5	2-D	239	VAL	CA-C	-6.27	1.45	1.52
5	3-D	239	VAL	CA-C	-6.27	1.45	1.52
1	1-A	346	PHE	CA-C	-6.26	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-G	844	SER	CA-C	-6.26	1.45	1.52
4	1-H	711	MET	CA-C	-6.26	1.44	1.52
1	2-A	346	PHE	CA-C	-6.26	1.44	1.52
7	2-G	844	SER	CA-C	-6.26	1.45	1.52
4	2-H	711	MET	CA-C	-6.26	1.44	1.52
1	3-A	346	PHE	CA-C	-6.26	1.44	1.52
7	3-G	844	SER	CA-C	-6.26	1.45	1.52
4	3-H	711	MET	CA-C	-6.26	1.44	1.52
4	1-C	272	GLU	CA-C	-6.26	1.44	1.52
7	1-G	509	ILE	N-CA	-6.26	1.38	1.46
7	1-K	167	LEU	N-CA	-6.26	1.38	1.46
4	2-C	272	GLU	CA-C	-6.26	1.44	1.52
7	2-G	509	ILE	N-CA	-6.26	1.38	1.46
7	2-K	167	LEU	N-CA	-6.26	1.38	1.46
4	3-C	272	GLU	CA-C	-6.26	1.44	1.52
7	3-G	509	ILE	N-CA	-6.26	1.38	1.46
7	3-K	167	LEU	N-CA	-6.26	1.38	1.46
1	1-A	487	LYS	CA-C	-6.26	1.45	1.52
7	1-G	149	VAL	N-CA	-6.26	1.39	1.46
7	1-G	521	ASP	CA-C	-6.26	1.45	1.53
1	2-A	487	LYS	CA-C	-6.26	1.45	1.52
7	2-G	149	VAL	N-CA	-6.26	1.39	1.46
7	2-G	521	ASP	CA-C	-6.26	1.45	1.53
1	3-A	487	LYS	CA-C	-6.26	1.45	1.52
7	3-G	149	VAL	N-CA	-6.26	1.39	1.46
7	3-G	521	ASP	CA-C	-6.26	1.45	1.53
4	1-C	255	ILE	CA-C	-6.26	1.45	1.52
4	2-C	255	ILE	CA-C	-6.26	1.45	1.52
4	3-C	255	ILE	CA-C	-6.26	1.45	1.52
4	1-C	711	MET	CA-C	-6.25	1.44	1.52
6	1-R	104	ARG	CA-C	-6.25	1.44	1.52
6	1-M	78	TRP	CA-C	-6.25	1.43	1.52
4	2-C	711	MET	CA-C	-6.25	1.44	1.52
6	2-R	104	ARG	CA-C	-6.25	1.44	1.52
6	2-M	78	TRP	CA-C	-6.25	1.43	1.52
4	3-C	711	MET	CA-C	-6.25	1.44	1.52
6	3-R	104	ARG	CA-C	-6.25	1.44	1.52
6	3-M	78	TRP	CA-C	-6.25	1.43	1.52
3	1-B	453	ILE	CA-C	-6.25	1.44	1.52
3	2-B	453	ILE	CA-C	-6.25	1.44	1.52
3	3-B	453	ILE	CA-C	-6.25	1.44	1.52
7	1-G	82	PRO	CA-C	-6.25	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	82	PRO	CA-C	-6.25	1.43	1.52
7	3-G	82	PRO	CA-C	-6.25	1.43	1.52
3	1-B	439	VAL	CA-C	-6.25	1.45	1.52
7	1-G	398	MET	CA-C	-6.25	1.44	1.52
3	2-B	439	VAL	CA-C	-6.25	1.45	1.52
7	2-G	398	MET	CA-C	-6.25	1.44	1.52
3	3-B	439	VAL	CA-C	-6.25	1.45	1.52
7	3-G	398	MET	CA-C	-6.25	1.44	1.52
3	1-B	834	LEU	CA-C	-6.24	1.44	1.52
3	1-B	941	HIS	N-CA	-6.24	1.38	1.46
4	1-H	498	ALA	CA-C	-6.24	1.44	1.52
3	2-B	834	LEU	CA-C	-6.24	1.44	1.52
3	2-B	941	HIS	N-CA	-6.24	1.38	1.46
4	2-H	498	ALA	CA-C	-6.24	1.44	1.52
3	3-B	834	LEU	CA-C	-6.24	1.44	1.52
3	3-B	941	HIS	N-CA	-6.24	1.38	1.46
4	3-H	498	ALA	CA-C	-6.24	1.44	1.52
1	1-A	200	VAL	CA-C	-6.24	1.45	1.52
7	1-K	828	LEU	N-CA	-6.24	1.38	1.46
3	1-N	474	LEU	CA-C	-6.24	1.44	1.52
1	2-A	200	VAL	CA-C	-6.24	1.45	1.52
7	2-K	828	LEU	N-CA	-6.24	1.38	1.46
3	2-N	474	LEU	CA-C	-6.24	1.44	1.52
1	3-A	200	VAL	CA-C	-6.24	1.45	1.52
7	3-K	828	LEU	N-CA	-6.24	1.38	1.46
3	3-N	474	LEU	CA-C	-6.24	1.44	1.52
7	1-G	828	LEU	CA-C	-6.24	1.45	1.52
8	1-Z	101	LEU	CA-C	-6.24	1.44	1.52
7	2-G	828	LEU	CA-C	-6.24	1.45	1.52
8	2-Z	101	LEU	CA-C	-6.24	1.44	1.52
7	3-G	828	LEU	CA-C	-6.24	1.45	1.52
8	3-Z	101	LEU	CA-C	-6.24	1.44	1.52
7	1-K	189	ASN	CA-C	-6.23	1.44	1.52
7	2-K	189	ASN	CA-C	-6.23	1.44	1.52
7	3-K	189	ASN	CA-C	-6.23	1.44	1.52
6	1-R	19	ARG	CA-C	-6.23	1.45	1.52
6	2-R	19	ARG	CA-C	-6.23	1.45	1.52
6	3-R	19	ARG	CA-C	-6.23	1.45	1.52
4	1-C	377	ILE	N-CA	-6.23	1.39	1.46
4	2-C	377	ILE	N-CA	-6.23	1.39	1.46
4	3-C	377	ILE	N-CA	-6.23	1.39	1.46
1	1-A	464	LEU	CA-C	-6.23	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	464	LEU	CA-C	-6.23	1.45	1.53
1	3-A	464	LEU	CA-C	-6.23	1.45	1.53
4	1-H	272	GLU	CA-C	-6.23	1.44	1.52
4	2-H	272	GLU	CA-C	-6.23	1.44	1.52
4	3-H	272	GLU	CA-C	-6.23	1.44	1.52
1	1-A	451	PRO	CA-C	-6.22	1.45	1.52
7	1-K	610	GLN	N-CA	-6.22	1.38	1.46
1	2-A	451	PRO	CA-C	-6.22	1.45	1.52
7	2-K	610	GLN	N-CA	-6.22	1.38	1.46
1	3-A	451	PRO	CA-C	-6.22	1.45	1.52
7	3-K	610	GLN	N-CA	-6.22	1.38	1.46
7	1-G	432	LYS	CA-C	-6.22	1.44	1.52
7	2-G	432	LYS	CA-C	-6.22	1.44	1.52
7	3-G	432	LYS	CA-C	-6.22	1.44	1.52
1	1-A	134	HIS	CA-C	-6.22	1.45	1.52
4	1-H	275	TRP	CA-C	-6.22	1.45	1.53
1	2-A	134	HIS	CA-C	-6.22	1.45	1.52
4	2-H	275	TRP	CA-C	-6.22	1.45	1.53
1	3-A	134	HIS	CA-C	-6.22	1.45	1.52
4	3-H	275	TRP	CA-C	-6.22	1.45	1.53
4	1-H	586	SER	CA-C	-6.22	1.44	1.52
4	2-H	586	SER	CA-C	-6.22	1.44	1.52
4	3-H	586	SER	CA-C	-6.22	1.44	1.52
8	1-L	93	VAL	CA-C	-6.22	1.44	1.52
8	2-L	93	VAL	CA-C	-6.22	1.44	1.52
8	3-L	93	VAL	CA-C	-6.22	1.44	1.52
7	1-G	456	LEU	CA-C	-6.21	1.45	1.52
7	1-K	174	VAL	N-CA	-6.21	1.39	1.46
3	1-N	307	GLU	CA-C	-6.21	1.45	1.52
5	1-I	14	LYS	N-CA	-6.21	1.38	1.46
7	2-G	456	LEU	CA-C	-6.21	1.45	1.52
7	2-K	174	VAL	N-CA	-6.21	1.39	1.46
3	2-N	307	GLU	CA-C	-6.21	1.45	1.52
5	2-I	14	LYS	N-CA	-6.21	1.38	1.46
7	3-G	456	LEU	CA-C	-6.21	1.45	1.52
7	3-K	174	VAL	N-CA	-6.21	1.39	1.46
3	3-N	307	GLU	CA-C	-6.21	1.45	1.52
5	3-I	14	LYS	N-CA	-6.21	1.38	1.46
7	1-K	116	LYS	CA-C	-6.21	1.44	1.52
7	2-K	116	LYS	CA-C	-6.21	1.44	1.52
7	3-K	116	LYS	CA-C	-6.21	1.44	1.52
6	1-R	43	ILE	C-N	6.21	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1-I	115	GLU	CA-C	-6.21	1.45	1.52
6	2-R	43	ILE	C-N	6.21	1.42	1.33
5	2-I	115	GLU	CA-C	-6.21	1.45	1.52
6	3-R	43	ILE	C-N	6.21	1.42	1.33
5	3-I	115	GLU	CA-C	-6.21	1.45	1.52
4	1-C	586	SER	CA-C	-6.21	1.44	1.52
4	2-C	586	SER	CA-C	-6.21	1.44	1.52
4	3-C	586	SER	CA-C	-6.21	1.44	1.52
7	1-G	71	PHE	CA-C	-6.21	1.44	1.52
7	2-G	71	PHE	CA-C	-6.21	1.44	1.52
7	3-G	71	PHE	CA-C	-6.21	1.44	1.52
1	1-A	343	GLN	CA-C	-6.20	1.44	1.52
7	1-G	118	ASP	N-CA	-6.20	1.38	1.46
8	1-Z	40	GLU	CA-C	-6.20	1.44	1.52
1	2-A	343	GLN	CA-C	-6.20	1.44	1.52
7	2-G	118	ASP	N-CA	-6.20	1.38	1.46
8	2-Z	40	GLU	CA-C	-6.20	1.44	1.52
1	3-A	343	GLN	CA-C	-6.20	1.44	1.52
7	3-G	118	ASP	N-CA	-6.20	1.38	1.46
8	3-Z	40	GLU	CA-C	-6.20	1.44	1.52
3	1-B	397	LEU	CA-C	-6.20	1.44	1.52
7	1-K	199	LEU	CA-C	-6.20	1.45	1.52
3	2-B	397	LEU	CA-C	-6.20	1.44	1.52
7	2-K	199	LEU	CA-C	-6.20	1.45	1.52
3	3-B	397	LEU	CA-C	-6.20	1.44	1.52
7	3-K	199	LEU	CA-C	-6.20	1.45	1.52
3	1-B	298	GLN	CA-C	-6.20	1.45	1.52
3	1-N	264	ILE	CA-C	-6.20	1.45	1.52
3	1-N	414	ALA	CA-C	-6.20	1.44	1.52
4	1-H	559	ARG	N-CA	-6.20	1.37	1.45
3	2-B	298	GLN	CA-C	-6.20	1.45	1.52
3	2-N	264	ILE	CA-C	-6.20	1.45	1.52
3	2-N	414	ALA	CA-C	-6.20	1.44	1.52
4	2-H	559	ARG	N-CA	-6.20	1.37	1.45
3	3-B	298	GLN	CA-C	-6.20	1.45	1.52
3	3-N	264	ILE	CA-C	-6.20	1.45	1.52
3	3-N	414	ALA	CA-C	-6.20	1.44	1.52
4	3-H	559	ARG	N-CA	-6.20	1.37	1.45
7	1-G	778	GLU	CA-C	-6.20	1.44	1.52
4	1-H	274	VAL	CA-C	-6.20	1.45	1.52
7	2-G	778	GLU	CA-C	-6.20	1.44	1.52
4	2-H	274	VAL	CA-C	-6.20	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3-G	778	GLU	CA-C	-6.20	1.44	1.52
4	3-H	274	VAL	CA-C	-6.20	1.45	1.52
8	1-Z	89	MET	CA-C	-6.19	1.44	1.52
7	1-K	152	VAL	N-CA	-6.19	1.42	1.46
8	2-Z	89	MET	CA-C	-6.19	1.44	1.52
7	2-K	152	VAL	N-CA	-6.19	1.42	1.46
8	3-Z	89	MET	CA-C	-6.19	1.44	1.52
7	3-K	152	VAL	N-CA	-6.19	1.42	1.46
7	1-K	206	ASN	N-CA	-6.19	1.38	1.46
7	2-K	206	ASN	N-CA	-6.19	1.38	1.46
7	3-K	206	ASN	N-CA	-6.19	1.38	1.46
3	1-B	474	LEU	CA-C	-6.19	1.45	1.52
7	1-G	142	ARG	CA-C	-6.19	1.45	1.52
8	1-L	142	VAL	N-CA	-6.19	1.39	1.46
4	1-H	377	ILE	N-CA	-6.19	1.39	1.46
3	2-B	474	LEU	CA-C	-6.19	1.45	1.52
7	2-G	142	ARG	CA-C	-6.19	1.45	1.52
8	2-L	142	VAL	N-CA	-6.19	1.39	1.46
4	2-H	377	ILE	N-CA	-6.19	1.39	1.46
3	3-B	474	LEU	CA-C	-6.19	1.45	1.52
7	3-G	142	ARG	CA-C	-6.19	1.45	1.52
8	3-L	142	VAL	N-CA	-6.19	1.39	1.46
4	3-H	377	ILE	N-CA	-6.19	1.39	1.46
6	1-M	170	LEU	CA-C	-6.19	1.44	1.52
4	1-H	715	LEU	CA-C	-6.19	1.44	1.52
6	2-M	170	LEU	CA-C	-6.19	1.44	1.52
4	2-H	715	LEU	CA-C	-6.19	1.44	1.52
6	3-M	170	LEU	CA-C	-6.19	1.44	1.52
4	3-H	715	LEU	CA-C	-6.19	1.44	1.52
5	1-D	117	VAL	N-CA	-6.19	1.38	1.46
5	2-D	117	VAL	N-CA	-6.19	1.38	1.46
5	3-D	117	VAL	N-CA	-6.19	1.38	1.46
6	1-F	26	ASP	CA-C	-6.18	1.44	1.52
7	1-G	289	VAL	CA-C	-6.18	1.45	1.52
3	1-N	135	THR	CA-C	-6.18	1.44	1.52
6	1-J	26	ASP	CA-C	-6.18	1.44	1.52
6	2-F	26	ASP	CA-C	-6.18	1.44	1.52
7	2-G	289	VAL	CA-C	-6.18	1.45	1.52
3	2-N	135	THR	CA-C	-6.18	1.44	1.52
6	2-J	26	ASP	CA-C	-6.18	1.44	1.52
6	3-F	26	ASP	CA-C	-6.18	1.44	1.52
7	3-G	289	VAL	CA-C	-6.18	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-N	135	THR	CA-C	-6.18	1.44	1.52
6	3-J	26	ASP	CA-C	-6.18	1.44	1.52
4	1-C	454	ASN	CA-C	-6.18	1.44	1.52
4	2-C	454	ASN	CA-C	-6.18	1.44	1.52
4	3-C	454	ASN	CA-C	-6.18	1.44	1.52
3	1-B	896	GLU	CA-C	-6.18	1.45	1.52
3	2-B	896	GLU	CA-C	-6.18	1.45	1.52
3	3-B	896	GLU	CA-C	-6.18	1.45	1.52
4	1-C	275	TRP	CA-C	-6.18	1.45	1.53
7	1-G	73	MET	CA-C	-6.18	1.44	1.52
6	1-R	108	GLN	N-CA	-6.18	1.38	1.46
8	1-L	97	LEU	N-CA	-6.18	1.39	1.46
4	2-C	275	TRP	CA-C	-6.18	1.45	1.53
7	2-G	73	MET	CA-C	-6.18	1.44	1.52
6	2-R	108	GLN	N-CA	-6.18	1.38	1.46
8	2-L	97	LEU	N-CA	-6.18	1.39	1.46
4	3-C	275	TRP	CA-C	-6.18	1.45	1.53
7	3-G	73	MET	CA-C	-6.18	1.44	1.52
6	3-R	108	GLN	N-CA	-6.18	1.38	1.46
8	3-L	97	LEU	N-CA	-6.18	1.39	1.46
8	1-Z	14	LYS	CA-C	-6.17	1.45	1.52
8	2-Z	14	LYS	CA-C	-6.17	1.45	1.52
8	3-Z	14	LYS	CA-C	-6.17	1.45	1.52
3	1-B	135	THR	CA-C	-6.17	1.44	1.52
3	2-B	135	THR	CA-C	-6.17	1.44	1.52
3	3-B	135	THR	CA-C	-6.17	1.44	1.52
1	1-A	542	ILE	CA-C	-6.17	1.45	1.52
1	2-A	542	ILE	CA-C	-6.17	1.45	1.52
1	3-A	542	ILE	CA-C	-6.17	1.45	1.52
4	1-C	274	VAL	CA-C	-6.17	1.45	1.52
7	1-G	80	ASN	N-CA	-6.17	1.39	1.46
4	2-C	274	VAL	CA-C	-6.17	1.45	1.52
7	2-G	80	ASN	N-CA	-6.17	1.39	1.46
4	3-C	274	VAL	CA-C	-6.17	1.45	1.52
7	3-G	80	ASN	N-CA	-6.17	1.39	1.46
6	1-R	86	GLU	N-CA	-6.17	1.38	1.46
7	1-K	779	VAL	N-CA	-6.17	1.39	1.46
6	2-R	86	GLU	N-CA	-6.17	1.38	1.46
7	2-K	779	VAL	N-CA	-6.17	1.39	1.46
6	3-R	86	GLU	N-CA	-6.17	1.38	1.46
7	3-K	779	VAL	N-CA	-6.17	1.39	1.46
1	1-A	614	MET	CA-C	-6.17	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	614	MET	CA-C	-6.17	1.44	1.52
1	3-A	614	MET	CA-C	-6.17	1.44	1.52
4	1-C	559	ARG	N-CA	-6.16	1.37	1.45
4	2-C	559	ARG	N-CA	-6.16	1.37	1.45
4	3-C	559	ARG	N-CA	-6.16	1.37	1.45
3	1-B	406	SER	N-CA	-6.16	1.39	1.46
3	2-B	406	SER	N-CA	-6.16	1.39	1.46
3	3-B	406	SER	N-CA	-6.16	1.39	1.46
7	1-K	303	LEU	CA-C	-6.16	1.44	1.52
7	2-K	303	LEU	CA-C	-6.16	1.44	1.52
7	3-K	303	LEU	CA-C	-6.16	1.44	1.52
7	1-G	294	LEU	CA-C	-6.16	1.45	1.52
7	2-G	294	LEU	CA-C	-6.16	1.45	1.52
7	3-G	294	LEU	CA-C	-6.16	1.45	1.52
6	1-R	126	ASN	CA-C	-6.16	1.44	1.53
6	1-M	37	LEU	N-CA	-6.16	1.39	1.46
6	2-R	126	ASN	CA-C	-6.16	1.44	1.53
6	2-M	37	LEU	N-CA	-6.16	1.39	1.46
6	3-R	126	ASN	CA-C	-6.16	1.44	1.53
6	3-M	37	LEU	N-CA	-6.16	1.39	1.46
3	1-N	473	ALA	CA-C	-6.15	1.45	1.52
3	2-N	473	ALA	CA-C	-6.15	1.45	1.52
3	3-N	473	ALA	CA-C	-6.15	1.45	1.52
4	1-C	498	ALA	CA-C	-6.15	1.44	1.52
7	1-G	235	VAL	CA-C	-6.15	1.45	1.52
4	2-C	498	ALA	CA-C	-6.15	1.44	1.52
7	2-G	235	VAL	CA-C	-6.15	1.45	1.52
4	3-C	498	ALA	CA-C	-6.15	1.44	1.52
7	3-G	235	VAL	CA-C	-6.15	1.45	1.52
8	1-L	50	ASN	N-CA	-6.15	1.39	1.46
8	2-L	50	ASN	N-CA	-6.15	1.39	1.46
8	3-L	50	ASN	N-CA	-6.15	1.39	1.46
7	1-K	167	LEU	CA-C	-6.15	1.44	1.52
7	2-K	167	LEU	CA-C	-6.15	1.44	1.52
7	3-K	167	LEU	CA-C	-6.15	1.44	1.52
7	1-G	67	THR	CA-C	-6.15	1.44	1.52
7	2-G	67	THR	CA-C	-6.15	1.44	1.52
7	3-G	67	THR	CA-C	-6.15	1.44	1.52
1	1-A	360	GLY	CA-C	-6.14	1.43	1.51
3	1-B	818	ILE	CA-C	-6.14	1.45	1.52
7	1-K	854	MET	CA-C	-6.14	1.45	1.52
3	1-N	117	CYS	CA-C	-6.14	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	360	GLY	CA-C	-6.14	1.43	1.51
3	2-B	818	ILE	CA-C	-6.14	1.45	1.52
7	2-K	854	MET	CA-C	-6.14	1.45	1.52
3	2-N	117	CYS	CA-C	-6.14	1.44	1.52
1	3-A	360	GLY	CA-C	-6.14	1.43	1.51
3	3-B	818	ILE	CA-C	-6.14	1.45	1.52
7	3-K	854	MET	CA-C	-6.14	1.45	1.52
3	3-N	117	CYS	CA-C	-6.14	1.44	1.52
7	1-G	484	HIS	N-CA	-6.14	1.38	1.46
6	1-R	99	ARG	CA-C	-6.14	1.44	1.52
3	1-N	411	ASP	CA-C	-6.14	1.47	1.53
7	2-G	484	HIS	N-CA	-6.14	1.38	1.46
6	2-R	99	ARG	CA-C	-6.14	1.44	1.52
3	2-N	411	ASP	CA-C	-6.14	1.47	1.53
7	3-G	484	HIS	N-CA	-6.14	1.38	1.46
6	3-R	99	ARG	CA-C	-6.14	1.44	1.52
3	3-N	411	ASP	CA-C	-6.14	1.47	1.53
7	1-G	417	ILE	CA-C	-6.14	1.45	1.52
7	2-G	417	ILE	CA-C	-6.14	1.45	1.52
7	3-G	417	ILE	CA-C	-6.14	1.45	1.52
3	1-B	54	THR	CA-C	-6.14	1.44	1.52
4	1-H	352	GLU	N-CA	-6.14	1.38	1.46
6	1-J	110	MET	CA-C	-6.14	1.44	1.52
3	2-B	54	THR	CA-C	-6.14	1.44	1.52
4	2-H	352	GLU	N-CA	-6.14	1.38	1.46
6	2-J	110	MET	CA-C	-6.14	1.44	1.52
3	3-B	54	THR	CA-C	-6.14	1.44	1.52
4	3-H	352	GLU	N-CA	-6.14	1.38	1.46
6	3-J	110	MET	CA-C	-6.14	1.44	1.52
4	1-C	224	THR	N-CA	-6.13	1.38	1.46
6	1-R	26	ASP	CA-C	-6.13	1.44	1.52
4	2-C	224	THR	N-CA	-6.13	1.38	1.46
6	2-R	26	ASP	CA-C	-6.13	1.44	1.52
4	3-C	224	THR	N-CA	-6.13	1.38	1.46
6	3-R	26	ASP	CA-C	-6.13	1.44	1.52
7	1-G	252	PHE	N-CA	-6.13	1.39	1.46
4	1-H	454	ASN	CA-C	-6.13	1.44	1.52
7	2-G	252	PHE	N-CA	-6.13	1.39	1.46
4	2-H	454	ASN	CA-C	-6.13	1.44	1.52
7	3-G	252	PHE	N-CA	-6.13	1.39	1.46
4	3-H	454	ASN	CA-C	-6.13	1.44	1.52
7	1-G	779	VAL	N-CA	-6.13	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	779	VAL	N-CA	-6.13	1.39	1.46
7	3-G	779	VAL	N-CA	-6.13	1.39	1.46
5	1-I	54	VAL	N-CA	-6.12	1.39	1.46
5	2-I	54	VAL	N-CA	-6.12	1.39	1.46
5	3-I	54	VAL	N-CA	-6.12	1.39	1.46
3	1-B	377	LYS	CA-C	-6.12	1.44	1.52
7	1-K	140	VAL	N-CA	-6.12	1.38	1.46
7	1-K	844	SER	N-CA	-6.12	1.39	1.46
3	2-B	377	LYS	CA-C	-6.12	1.44	1.52
7	2-K	140	VAL	N-CA	-6.12	1.38	1.46
7	2-K	844	SER	N-CA	-6.12	1.39	1.46
3	3-B	377	LYS	CA-C	-6.12	1.44	1.52
7	3-K	140	VAL	N-CA	-6.12	1.38	1.46
7	3-K	844	SER	N-CA	-6.12	1.39	1.46
8	1-L	77	PHE	N-CA	-6.12	1.38	1.46
8	2-L	77	PHE	N-CA	-6.12	1.38	1.46
8	3-L	77	PHE	N-CA	-6.12	1.38	1.46
3	1-B	212	LEU	CA-C	-6.12	1.45	1.52
3	1-B	858	MET	N-CA	-6.12	1.38	1.46
4	1-C	715	LEU	CA-C	-6.12	1.44	1.52
3	2-B	212	LEU	CA-C	-6.12	1.45	1.52
3	2-B	858	MET	N-CA	-6.12	1.38	1.46
4	2-C	715	LEU	CA-C	-6.12	1.44	1.52
3	3-B	212	LEU	CA-C	-6.12	1.45	1.52
3	3-B	858	MET	N-CA	-6.12	1.38	1.46
4	3-C	715	LEU	CA-C	-6.12	1.44	1.52
6	1-M	48	THR	CA-C	-6.12	1.45	1.52
6	2-M	48	THR	CA-C	-6.12	1.45	1.52
6	3-M	48	THR	CA-C	-6.12	1.45	1.52
1	1-A	37	ASP	CA-C	-6.12	1.45	1.53
3	1-B	264	ILE	CA-C	-6.12	1.45	1.52
8	1-Z	26	LEU	CA-C	-6.12	1.45	1.52
1	2-A	37	ASP	CA-C	-6.12	1.45	1.53
3	2-B	264	ILE	CA-C	-6.12	1.45	1.52
8	2-Z	26	LEU	CA-C	-6.12	1.45	1.52
1	3-A	37	ASP	CA-C	-6.12	1.45	1.53
3	3-B	264	ILE	CA-C	-6.12	1.45	1.52
8	3-Z	26	LEU	CA-C	-6.12	1.45	1.52
7	1-G	169	CYS	N-CA	-6.11	1.39	1.46
7	1-K	778	GLU	CA-C	-6.11	1.44	1.52
7	2-G	169	CYS	N-CA	-6.11	1.39	1.46
7	2-K	778	GLU	CA-C	-6.11	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3-G	169	CYS	N-CA	-6.11	1.39	1.46
7	3-K	778	GLU	CA-C	-6.11	1.44	1.52
3	1-N	139	LEU	N-CA	-6.11	1.38	1.46
3	2-N	139	LEU	N-CA	-6.11	1.38	1.46
3	3-N	139	LEU	N-CA	-6.11	1.38	1.46
7	1-G	854	MET	CA-C	-6.11	1.45	1.52
7	2-G	854	MET	CA-C	-6.11	1.45	1.52
7	3-G	854	MET	CA-C	-6.11	1.45	1.52
1	1-A	601	LEU	N-CA	-6.11	1.39	1.46
1	2-A	601	LEU	N-CA	-6.11	1.39	1.46
1	3-A	601	LEU	N-CA	-6.11	1.39	1.46
4	1-H	224	THR	N-CA	-6.10	1.38	1.46
4	2-H	224	THR	N-CA	-6.10	1.38	1.46
4	3-H	224	THR	N-CA	-6.10	1.38	1.46
8	1-Z	66	THR	N-CA	-6.10	1.37	1.46
8	2-Z	66	THR	N-CA	-6.10	1.37	1.46
8	3-Z	66	THR	N-CA	-6.10	1.37	1.46
7	1-G	307	ALA	CA-C	-6.10	1.44	1.52
8	1-Z	31	TYR	CA-C	-6.10	1.45	1.52
8	1-Z	125	VAL	CA-C	-6.10	1.45	1.52
7	2-G	307	ALA	CA-C	-6.10	1.44	1.52
8	2-Z	31	TYR	CA-C	-6.10	1.45	1.52
8	2-Z	125	VAL	CA-C	-6.10	1.45	1.52
7	3-G	307	ALA	CA-C	-6.10	1.44	1.52
8	3-Z	31	TYR	CA-C	-6.10	1.45	1.52
8	3-Z	125	VAL	CA-C	-6.10	1.45	1.52
1	1-A	10	ALA	CA-C	-6.10	1.44	1.52
1	2-A	10	ALA	CA-C	-6.10	1.44	1.52
1	3-A	10	ALA	CA-C	-6.10	1.44	1.52
4	1-C	472	ASP	N-CA	-6.10	1.38	1.46
4	2-C	472	ASP	N-CA	-6.10	1.38	1.46
4	3-C	472	ASP	N-CA	-6.10	1.38	1.46
1	1-A	244	THR	CA-C	-6.09	1.45	1.52
3	1-N	298	GLN	CA-C	-6.09	1.45	1.52
1	2-A	244	THR	CA-C	-6.09	1.45	1.52
3	2-N	298	GLN	CA-C	-6.09	1.45	1.52
1	3-A	244	THR	CA-C	-6.09	1.45	1.52
3	3-N	298	GLN	CA-C	-6.09	1.45	1.52
7	1-G	529	THR	CA-C	-6.09	1.45	1.52
7	2-G	529	THR	CA-C	-6.09	1.45	1.52
7	3-G	529	THR	CA-C	-6.09	1.45	1.52
1	1-A	453	CYS	N-CA	-6.09	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	473	ALA	CA-C	-6.09	1.45	1.52
7	1-K	109	LEU	N-CA	-6.09	1.38	1.46
3	1-N	54	THR	CA-C	-6.09	1.44	1.52
1	2-A	453	CYS	N-CA	-6.09	1.39	1.46
3	2-B	473	ALA	CA-C	-6.09	1.45	1.52
7	2-K	109	LEU	N-CA	-6.09	1.38	1.46
3	2-N	54	THR	CA-C	-6.09	1.44	1.52
1	3-A	453	CYS	N-CA	-6.09	1.39	1.46
3	3-B	473	ALA	CA-C	-6.09	1.45	1.52
7	3-K	109	LEU	N-CA	-6.09	1.38	1.46
3	3-N	54	THR	CA-C	-6.09	1.44	1.52
3	1-B	139	LEU	N-CA	-6.08	1.38	1.46
8	1-L	90	LEU	CA-C	-6.08	1.45	1.52
3	2-B	139	LEU	N-CA	-6.08	1.38	1.46
8	2-L	90	LEU	CA-C	-6.08	1.45	1.52
3	3-B	139	LEU	N-CA	-6.08	1.38	1.46
8	3-L	90	LEU	CA-C	-6.08	1.45	1.52
4	1-C	264	GLU	N-CA	-6.08	1.38	1.46
4	2-C	264	GLU	N-CA	-6.08	1.38	1.46
4	3-C	264	GLU	N-CA	-6.08	1.38	1.46
3	1-B	259	ARG	CA-C	-6.08	1.44	1.52
7	1-G	470	SER	CA-C	-6.08	1.44	1.52
3	2-B	259	ARG	CA-C	-6.08	1.44	1.52
7	2-G	470	SER	CA-C	-6.08	1.44	1.52
3	3-B	259	ARG	CA-C	-6.08	1.44	1.52
7	3-G	470	SER	CA-C	-6.08	1.44	1.52
7	1-K	188	ASP	CA-C	-6.08	1.45	1.53
7	2-K	188	ASP	CA-C	-6.08	1.45	1.53
7	3-K	188	ASP	CA-C	-6.08	1.45	1.53
6	1-F	102	GLU	N-CA	-6.08	1.38	1.46
6	2-F	102	GLU	N-CA	-6.08	1.38	1.46
6	3-F	102	GLU	N-CA	-6.08	1.38	1.46
4	1-H	417	ASN	CA-C	-6.07	1.44	1.53
6	1-J	85	THR	CA-C	-6.07	1.44	1.53
4	2-H	417	ASN	CA-C	-6.07	1.44	1.53
6	2-J	85	THR	CA-C	-6.07	1.44	1.53
4	3-H	417	ASN	CA-C	-6.07	1.44	1.53
6	3-J	85	THR	CA-C	-6.07	1.44	1.53
3	1-B	55	GLU	CA-C	-6.07	1.45	1.52
3	1-B	117	CYS	CA-C	-6.07	1.44	1.52
7	1-G	348	LEU	N-CA	-6.07	1.38	1.46
3	2-B	55	GLU	CA-C	-6.07	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	117	CYS	CA-C	-6.07	1.44	1.52
7	2-G	348	LEU	N-CA	-6.07	1.38	1.46
3	3-B	55	GLU	CA-C	-6.07	1.45	1.52
3	3-B	117	CYS	CA-C	-6.07	1.44	1.52
7	3-G	348	LEU	N-CA	-6.07	1.38	1.46
4	1-C	417	ASN	CA-C	-6.07	1.44	1.53
4	1-H	264	GLU	N-CA	-6.07	1.38	1.46
4	2-C	417	ASN	CA-C	-6.07	1.44	1.53
4	2-H	264	GLU	N-CA	-6.07	1.38	1.46
4	3-C	417	ASN	CA-C	-6.07	1.44	1.53
4	3-H	264	GLU	N-CA	-6.07	1.38	1.46
4	1-C	5	LEU	CA-C	-6.07	1.45	1.52
7	1-G	46	HIS	CA-C	-6.07	1.44	1.52
3	1-N	212	LEU	CA-C	-6.07	1.45	1.52
4	2-C	5	LEU	CA-C	-6.07	1.45	1.52
7	2-G	46	HIS	CA-C	-6.07	1.44	1.52
3	2-N	212	LEU	CA-C	-6.07	1.45	1.52
4	3-C	5	LEU	CA-C	-6.07	1.45	1.52
7	3-G	46	HIS	CA-C	-6.07	1.44	1.52
3	3-N	212	LEU	CA-C	-6.07	1.45	1.52
3	1-B	804	VAL	CA-C	-6.06	1.45	1.52
3	2-B	804	VAL	CA-C	-6.06	1.45	1.52
3	3-B	804	VAL	CA-C	-6.06	1.45	1.52
4	1-C	775	GLU	CA-C	-6.06	1.44	1.52
4	2-C	775	GLU	CA-C	-6.06	1.44	1.52
4	3-C	775	GLU	CA-C	-6.06	1.44	1.52
7	1-K	670	ASN	C-N	6.06	1.41	1.33
7	2-K	670	ASN	C-N	6.06	1.41	1.33
7	3-K	670	ASN	C-N	6.06	1.41	1.33
3	1-B	826	ALA	CA-C	-6.06	1.44	1.52
4	1-C	352	GLU	N-CA	-6.06	1.38	1.46
7	1-G	143	TYR	N-CA	-6.06	1.39	1.46
4	1-H	5	LEU	CA-C	-6.06	1.45	1.52
6	1-J	102	GLU	N-CA	-6.06	1.39	1.46
3	2-B	826	ALA	CA-C	-6.06	1.44	1.52
4	2-C	352	GLU	N-CA	-6.06	1.38	1.46
7	2-G	143	TYR	N-CA	-6.06	1.39	1.46
4	2-H	5	LEU	CA-C	-6.06	1.45	1.52
6	2-J	102	GLU	N-CA	-6.06	1.39	1.46
3	3-B	826	ALA	CA-C	-6.06	1.44	1.52
4	3-C	352	GLU	N-CA	-6.06	1.38	1.46
7	3-G	143	TYR	N-CA	-6.06	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-H	5	LEU	CA-C	-6.06	1.45	1.52
6	3-J	102	GLU	N-CA	-6.06	1.39	1.46
7	1-G	141	GLU	CA-C	-6.05	1.44	1.52
7	2-G	141	GLU	CA-C	-6.05	1.44	1.52
7	3-G	141	GLU	CA-C	-6.05	1.44	1.52
7	1-G	254	PHE	N-CA	-6.05	1.39	1.46
8	1-Z	141	GLN	N-CA	-6.05	1.39	1.46
7	2-G	254	PHE	N-CA	-6.05	1.39	1.46
8	2-Z	141	GLN	N-CA	-6.05	1.39	1.46
7	3-G	254	PHE	N-CA	-6.05	1.39	1.46
8	3-Z	141	GLN	N-CA	-6.05	1.39	1.46
7	1-K	259	LEU	N-CA	-6.05	1.39	1.46
3	1-N	259	ARG	CA-C	-6.05	1.45	1.52
3	1-N	402	LEU	N-CA	-6.05	1.39	1.46
7	2-K	259	LEU	N-CA	-6.05	1.39	1.46
3	2-N	259	ARG	CA-C	-6.05	1.45	1.52
3	2-N	402	LEU	N-CA	-6.05	1.39	1.46
7	3-K	259	LEU	N-CA	-6.05	1.39	1.46
3	3-N	259	ARG	CA-C	-6.05	1.45	1.52
3	3-N	402	LEU	N-CA	-6.05	1.39	1.46
1	1-A	599	PHE	CA-C	-6.05	1.45	1.52
4	1-C	131	LYS	CA-C	-6.05	1.44	1.52
4	1-H	131	LYS	CA-C	-6.05	1.44	1.52
1	2-A	599	PHE	CA-C	-6.05	1.45	1.52
4	2-C	131	LYS	CA-C	-6.05	1.44	1.52
4	2-H	131	LYS	CA-C	-6.05	1.44	1.52
1	3-A	599	PHE	CA-C	-6.05	1.45	1.52
4	3-C	131	LYS	CA-C	-6.05	1.44	1.52
4	3-H	131	LYS	CA-C	-6.05	1.44	1.52
3	1-B	402	LEU	N-CA	-6.05	1.39	1.46
3	2-B	402	LEU	N-CA	-6.05	1.39	1.46
3	3-B	402	LEU	N-CA	-6.05	1.39	1.46
7	1-G	473	ILE	CA-C	-6.05	1.45	1.52
5	1-I	83	LEU	CA-C	-6.05	1.45	1.52
7	2-G	473	ILE	CA-C	-6.05	1.45	1.52
5	2-I	83	LEU	CA-C	-6.05	1.45	1.52
7	3-G	473	ILE	CA-C	-6.05	1.45	1.52
5	3-I	83	LEU	CA-C	-6.05	1.45	1.52
5	1-D	54	VAL	N-CA	-6.04	1.39	1.46
5	2-D	54	VAL	N-CA	-6.04	1.39	1.46
5	3-D	54	VAL	N-CA	-6.04	1.39	1.46
4	1-C	185	GLU	CA-C	-6.04	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-H	358	ILE	N-CA	-6.04	1.39	1.46
4	2-C	185	GLU	CA-C	-6.04	1.45	1.52
4	2-H	358	ILE	N-CA	-6.04	1.39	1.46
4	3-C	185	GLU	CA-C	-6.04	1.45	1.52
4	3-H	358	ILE	N-CA	-6.04	1.39	1.46
6	1-F	110	MET	CA-C	-6.04	1.45	1.52
4	1-H	719	ALA	CA-C	-6.04	1.45	1.52
6	2-F	110	MET	CA-C	-6.04	1.45	1.52
4	2-H	719	ALA	CA-C	-6.04	1.45	1.52
6	3-F	110	MET	CA-C	-6.04	1.45	1.52
4	3-H	719	ALA	CA-C	-6.04	1.45	1.52
3	1-B	78	ILE	N-CA	-6.04	1.39	1.46
3	1-B	458	LEU	CA-C	-6.04	1.45	1.52
4	1-C	590	SER	CA-C	-6.04	1.45	1.52
4	1-C	618	ARG	CA-C	-6.04	1.45	1.52
3	2-B	78	ILE	N-CA	-6.04	1.39	1.46
3	2-B	458	LEU	CA-C	-6.04	1.45	1.52
4	2-C	590	SER	CA-C	-6.04	1.45	1.52
4	2-C	618	ARG	CA-C	-6.04	1.45	1.52
3	3-B	78	ILE	N-CA	-6.04	1.39	1.46
3	3-B	458	LEU	CA-C	-6.04	1.45	1.52
4	3-C	590	SER	CA-C	-6.04	1.45	1.52
4	3-C	618	ARG	CA-C	-6.04	1.45	1.52
4	1-C	719	ALA	CA-C	-6.03	1.45	1.52
7	1-G	211	VAL	N-CA	-6.03	1.39	1.46
7	1-G	670	ASN	C-N	6.03	1.41	1.33
4	2-C	719	ALA	CA-C	-6.03	1.45	1.52
7	2-G	211	VAL	N-CA	-6.03	1.39	1.46
7	2-G	670	ASN	C-N	6.03	1.41	1.33
4	3-C	719	ALA	CA-C	-6.03	1.45	1.52
7	3-G	211	VAL	N-CA	-6.03	1.39	1.46
7	3-G	670	ASN	C-N	6.03	1.41	1.33
4	1-H	590	SER	CA-C	-6.03	1.45	1.52
4	2-H	590	SER	CA-C	-6.03	1.45	1.52
4	3-H	590	SER	CA-C	-6.03	1.45	1.52
3	1-B	924	VAL	N-CA	-6.03	1.39	1.46
3	1-N	55	GLU	CA-C	-6.03	1.45	1.52
6	1-J	60	ASN	N-CA	-6.03	1.37	1.46
3	2-B	924	VAL	N-CA	-6.03	1.39	1.46
3	2-N	55	GLU	CA-C	-6.03	1.45	1.52
6	2-J	60	ASN	N-CA	-6.03	1.37	1.46
3	3-B	924	VAL	N-CA	-6.03	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-N	55	GLU	CA-C	-6.03	1.45	1.52
6	3-J	60	ASN	N-CA	-6.03	1.37	1.46
4	1-C	358	ILE	N-CA	-6.03	1.39	1.46
4	1-H	185	GLU	CA-C	-6.03	1.45	1.52
4	2-C	358	ILE	N-CA	-6.03	1.39	1.46
4	2-H	185	GLU	CA-C	-6.03	1.45	1.52
4	3-C	358	ILE	N-CA	-6.03	1.39	1.46
4	3-H	185	GLU	CA-C	-6.03	1.45	1.52
7	1-G	108	SER	CA-C	-6.03	1.45	1.52
7	2-G	108	SER	CA-C	-6.03	1.45	1.52
7	3-G	108	SER	CA-C	-6.03	1.45	1.52
1	1-A	648	ARG	CA-C	-6.02	1.45	1.52
1	2-A	648	ARG	CA-C	-6.02	1.45	1.52
1	3-A	648	ARG	CA-C	-6.02	1.45	1.52
4	1-C	312	GLY	CA-C	-6.02	1.43	1.51
4	1-C	620	ARG	CA-C	-6.02	1.45	1.52
4	2-C	312	GLY	CA-C	-6.02	1.43	1.51
4	2-C	620	ARG	CA-C	-6.02	1.45	1.52
4	3-C	312	GLY	CA-C	-6.02	1.43	1.51
4	3-C	620	ARG	CA-C	-6.02	1.45	1.52
3	1-N	406	SER	N-CA	-6.02	1.38	1.46
3	2-N	406	SER	N-CA	-6.02	1.38	1.46
3	3-N	406	SER	N-CA	-6.02	1.38	1.46
3	1-B	467	VAL	CA-C	-6.02	1.45	1.52
3	1-N	377	LYS	CA-C	-6.02	1.45	1.52
3	1-N	458	LEU	CA-C	-6.02	1.45	1.52
4	1-H	472	ASP	N-CA	-6.02	1.38	1.46
3	2-B	467	VAL	CA-C	-6.02	1.45	1.52
3	2-N	377	LYS	CA-C	-6.02	1.45	1.52
3	2-N	458	LEU	CA-C	-6.02	1.45	1.52
4	2-H	472	ASP	N-CA	-6.02	1.38	1.46
3	3-B	467	VAL	CA-C	-6.02	1.45	1.52
3	3-N	377	LYS	CA-C	-6.02	1.45	1.52
3	3-N	458	LEU	CA-C	-6.02	1.45	1.52
4	3-H	472	ASP	N-CA	-6.02	1.38	1.46
1	1-A	431	ARG	CA-C	-6.02	1.46	1.53
1	2-A	431	ARG	CA-C	-6.02	1.46	1.53
1	3-A	431	ARG	CA-C	-6.02	1.46	1.53
1	1-A	283	GLY	CA-C	-6.01	1.43	1.51
1	2-A	283	GLY	CA-C	-6.01	1.43	1.51
1	3-A	283	GLY	CA-C	-6.01	1.43	1.51
3	1-B	121	ARG	CA-C	-6.01	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	121	ARG	CA-C	-6.01	1.45	1.52
3	3-B	121	ARG	CA-C	-6.01	1.45	1.52
3	1-B	392	ASP	N-CA	-6.01	1.39	1.46
3	2-B	392	ASP	N-CA	-6.01	1.39	1.46
3	3-B	392	ASP	N-CA	-6.01	1.39	1.46
6	1-F	85	THR	CA-C	-6.01	1.44	1.53
7	1-K	191	MET	N-CA	-6.01	1.39	1.46
4	1-H	81	ILE	N-CA	-6.01	1.39	1.46
4	1-H	134	CYS	CA-C	-6.01	1.45	1.52
6	2-F	85	THR	CA-C	-6.01	1.44	1.53
7	2-K	191	MET	N-CA	-6.01	1.39	1.46
4	2-H	81	ILE	N-CA	-6.01	1.39	1.46
4	2-H	134	CYS	CA-C	-6.01	1.45	1.52
6	3-F	85	THR	CA-C	-6.01	1.44	1.53
7	3-K	191	MET	N-CA	-6.01	1.39	1.46
4	3-H	81	ILE	N-CA	-6.01	1.39	1.46
4	3-H	134	CYS	CA-C	-6.01	1.45	1.52
7	1-G	250	PRO	CA-C	-6.01	1.43	1.52
3	1-N	78	ILE	N-CA	-6.01	1.39	1.46
7	2-G	250	PRO	CA-C	-6.01	1.43	1.52
3	2-N	78	ILE	N-CA	-6.01	1.39	1.46
7	3-G	250	PRO	CA-C	-6.01	1.43	1.52
3	3-N	78	ILE	N-CA	-6.01	1.39	1.46
3	1-B	155	ILE	CA-C	-6.00	1.45	1.52
3	2-B	155	ILE	CA-C	-6.00	1.45	1.52
3	3-B	155	ILE	CA-C	-6.00	1.45	1.52
3	1-B	398	LEU	N-CA	-6.00	1.39	1.46
3	2-B	398	LEU	N-CA	-6.00	1.39	1.46
3	3-B	398	LEU	N-CA	-6.00	1.39	1.46
3	1-N	388	HIS	CA-C	-6.00	1.45	1.52
3	1-N	459	GLU	N-CA	-6.00	1.39	1.46
3	2-N	388	HIS	CA-C	-6.00	1.45	1.52
3	2-N	459	GLU	N-CA	-6.00	1.39	1.46
3	3-N	388	HIS	CA-C	-6.00	1.45	1.52
3	3-N	459	GLU	N-CA	-6.00	1.39	1.46
3	1-B	764	THR	CA-C	-6.00	1.44	1.52
3	2-B	764	THR	CA-C	-6.00	1.44	1.52
3	3-B	764	THR	CA-C	-6.00	1.44	1.52
7	1-G	75	LYS	N-CA	-6.00	1.38	1.46
7	2-G	75	LYS	N-CA	-6.00	1.38	1.46
7	3-G	75	LYS	N-CA	-6.00	1.38	1.46
7	1-G	231	MET	CA-C	-6.00	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	231	MET	CA-C	-6.00	1.45	1.52
7	3-G	231	MET	CA-C	-6.00	1.45	1.52
3	1-B	388	HIS	CA-C	-5.99	1.45	1.52
6	1-R	107	MET	N-CA	-5.99	1.38	1.46
3	2-B	388	HIS	CA-C	-5.99	1.45	1.52
6	2-R	107	MET	N-CA	-5.99	1.38	1.46
3	3-B	388	HIS	CA-C	-5.99	1.45	1.52
6	3-R	107	MET	N-CA	-5.99	1.38	1.46
6	1-R	46	ILE	N-CA	-5.99	1.41	1.47
7	1-K	864	LEU	N-CA	-5.99	1.40	1.46
6	2-R	46	ILE	N-CA	-5.99	1.41	1.47
7	2-K	864	LEU	N-CA	-5.99	1.40	1.46
6	3-R	46	ILE	N-CA	-5.99	1.41	1.47
7	3-K	864	LEU	N-CA	-5.99	1.40	1.46
7	1-G	215	ILE	N-CA	-5.99	1.39	1.46
7	1-G	486	GLU	N-CA	-5.99	1.39	1.46
7	2-G	215	ILE	N-CA	-5.99	1.39	1.46
7	2-G	486	GLU	N-CA	-5.99	1.39	1.46
7	3-G	215	ILE	N-CA	-5.99	1.39	1.46
7	3-G	486	GLU	N-CA	-5.99	1.39	1.46
8	1-Z	143	VAL	CA-C	-5.98	1.45	1.52
8	2-Z	143	VAL	CA-C	-5.98	1.45	1.52
8	3-Z	143	VAL	CA-C	-5.98	1.45	1.52
3	1-N	155	ILE	CA-C	-5.98	1.45	1.52
3	2-N	155	ILE	CA-C	-5.98	1.45	1.52
3	3-N	155	ILE	CA-C	-5.98	1.45	1.52
1	1-A	246	ARG	CA-C	-5.98	1.45	1.52
1	2-A	246	ARG	CA-C	-5.98	1.45	1.52
1	3-A	246	ARG	CA-C	-5.98	1.45	1.52
7	1-G	138	GLN	CA-C	-5.97	1.45	1.52
4	1-H	618	ARG	CA-C	-5.97	1.45	1.52
7	2-G	138	GLN	CA-C	-5.97	1.45	1.52
4	2-H	618	ARG	CA-C	-5.97	1.45	1.52
7	3-G	138	GLN	CA-C	-5.97	1.45	1.52
4	3-H	618	ARG	CA-C	-5.97	1.45	1.52
1	1-A	464	LEU	N-CA	-5.97	1.41	1.46
3	1-B	459	GLU	N-CA	-5.97	1.39	1.46
5	1-D	83	LEU	CA-C	-5.97	1.45	1.52
7	1-G	844	SER	N-CA	-5.97	1.39	1.46
1	2-A	464	LEU	N-CA	-5.97	1.41	1.46
3	2-B	459	GLU	N-CA	-5.97	1.39	1.46
5	2-D	83	LEU	CA-C	-5.97	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	844	SER	N-CA	-5.97	1.39	1.46
1	3-A	464	LEU	N-CA	-5.97	1.41	1.46
3	3-B	459	GLU	N-CA	-5.97	1.39	1.46
5	3-D	83	LEU	CA-C	-5.97	1.45	1.52
7	3-G	844	SER	N-CA	-5.97	1.39	1.46
4	1-C	575	LEU	N-CA	-5.97	1.38	1.45
4	2-C	575	LEU	N-CA	-5.97	1.38	1.45
4	3-C	575	LEU	N-CA	-5.97	1.38	1.45
3	1-N	100	VAL	CA-C	-5.97	1.46	1.52
3	2-N	100	VAL	CA-C	-5.97	1.46	1.52
3	3-N	100	VAL	CA-C	-5.97	1.46	1.52
1	1-A	544	THR	CA-C	-5.97	1.45	1.52
3	1-B	743	ALA	CA-C	-5.97	1.45	1.52
3	1-B	845	ILE	CA-C	-5.97	1.45	1.52
4	1-H	499	GLN	CA-C	-5.97	1.45	1.52
1	2-A	544	THR	CA-C	-5.97	1.45	1.52
3	2-B	743	ALA	CA-C	-5.97	1.45	1.52
3	2-B	845	ILE	CA-C	-5.97	1.45	1.52
4	2-H	499	GLN	CA-C	-5.97	1.45	1.52
1	3-A	544	THR	CA-C	-5.97	1.45	1.52
3	3-B	743	ALA	CA-C	-5.97	1.45	1.52
3	3-B	845	ILE	CA-C	-5.97	1.45	1.52
4	3-H	499	GLN	CA-C	-5.97	1.45	1.52
3	1-B	784	VAL	N-CA	-5.96	1.38	1.46
8	1-L	29	LYS	CA-C	-5.96	1.45	1.52
3	2-B	784	VAL	N-CA	-5.96	1.38	1.46
8	2-L	29	LYS	CA-C	-5.96	1.45	1.52
3	3-B	784	VAL	N-CA	-5.96	1.38	1.46
8	3-L	29	LYS	CA-C	-5.96	1.45	1.52
4	1-C	499	GLN	CA-C	-5.96	1.45	1.52
4	2-C	499	GLN	CA-C	-5.96	1.45	1.52
4	3-C	499	GLN	CA-C	-5.96	1.45	1.52
4	1-C	105	ILE	CA-C	-5.96	1.45	1.52
3	1-N	305	ILE	N-CA	-5.96	1.39	1.46
4	1-H	312	GLY	CA-C	-5.96	1.43	1.51
4	1-H	620	ARG	CA-C	-5.96	1.45	1.52
4	2-C	105	ILE	CA-C	-5.96	1.45	1.52
3	2-N	305	ILE	N-CA	-5.96	1.39	1.46
4	2-H	312	GLY	CA-C	-5.96	1.43	1.51
4	2-H	620	ARG	CA-C	-5.96	1.45	1.52
4	3-C	105	ILE	CA-C	-5.96	1.45	1.52
3	3-N	305	ILE	N-CA	-5.96	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-H	312	GLY	CA-C	-5.96	1.43	1.51
4	3-H	620	ARG	CA-C	-5.96	1.45	1.52
3	1-B	137	ARG	CA-C	-5.96	1.45	1.52
7	1-G	136	MET	N-CA	-5.96	1.38	1.46
3	2-B	137	ARG	CA-C	-5.96	1.45	1.52
7	2-G	136	MET	N-CA	-5.96	1.38	1.46
3	3-B	137	ARG	CA-C	-5.96	1.45	1.52
7	3-G	136	MET	N-CA	-5.96	1.38	1.46
3	1-N	405	CYS	CA-C	-5.96	1.45	1.52
3	2-N	405	CYS	CA-C	-5.96	1.45	1.52
3	3-N	405	CYS	CA-C	-5.96	1.45	1.52
7	1-G	864	LEU	N-CA	-5.96	1.40	1.46
7	2-G	864	LEU	N-CA	-5.96	1.40	1.46
7	3-G	864	LEU	N-CA	-5.96	1.40	1.46
6	1-M	171	GLU	N-CA	-5.95	1.39	1.46
6	2-M	171	GLU	N-CA	-5.95	1.39	1.46
6	3-M	171	GLU	N-CA	-5.95	1.39	1.46
3	1-B	839	ILE	CA-C	-5.95	1.45	1.52
7	1-G	292	LEU	N-CA	-5.95	1.39	1.46
3	2-B	839	ILE	CA-C	-5.95	1.45	1.52
7	2-G	292	LEU	N-CA	-5.95	1.39	1.46
3	3-B	839	ILE	CA-C	-5.95	1.45	1.52
7	3-G	292	LEU	N-CA	-5.95	1.39	1.46
4	1-C	134	CYS	CA-C	-5.95	1.45	1.52
4	2-C	134	CYS	CA-C	-5.95	1.45	1.52
4	3-C	134	CYS	CA-C	-5.95	1.45	1.52
1	1-A	628	TYR	N-CA	-5.95	1.38	1.46
3	1-N	398	LEU	N-CA	-5.95	1.39	1.46
1	2-A	628	TYR	N-CA	-5.95	1.38	1.46
3	2-N	398	LEU	N-CA	-5.95	1.39	1.46
1	3-A	628	TYR	N-CA	-5.95	1.38	1.46
3	3-N	398	LEU	N-CA	-5.95	1.39	1.46
7	1-G	151	LYS	CA-C	-5.94	1.44	1.52
7	2-G	151	LYS	CA-C	-5.94	1.44	1.52
7	3-G	151	LYS	CA-C	-5.94	1.44	1.52
3	1-B	138	PHE	N-CA	-5.94	1.39	1.46
3	2-B	138	PHE	N-CA	-5.94	1.39	1.46
3	3-B	138	PHE	N-CA	-5.94	1.39	1.46
8	1-Z	37	SER	CA-C	-5.94	1.44	1.52
3	1-N	392	ASP	N-CA	-5.94	1.39	1.46
8	2-Z	37	SER	CA-C	-5.94	1.44	1.52
3	2-N	392	ASP	N-CA	-5.94	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	3-Z	37	SER	CA-C	-5.94	1.44	1.52
3	3-N	392	ASP	N-CA	-5.94	1.39	1.46
3	1-B	405	CYS	CA-C	-5.94	1.45	1.52
7	1-G	79	SER	CA-C	-5.94	1.44	1.53
3	1-N	467	VAL	CA-C	-5.94	1.45	1.52
3	2-B	405	CYS	CA-C	-5.94	1.45	1.52
7	2-G	79	SER	CA-C	-5.94	1.44	1.53
3	2-N	467	VAL	CA-C	-5.94	1.45	1.52
3	3-B	405	CYS	CA-C	-5.94	1.45	1.52
7	3-G	79	SER	CA-C	-5.94	1.44	1.53
3	3-N	467	VAL	CA-C	-5.94	1.45	1.52
4	1-H	562	TYR	CA-C	-5.93	1.45	1.52
4	2-H	562	TYR	CA-C	-5.93	1.45	1.52
4	3-H	562	TYR	CA-C	-5.93	1.45	1.52
5	1-I	159	MET	CA-C	-5.93	1.45	1.52
5	2-I	159	MET	CA-C	-5.93	1.45	1.52
5	3-I	159	MET	CA-C	-5.93	1.45	1.52
8	1-L	84	TYR	N-CA	-5.93	1.38	1.46
8	2-L	84	TYR	N-CA	-5.93	1.38	1.46
8	3-L	84	TYR	N-CA	-5.93	1.38	1.46
4	1-C	236	SER	CA-C	-5.93	1.45	1.52
4	2-C	236	SER	CA-C	-5.93	1.45	1.52
4	3-C	236	SER	CA-C	-5.93	1.45	1.52
7	1-G	191	MET	N-CA	-5.93	1.39	1.46
8	1-Z	16	ILE	CA-C	-5.93	1.45	1.52
7	1-K	52	LEU	CA-C	-5.93	1.45	1.52
4	1-H	316	TRP	N-CA	-5.93	1.38	1.45
7	2-G	191	MET	N-CA	-5.93	1.39	1.46
8	2-Z	16	ILE	CA-C	-5.93	1.45	1.52
7	2-K	52	LEU	CA-C	-5.93	1.45	1.52
4	2-H	316	TRP	N-CA	-5.93	1.38	1.45
7	3-G	191	MET	N-CA	-5.93	1.39	1.46
8	3-Z	16	ILE	CA-C	-5.93	1.45	1.52
7	3-K	52	LEU	CA-C	-5.93	1.45	1.52
4	3-H	316	TRP	N-CA	-5.93	1.38	1.45
5	1-D	55	ARG	N-CA	-5.92	1.38	1.46
3	1-N	121	ARG	CA-C	-5.92	1.45	1.52
3	1-N	138	PHE	N-CA	-5.92	1.39	1.46
5	2-D	55	ARG	N-CA	-5.92	1.38	1.46
3	2-N	121	ARG	CA-C	-5.92	1.45	1.52
3	2-N	138	PHE	N-CA	-5.92	1.39	1.46
5	3-D	55	ARG	N-CA	-5.92	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-N	121	ARG	CA-C	-5.92	1.45	1.52
3	3-N	138	PHE	N-CA	-5.92	1.39	1.46
3	1-B	856	ARG	CA-C	-5.92	1.45	1.52
3	2-B	856	ARG	CA-C	-5.92	1.45	1.52
3	3-B	856	ARG	CA-C	-5.92	1.45	1.52
4	1-C	316	TRP	N-CA	-5.92	1.38	1.45
4	2-C	316	TRP	N-CA	-5.92	1.38	1.45
4	3-C	316	TRP	N-CA	-5.92	1.38	1.45
1	1-A	254	CYS	CA-C	-5.92	1.45	1.52
7	1-K	707	TYR	N-CA	-5.92	1.38	1.45
1	2-A	254	CYS	CA-C	-5.92	1.45	1.52
7	2-K	707	TYR	N-CA	-5.92	1.38	1.45
1	3-A	254	CYS	CA-C	-5.92	1.45	1.52
7	3-K	707	TYR	N-CA	-5.92	1.38	1.45
1	1-A	146	SER	CA-C	-5.92	1.44	1.52
1	1-A	231	ILE	CA-C	-5.92	1.45	1.52
3	1-B	204	CYS	N-CA	-5.92	1.39	1.46
3	1-B	305	ILE	N-CA	-5.92	1.39	1.46
1	2-A	146	SER	CA-C	-5.92	1.44	1.52
1	2-A	231	ILE	CA-C	-5.92	1.45	1.52
3	2-B	204	CYS	N-CA	-5.92	1.39	1.46
3	2-B	305	ILE	N-CA	-5.92	1.39	1.46
1	3-A	146	SER	CA-C	-5.92	1.44	1.52
1	3-A	231	ILE	CA-C	-5.92	1.45	1.52
3	3-B	204	CYS	N-CA	-5.92	1.39	1.46
3	3-B	305	ILE	N-CA	-5.92	1.39	1.46
3	1-B	79	ARG	CA-C	-5.91	1.45	1.52
3	1-B	140	CYS	CA-C	-5.91	1.45	1.52
4	1-C	556	HIS	N-CA	-5.91	1.38	1.46
4	1-C	809	GLU	CA-C	-5.91	1.45	1.52
5	1-D	159	MET	CA-C	-5.91	1.45	1.52
3	2-B	79	ARG	CA-C	-5.91	1.45	1.52
3	2-B	140	CYS	CA-C	-5.91	1.45	1.52
4	2-C	556	HIS	N-CA	-5.91	1.38	1.46
4	2-C	809	GLU	CA-C	-5.91	1.45	1.52
5	2-D	159	MET	CA-C	-5.91	1.45	1.52
3	3-B	79	ARG	CA-C	-5.91	1.45	1.52
3	3-B	140	CYS	CA-C	-5.91	1.45	1.52
4	3-C	556	HIS	N-CA	-5.91	1.38	1.46
4	3-C	809	GLU	CA-C	-5.91	1.45	1.52
5	3-D	159	MET	CA-C	-5.91	1.45	1.52
1	1-A	47	PHE	CA-C	-5.91	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	267	ASN	N-CA	-5.91	1.38	1.45
4	1-C	81	ILE	N-CA	-5.91	1.39	1.46
1	2-A	47	PHE	CA-C	-5.91	1.45	1.52
1	2-A	267	ASN	N-CA	-5.91	1.38	1.45
4	2-C	81	ILE	N-CA	-5.91	1.39	1.46
1	3-A	47	PHE	CA-C	-5.91	1.45	1.52
1	3-A	267	ASN	N-CA	-5.91	1.38	1.45
4	3-C	81	ILE	N-CA	-5.91	1.39	1.46
7	1-G	539	GLN	CA-C	-5.91	1.44	1.52
7	2-G	539	GLN	CA-C	-5.91	1.44	1.52
7	3-G	539	GLN	CA-C	-5.91	1.44	1.52
6	1-R	28	ALA	CA-C	-5.91	1.45	1.52
3	1-N	357	GLN	CA-C	-5.91	1.45	1.52
5	1-I	55	ARG	N-CA	-5.91	1.38	1.46
6	2-R	28	ALA	CA-C	-5.91	1.45	1.52
3	2-N	357	GLN	CA-C	-5.91	1.45	1.52
5	2-I	55	ARG	N-CA	-5.91	1.38	1.46
6	3-R	28	ALA	CA-C	-5.91	1.45	1.52
3	3-N	357	GLN	CA-C	-5.91	1.45	1.52
5	3-I	55	ARG	N-CA	-5.91	1.38	1.46
7	1-G	857	THR	CA-C	-5.91	1.45	1.52
8	1-Z	129	VAL	N-CA	-5.91	1.39	1.46
7	2-G	857	THR	CA-C	-5.91	1.45	1.52
8	2-Z	129	VAL	N-CA	-5.91	1.39	1.46
7	3-G	857	THR	CA-C	-5.91	1.45	1.52
8	3-Z	129	VAL	N-CA	-5.91	1.39	1.46
4	1-H	556	HIS	N-CA	-5.90	1.38	1.46
4	2-H	556	HIS	N-CA	-5.90	1.38	1.46
4	3-H	556	HIS	N-CA	-5.90	1.38	1.46
3	1-B	100	VAL	CA-C	-5.90	1.46	1.52
3	2-B	100	VAL	CA-C	-5.90	1.46	1.52
3	3-B	100	VAL	CA-C	-5.90	1.46	1.52
1	1-A	36	TRP	N-CA	-5.90	1.38	1.46
1	1-A	722	ILE	CA-C	-5.90	1.45	1.52
3	1-B	123	ASP	CA-C	-5.90	1.45	1.52
4	1-H	369	VAL	N-CA	-5.90	1.39	1.46
1	2-A	36	TRP	N-CA	-5.90	1.38	1.46
1	2-A	722	ILE	CA-C	-5.90	1.45	1.52
3	2-B	123	ASP	CA-C	-5.90	1.45	1.52
4	2-H	369	VAL	N-CA	-5.90	1.39	1.46
1	3-A	36	TRP	N-CA	-5.90	1.38	1.46
1	3-A	722	ILE	CA-C	-5.90	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	123	ASP	CA-C	-5.90	1.45	1.52
4	3-H	369	VAL	N-CA	-5.90	1.39	1.46
7	1-K	732	VAL	N-CA	-5.90	1.39	1.46
7	2-K	732	VAL	N-CA	-5.90	1.39	1.46
7	3-K	732	VAL	N-CA	-5.90	1.39	1.46
4	1-H	236	SER	CA-C	-5.90	1.45	1.52
4	1-H	575	LEU	N-CA	-5.90	1.38	1.45
4	2-H	236	SER	CA-C	-5.90	1.45	1.52
4	2-H	575	LEU	N-CA	-5.90	1.38	1.45
4	3-H	236	SER	CA-C	-5.90	1.45	1.52
4	3-H	575	LEU	N-CA	-5.90	1.38	1.45
4	1-C	736	GLY	CA-C	-5.89	1.43	1.51
7	1-K	83	THR	N-CA	-5.89	1.38	1.46
4	2-C	736	GLY	CA-C	-5.89	1.43	1.51
7	2-K	83	THR	N-CA	-5.89	1.38	1.46
4	3-C	736	GLY	CA-C	-5.89	1.43	1.51
7	3-K	83	THR	N-CA	-5.89	1.38	1.46
3	1-B	762	ASN	N-CA	-5.89	1.39	1.46
8	1-L	14	LYS	CA-C	-5.89	1.45	1.52
8	1-L	38	VAL	CA-C	-5.89	1.45	1.52
3	1-N	191	LEU	CA-C	-5.89	1.45	1.52
3	2-B	762	ASN	N-CA	-5.89	1.39	1.46
8	2-L	14	LYS	CA-C	-5.89	1.45	1.52
8	2-L	38	VAL	CA-C	-5.89	1.45	1.52
3	2-N	191	LEU	CA-C	-5.89	1.45	1.52
3	3-B	762	ASN	N-CA	-5.89	1.39	1.46
8	3-L	14	LYS	CA-C	-5.89	1.45	1.52
8	3-L	38	VAL	CA-C	-5.89	1.45	1.52
3	3-N	191	LEU	CA-C	-5.89	1.45	1.52
7	1-K	174	VAL	CA-C	-5.89	1.45	1.52
7	2-K	174	VAL	CA-C	-5.89	1.45	1.52
7	3-K	174	VAL	CA-C	-5.89	1.45	1.52
4	1-C	109	PRO	CA-C	-5.89	1.44	1.52
8	1-Z	143	VAL	N-CA	-5.89	1.39	1.46
4	2-C	109	PRO	CA-C	-5.89	1.44	1.52
8	2-Z	143	VAL	N-CA	-5.89	1.39	1.46
4	3-C	109	PRO	CA-C	-5.89	1.44	1.52
8	3-Z	143	VAL	N-CA	-5.89	1.39	1.46
3	1-B	357	GLN	CA-C	-5.89	1.45	1.52
7	1-K	289	VAL	N-CA	-5.89	1.39	1.46
3	2-B	357	GLN	CA-C	-5.89	1.45	1.52
7	2-K	289	VAL	N-CA	-5.89	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	357	GLN	CA-C	-5.89	1.45	1.52
7	3-K	289	VAL	N-CA	-5.89	1.39	1.46
7	1-K	92	ILE	CA-C	-5.88	1.45	1.52
7	2-K	92	ILE	CA-C	-5.88	1.45	1.52
7	3-K	92	ILE	CA-C	-5.88	1.45	1.52
1	1-A	224	ALA	CA-C	-5.88	1.45	1.52
4	1-C	780	VAL	CA-C	-5.88	1.45	1.52
1	2-A	224	ALA	CA-C	-5.88	1.45	1.52
4	2-C	780	VAL	CA-C	-5.88	1.45	1.52
1	3-A	224	ALA	CA-C	-5.88	1.45	1.52
4	3-C	780	VAL	CA-C	-5.88	1.45	1.52
5	1-I	118	ALA	CA-C	-5.88	1.45	1.52
5	2-I	118	ALA	CA-C	-5.88	1.45	1.52
5	3-I	118	ALA	CA-C	-5.88	1.45	1.52
3	1-B	61	ILE	N-CA	-5.88	1.39	1.46
3	1-B	863	GLU	CA-C	-5.88	1.45	1.52
3	1-N	399	VAL	CA-C	-5.88	1.45	1.52
3	2-B	61	ILE	N-CA	-5.88	1.39	1.46
3	2-B	863	GLU	CA-C	-5.88	1.45	1.52
3	2-N	399	VAL	CA-C	-5.88	1.45	1.52
3	3-B	61	ILE	N-CA	-5.88	1.39	1.46
3	3-B	863	GLU	CA-C	-5.88	1.45	1.52
3	3-N	399	VAL	CA-C	-5.88	1.45	1.52
7	1-G	707	TYR	N-CA	-5.88	1.38	1.45
3	1-N	137	ARG	CA-C	-5.88	1.45	1.52
4	1-H	322	VAL	CA-C	-5.88	1.46	1.53
7	2-G	707	TYR	N-CA	-5.88	1.38	1.45
3	2-N	137	ARG	CA-C	-5.88	1.45	1.52
4	2-H	322	VAL	CA-C	-5.88	1.46	1.53
7	3-G	707	TYR	N-CA	-5.88	1.38	1.45
3	3-N	137	ARG	CA-C	-5.88	1.45	1.52
4	3-H	322	VAL	CA-C	-5.88	1.46	1.53
4	1-H	105	ILE	CA-C	-5.88	1.45	1.52
4	2-H	105	ILE	CA-C	-5.88	1.45	1.52
4	3-H	105	ILE	CA-C	-5.88	1.45	1.52
7	1-G	442	PHE	N-CA	-5.87	1.39	1.46
7	1-G	622	GLU	CA-C	-5.87	1.44	1.52
7	1-K	176	ARG	CA-C	-5.87	1.44	1.52
7	2-G	442	PHE	N-CA	-5.87	1.39	1.46
7	2-G	622	GLU	CA-C	-5.87	1.44	1.52
7	2-K	176	ARG	CA-C	-5.87	1.44	1.52
7	3-G	442	PHE	N-CA	-5.87	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3-G	622	GLU	CA-C	-5.87	1.44	1.52
7	3-K	176	ARG	CA-C	-5.87	1.44	1.52
8	1-Z	47	ASN	CA-C	-5.87	1.45	1.52
3	1-N	123	ASP	CA-C	-5.87	1.45	1.52
8	2-Z	47	ASN	CA-C	-5.87	1.45	1.52
3	2-N	123	ASP	CA-C	-5.87	1.45	1.52
8	3-Z	47	ASN	CA-C	-5.87	1.45	1.52
3	3-N	123	ASP	CA-C	-5.87	1.45	1.52
7	1-K	857	THR	CA-C	-5.87	1.45	1.52
3	1-N	61	ILE	N-CA	-5.87	1.39	1.46
3	1-N	79	ARG	CA-C	-5.87	1.45	1.52
7	2-K	857	THR	CA-C	-5.87	1.45	1.52
3	2-N	61	ILE	N-CA	-5.87	1.39	1.46
3	2-N	79	ARG	CA-C	-5.87	1.45	1.52
7	3-K	857	THR	CA-C	-5.87	1.45	1.52
3	3-N	61	ILE	N-CA	-5.87	1.39	1.46
3	3-N	79	ARG	CA-C	-5.87	1.45	1.52
3	1-N	321	VAL	N-CA	-5.87	1.39	1.46
4	1-H	109	PRO	CA-C	-5.87	1.44	1.52
3	2-N	321	VAL	N-CA	-5.87	1.39	1.46
4	2-H	109	PRO	CA-C	-5.87	1.44	1.52
3	3-N	321	VAL	N-CA	-5.87	1.39	1.46
4	3-H	109	PRO	CA-C	-5.87	1.44	1.52
3	1-B	834	LEU	N-CA	-5.86	1.38	1.45
7	1-K	640	THR	CA-C	-5.86	1.45	1.52
3	2-B	834	LEU	N-CA	-5.86	1.38	1.45
7	2-K	640	THR	CA-C	-5.86	1.45	1.52
3	3-B	834	LEU	N-CA	-5.86	1.38	1.45
7	3-K	640	THR	CA-C	-5.86	1.45	1.52
7	1-G	732	VAL	N-CA	-5.86	1.39	1.46
7	2-G	732	VAL	N-CA	-5.86	1.39	1.46
7	3-G	732	VAL	N-CA	-5.86	1.39	1.46
8	1-L	117	ASN	CA-C	-5.86	1.45	1.52
8	1-L	139	PRO	CA-C	-5.86	1.42	1.52
8	2-L	117	ASN	CA-C	-5.86	1.45	1.52
8	2-L	139	PRO	CA-C	-5.86	1.42	1.52
8	3-L	117	ASN	CA-C	-5.86	1.45	1.52
8	3-L	139	PRO	CA-C	-5.86	1.42	1.52
6	1-R	33	VAL	CA-C	-5.86	1.45	1.52
6	2-R	33	VAL	CA-C	-5.86	1.45	1.52
6	3-R	33	VAL	CA-C	-5.86	1.45	1.52
6	1-F	67	ASP	CA-C	-5.85	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2-F	67	ASP	CA-C	-5.85	1.45	1.52
6	3-F	67	ASP	CA-C	-5.85	1.45	1.52
5	1-D	118	ALA	CA-C	-5.85	1.45	1.52
6	1-R	47	PRO	CA-C	-5.85	1.44	1.52
7	1-K	179	ASN	N-CA	-5.85	1.39	1.46
5	2-D	118	ALA	CA-C	-5.85	1.45	1.52
6	2-R	47	PRO	CA-C	-5.85	1.44	1.52
7	2-K	179	ASN	N-CA	-5.85	1.39	1.46
5	3-D	118	ALA	CA-C	-5.85	1.45	1.52
6	3-R	47	PRO	CA-C	-5.85	1.44	1.52
7	3-K	179	ASN	N-CA	-5.85	1.39	1.46
7	1-K	139	ALA	N-CA	-5.85	1.39	1.46
7	1-K	622	GLU	CA-C	-5.85	1.44	1.52
3	1-N	315	ILE	CA-C	-5.85	1.45	1.52
4	1-H	603	PHE	N-CA	-5.85	1.39	1.46
7	2-K	139	ALA	N-CA	-5.85	1.39	1.46
7	2-K	622	GLU	CA-C	-5.85	1.44	1.52
3	2-N	315	ILE	CA-C	-5.85	1.45	1.52
4	2-H	603	PHE	N-CA	-5.85	1.39	1.46
7	3-K	139	ALA	N-CA	-5.85	1.39	1.46
7	3-K	622	GLU	CA-C	-5.85	1.44	1.52
3	3-N	315	ILE	CA-C	-5.85	1.45	1.52
4	3-H	603	PHE	N-CA	-5.85	1.39	1.46
1	1-A	680	VAL	N-CA	-5.85	1.39	1.46
3	1-B	191	LEU	CA-C	-5.85	1.45	1.52
1	2-A	680	VAL	N-CA	-5.85	1.39	1.46
3	2-B	191	LEU	CA-C	-5.85	1.45	1.52
1	3-A	680	VAL	N-CA	-5.85	1.39	1.46
3	3-B	191	LEU	CA-C	-5.85	1.45	1.52
6	1-R	105	GLU	N-CA	-5.84	1.39	1.46
4	1-H	551	ILE	N-CA	-5.84	1.39	1.46
6	2-R	105	GLU	N-CA	-5.84	1.39	1.46
4	2-H	551	ILE	N-CA	-5.84	1.39	1.46
6	3-R	105	GLU	N-CA	-5.84	1.39	1.46
4	3-H	551	ILE	N-CA	-5.84	1.39	1.46
3	1-B	315	ILE	CA-C	-5.84	1.45	1.52
3	2-B	315	ILE	CA-C	-5.84	1.45	1.52
3	3-B	315	ILE	CA-C	-5.84	1.45	1.52
3	1-B	395	ARG	CA-C	-5.84	1.45	1.52
4	1-C	562	TYR	CA-C	-5.84	1.45	1.52
4	1-H	550	GLU	N-CA	-5.84	1.38	1.45
3	2-B	395	ARG	CA-C	-5.84	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-C	562	TYR	CA-C	-5.84	1.45	1.52
4	2-H	550	GLU	N-CA	-5.84	1.38	1.45
3	3-B	395	ARG	CA-C	-5.84	1.45	1.52
4	3-C	562	TYR	CA-C	-5.84	1.45	1.52
4	3-H	550	GLU	N-CA	-5.84	1.38	1.45
4	1-C	369	VAL	N-CA	-5.84	1.39	1.46
7	1-G	640	THR	CA-C	-5.84	1.45	1.52
4	2-C	369	VAL	N-CA	-5.84	1.39	1.46
7	2-G	640	THR	CA-C	-5.84	1.45	1.52
4	3-C	369	VAL	N-CA	-5.84	1.39	1.46
7	3-G	640	THR	CA-C	-5.84	1.45	1.52
3	1-B	399	VAL	CA-C	-5.84	1.45	1.52
3	2-B	399	VAL	CA-C	-5.84	1.45	1.52
3	3-B	399	VAL	CA-C	-5.84	1.45	1.52
6	1-R	145	LEU	CA-C	-5.84	1.45	1.52
6	2-R	145	LEU	CA-C	-5.84	1.45	1.52
6	3-R	145	LEU	CA-C	-5.84	1.45	1.52
3	1-N	234	PHE	CA-C	-5.83	1.45	1.52
3	2-N	234	PHE	CA-C	-5.83	1.45	1.52
3	3-N	234	PHE	CA-C	-5.83	1.45	1.52
1	1-A	589	VAL	CA-C	-5.83	1.45	1.52
3	1-N	136	LEU	CA-C	-5.83	1.45	1.52
1	2-A	589	VAL	CA-C	-5.83	1.45	1.52
3	2-N	136	LEU	CA-C	-5.83	1.45	1.52
1	3-A	589	VAL	CA-C	-5.83	1.45	1.52
3	3-N	136	LEU	CA-C	-5.83	1.45	1.52
3	1-N	204	CYS	N-CA	-5.83	1.39	1.46
3	1-N	286	LEU	N-CA	-5.83	1.39	1.46
3	2-N	204	CYS	N-CA	-5.83	1.39	1.46
3	2-N	286	LEU	N-CA	-5.83	1.39	1.46
3	3-N	204	CYS	N-CA	-5.83	1.39	1.46
3	3-N	286	LEU	N-CA	-5.83	1.39	1.46
3	1-B	75	MET	N-CA	-5.83	1.39	1.46
3	2-B	75	MET	N-CA	-5.83	1.39	1.46
3	3-B	75	MET	N-CA	-5.83	1.39	1.46
5	1-I	81	GLU	N-CA	-5.83	1.39	1.46
5	2-I	81	GLU	N-CA	-5.83	1.39	1.46
5	3-I	81	GLU	N-CA	-5.83	1.39	1.46
7	1-G	162	SER	N-CA	-5.83	1.39	1.46
3	1-N	140	CYS	CA-C	-5.83	1.45	1.52
4	1-H	625	LEU	CA-C	-5.83	1.45	1.52
7	2-G	162	SER	N-CA	-5.83	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-N	140	CYS	CA-C	-5.83	1.45	1.52
4	2-H	625	LEU	CA-C	-5.83	1.45	1.52
7	3-G	162	SER	N-CA	-5.83	1.39	1.46
3	3-N	140	CYS	CA-C	-5.83	1.45	1.52
4	3-H	625	LEU	CA-C	-5.83	1.45	1.52
4	1-C	15	SER	N-CA	-5.83	1.40	1.46
4	2-C	15	SER	N-CA	-5.83	1.40	1.46
4	3-C	15	SER	N-CA	-5.83	1.40	1.46
7	1-G	662	GLN	CA-C	-5.82	1.45	1.52
7	1-K	233	ILE	CA-C	-5.82	1.45	1.52
7	2-G	662	GLN	CA-C	-5.82	1.45	1.52
7	2-K	233	ILE	CA-C	-5.82	1.45	1.52
7	3-G	662	GLN	CA-C	-5.82	1.45	1.52
7	3-K	233	ILE	CA-C	-5.82	1.45	1.52
3	1-B	283	LEU	CA-C	-5.82	1.45	1.52
4	1-C	603	PHE	N-CA	-5.82	1.39	1.46
3	2-B	283	LEU	CA-C	-5.82	1.45	1.52
4	2-C	603	PHE	N-CA	-5.82	1.39	1.46
3	3-B	283	LEU	CA-C	-5.82	1.45	1.52
4	3-C	603	PHE	N-CA	-5.82	1.39	1.46
3	1-B	263	CYS	CA-C	-5.82	1.45	1.52
4	1-C	550	GLU	N-CA	-5.82	1.39	1.45
7	1-G	378	VAL	CA-C	-5.82	1.45	1.52
7	1-K	241	GLU	CA-C	-5.82	1.44	1.52
4	1-H	587	LEU	CA-C	-5.82	1.45	1.52
3	2-B	263	CYS	CA-C	-5.82	1.45	1.52
4	2-C	550	GLU	N-CA	-5.82	1.39	1.45
7	2-G	378	VAL	CA-C	-5.82	1.45	1.52
7	2-K	241	GLU	CA-C	-5.82	1.44	1.52
4	2-H	587	LEU	CA-C	-5.82	1.45	1.52
3	3-B	263	CYS	CA-C	-5.82	1.45	1.52
4	3-C	550	GLU	N-CA	-5.82	1.39	1.45
7	3-G	378	VAL	CA-C	-5.82	1.45	1.52
7	3-K	241	GLU	CA-C	-5.82	1.44	1.52
4	3-H	587	LEU	CA-C	-5.82	1.45	1.52
3	1-B	172	LEU	CA-C	-5.82	1.45	1.52
7	1-G	508	SER	CA-C	-5.82	1.45	1.52
3	2-B	172	LEU	CA-C	-5.82	1.45	1.52
7	2-G	508	SER	CA-C	-5.82	1.45	1.52
3	3-B	172	LEU	CA-C	-5.82	1.45	1.52
7	3-G	508	SER	CA-C	-5.82	1.45	1.52
1	1-A	683	LEU	CA-C	-5.82	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	851	THR	CA-C	-5.82	1.45	1.52
5	1-D	6	ALA	CA-C	-5.82	1.45	1.52
7	1-G	136	MET	CA-C	-5.82	1.44	1.52
7	1-G	531	TYR	CA-C	-5.82	1.45	1.52
5	1-I	6	ALA	CA-C	-5.82	1.45	1.52
1	2-A	683	LEU	CA-C	-5.82	1.45	1.52
3	2-B	851	THR	CA-C	-5.82	1.45	1.52
5	2-D	6	ALA	CA-C	-5.82	1.45	1.52
7	2-G	136	MET	CA-C	-5.82	1.44	1.52
7	2-G	531	TYR	CA-C	-5.82	1.45	1.52
5	2-I	6	ALA	CA-C	-5.82	1.45	1.52
1	3-A	683	LEU	CA-C	-5.82	1.45	1.52
3	3-B	851	THR	CA-C	-5.82	1.45	1.52
5	3-D	6	ALA	CA-C	-5.82	1.45	1.52
7	3-G	136	MET	CA-C	-5.82	1.44	1.52
7	3-G	531	TYR	CA-C	-5.82	1.45	1.52
5	3-I	6	ALA	CA-C	-5.82	1.45	1.52
6	1-J	67	ASP	CA-C	-5.81	1.45	1.52
6	2-J	67	ASP	CA-C	-5.81	1.45	1.52
6	3-J	67	ASP	CA-C	-5.81	1.45	1.52
3	1-B	441	GLU	CA-C	-5.81	1.45	1.52
4	1-C	587	LEU	CA-C	-5.81	1.45	1.52
3	1-N	263	CYS	CA-C	-5.81	1.45	1.52
3	2-B	441	GLU	CA-C	-5.81	1.45	1.52
4	2-C	587	LEU	CA-C	-5.81	1.45	1.52
3	2-N	263	CYS	CA-C	-5.81	1.45	1.52
3	3-B	441	GLU	CA-C	-5.81	1.45	1.52
4	3-C	587	LEU	CA-C	-5.81	1.45	1.52
3	3-N	263	CYS	CA-C	-5.81	1.45	1.52
7	1-G	81	ASP	CA-C	-5.81	1.45	1.52
7	2-G	81	ASP	CA-C	-5.81	1.45	1.52
7	3-G	81	ASP	CA-C	-5.81	1.45	1.52
3	1-N	283	LEU	CA-C	-5.81	1.45	1.52
3	1-N	372	VAL	C-N	-5.81	1.26	1.33
3	2-N	283	LEU	CA-C	-5.81	1.45	1.52
3	2-N	372	VAL	C-N	-5.81	1.26	1.33
3	3-N	283	LEU	CA-C	-5.81	1.45	1.52
3	3-N	372	VAL	C-N	-5.81	1.26	1.33
4	1-C	551	ILE	N-CA	-5.81	1.39	1.46
7	1-G	249	SER	C-O	-5.81	1.19	1.24
4	2-C	551	ILE	N-CA	-5.81	1.39	1.46
7	2-G	249	SER	C-O	-5.81	1.19	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-C	551	ILE	N-CA	-5.81	1.39	1.46
7	3-G	249	SER	C-O	-5.81	1.19	1.24
3	1-N	428	ASN	CA-C	-5.80	1.45	1.52
3	1-N	441	GLU	CA-C	-5.80	1.45	1.52
3	2-N	428	ASN	CA-C	-5.80	1.45	1.52
3	2-N	441	GLU	CA-C	-5.80	1.45	1.52
3	3-N	428	ASN	CA-C	-5.80	1.45	1.52
3	3-N	441	GLU	CA-C	-5.80	1.45	1.52
3	1-N	395	ARG	CA-C	-5.80	1.45	1.52
3	2-N	395	ARG	CA-C	-5.80	1.45	1.52
3	3-N	395	ARG	CA-C	-5.80	1.45	1.52
3	1-B	234	PHE	CA-C	-5.80	1.45	1.52
3	1-B	428	ASN	CA-C	-5.80	1.45	1.52
7	1-K	769	LYS	CA-C	-5.80	1.45	1.52
3	2-B	234	PHE	CA-C	-5.80	1.45	1.52
3	2-B	428	ASN	CA-C	-5.80	1.45	1.52
7	2-K	769	LYS	CA-C	-5.80	1.45	1.52
3	3-B	234	PHE	CA-C	-5.80	1.45	1.52
3	3-B	428	ASN	CA-C	-5.80	1.45	1.52
7	3-K	769	LYS	CA-C	-5.80	1.45	1.52
3	1-B	855	PHE	CA-C	-5.79	1.45	1.52
6	1-J	71	GLN	CA-C	-5.79	1.45	1.53
3	2-B	855	PHE	CA-C	-5.79	1.45	1.52
6	2-J	71	GLN	CA-C	-5.79	1.45	1.53
3	3-B	855	PHE	CA-C	-5.79	1.45	1.52
6	3-J	71	GLN	CA-C	-5.79	1.45	1.53
3	1-N	172	LEU	CA-C	-5.79	1.45	1.52
5	1-I	82	THR	N-CA	-5.79	1.39	1.46
3	2-N	172	LEU	CA-C	-5.79	1.45	1.52
5	2-I	82	THR	N-CA	-5.79	1.39	1.46
3	3-N	172	LEU	CA-C	-5.79	1.45	1.52
5	3-I	82	THR	N-CA	-5.79	1.39	1.46
1	1-A	212	ALA	CA-C	-5.79	1.45	1.52
1	1-A	682	LEU	CA-C	-5.79	1.45	1.52
1	2-A	212	ALA	CA-C	-5.79	1.45	1.52
1	2-A	682	LEU	CA-C	-5.79	1.45	1.52
1	3-A	212	ALA	CA-C	-5.79	1.45	1.52
1	3-A	682	LEU	CA-C	-5.79	1.45	1.52
8	1-Z	119	GLU	CA-C	-5.79	1.45	1.52
8	2-Z	119	GLU	CA-C	-5.79	1.45	1.52
8	3-Z	119	GLU	CA-C	-5.79	1.45	1.52
7	1-G	137	LEU	N-CA	-5.79	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1-Z	146	VAL	CA-C	-5.79	1.46	1.52
3	1-N	75	MET	N-CA	-5.79	1.39	1.46
7	2-G	137	LEU	N-CA	-5.79	1.39	1.46
8	2-Z	146	VAL	CA-C	-5.79	1.46	1.52
3	2-N	75	MET	N-CA	-5.79	1.39	1.46
7	3-G	137	LEU	N-CA	-5.79	1.39	1.46
8	3-Z	146	VAL	CA-C	-5.79	1.46	1.52
3	3-N	75	MET	N-CA	-5.79	1.39	1.46
6	1-F	92	VAL	CA-C	-5.79	1.45	1.52
6	2-F	92	VAL	CA-C	-5.79	1.45	1.52
6	3-F	92	VAL	CA-C	-5.79	1.45	1.52
7	1-G	164	LEU	CA-C	-5.78	1.45	1.52
6	1-J	92	VAL	CA-C	-5.78	1.45	1.52
7	2-G	164	LEU	CA-C	-5.78	1.45	1.52
6	2-J	92	VAL	CA-C	-5.78	1.45	1.52
7	3-G	164	LEU	CA-C	-5.78	1.45	1.52
6	3-J	92	VAL	CA-C	-5.78	1.45	1.52
1	1-A	620	LEU	CA-C	-5.78	1.45	1.52
7	1-K	64	THR	CA-C	-5.78	1.45	1.52
7	1-K	732	VAL	CA-C	-5.78	1.45	1.52
1	2-A	620	LEU	CA-C	-5.78	1.45	1.52
7	2-K	64	THR	CA-C	-5.78	1.45	1.52
7	2-K	732	VAL	CA-C	-5.78	1.45	1.52
1	3-A	620	LEU	CA-C	-5.78	1.45	1.52
7	3-K	64	THR	CA-C	-5.78	1.45	1.52
7	3-K	732	VAL	CA-C	-5.78	1.45	1.52
4	1-H	298	LYS	CA-C	-5.78	1.45	1.52
4	2-H	298	LYS	CA-C	-5.78	1.45	1.52
4	3-H	298	LYS	CA-C	-5.78	1.45	1.52
3	1-B	372	VAL	C-N	-5.78	1.26	1.33
3	2-B	372	VAL	C-N	-5.78	1.26	1.33
3	3-B	372	VAL	C-N	-5.78	1.26	1.33
6	1-F	38	LYS	CA-C	-5.78	1.45	1.52
6	2-F	38	LYS	CA-C	-5.78	1.45	1.52
6	3-F	38	LYS	CA-C	-5.78	1.45	1.52
7	1-G	443	ILE	CA-C	-5.77	1.45	1.52
7	2-G	443	ILE	CA-C	-5.77	1.45	1.52
7	3-G	443	ILE	CA-C	-5.77	1.45	1.52
4	1-C	521	GLN	N-CA	-5.77	1.39	1.46
8	1-Z	62	LEU	N-CA	-5.77	1.38	1.46
7	1-K	662	GLN	CA-C	-5.77	1.45	1.52
4	2-C	521	GLN	N-CA	-5.77	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2-Z	62	LEU	N-CA	-5.77	1.38	1.46
7	2-K	662	GLN	CA-C	-5.77	1.45	1.52
4	3-C	521	GLN	N-CA	-5.77	1.39	1.46
8	3-Z	62	LEU	N-CA	-5.77	1.38	1.46
7	3-K	662	GLN	CA-C	-5.77	1.45	1.52
4	1-C	625	LEU	CA-C	-5.77	1.45	1.52
4	2-C	625	LEU	CA-C	-5.77	1.45	1.52
4	3-C	625	LEU	CA-C	-5.77	1.45	1.52
1	1-A	564	LEU	CA-C	-5.77	1.45	1.52
1	1-A	630	GLN	N-CA	-5.77	1.38	1.46
3	1-B	262	ARG	N-CA	-5.77	1.39	1.46
6	1-R	25	LEU	CA-C	-5.77	1.45	1.53
7	1-K	194	TYR	N-CA	-5.77	1.39	1.46
1	2-A	564	LEU	CA-C	-5.77	1.45	1.52
1	2-A	630	GLN	N-CA	-5.77	1.38	1.46
3	2-B	262	ARG	N-CA	-5.77	1.39	1.46
6	2-R	25	LEU	CA-C	-5.77	1.45	1.53
7	2-K	194	TYR	N-CA	-5.77	1.39	1.46
1	3-A	564	LEU	CA-C	-5.77	1.45	1.52
1	3-A	630	GLN	N-CA	-5.77	1.38	1.46
3	3-B	262	ARG	N-CA	-5.77	1.39	1.46
6	3-R	25	LEU	CA-C	-5.77	1.45	1.53
7	3-K	194	TYR	N-CA	-5.77	1.39	1.46
4	1-C	783	LYS	CA-C	-5.76	1.45	1.52
7	1-G	234	ARG	C-N	-5.76	1.26	1.33
3	1-N	258	ALA	CA-C	-5.76	1.45	1.52
3	1-N	262	ARG	N-CA	-5.76	1.39	1.46
4	2-C	783	LYS	CA-C	-5.76	1.45	1.52
7	2-G	234	ARG	C-N	-5.76	1.26	1.33
3	2-N	258	ALA	CA-C	-5.76	1.45	1.52
3	2-N	262	ARG	N-CA	-5.76	1.39	1.46
4	3-C	783	LYS	CA-C	-5.76	1.45	1.52
7	3-G	234	ARG	C-N	-5.76	1.26	1.33
3	3-N	258	ALA	CA-C	-5.76	1.45	1.52
3	3-N	262	ARG	N-CA	-5.76	1.39	1.46
3	1-B	267	LEU	CA-C	-5.76	1.44	1.52
3	1-B	802	ALA	CA-C	-5.76	1.45	1.52
4	1-C	322	VAL	CA-C	-5.76	1.46	1.53
3	2-B	267	LEU	CA-C	-5.76	1.44	1.52
3	2-B	802	ALA	CA-C	-5.76	1.45	1.52
4	2-C	322	VAL	CA-C	-5.76	1.46	1.53
3	3-B	267	LEU	CA-C	-5.76	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	802	ALA	CA-C	-5.76	1.45	1.52
4	3-C	322	VAL	CA-C	-5.76	1.46	1.53
7	1-K	46	HIS	CA-C	-5.76	1.45	1.52
7	1-K	202	HIS	N-CA	-5.76	1.39	1.46
7	1-K	674	LEU	CA-C	-5.76	1.45	1.52
8	1-L	83	SER	N-CA	-5.76	1.38	1.46
7	2-K	46	HIS	CA-C	-5.76	1.45	1.52
7	2-K	202	HIS	N-CA	-5.76	1.39	1.46
7	2-K	674	LEU	CA-C	-5.76	1.45	1.52
8	2-L	83	SER	N-CA	-5.76	1.38	1.46
7	3-K	46	HIS	CA-C	-5.76	1.45	1.52
7	3-K	202	HIS	N-CA	-5.76	1.39	1.46
7	3-K	674	LEU	CA-C	-5.76	1.45	1.52
8	3-L	83	SER	N-CA	-5.76	1.38	1.46
3	1-B	136	LEU	CA-C	-5.76	1.45	1.52
3	2-B	136	LEU	CA-C	-5.76	1.45	1.52
3	3-B	136	LEU	CA-C	-5.76	1.45	1.52
6	1-R	122	LEU	CA-C	-5.76	1.45	1.52
6	2-R	122	LEU	CA-C	-5.76	1.45	1.52
6	3-R	122	LEU	CA-C	-5.76	1.45	1.52
3	1-B	321	VAL	N-CA	-5.76	1.39	1.46
3	2-B	321	VAL	N-CA	-5.76	1.39	1.46
3	3-B	321	VAL	N-CA	-5.76	1.39	1.46
7	1-K	107	SER	CA-C	-5.75	1.45	1.52
7	2-K	107	SER	CA-C	-5.75	1.45	1.52
7	3-K	107	SER	CA-C	-5.75	1.45	1.52
3	1-B	376	LYS	CA-C	-5.75	1.45	1.52
3	2-B	376	LYS	CA-C	-5.75	1.45	1.52
3	3-B	376	LYS	CA-C	-5.75	1.45	1.52
3	1-N	376	LYS	CA-C	-5.75	1.45	1.52
4	1-H	15	SER	N-CA	-5.75	1.40	1.46
3	2-N	376	LYS	CA-C	-5.75	1.45	1.52
4	2-H	15	SER	N-CA	-5.75	1.40	1.46
3	3-N	376	LYS	CA-C	-5.75	1.45	1.52
4	3-H	15	SER	N-CA	-5.75	1.40	1.46
3	1-B	188	ALA	N-CA	-5.75	1.41	1.46
3	2-B	188	ALA	N-CA	-5.75	1.41	1.46
3	3-B	188	ALA	N-CA	-5.75	1.41	1.46
8	1-Z	44	PHE	CA-C	-5.75	1.45	1.52
7	1-K	155	VAL	N-CA	-5.75	1.39	1.46
8	2-Z	44	PHE	CA-C	-5.75	1.45	1.52
7	2-K	155	VAL	N-CA	-5.75	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	3-Z	44	PHE	CA-C	-5.75	1.45	1.52
7	3-K	155	VAL	N-CA	-5.75	1.39	1.46
7	1-G	732	VAL	CA-C	-5.75	1.45	1.52
6	1-R	110	MET	N-CA	-5.75	1.39	1.46
7	2-G	732	VAL	CA-C	-5.75	1.45	1.52
6	2-R	110	MET	N-CA	-5.75	1.39	1.46
7	3-G	732	VAL	CA-C	-5.75	1.45	1.52
6	3-R	110	MET	N-CA	-5.75	1.39	1.46
3	1-B	414	ALA	C-O	-5.74	1.17	1.24
7	1-K	184	ALA	N-CA	-5.74	1.39	1.46
3	2-B	414	ALA	C-O	-5.74	1.17	1.24
7	2-K	184	ALA	N-CA	-5.74	1.39	1.46
3	3-B	414	ALA	C-O	-5.74	1.17	1.24
7	3-K	184	ALA	N-CA	-5.74	1.39	1.46
4	1-H	249	GLU	CA-C	-5.74	1.45	1.53
4	2-H	249	GLU	CA-C	-5.74	1.45	1.53
4	3-H	249	GLU	CA-C	-5.74	1.45	1.53
6	1-R	122	LEU	N-CA	-5.74	1.39	1.46
6	2-R	122	LEU	N-CA	-5.74	1.39	1.46
6	3-R	122	LEU	N-CA	-5.74	1.39	1.46
1	1-A	38	TYR	CA-C	-5.74	1.45	1.52
1	1-A	521	LEU	CA-C	-5.74	1.45	1.52
5	1-D	82	THR	N-CA	-5.74	1.39	1.46
7	1-G	650	CYS	CA-C	-5.74	1.45	1.52
6	1-J	38	LYS	CA-C	-5.74	1.45	1.52
1	2-A	38	TYR	CA-C	-5.74	1.45	1.52
1	2-A	521	LEU	CA-C	-5.74	1.45	1.52
5	2-D	82	THR	N-CA	-5.74	1.39	1.46
7	2-G	650	CYS	CA-C	-5.74	1.45	1.52
6	2-J	38	LYS	CA-C	-5.74	1.45	1.52
1	3-A	38	TYR	CA-C	-5.74	1.45	1.52
1	3-A	521	LEU	CA-C	-5.74	1.45	1.52
5	3-D	82	THR	N-CA	-5.74	1.39	1.46
7	3-G	650	CYS	CA-C	-5.74	1.45	1.52
6	3-J	38	LYS	CA-C	-5.74	1.45	1.52
3	1-B	361	ASP	N-CA	-5.73	1.39	1.46
3	1-B	391	THR	CA-C	-5.73	1.44	1.52
7	1-G	721	ALA	CA-C	-5.73	1.45	1.52
7	1-K	67	THR	CA-C	-5.73	1.45	1.52
3	2-B	361	ASP	N-CA	-5.73	1.39	1.46
3	2-B	391	THR	CA-C	-5.73	1.44	1.52
7	2-G	721	ALA	CA-C	-5.73	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-K	67	THR	CA-C	-5.73	1.45	1.52
3	3-B	361	ASP	N-CA	-5.73	1.39	1.46
3	3-B	391	THR	CA-C	-5.73	1.44	1.52
7	3-G	721	ALA	CA-C	-5.73	1.45	1.52
7	3-K	67	THR	CA-C	-5.73	1.45	1.52
5	1-D	81	GLU	N-CA	-5.73	1.39	1.46
8	1-L	40	GLU	CA-C	-5.73	1.45	1.52
3	1-N	267	LEU	CA-C	-5.73	1.44	1.52
4	1-H	7	ILE	N-CA	-5.73	1.39	1.46
5	2-D	81	GLU	N-CA	-5.73	1.39	1.46
8	2-L	40	GLU	CA-C	-5.73	1.45	1.52
3	2-N	267	LEU	CA-C	-5.73	1.44	1.52
4	2-H	7	ILE	N-CA	-5.73	1.39	1.46
5	3-D	81	GLU	N-CA	-5.73	1.39	1.46
8	3-L	40	GLU	CA-C	-5.73	1.45	1.52
3	3-N	267	LEU	CA-C	-5.73	1.44	1.52
4	3-H	7	ILE	N-CA	-5.73	1.39	1.46
7	1-G	751	TYR	CA-C	-5.73	1.45	1.52
7	2-G	751	TYR	CA-C	-5.73	1.45	1.52
7	3-G	751	TYR	CA-C	-5.73	1.45	1.52
1	1-A	679	GLU	N-CA	-5.73	1.39	1.46
3	1-B	286	LEU	N-CA	-5.73	1.39	1.46
7	1-G	674	LEU	CA-C	-5.73	1.45	1.52
1	2-A	679	GLU	N-CA	-5.73	1.39	1.46
3	2-B	286	LEU	N-CA	-5.73	1.39	1.46
7	2-G	674	LEU	CA-C	-5.73	1.45	1.52
1	3-A	679	GLU	N-CA	-5.73	1.39	1.46
3	3-B	286	LEU	N-CA	-5.73	1.39	1.46
7	3-G	674	LEU	CA-C	-5.73	1.45	1.52
4	1-C	7	ILE	N-CA	-5.73	1.39	1.46
4	2-C	7	ILE	N-CA	-5.73	1.39	1.46
4	3-C	7	ILE	N-CA	-5.73	1.39	1.46
4	1-C	249	GLU	CA-C	-5.72	1.45	1.53
4	1-C	259	SER	CA-C	-5.72	1.45	1.52
4	1-C	402	GLU	CA-C	-5.72	1.45	1.52
4	1-H	406	ARG	CA-C	-5.72	1.45	1.52
4	2-C	249	GLU	CA-C	-5.72	1.45	1.53
4	2-C	259	SER	CA-C	-5.72	1.45	1.52
4	2-C	402	GLU	CA-C	-5.72	1.45	1.52
4	2-H	406	ARG	CA-C	-5.72	1.45	1.52
4	3-C	249	GLU	CA-C	-5.72	1.45	1.53
4	3-C	259	SER	CA-C	-5.72	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-C	402	GLU	CA-C	-5.72	1.45	1.52
4	3-H	406	ARG	CA-C	-5.72	1.45	1.52
7	1-G	683	PRO	C-N	5.72	1.41	1.33
7	1-G	769	LYS	CA-C	-5.72	1.45	1.52
7	2-G	683	PRO	C-N	5.72	1.41	1.33
7	2-G	769	LYS	CA-C	-5.72	1.45	1.52
7	3-G	683	PRO	C-N	5.72	1.41	1.33
7	3-G	769	LYS	CA-C	-5.72	1.45	1.52
4	1-C	836	MET	CA-C	-5.72	1.45	1.52
4	2-C	836	MET	CA-C	-5.72	1.45	1.52
4	3-C	836	MET	CA-C	-5.72	1.45	1.52
1	1-A	325	ALA	C-N	5.71	1.40	1.33
8	1-Z	70	LYS	N-CA	-5.71	1.38	1.46
1	2-A	325	ALA	C-N	5.71	1.40	1.33
8	2-Z	70	LYS	N-CA	-5.71	1.38	1.46
1	3-A	325	ALA	C-N	5.71	1.40	1.33
8	3-Z	70	LYS	N-CA	-5.71	1.38	1.46
1	1-A	496	TRP	CA-C	-5.71	1.45	1.52
4	1-H	182	GLU	CA-C	-5.71	1.45	1.53
1	2-A	496	TRP	CA-C	-5.71	1.45	1.52
4	2-H	182	GLU	CA-C	-5.71	1.45	1.53
1	3-A	496	TRP	CA-C	-5.71	1.45	1.52
4	3-H	182	GLU	CA-C	-5.71	1.45	1.53
4	1-H	521	GLN	N-CA	-5.71	1.39	1.46
4	2-H	521	GLN	N-CA	-5.71	1.39	1.46
4	3-H	521	GLN	N-CA	-5.71	1.39	1.46
3	1-B	781	LEU	N-CA	-5.71	1.39	1.46
4	1-C	510	ILE	CA-C	-5.71	1.45	1.52
6	1-R	113	GLU	N-CA	-5.71	1.38	1.46
3	2-B	781	LEU	N-CA	-5.71	1.39	1.46
4	2-C	510	ILE	CA-C	-5.71	1.45	1.52
6	2-R	113	GLU	N-CA	-5.71	1.38	1.46
3	3-B	781	LEU	N-CA	-5.71	1.39	1.46
4	3-C	510	ILE	CA-C	-5.71	1.45	1.52
6	3-R	113	GLU	N-CA	-5.71	1.38	1.46
8	1-L	144	HIS	CA-C	-5.71	1.45	1.52
8	2-L	144	HIS	CA-C	-5.71	1.45	1.52
8	3-L	144	HIS	CA-C	-5.71	1.45	1.52
3	1-B	953	LEU	CA-C	-5.70	1.45	1.52
5	1-D	147	VAL	CA-C	-5.70	1.45	1.52
6	1-M	25	LEU	CA-C	-5.70	1.45	1.53
3	1-N	391	THR	CA-C	-5.70	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	953	LEU	CA-C	-5.70	1.45	1.52
5	2-D	147	VAL	CA-C	-5.70	1.45	1.52
6	2-M	25	LEU	CA-C	-5.70	1.45	1.53
3	2-N	391	THR	CA-C	-5.70	1.44	1.52
3	3-B	953	LEU	CA-C	-5.70	1.45	1.52
5	3-D	147	VAL	CA-C	-5.70	1.45	1.52
6	3-M	25	LEU	CA-C	-5.70	1.45	1.53
3	3-N	391	THR	CA-C	-5.70	1.44	1.52
4	1-C	182	GLU	CA-C	-5.70	1.45	1.53
4	2-C	182	GLU	CA-C	-5.70	1.45	1.53
4	3-C	182	GLU	CA-C	-5.70	1.45	1.53
4	1-C	214	TRP	CA-C	-5.70	1.45	1.52
7	1-K	683	PRO	C-N	5.70	1.41	1.33
4	2-C	214	TRP	CA-C	-5.70	1.45	1.52
7	2-K	683	PRO	C-N	5.70	1.41	1.33
4	3-C	214	TRP	CA-C	-5.70	1.45	1.52
7	3-K	683	PRO	C-N	5.70	1.41	1.33
5	1-D	144	PHE	CA-C	-5.70	1.45	1.52
3	1-N	94	LEU	N-CA	-5.70	1.39	1.46
5	2-D	144	PHE	CA-C	-5.70	1.45	1.52
3	2-N	94	LEU	N-CA	-5.70	1.39	1.46
5	3-D	144	PHE	CA-C	-5.70	1.45	1.52
3	3-N	94	LEU	N-CA	-5.70	1.39	1.46
4	1-C	737	LYS	CA-C	-5.70	1.45	1.52
4	2-C	737	LYS	CA-C	-5.70	1.45	1.52
4	3-C	737	LYS	CA-C	-5.70	1.45	1.52
4	1-C	298	LYS	CA-C	-5.70	1.45	1.52
4	2-C	298	LYS	CA-C	-5.70	1.45	1.52
4	3-C	298	LYS	CA-C	-5.70	1.45	1.52
3	1-B	310	ASN	N-CA	-5.69	1.39	1.46
4	1-C	841	GLY	CA-C	-5.69	1.45	1.51
7	1-K	217	LYS	N-CA	-5.69	1.39	1.46
7	1-K	650	CYS	CA-C	-5.69	1.45	1.52
3	1-N	415	ASN	N-CA	-5.69	1.39	1.46
3	2-B	310	ASN	N-CA	-5.69	1.39	1.46
4	2-C	841	GLY	CA-C	-5.69	1.45	1.51
7	2-K	217	LYS	N-CA	-5.69	1.39	1.46
7	2-K	650	CYS	CA-C	-5.69	1.45	1.52
3	2-N	415	ASN	N-CA	-5.69	1.39	1.46
3	3-B	310	ASN	N-CA	-5.69	1.39	1.46
4	3-C	841	GLY	CA-C	-5.69	1.45	1.51
7	3-K	217	LYS	N-CA	-5.69	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3-K	650	CYS	CA-C	-5.69	1.45	1.52
3	3-N	415	ASN	N-CA	-5.69	1.39	1.46
6	1-F	71	GLN	CA-C	-5.69	1.45	1.53
8	1-Z	124	ALA	CA-C	-5.69	1.45	1.52
3	1-N	361	ASP	N-CA	-5.69	1.39	1.46
6	2-F	71	GLN	CA-C	-5.69	1.45	1.53
8	2-Z	124	ALA	CA-C	-5.69	1.45	1.52
3	2-N	361	ASP	N-CA	-5.69	1.39	1.46
6	3-F	71	GLN	CA-C	-5.69	1.45	1.53
8	3-Z	124	ALA	CA-C	-5.69	1.45	1.52
3	3-N	361	ASP	N-CA	-5.69	1.39	1.46
3	1-B	258	ALA	CA-C	-5.69	1.45	1.52
7	1-K	256	GLU	CA-C	-5.69	1.45	1.52
3	2-B	258	ALA	CA-C	-5.69	1.45	1.52
7	2-K	256	GLU	CA-C	-5.69	1.45	1.52
3	3-B	258	ALA	CA-C	-5.69	1.45	1.52
7	3-K	256	GLU	CA-C	-5.69	1.45	1.52
1	1-A	536	ASP	CA-C	-5.69	1.45	1.52
5	1-D	77	LEU	CA-C	-5.69	1.45	1.52
4	1-H	644	ARG	CA-C	-5.69	1.45	1.52
1	2-A	536	ASP	CA-C	-5.69	1.45	1.52
5	2-D	77	LEU	CA-C	-5.69	1.45	1.52
4	2-H	644	ARG	CA-C	-5.69	1.45	1.52
1	3-A	536	ASP	CA-C	-5.69	1.45	1.52
5	3-D	77	LEU	CA-C	-5.69	1.45	1.52
4	3-H	644	ARG	CA-C	-5.69	1.45	1.52
3	1-B	94	LEU	N-CA	-5.68	1.39	1.46
3	1-B	303	LEU	N-CA	-5.68	1.39	1.46
3	2-B	94	LEU	N-CA	-5.68	1.39	1.46
3	2-B	303	LEU	N-CA	-5.68	1.39	1.46
3	3-B	94	LEU	N-CA	-5.68	1.39	1.46
3	3-B	303	LEU	N-CA	-5.68	1.39	1.46
7	1-G	776	TRP	N-CA	-5.68	1.39	1.46
7	1-K	231	MET	CA-C	-5.68	1.45	1.52
7	1-K	632	SER	CA-C	-5.68	1.45	1.52
7	2-G	776	TRP	N-CA	-5.68	1.39	1.46
7	2-K	231	MET	CA-C	-5.68	1.45	1.52
7	2-K	632	SER	CA-C	-5.68	1.45	1.52
7	3-G	776	TRP	N-CA	-5.68	1.39	1.46
7	3-K	231	MET	CA-C	-5.68	1.45	1.52
7	3-K	632	SER	CA-C	-5.68	1.45	1.52
1	1-A	594	PRO	C-N	-5.68	1.26	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	374	VAL	C-O	-5.68	1.17	1.24
3	1-B	439	VAL	N-CA	-5.68	1.40	1.46
1	2-A	594	PRO	C-N	-5.68	1.26	1.34
3	2-B	374	VAL	C-O	-5.68	1.17	1.24
3	2-B	439	VAL	N-CA	-5.68	1.40	1.46
1	3-A	594	PRO	C-N	-5.68	1.26	1.34
3	3-B	374	VAL	C-O	-5.68	1.17	1.24
3	3-B	439	VAL	N-CA	-5.68	1.40	1.46
7	1-G	104	ILE	CA-C	-5.68	1.45	1.52
5	1-I	102	ILE	CA-C	-5.68	1.45	1.52
7	2-G	104	ILE	CA-C	-5.68	1.45	1.52
5	2-I	102	ILE	CA-C	-5.68	1.45	1.52
7	3-G	104	ILE	CA-C	-5.68	1.45	1.52
5	3-I	102	ILE	CA-C	-5.68	1.45	1.52
3	1-B	415	ASN	N-CA	-5.68	1.39	1.46
5	1-I	132	THR	CA-C	-5.68	1.45	1.52
3	2-B	415	ASN	N-CA	-5.68	1.39	1.46
5	2-I	132	THR	CA-C	-5.68	1.45	1.52
3	3-B	415	ASN	N-CA	-5.68	1.39	1.46
5	3-I	132	THR	CA-C	-5.68	1.45	1.52
7	1-G	383	ILE	CA-C	-5.67	1.45	1.52
8	1-Z	28	ALA	N-CA	-5.67	1.39	1.46
4	1-H	259	SER	CA-C	-5.67	1.45	1.52
7	2-G	383	ILE	CA-C	-5.67	1.45	1.52
8	2-Z	28	ALA	N-CA	-5.67	1.39	1.46
4	2-H	259	SER	CA-C	-5.67	1.45	1.52
7	3-G	383	ILE	CA-C	-5.67	1.45	1.52
8	3-Z	28	ALA	N-CA	-5.67	1.39	1.46
4	3-H	259	SER	CA-C	-5.67	1.45	1.52
4	1-H	510	ILE	CA-C	-5.67	1.46	1.52
4	2-H	510	ILE	CA-C	-5.67	1.46	1.52
4	3-H	510	ILE	CA-C	-5.67	1.46	1.52
4	1-H	241	LEU	CA-C	-5.67	1.45	1.52
4	1-H	555	ALA	N-CA	-5.67	1.38	1.46
4	2-H	241	LEU	CA-C	-5.67	1.45	1.52
4	2-H	555	ALA	N-CA	-5.67	1.38	1.46
4	3-H	241	LEU	CA-C	-5.67	1.45	1.52
4	3-H	555	ALA	N-CA	-5.67	1.38	1.46
3	1-N	422	GLU	N-CA	-5.67	1.39	1.46
4	1-H	214	TRP	CA-C	-5.67	1.45	1.52
3	2-N	422	GLU	N-CA	-5.67	1.39	1.46
4	2-H	214	TRP	CA-C	-5.67	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-N	422	GLU	N-CA	-5.67	1.39	1.46
4	3-H	214	TRP	CA-C	-5.67	1.45	1.52
3	1-B	124	LEU	CA-C	-5.67	1.45	1.52
3	2-B	124	LEU	CA-C	-5.67	1.45	1.52
3	3-B	124	LEU	CA-C	-5.67	1.45	1.52
7	1-G	93	LYS	N-CA	-5.66	1.39	1.46
8	1-L	98	PHE	CA-C	-5.66	1.45	1.52
7	2-G	93	LYS	N-CA	-5.66	1.39	1.46
8	2-L	98	PHE	CA-C	-5.66	1.45	1.52
7	3-G	93	LYS	N-CA	-5.66	1.39	1.46
8	3-L	98	PHE	CA-C	-5.66	1.45	1.52
5	1-D	102	ILE	CA-C	-5.66	1.45	1.52
7	1-G	76	LEU	CA-C	-5.66	1.45	1.52
5	2-D	102	ILE	CA-C	-5.66	1.45	1.52
7	2-G	76	LEU	CA-C	-5.66	1.45	1.52
5	3-D	102	ILE	CA-C	-5.66	1.45	1.52
7	3-G	76	LEU	CA-C	-5.66	1.45	1.52
3	1-B	778	LEU	CA-C	-5.66	1.45	1.52
4	1-C	458	ILE	N-CA	-5.66	1.39	1.46
4	1-C	644	ARG	CA-C	-5.66	1.45	1.52
8	1-L	49	PHE	N-CA	-5.66	1.39	1.46
3	2-B	778	LEU	CA-C	-5.66	1.45	1.52
4	2-C	458	ILE	N-CA	-5.66	1.39	1.46
4	2-C	644	ARG	CA-C	-5.66	1.45	1.52
8	2-L	49	PHE	N-CA	-5.66	1.39	1.46
3	3-B	778	LEU	CA-C	-5.66	1.45	1.52
4	3-C	458	ILE	N-CA	-5.66	1.39	1.46
4	3-C	644	ARG	CA-C	-5.66	1.45	1.52
8	3-L	49	PHE	N-CA	-5.66	1.39	1.46
4	1-H	677	ALA	CA-C	-5.66	1.45	1.52
4	2-H	677	ALA	CA-C	-5.66	1.45	1.52
4	3-H	677	ALA	CA-C	-5.66	1.45	1.52
5	1-D	57	VAL	N-CA	-5.66	1.39	1.46
7	1-G	727	VAL	CA-C	-5.66	1.45	1.52
7	1-G	840	ILE	CA-C	-5.66	1.45	1.52
7	1-K	776	TRP	N-CA	-5.66	1.39	1.46
8	1-L	92	ALA	CA-C	-5.66	1.45	1.52
5	1-I	57	VAL	N-CA	-5.66	1.39	1.46
5	2-D	57	VAL	N-CA	-5.66	1.39	1.46
7	2-G	727	VAL	CA-C	-5.66	1.45	1.52
7	2-G	840	ILE	CA-C	-5.66	1.45	1.52
7	2-K	776	TRP	N-CA	-5.66	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2-L	92	ALA	CA-C	-5.66	1.45	1.52
5	2-I	57	VAL	N-CA	-5.66	1.39	1.46
5	3-D	57	VAL	N-CA	-5.66	1.39	1.46
7	3-G	727	VAL	CA-C	-5.66	1.45	1.52
7	3-G	840	ILE	CA-C	-5.66	1.45	1.52
7	3-K	776	TRP	N-CA	-5.66	1.39	1.46
8	3-L	92	ALA	CA-C	-5.66	1.45	1.52
5	3-I	57	VAL	N-CA	-5.66	1.39	1.46
1	1-A	663	GLU	N-CA	-5.65	1.39	1.46
4	1-C	542	ARG	CA-C	-5.65	1.46	1.52
1	2-A	663	GLU	N-CA	-5.65	1.39	1.46
4	2-C	542	ARG	CA-C	-5.65	1.46	1.52
1	3-A	663	GLU	N-CA	-5.65	1.39	1.46
4	3-C	542	ARG	CA-C	-5.65	1.46	1.52
8	1-L	144	HIS	N-CA	-5.65	1.39	1.46
8	2-L	144	HIS	N-CA	-5.65	1.39	1.46
8	3-L	144	HIS	N-CA	-5.65	1.39	1.46
1	1-A	436	LEU	N-CA	-5.65	1.39	1.45
4	1-C	610	LEU	N-CA	-5.65	1.40	1.46
7	1-K	162	SER	CA-C	-5.65	1.45	1.52
8	1-L	39	LYS	CA-C	-5.65	1.45	1.52
1	2-A	436	LEU	N-CA	-5.65	1.39	1.45
4	2-C	610	LEU	N-CA	-5.65	1.40	1.46
7	2-K	162	SER	CA-C	-5.65	1.45	1.52
8	2-L	39	LYS	CA-C	-5.65	1.45	1.52
1	3-A	436	LEU	N-CA	-5.65	1.39	1.45
4	3-C	610	LEU	N-CA	-5.65	1.40	1.46
7	3-K	162	SER	CA-C	-5.65	1.45	1.52
8	3-L	39	LYS	CA-C	-5.65	1.45	1.52
1	1-A	506	LEU	N-CA	-5.65	1.39	1.45
7	1-K	727	VAL	CA-C	-5.65	1.45	1.52
1	2-A	506	LEU	N-CA	-5.65	1.39	1.45
7	2-K	727	VAL	CA-C	-5.65	1.45	1.52
1	3-A	506	LEU	N-CA	-5.65	1.39	1.45
7	3-K	727	VAL	CA-C	-5.65	1.45	1.52
4	1-C	291	ASP	CA-C	-5.65	1.45	1.52
4	1-C	406	ARG	CA-C	-5.65	1.45	1.52
6	1-M	100	ILE	N-CA	-5.65	1.39	1.46
3	1-N	124	LEU	CA-C	-5.65	1.45	1.52
5	1-I	77	LEU	CA-C	-5.65	1.45	1.52
4	2-C	291	ASP	CA-C	-5.65	1.45	1.52
4	2-C	406	ARG	CA-C	-5.65	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2-M	100	ILE	N-CA	-5.65	1.39	1.46
3	2-N	124	LEU	CA-C	-5.65	1.45	1.52
5	2-I	77	LEU	CA-C	-5.65	1.45	1.52
4	3-C	291	ASP	CA-C	-5.65	1.45	1.52
4	3-C	406	ARG	CA-C	-5.65	1.45	1.52
6	3-M	100	ILE	N-CA	-5.65	1.39	1.46
3	3-N	124	LEU	CA-C	-5.65	1.45	1.52
5	3-I	77	LEU	CA-C	-5.65	1.45	1.52
5	1-D	132	THR	CA-C	-5.65	1.45	1.52
3	1-N	310	ASN	N-CA	-5.65	1.39	1.46
4	1-H	542	ARG	CA-C	-5.65	1.46	1.52
5	2-D	132	THR	CA-C	-5.65	1.45	1.52
3	2-N	310	ASN	N-CA	-5.65	1.39	1.46
4	2-H	542	ARG	CA-C	-5.65	1.46	1.52
5	3-D	132	THR	CA-C	-5.65	1.45	1.52
3	3-N	310	ASN	N-CA	-5.65	1.39	1.46
4	3-H	542	ARG	CA-C	-5.65	1.46	1.52
6	1-F	93	ASP	CA-C	-5.64	1.45	1.52
8	1-Z	49	PHE	CA-C	-5.64	1.45	1.52
7	1-K	721	ALA	CA-C	-5.64	1.45	1.52
7	1-K	752	VAL	CA-C	-5.64	1.45	1.52
6	2-F	93	ASP	CA-C	-5.64	1.45	1.52
8	2-Z	49	PHE	CA-C	-5.64	1.45	1.52
7	2-K	721	ALA	CA-C	-5.64	1.45	1.52
7	2-K	752	VAL	CA-C	-5.64	1.45	1.52
6	3-F	93	ASP	CA-C	-5.64	1.45	1.52
8	3-Z	49	PHE	CA-C	-5.64	1.45	1.52
7	3-K	721	ALA	CA-C	-5.64	1.45	1.52
7	3-K	752	VAL	CA-C	-5.64	1.45	1.52
6	1-F	141	GLU	CA-C	-5.64	1.45	1.52
4	1-H	536	TYR	CA-C	-5.64	1.45	1.52
6	2-F	141	GLU	CA-C	-5.64	1.45	1.52
4	2-H	536	TYR	CA-C	-5.64	1.45	1.52
6	3-F	141	GLU	CA-C	-5.64	1.45	1.52
4	3-H	536	TYR	CA-C	-5.64	1.45	1.52
1	1-A	445	THR	CA-C	-5.64	1.45	1.52
7	1-G	249	SER	C-N	-5.64	1.26	1.33
1	2-A	445	THR	CA-C	-5.64	1.45	1.52
7	2-G	249	SER	C-N	-5.64	1.26	1.33
1	3-A	445	THR	CA-C	-5.64	1.45	1.52
7	3-G	249	SER	C-N	-5.64	1.26	1.33
1	1-A	586	ARG	C-N	5.64	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	586	ARG	C-N	5.64	1.40	1.33
1	3-A	586	ARG	C-N	5.64	1.40	1.33
7	1-G	243	GLU	CA-C	-5.64	1.45	1.52
7	1-K	638	ALA	CA-C	-5.64	1.45	1.52
3	1-N	374	VAL	C-O	-5.64	1.17	1.24
7	2-G	243	GLU	CA-C	-5.64	1.45	1.52
7	2-K	638	ALA	CA-C	-5.64	1.45	1.52
3	2-N	374	VAL	C-O	-5.64	1.17	1.24
7	3-G	243	GLU	CA-C	-5.64	1.45	1.52
7	3-K	638	ALA	CA-C	-5.64	1.45	1.52
3	3-N	374	VAL	C-O	-5.64	1.17	1.24
6	1-F	42	VAL	CA-C	-5.63	1.47	1.52
4	1-H	232	VAL	N-CA	-5.63	1.39	1.46
5	1-I	144	PHE	CA-C	-5.63	1.45	1.52
6	2-F	42	VAL	CA-C	-5.63	1.47	1.52
4	2-H	232	VAL	N-CA	-5.63	1.39	1.46
5	2-I	144	PHE	CA-C	-5.63	1.45	1.52
6	3-F	42	VAL	CA-C	-5.63	1.47	1.52
4	3-H	232	VAL	N-CA	-5.63	1.39	1.46
5	3-I	144	PHE	CA-C	-5.63	1.45	1.52
7	1-K	154	SER	CA-C	-5.63	1.45	1.52
7	2-K	154	SER	CA-C	-5.63	1.45	1.52
7	3-K	154	SER	CA-C	-5.63	1.45	1.52
6	1-F	19	ARG	N-CA	-5.63	1.39	1.46
6	2-F	19	ARG	N-CA	-5.63	1.39	1.46
6	3-F	19	ARG	N-CA	-5.63	1.39	1.46
1	1-A	660	ILE	N-CA	-5.63	1.39	1.46
4	1-C	241	LEU	CA-C	-5.63	1.45	1.52
3	1-N	95	VAL	CA-C	-5.63	1.45	1.52
1	2-A	660	ILE	N-CA	-5.63	1.39	1.46
4	2-C	241	LEU	CA-C	-5.63	1.45	1.52
3	2-N	95	VAL	CA-C	-5.63	1.45	1.52
1	3-A	660	ILE	N-CA	-5.63	1.39	1.46
4	3-C	241	LEU	CA-C	-5.63	1.45	1.52
3	3-N	95	VAL	CA-C	-5.63	1.45	1.52
7	1-G	256	GLU	CA-C	-5.63	1.45	1.52
7	1-G	632	SER	CA-C	-5.63	1.45	1.52
7	2-G	256	GLU	CA-C	-5.63	1.45	1.52
7	2-G	632	SER	CA-C	-5.63	1.45	1.52
7	3-G	256	GLU	CA-C	-5.63	1.45	1.52
7	3-G	632	SER	CA-C	-5.63	1.45	1.52
4	1-C	538	SER	CA-C	-5.62	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-K	212	SER	N-CA	-5.62	1.39	1.46
4	2-C	538	SER	CA-C	-5.62	1.45	1.52
7	2-K	212	SER	N-CA	-5.62	1.39	1.46
4	3-C	538	SER	CA-C	-5.62	1.45	1.52
7	3-K	212	SER	N-CA	-5.62	1.39	1.46
7	1-K	192	VAL	N-CA	-5.62	1.39	1.46
7	2-K	192	VAL	N-CA	-5.62	1.39	1.46
7	3-K	192	VAL	N-CA	-5.62	1.39	1.46
4	1-H	433	ILE	CA-C	-5.62	1.45	1.52
4	2-H	433	ILE	CA-C	-5.62	1.45	1.52
4	3-H	433	ILE	CA-C	-5.62	1.45	1.52
1	1-A	201	LEU	CA-C	-5.62	1.46	1.52
1	1-A	560	ILE	CA-C	-5.62	1.45	1.52
1	1-A	570	VAL	C-O	-5.62	1.18	1.24
4	1-C	677	ALA	CA-C	-5.62	1.45	1.52
8	1-Z	82	SER	CA-C	-5.62	1.45	1.52
5	1-I	147	VAL	CA-C	-5.62	1.46	1.52
1	2-A	201	LEU	CA-C	-5.62	1.46	1.52
1	2-A	560	ILE	CA-C	-5.62	1.45	1.52
1	2-A	570	VAL	C-O	-5.62	1.18	1.24
4	2-C	677	ALA	CA-C	-5.62	1.45	1.52
8	2-Z	82	SER	CA-C	-5.62	1.45	1.52
5	2-I	147	VAL	CA-C	-5.62	1.46	1.52
1	3-A	201	LEU	CA-C	-5.62	1.46	1.52
1	3-A	560	ILE	CA-C	-5.62	1.45	1.52
1	3-A	570	VAL	C-O	-5.62	1.18	1.24
4	3-C	677	ALA	CA-C	-5.62	1.45	1.52
8	3-Z	82	SER	CA-C	-5.62	1.45	1.52
5	3-I	147	VAL	CA-C	-5.62	1.46	1.52
6	1-J	141	GLU	CA-C	-5.62	1.45	1.52
6	2-J	141	GLU	CA-C	-5.62	1.45	1.52
6	3-J	141	GLU	CA-C	-5.62	1.45	1.52
3	1-B	57	LEU	CA-C	-5.61	1.45	1.52
3	1-B	95	VAL	CA-C	-5.61	1.45	1.52
7	1-G	152	VAL	CA-C	-5.61	1.47	1.52
8	1-Z	126	ASP	CA-C	-5.61	1.45	1.52
3	2-B	57	LEU	CA-C	-5.61	1.45	1.52
3	2-B	95	VAL	CA-C	-5.61	1.45	1.52
7	2-G	152	VAL	CA-C	-5.61	1.47	1.52
8	2-Z	126	ASP	CA-C	-5.61	1.45	1.52
3	3-B	57	LEU	CA-C	-5.61	1.45	1.52
3	3-B	95	VAL	CA-C	-5.61	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3-G	152	VAL	CA-C	-5.61	1.47	1.52
8	3-Z	126	ASP	CA-C	-5.61	1.45	1.52
1	1-A	658	ILE	CA-C	-5.61	1.43	1.52
1	2-A	658	ILE	CA-C	-5.61	1.43	1.52
1	3-A	658	ILE	CA-C	-5.61	1.43	1.52
1	1-A	80	TYR	CA-C	-5.61	1.46	1.52
1	1-A	145	PRO	CA-C	-5.61	1.44	1.52
3	1-B	793	ALA	C-N	-5.61	1.26	1.33
8	1-Z	30	TYR	N-CA	-5.61	1.39	1.46
7	1-K	216	SER	CA-C	-5.61	1.45	1.52
1	2-A	80	TYR	CA-C	-5.61	1.46	1.52
1	2-A	145	PRO	CA-C	-5.61	1.44	1.52
3	2-B	793	ALA	C-N	-5.61	1.26	1.33
8	2-Z	30	TYR	N-CA	-5.61	1.39	1.46
7	2-K	216	SER	CA-C	-5.61	1.45	1.52
1	3-A	80	TYR	CA-C	-5.61	1.46	1.52
1	3-A	145	PRO	CA-C	-5.61	1.44	1.52
3	3-B	793	ALA	C-N	-5.61	1.26	1.33
8	3-Z	30	TYR	N-CA	-5.61	1.39	1.46
7	3-K	216	SER	CA-C	-5.61	1.45	1.52
4	1-C	536	TYR	CA-C	-5.61	1.45	1.52
7	1-G	638	ALA	CA-C	-5.61	1.45	1.52
4	1-H	612	THR	N-CA	-5.61	1.39	1.46
4	2-C	536	TYR	CA-C	-5.61	1.45	1.52
7	2-G	638	ALA	CA-C	-5.61	1.45	1.52
4	2-H	612	THR	N-CA	-5.61	1.39	1.46
4	3-C	536	TYR	CA-C	-5.61	1.45	1.52
7	3-G	638	ALA	CA-C	-5.61	1.45	1.52
4	3-H	612	THR	N-CA	-5.61	1.39	1.46
1	1-A	452	ASN	CA-C	-5.61	1.45	1.52
1	2-A	452	ASN	CA-C	-5.61	1.45	1.52
1	3-A	452	ASN	CA-C	-5.61	1.45	1.52
3	1-B	138	PHE	CA-C	-5.61	1.45	1.52
4	1-C	433	ILE	CA-C	-5.61	1.45	1.52
6	1-R	109	ARG	N-CA	-5.61	1.38	1.46
3	2-B	138	PHE	CA-C	-5.61	1.45	1.52
4	2-C	433	ILE	CA-C	-5.61	1.45	1.52
6	2-R	109	ARG	N-CA	-5.61	1.38	1.46
3	3-B	138	PHE	CA-C	-5.61	1.45	1.52
4	3-C	433	ILE	CA-C	-5.61	1.45	1.52
6	3-R	109	ARG	N-CA	-5.61	1.38	1.46
7	1-G	804	ILE	C-N	5.60	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	804	ILE	C-N	5.60	1.40	1.33
7	3-G	804	ILE	C-N	5.60	1.40	1.33
7	1-G	92	ILE	N-CA	-5.60	1.39	1.46
7	1-G	421	ILE	CA-C	-5.60	1.46	1.52
8	1-Z	145	ARG	CA-C	-5.60	1.45	1.52
4	1-H	688	GLU	CA-C	-5.60	1.45	1.52
6	1-J	93	ASP	CA-C	-5.60	1.46	1.52
7	2-G	92	ILE	N-CA	-5.60	1.39	1.46
7	2-G	421	ILE	CA-C	-5.60	1.46	1.52
8	2-Z	145	ARG	CA-C	-5.60	1.45	1.52
4	2-H	688	GLU	CA-C	-5.60	1.45	1.52
6	2-J	93	ASP	CA-C	-5.60	1.46	1.52
7	3-G	92	ILE	N-CA	-5.60	1.39	1.46
7	3-G	421	ILE	CA-C	-5.60	1.46	1.52
8	3-Z	145	ARG	CA-C	-5.60	1.45	1.52
4	3-H	688	GLU	CA-C	-5.60	1.45	1.52
6	3-J	93	ASP	CA-C	-5.60	1.46	1.52
1	1-A	681	ALA	N-CA	-5.60	1.39	1.46
7	1-K	840	ILE	CA-C	-5.60	1.45	1.52
3	1-N	57	LEU	CA-C	-5.60	1.45	1.52
4	1-H	207	ASP	CA-C	-5.60	1.44	1.52
6	1-J	42	VAL	CA-C	-5.60	1.47	1.52
1	2-A	681	ALA	N-CA	-5.60	1.39	1.46
7	2-K	840	ILE	CA-C	-5.60	1.45	1.52
3	2-N	57	LEU	CA-C	-5.60	1.45	1.52
4	2-H	207	ASP	CA-C	-5.60	1.44	1.52
6	2-J	42	VAL	CA-C	-5.60	1.47	1.52
1	3-A	681	ALA	N-CA	-5.60	1.39	1.46
7	3-K	840	ILE	CA-C	-5.60	1.45	1.52
3	3-N	57	LEU	CA-C	-5.60	1.45	1.52
4	3-H	207	ASP	CA-C	-5.60	1.44	1.52
6	3-J	42	VAL	CA-C	-5.60	1.47	1.52
7	1-G	403	THR	CA-C	-5.60	1.45	1.52
5	1-I	49	VAL	CA-C	-5.60	1.45	1.52
7	2-G	403	THR	CA-C	-5.60	1.45	1.52
5	2-I	49	VAL	CA-C	-5.60	1.45	1.52
7	3-G	403	THR	CA-C	-5.60	1.45	1.52
5	3-I	49	VAL	CA-C	-5.60	1.45	1.52
6	1-R	172	TRP	CA-C	-5.60	1.45	1.52
6	2-R	172	TRP	CA-C	-5.60	1.45	1.52
6	3-R	172	TRP	CA-C	-5.60	1.45	1.52
3	1-N	303	LEU	N-CA	-5.59	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-N	326	HIS	N-CA	-5.59	1.40	1.46
4	1-H	458	ILE	N-CA	-5.59	1.39	1.46
3	2-N	303	LEU	N-CA	-5.59	1.39	1.46
3	2-N	326	HIS	N-CA	-5.59	1.40	1.46
4	2-H	458	ILE	N-CA	-5.59	1.39	1.46
3	3-N	303	LEU	N-CA	-5.59	1.39	1.46
3	3-N	326	HIS	N-CA	-5.59	1.40	1.46
4	3-H	458	ILE	N-CA	-5.59	1.39	1.46
7	1-K	751	TYR	CA-C	-5.59	1.45	1.52
7	2-K	751	TYR	CA-C	-5.59	1.45	1.52
7	3-K	751	TYR	CA-C	-5.59	1.45	1.52
7	1-G	682	GLU	CA-C	5.59	1.59	1.52
3	1-N	413	ALA	CA-C	-5.59	1.45	1.52
4	1-H	291	ASP	CA-C	-5.59	1.45	1.52
7	2-G	682	GLU	CA-C	5.59	1.59	1.52
3	2-N	413	ALA	CA-C	-5.59	1.45	1.52
4	2-H	291	ASP	CA-C	-5.59	1.45	1.52
7	3-G	682	GLU	CA-C	5.59	1.59	1.52
3	3-N	413	ALA	CA-C	-5.59	1.45	1.52
4	3-H	291	ASP	CA-C	-5.59	1.45	1.52
3	1-B	413	ALA	CA-C	-5.59	1.45	1.52
4	1-C	193	TYR	CA-C	-5.59	1.46	1.52
3	2-B	413	ALA	CA-C	-5.59	1.45	1.52
4	2-C	193	TYR	CA-C	-5.59	1.46	1.52
3	3-B	413	ALA	CA-C	-5.59	1.45	1.52
4	3-C	193	TYR	CA-C	-5.59	1.46	1.52
4	1-C	777	LEU	CA-C	-5.59	1.45	1.52
4	2-C	777	LEU	CA-C	-5.59	1.45	1.52
4	3-C	777	LEU	CA-C	-5.59	1.45	1.52
3	1-B	835	SER	CA-C	-5.59	1.46	1.52
5	1-D	49	VAL	CA-C	-5.59	1.45	1.52
7	1-G	374	GLU	CA-C	-5.59	1.48	1.53
3	2-B	835	SER	CA-C	-5.59	1.46	1.52
5	2-D	49	VAL	CA-C	-5.59	1.45	1.52
7	2-G	374	GLU	CA-C	-5.59	1.48	1.53
3	3-B	835	SER	CA-C	-5.59	1.46	1.52
5	3-D	49	VAL	CA-C	-5.59	1.45	1.52
7	3-G	374	GLU	CA-C	-5.59	1.48	1.53
8	1-L	82	SER	CA-C	-5.58	1.46	1.52
8	2-L	82	SER	CA-C	-5.58	1.46	1.52
8	3-L	82	SER	CA-C	-5.58	1.46	1.52
1	1-A	609	ASP	CA-C	-5.58	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	422	GLU	N-CA	-5.58	1.39	1.46
4	1-H	402	GLU	CA-C	-5.58	1.45	1.52
4	1-H	655	LYS	CA-C	-5.58	1.45	1.52
1	2-A	609	ASP	CA-C	-5.58	1.45	1.52
3	2-B	422	GLU	N-CA	-5.58	1.39	1.46
4	2-H	402	GLU	CA-C	-5.58	1.45	1.52
4	2-H	655	LYS	CA-C	-5.58	1.45	1.52
1	3-A	609	ASP	CA-C	-5.58	1.45	1.52
3	3-B	422	GLU	N-CA	-5.58	1.39	1.46
4	3-H	402	GLU	CA-C	-5.58	1.45	1.52
4	3-H	655	LYS	CA-C	-5.58	1.45	1.52
3	1-B	871	ASN	N-CA	-5.58	1.39	1.46
3	2-B	871	ASN	N-CA	-5.58	1.39	1.46
3	3-B	871	ASN	N-CA	-5.58	1.39	1.46
1	1-A	744	GLU	CA-C	-5.58	1.45	1.52
4	1-C	232	VAL	N-CA	-5.58	1.39	1.46
1	2-A	744	GLU	CA-C	-5.58	1.45	1.52
4	2-C	232	VAL	N-CA	-5.58	1.39	1.46
1	3-A	744	GLU	CA-C	-5.58	1.45	1.52
4	3-C	232	VAL	N-CA	-5.58	1.39	1.46
7	1-K	155	VAL	CA-C	-5.58	1.45	1.52
7	1-K	302	ALA	N-CA	-5.58	1.39	1.46
7	2-K	155	VAL	CA-C	-5.58	1.45	1.52
7	2-K	302	ALA	N-CA	-5.58	1.39	1.46
7	3-K	155	VAL	CA-C	-5.58	1.45	1.52
7	3-K	302	ALA	N-CA	-5.58	1.39	1.46
6	1-M	89	ILE	N-CA	-5.57	1.39	1.46
4	1-H	398	HIS	CA-C	-5.57	1.45	1.52
6	2-M	89	ILE	N-CA	-5.57	1.39	1.46
4	2-H	398	HIS	CA-C	-5.57	1.45	1.52
6	3-M	89	ILE	N-CA	-5.57	1.39	1.46
4	3-H	398	HIS	CA-C	-5.57	1.45	1.52
4	1-C	110	THR	CA-C	-5.57	1.45	1.52
7	1-G	88	CYS	N-CA	-5.57	1.39	1.46
7	1-G	309	ARG	CA-C	-5.57	1.45	1.52
6	1-R	127	LYS	CA-C	-5.57	1.46	1.53
7	1-K	52	LEU	N-CA	-5.57	1.39	1.46
4	2-C	110	THR	CA-C	-5.57	1.45	1.52
7	2-G	88	CYS	N-CA	-5.57	1.39	1.46
7	2-G	309	ARG	CA-C	-5.57	1.45	1.52
6	2-R	127	LYS	CA-C	-5.57	1.46	1.53
7	2-K	52	LEU	N-CA	-5.57	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-C	110	THR	CA-C	-5.57	1.45	1.52
7	3-G	88	CYS	N-CA	-5.57	1.39	1.46
7	3-G	309	ARG	CA-C	-5.57	1.45	1.52
6	3-R	127	LYS	CA-C	-5.57	1.46	1.53
7	3-K	52	LEU	N-CA	-5.57	1.39	1.46
1	1-A	578	VAL	C-N	5.57	1.41	1.33
1	2-A	578	VAL	C-N	5.57	1.41	1.33
1	3-A	578	VAL	C-N	5.57	1.41	1.33
4	1-H	110	THR	CA-C	-5.57	1.45	1.52
4	2-H	110	THR	CA-C	-5.57	1.45	1.52
4	3-H	110	THR	CA-C	-5.57	1.45	1.52
3	1-B	99	ILE	CA-C	-5.57	1.45	1.52
4	1-C	612	THR	N-CA	-5.57	1.39	1.46
7	1-G	192	VAL	N-CA	-5.57	1.39	1.46
3	1-N	138	PHE	CA-C	-5.57	1.45	1.52
3	2-B	99	ILE	CA-C	-5.57	1.45	1.52
4	2-C	612	THR	N-CA	-5.57	1.39	1.46
7	2-G	192	VAL	N-CA	-5.57	1.39	1.46
3	2-N	138	PHE	CA-C	-5.57	1.45	1.52
3	3-B	99	ILE	CA-C	-5.57	1.45	1.52
4	3-C	612	THR	N-CA	-5.57	1.39	1.46
7	3-G	192	VAL	N-CA	-5.57	1.39	1.46
3	3-N	138	PHE	CA-C	-5.57	1.45	1.52
4	1-C	357	THR	CA-C	-5.56	1.45	1.52
3	1-N	414	ALA	C-O	-5.56	1.17	1.24
4	2-C	357	THR	CA-C	-5.56	1.45	1.52
3	2-N	414	ALA	C-O	-5.56	1.17	1.24
4	3-C	357	THR	CA-C	-5.56	1.45	1.52
3	3-N	414	ALA	C-O	-5.56	1.17	1.24
1	1-A	220	ILE	CA-C	-5.56	1.46	1.52
4	1-C	436	GLY	CA-C	-5.56	1.45	1.52
7	1-K	702	GLN	CA-C	-5.56	1.45	1.52
3	1-N	188	ALA	N-CA	-5.56	1.41	1.46
1	2-A	220	ILE	CA-C	-5.56	1.46	1.52
4	2-C	436	GLY	CA-C	-5.56	1.45	1.52
7	2-K	702	GLN	CA-C	-5.56	1.45	1.52
3	2-N	188	ALA	N-CA	-5.56	1.41	1.46
1	3-A	220	ILE	CA-C	-5.56	1.46	1.52
4	3-C	436	GLY	CA-C	-5.56	1.45	1.52
7	3-K	702	GLN	CA-C	-5.56	1.45	1.52
3	3-N	188	ALA	N-CA	-5.56	1.41	1.46
4	1-C	556	HIS	CA-C	-5.56	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1-R	101	GLY	CA-C	-5.56	1.45	1.52
7	1-K	44	CYS	N-CA	-5.56	1.39	1.46
4	2-C	556	HIS	CA-C	-5.56	1.45	1.52
6	2-R	101	GLY	CA-C	-5.56	1.45	1.52
7	2-K	44	CYS	N-CA	-5.56	1.39	1.46
4	3-C	556	HIS	CA-C	-5.56	1.45	1.52
6	3-R	101	GLY	CA-C	-5.56	1.45	1.52
7	3-K	44	CYS	N-CA	-5.56	1.39	1.46
8	1-L	14	LYS	N-CA	-5.56	1.39	1.46
4	1-H	254	ARG	CA-C	-5.56	1.45	1.52
8	2-L	14	LYS	N-CA	-5.56	1.39	1.46
4	2-H	254	ARG	CA-C	-5.56	1.45	1.52
8	3-L	14	LYS	N-CA	-5.56	1.39	1.46
4	3-H	254	ARG	CA-C	-5.56	1.45	1.52
6	1-R	123	VAL	N-CA	-5.55	1.39	1.46
7	1-K	111	LYS	N-CA	-5.55	1.39	1.46
3	1-N	439	VAL	N-CA	-5.55	1.40	1.46
6	2-R	123	VAL	N-CA	-5.55	1.39	1.46
7	2-K	111	LYS	N-CA	-5.55	1.39	1.46
3	2-N	439	VAL	N-CA	-5.55	1.40	1.46
6	3-R	123	VAL	N-CA	-5.55	1.39	1.46
7	3-K	111	LYS	N-CA	-5.55	1.39	1.46
3	3-N	439	VAL	N-CA	-5.55	1.40	1.46
4	1-C	506	THR	CA-C	-5.55	1.46	1.52
4	2-C	506	THR	CA-C	-5.55	1.46	1.52
4	3-C	506	THR	CA-C	-5.55	1.46	1.52
6	1-R	34	LEU	CA-C	-5.55	1.45	1.52
6	1-J	19	ARG	N-CA	-5.55	1.39	1.46
6	2-R	34	LEU	CA-C	-5.55	1.45	1.52
6	2-J	19	ARG	N-CA	-5.55	1.39	1.46
6	3-R	34	LEU	CA-C	-5.55	1.45	1.52
6	3-J	19	ARG	N-CA	-5.55	1.39	1.46
6	1-R	22	MET	CA-C	-5.55	1.45	1.52
7	1-K	91	THR	CA-C	-5.55	1.45	1.52
6	2-R	22	MET	CA-C	-5.55	1.45	1.52
7	2-K	91	THR	CA-C	-5.55	1.45	1.52
6	3-R	22	MET	CA-C	-5.55	1.45	1.52
7	3-K	91	THR	CA-C	-5.55	1.45	1.52
4	1-C	555	ALA	N-CA	-5.55	1.39	1.46
4	2-C	555	ALA	N-CA	-5.55	1.39	1.46
4	3-C	555	ALA	N-CA	-5.55	1.39	1.46
3	1-B	803	ASN	N-CA	-5.55	1.38	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-H	610	LEU	N-CA	-5.55	1.40	1.46
3	2-B	803	ASN	N-CA	-5.55	1.38	1.45
4	2-H	610	LEU	N-CA	-5.55	1.40	1.46
3	3-B	803	ASN	N-CA	-5.55	1.38	1.45
4	3-H	610	LEU	N-CA	-5.55	1.40	1.46
1	1-A	623	GLN	N-CA	-5.54	1.39	1.46
7	1-G	543	ASN	CA-C	-5.54	1.45	1.52
7	1-K	147	ALA	CA-C	-5.54	1.45	1.52
3	1-N	148	LEU	CA-C	-5.54	1.45	1.52
1	2-A	623	GLN	N-CA	-5.54	1.39	1.46
7	2-G	543	ASN	CA-C	-5.54	1.45	1.52
7	2-K	147	ALA	CA-C	-5.54	1.45	1.52
3	2-N	148	LEU	CA-C	-5.54	1.45	1.52
1	3-A	623	GLN	N-CA	-5.54	1.39	1.46
7	3-G	543	ASN	CA-C	-5.54	1.45	1.52
7	3-K	147	ALA	CA-C	-5.54	1.45	1.52
3	3-N	148	LEU	CA-C	-5.54	1.45	1.52
4	1-H	357	THR	CA-C	-5.54	1.46	1.52
4	2-H	357	THR	CA-C	-5.54	1.46	1.52
4	3-H	357	THR	CA-C	-5.54	1.46	1.52
8	1-L	28	ALA	CA-C	-5.54	1.45	1.52
4	1-H	193	TYR	CA-C	-5.54	1.46	1.52
8	2-L	28	ALA	CA-C	-5.54	1.45	1.52
4	2-H	193	TYR	CA-C	-5.54	1.46	1.52
8	3-L	28	ALA	CA-C	-5.54	1.45	1.52
4	3-H	193	TYR	CA-C	-5.54	1.46	1.52
3	1-N	356	LEU	CA-C	-5.54	1.45	1.52
3	2-N	356	LEU	CA-C	-5.54	1.45	1.52
3	3-N	356	LEU	CA-C	-5.54	1.45	1.52
1	1-A	794	LEU	CA-C	-5.53	1.47	1.53
4	1-H	440	GLY	CA-C	-5.53	1.48	1.52
1	2-A	794	LEU	CA-C	-5.53	1.47	1.53
4	2-H	440	GLY	CA-C	-5.53	1.48	1.52
1	3-A	794	LEU	CA-C	-5.53	1.47	1.53
4	3-H	440	GLY	CA-C	-5.53	1.48	1.52
1	1-A	705	PHE	CA-C	-5.53	1.45	1.52
1	1-A	718	LYS	CA-C	-5.53	1.45	1.52
7	1-K	106	THR	N-CA	-5.53	1.39	1.46
1	2-A	705	PHE	CA-C	-5.53	1.45	1.52
1	2-A	718	LYS	CA-C	-5.53	1.45	1.52
7	2-K	106	THR	N-CA	-5.53	1.39	1.46
1	3-A	705	PHE	CA-C	-5.53	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-A	718	LYS	CA-C	-5.53	1.45	1.52
7	3-K	106	THR	N-CA	-5.53	1.39	1.46
3	1-N	353	LYS	N-CA	-5.53	1.39	1.46
4	1-H	538	SER	CA-C	-5.53	1.45	1.52
3	2-N	353	LYS	N-CA	-5.53	1.39	1.46
4	2-H	538	SER	CA-C	-5.53	1.45	1.52
3	3-N	353	LYS	N-CA	-5.53	1.39	1.46
4	3-H	538	SER	CA-C	-5.53	1.45	1.52
7	1-G	160	LEU	CA-C	-5.53	1.45	1.52
7	2-G	160	LEU	CA-C	-5.53	1.45	1.52
7	3-G	160	LEU	CA-C	-5.53	1.45	1.52
3	1-B	950	GLY	CA-C	-5.53	1.45	1.52
3	2-B	950	GLY	CA-C	-5.53	1.45	1.52
3	3-B	950	GLY	CA-C	-5.53	1.45	1.52
3	1-B	312	VAL	CA-C	-5.53	1.45	1.52
4	1-C	207	ASP	CA-C	-5.53	1.44	1.52
4	1-C	398	HIS	CA-C	-5.53	1.45	1.52
4	1-C	688	GLU	CA-C	-5.53	1.45	1.52
6	1-R	134	MET	C-N	5.53	1.41	1.33
3	2-B	312	VAL	CA-C	-5.53	1.45	1.52
4	2-C	207	ASP	CA-C	-5.53	1.44	1.52
4	2-C	398	HIS	CA-C	-5.53	1.45	1.52
4	2-C	688	GLU	CA-C	-5.53	1.45	1.52
6	2-R	134	MET	C-N	5.53	1.41	1.33
3	3-B	312	VAL	CA-C	-5.53	1.45	1.52
4	3-C	207	ASP	CA-C	-5.53	1.44	1.52
4	3-C	398	HIS	CA-C	-5.53	1.45	1.52
4	3-C	688	GLU	CA-C	-5.53	1.45	1.52
6	3-R	134	MET	C-N	5.53	1.41	1.33
5	1-D	78	GLU	N-CA	-5.52	1.39	1.46
5	2-D	78	GLU	N-CA	-5.52	1.39	1.46
5	3-D	78	GLU	N-CA	-5.52	1.39	1.46
1	1-A	313	GLY	CA-C	-5.52	1.44	1.52
3	1-B	148	LEU	CA-C	-5.52	1.45	1.52
4	1-C	825	PRO	C-N	5.52	1.40	1.33
7	1-G	215	ILE	C-O	-5.52	1.18	1.24
7	1-K	804	ILE	C-N	5.52	1.40	1.33
1	2-A	313	GLY	CA-C	-5.52	1.44	1.52
3	2-B	148	LEU	CA-C	-5.52	1.45	1.52
4	2-C	825	PRO	C-N	5.52	1.40	1.33
7	2-G	215	ILE	C-O	-5.52	1.18	1.24
7	2-K	804	ILE	C-N	5.52	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-A	313	GLY	CA-C	-5.52	1.44	1.52
3	3-B	148	LEU	CA-C	-5.52	1.45	1.52
4	3-C	825	PRO	C-N	5.52	1.40	1.33
7	3-G	215	ILE	C-O	-5.52	1.18	1.24
7	3-K	804	ILE	C-N	5.52	1.40	1.33
7	1-G	532	LEU	N-CA	-5.52	1.39	1.46
7	2-G	532	LEU	N-CA	-5.52	1.39	1.46
7	3-G	532	LEU	N-CA	-5.52	1.39	1.46
1	1-A	680	VAL	CA-C	-5.52	1.45	1.52
3	1-B	326	HIS	N-CA	-5.52	1.40	1.46
8	1-Z	66	THR	CA-C	-5.52	1.45	1.52
1	2-A	680	VAL	CA-C	-5.52	1.45	1.52
3	2-B	326	HIS	N-CA	-5.52	1.40	1.46
8	2-Z	66	THR	CA-C	-5.52	1.45	1.52
1	3-A	680	VAL	CA-C	-5.52	1.45	1.52
3	3-B	326	HIS	N-CA	-5.52	1.40	1.46
8	3-Z	66	THR	CA-C	-5.52	1.45	1.52
1	1-A	716	LEU	N-CA	-5.52	1.39	1.46
4	1-C	248	SER	CA-C	-5.52	1.45	1.52
7	1-G	84	LEU	CA-C	-5.52	1.45	1.52
1	2-A	716	LEU	N-CA	-5.52	1.39	1.46
4	2-C	248	SER	CA-C	-5.52	1.45	1.52
7	2-G	84	LEU	CA-C	-5.52	1.45	1.52
1	3-A	716	LEU	N-CA	-5.52	1.39	1.46
4	3-C	248	SER	CA-C	-5.52	1.45	1.52
7	3-G	84	LEU	CA-C	-5.52	1.45	1.52
1	1-A	692	MET	CA-C	-5.52	1.45	1.52
1	2-A	692	MET	CA-C	-5.52	1.45	1.52
1	3-A	692	MET	CA-C	-5.52	1.45	1.52
7	1-G	55	ILE	N-CA	-5.51	1.39	1.46
7	2-G	55	ILE	N-CA	-5.51	1.39	1.46
7	3-G	55	ILE	N-CA	-5.51	1.39	1.46
3	1-N	302	ASP	CA-C	-5.51	1.45	1.52
3	2-N	302	ASP	CA-C	-5.51	1.45	1.52
3	3-N	302	ASP	CA-C	-5.51	1.45	1.52
3	1-N	461	PHE	CA-C	-5.51	1.45	1.52
3	2-N	461	PHE	CA-C	-5.51	1.45	1.52
3	3-N	461	PHE	CA-C	-5.51	1.45	1.52
3	1-N	99	ILE	CA-C	-5.51	1.45	1.52
3	2-N	99	ILE	CA-C	-5.51	1.45	1.52
3	3-N	99	ILE	CA-C	-5.51	1.45	1.52
4	1-C	537	THR	CA-C	-5.50	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-G	191	MET	CA-C	-5.50	1.45	1.52
8	1-L	110	GLU	CA-C	-5.50	1.45	1.53
3	1-N	350	GLU	N-CA	-5.50	1.39	1.46
4	2-C	537	THR	CA-C	-5.50	1.45	1.52
7	2-G	191	MET	CA-C	-5.50	1.45	1.52
8	2-L	110	GLU	CA-C	-5.50	1.45	1.53
3	2-N	350	GLU	N-CA	-5.50	1.39	1.46
4	3-C	537	THR	CA-C	-5.50	1.45	1.52
7	3-G	191	MET	CA-C	-5.50	1.45	1.52
8	3-L	110	GLU	CA-C	-5.50	1.45	1.53
3	3-N	350	GLU	N-CA	-5.50	1.39	1.46
1	1-A	253	SER	CA-C	-5.50	1.45	1.52
1	2-A	253	SER	CA-C	-5.50	1.45	1.52
1	3-A	253	SER	CA-C	-5.50	1.45	1.52
1	1-A	285	GLN	N-CA	-5.50	1.39	1.46
7	1-K	56	ASN	CA-C	-5.50	1.45	1.52
1	2-A	285	GLN	N-CA	-5.50	1.39	1.46
7	2-K	56	ASN	CA-C	-5.50	1.45	1.52
1	3-A	285	GLN	N-CA	-5.50	1.39	1.46
7	3-K	56	ASN	CA-C	-5.50	1.45	1.52
3	1-B	304	ILE	CA-C	-5.50	1.45	1.52
3	1-B	857	GLN	N-CA	-5.50	1.39	1.46
7	1-K	148	ILE	CA-C	-5.50	1.45	1.52
3	2-B	304	ILE	CA-C	-5.50	1.45	1.52
3	2-B	857	GLN	N-CA	-5.50	1.39	1.46
7	2-K	148	ILE	CA-C	-5.50	1.45	1.52
3	3-B	304	ILE	CA-C	-5.50	1.45	1.52
3	3-B	857	GLN	N-CA	-5.50	1.39	1.46
7	3-K	148	ILE	CA-C	-5.50	1.45	1.52
1	1-A	439	ASN	CA-C	-5.49	1.45	1.52
4	1-H	556	HIS	CA-C	-5.49	1.46	1.52
1	2-A	439	ASN	CA-C	-5.49	1.45	1.52
4	2-H	556	HIS	CA-C	-5.49	1.46	1.52
1	3-A	439	ASN	CA-C	-5.49	1.45	1.52
4	3-H	556	HIS	CA-C	-5.49	1.46	1.52
8	1-Z	17	LEU	N-CA	-5.49	1.39	1.45
3	1-N	312	VAL	CA-C	-5.49	1.45	1.52
8	2-Z	17	LEU	N-CA	-5.49	1.39	1.45
3	2-N	312	VAL	CA-C	-5.49	1.45	1.52
8	3-Z	17	LEU	N-CA	-5.49	1.39	1.45
3	3-N	312	VAL	CA-C	-5.49	1.45	1.52
5	1-I	78	GLU	N-CA	-5.49	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2-I	78	GLU	N-CA	-5.49	1.39	1.46
5	3-I	78	GLU	N-CA	-5.49	1.39	1.46
7	1-K	682	GLU	CA-C	5.49	1.59	1.52
4	1-H	203	ILE	N-CA	-5.49	1.39	1.46
7	2-K	682	GLU	CA-C	5.49	1.59	1.52
4	2-H	203	ILE	N-CA	-5.49	1.39	1.46
7	3-K	682	GLU	CA-C	5.49	1.59	1.52
4	3-H	203	ILE	N-CA	-5.49	1.39	1.46
3	1-B	287	SER	CA-C	-5.49	1.45	1.52
3	2-B	287	SER	CA-C	-5.49	1.45	1.52
3	3-B	287	SER	CA-C	-5.49	1.45	1.52
3	1-B	302	ASP	CA-C	-5.49	1.45	1.52
3	1-B	476	ILE	CA-C	-5.49	1.45	1.52
6	1-R	55	THR	N-CA	-5.49	1.39	1.46
4	1-H	218	ASN	CA-C	-5.49	1.45	1.52
3	2-B	302	ASP	CA-C	-5.49	1.45	1.52
3	2-B	476	ILE	CA-C	-5.49	1.45	1.52
6	2-R	55	THR	N-CA	-5.49	1.39	1.46
4	2-H	218	ASN	CA-C	-5.49	1.45	1.52
3	3-B	302	ASP	CA-C	-5.49	1.45	1.52
3	3-B	476	ILE	CA-C	-5.49	1.45	1.52
6	3-R	55	THR	N-CA	-5.49	1.39	1.46
4	3-H	218	ASN	CA-C	-5.49	1.45	1.52
7	1-K	265	MET	N-CA	-5.48	1.39	1.46
7	2-K	265	MET	N-CA	-5.48	1.39	1.46
7	3-K	265	MET	N-CA	-5.48	1.39	1.46
4	1-C	522	GLU	CA-C	-5.48	1.46	1.52
5	1-D	240	ASP	CA-C	-5.48	1.45	1.52
3	1-N	98	GLU	CA-C	-5.48	1.46	1.52
3	1-N	304	ILE	CA-C	-5.48	1.45	1.52
4	2-C	522	GLU	CA-C	-5.48	1.46	1.52
5	2-D	240	ASP	CA-C	-5.48	1.45	1.52
3	2-N	98	GLU	CA-C	-5.48	1.46	1.52
3	2-N	304	ILE	CA-C	-5.48	1.45	1.52
4	3-C	522	GLU	CA-C	-5.48	1.46	1.52
5	3-D	240	ASP	CA-C	-5.48	1.45	1.52
3	3-N	98	GLU	CA-C	-5.48	1.46	1.52
3	3-N	304	ILE	CA-C	-5.48	1.45	1.52
3	1-B	421	MET	CA-C	-5.48	1.45	1.52
3	1-B	461	PHE	CA-C	-5.48	1.45	1.52
4	1-C	655	LYS	CA-C	-5.48	1.45	1.52
7	1-G	691	SER	C-N	5.48	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	421	MET	CA-C	-5.48	1.45	1.52
3	2-B	461	PHE	CA-C	-5.48	1.45	1.52
4	2-C	655	LYS	CA-C	-5.48	1.45	1.52
7	2-G	691	SER	C-N	5.48	1.40	1.33
3	3-B	421	MET	CA-C	-5.48	1.45	1.52
3	3-B	461	PHE	CA-C	-5.48	1.45	1.52
4	3-C	655	LYS	CA-C	-5.48	1.45	1.52
7	3-G	691	SER	C-N	5.48	1.40	1.33
1	1-A	147	GLU	N-CA	-5.48	1.39	1.46
4	1-C	440	GLY	CA-C	-5.48	1.48	1.52
7	1-G	178	VAL	CA-C	-5.48	1.45	1.52
3	1-N	333	LEU	CA-C	-5.48	1.45	1.52
5	1-I	240	ASP	CA-C	-5.48	1.45	1.52
1	2-A	147	GLU	N-CA	-5.48	1.39	1.46
4	2-C	440	GLY	CA-C	-5.48	1.48	1.52
7	2-G	178	VAL	CA-C	-5.48	1.45	1.52
3	2-N	333	LEU	CA-C	-5.48	1.45	1.52
5	2-I	240	ASP	CA-C	-5.48	1.45	1.52
1	3-A	147	GLU	N-CA	-5.48	1.39	1.46
4	3-C	440	GLY	CA-C	-5.48	1.48	1.52
7	3-G	178	VAL	CA-C	-5.48	1.45	1.52
3	3-N	333	LEU	CA-C	-5.48	1.45	1.52
5	3-I	240	ASP	CA-C	-5.48	1.45	1.52
3	1-B	353	LYS	N-CA	-5.48	1.39	1.46
7	1-K	102	VAL	N-CA	-5.48	1.39	1.46
3	1-N	318	ASP	N-CA	-5.48	1.39	1.46
3	2-B	353	LYS	N-CA	-5.48	1.39	1.46
7	2-K	102	VAL	N-CA	-5.48	1.39	1.46
3	2-N	318	ASP	N-CA	-5.48	1.39	1.46
3	3-B	353	LYS	N-CA	-5.48	1.39	1.46
7	3-K	102	VAL	N-CA	-5.48	1.39	1.46
3	3-N	318	ASP	N-CA	-5.48	1.39	1.46
1	1-A	75	ILE	N-CA	-5.48	1.39	1.46
4	1-C	570	ASP	CA-C	-5.48	1.45	1.52
1	2-A	75	ILE	N-CA	-5.48	1.39	1.46
4	2-C	570	ASP	CA-C	-5.48	1.45	1.52
1	3-A	75	ILE	N-CA	-5.48	1.39	1.46
4	3-C	570	ASP	CA-C	-5.48	1.45	1.52
3	1-N	192	ILE	CA-C	-5.47	1.46	1.52
3	1-N	337	VAL	N-CA	-5.47	1.40	1.46
4	1-H	607	ASP	CA-C	-5.47	1.45	1.52
3	2-N	192	ILE	CA-C	-5.47	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-N	337	VAL	N-CA	-5.47	1.40	1.46
4	2-H	607	ASP	CA-C	-5.47	1.45	1.52
3	3-N	192	ILE	CA-C	-5.47	1.46	1.52
3	3-N	337	VAL	N-CA	-5.47	1.40	1.46
4	3-H	607	ASP	CA-C	-5.47	1.45	1.52
1	1-A	595	THR	C-N	-5.47	1.26	1.34
3	1-B	274	ALA	CA-C	-5.47	1.45	1.52
3	1-N	408	ARG	N-CA	-5.47	1.39	1.46
4	1-H	400	SER	CA-C	-5.47	1.45	1.52
4	1-H	506	THR	CA-C	-5.47	1.46	1.52
1	2-A	595	THR	C-N	-5.47	1.26	1.34
3	2-B	274	ALA	CA-C	-5.47	1.45	1.52
3	2-N	408	ARG	N-CA	-5.47	1.39	1.46
4	2-H	400	SER	CA-C	-5.47	1.45	1.52
4	2-H	506	THR	CA-C	-5.47	1.46	1.52
1	3-A	595	THR	C-N	-5.47	1.26	1.34
3	3-B	274	ALA	CA-C	-5.47	1.45	1.52
3	3-N	408	ARG	N-CA	-5.47	1.39	1.46
4	3-H	400	SER	CA-C	-5.47	1.45	1.52
4	3-H	506	THR	CA-C	-5.47	1.46	1.52
7	1-G	188	ASP	CA-C	-5.47	1.46	1.53
4	1-H	176	SER	N-CA	-5.47	1.41	1.46
7	2-G	188	ASP	CA-C	-5.47	1.46	1.53
4	2-H	176	SER	N-CA	-5.47	1.41	1.46
7	3-G	188	ASP	CA-C	-5.47	1.46	1.53
4	3-H	176	SER	N-CA	-5.47	1.41	1.46
1	1-A	694	TYR	N-CA	-5.47	1.39	1.46
4	1-C	203	ILE	N-CA	-5.47	1.39	1.46
4	1-C	254	ARG	CA-C	-5.47	1.46	1.52
4	1-H	248	SER	CA-C	-5.47	1.45	1.52
1	2-A	694	TYR	N-CA	-5.47	1.39	1.46
4	2-C	203	ILE	N-CA	-5.47	1.39	1.46
4	2-C	254	ARG	CA-C	-5.47	1.46	1.52
4	2-H	248	SER	CA-C	-5.47	1.45	1.52
1	3-A	694	TYR	N-CA	-5.47	1.39	1.46
4	3-C	203	ILE	N-CA	-5.47	1.39	1.46
4	3-C	254	ARG	CA-C	-5.47	1.46	1.52
4	3-H	248	SER	CA-C	-5.47	1.45	1.52
6	1-M	20	ILE	CA-C	-5.47	1.45	1.52
3	1-N	326	HIS	CA-C	-5.47	1.46	1.52
3	1-N	431	ALA	CA-C	-5.47	1.45	1.52
6	2-M	20	ILE	CA-C	-5.47	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-N	326	HIS	CA-C	-5.47	1.46	1.52
3	2-N	431	ALA	CA-C	-5.47	1.45	1.52
6	3-M	20	ILE	CA-C	-5.47	1.45	1.52
3	3-N	326	HIS	CA-C	-5.47	1.46	1.52
3	3-N	431	ALA	CA-C	-5.47	1.45	1.52
3	1-B	98	GLU	CA-C	-5.47	1.46	1.52
3	1-B	337	VAL	N-CA	-5.47	1.40	1.46
4	1-C	718	GLY	CA-C	-5.47	1.46	1.52
6	1-R	65	VAL	CA-C	-5.47	1.45	1.52
7	1-K	772	PHE	CA-C	-5.47	1.46	1.52
3	1-N	359	ALA	N-CA	-5.47	1.39	1.46
3	2-B	98	GLU	CA-C	-5.47	1.46	1.52
3	2-B	337	VAL	N-CA	-5.47	1.40	1.46
4	2-C	718	GLY	CA-C	-5.47	1.46	1.52
6	2-R	65	VAL	CA-C	-5.47	1.45	1.52
7	2-K	772	PHE	CA-C	-5.47	1.46	1.52
3	2-N	359	ALA	N-CA	-5.47	1.39	1.46
3	3-B	98	GLU	CA-C	-5.47	1.46	1.52
3	3-B	337	VAL	N-CA	-5.47	1.40	1.46
4	3-C	718	GLY	CA-C	-5.47	1.46	1.52
6	3-R	65	VAL	CA-C	-5.47	1.45	1.52
7	3-K	772	PHE	CA-C	-5.47	1.46	1.52
3	3-N	359	ALA	N-CA	-5.47	1.39	1.46
3	1-B	408	ARG	N-CA	-5.46	1.39	1.46
6	1-F	29	GLY	N-CA	-5.46	1.37	1.45
3	2-B	408	ARG	N-CA	-5.46	1.39	1.46
6	2-F	29	GLY	N-CA	-5.46	1.37	1.45
3	3-B	408	ARG	N-CA	-5.46	1.39	1.46
6	3-F	29	GLY	N-CA	-5.46	1.37	1.45
1	1-A	701	ASP	CA-C	-5.46	1.45	1.52
1	2-A	701	ASP	CA-C	-5.46	1.45	1.52
1	3-A	701	ASP	CA-C	-5.46	1.45	1.52
3	1-B	431	ALA	CA-C	-5.46	1.45	1.52
7	1-G	249	SER	N-CA	-5.46	1.42	1.46
4	1-H	718	GLY	CA-C	-5.46	1.46	1.52
3	2-B	431	ALA	CA-C	-5.46	1.45	1.52
7	2-G	249	SER	N-CA	-5.46	1.42	1.46
4	2-H	718	GLY	CA-C	-5.46	1.46	1.52
3	3-B	431	ALA	CA-C	-5.46	1.45	1.52
7	3-G	249	SER	N-CA	-5.46	1.42	1.46
4	3-H	718	GLY	CA-C	-5.46	1.46	1.52
1	1-A	229	VAL	N-CA	-5.46	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	229	VAL	N-CA	-5.46	1.39	1.46
1	3-A	229	VAL	N-CA	-5.46	1.39	1.46
8	1-Z	41	GLN	N-CA	-5.46	1.39	1.46
8	2-Z	41	GLN	N-CA	-5.46	1.39	1.46
8	3-Z	41	GLN	N-CA	-5.46	1.39	1.46
7	1-K	104	ILE	CA-C	-5.46	1.45	1.52
7	2-K	104	ILE	CA-C	-5.46	1.45	1.52
7	3-K	104	ILE	CA-C	-5.46	1.45	1.52
1	1-A	499	ASP	CA-C	-5.46	1.45	1.52
1	2-A	499	ASP	CA-C	-5.46	1.45	1.52
1	3-A	499	ASP	CA-C	-5.46	1.45	1.52
4	1-H	570	ASP	CA-C	-5.45	1.45	1.52
4	2-H	570	ASP	CA-C	-5.45	1.45	1.52
4	3-H	570	ASP	CA-C	-5.45	1.45	1.52
1	1-A	722	ILE	N-CA	-5.45	1.39	1.46
3	1-B	910	LEU	CA-C	-5.45	1.46	1.52
7	1-G	230	CYS	CA-C	-5.45	1.45	1.52
1	2-A	722	ILE	N-CA	-5.45	1.39	1.46
3	2-B	910	LEU	CA-C	-5.45	1.46	1.52
7	2-G	230	CYS	CA-C	-5.45	1.45	1.52
1	3-A	722	ILE	N-CA	-5.45	1.39	1.46
3	3-B	910	LEU	CA-C	-5.45	1.46	1.52
7	3-G	230	CYS	CA-C	-5.45	1.45	1.52
3	1-B	35	PRO	CA-C	5.45	1.57	1.52
4	1-C	756	PHE	CA-C	-5.45	1.45	1.52
7	1-K	133	ASP	CA-C	-5.45	1.45	1.52
3	2-B	35	PRO	CA-C	5.45	1.57	1.52
4	2-C	756	PHE	CA-C	-5.45	1.45	1.52
7	2-K	133	ASP	CA-C	-5.45	1.45	1.52
3	3-B	35	PRO	CA-C	5.45	1.57	1.52
4	3-C	756	PHE	CA-C	-5.45	1.45	1.52
7	3-K	133	ASP	CA-C	-5.45	1.45	1.52
4	1-C	640	ASP	CA-C	-5.45	1.46	1.52
4	2-C	640	ASP	CA-C	-5.45	1.46	1.52
4	3-C	640	ASP	CA-C	-5.45	1.46	1.52
8	1-Z	76	TYR	CA-C	-5.45	1.46	1.52
6	1-M	91	VAL	CA-C	-5.45	1.46	1.52
3	1-N	316	VAL	CA-C	-5.45	1.44	1.52
8	2-Z	76	TYR	CA-C	-5.45	1.46	1.52
6	2-M	91	VAL	CA-C	-5.45	1.46	1.52
3	2-N	316	VAL	CA-C	-5.45	1.44	1.52
8	3-Z	76	TYR	CA-C	-5.45	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	3-M	91	VAL	CA-C	-5.45	1.46	1.52
3	3-N	316	VAL	CA-C	-5.45	1.44	1.52
7	1-K	258	CYS	CA-C	-5.44	1.45	1.52
7	2-K	258	CYS	CA-C	-5.44	1.45	1.52
7	3-K	258	CYS	CA-C	-5.44	1.45	1.52
1	1-A	512	VAL	CA-C	-5.44	1.46	1.52
4	1-H	554	ILE	N-CA	-5.44	1.40	1.46
1	2-A	512	VAL	CA-C	-5.44	1.46	1.52
4	2-H	554	ILE	N-CA	-5.44	1.40	1.46
1	3-A	512	VAL	CA-C	-5.44	1.46	1.52
4	3-H	554	ILE	N-CA	-5.44	1.40	1.46
3	1-B	318	ASP	N-CA	-5.44	1.39	1.46
4	1-C	400	SER	CA-C	-5.44	1.45	1.52
7	1-K	166	LEU	C-O	-5.44	1.17	1.24
3	2-B	318	ASP	N-CA	-5.44	1.39	1.46
4	2-C	400	SER	CA-C	-5.44	1.45	1.52
7	2-K	166	LEU	C-O	-5.44	1.17	1.24
3	3-B	318	ASP	N-CA	-5.44	1.39	1.46
4	3-C	400	SER	CA-C	-5.44	1.45	1.52
7	3-K	166	LEU	C-O	-5.44	1.17	1.24
3	1-B	356	LEU	CA-C	-5.44	1.45	1.52
7	1-G	365	SER	CA-C	-5.44	1.45	1.52
3	2-B	356	LEU	CA-C	-5.44	1.45	1.52
7	2-G	365	SER	CA-C	-5.44	1.45	1.52
3	3-B	356	LEU	CA-C	-5.44	1.45	1.52
7	3-G	365	SER	CA-C	-5.44	1.45	1.52
3	1-B	796	ASP	CA-C	-5.44	1.46	1.52
3	2-B	796	ASP	CA-C	-5.44	1.46	1.52
3	3-B	796	ASP	CA-C	-5.44	1.46	1.52
4	1-H	436	GLY	CA-C	-5.44	1.45	1.52
4	2-H	436	GLY	CA-C	-5.44	1.45	1.52
4	3-H	436	GLY	CA-C	-5.44	1.45	1.52
3	1-B	333	LEU	CA-C	-5.43	1.45	1.52
3	2-B	333	LEU	CA-C	-5.43	1.45	1.52
3	3-B	333	LEU	CA-C	-5.43	1.45	1.52
3	1-B	126	HIS	C-N	-5.43	1.25	1.33
3	2-B	126	HIS	C-N	-5.43	1.25	1.33
3	3-B	126	HIS	C-N	-5.43	1.25	1.33
3	1-B	852	ASP	N-CA	-5.43	1.39	1.46
3	2-B	852	ASP	N-CA	-5.43	1.39	1.46
3	3-B	852	ASP	N-CA	-5.43	1.39	1.46
1	1-A	651	LEU	CA-C	-5.43	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	369	GLU	C-N	-5.43	1.26	1.33
7	1-K	771	ASN	N-CA	-5.43	1.39	1.46
4	1-H	537	THR	CA-C	-5.43	1.45	1.52
1	2-A	651	LEU	CA-C	-5.43	1.45	1.52
3	2-B	369	GLU	C-N	-5.43	1.26	1.33
7	2-K	771	ASN	N-CA	-5.43	1.39	1.46
4	2-H	537	THR	CA-C	-5.43	1.45	1.52
1	3-A	651	LEU	CA-C	-5.43	1.45	1.52
3	3-B	369	GLU	C-N	-5.43	1.26	1.33
7	3-K	771	ASN	N-CA	-5.43	1.39	1.46
4	3-H	537	THR	CA-C	-5.43	1.45	1.52
6	1-J	29	GLY	N-CA	-5.43	1.37	1.45
6	1-J	65	VAL	N-CA	-5.43	1.39	1.46
6	2-J	29	GLY	N-CA	-5.43	1.37	1.45
6	2-J	65	VAL	N-CA	-5.43	1.39	1.46
6	3-J	29	GLY	N-CA	-5.43	1.37	1.45
6	3-J	65	VAL	N-CA	-5.43	1.39	1.46
3	1-B	97	TRP	CA-C	-5.43	1.45	1.52
4	1-C	323	GLN	CA-C	-5.43	1.46	1.52
8	1-Z	122	PHE	N-CA	-5.43	1.40	1.46
3	1-N	476	ILE	CA-C	-5.43	1.45	1.52
3	2-B	97	TRP	CA-C	-5.43	1.45	1.52
4	2-C	323	GLN	CA-C	-5.43	1.46	1.52
8	2-Z	122	PHE	N-CA	-5.43	1.40	1.46
3	2-N	476	ILE	CA-C	-5.43	1.45	1.52
3	3-B	97	TRP	CA-C	-5.43	1.45	1.52
4	3-C	323	GLN	CA-C	-5.43	1.46	1.52
8	3-Z	122	PHE	N-CA	-5.43	1.40	1.46
3	3-N	476	ILE	CA-C	-5.43	1.45	1.52
3	1-B	192	ILE	CA-C	-5.42	1.46	1.52
4	1-C	554	ILE	N-CA	-5.42	1.40	1.46
7	1-K	250	PRO	CA-C	-5.42	1.44	1.52
3	1-N	274	ALA	CA-C	-5.42	1.45	1.52
3	1-N	276	LYS	N-CA	-5.42	1.39	1.46
3	2-B	192	ILE	CA-C	-5.42	1.46	1.52
4	2-C	554	ILE	N-CA	-5.42	1.40	1.46
7	2-K	250	PRO	CA-C	-5.42	1.44	1.52
3	2-N	274	ALA	CA-C	-5.42	1.45	1.52
3	2-N	276	LYS	N-CA	-5.42	1.39	1.46
3	3-B	192	ILE	CA-C	-5.42	1.46	1.52
4	3-C	554	ILE	N-CA	-5.42	1.40	1.46
7	3-K	250	PRO	CA-C	-5.42	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-N	274	ALA	CA-C	-5.42	1.45	1.52
3	3-N	276	LYS	N-CA	-5.42	1.39	1.46
4	1-C	181	LEU	N-CA	-5.42	1.39	1.45
7	1-K	180	GLU	CA-C	-5.42	1.45	1.52
3	1-N	287	SER	CA-C	-5.42	1.45	1.52
4	2-C	181	LEU	N-CA	-5.42	1.39	1.45
7	2-K	180	GLU	CA-C	-5.42	1.45	1.52
3	2-N	287	SER	CA-C	-5.42	1.45	1.52
4	3-C	181	LEU	N-CA	-5.42	1.39	1.45
7	3-K	180	GLU	CA-C	-5.42	1.45	1.52
3	3-N	287	SER	CA-C	-5.42	1.45	1.52
4	1-C	478	CYS	N-CA	-5.42	1.39	1.46
4	2-C	478	CYS	N-CA	-5.42	1.39	1.46
4	3-C	478	CYS	N-CA	-5.42	1.39	1.46
3	1-B	359	ALA	N-CA	-5.42	1.39	1.46
4	1-H	27	GLU	CA-C	-5.42	1.46	1.52
4	1-H	323	GLN	CA-C	-5.42	1.46	1.52
3	2-B	359	ALA	N-CA	-5.42	1.39	1.46
4	2-H	27	GLU	CA-C	-5.42	1.46	1.52
4	2-H	323	GLN	CA-C	-5.42	1.46	1.52
3	3-B	359	ALA	N-CA	-5.42	1.39	1.46
4	3-H	27	GLU	CA-C	-5.42	1.46	1.52
4	3-H	323	GLN	CA-C	-5.42	1.46	1.52
1	1-A	598	LYS	N-CA	-5.41	1.39	1.46
4	1-C	143	HIS	N-CA	-5.41	1.40	1.46
4	1-C	607	ASP	CA-C	-5.41	1.45	1.52
7	1-K	691	SER	C-N	5.41	1.40	1.33
8	1-L	15	ALA	CA-C	-5.41	1.46	1.52
5	1-I	3	LEU	CA-C	-5.41	1.46	1.52
1	2-A	598	LYS	N-CA	-5.41	1.39	1.46
4	2-C	143	HIS	N-CA	-5.41	1.40	1.46
4	2-C	607	ASP	CA-C	-5.41	1.45	1.52
7	2-K	691	SER	C-N	5.41	1.40	1.33
8	2-L	15	ALA	CA-C	-5.41	1.46	1.52
5	2-I	3	LEU	CA-C	-5.41	1.46	1.52
1	3-A	598	LYS	N-CA	-5.41	1.39	1.46
4	3-C	143	HIS	N-CA	-5.41	1.40	1.46
4	3-C	607	ASP	CA-C	-5.41	1.45	1.52
7	3-K	691	SER	C-N	5.41	1.40	1.33
8	3-L	15	ALA	CA-C	-5.41	1.46	1.52
5	3-I	3	LEU	CA-C	-5.41	1.46	1.52
3	1-B	350	GLU	N-CA	-5.41	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	350	GLU	N-CA	-5.41	1.39	1.46
3	3-B	350	GLU	N-CA	-5.41	1.39	1.46
3	1-N	340	ILE	CA-C	-5.41	1.46	1.52
3	2-N	340	ILE	CA-C	-5.41	1.46	1.52
3	3-N	340	ILE	CA-C	-5.41	1.46	1.52
4	1-H	522	GLU	CA-C	-5.41	1.46	1.52
4	2-H	522	GLU	CA-C	-5.41	1.46	1.52
4	3-H	522	GLU	CA-C	-5.41	1.46	1.52
3	1-B	276	LYS	N-CA	-5.41	1.39	1.46
3	1-N	421	MET	CA-C	-5.41	1.45	1.52
3	2-B	276	LYS	N-CA	-5.41	1.39	1.46
3	2-N	421	MET	CA-C	-5.41	1.45	1.52
3	3-B	276	LYS	N-CA	-5.41	1.39	1.46
3	3-N	421	MET	CA-C	-5.41	1.45	1.52
6	1-F	65	VAL	N-CA	-5.41	1.39	1.46
8	1-L	123	LEU	N-CA	-5.41	1.39	1.46
6	2-F	65	VAL	N-CA	-5.41	1.39	1.46
8	2-L	123	LEU	N-CA	-5.41	1.39	1.46
6	3-F	65	VAL	N-CA	-5.41	1.39	1.46
8	3-L	123	LEU	N-CA	-5.41	1.39	1.46
7	1-G	68	GLU	CA-C	-5.40	1.45	1.52
8	1-L	28	ALA	N-CA	-5.40	1.39	1.46
7	2-G	68	GLU	CA-C	-5.40	1.45	1.52
8	2-L	28	ALA	N-CA	-5.40	1.39	1.46
7	3-G	68	GLU	CA-C	-5.40	1.45	1.52
8	3-L	28	ALA	N-CA	-5.40	1.39	1.46
3	1-B	449	LEU	CA-C	-5.40	1.45	1.52
5	1-I	114	ASP	CA-C	-5.40	1.45	1.52
3	2-B	449	LEU	CA-C	-5.40	1.45	1.52
5	2-I	114	ASP	CA-C	-5.40	1.45	1.52
3	3-B	449	LEU	CA-C	-5.40	1.45	1.52
5	3-I	114	ASP	CA-C	-5.40	1.45	1.52
8	1-Z	91	MET	N-CA	-5.40	1.39	1.46
8	2-Z	91	MET	N-CA	-5.40	1.39	1.46
8	3-Z	91	MET	N-CA	-5.40	1.39	1.46
8	1-L	120	GLY	CA-C	-5.39	1.46	1.52
8	2-L	120	GLY	CA-C	-5.39	1.46	1.52
8	3-L	120	GLY	CA-C	-5.39	1.46	1.52
4	1-C	27	GLU	CA-C	-5.39	1.46	1.52
4	2-C	27	GLU	CA-C	-5.39	1.46	1.52
4	3-C	27	GLU	CA-C	-5.39	1.46	1.52
3	1-B	77	ILE	N-CA	-5.39	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	77	ILE	N-CA	-5.39	1.40	1.46
3	3-B	77	ILE	N-CA	-5.39	1.40	1.46
3	1-B	922	ALA	CA-C	-5.39	1.46	1.52
7	1-K	751	TYR	N-CA	-5.39	1.39	1.46
3	1-N	97	TRP	CA-C	-5.39	1.45	1.52
4	1-H	483	GLU	CA-C	-5.39	1.45	1.52
3	2-B	922	ALA	CA-C	-5.39	1.46	1.52
7	2-K	751	TYR	N-CA	-5.39	1.39	1.46
3	2-N	97	TRP	CA-C	-5.39	1.45	1.52
4	2-H	483	GLU	CA-C	-5.39	1.45	1.52
3	3-B	922	ALA	CA-C	-5.39	1.46	1.52
7	3-K	751	TYR	N-CA	-5.39	1.39	1.46
3	3-N	97	TRP	CA-C	-5.39	1.45	1.52
4	3-H	483	GLU	CA-C	-5.39	1.45	1.52
3	1-B	810	GLU	N-CA	-5.39	1.38	1.46
4	1-C	176	SER	N-CA	-5.39	1.41	1.46
4	1-C	483	GLU	CA-C	-5.39	1.45	1.52
3	2-B	810	GLU	N-CA	-5.39	1.38	1.46
4	2-C	176	SER	N-CA	-5.39	1.41	1.46
4	2-C	483	GLU	CA-C	-5.39	1.45	1.52
3	3-B	810	GLU	N-CA	-5.39	1.38	1.46
4	3-C	176	SER	N-CA	-5.39	1.41	1.46
4	3-C	483	GLU	CA-C	-5.39	1.45	1.52
4	1-C	505	VAL	CA-C	-5.38	1.46	1.52
4	1-H	143	HIS	N-CA	-5.38	1.40	1.46
4	2-C	505	VAL	CA-C	-5.38	1.46	1.52
4	2-H	143	HIS	N-CA	-5.38	1.40	1.46
4	3-C	505	VAL	CA-C	-5.38	1.46	1.52
4	3-H	143	HIS	N-CA	-5.38	1.40	1.46
7	1-G	647	VAL	CA-C	-5.38	1.46	1.52
8	1-L	114	LEU	N-CA	-5.38	1.40	1.46
7	2-G	647	VAL	CA-C	-5.38	1.46	1.52
8	2-L	114	LEU	N-CA	-5.38	1.40	1.46
7	3-G	647	VAL	CA-C	-5.38	1.46	1.52
8	3-L	114	LEU	N-CA	-5.38	1.40	1.46
4	1-C	734	LEU	CA-C	-5.38	1.45	1.52
4	1-H	459	ARG	N-CA	-5.38	1.39	1.46
6	1-J	77	LEU	N-CA	-5.38	1.39	1.46
4	2-C	734	LEU	CA-C	-5.38	1.45	1.52
4	2-H	459	ARG	N-CA	-5.38	1.39	1.46
6	2-J	77	LEU	N-CA	-5.38	1.39	1.46
4	3-C	734	LEU	CA-C	-5.38	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-H	459	ARG	N-CA	-5.38	1.39	1.46
6	3-J	77	LEU	N-CA	-5.38	1.39	1.46
7	1-G	520	ASP	CA-C	-5.38	1.45	1.52
4	1-H	70	ASN	CA-C	-5.38	1.46	1.52
7	2-G	520	ASP	CA-C	-5.38	1.45	1.52
4	2-H	70	ASN	CA-C	-5.38	1.46	1.52
7	3-G	520	ASP	CA-C	-5.38	1.45	1.52
4	3-H	70	ASN	CA-C	-5.38	1.46	1.52
3	1-B	326	HIS	CA-C	-5.38	1.46	1.52
3	1-N	126	HIS	C-N	-5.38	1.25	1.33
3	1-N	305	ILE	CA-C	-5.38	1.45	1.52
4	1-H	640	ASP	CA-C	-5.38	1.46	1.52
3	2-B	326	HIS	CA-C	-5.38	1.46	1.52
3	2-N	126	HIS	C-N	-5.38	1.25	1.33
3	2-N	305	ILE	CA-C	-5.38	1.45	1.52
4	2-H	640	ASP	CA-C	-5.38	1.46	1.52
3	3-B	326	HIS	CA-C	-5.38	1.46	1.52
3	3-N	126	HIS	C-N	-5.38	1.25	1.33
3	3-N	305	ILE	CA-C	-5.38	1.45	1.52
4	3-H	640	ASP	CA-C	-5.38	1.46	1.52
7	1-K	859	ARG	CA-C	-5.38	1.46	1.52
7	2-K	859	ARG	CA-C	-5.38	1.46	1.52
7	3-K	859	ARG	CA-C	-5.38	1.46	1.52
1	1-A	428	VAL	CA-C	-5.37	1.46	1.52
4	1-H	337	ASP	CA-C	-5.37	1.45	1.52
1	2-A	428	VAL	CA-C	-5.37	1.46	1.52
4	2-H	337	ASP	CA-C	-5.37	1.45	1.52
1	3-A	428	VAL	CA-C	-5.37	1.46	1.52
4	3-H	337	ASP	CA-C	-5.37	1.45	1.52
1	1-A	444	ILE	CA-C	-5.37	1.47	1.53
1	1-A	677	LEU	CA-C	-5.37	1.45	1.52
5	1-D	114	ASP	CA-C	-5.37	1.45	1.52
7	1-G	262	LYS	CA-C	-5.37	1.45	1.52
8	1-Z	24	ASP	N-CA	-5.37	1.38	1.45
7	1-K	169	CYS	N-CA	-5.37	1.40	1.46
3	1-N	74	LEU	CA-C	-5.37	1.45	1.52
5	1-I	58	TYR	CA-C	-5.37	1.46	1.52
1	2-A	444	ILE	CA-C	-5.37	1.47	1.53
1	2-A	677	LEU	CA-C	-5.37	1.45	1.52
5	2-D	114	ASP	CA-C	-5.37	1.45	1.52
7	2-G	262	LYS	CA-C	-5.37	1.45	1.52
8	2-Z	24	ASP	N-CA	-5.37	1.38	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-K	169	CYS	N-CA	-5.37	1.40	1.46
3	2-N	74	LEU	CA-C	-5.37	1.45	1.52
5	2-I	58	TYR	CA-C	-5.37	1.46	1.52
1	3-A	444	ILE	CA-C	-5.37	1.47	1.53
1	3-A	677	LEU	CA-C	-5.37	1.45	1.52
5	3-D	114	ASP	CA-C	-5.37	1.45	1.52
7	3-G	262	LYS	CA-C	-5.37	1.45	1.52
8	3-Z	24	ASP	N-CA	-5.37	1.38	1.45
7	3-K	169	CYS	N-CA	-5.37	1.40	1.46
3	3-N	74	LEU	CA-C	-5.37	1.45	1.52
5	3-I	58	TYR	CA-C	-5.37	1.46	1.52
3	1-N	77	ILE	N-CA	-5.37	1.40	1.46
3	2-N	77	ILE	N-CA	-5.37	1.40	1.46
3	3-N	77	ILE	N-CA	-5.37	1.40	1.46
3	1-B	305	ILE	CA-C	-5.37	1.45	1.52
4	1-C	218	ASN	CA-C	-5.37	1.46	1.52
7	1-G	848	LEU	CA-C	-5.37	1.46	1.52
8	1-Z	128	ILE	CA-C	-5.37	1.46	1.52
3	2-B	305	ILE	CA-C	-5.37	1.45	1.52
4	2-C	218	ASN	CA-C	-5.37	1.46	1.52
7	2-G	848	LEU	CA-C	-5.37	1.46	1.52
8	2-Z	128	ILE	CA-C	-5.37	1.46	1.52
3	3-B	305	ILE	CA-C	-5.37	1.45	1.52
4	3-C	218	ASN	CA-C	-5.37	1.46	1.52
7	3-G	848	LEU	CA-C	-5.37	1.46	1.52
8	3-Z	128	ILE	CA-C	-5.37	1.46	1.52
7	1-G	478	ASN	CA-C	-5.37	1.45	1.52
8	1-Z	78	TYR	CA-C	-5.37	1.46	1.52
4	1-H	122	LEU	CA-C	-5.37	1.46	1.52
7	2-G	478	ASN	CA-C	-5.37	1.45	1.52
8	2-Z	78	TYR	CA-C	-5.37	1.46	1.52
4	2-H	122	LEU	CA-C	-5.37	1.46	1.52
7	3-G	478	ASN	CA-C	-5.37	1.45	1.52
8	3-Z	78	TYR	CA-C	-5.37	1.46	1.52
4	3-H	122	LEU	CA-C	-5.37	1.46	1.52
7	1-G	68	GLU	N-CA	-5.37	1.39	1.46
4	1-H	237	PHE	CA-C	-5.37	1.46	1.52
5	1-I	149	GLU	N-CA	-5.37	1.40	1.46
7	2-G	68	GLU	N-CA	-5.37	1.39	1.46
4	2-H	237	PHE	CA-C	-5.37	1.46	1.52
5	2-I	149	GLU	N-CA	-5.37	1.40	1.46
7	3-G	68	GLU	N-CA	-5.37	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-H	237	PHE	CA-C	-5.37	1.46	1.52
5	3-I	149	GLU	N-CA	-5.37	1.40	1.46
4	1-C	662	VAL	CA-C	-5.36	1.46	1.52
8	1-Z	127	GLU	N-CA	-5.36	1.39	1.46
7	1-K	90	LEU	N-CA	-5.36	1.40	1.46
4	2-C	662	VAL	CA-C	-5.36	1.46	1.52
8	2-Z	127	GLU	N-CA	-5.36	1.39	1.46
7	2-K	90	LEU	N-CA	-5.36	1.40	1.46
4	3-C	662	VAL	CA-C	-5.36	1.46	1.52
8	3-Z	127	GLU	N-CA	-5.36	1.39	1.46
7	3-K	90	LEU	N-CA	-5.36	1.40	1.46
7	1-K	848	LEU	CA-C	-5.36	1.46	1.52
7	2-K	848	LEU	CA-C	-5.36	1.46	1.52
7	3-K	848	LEU	CA-C	-5.36	1.46	1.52
4	1-C	122	LEU	CA-C	-5.36	1.46	1.52
7	1-G	859	ARG	CA-C	-5.36	1.46	1.52
4	2-C	122	LEU	CA-C	-5.36	1.46	1.52
7	2-G	859	ARG	CA-C	-5.36	1.46	1.52
4	3-C	122	LEU	CA-C	-5.36	1.46	1.52
7	3-G	859	ARG	CA-C	-5.36	1.46	1.52
1	1-A	255	ALA	N-CA	-5.36	1.40	1.46
3	1-B	819	VAL	N-CA	-5.36	1.39	1.46
7	1-G	771	ASN	N-CA	-5.36	1.40	1.46
7	1-K	148	ILE	N-CA	-5.36	1.40	1.46
4	1-H	478	CYS	N-CA	-5.36	1.39	1.46
1	2-A	255	ALA	N-CA	-5.36	1.40	1.46
3	2-B	819	VAL	N-CA	-5.36	1.39	1.46
7	2-G	771	ASN	N-CA	-5.36	1.40	1.46
7	2-K	148	ILE	N-CA	-5.36	1.40	1.46
4	2-H	478	CYS	N-CA	-5.36	1.39	1.46
1	3-A	255	ALA	N-CA	-5.36	1.40	1.46
3	3-B	819	VAL	N-CA	-5.36	1.39	1.46
7	3-G	771	ASN	N-CA	-5.36	1.40	1.46
7	3-K	148	ILE	N-CA	-5.36	1.40	1.46
4	3-H	478	CYS	N-CA	-5.36	1.39	1.46
7	1-G	293	GLN	CA-C	-5.36	1.46	1.52
7	2-G	293	GLN	CA-C	-5.36	1.46	1.52
7	3-G	293	GLN	CA-C	-5.36	1.46	1.52
3	1-B	316	VAL	CA-C	-5.36	1.45	1.52
7	1-G	772	PHE	CA-C	-5.36	1.46	1.52
3	2-B	316	VAL	CA-C	-5.36	1.45	1.52
7	2-G	772	PHE	CA-C	-5.36	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	316	VAL	CA-C	-5.36	1.45	1.52
7	3-G	772	PHE	CA-C	-5.36	1.46	1.52
4	1-C	761	TYR	N-CA	-5.35	1.40	1.46
4	2-C	761	TYR	N-CA	-5.35	1.40	1.46
4	3-C	761	TYR	N-CA	-5.35	1.40	1.46
1	1-A	669	ASP	N-CA	-5.35	1.39	1.46
3	1-B	311	ASN	CA-C	-5.35	1.45	1.52
3	1-B	340	ILE	CA-C	-5.35	1.46	1.52
4	1-C	90	GLU	CA-C	-5.35	1.46	1.52
4	1-H	662	VAL	CA-C	-5.35	1.46	1.52
1	2-A	669	ASP	N-CA	-5.35	1.39	1.46
3	2-B	311	ASN	CA-C	-5.35	1.45	1.52
3	2-B	340	ILE	CA-C	-5.35	1.46	1.52
4	2-C	90	GLU	CA-C	-5.35	1.46	1.52
4	2-H	662	VAL	CA-C	-5.35	1.46	1.52
1	3-A	669	ASP	N-CA	-5.35	1.39	1.46
3	3-B	311	ASN	CA-C	-5.35	1.45	1.52
3	3-B	340	ILE	CA-C	-5.35	1.46	1.52
4	3-C	90	GLU	CA-C	-5.35	1.46	1.52
4	3-H	662	VAL	CA-C	-5.35	1.46	1.52
4	1-C	424	PHE	N-CA	-5.35	1.39	1.46
5	1-D	149	GLU	N-CA	-5.35	1.40	1.46
8	1-L	25	ARG	CA-C	-5.35	1.46	1.52
3	1-N	311	ASN	CA-C	-5.35	1.45	1.52
4	2-C	424	PHE	N-CA	-5.35	1.39	1.46
5	2-D	149	GLU	N-CA	-5.35	1.40	1.46
8	2-L	25	ARG	CA-C	-5.35	1.46	1.52
3	2-N	311	ASN	CA-C	-5.35	1.45	1.52
4	3-C	424	PHE	N-CA	-5.35	1.39	1.46
5	3-D	149	GLU	N-CA	-5.35	1.40	1.46
8	3-L	25	ARG	CA-C	-5.35	1.46	1.52
3	3-N	311	ASN	CA-C	-5.35	1.45	1.52
4	1-C	70	ASN	CA-C	-5.35	1.46	1.52
4	2-C	70	ASN	CA-C	-5.35	1.46	1.52
4	3-C	70	ASN	CA-C	-5.35	1.46	1.52
1	1-A	267	ASN	CA-C	-5.34	1.46	1.52
3	1-B	317	LEU	C-N	-5.34	1.26	1.34
3	1-N	369	GLU	C-N	-5.34	1.26	1.33
3	1-N	449	LEU	CA-C	-5.34	1.45	1.52
3	1-N	454	VAL	N-CA	-5.34	1.40	1.46
4	1-H	83	VAL	CA-C	-5.34	1.46	1.52
1	2-A	267	ASN	CA-C	-5.34	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	317	LEU	C-N	-5.34	1.26	1.34
3	2-N	369	GLU	C-N	-5.34	1.26	1.33
3	2-N	449	LEU	CA-C	-5.34	1.45	1.52
3	2-N	454	VAL	N-CA	-5.34	1.40	1.46
4	2-H	83	VAL	CA-C	-5.34	1.46	1.52
1	3-A	267	ASN	CA-C	-5.34	1.46	1.52
3	3-B	317	LEU	C-N	-5.34	1.26	1.34
3	3-N	369	GLU	C-N	-5.34	1.26	1.33
3	3-N	449	LEU	CA-C	-5.34	1.45	1.52
3	3-N	454	VAL	N-CA	-5.34	1.40	1.46
4	3-H	83	VAL	CA-C	-5.34	1.46	1.52
7	1-G	800	ALA	CA-C	-5.34	1.45	1.52
7	2-G	800	ALA	CA-C	-5.34	1.45	1.52
7	3-G	800	ALA	CA-C	-5.34	1.45	1.52
4	1-H	181	LEU	N-CA	-5.34	1.39	1.45
4	2-H	181	LEU	N-CA	-5.34	1.39	1.45
4	3-H	181	LEU	N-CA	-5.34	1.39	1.45
3	1-B	130	PHE	CA-C	-5.34	1.45	1.52
7	1-K	305	TYR	CA-C	-5.34	1.46	1.52
4	1-H	143	HIS	CA-C	-5.34	1.46	1.52
3	2-B	130	PHE	CA-C	-5.34	1.45	1.52
7	2-K	305	TYR	CA-C	-5.34	1.46	1.52
4	2-H	143	HIS	CA-C	-5.34	1.46	1.52
3	3-B	130	PHE	CA-C	-5.34	1.45	1.52
7	3-K	305	TYR	CA-C	-5.34	1.46	1.52
4	3-H	143	HIS	CA-C	-5.34	1.46	1.52
3	1-N	35	PRO	CA-C	5.34	1.57	1.52
3	2-N	35	PRO	CA-C	5.34	1.57	1.52
3	3-N	35	PRO	CA-C	5.34	1.57	1.52
5	1-D	3	LEU	CA-C	-5.34	1.46	1.52
4	1-H	90	GLU	CA-C	-5.34	1.46	1.52
5	2-D	3	LEU	CA-C	-5.34	1.46	1.52
4	2-H	90	GLU	CA-C	-5.34	1.46	1.52
5	3-D	3	LEU	CA-C	-5.34	1.46	1.52
4	3-H	90	GLU	CA-C	-5.34	1.46	1.52
4	1-C	773	TRP	CA-C	-5.33	1.46	1.52
4	2-C	773	TRP	CA-C	-5.33	1.46	1.52
4	3-C	773	TRP	CA-C	-5.33	1.46	1.52
1	1-A	689	ILE	N-CA	-5.33	1.40	1.46
3	1-B	74	LEU	CA-C	-5.33	1.45	1.52
3	1-B	755	VAL	CA-C	-5.33	1.46	1.52
1	2-A	689	ILE	N-CA	-5.33	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	74	LEU	CA-C	-5.33	1.45	1.52
3	2-B	755	VAL	CA-C	-5.33	1.46	1.52
1	3-A	689	ILE	N-CA	-5.33	1.40	1.46
3	3-B	74	LEU	CA-C	-5.33	1.45	1.52
3	3-B	755	VAL	CA-C	-5.33	1.46	1.52
1	1-A	107	TRP	C-N	5.33	1.41	1.33
7	1-G	137	LEU	CA-C	-5.33	1.45	1.52
1	2-A	107	TRP	C-N	5.33	1.41	1.33
7	2-G	137	LEU	CA-C	-5.33	1.45	1.52
1	3-A	107	TRP	C-N	5.33	1.41	1.33
7	3-G	137	LEU	CA-C	-5.33	1.45	1.52
1	1-A	626	ILE	N-CA	-5.33	1.39	1.46
3	1-N	151	LEU	N-CA	-5.33	1.39	1.46
4	1-H	376	ILE	CA-C	-5.33	1.46	1.52
4	1-H	647	LEU	CA-C	-5.33	1.45	1.52
5	1-I	163	ALA	CA-C	-5.33	1.46	1.52
1	2-A	626	ILE	N-CA	-5.33	1.39	1.46
3	2-N	151	LEU	N-CA	-5.33	1.39	1.46
4	2-H	376	ILE	CA-C	-5.33	1.46	1.52
4	2-H	647	LEU	CA-C	-5.33	1.45	1.52
5	2-I	163	ALA	CA-C	-5.33	1.46	1.52
1	3-A	626	ILE	N-CA	-5.33	1.39	1.46
3	3-N	151	LEU	N-CA	-5.33	1.39	1.46
4	3-H	376	ILE	CA-C	-5.33	1.46	1.52
4	3-H	647	LEU	CA-C	-5.33	1.45	1.52
5	3-I	163	ALA	CA-C	-5.33	1.46	1.52
7	1-K	198	GLY	CA-C	-5.33	1.46	1.52
7	1-K	295	PHE	CA-C	-5.33	1.45	1.52
7	2-K	198	GLY	CA-C	-5.33	1.46	1.52
7	2-K	295	PHE	CA-C	-5.33	1.45	1.52
7	3-K	198	GLY	CA-C	-5.33	1.46	1.52
7	3-K	295	PHE	CA-C	-5.33	1.45	1.52
7	1-G	212	SER	CA-C	-5.33	1.46	1.52
7	2-G	212	SER	CA-C	-5.33	1.46	1.52
7	3-G	212	SER	CA-C	-5.33	1.46	1.52
4	1-C	642	GLU	N-CA	-5.32	1.40	1.46
4	1-C	781	ASN	CA-C	-5.32	1.45	1.52
7	1-G	723	THR	CA-C	-5.32	1.46	1.52
7	1-K	800	ALA	CA-C	-5.32	1.45	1.52
4	2-C	642	GLU	N-CA	-5.32	1.40	1.46
4	2-C	781	ASN	CA-C	-5.32	1.45	1.52
7	2-G	723	THR	CA-C	-5.32	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-K	800	ALA	CA-C	-5.32	1.45	1.52
4	3-C	642	GLU	N-CA	-5.32	1.40	1.46
4	3-C	781	ASN	CA-C	-5.32	1.45	1.52
7	3-G	723	THR	CA-C	-5.32	1.46	1.52
7	3-K	800	ALA	CA-C	-5.32	1.45	1.52
3	1-B	454	VAL	N-CA	-5.32	1.40	1.46
3	2-B	454	VAL	N-CA	-5.32	1.40	1.46
3	3-B	454	VAL	N-CA	-5.32	1.40	1.46
4	1-C	237	PHE	CA-C	-5.32	1.46	1.52
4	2-C	237	PHE	CA-C	-5.32	1.46	1.52
4	3-C	237	PHE	CA-C	-5.32	1.46	1.52
3	1-B	193	HIS	N-CA	-5.32	1.40	1.46
7	1-G	532	LEU	CA-C	-5.32	1.46	1.52
7	1-K	856	VAL	CA-C	-5.32	1.46	1.52
3	2-B	193	HIS	N-CA	-5.32	1.40	1.46
7	2-G	532	LEU	CA-C	-5.32	1.46	1.52
7	2-K	856	VAL	CA-C	-5.32	1.46	1.52
3	3-B	193	HIS	N-CA	-5.32	1.40	1.46
7	3-G	532	LEU	CA-C	-5.32	1.46	1.52
7	3-K	856	VAL	CA-C	-5.32	1.46	1.52
1	1-A	133	GLY	CA-C	-5.32	1.44	1.51
4	1-C	57	ASP	CA-C	-5.32	1.46	1.52
1	2-A	133	GLY	CA-C	-5.32	1.44	1.51
4	2-C	57	ASP	CA-C	-5.32	1.46	1.52
1	3-A	133	GLY	CA-C	-5.32	1.44	1.51
4	3-C	57	ASP	CA-C	-5.32	1.46	1.52
4	1-C	459	ARG	N-CA	-5.31	1.39	1.46
5	1-D	7	ALA	CA-C	-5.31	1.46	1.52
4	2-C	459	ARG	N-CA	-5.31	1.39	1.46
5	2-D	7	ALA	CA-C	-5.31	1.46	1.52
4	3-C	459	ARG	N-CA	-5.31	1.39	1.46
5	3-D	7	ALA	CA-C	-5.31	1.46	1.52
3	1-B	381	LYS	CA-C	-5.31	1.45	1.52
4	1-C	143	HIS	CA-C	-5.31	1.46	1.52
4	1-C	337	ASP	CA-C	-5.31	1.45	1.52
6	1-R	116	LEU	CA-C	-5.31	1.45	1.52
4	1-H	642	GLU	N-CA	-5.31	1.40	1.46
3	2-B	381	LYS	CA-C	-5.31	1.45	1.52
4	2-C	143	HIS	CA-C	-5.31	1.46	1.52
4	2-C	337	ASP	CA-C	-5.31	1.45	1.52
6	2-R	116	LEU	CA-C	-5.31	1.45	1.52
4	2-H	642	GLU	N-CA	-5.31	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	381	LYS	CA-C	-5.31	1.45	1.52
4	3-C	143	HIS	CA-C	-5.31	1.46	1.52
4	3-C	337	ASP	CA-C	-5.31	1.45	1.52
6	3-R	116	LEU	CA-C	-5.31	1.45	1.52
4	3-H	642	GLU	N-CA	-5.31	1.40	1.46
5	1-D	58	TYR	CA-C	-5.31	1.46	1.52
5	2-D	58	TYR	CA-C	-5.31	1.46	1.52
5	3-D	58	TYR	CA-C	-5.31	1.46	1.52
3	1-B	800	ILE	N-CA	-5.30	1.40	1.46
4	1-C	213	ILE	N-CA	-5.30	1.40	1.46
6	1-M	26	ASP	CA-C	-5.30	1.46	1.52
4	1-H	424	PHE	N-CA	-5.30	1.39	1.46
4	1-H	632	GLN	CA-C	-5.30	1.46	1.52
3	2-B	800	ILE	N-CA	-5.30	1.40	1.46
4	2-C	213	ILE	N-CA	-5.30	1.40	1.46
6	2-M	26	ASP	CA-C	-5.30	1.46	1.52
4	2-H	424	PHE	N-CA	-5.30	1.39	1.46
4	2-H	632	GLN	CA-C	-5.30	1.46	1.52
3	3-B	800	ILE	N-CA	-5.30	1.40	1.46
4	3-C	213	ILE	N-CA	-5.30	1.40	1.46
6	3-M	26	ASP	CA-C	-5.30	1.46	1.52
4	3-H	424	PHE	N-CA	-5.30	1.39	1.46
4	3-H	632	GLN	CA-C	-5.30	1.46	1.52
4	1-C	262	ARG	N-CA	-5.30	1.39	1.45
4	2-C	262	ARG	N-CA	-5.30	1.39	1.45
4	3-C	262	ARG	N-CA	-5.30	1.39	1.45
6	1-F	77	LEU	N-CA	-5.30	1.39	1.46
6	1-R	119	ALA	CA-C	-5.30	1.46	1.52
6	2-F	77	LEU	N-CA	-5.30	1.39	1.46
6	2-R	119	ALA	CA-C	-5.30	1.46	1.52
6	3-F	77	LEU	N-CA	-5.30	1.39	1.46
6	3-R	119	ALA	CA-C	-5.30	1.46	1.52
3	1-N	381	LYS	CA-C	-5.30	1.45	1.52
3	2-N	381	LYS	CA-C	-5.30	1.45	1.52
3	3-N	381	LYS	CA-C	-5.30	1.45	1.52
7	1-G	480	VAL	N-CA	-5.30	1.40	1.46
7	1-K	683	PRO	CA-C	5.30	1.58	1.52
6	1-M	53	VAL	CA-C	-5.30	1.46	1.52
4	1-H	262	ARG	N-CA	-5.30	1.39	1.45
7	2-G	480	VAL	N-CA	-5.30	1.40	1.46
7	2-K	683	PRO	CA-C	5.30	1.58	1.52
6	2-M	53	VAL	CA-C	-5.30	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-H	262	ARG	N-CA	-5.30	1.39	1.45
7	3-G	480	VAL	N-CA	-5.30	1.40	1.46
7	3-K	683	PRO	CA-C	5.30	1.58	1.52
6	3-M	53	VAL	CA-C	-5.30	1.46	1.52
4	3-H	262	ARG	N-CA	-5.30	1.39	1.45
1	1-A	662	LEU	C-N	-5.29	1.26	1.33
3	1-N	419	VAL	N-CA	-5.29	1.40	1.46
1	2-A	662	LEU	C-N	-5.29	1.26	1.33
3	2-N	419	VAL	N-CA	-5.29	1.40	1.46
1	3-A	662	LEU	C-N	-5.29	1.26	1.33
3	3-N	419	VAL	N-CA	-5.29	1.40	1.46
7	1-G	56	ASN	CA-C	-5.29	1.46	1.52
4	1-H	57	ASP	CA-C	-5.29	1.46	1.52
7	2-G	56	ASN	CA-C	-5.29	1.46	1.52
4	2-H	57	ASP	CA-C	-5.29	1.46	1.52
7	3-G	56	ASN	CA-C	-5.29	1.46	1.52
4	3-H	57	ASP	CA-C	-5.29	1.46	1.52
4	1-H	213	ILE	N-CA	-5.29	1.40	1.46
4	2-H	213	ILE	N-CA	-5.29	1.40	1.46
4	3-H	213	ILE	N-CA	-5.29	1.40	1.46
1	1-A	91	GLY	CA-C	-5.29	1.47	1.52
4	1-C	512	ASP	CA-C	-5.29	1.47	1.53
6	1-R	30	LYS	N-CA	-5.29	1.40	1.46
1	2-A	91	GLY	CA-C	-5.29	1.47	1.52
4	2-C	512	ASP	CA-C	-5.29	1.47	1.53
6	2-R	30	LYS	N-CA	-5.29	1.40	1.46
1	3-A	91	GLY	CA-C	-5.29	1.47	1.52
4	3-C	512	ASP	CA-C	-5.29	1.47	1.53
6	3-R	30	LYS	N-CA	-5.29	1.40	1.46
4	1-C	83	VAL	CA-C	-5.29	1.46	1.52
4	2-C	83	VAL	CA-C	-5.29	1.46	1.52
4	3-C	83	VAL	CA-C	-5.29	1.46	1.52
4	1-C	632	GLN	CA-C	-5.29	1.46	1.52
6	1-F	76	SER	CA-C	-5.29	1.45	1.52
3	1-N	317	LEU	C-N	-5.29	1.26	1.34
4	2-C	632	GLN	CA-C	-5.29	1.46	1.52
6	2-F	76	SER	CA-C	-5.29	1.45	1.52
3	2-N	317	LEU	C-N	-5.29	1.26	1.34
4	3-C	632	GLN	CA-C	-5.29	1.46	1.52
6	3-F	76	SER	CA-C	-5.29	1.45	1.52
3	3-N	317	LEU	C-N	-5.29	1.26	1.34
4	1-C	810	TRP	N-CA	-5.28	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1-D	163	ALA	CA-C	-5.28	1.46	1.52
7	1-G	533	ASN	N-CA	-5.28	1.39	1.46
8	1-Z	29	LYS	N-CA	-5.28	1.39	1.46
7	1-K	723	THR	CA-C	-5.28	1.46	1.52
8	1-L	91	MET	N-CA	-5.28	1.39	1.46
4	2-C	810	TRP	N-CA	-5.28	1.40	1.46
5	2-D	163	ALA	CA-C	-5.28	1.46	1.52
7	2-G	533	ASN	N-CA	-5.28	1.39	1.46
8	2-Z	29	LYS	N-CA	-5.28	1.39	1.46
7	2-K	723	THR	CA-C	-5.28	1.46	1.52
8	2-L	91	MET	N-CA	-5.28	1.39	1.46
4	3-C	810	TRP	N-CA	-5.28	1.40	1.46
5	3-D	163	ALA	CA-C	-5.28	1.46	1.52
7	3-G	533	ASN	N-CA	-5.28	1.39	1.46
8	3-Z	29	LYS	N-CA	-5.28	1.39	1.46
7	3-K	723	THR	CA-C	-5.28	1.46	1.52
8	3-L	91	MET	N-CA	-5.28	1.39	1.46
3	1-B	93	LEU	CA-C	-5.28	1.46	1.52
4	1-H	437	PHE	CA-C	-5.28	1.45	1.52
3	2-B	93	LEU	CA-C	-5.28	1.46	1.52
4	2-H	437	PHE	CA-C	-5.28	1.45	1.52
3	3-B	93	LEU	CA-C	-5.28	1.46	1.52
4	3-H	437	PHE	CA-C	-5.28	1.45	1.52
7	1-G	399	ASN	CA-C	-5.28	1.46	1.52
7	2-G	399	ASN	CA-C	-5.28	1.46	1.52
7	3-G	399	ASN	CA-C	-5.28	1.46	1.52
3	1-B	151	LEU	N-CA	-5.28	1.39	1.46
7	1-K	637	VAL	CA-C	-5.28	1.46	1.52
8	1-L	94	LEU	N-CA	-5.28	1.40	1.46
3	2-B	151	LEU	N-CA	-5.28	1.39	1.46
7	2-K	637	VAL	CA-C	-5.28	1.46	1.52
8	2-L	94	LEU	N-CA	-5.28	1.40	1.46
3	3-B	151	LEU	N-CA	-5.28	1.39	1.46
7	3-K	637	VAL	CA-C	-5.28	1.46	1.52
8	3-L	94	LEU	N-CA	-5.28	1.40	1.46
7	1-K	108	SER	CA-C	-5.28	1.46	1.52
3	1-N	268	LEU	CA-C	-5.28	1.45	1.53
4	1-H	425	LYS	CA-C	-5.28	1.46	1.52
4	1-H	505	VAL	CA-C	-5.28	1.46	1.52
7	2-K	108	SER	CA-C	-5.28	1.46	1.52
3	2-N	268	LEU	CA-C	-5.28	1.45	1.53
4	2-H	425	LYS	CA-C	-5.28	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-H	505	VAL	CA-C	-5.28	1.46	1.52
7	3-K	108	SER	CA-C	-5.28	1.46	1.52
3	3-N	268	LEU	CA-C	-5.28	1.45	1.53
4	3-H	425	LYS	CA-C	-5.28	1.46	1.52
4	3-H	505	VAL	CA-C	-5.28	1.46	1.52
8	1-L	66	THR	CA-C	-5.27	1.46	1.52
8	2-L	66	THR	CA-C	-5.27	1.46	1.52
8	3-L	66	THR	CA-C	-5.27	1.46	1.52
4	1-C	469	PHE	N-CA	-5.27	1.39	1.46
4	1-C	481	THR	CA-C	-5.27	1.47	1.53
7	1-K	40	ASN	CA-C	-5.27	1.46	1.52
4	2-C	469	PHE	N-CA	-5.27	1.39	1.46
4	2-C	481	THR	CA-C	-5.27	1.47	1.53
7	2-K	40	ASN	CA-C	-5.27	1.46	1.52
4	3-C	469	PHE	N-CA	-5.27	1.39	1.46
4	3-C	481	THR	CA-C	-5.27	1.47	1.53
7	3-K	40	ASN	CA-C	-5.27	1.46	1.52
1	1-A	430	ASP	CA-C	-5.27	1.46	1.52
3	1-B	62	ILE	N-CA	-5.27	1.40	1.46
4	1-H	368	VAL	N-CA	-5.27	1.40	1.46
1	2-A	430	ASP	CA-C	-5.27	1.46	1.52
3	2-B	62	ILE	N-CA	-5.27	1.40	1.46
4	2-H	368	VAL	N-CA	-5.27	1.40	1.46
1	3-A	430	ASP	CA-C	-5.27	1.46	1.52
3	3-B	62	ILE	N-CA	-5.27	1.40	1.46
4	3-H	368	VAL	N-CA	-5.27	1.40	1.46
3	1-B	419	VAL	N-CA	-5.27	1.40	1.46
4	1-C	368	VAL	N-CA	-5.27	1.40	1.46
3	2-B	419	VAL	N-CA	-5.27	1.40	1.46
4	2-C	368	VAL	N-CA	-5.27	1.40	1.46
3	3-B	419	VAL	N-CA	-5.27	1.40	1.46
4	3-C	368	VAL	N-CA	-5.27	1.40	1.46
1	1-A	657	ASN	CA-C	-5.27	1.45	1.52
1	2-A	657	ASN	CA-C	-5.27	1.45	1.52
1	3-A	657	ASN	CA-C	-5.27	1.45	1.52
1	1-A	668	LEU	CA-C	-5.26	1.45	1.52
7	1-G	637	VAL	CA-C	-5.26	1.46	1.52
1	2-A	668	LEU	CA-C	-5.26	1.45	1.52
7	2-G	637	VAL	CA-C	-5.26	1.46	1.52
1	3-A	668	LEU	CA-C	-5.26	1.45	1.52
7	3-G	637	VAL	CA-C	-5.26	1.46	1.52
7	1-G	291	VAL	CA-C	-5.26	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-K	84	LEU	N-CA	-5.26	1.40	1.46
7	1-K	163	SER	N-CA	-5.26	1.40	1.46
7	2-G	291	VAL	CA-C	-5.26	1.46	1.52
7	2-K	84	LEU	N-CA	-5.26	1.40	1.46
7	2-K	163	SER	N-CA	-5.26	1.40	1.46
7	3-G	291	VAL	CA-C	-5.26	1.46	1.52
7	3-K	84	LEU	N-CA	-5.26	1.40	1.46
7	3-K	163	SER	N-CA	-5.26	1.40	1.46
4	1-C	678	ILE	N-CA	-5.26	1.40	1.46
4	2-C	678	ILE	N-CA	-5.26	1.40	1.46
4	3-C	678	ILE	N-CA	-5.26	1.40	1.46
4	1-C	815	HIS	N-CA	-5.25	1.40	1.46
4	2-C	815	HIS	N-CA	-5.25	1.40	1.46
4	3-C	815	HIS	N-CA	-5.25	1.40	1.46
3	1-B	235	GLY	CA-C	-5.25	1.47	1.52
3	1-B	771	CYS	CA-C	-5.25	1.45	1.52
3	2-B	235	GLY	CA-C	-5.25	1.47	1.52
3	2-B	771	CYS	CA-C	-5.25	1.45	1.52
3	3-B	235	GLY	CA-C	-5.25	1.47	1.52
3	3-B	771	CYS	CA-C	-5.25	1.45	1.52
1	1-A	442	ASN	CA-C	-5.25	1.45	1.53
8	1-L	80	ILE	CA-C	-5.25	1.46	1.52
1	2-A	442	ASN	CA-C	-5.25	1.45	1.53
8	2-L	80	ILE	CA-C	-5.25	1.46	1.52
1	3-A	442	ASN	CA-C	-5.25	1.45	1.53
8	3-L	80	ILE	CA-C	-5.25	1.46	1.52
3	1-B	966	THR	CA-C	5.25	1.59	1.52
4	1-H	271	MET	CA-C	-5.25	1.44	1.52
3	2-B	966	THR	CA-C	5.25	1.59	1.52
4	2-H	271	MET	CA-C	-5.25	1.44	1.52
3	3-B	966	THR	CA-C	5.25	1.59	1.52
4	3-H	271	MET	CA-C	-5.25	1.44	1.52
4	1-C	739	ASP	N-CA	-5.25	1.40	1.46
3	1-N	235	GLY	CA-C	-5.25	1.47	1.52
5	1-I	7	ALA	CA-C	-5.25	1.46	1.52
4	2-C	739	ASP	N-CA	-5.25	1.40	1.46
3	2-N	235	GLY	CA-C	-5.25	1.47	1.52
5	2-I	7	ALA	CA-C	-5.25	1.46	1.52
4	3-C	739	ASP	N-CA	-5.25	1.40	1.46
3	3-N	235	GLY	CA-C	-5.25	1.47	1.52
5	3-I	7	ALA	CA-C	-5.25	1.46	1.52
1	1-A	639	LEU	N-CA	-5.25	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-K	202	HIS	C-N	-5.25	1.27	1.33
3	1-N	193	HIS	N-CA	-5.25	1.40	1.46
1	2-A	639	LEU	N-CA	-5.25	1.40	1.46
7	2-K	202	HIS	C-N	-5.25	1.27	1.33
3	2-N	193	HIS	N-CA	-5.25	1.40	1.46
1	3-A	639	LEU	N-CA	-5.25	1.40	1.46
7	3-K	202	HIS	C-N	-5.25	1.27	1.33
3	3-N	193	HIS	N-CA	-5.25	1.40	1.46
7	1-G	751	TYR	N-CA	-5.24	1.39	1.45
7	2-G	751	TYR	N-CA	-5.24	1.39	1.45
7	3-G	751	TYR	N-CA	-5.24	1.39	1.45
4	1-C	437	PHE	CA-C	-5.24	1.46	1.52
3	1-N	382	THR	CA-C	-5.24	1.45	1.52
4	2-C	437	PHE	CA-C	-5.24	1.46	1.52
3	2-N	382	THR	CA-C	-5.24	1.45	1.52
4	3-C	437	PHE	CA-C	-5.24	1.46	1.52
3	3-N	382	THR	CA-C	-5.24	1.45	1.52
1	1-A	474	LEU	C-N	5.24	1.40	1.33
1	1-A	587	PRO	C-N	5.24	1.40	1.33
1	2-A	474	LEU	C-N	5.24	1.40	1.33
1	2-A	587	PRO	C-N	5.24	1.40	1.33
1	3-A	474	LEU	C-N	5.24	1.40	1.33
1	3-A	587	PRO	C-N	5.24	1.40	1.33
7	1-G	830	LEU	C-N	5.24	1.40	1.33
4	1-H	153	LYS	CA-C	-5.24	1.46	1.52
7	2-G	830	LEU	C-N	5.24	1.40	1.33
4	2-H	153	LYS	CA-C	-5.24	1.46	1.52
7	3-G	830	LEU	C-N	5.24	1.40	1.33
4	3-H	153	LYS	CA-C	-5.24	1.46	1.52
3	1-B	205	LYS	CA-C	-5.24	1.46	1.52
3	2-B	205	LYS	CA-C	-5.24	1.46	1.52
3	3-B	205	LYS	CA-C	-5.24	1.46	1.52
7	1-G	297	SER	CA-C	-5.24	1.45	1.52
8	1-Z	124	ALA	N-CA	-5.24	1.40	1.46
4	1-H	450	TYR	N-CA	-5.24	1.39	1.45
7	2-G	297	SER	CA-C	-5.24	1.45	1.52
8	2-Z	124	ALA	N-CA	-5.24	1.40	1.46
4	2-H	450	TYR	N-CA	-5.24	1.39	1.45
7	3-G	297	SER	CA-C	-5.24	1.45	1.52
8	3-Z	124	ALA	N-CA	-5.24	1.40	1.46
4	3-H	450	TYR	N-CA	-5.24	1.39	1.45
8	1-L	94	LEU	CA-C	-5.23	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2-L	94	LEU	CA-C	-5.23	1.46	1.52
8	3-L	94	LEU	CA-C	-5.23	1.46	1.52
1	1-A	438	LYS	CA-C	-5.23	1.46	1.52
3	1-B	301	ILE	N-CA	-5.23	1.40	1.46
3	1-B	817	ASN	N-CA	-5.23	1.39	1.46
4	1-C	273	ARG	N-CA	-5.23	1.39	1.46
7	1-G	63	THR	CA-C	-5.23	1.46	1.52
7	1-G	174	VAL	C-N	-5.23	1.27	1.33
3	1-N	130	PHE	CA-C	-5.23	1.46	1.52
1	2-A	438	LYS	CA-C	-5.23	1.46	1.52
3	2-B	301	ILE	N-CA	-5.23	1.40	1.46
3	2-B	817	ASN	N-CA	-5.23	1.39	1.46
4	2-C	273	ARG	N-CA	-5.23	1.39	1.46
7	2-G	63	THR	CA-C	-5.23	1.46	1.52
7	2-G	174	VAL	C-N	-5.23	1.27	1.33
3	2-N	130	PHE	CA-C	-5.23	1.46	1.52
1	3-A	438	LYS	CA-C	-5.23	1.46	1.52
3	3-B	301	ILE	N-CA	-5.23	1.40	1.46
3	3-B	817	ASN	N-CA	-5.23	1.39	1.46
4	3-C	273	ARG	N-CA	-5.23	1.39	1.46
7	3-G	63	THR	CA-C	-5.23	1.46	1.52
7	3-G	174	VAL	C-N	-5.23	1.27	1.33
3	3-N	130	PHE	CA-C	-5.23	1.46	1.52
1	1-A	265	LEU	CA-C	-5.23	1.46	1.52
1	1-A	412	ARG	CA-C	-5.23	1.46	1.52
4	1-C	271	MET	CA-C	-5.23	1.44	1.52
1	2-A	265	LEU	CA-C	-5.23	1.46	1.52
1	2-A	412	ARG	CA-C	-5.23	1.46	1.52
4	2-C	271	MET	CA-C	-5.23	1.44	1.52
1	3-A	265	LEU	CA-C	-5.23	1.46	1.52
1	3-A	412	ARG	CA-C	-5.23	1.46	1.52
4	3-C	271	MET	CA-C	-5.23	1.44	1.52
1	1-A	392	ASP	N-CA	-5.23	1.39	1.46
3	1-B	192	ILE	N-CA	-5.23	1.40	1.46
3	1-B	375	LEU	N-CA	-5.23	1.40	1.46
7	1-K	216	SER	N-CA	-5.23	1.39	1.46
6	1-M	72	ASP	CA-C	-5.23	1.46	1.52
4	1-H	492	SER	CA-C	-5.23	1.46	1.52
1	2-A	392	ASP	N-CA	-5.23	1.39	1.46
3	2-B	192	ILE	N-CA	-5.23	1.40	1.46
3	2-B	375	LEU	N-CA	-5.23	1.40	1.46
7	2-K	216	SER	N-CA	-5.23	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2-M	72	ASP	CA-C	-5.23	1.46	1.52
4	2-H	492	SER	CA-C	-5.23	1.46	1.52
1	3-A	392	ASP	N-CA	-5.23	1.39	1.46
3	3-B	192	ILE	N-CA	-5.23	1.40	1.46
3	3-B	375	LEU	N-CA	-5.23	1.40	1.46
7	3-K	216	SER	N-CA	-5.23	1.39	1.46
6	3-M	72	ASP	CA-C	-5.23	1.46	1.52
4	3-H	492	SER	CA-C	-5.23	1.46	1.52
3	1-B	382	THR	CA-C	-5.23	1.45	1.52
4	1-C	450	TYR	N-CA	-5.23	1.39	1.45
3	2-B	382	THR	CA-C	-5.23	1.45	1.52
4	2-C	450	TYR	N-CA	-5.23	1.39	1.45
3	3-B	382	THR	CA-C	-5.23	1.45	1.52
4	3-C	450	TYR	N-CA	-5.23	1.39	1.45
5	1-I	106	CYS	CA-C	-5.23	1.46	1.52
5	2-I	106	CYS	CA-C	-5.23	1.46	1.52
5	3-I	106	CYS	CA-C	-5.23	1.46	1.52
7	1-G	856	VAL	CA-C	-5.22	1.46	1.52
4	1-H	656	ILE	N-CA	-5.22	1.40	1.46
7	2-G	856	VAL	CA-C	-5.22	1.46	1.52
4	2-H	656	ILE	N-CA	-5.22	1.40	1.46
7	3-G	856	VAL	CA-C	-5.22	1.46	1.52
4	3-H	656	ILE	N-CA	-5.22	1.40	1.46
1	1-A	391	TYR	N-CA	-5.22	1.39	1.46
7	1-G	725	SER	CA-C	-5.22	1.46	1.52
1	2-A	391	TYR	N-CA	-5.22	1.39	1.46
7	2-G	725	SER	CA-C	-5.22	1.46	1.52
1	3-A	391	TYR	N-CA	-5.22	1.39	1.46
7	3-G	725	SER	CA-C	-5.22	1.46	1.52
3	1-B	202	ALA	CA-C	-5.22	1.46	1.52
3	1-B	959	ILE	N-CA	-5.22	1.40	1.46
3	2-B	202	ALA	CA-C	-5.22	1.46	1.52
3	2-B	959	ILE	N-CA	-5.22	1.40	1.46
3	3-B	202	ALA	CA-C	-5.22	1.46	1.52
3	3-B	959	ILE	N-CA	-5.22	1.40	1.46
1	1-A	519	ASP	N-CA	-5.22	1.40	1.46
7	1-G	73	MET	N-CA	-5.22	1.40	1.46
1	2-A	519	ASP	N-CA	-5.22	1.40	1.46
7	2-G	73	MET	N-CA	-5.22	1.40	1.46
1	3-A	519	ASP	N-CA	-5.22	1.40	1.46
7	3-G	73	MET	N-CA	-5.22	1.40	1.46
1	1-A	615	VAL	CA-C	-5.22	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-C	340	ARG	C-N	5.22	1.39	1.32
7	1-K	233	ILE	N-CA	-5.22	1.40	1.46
1	2-A	615	VAL	CA-C	-5.22	1.46	1.52
4	2-C	340	ARG	C-N	5.22	1.39	1.32
7	2-K	233	ILE	N-CA	-5.22	1.40	1.46
1	3-A	615	VAL	CA-C	-5.22	1.46	1.52
4	3-C	340	ARG	C-N	5.22	1.39	1.32
7	3-K	233	ILE	N-CA	-5.22	1.40	1.46
3	1-B	938	VAL	N-CA	-5.22	1.39	1.46
3	1-N	192	ILE	N-CA	-5.22	1.40	1.46
4	1-H	186	LYS	N-CA	-5.22	1.39	1.46
3	2-B	938	VAL	N-CA	-5.22	1.39	1.46
3	2-N	192	ILE	N-CA	-5.22	1.40	1.46
4	2-H	186	LYS	N-CA	-5.22	1.39	1.46
3	3-B	938	VAL	N-CA	-5.22	1.39	1.46
3	3-N	192	ILE	N-CA	-5.22	1.40	1.46
4	3-H	186	LYS	N-CA	-5.22	1.39	1.46
1	1-A	429	LEU	CA-C	-5.21	1.46	1.52
4	1-C	647	LEU	CA-C	-5.21	1.46	1.52
5	1-D	162	LYS	CA-C	-5.21	1.46	1.52
7	1-K	86	ARG	CA-C	-5.21	1.45	1.52
6	1-M	159	CYS	N-CA	-5.21	1.39	1.46
1	2-A	429	LEU	CA-C	-5.21	1.46	1.52
4	2-C	647	LEU	CA-C	-5.21	1.46	1.52
5	2-D	162	LYS	CA-C	-5.21	1.46	1.52
7	2-K	86	ARG	CA-C	-5.21	1.45	1.52
6	2-M	159	CYS	N-CA	-5.21	1.39	1.46
1	3-A	429	LEU	CA-C	-5.21	1.46	1.52
4	3-C	647	LEU	CA-C	-5.21	1.46	1.52
5	3-D	162	LYS	CA-C	-5.21	1.46	1.52
7	3-K	86	ARG	CA-C	-5.21	1.45	1.52
6	3-M	159	CYS	N-CA	-5.21	1.39	1.46
4	1-C	258	SER	N-CA	-5.21	1.39	1.46
4	1-C	443	SER	CA-C	-5.21	1.45	1.52
3	1-N	301	ILE	N-CA	-5.21	1.40	1.46
4	2-C	258	SER	N-CA	-5.21	1.39	1.46
4	2-C	443	SER	CA-C	-5.21	1.45	1.52
3	2-N	301	ILE	N-CA	-5.21	1.40	1.46
4	3-C	258	SER	N-CA	-5.21	1.39	1.46
4	3-C	443	SER	CA-C	-5.21	1.45	1.52
3	3-N	301	ILE	N-CA	-5.21	1.40	1.46
7	1-G	477	TYR	N-CA	-5.21	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	477	TYR	N-CA	-5.21	1.40	1.46
7	3-G	477	TYR	N-CA	-5.21	1.40	1.46
1	1-A	147	GLU	CA-C	-5.21	1.46	1.52
1	1-A	263	LEU	CA-C	-5.21	1.46	1.52
6	1-F	138	GLU	CA-C	-5.21	1.46	1.52
7	1-G	210	ALA	N-CA	-5.21	1.40	1.46
7	1-K	51	ILE	CA-C	-5.21	1.46	1.52
7	1-K	237	SER	CA-C	-5.21	1.46	1.52
6	1-J	76	SER	CA-C	-5.21	1.45	1.52
1	2-A	147	GLU	CA-C	-5.21	1.46	1.52
1	2-A	263	LEU	CA-C	-5.21	1.46	1.52
6	2-F	138	GLU	CA-C	-5.21	1.46	1.52
7	2-G	210	ALA	N-CA	-5.21	1.40	1.46
7	2-K	51	ILE	CA-C	-5.21	1.46	1.52
7	2-K	237	SER	CA-C	-5.21	1.46	1.52
6	2-J	76	SER	CA-C	-5.21	1.45	1.52
1	3-A	147	GLU	CA-C	-5.21	1.46	1.52
1	3-A	263	LEU	CA-C	-5.21	1.46	1.52
6	3-F	138	GLU	CA-C	-5.21	1.46	1.52
7	3-G	210	ALA	N-CA	-5.21	1.40	1.46
7	3-K	51	ILE	CA-C	-5.21	1.46	1.52
7	3-K	237	SER	CA-C	-5.21	1.46	1.52
6	3-J	76	SER	CA-C	-5.21	1.45	1.52
1	1-A	471	SER	CA-C	-5.21	1.45	1.52
4	1-C	656	ILE	N-CA	-5.21	1.40	1.46
7	1-G	683	PRO	CA-C	5.21	1.57	1.52
3	1-N	117	CYS	N-CA	-5.21	1.40	1.46
3	1-N	375	LEU	N-CA	-5.21	1.40	1.46
4	1-H	273	ARG	N-CA	-5.21	1.39	1.46
1	2-A	471	SER	CA-C	-5.21	1.45	1.52
4	2-C	656	ILE	N-CA	-5.21	1.40	1.46
7	2-G	683	PRO	CA-C	5.21	1.57	1.52
3	2-N	117	CYS	N-CA	-5.21	1.40	1.46
3	2-N	375	LEU	N-CA	-5.21	1.40	1.46
4	2-H	273	ARG	N-CA	-5.21	1.39	1.46
1	3-A	471	SER	CA-C	-5.21	1.45	1.52
4	3-C	656	ILE	N-CA	-5.21	1.40	1.46
7	3-G	683	PRO	CA-C	5.21	1.57	1.52
3	3-N	117	CYS	N-CA	-5.21	1.40	1.46
3	3-N	375	LEU	N-CA	-5.21	1.40	1.46
4	3-H	273	ARG	N-CA	-5.21	1.39	1.46
4	1-H	292	GLU	CA-C	-5.21	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-H	292	GLU	CA-C	-5.21	1.45	1.52
4	3-H	292	GLU	CA-C	-5.21	1.45	1.52
3	1-B	272	SER	C-N	-5.20	1.27	1.34
4	1-C	186	LYS	N-CA	-5.20	1.39	1.46
4	1-H	258	SER	N-CA	-5.20	1.40	1.46
4	1-H	469	PHE	N-CA	-5.20	1.39	1.46
3	2-B	272	SER	C-N	-5.20	1.27	1.34
4	2-C	186	LYS	N-CA	-5.20	1.39	1.46
4	2-H	258	SER	N-CA	-5.20	1.40	1.46
4	2-H	469	PHE	N-CA	-5.20	1.39	1.46
3	3-B	272	SER	C-N	-5.20	1.27	1.34
4	3-C	186	LYS	N-CA	-5.20	1.39	1.46
4	3-H	258	SER	N-CA	-5.20	1.40	1.46
4	3-H	469	PHE	N-CA	-5.20	1.39	1.46
4	1-C	557	LEU	CA-C	-5.20	1.46	1.52
4	2-C	557	LEU	CA-C	-5.20	1.46	1.52
4	3-C	557	LEU	CA-C	-5.20	1.46	1.52
3	1-B	268	LEU	CA-C	-5.20	1.46	1.53
3	1-B	811	ASN	N-CA	-5.20	1.39	1.46
8	1-L	39	LYS	N-CA	-5.20	1.40	1.46
6	1-M	78	TRP	N-CA	-5.20	1.39	1.46
3	1-N	190	GLU	N-CA	-5.20	1.40	1.46
3	2-B	268	LEU	CA-C	-5.20	1.46	1.53
3	2-B	811	ASN	N-CA	-5.20	1.39	1.46
8	2-L	39	LYS	N-CA	-5.20	1.40	1.46
6	2-M	78	TRP	N-CA	-5.20	1.39	1.46
3	2-N	190	GLU	N-CA	-5.20	1.40	1.46
3	3-B	268	LEU	CA-C	-5.20	1.46	1.53
3	3-B	811	ASN	N-CA	-5.20	1.39	1.46
8	3-L	39	LYS	N-CA	-5.20	1.40	1.46
6	3-M	78	TRP	N-CA	-5.20	1.39	1.46
3	3-N	190	GLU	N-CA	-5.20	1.40	1.46
1	1-A	661	ALA	CA-C	-5.20	1.46	1.52
3	1-B	394	TYR	N-CA	-5.20	1.40	1.46
7	1-G	34	PHE	CA-C	-5.20	1.45	1.52
6	1-R	40	GLY	CA-C	-5.20	1.44	1.51
1	2-A	661	ALA	CA-C	-5.20	1.46	1.52
3	2-B	394	TYR	N-CA	-5.20	1.40	1.46
7	2-G	34	PHE	CA-C	-5.20	1.45	1.52
6	2-R	40	GLY	CA-C	-5.20	1.44	1.51
1	3-A	661	ALA	CA-C	-5.20	1.46	1.52
3	3-B	394	TYR	N-CA	-5.20	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	3-G	34	PHE	CA-C	-5.20	1.45	1.52
6	3-R	40	GLY	CA-C	-5.20	1.44	1.51
3	1-B	284	VAL	CA-C	-5.20	1.45	1.52
4	1-C	492	SER	CA-C	-5.20	1.46	1.52
6	1-M	20	ILE	N-CA	-5.20	1.40	1.46
3	1-N	62	ILE	N-CA	-5.20	1.40	1.46
4	1-H	481	THR	CA-C	-5.20	1.47	1.53
3	2-B	284	VAL	CA-C	-5.20	1.45	1.52
4	2-C	492	SER	CA-C	-5.20	1.46	1.52
6	2-M	20	ILE	N-CA	-5.20	1.40	1.46
3	2-N	62	ILE	N-CA	-5.20	1.40	1.46
4	2-H	481	THR	CA-C	-5.20	1.47	1.53
3	3-B	284	VAL	CA-C	-5.20	1.45	1.52
4	3-C	492	SER	CA-C	-5.20	1.46	1.52
6	3-M	20	ILE	N-CA	-5.20	1.40	1.46
3	3-N	62	ILE	N-CA	-5.20	1.40	1.46
4	3-H	481	THR	CA-C	-5.20	1.47	1.53
1	1-A	120	TRP	C-N	5.19	1.40	1.33
7	1-K	237	SER	N-CA	-5.19	1.40	1.46
1	2-A	120	TRP	C-N	5.19	1.40	1.33
7	2-K	237	SER	N-CA	-5.19	1.40	1.46
1	3-A	120	TRP	C-N	5.19	1.40	1.33
7	3-K	237	SER	N-CA	-5.19	1.40	1.46
7	1-G	146	GLN	N-CA	-5.19	1.40	1.46
7	2-G	146	GLN	N-CA	-5.19	1.40	1.46
7	3-G	146	GLN	N-CA	-5.19	1.40	1.46
3	1-B	52	SER	N-CA	-5.19	1.40	1.46
4	1-C	530	VAL	N-CA	-5.19	1.39	1.46
3	2-B	52	SER	N-CA	-5.19	1.40	1.46
4	2-C	530	VAL	N-CA	-5.19	1.39	1.46
3	3-B	52	SER	N-CA	-5.19	1.40	1.46
4	3-C	530	VAL	N-CA	-5.19	1.39	1.46
8	1-L	95	ASN	CA-C	-5.19	1.46	1.52
8	1-L	139	PRO	N-CA	-5.19	1.40	1.47
8	2-L	95	ASN	CA-C	-5.19	1.46	1.52
8	2-L	139	PRO	N-CA	-5.19	1.40	1.47
8	3-L	95	ASN	CA-C	-5.19	1.46	1.52
8	3-L	139	PRO	N-CA	-5.19	1.40	1.47
8	1-L	146	VAL	CA-C	-5.19	1.46	1.53
4	1-H	317	ALA	CA-C	-5.19	1.46	1.52
4	1-H	512	ASP	CA-C	-5.19	1.47	1.53
8	2-L	146	VAL	CA-C	-5.19	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-H	317	ALA	CA-C	-5.19	1.46	1.52
4	2-H	512	ASP	CA-C	-5.19	1.47	1.53
8	3-L	146	VAL	CA-C	-5.19	1.46	1.53
4	3-H	317	ALA	CA-C	-5.19	1.46	1.52
4	3-H	512	ASP	CA-C	-5.19	1.47	1.53
1	1-A	641	PHE	CA-C	-5.19	1.46	1.52
4	1-C	292	GLU	CA-C	-5.19	1.45	1.52
6	1-F	31	THR	N-CA	-5.19	1.40	1.46
1	2-A	641	PHE	CA-C	-5.19	1.46	1.52
4	2-C	292	GLU	CA-C	-5.19	1.45	1.52
6	2-F	31	THR	N-CA	-5.19	1.40	1.46
1	3-A	641	PHE	CA-C	-5.19	1.46	1.52
4	3-C	292	GLU	CA-C	-5.19	1.45	1.52
6	3-F	31	THR	N-CA	-5.19	1.40	1.46
1	1-A	344	LEU	N-CA	-5.18	1.38	1.46
1	1-A	704	SER	CA-C	-5.18	1.46	1.52
3	1-B	181	PHE	N-CA	-5.18	1.39	1.46
8	1-L	15	ALA	N-CA	-5.18	1.39	1.46
8	1-L	89	MET	N-CA	-5.18	1.40	1.46
6	1-M	48	THR	N-CA	-5.18	1.39	1.46
3	1-N	394	TYR	N-CA	-5.18	1.40	1.46
4	1-H	51	LYS	CA-C	-5.18	1.46	1.52
4	1-H	529	TRP	N-CA	-5.18	1.39	1.46
4	1-H	530	VAL	N-CA	-5.18	1.39	1.46
1	2-A	344	LEU	N-CA	-5.18	1.38	1.46
1	2-A	704	SER	CA-C	-5.18	1.46	1.52
3	2-B	181	PHE	N-CA	-5.18	1.39	1.46
8	2-L	15	ALA	N-CA	-5.18	1.39	1.46
8	2-L	89	MET	N-CA	-5.18	1.40	1.46
6	2-M	48	THR	N-CA	-5.18	1.39	1.46
3	2-N	394	TYR	N-CA	-5.18	1.40	1.46
4	2-H	51	LYS	CA-C	-5.18	1.46	1.52
4	2-H	529	TRP	N-CA	-5.18	1.39	1.46
4	2-H	530	VAL	N-CA	-5.18	1.39	1.46
1	3-A	344	LEU	N-CA	-5.18	1.38	1.46
1	3-A	704	SER	CA-C	-5.18	1.46	1.52
3	3-B	181	PHE	N-CA	-5.18	1.39	1.46
8	3-L	15	ALA	N-CA	-5.18	1.39	1.46
8	3-L	89	MET	N-CA	-5.18	1.40	1.46
6	3-M	48	THR	N-CA	-5.18	1.39	1.46
3	3-N	394	TYR	N-CA	-5.18	1.40	1.46
4	3-H	51	LYS	CA-C	-5.18	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-H	529	TRP	N-CA	-5.18	1.39	1.46
4	3-H	530	VAL	N-CA	-5.18	1.39	1.46
3	1-N	52	SER	N-CA	-5.18	1.40	1.46
3	2-N	52	SER	N-CA	-5.18	1.40	1.46
3	3-N	52	SER	N-CA	-5.18	1.40	1.46
4	1-C	782	GLN	CA-C	-5.18	1.45	1.52
4	2-C	782	GLN	CA-C	-5.18	1.45	1.52
4	3-C	782	GLN	CA-C	-5.18	1.45	1.52
1	1-A	626	ILE	CA-C	-5.18	1.46	1.52
7	1-G	27	VAL	N-CA	-5.18	1.40	1.46
7	1-G	294	LEU	N-CA	-5.18	1.40	1.46
8	1-L	135	LEU	N-CA	-5.18	1.39	1.46
4	1-H	194	TYR	CA-C	-5.18	1.46	1.52
1	2-A	626	ILE	CA-C	-5.18	1.46	1.52
7	2-G	27	VAL	N-CA	-5.18	1.40	1.46
7	2-G	294	LEU	N-CA	-5.18	1.40	1.46
8	2-L	135	LEU	N-CA	-5.18	1.39	1.46
4	2-H	194	TYR	CA-C	-5.18	1.46	1.52
1	3-A	626	ILE	CA-C	-5.18	1.46	1.52
7	3-G	27	VAL	N-CA	-5.18	1.40	1.46
7	3-G	294	LEU	N-CA	-5.18	1.40	1.46
8	3-L	135	LEU	N-CA	-5.18	1.39	1.46
4	3-H	194	TYR	CA-C	-5.18	1.46	1.52
3	1-B	201	ASP	CA-C	-5.18	1.46	1.52
3	1-N	93	LEU	CA-C	-5.18	1.46	1.52
3	2-B	201	ASP	CA-C	-5.18	1.46	1.52
3	2-N	93	LEU	CA-C	-5.18	1.46	1.52
3	3-B	201	ASP	CA-C	-5.18	1.46	1.52
3	3-N	93	LEU	CA-C	-5.18	1.46	1.52
4	1-C	153	LYS	CA-C	-5.17	1.46	1.52
4	1-H	443	SER	CA-C	-5.17	1.46	1.52
6	1-J	138	GLU	CA-C	-5.17	1.46	1.52
4	2-C	153	LYS	CA-C	-5.17	1.46	1.52
4	2-H	443	SER	CA-C	-5.17	1.46	1.52
6	2-J	138	GLU	CA-C	-5.17	1.46	1.52
4	3-C	153	LYS	CA-C	-5.17	1.46	1.52
4	3-H	443	SER	CA-C	-5.17	1.46	1.52
6	3-J	138	GLU	CA-C	-5.17	1.46	1.52
1	1-A	681	ALA	C-O	-5.17	1.18	1.24
3	1-B	782	LYS	N-CA	-5.17	1.39	1.45
7	1-G	850	ASP	CA-C	-5.17	1.45	1.52
1	2-A	681	ALA	C-O	-5.17	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-B	782	LYS	N-CA	-5.17	1.39	1.45
7	2-G	850	ASP	CA-C	-5.17	1.45	1.52
1	3-A	681	ALA	C-O	-5.17	1.18	1.24
3	3-B	782	LYS	N-CA	-5.17	1.39	1.45
7	3-G	850	ASP	CA-C	-5.17	1.45	1.52
3	1-B	90	LYS	CA-C	-5.17	1.46	1.52
4	1-C	468	ILE	CA-C	-5.17	1.46	1.52
4	1-H	340	ARG	C-N	5.17	1.39	1.32
3	2-B	90	LYS	CA-C	-5.17	1.46	1.52
4	2-C	468	ILE	CA-C	-5.17	1.46	1.52
4	2-H	340	ARG	C-N	5.17	1.39	1.32
3	3-B	90	LYS	CA-C	-5.17	1.46	1.52
4	3-C	468	ILE	CA-C	-5.17	1.46	1.52
4	3-H	340	ARG	C-N	5.17	1.39	1.32
1	1-A	465	LEU	CA-C	-5.17	1.45	1.52
1	1-A	553	VAL	C-N	5.17	1.40	1.33
7	1-G	90	LEU	N-CA	-5.17	1.40	1.46
6	1-J	31	THR	N-CA	-5.17	1.40	1.46
1	2-A	465	LEU	CA-C	-5.17	1.45	1.52
1	2-A	553	VAL	C-N	5.17	1.40	1.33
7	2-G	90	LEU	N-CA	-5.17	1.40	1.46
6	2-J	31	THR	N-CA	-5.17	1.40	1.46
1	3-A	465	LEU	CA-C	-5.17	1.45	1.52
1	3-A	553	VAL	C-N	5.17	1.40	1.33
7	3-G	90	LEU	N-CA	-5.17	1.40	1.46
6	3-J	31	THR	N-CA	-5.17	1.40	1.46
8	1-Z	110	GLU	CA-C	-5.17	1.46	1.52
3	1-N	90	LYS	CA-C	-5.17	1.46	1.52
8	2-Z	110	GLU	CA-C	-5.17	1.46	1.52
3	2-N	90	LYS	CA-C	-5.17	1.46	1.52
8	3-Z	110	GLU	CA-C	-5.17	1.46	1.52
3	3-N	90	LYS	CA-C	-5.17	1.46	1.52
7	1-K	725	SER	CA-C	-5.17	1.46	1.52
5	1-I	241	LYS	CA-C	-5.17	1.46	1.52
7	2-K	725	SER	CA-C	-5.17	1.46	1.52
5	2-I	241	LYS	CA-C	-5.17	1.46	1.52
7	3-K	725	SER	CA-C	-5.17	1.46	1.52
5	3-I	241	LYS	CA-C	-5.17	1.46	1.52
3	1-B	855	PHE	N-CA	-5.16	1.40	1.46
4	1-C	376	ILE	CA-C	-5.16	1.46	1.52
7	1-G	113	MET	N-CA	-5.16	1.40	1.46
3	2-B	855	PHE	N-CA	-5.16	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-C	376	ILE	CA-C	-5.16	1.46	1.52
7	2-G	113	MET	N-CA	-5.16	1.40	1.46
3	3-B	855	PHE	N-CA	-5.16	1.40	1.46
4	3-C	376	ILE	CA-C	-5.16	1.46	1.52
7	3-G	113	MET	N-CA	-5.16	1.40	1.46
3	1-B	776	ALA	CA-C	-5.16	1.45	1.52
5	1-D	241	LYS	CA-C	-5.16	1.46	1.52
5	1-I	128	ALA	CA-C	-5.16	1.46	1.52
3	2-B	776	ALA	CA-C	-5.16	1.45	1.52
5	2-D	241	LYS	CA-C	-5.16	1.46	1.52
5	2-I	128	ALA	CA-C	-5.16	1.46	1.52
3	3-B	776	ALA	CA-C	-5.16	1.45	1.52
5	3-D	241	LYS	CA-C	-5.16	1.46	1.52
5	3-I	128	ALA	CA-C	-5.16	1.46	1.52
1	1-A	286	THR	N-CA	-5.16	1.39	1.46
8	1-L	38	VAL	N-CA	-5.16	1.40	1.46
3	1-N	52	SER	CA-C	-5.16	1.46	1.52
3	1-N	471	ARG	N-CA	-5.16	1.40	1.46
3	1-N	474	LEU	N-CA	-5.16	1.40	1.46
4	1-H	468	ILE	CA-C	-5.16	1.46	1.52
1	2-A	286	THR	N-CA	-5.16	1.39	1.46
8	2-L	38	VAL	N-CA	-5.16	1.40	1.46
3	2-N	52	SER	CA-C	-5.16	1.46	1.52
3	2-N	471	ARG	N-CA	-5.16	1.40	1.46
3	2-N	474	LEU	N-CA	-5.16	1.40	1.46
4	2-H	468	ILE	CA-C	-5.16	1.46	1.52
1	3-A	286	THR	N-CA	-5.16	1.39	1.46
8	3-L	38	VAL	N-CA	-5.16	1.40	1.46
3	3-N	52	SER	CA-C	-5.16	1.46	1.52
3	3-N	471	ARG	N-CA	-5.16	1.40	1.46
3	3-N	474	LEU	N-CA	-5.16	1.40	1.46
4	3-H	468	ILE	CA-C	-5.16	1.46	1.52
1	1-A	211	ALA	CA-C	-5.16	1.46	1.52
7	1-G	639	LEU	CA-C	-5.16	1.45	1.52
1	2-A	211	ALA	CA-C	-5.16	1.46	1.52
7	2-G	639	LEU	CA-C	-5.16	1.45	1.52
1	3-A	211	ALA	CA-C	-5.16	1.46	1.52
7	3-G	639	LEU	CA-C	-5.16	1.45	1.52
4	1-C	144	TYR	CA-C	-5.16	1.46	1.52
3	1-N	272	SER	C-N	-5.16	1.27	1.34
4	2-C	144	TYR	CA-C	-5.16	1.46	1.52
3	2-N	272	SER	C-N	-5.16	1.27	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-C	144	TYR	CA-C	-5.16	1.46	1.52
3	3-N	272	SER	C-N	-5.16	1.27	1.34
5	1-D	128	ALA	CA-C	-5.16	1.46	1.52
5	2-D	128	ALA	CA-C	-5.16	1.46	1.52
5	3-D	128	ALA	CA-C	-5.16	1.46	1.52
3	1-N	403	HIS	CA-C	-5.15	1.46	1.52
4	1-H	557	LEU	CA-C	-5.15	1.46	1.52
3	2-N	403	HIS	CA-C	-5.15	1.46	1.52
4	2-H	557	LEU	CA-C	-5.15	1.46	1.52
3	3-N	403	HIS	CA-C	-5.15	1.46	1.52
4	3-H	557	LEU	CA-C	-5.15	1.46	1.52
4	1-C	817	ASP	CA-C	-5.15	1.45	1.52
7	1-G	147	ALA	N-CA	-5.15	1.40	1.46
7	1-K	119	ASN	N-CA	-5.15	1.40	1.46
6	1-M	35	TYR	N-CA	-5.15	1.39	1.46
5	1-I	79	ASP	N-CA	-5.15	1.40	1.46
5	1-I	162	LYS	CA-C	-5.15	1.46	1.52
4	2-C	817	ASP	CA-C	-5.15	1.45	1.52
7	2-G	147	ALA	N-CA	-5.15	1.40	1.46
7	2-K	119	ASN	N-CA	-5.15	1.40	1.46
6	2-M	35	TYR	N-CA	-5.15	1.39	1.46
5	2-I	79	ASP	N-CA	-5.15	1.40	1.46
5	2-I	162	LYS	CA-C	-5.15	1.46	1.52
4	3-C	817	ASP	CA-C	-5.15	1.45	1.52
7	3-G	147	ALA	N-CA	-5.15	1.40	1.46
7	3-K	119	ASN	N-CA	-5.15	1.40	1.46
6	3-M	35	TYR	N-CA	-5.15	1.39	1.46
5	3-I	79	ASP	N-CA	-5.15	1.40	1.46
5	3-I	162	LYS	CA-C	-5.15	1.46	1.52
1	1-A	758	ALA	N-CA	-5.15	1.40	1.46
3	1-B	52	SER	CA-C	-5.15	1.46	1.52
7	1-K	227	PHE	N-CA	-5.15	1.39	1.46
3	1-N	202	ALA	CA-C	-5.15	1.46	1.52
3	1-N	260	PHE	CA-C	-5.15	1.46	1.52
3	1-N	304	ILE	N-CA	-5.15	1.40	1.46
1	2-A	758	ALA	N-CA	-5.15	1.40	1.46
3	2-B	52	SER	CA-C	-5.15	1.46	1.52
7	2-K	227	PHE	N-CA	-5.15	1.39	1.46
3	2-N	202	ALA	CA-C	-5.15	1.46	1.52
3	2-N	260	PHE	CA-C	-5.15	1.46	1.52
3	2-N	304	ILE	N-CA	-5.15	1.40	1.46
1	3-A	758	ALA	N-CA	-5.15	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	52	SER	CA-C	-5.15	1.46	1.52
7	3-K	227	PHE	N-CA	-5.15	1.39	1.46
3	3-N	202	ALA	CA-C	-5.15	1.46	1.52
3	3-N	260	PHE	CA-C	-5.15	1.46	1.52
3	3-N	304	ILE	N-CA	-5.15	1.40	1.46
7	1-K	830	LEU	C-N	5.15	1.40	1.33
7	2-K	830	LEU	C-N	5.15	1.40	1.33
7	3-K	830	LEU	C-N	5.15	1.40	1.33
7	1-K	683	PRO	N-CA	5.15	1.52	1.46
5	1-I	9	CYS	CA-C	-5.15	1.46	1.52
7	2-K	683	PRO	N-CA	5.15	1.52	1.46
5	2-I	9	CYS	CA-C	-5.15	1.46	1.52
7	3-K	683	PRO	N-CA	5.15	1.52	1.46
5	3-I	9	CYS	CA-C	-5.15	1.46	1.52
6	1-R	128	GLN	CA-C	-5.15	1.46	1.52
6	2-R	128	GLN	CA-C	-5.15	1.46	1.52
6	3-R	128	GLN	CA-C	-5.15	1.46	1.52
7	1-K	34	PHE	CA-C	-5.14	1.46	1.52
6	1-J	96	ASP	CA-C	-5.14	1.46	1.52
7	2-K	34	PHE	CA-C	-5.14	1.46	1.52
6	2-J	96	ASP	CA-C	-5.14	1.46	1.52
7	3-K	34	PHE	CA-C	-5.14	1.46	1.52
6	3-J	96	ASP	CA-C	-5.14	1.46	1.52
3	1-B	304	ILE	N-CA	-5.14	1.40	1.46
3	1-B	306	LYS	N-CA	-5.14	1.40	1.46
5	1-D	106	CYS	CA-C	-5.14	1.46	1.52
7	1-G	872	SER	C-O	-5.14	1.18	1.24
3	2-B	304	ILE	N-CA	-5.14	1.40	1.46
3	2-B	306	LYS	N-CA	-5.14	1.40	1.46
5	2-D	106	CYS	CA-C	-5.14	1.46	1.52
7	2-G	872	SER	C-O	-5.14	1.18	1.24
3	3-B	304	ILE	N-CA	-5.14	1.40	1.46
3	3-B	306	LYS	N-CA	-5.14	1.40	1.46
5	3-D	106	CYS	CA-C	-5.14	1.46	1.52
7	3-G	872	SER	C-O	-5.14	1.18	1.24
3	1-N	201	ASP	CA-C	-5.14	1.46	1.52
3	1-N	284	VAL	CA-C	-5.14	1.45	1.52
3	2-N	201	ASP	CA-C	-5.14	1.46	1.52
3	2-N	284	VAL	CA-C	-5.14	1.45	1.52
3	3-N	201	ASP	CA-C	-5.14	1.46	1.52
3	3-N	284	VAL	CA-C	-5.14	1.45	1.52
1	1-A	466	LEU	N-CA	-5.14	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	693	CYS	CA-C	-5.14	1.46	1.52
3	1-B	403	HIS	CA-C	-5.14	1.46	1.52
1	2-A	466	LEU	N-CA	-5.14	1.39	1.46
1	2-A	693	CYS	CA-C	-5.14	1.46	1.52
3	2-B	403	HIS	CA-C	-5.14	1.46	1.52
1	3-A	466	LEU	N-CA	-5.14	1.39	1.46
1	3-A	693	CYS	CA-C	-5.14	1.46	1.52
3	3-B	403	HIS	CA-C	-5.14	1.46	1.52
3	1-B	473	ALA	N-CA	-5.14	1.40	1.46
6	1-J	28	ALA	CA-C	-5.14	1.45	1.52
3	2-B	473	ALA	N-CA	-5.14	1.40	1.46
6	2-J	28	ALA	CA-C	-5.14	1.45	1.52
3	3-B	473	ALA	N-CA	-5.14	1.40	1.46
6	3-J	28	ALA	CA-C	-5.14	1.45	1.52
8	1-Z	80	ILE	CA-C	-5.14	1.46	1.52
8	2-Z	80	ILE	CA-C	-5.14	1.46	1.52
8	3-Z	80	ILE	CA-C	-5.14	1.46	1.52
7	1-G	145	LYS	N-CA	-5.13	1.40	1.46
8	1-Z	45	GLU	N-CA	-5.13	1.40	1.46
8	1-Z	88	LEU	N-CA	-5.13	1.40	1.46
7	2-G	145	LYS	N-CA	-5.13	1.40	1.46
8	2-Z	45	GLU	N-CA	-5.13	1.40	1.46
8	2-Z	88	LEU	N-CA	-5.13	1.40	1.46
7	3-G	145	LYS	N-CA	-5.13	1.40	1.46
8	3-Z	45	GLU	N-CA	-5.13	1.40	1.46
8	3-Z	88	LEU	N-CA	-5.13	1.40	1.46
3	1-B	474	LEU	N-CA	-5.13	1.40	1.46
4	1-C	51	LYS	CA-C	-5.13	1.46	1.52
7	1-K	85	ARG	N-CA	-5.13	1.40	1.46
3	1-N	181	PHE	N-CA	-5.13	1.39	1.46
3	1-N	295	ALA	CA-C	-5.13	1.46	1.52
4	1-H	144	TYR	CA-C	-5.13	1.46	1.52
3	2-B	474	LEU	N-CA	-5.13	1.40	1.46
4	2-C	51	LYS	CA-C	-5.13	1.46	1.52
7	2-K	85	ARG	N-CA	-5.13	1.40	1.46
3	2-N	181	PHE	N-CA	-5.13	1.39	1.46
3	2-N	295	ALA	CA-C	-5.13	1.46	1.52
4	2-H	144	TYR	CA-C	-5.13	1.46	1.52
3	3-B	474	LEU	N-CA	-5.13	1.40	1.46
4	3-C	51	LYS	CA-C	-5.13	1.46	1.52
7	3-K	85	ARG	N-CA	-5.13	1.40	1.46
3	3-N	181	PHE	N-CA	-5.13	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-N	295	ALA	CA-C	-5.13	1.46	1.52
4	3-H	144	TYR	CA-C	-5.13	1.46	1.52
1	1-A	110	SER	CA-C	-5.13	1.46	1.52
4	1-C	621	VAL	N-CA	-5.13	1.40	1.46
4	1-C	646	GLU	CA-C	-5.13	1.46	1.52
4	1-H	678	ILE	N-CA	-5.13	1.40	1.46
1	2-A	110	SER	CA-C	-5.13	1.46	1.52
4	2-C	621	VAL	N-CA	-5.13	1.40	1.46
4	2-C	646	GLU	CA-C	-5.13	1.46	1.52
4	2-H	678	ILE	N-CA	-5.13	1.40	1.46
1	3-A	110	SER	CA-C	-5.13	1.46	1.52
4	3-C	621	VAL	N-CA	-5.13	1.40	1.46
4	3-C	646	GLU	CA-C	-5.13	1.46	1.52
4	3-H	678	ILE	N-CA	-5.13	1.40	1.46
1	1-A	162	TRP	CA-C	-5.13	1.46	1.52
4	1-C	194	TYR	CA-C	-5.13	1.46	1.52
1	2-A	162	TRP	CA-C	-5.13	1.46	1.52
4	2-C	194	TYR	CA-C	-5.13	1.46	1.52
1	3-A	162	TRP	CA-C	-5.13	1.46	1.52
4	3-C	194	TYR	CA-C	-5.13	1.46	1.52
1	1-A	476	ASP	CA-C	5.13	1.55	1.52
4	1-C	425	LYS	CA-C	-5.13	1.46	1.52
6	1-R	35	TYR	N-CA	-5.13	1.39	1.46
4	1-H	621	VAL	N-CA	-5.13	1.40	1.46
1	2-A	476	ASP	CA-C	5.13	1.55	1.52
4	2-C	425	LYS	CA-C	-5.13	1.46	1.52
6	2-R	35	TYR	N-CA	-5.13	1.39	1.46
4	2-H	621	VAL	N-CA	-5.13	1.40	1.46
1	3-A	476	ASP	CA-C	5.13	1.55	1.52
4	3-C	425	LYS	CA-C	-5.13	1.46	1.52
6	3-R	35	TYR	N-CA	-5.13	1.39	1.46
4	3-H	621	VAL	N-CA	-5.13	1.40	1.46
5	1-D	79	ASP	N-CA	-5.13	1.40	1.46
7	1-K	44	CYS	CA-C	-5.13	1.46	1.52
4	1-H	179	PHE	CA-C	-5.13	1.46	1.52
5	2-D	79	ASP	N-CA	-5.13	1.40	1.46
7	2-K	44	CYS	CA-C	-5.13	1.46	1.52
4	2-H	179	PHE	CA-C	-5.13	1.46	1.52
5	3-D	79	ASP	N-CA	-5.13	1.40	1.46
7	3-K	44	CYS	CA-C	-5.13	1.46	1.52
4	3-H	179	PHE	CA-C	-5.13	1.46	1.52
6	1-F	28	ALA	CA-C	-5.12	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2-F	28	ALA	CA-C	-5.12	1.45	1.52
6	3-F	28	ALA	CA-C	-5.12	1.45	1.52
7	1-K	872	SER	C-O	-5.12	1.18	1.24
4	1-H	646	GLU	CA-C	-5.12	1.46	1.52
5	1-I	9	CYS	N-CA	-5.12	1.39	1.45
5	1-I	129	GLN	N-CA	-5.12	1.40	1.46
7	2-K	872	SER	C-O	-5.12	1.18	1.24
4	2-H	646	GLU	CA-C	-5.12	1.46	1.52
5	2-I	9	CYS	N-CA	-5.12	1.39	1.45
5	2-I	129	GLN	N-CA	-5.12	1.40	1.46
7	3-K	872	SER	C-O	-5.12	1.18	1.24
4	3-H	646	GLU	CA-C	-5.12	1.46	1.52
5	3-I	9	CYS	N-CA	-5.12	1.39	1.45
5	3-I	129	GLN	N-CA	-5.12	1.40	1.46
1	1-A	561	ILE	CA-C	-5.12	1.46	1.52
7	1-G	440	CYS	CA-C	-5.12	1.46	1.52
1	2-A	561	ILE	CA-C	-5.12	1.46	1.52
7	2-G	440	CYS	CA-C	-5.12	1.46	1.52
1	3-A	561	ILE	CA-C	-5.12	1.46	1.52
7	3-G	440	CYS	CA-C	-5.12	1.46	1.52
4	1-C	156	ASN	N-CA	-5.12	1.39	1.46
7	1-K	300	LYS	CA-C	-5.12	1.45	1.53
4	2-C	156	ASN	N-CA	-5.12	1.39	1.46
7	2-K	300	LYS	CA-C	-5.12	1.45	1.53
4	3-C	156	ASN	N-CA	-5.12	1.39	1.46
7	3-K	300	LYS	CA-C	-5.12	1.45	1.53
6	1-M	75	ARG	N-CA	-5.12	1.40	1.46
6	2-M	75	ARG	N-CA	-5.12	1.40	1.46
6	3-M	75	ARG	N-CA	-5.12	1.40	1.46
5	1-D	27	THR	C-O	-5.12	1.17	1.24
7	1-G	683	PRO	N-CA	5.12	1.52	1.46
7	1-K	639	LEU	CA-C	-5.12	1.45	1.52
5	2-D	27	THR	C-O	-5.12	1.17	1.24
7	2-G	683	PRO	N-CA	5.12	1.52	1.46
7	2-K	639	LEU	CA-C	-5.12	1.45	1.52
5	3-D	27	THR	C-O	-5.12	1.17	1.24
7	3-G	683	PRO	N-CA	5.12	1.52	1.46
7	3-K	639	LEU	CA-C	-5.12	1.45	1.52
4	1-C	179	PHE	CA-C	-5.11	1.46	1.52
8	1-L	125	VAL	N-CA	-5.11	1.40	1.46
4	1-H	325	ALA	N-CA	-5.11	1.39	1.46
4	2-C	179	PHE	CA-C	-5.11	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2-L	125	VAL	N-CA	-5.11	1.40	1.46
4	2-H	325	ALA	N-CA	-5.11	1.39	1.46
4	3-C	179	PHE	CA-C	-5.11	1.46	1.52
8	3-L	125	VAL	N-CA	-5.11	1.40	1.46
4	3-H	325	ALA	N-CA	-5.11	1.39	1.46
6	1-R	61	ILE	CA-C	-5.11	1.46	1.52
6	1-R	154	PHE	N-CA	-5.11	1.39	1.46
6	2-R	61	ILE	CA-C	-5.11	1.46	1.52
6	2-R	154	PHE	N-CA	-5.11	1.39	1.46
6	3-R	61	ILE	CA-C	-5.11	1.46	1.52
6	3-R	154	PHE	N-CA	-5.11	1.39	1.46
3	1-B	260	PHE	CA-C	-5.11	1.46	1.52
3	1-B	963	GLN	CA-C	-5.11	1.46	1.52
6	1-R	85	THR	N-CA	-5.11	1.39	1.45
6	1-R	97	ARG	N-CA	-5.11	1.39	1.46
3	2-B	260	PHE	CA-C	-5.11	1.46	1.52
3	2-B	963	GLN	CA-C	-5.11	1.46	1.52
6	2-R	85	THR	N-CA	-5.11	1.39	1.45
6	2-R	97	ARG	N-CA	-5.11	1.39	1.46
3	3-B	260	PHE	CA-C	-5.11	1.46	1.52
3	3-B	963	GLN	CA-C	-5.11	1.46	1.52
6	3-R	85	THR	N-CA	-5.11	1.39	1.45
6	3-R	97	ARG	N-CA	-5.11	1.39	1.46
3	1-B	117	CYS	N-CA	-5.10	1.40	1.46
7	1-G	239	GLN	CA-C	-5.10	1.46	1.52
7	1-K	301	ALA	CA-C	-5.10	1.46	1.52
8	1-L	109	VAL	CA-C	-5.10	1.45	1.52
3	2-B	117	CYS	N-CA	-5.10	1.40	1.46
7	2-G	239	GLN	CA-C	-5.10	1.46	1.52
7	2-K	301	ALA	CA-C	-5.10	1.46	1.52
8	2-L	109	VAL	CA-C	-5.10	1.45	1.52
3	3-B	117	CYS	N-CA	-5.10	1.40	1.46
7	3-G	239	GLN	CA-C	-5.10	1.46	1.52
7	3-K	301	ALA	CA-C	-5.10	1.46	1.52
8	3-L	109	VAL	CA-C	-5.10	1.45	1.52
1	1-A	34	GLN	CA-C	-5.10	1.46	1.52
1	1-A	552	ALA	N-CA	-5.10	1.40	1.46
3	1-B	190	GLU	N-CA	-5.10	1.40	1.46
7	1-G	48	LEU	CA-C	-5.10	1.46	1.52
7	1-G	227	PHE	N-CA	-5.10	1.40	1.46
7	1-K	43	LYS	CA-C	-5.10	1.46	1.52
3	1-N	205	LYS	CA-C	-5.10	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-H	65	PHE	CA-C	-5.10	1.46	1.52
5	1-I	129	GLN	CA-C	-5.10	1.46	1.52
1	2-A	34	GLN	CA-C	-5.10	1.46	1.52
1	2-A	552	ALA	N-CA	-5.10	1.40	1.46
3	2-B	190	GLU	N-CA	-5.10	1.40	1.46
7	2-G	48	LEU	CA-C	-5.10	1.46	1.52
7	2-G	227	PHE	N-CA	-5.10	1.40	1.46
7	2-K	43	LYS	CA-C	-5.10	1.46	1.52
3	2-N	205	LYS	CA-C	-5.10	1.46	1.52
4	2-H	65	PHE	CA-C	-5.10	1.46	1.52
5	2-I	129	GLN	CA-C	-5.10	1.46	1.52
1	3-A	34	GLN	CA-C	-5.10	1.46	1.52
1	3-A	552	ALA	N-CA	-5.10	1.40	1.46
3	3-B	190	GLU	N-CA	-5.10	1.40	1.46
7	3-G	48	LEU	CA-C	-5.10	1.46	1.52
7	3-G	227	PHE	N-CA	-5.10	1.40	1.46
7	3-K	43	LYS	CA-C	-5.10	1.46	1.52
3	3-N	205	LYS	CA-C	-5.10	1.46	1.52
4	3-H	65	PHE	CA-C	-5.10	1.46	1.52
5	3-I	129	GLN	CA-C	-5.10	1.46	1.52
1	1-A	658	ILE	N-CA	-5.10	1.39	1.46
3	1-N	319	ARG	N-CA	-5.10	1.40	1.46
1	2-A	658	ILE	N-CA	-5.10	1.39	1.46
3	2-N	319	ARG	N-CA	-5.10	1.40	1.46
1	3-A	658	ILE	N-CA	-5.10	1.39	1.46
3	3-N	319	ARG	N-CA	-5.10	1.40	1.46
4	1-C	65	PHE	CA-C	-5.10	1.46	1.52
5	1-D	129	GLN	CA-C	-5.10	1.46	1.52
6	1-M	47	PRO	N-CA	-5.10	1.41	1.47
4	1-H	544	ASN	N-CA	-5.10	1.39	1.45
4	2-C	65	PHE	CA-C	-5.10	1.46	1.52
5	2-D	129	GLN	CA-C	-5.10	1.46	1.52
6	2-M	47	PRO	N-CA	-5.10	1.41	1.47
4	2-H	544	ASN	N-CA	-5.10	1.39	1.45
4	3-C	65	PHE	CA-C	-5.10	1.46	1.52
5	3-D	129	GLN	CA-C	-5.10	1.46	1.52
6	3-M	47	PRO	N-CA	-5.10	1.41	1.47
4	3-H	544	ASN	N-CA	-5.10	1.39	1.45
4	1-C	317	ALA	CA-C	-5.10	1.46	1.52
7	1-G	75	LYS	CA-C	-5.10	1.45	1.52
7	1-G	121	ARG	N-CA	-5.10	1.40	1.46
4	2-C	317	ALA	CA-C	-5.10	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	75	LYS	CA-C	-5.10	1.45	1.52
7	2-G	121	ARG	N-CA	-5.10	1.40	1.46
4	3-C	317	ALA	CA-C	-5.10	1.46	1.52
7	3-G	75	LYS	CA-C	-5.10	1.45	1.52
7	3-G	121	ARG	N-CA	-5.10	1.40	1.46
1	1-A	638	ALA	CA-C	-5.10	1.46	1.52
4	1-C	689	CYS	CA-C	-5.10	1.46	1.52
7	1-G	214	MET	N-CA	-5.10	1.40	1.46
1	2-A	638	ALA	CA-C	-5.10	1.46	1.52
4	2-C	689	CYS	CA-C	-5.10	1.46	1.52
7	2-G	214	MET	N-CA	-5.10	1.40	1.46
1	3-A	638	ALA	CA-C	-5.10	1.46	1.52
4	3-C	689	CYS	CA-C	-5.10	1.46	1.52
7	3-G	214	MET	N-CA	-5.10	1.40	1.46
7	1-G	798	GLU	CA-C	-5.09	1.46	1.52
6	1-R	84	ASN	N-CA	-5.09	1.39	1.46
5	1-I	162	LYS	N-CA	-5.09	1.40	1.46
7	2-G	798	GLU	CA-C	-5.09	1.46	1.52
6	2-R	84	ASN	N-CA	-5.09	1.39	1.46
5	2-I	162	LYS	N-CA	-5.09	1.40	1.46
7	3-G	798	GLU	CA-C	-5.09	1.46	1.52
6	3-R	84	ASN	N-CA	-5.09	1.39	1.46
5	3-I	162	LYS	N-CA	-5.09	1.40	1.46
4	1-H	397	ALA	N-CA	-5.09	1.40	1.46
4	1-H	420	GLU	CA-C	-5.09	1.46	1.52
4	2-H	397	ALA	N-CA	-5.09	1.40	1.46
4	2-H	420	GLU	CA-C	-5.09	1.46	1.52
4	3-H	397	ALA	N-CA	-5.09	1.40	1.46
4	3-H	420	GLU	CA-C	-5.09	1.46	1.52
1	1-A	629	LEU	N-CA	-5.09	1.39	1.46
7	1-K	166	LEU	N-CA	-5.09	1.39	1.46
4	1-H	399	ASP	N-CA	-5.09	1.40	1.46
1	2-A	629	LEU	N-CA	-5.09	1.39	1.46
7	2-K	166	LEU	N-CA	-5.09	1.39	1.46
4	2-H	399	ASP	N-CA	-5.09	1.40	1.46
1	3-A	629	LEU	N-CA	-5.09	1.39	1.46
7	3-K	166	LEU	N-CA	-5.09	1.39	1.46
4	3-H	399	ASP	N-CA	-5.09	1.40	1.46
4	1-C	399	ASP	N-CA	-5.09	1.40	1.46
5	1-D	9	CYS	N-CA	-5.09	1.39	1.45
7	1-K	88	CYS	N-CA	-5.09	1.40	1.46
4	2-C	399	ASP	N-CA	-5.09	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2-D	9	CYS	N-CA	-5.09	1.39	1.45
7	2-K	88	CYS	N-CA	-5.09	1.40	1.46
4	3-C	399	ASP	N-CA	-5.09	1.40	1.46
5	3-D	9	CYS	N-CA	-5.09	1.39	1.45
7	3-K	88	CYS	N-CA	-5.09	1.40	1.46
4	1-C	420	GLU	CA-C	-5.08	1.46	1.52
4	1-H	506	THR	N-CA	-5.08	1.40	1.46
4	2-C	420	GLU	CA-C	-5.08	1.46	1.52
4	2-H	506	THR	N-CA	-5.08	1.40	1.46
4	3-C	420	GLU	CA-C	-5.08	1.46	1.52
4	3-H	506	THR	N-CA	-5.08	1.40	1.46
4	1-C	644	ARG	N-CA	-5.08	1.40	1.46
7	1-G	156	SER	N-CA	-5.08	1.40	1.46
7	1-G	307	ALA	N-CA	-5.08	1.40	1.46
8	1-L	66	THR	N-CA	-5.08	1.39	1.46
4	2-C	644	ARG	N-CA	-5.08	1.40	1.46
7	2-G	156	SER	N-CA	-5.08	1.40	1.46
7	2-G	307	ALA	N-CA	-5.08	1.40	1.46
8	2-L	66	THR	N-CA	-5.08	1.39	1.46
4	3-C	644	ARG	N-CA	-5.08	1.40	1.46
7	3-G	156	SER	N-CA	-5.08	1.40	1.46
7	3-G	307	ALA	N-CA	-5.08	1.40	1.46
8	3-L	66	THR	N-CA	-5.08	1.39	1.46
5	1-D	129	GLN	N-CA	-5.08	1.40	1.46
7	1-G	175	LYS	C-N	-5.08	1.27	1.34
5	2-D	129	GLN	N-CA	-5.08	1.40	1.46
7	2-G	175	LYS	C-N	-5.08	1.27	1.34
5	3-D	129	GLN	N-CA	-5.08	1.40	1.46
7	3-G	175	LYS	C-N	-5.08	1.27	1.34
6	1-F	118	ASN	CA-C	-5.08	1.47	1.53
6	2-F	118	ASN	CA-C	-5.08	1.47	1.53
6	3-F	118	ASN	CA-C	-5.08	1.47	1.53
5	1-D	162	LYS	N-CA	-5.08	1.40	1.46
5	2-D	162	LYS	N-CA	-5.08	1.40	1.46
5	3-D	162	LYS	N-CA	-5.08	1.40	1.46
7	1-G	534	VAL	CA-C	-5.07	1.46	1.52
7	1-G	766	LYS	CA-C	-5.07	1.46	1.52
7	1-K	658	HIS	CA-C	-5.07	1.46	1.52
3	1-N	473	ALA	N-CA	-5.07	1.40	1.46
7	2-G	534	VAL	CA-C	-5.07	1.46	1.52
7	2-G	766	LYS	CA-C	-5.07	1.46	1.52
7	2-K	658	HIS	CA-C	-5.07	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-N	473	ALA	N-CA	-5.07	1.40	1.46
7	3-G	534	VAL	CA-C	-5.07	1.46	1.52
7	3-G	766	LYS	CA-C	-5.07	1.46	1.52
7	3-K	658	HIS	CA-C	-5.07	1.46	1.52
3	3-N	473	ALA	N-CA	-5.07	1.40	1.46
4	1-C	259	SER	N-CA	-5.07	1.39	1.46
4	1-C	325	ALA	N-CA	-5.07	1.39	1.46
4	2-C	259	SER	N-CA	-5.07	1.39	1.46
4	2-C	325	ALA	N-CA	-5.07	1.39	1.46
4	3-C	259	SER	N-CA	-5.07	1.39	1.46
4	3-C	325	ALA	N-CA	-5.07	1.39	1.46
3	1-B	832	VAL	CA-C	-5.07	1.46	1.52
4	1-C	616	GLU	N-CA	-5.07	1.40	1.46
7	1-G	146	GLN	CA-C	-5.07	1.46	1.52
3	2-B	832	VAL	CA-C	-5.07	1.46	1.52
4	2-C	616	GLU	N-CA	-5.07	1.40	1.46
7	2-G	146	GLN	CA-C	-5.07	1.46	1.52
3	3-B	832	VAL	CA-C	-5.07	1.46	1.52
4	3-C	616	GLU	N-CA	-5.07	1.40	1.46
7	3-G	146	GLN	CA-C	-5.07	1.46	1.52
7	1-K	144	MET	CA-C	-5.07	1.46	1.52
7	1-K	850	ASP	CA-C	-5.07	1.46	1.52
7	2-K	144	MET	CA-C	-5.07	1.46	1.52
7	2-K	850	ASP	CA-C	-5.07	1.46	1.52
7	3-K	144	MET	CA-C	-5.07	1.46	1.52
7	3-K	850	ASP	CA-C	-5.07	1.46	1.52
3	1-B	471	ARG	N-CA	-5.07	1.40	1.46
4	1-C	361	ASN	N-CA	-5.07	1.38	1.45
6	1-R	125	ALA	CA-C	-5.07	1.46	1.52
3	1-N	269	GLN	N-CA	-5.07	1.39	1.46
3	2-B	471	ARG	N-CA	-5.07	1.40	1.46
4	2-C	361	ASN	N-CA	-5.07	1.38	1.45
6	2-R	125	ALA	CA-C	-5.07	1.46	1.52
3	2-N	269	GLN	N-CA	-5.07	1.39	1.46
3	3-B	471	ARG	N-CA	-5.07	1.40	1.46
4	3-C	361	ASN	N-CA	-5.07	1.38	1.45
6	3-R	125	ALA	CA-C	-5.07	1.46	1.52
3	3-N	269	GLN	N-CA	-5.07	1.39	1.46
4	1-H	111	GLN	CA-C	-5.07	1.45	1.52
4	1-H	644	ARG	N-CA	-5.07	1.40	1.46
4	2-H	111	GLN	CA-C	-5.07	1.45	1.52
4	2-H	644	ARG	N-CA	-5.07	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3-H	111	GLN	CA-C	-5.07	1.45	1.52
4	3-H	644	ARG	N-CA	-5.07	1.40	1.46
3	1-B	224	LEU	CA-C	-5.06	1.46	1.52
3	2-B	224	LEU	CA-C	-5.06	1.46	1.52
3	3-B	224	LEU	CA-C	-5.06	1.46	1.52
1	1-A	521	LEU	N-CA	-5.06	1.40	1.46
3	1-B	269	GLN	N-CA	-5.06	1.39	1.46
4	1-C	9	ARG	CA-C	-5.06	1.46	1.52
4	1-C	397	ALA	N-CA	-5.06	1.40	1.46
7	1-G	39	ILE	N-CA	-5.06	1.41	1.46
7	1-K	287	PRO	CA-C	-5.06	1.45	1.52
1	2-A	521	LEU	N-CA	-5.06	1.40	1.46
3	2-B	269	GLN	N-CA	-5.06	1.39	1.46
4	2-C	9	ARG	CA-C	-5.06	1.46	1.52
4	2-C	397	ALA	N-CA	-5.06	1.40	1.46
7	2-G	39	ILE	N-CA	-5.06	1.41	1.46
7	2-K	287	PRO	CA-C	-5.06	1.45	1.52
1	3-A	521	LEU	N-CA	-5.06	1.40	1.46
3	3-B	269	GLN	N-CA	-5.06	1.39	1.46
4	3-C	9	ARG	CA-C	-5.06	1.46	1.52
4	3-C	397	ALA	N-CA	-5.06	1.40	1.46
7	3-G	39	ILE	N-CA	-5.06	1.41	1.46
7	3-K	287	PRO	CA-C	-5.06	1.45	1.52
1	1-A	65	LEU	CA-C	-5.06	1.46	1.52
1	2-A	65	LEU	CA-C	-5.06	1.46	1.52
1	3-A	65	LEU	CA-C	-5.06	1.46	1.52
8	1-L	145	ARG	N-CA	-5.06	1.39	1.46
5	1-I	90	ILE	CA-C	-5.06	1.47	1.52
6	1-J	111	LEU	CA-C	-5.06	1.45	1.52
8	2-L	145	ARG	N-CA	-5.06	1.39	1.46
5	2-I	90	ILE	CA-C	-5.06	1.47	1.52
6	2-J	111	LEU	CA-C	-5.06	1.45	1.52
8	3-L	145	ARG	N-CA	-5.06	1.39	1.46
5	3-I	90	ILE	CA-C	-5.06	1.47	1.52
6	3-J	111	LEU	CA-C	-5.06	1.45	1.52
1	1-A	682	LEU	N-CA	-5.06	1.40	1.46
7	1-G	401	LEU	N-CA	-5.06	1.40	1.46
7	1-G	483	GLU	CA-C	-5.06	1.46	1.53
7	1-K	766	LYS	CA-C	-5.06	1.46	1.52
7	1-K	798	GLU	CA-C	-5.06	1.46	1.52
1	2-A	682	LEU	N-CA	-5.06	1.40	1.46
7	2-G	401	LEU	N-CA	-5.06	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	2-G	483	GLU	CA-C	-5.06	1.46	1.53
7	2-K	766	LYS	CA-C	-5.06	1.46	1.52
7	2-K	798	GLU	CA-C	-5.06	1.46	1.52
1	3-A	682	LEU	N-CA	-5.06	1.40	1.46
7	3-G	401	LEU	N-CA	-5.06	1.40	1.46
7	3-G	483	GLU	CA-C	-5.06	1.46	1.53
7	3-K	766	LYS	CA-C	-5.06	1.46	1.52
7	3-K	798	GLU	CA-C	-5.06	1.46	1.52
7	1-G	658	HIS	CA-C	-5.05	1.46	1.52
4	1-H	156	ASN	N-CA	-5.05	1.39	1.46
7	2-G	658	HIS	CA-C	-5.05	1.46	1.52
4	2-H	156	ASN	N-CA	-5.05	1.39	1.46
7	3-G	658	HIS	CA-C	-5.05	1.46	1.52
4	3-H	156	ASN	N-CA	-5.05	1.39	1.46
3	1-B	845	ILE	N-CA	-5.05	1.40	1.46
4	1-C	529	TRP	N-CA	-5.05	1.39	1.46
4	1-C	544	ASN	N-CA	-5.05	1.39	1.45
3	2-B	845	ILE	N-CA	-5.05	1.40	1.46
4	2-C	529	TRP	N-CA	-5.05	1.39	1.46
4	2-C	544	ASN	N-CA	-5.05	1.39	1.45
3	3-B	845	ILE	N-CA	-5.05	1.40	1.46
4	3-C	529	TRP	N-CA	-5.05	1.39	1.46
4	3-C	544	ASN	N-CA	-5.05	1.39	1.45
1	1-A	508	LYS	CA-C	-5.05	1.46	1.52
3	1-B	265	TYR	N-CA	-5.05	1.40	1.46
3	1-B	375	LEU	C-N	-5.05	1.27	1.33
3	1-B	385	VAL	CA-C	-5.05	1.46	1.52
3	1-B	434	ASP	C-N	-5.05	1.27	1.33
3	1-B	946	ALA	CA-C	-5.05	1.46	1.52
7	1-K	835	ARG	CA-C	-5.05	1.46	1.52
4	1-H	457	LEU	CA-C	-5.05	1.46	1.52
1	2-A	508	LYS	CA-C	-5.05	1.46	1.52
3	2-B	265	TYR	N-CA	-5.05	1.40	1.46
3	2-B	375	LEU	C-N	-5.05	1.27	1.33
3	2-B	385	VAL	CA-C	-5.05	1.46	1.52
3	2-B	434	ASP	C-N	-5.05	1.27	1.33
3	2-B	946	ALA	CA-C	-5.05	1.46	1.52
7	2-K	835	ARG	CA-C	-5.05	1.46	1.52
4	2-H	457	LEU	CA-C	-5.05	1.46	1.52
1	3-A	508	LYS	CA-C	-5.05	1.46	1.52
3	3-B	265	TYR	N-CA	-5.05	1.40	1.46
3	3-B	375	LEU	C-N	-5.05	1.27	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-B	385	VAL	CA-C	-5.05	1.46	1.52
3	3-B	434	ASP	C-N	-5.05	1.27	1.33
3	3-B	946	ALA	CA-C	-5.05	1.46	1.52
7	3-K	835	ARG	CA-C	-5.05	1.46	1.52
4	3-H	457	LEU	CA-C	-5.05	1.46	1.52
4	1-C	780	VAL	N-CA	-5.04	1.40	1.46
4	2-C	780	VAL	N-CA	-5.04	1.40	1.46
4	3-C	780	VAL	N-CA	-5.04	1.40	1.46
4	1-C	38	SER	CA-C	-5.04	1.46	1.52
7	1-G	835	ARG	CA-C	-5.04	1.46	1.52
7	1-G	868	ILE	CA-C	-5.04	1.46	1.52
6	1-M	130	LEU	CA-C	-5.04	1.47	1.52
3	1-N	535	THR	C-N	5.04	1.40	1.33
4	1-H	616	GLU	N-CA	-5.04	1.40	1.46
4	2-C	38	SER	CA-C	-5.04	1.46	1.52
7	2-G	835	ARG	CA-C	-5.04	1.46	1.52
7	2-G	868	ILE	CA-C	-5.04	1.46	1.52
6	2-M	130	LEU	CA-C	-5.04	1.47	1.52
3	2-N	535	THR	C-N	5.04	1.40	1.33
4	2-H	616	GLU	N-CA	-5.04	1.40	1.46
4	3-C	38	SER	CA-C	-5.04	1.46	1.52
7	3-G	835	ARG	CA-C	-5.04	1.46	1.52
7	3-G	868	ILE	CA-C	-5.04	1.46	1.52
6	3-M	130	LEU	CA-C	-5.04	1.47	1.52
3	3-N	535	THR	C-N	5.04	1.40	1.33
4	3-H	616	GLU	N-CA	-5.04	1.40	1.46
5	1-D	9	CYS	CA-C	-5.04	1.46	1.52
8	1-Z	125	VAL	N-CA	-5.04	1.40	1.46
3	1-N	165	TYR	CA-C	-5.04	1.46	1.52
5	2-D	9	CYS	CA-C	-5.04	1.46	1.52
8	2-Z	125	VAL	N-CA	-5.04	1.40	1.46
3	2-N	165	TYR	CA-C	-5.04	1.46	1.52
5	3-D	9	CYS	CA-C	-5.04	1.46	1.52
8	3-Z	125	VAL	N-CA	-5.04	1.40	1.46
3	3-N	165	TYR	CA-C	-5.04	1.46	1.52
3	1-B	417	ILE	N-CA	-5.04	1.40	1.46
7	1-G	242	GLU	CA-C	-5.04	1.46	1.52
3	2-B	417	ILE	N-CA	-5.04	1.40	1.46
7	2-G	242	GLU	CA-C	-5.04	1.46	1.52
3	3-B	417	ILE	N-CA	-5.04	1.40	1.46
7	3-G	242	GLU	CA-C	-5.04	1.46	1.52
4	1-C	314	ILE	C-N	-5.04	1.27	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1-G	479	ARG	CA-C	-5.04	1.46	1.52
7	1-G	509	ILE	CA-C	-5.04	1.45	1.52
7	1-K	228	ALA	CA-C	-5.04	1.46	1.52
7	1-K	255	ILE	N-CA	-5.04	1.40	1.46
4	2-C	314	ILE	C-N	-5.04	1.27	1.33
7	2-G	479	ARG	CA-C	-5.04	1.46	1.52
7	2-G	509	ILE	CA-C	-5.04	1.45	1.52
7	2-K	228	ALA	CA-C	-5.04	1.46	1.52
7	2-K	255	ILE	N-CA	-5.04	1.40	1.46
4	3-C	314	ILE	C-N	-5.04	1.27	1.33
7	3-G	479	ARG	CA-C	-5.04	1.46	1.52
7	3-G	509	ILE	CA-C	-5.04	1.45	1.52
7	3-K	228	ALA	CA-C	-5.04	1.46	1.52
7	3-K	255	ILE	N-CA	-5.04	1.40	1.46
7	1-K	141	GLU	CA-C	-5.04	1.46	1.52
7	1-K	868	ILE	CA-C	-5.04	1.46	1.52
4	1-H	125	LEU	CA-C	-5.04	1.46	1.52
7	2-K	141	GLU	CA-C	-5.04	1.46	1.52
7	2-K	868	ILE	CA-C	-5.04	1.46	1.52
4	2-H	125	LEU	CA-C	-5.04	1.46	1.52
7	3-K	141	GLU	CA-C	-5.04	1.46	1.52
7	3-K	868	ILE	CA-C	-5.04	1.46	1.52
4	3-H	125	LEU	CA-C	-5.04	1.46	1.52
4	1-C	457	LEU	CA-C	-5.04	1.46	1.52
8	1-L	105	LEU	N-CA	-5.04	1.39	1.46
4	2-C	457	LEU	CA-C	-5.04	1.46	1.52
8	2-L	105	LEU	N-CA	-5.04	1.39	1.46
4	3-C	457	LEU	CA-C	-5.04	1.46	1.52
8	3-L	105	LEU	N-CA	-5.04	1.39	1.46
3	1-B	314	LEU	N-CA	-5.03	1.40	1.46
7	1-K	197	LEU	CA-C	-5.03	1.45	1.52
3	2-B	314	LEU	N-CA	-5.03	1.40	1.46
7	2-K	197	LEU	CA-C	-5.03	1.45	1.52
3	3-B	314	LEU	N-CA	-5.03	1.40	1.46
7	3-K	197	LEU	CA-C	-5.03	1.45	1.52
4	1-C	111	GLN	CA-C	-5.03	1.45	1.52
3	1-N	375	LEU	C-N	-5.03	1.27	1.33
4	1-H	11	LEU	CA-C	-5.03	1.46	1.52
4	1-H	259	SER	N-CA	-5.03	1.39	1.46
4	2-C	111	GLN	CA-C	-5.03	1.45	1.52
3	2-N	375	LEU	C-N	-5.03	1.27	1.33
4	2-H	11	LEU	CA-C	-5.03	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-H	259	SER	N-CA	-5.03	1.39	1.46
4	3-C	111	GLN	CA-C	-5.03	1.45	1.52
3	3-N	375	LEU	C-N	-5.03	1.27	1.33
4	3-H	11	LEU	CA-C	-5.03	1.46	1.52
4	3-H	259	SER	N-CA	-5.03	1.39	1.46
3	1-B	165	TYR	CA-C	-5.03	1.46	1.52
3	1-B	295	ALA	CA-C	-5.03	1.46	1.52
3	1-B	317	LEU	C-O	-5.03	1.18	1.24
4	1-C	222	VAL	CA-C	-5.03	1.47	1.52
8	1-Z	141	GLN	CA-C	-5.03	1.46	1.52
4	1-H	314	ILE	N-CA	-5.03	1.40	1.46
3	2-B	165	TYR	CA-C	-5.03	1.46	1.52
3	2-B	295	ALA	CA-C	-5.03	1.46	1.52
3	2-B	317	LEU	C-O	-5.03	1.18	1.24
4	2-C	222	VAL	CA-C	-5.03	1.47	1.52
8	2-Z	141	GLN	CA-C	-5.03	1.46	1.52
4	2-H	314	ILE	N-CA	-5.03	1.40	1.46
3	3-B	165	TYR	CA-C	-5.03	1.46	1.52
3	3-B	295	ALA	CA-C	-5.03	1.46	1.52
3	3-B	317	LEU	C-O	-5.03	1.18	1.24
4	3-C	222	VAL	CA-C	-5.03	1.47	1.52
8	3-Z	141	GLN	CA-C	-5.03	1.46	1.52
4	3-H	314	ILE	N-CA	-5.03	1.40	1.46
3	1-N	417	ILE	N-CA	-5.03	1.40	1.46
3	2-N	417	ILE	N-CA	-5.03	1.40	1.46
3	3-N	417	ILE	N-CA	-5.03	1.40	1.46
3	1-N	337	VAL	CA-C	-5.03	1.46	1.52
4	1-H	361	ASN	N-CA	-5.03	1.38	1.45
3	2-N	337	VAL	CA-C	-5.03	1.46	1.52
4	2-H	361	ASN	N-CA	-5.03	1.38	1.45
3	3-N	337	VAL	CA-C	-5.03	1.46	1.52
4	3-H	361	ASN	N-CA	-5.03	1.38	1.45
3	1-B	319	ARG	N-CA	-5.03	1.40	1.46
6	1-M	19	ARG	N-CA	-5.03	1.40	1.46
3	2-B	319	ARG	N-CA	-5.03	1.40	1.46
6	2-M	19	ARG	N-CA	-5.03	1.40	1.46
3	3-B	319	ARG	N-CA	-5.03	1.40	1.46
6	3-M	19	ARG	N-CA	-5.03	1.40	1.46
7	1-K	306	ALA	N-CA	-5.02	1.40	1.46
3	1-N	265	TYR	N-CA	-5.02	1.40	1.46
5	1-I	27	THR	C-O	-5.02	1.17	1.24
7	2-K	306	ALA	N-CA	-5.02	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-N	265	TYR	N-CA	-5.02	1.40	1.46
5	2-I	27	THR	C-O	-5.02	1.17	1.24
7	3-K	306	ALA	N-CA	-5.02	1.40	1.46
3	3-N	265	TYR	N-CA	-5.02	1.40	1.46
5	3-I	27	THR	C-O	-5.02	1.17	1.24
5	1-D	66	MET	CA-C	-5.02	1.46	1.52
5	2-D	66	MET	CA-C	-5.02	1.46	1.52
5	3-D	66	MET	CA-C	-5.02	1.46	1.52
3	1-B	278	GLU	N-CA	-5.02	1.40	1.46
3	1-B	835	SER	N-CA	-5.02	1.39	1.45
5	1-D	90	ILE	CA-C	-5.02	1.47	1.52
6	1-F	111	LEU	CA-C	-5.02	1.45	1.52
3	1-N	124	LEU	N-CA	-5.02	1.39	1.46
3	2-B	278	GLU	N-CA	-5.02	1.40	1.46
3	2-B	835	SER	N-CA	-5.02	1.39	1.45
5	2-D	90	ILE	CA-C	-5.02	1.47	1.52
6	2-F	111	LEU	CA-C	-5.02	1.45	1.52
3	2-N	124	LEU	N-CA	-5.02	1.39	1.46
3	3-B	278	GLU	N-CA	-5.02	1.40	1.46
3	3-B	835	SER	N-CA	-5.02	1.39	1.45
5	3-D	90	ILE	CA-C	-5.02	1.47	1.52
6	3-F	111	LEU	CA-C	-5.02	1.45	1.52
3	3-N	124	LEU	N-CA	-5.02	1.39	1.46
3	1-B	436	LEU	CA-C	-5.02	1.46	1.52
7	1-K	269	GLU	N-CA	-5.02	1.40	1.46
3	2-B	436	LEU	CA-C	-5.02	1.46	1.52
7	2-K	269	GLU	N-CA	-5.02	1.40	1.46
3	3-B	436	LEU	CA-C	-5.02	1.46	1.52
7	3-K	269	GLU	N-CA	-5.02	1.40	1.46
3	1-B	535	THR	C-N	5.02	1.40	1.33
5	1-I	66	MET	CA-C	-5.02	1.46	1.52
3	2-B	535	THR	C-N	5.02	1.40	1.33
5	2-I	66	MET	CA-C	-5.02	1.46	1.52
3	3-B	535	THR	C-N	5.02	1.40	1.33
5	3-I	66	MET	CA-C	-5.02	1.46	1.52
1	1-A	74	LYS	N-CA	-5.01	1.39	1.46
3	1-B	294	LYS	N-CA	-5.01	1.40	1.46
7	1-G	668	THR	CA-C	-5.01	1.46	1.52
4	1-H	38	SER	CA-C	-5.01	1.46	1.52
1	2-A	74	LYS	N-CA	-5.01	1.39	1.46
3	2-B	294	LYS	N-CA	-5.01	1.40	1.46
7	2-G	668	THR	CA-C	-5.01	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-H	38	SER	CA-C	-5.01	1.46	1.52
1	3-A	74	LYS	N-CA	-5.01	1.39	1.46
3	3-B	294	LYS	N-CA	-5.01	1.40	1.46
7	3-G	668	THR	CA-C	-5.01	1.46	1.52
4	3-H	38	SER	CA-C	-5.01	1.46	1.52
8	1-L	30	TYR	N-CA	-5.01	1.40	1.46
3	1-N	371	LEU	C-O	-5.01	1.18	1.24
4	1-H	9	ARG	CA-C	-5.01	1.46	1.52
8	2-L	30	TYR	N-CA	-5.01	1.40	1.46
3	2-N	371	LEU	C-O	-5.01	1.18	1.24
4	2-H	9	ARG	CA-C	-5.01	1.46	1.52
8	3-L	30	TYR	N-CA	-5.01	1.40	1.46
3	3-N	371	LEU	C-O	-5.01	1.18	1.24
4	3-H	9	ARG	CA-C	-5.01	1.46	1.52
6	1-F	96	ASP	CA-C	-5.01	1.46	1.52
6	2-F	96	ASP	CA-C	-5.01	1.46	1.52
6	3-F	96	ASP	CA-C	-5.01	1.46	1.52
3	1-N	211	MET	N-CA	-5.01	1.40	1.46
3	2-N	211	MET	N-CA	-5.01	1.40	1.46
3	3-N	211	MET	N-CA	-5.01	1.40	1.46
3	1-B	358	LEU	CA-C	-5.01	1.46	1.52
3	1-B	746	TYR	CA-C	-5.01	1.46	1.52
7	1-K	839	ASP	N-CA	-5.01	1.39	1.45
8	1-L	37	SER	N-CA	-5.01	1.39	1.46
3	2-B	358	LEU	CA-C	-5.01	1.46	1.52
3	2-B	746	TYR	CA-C	-5.01	1.46	1.52
7	2-K	839	ASP	N-CA	-5.01	1.39	1.45
8	2-L	37	SER	N-CA	-5.01	1.39	1.46
3	3-B	358	LEU	CA-C	-5.01	1.46	1.52
3	3-B	746	TYR	CA-C	-5.01	1.46	1.52
7	3-K	839	ASP	N-CA	-5.01	1.39	1.45
8	3-L	37	SER	N-CA	-5.01	1.39	1.46
3	1-B	371	LEU	C-O	-5.00	1.18	1.24
6	1-R	30	LYS	CA-C	-5.00	1.46	1.52
4	1-H	334	GLU	C-N	5.00	1.40	1.33
3	2-B	371	LEU	C-O	-5.00	1.18	1.24
6	2-R	30	LYS	CA-C	-5.00	1.46	1.52
4	2-H	334	GLU	C-N	5.00	1.40	1.33
3	3-B	371	LEU	C-O	-5.00	1.18	1.24
6	3-R	30	LYS	CA-C	-5.00	1.46	1.52
4	3-H	334	GLU	C-N	5.00	1.40	1.33
1	1-A	304	ASN	CA-C	-5.00	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-C	178	ASN	CA-C	-5.00	1.46	1.52
5	1-D	20	GLN	N-CA	-5.00	1.40	1.46
7	1-K	80	ASN	CA-C	-5.00	1.46	1.52
4	1-H	94	MET	CA-C	-5.00	1.46	1.52
1	2-A	304	ASN	CA-C	-5.00	1.46	1.52
4	2-C	178	ASN	CA-C	-5.00	1.46	1.52
5	2-D	20	GLN	N-CA	-5.00	1.40	1.46
7	2-K	80	ASN	CA-C	-5.00	1.46	1.52
4	2-H	94	MET	CA-C	-5.00	1.46	1.52
1	3-A	304	ASN	CA-C	-5.00	1.46	1.52
4	3-C	178	ASN	CA-C	-5.00	1.46	1.52
5	3-D	20	GLN	N-CA	-5.00	1.40	1.46
7	3-K	80	ASN	CA-C	-5.00	1.46	1.52
4	3-H	94	MET	CA-C	-5.00	1.46	1.52
4	1-C	68	ARG	CA-C	-5.00	1.46	1.52
7	1-G	679	VAL	CA-C	-5.00	1.46	1.52
3	1-N	224	LEU	CA-C	-5.00	1.46	1.52
4	2-C	68	ARG	CA-C	-5.00	1.46	1.52
7	2-G	679	VAL	CA-C	-5.00	1.46	1.52
3	2-N	224	LEU	CA-C	-5.00	1.46	1.52
4	3-C	68	ARG	CA-C	-5.00	1.46	1.52
7	3-G	679	VAL	CA-C	-5.00	1.46	1.52
3	3-N	224	LEU	CA-C	-5.00	1.46	1.52

All (8208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	693	VAL	CA-C-N	-22.64	91.53	119.84
7	1-G	693	VAL	C-N-CA	-22.64	91.53	119.84
7	2-G	693	VAL	CA-C-N	-22.64	91.53	119.84
7	2-G	693	VAL	C-N-CA	-22.64	91.53	119.84
7	3-G	693	VAL	CA-C-N	-22.64	91.53	119.84
7	3-G	693	VAL	C-N-CA	-22.64	91.53	119.84
7	1-G	277	LEU	CA-C-N	-19.07	96.01	119.84
7	1-G	277	LEU	C-N-CA	-19.07	96.01	119.84
7	2-G	277	LEU	CA-C-N	-19.07	96.01	119.84
7	2-G	277	LEU	C-N-CA	-19.07	96.01	119.84
7	3-G	277	LEU	CA-C-N	-19.07	96.01	119.84
7	3-G	277	LEU	C-N-CA	-19.07	96.01	119.84
3	1-B	933	GLY	CA-C-N	-19.00	96.09	119.84
3	1-B	933	GLY	C-N-CA	-19.00	96.09	119.84
3	2-B	933	GLY	CA-C-N	-19.00	96.09	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2-B	933	GLY	C-N-CA	-19.00	96.09	119.84
3	3-B	933	GLY	CA-C-N	-19.00	96.09	119.84
3	3-B	933	GLY	C-N-CA	-19.00	96.09	119.84
1	1-A	586	ARG	CA-C-N	18.91	141.27	120.66
1	1-A	586	ARG	C-N-CA	18.91	141.27	120.66
1	2-A	586	ARG	CA-C-N	18.91	141.27	120.66
1	2-A	586	ARG	C-N-CA	18.91	141.27	120.66
1	3-A	586	ARG	CA-C-N	18.91	141.27	120.66
1	3-A	586	ARG	C-N-CA	18.91	141.27	120.66
7	1-K	117	GLU	CA-C-N	18.14	146.05	120.29
7	1-K	117	GLU	C-N-CA	18.14	146.05	120.29
7	2-K	117	GLU	CA-C-N	18.14	146.05	120.29
7	2-K	117	GLU	C-N-CA	18.14	146.05	120.29
7	3-K	117	GLU	CA-C-N	18.14	146.05	120.29
7	3-K	117	GLU	C-N-CA	18.14	146.05	120.29
3	1-B	326	HIS	N-CA-C	-16.41	85.13	108.76
3	2-B	326	HIS	N-CA-C	-16.41	85.13	108.76
3	3-B	326	HIS	N-CA-C	-16.41	85.13	108.76
3	1-N	326	HIS	N-CA-C	-16.41	85.14	108.76
3	2-N	326	HIS	N-CA-C	-16.41	85.14	108.76
3	3-N	326	HIS	N-CA-C	-16.41	85.14	108.76
7	1-K	225	SER	CA-C-N	16.07	139.93	119.84
7	1-K	225	SER	C-N-CA	16.07	139.93	119.84
7	2-K	225	SER	CA-C-N	16.07	139.93	119.84
7	2-K	225	SER	C-N-CA	16.07	139.93	119.84
7	3-K	225	SER	CA-C-N	16.07	139.93	119.84
7	3-K	225	SER	C-N-CA	16.07	139.93	119.84
3	1-B	841	ILE	N-CA-C	15.44	126.31	110.72
3	2-B	841	ILE	N-CA-C	15.44	126.31	110.72
3	3-B	841	ILE	N-CA-C	15.44	126.31	110.72
1	1-A	338	ASP	N-CA-C	-15.32	91.48	111.24
1	2-A	338	ASP	N-CA-C	-15.32	91.48	111.24
1	3-A	338	ASP	N-CA-C	-15.32	91.48	111.24
7	1-G	804	ILE	N-CA-C	15.13	124.76	110.53
7	2-G	804	ILE	N-CA-C	15.13	124.76	110.53
7	3-G	804	ILE	N-CA-C	15.13	124.76	110.53
7	1-K	804	ILE	N-CA-C	14.98	124.61	110.53
7	2-K	804	ILE	N-CA-C	14.98	124.61	110.53
7	3-K	804	ILE	N-CA-C	14.98	124.61	110.53
7	1-K	277	LEU	CA-C-N	-14.86	101.27	119.84
7	1-K	277	LEU	C-N-CA	-14.86	101.27	119.84
7	2-K	277	LEU	CA-C-N	-14.86	101.27	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-K	277	LEU	C-N-CA	-14.86	101.27	119.84
7	3-K	277	LEU	CA-C-N	-14.86	101.27	119.84
7	3-K	277	LEU	C-N-CA	-14.86	101.27	119.84
1	1-A	595	THR	CA-C-O	14.76	130.16	119.68
1	2-A	595	THR	CA-C-O	14.76	130.16	119.68
1	3-A	595	THR	CA-C-O	14.76	130.16	119.68
3	1-B	325	GLU	CA-C-N	14.73	136.07	122.37
3	1-B	325	GLU	C-N-CA	14.73	136.07	122.37
3	2-B	325	GLU	CA-C-N	14.73	136.07	122.37
3	2-B	325	GLU	C-N-CA	14.73	136.07	122.37
3	3-B	325	GLU	CA-C-N	14.73	136.07	122.37
3	3-B	325	GLU	C-N-CA	14.73	136.07	122.37
3	1-N	325	GLU	CA-C-N	14.72	136.06	122.37
3	1-N	325	GLU	C-N-CA	14.72	136.06	122.37
3	2-N	325	GLU	CA-C-N	14.72	136.06	122.37
3	2-N	325	GLU	C-N-CA	14.72	136.06	122.37
3	3-N	325	GLU	CA-C-N	14.72	136.06	122.37
3	3-N	325	GLU	C-N-CA	14.72	136.06	122.37
1	1-A	214	HIS	CA-C-N	14.59	138.08	119.84
1	1-A	214	HIS	C-N-CA	14.59	138.08	119.84
1	2-A	214	HIS	CA-C-N	14.59	138.08	119.84
1	2-A	214	HIS	C-N-CA	14.59	138.08	119.84
1	3-A	214	HIS	CA-C-N	14.59	138.08	119.84
1	3-A	214	HIS	C-N-CA	14.59	138.08	119.84
1	1-A	229	VAL	N-CA-C	-14.47	87.86	108.11
1	2-A	229	VAL	N-CA-C	-14.47	87.86	108.11
1	3-A	229	VAL	N-CA-C	-14.47	87.86	108.11
3	1-B	760	VAL	N-CA-C	-14.43	87.91	108.11
3	2-B	760	VAL	N-CA-C	-14.43	87.91	108.11
3	3-B	760	VAL	N-CA-C	-14.43	87.91	108.11
1	1-A	227	ARG	N-CA-C	-14.23	95.84	111.07
1	2-A	227	ARG	N-CA-C	-14.23	95.84	111.07
1	3-A	227	ARG	N-CA-C	-14.23	95.84	111.07
6	1-J	121	TRP	N-CA-C	14.15	130.07	109.69
6	2-J	121	TRP	N-CA-C	14.15	130.07	109.69
6	3-J	121	TRP	N-CA-C	14.15	130.07	109.69
6	1-F	121	TRP	N-CA-C	14.15	130.06	109.69
6	2-F	121	TRP	N-CA-C	14.15	130.06	109.69
6	3-F	121	TRP	N-CA-C	14.15	130.06	109.69
7	1-G	609	ARG	CA-C-N	14.12	139.20	120.28
7	1-G	609	ARG	C-N-CA	14.12	139.20	120.28
7	2-G	609	ARG	CA-C-N	14.12	139.20	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-G	609	ARG	C-N-CA	14.12	139.20	120.28
7	3-G	609	ARG	CA-C-N	14.12	139.20	120.28
7	3-G	609	ARG	C-N-CA	14.12	139.20	120.28
7	1-G	665	CYS	N-CA-C	14.11	127.77	107.88
6	1-J	59	LYS	CA-C-N	14.11	142.35	122.46
6	1-J	59	LYS	C-N-CA	14.11	142.35	122.46
7	2-G	665	CYS	N-CA-C	14.11	127.77	107.88
6	2-J	59	LYS	CA-C-N	14.11	142.35	122.46
6	2-J	59	LYS	C-N-CA	14.11	142.35	122.46
7	3-G	665	CYS	N-CA-C	14.11	127.77	107.88
6	3-J	59	LYS	CA-C-N	14.11	142.35	122.46
6	3-J	59	LYS	C-N-CA	14.11	142.35	122.46
7	1-K	609	ARG	CA-C-N	14.10	139.17	120.28
7	1-K	609	ARG	C-N-CA	14.10	139.17	120.28
7	2-K	609	ARG	CA-C-N	14.10	139.17	120.28
7	2-K	609	ARG	C-N-CA	14.10	139.17	120.28
7	3-K	609	ARG	CA-C-N	14.10	139.17	120.28
7	3-K	609	ARG	C-N-CA	14.10	139.17	120.28
6	1-R	88	VAL	N-CA-C	14.09	126.09	108.06
6	2-R	88	VAL	N-CA-C	14.09	126.09	108.06
6	3-R	88	VAL	N-CA-C	14.09	126.09	108.06
1	1-A	630	GLN	N-CA-C	-13.99	96.69	114.04
1	2-A	630	GLN	N-CA-C	-13.99	96.69	114.04
1	3-A	630	GLN	N-CA-C	-13.99	96.69	114.04
1	1-A	797	PRO	CA-C-N	-13.91	102.45	119.84
1	1-A	797	PRO	C-N-CA	-13.91	102.45	119.84
1	2-A	797	PRO	CA-C-N	-13.91	102.45	119.84
1	2-A	797	PRO	C-N-CA	-13.91	102.45	119.84
1	3-A	797	PRO	CA-C-N	-13.91	102.45	119.84
1	3-A	797	PRO	C-N-CA	-13.91	102.45	119.84
7	1-G	178	VAL	N-CA-C	13.76	126.30	110.62
7	2-G	178	VAL	N-CA-C	13.76	126.30	110.62
7	3-G	178	VAL	N-CA-C	13.76	126.30	110.62
8	1-Z	58	GLU	N-CA-C	-13.63	95.90	111.03
8	2-Z	58	GLU	N-CA-C	-13.63	95.90	111.03
8	3-Z	58	GLU	N-CA-C	-13.63	95.90	111.03
4	1-H	416	LYS	N-CA-C	-13.44	87.00	108.90
4	2-H	416	LYS	N-CA-C	-13.44	87.00	108.90
4	3-H	416	LYS	N-CA-C	-13.44	87.00	108.90
4	1-C	416	LYS	N-CA-C	-13.43	87.01	108.90
4	2-C	416	LYS	N-CA-C	-13.43	87.01	108.90
4	3-C	416	LYS	N-CA-C	-13.43	87.01	108.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	736	ALA	N-CA-C	13.25	125.80	111.36
1	2-A	736	ALA	N-CA-C	13.25	125.80	111.36
1	3-A	736	ALA	N-CA-C	13.25	125.80	111.36
7	1-K	629	LEU	CA-C-N	13.09	138.24	120.44
7	1-K	629	LEU	C-N-CA	13.09	138.24	120.44
7	2-K	629	LEU	CA-C-N	13.09	138.24	120.44
7	2-K	629	LEU	C-N-CA	13.09	138.24	120.44
7	3-K	629	LEU	CA-C-N	13.09	138.24	120.44
7	3-K	629	LEU	C-N-CA	13.09	138.24	120.44
7	1-G	629	LEU	CA-C-N	13.08	138.23	120.44
7	1-G	629	LEU	C-N-CA	13.08	138.23	120.44
7	2-G	629	LEU	CA-C-N	13.08	138.23	120.44
7	2-G	629	LEU	C-N-CA	13.08	138.23	120.44
7	3-G	629	LEU	CA-C-N	13.08	138.23	120.44
7	3-G	629	LEU	C-N-CA	13.08	138.23	120.44
1	1-A	768	ASP	CA-C-N	13.04	137.39	120.44
1	1-A	768	ASP	C-N-CA	13.04	137.39	120.44
1	2-A	768	ASP	CA-C-N	13.04	137.39	120.44
1	2-A	768	ASP	C-N-CA	13.04	137.39	120.44
1	3-A	768	ASP	CA-C-N	13.04	137.39	120.44
1	3-A	768	ASP	C-N-CA	13.04	137.39	120.44
3	1-B	414	ALA	CA-C-N	12.88	137.54	120.28
3	1-B	414	ALA	C-N-CA	12.88	137.54	120.28
3	2-B	414	ALA	CA-C-N	12.88	137.54	120.28
3	2-B	414	ALA	C-N-CA	12.88	137.54	120.28
3	3-B	414	ALA	CA-C-N	12.88	137.54	120.28
3	3-B	414	ALA	C-N-CA	12.88	137.54	120.28
3	1-N	414	ALA	CA-C-N	12.86	137.52	120.28
3	1-N	414	ALA	C-N-CA	12.86	137.52	120.28
3	2-N	414	ALA	CA-C-N	12.86	137.52	120.28
3	2-N	414	ALA	C-N-CA	12.86	137.52	120.28
3	3-N	414	ALA	CA-C-N	12.86	137.52	120.28
3	3-N	414	ALA	C-N-CA	12.86	137.52	120.28
3	1-B	940	GLY	N-CA-C	-12.81	90.50	111.38
3	2-B	940	GLY	N-CA-C	-12.81	90.50	111.38
3	3-B	940	GLY	N-CA-C	-12.81	90.50	111.38
6	1-R	159	CYS	N-CA-C	-12.70	90.64	108.54
6	2-R	159	CYS	N-CA-C	-12.70	90.64	108.54
6	3-R	159	CYS	N-CA-C	-12.70	90.64	108.54
3	1-B	926	ILE	N-CA-C	12.56	126.20	108.12
3	2-B	926	ILE	N-CA-C	12.56	126.20	108.12
3	3-B	926	ILE	N-CA-C	12.56	126.20	108.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-K	665	CYS	N-CA-C	12.44	127.58	108.42
7	2-K	665	CYS	N-CA-C	12.44	127.58	108.42
7	3-K	665	CYS	N-CA-C	12.44	127.58	108.42
1	1-A	343	GLN	N-CA-C	-12.39	84.41	110.80
1	2-A	343	GLN	N-CA-C	-12.39	84.41	110.80
1	3-A	343	GLN	N-CA-C	-12.39	84.41	110.80
1	1-A	504	ALA	N-CA-C	-12.27	89.40	109.40
1	2-A	504	ALA	N-CA-C	-12.27	89.40	109.40
1	3-A	504	ALA	N-CA-C	-12.27	89.40	109.40
6	1-F	61	ILE	N-CA-C	-12.26	90.83	108.36
6	2-F	61	ILE	N-CA-C	-12.26	90.83	108.36
6	3-F	61	ILE	N-CA-C	-12.26	90.83	108.36
6	1-J	61	ILE	N-CA-C	-12.25	90.84	108.36
6	2-J	61	ILE	N-CA-C	-12.25	90.84	108.36
6	3-J	61	ILE	N-CA-C	-12.25	90.84	108.36
4	1-C	246	THR	CA-C-N	12.20	133.92	121.35
4	1-C	246	THR	C-N-CA	12.20	133.92	121.35
4	2-C	246	THR	CA-C-N	12.20	133.92	121.35
4	2-C	246	THR	C-N-CA	12.20	133.92	121.35
4	3-C	246	THR	CA-C-N	12.20	133.92	121.35
4	3-C	246	THR	C-N-CA	12.20	133.92	121.35
4	1-H	441	VAL	N-CA-C	-12.19	90.30	108.46
4	2-H	441	VAL	N-CA-C	-12.19	90.30	108.46
4	3-H	441	VAL	N-CA-C	-12.19	90.30	108.46
4	1-H	246	THR	CA-C-N	12.18	133.90	121.35
4	1-H	246	THR	C-N-CA	12.18	133.90	121.35
4	2-H	246	THR	CA-C-N	12.18	133.90	121.35
4	2-H	246	THR	C-N-CA	12.18	133.90	121.35
4	3-H	246	THR	CA-C-N	12.18	133.90	121.35
4	3-H	246	THR	C-N-CA	12.18	133.90	121.35
8	1-L	58	GLU	N-CA-C	-12.18	97.51	111.03
8	2-L	58	GLU	N-CA-C	-12.18	97.51	111.03
8	3-L	58	GLU	N-CA-C	-12.18	97.51	111.03
4	1-C	441	VAL	N-CA-C	-12.15	90.35	108.46
4	2-C	441	VAL	N-CA-C	-12.15	90.35	108.46
4	3-C	441	VAL	N-CA-C	-12.15	90.35	108.46
3	1-N	257	ARG	N-CA-C	12.09	125.61	111.11
3	2-N	257	ARG	N-CA-C	12.09	125.61	111.11
3	3-N	257	ARG	N-CA-C	12.09	125.61	111.11
3	1-B	759	LEU	N-CA-C	-12.08	89.20	108.90
7	1-G	225	SER	CA-C-O	-12.08	111.44	119.29
3	2-B	759	LEU	N-CA-C	-12.08	89.20	108.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-G	225	SER	CA-C-O	-12.08	111.44	119.29
3	3-B	759	LEU	N-CA-C	-12.08	89.20	108.90
7	3-G	225	SER	CA-C-O	-12.08	111.44	119.29
3	1-B	257	ARG	N-CA-C	12.07	125.60	111.11
3	2-B	257	ARG	N-CA-C	12.07	125.60	111.11
3	3-B	257	ARG	N-CA-C	12.07	125.60	111.11
7	1-G	459	LEU	CA-C-N	12.07	133.63	119.99
7	1-G	459	LEU	C-N-CA	12.07	133.63	119.99
7	2-G	459	LEU	CA-C-N	12.07	133.63	119.99
7	2-G	459	LEU	C-N-CA	12.07	133.63	119.99
7	3-G	459	LEU	CA-C-N	12.07	133.63	119.99
7	3-G	459	LEU	C-N-CA	12.07	133.63	119.99
1	1-A	242	VAL	N-CA-C	-12.06	93.31	106.21
1	2-A	242	VAL	N-CA-C	-12.06	93.31	106.21
1	3-A	242	VAL	N-CA-C	-12.06	93.31	106.21
4	1-H	559	ARG	N-CA-C	-12.02	91.23	109.14
4	2-H	559	ARG	N-CA-C	-12.02	91.23	109.14
4	3-H	559	ARG	N-CA-C	-12.02	91.23	109.14
4	1-C	559	ARG	N-CA-C	-12.01	91.24	109.14
4	2-C	559	ARG	N-CA-C	-12.01	91.24	109.14
4	3-C	559	ARG	N-CA-C	-12.01	91.24	109.14
3	1-N	145	ALA	N-CA-C	11.90	124.25	111.28
3	2-N	145	ALA	N-CA-C	11.90	124.25	111.28
3	3-N	145	ALA	N-CA-C	11.90	124.25	111.28
3	1-B	145	ALA	N-CA-C	11.88	124.23	111.28
3	2-B	145	ALA	N-CA-C	11.88	124.23	111.28
3	3-B	145	ALA	N-CA-C	11.88	124.23	111.28
7	1-K	247	ARG	N-CA-C	-11.84	96.95	111.40
7	2-K	247	ARG	N-CA-C	-11.84	96.95	111.40
7	3-K	247	ARG	N-CA-C	-11.84	96.95	111.40
7	1-K	240	LEU	CA-C-N	11.72	136.44	120.38
7	1-K	240	LEU	C-N-CA	11.72	136.44	120.38
7	2-K	240	LEU	CA-C-N	11.72	136.44	120.38
7	2-K	240	LEU	C-N-CA	11.72	136.44	120.38
7	3-K	240	LEU	CA-C-N	11.72	136.44	120.38
7	3-K	240	LEU	C-N-CA	11.72	136.44	120.38
3	1-B	761	VAL	N-CA-C	-11.71	91.62	108.48
3	2-B	761	VAL	N-CA-C	-11.71	91.62	108.48
3	3-B	761	VAL	N-CA-C	-11.71	91.62	108.48
7	1-G	96	SER	N-CA-C	11.62	135.55	110.80
7	2-G	96	SER	N-CA-C	11.62	135.55	110.80
7	3-G	96	SER	N-CA-C	11.62	135.55	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-K	24	LYS	N-CA-C	11.59	124.00	111.36
7	2-K	24	LYS	N-CA-C	11.59	124.00	111.36
7	3-K	24	LYS	N-CA-C	11.59	124.00	111.36
7	1-G	205	LYS	N-CA-C	-11.56	98.66	111.14
7	2-G	205	LYS	N-CA-C	-11.56	98.66	111.14
7	3-G	205	LYS	N-CA-C	-11.56	98.66	111.14
5	1-D	19	ARG	CA-C-N	11.50	137.79	122.84
5	1-D	19	ARG	C-N-CA	11.50	137.79	122.84
5	2-D	19	ARG	CA-C-N	11.50	137.79	122.84
5	2-D	19	ARG	C-N-CA	11.50	137.79	122.84
5	3-D	19	ARG	CA-C-N	11.50	137.79	122.84
5	3-D	19	ARG	C-N-CA	11.50	137.79	122.84
5	1-I	19	ARG	CA-C-N	11.48	137.77	122.84
5	1-I	19	ARG	C-N-CA	11.48	137.77	122.84
5	2-I	19	ARG	CA-C-N	11.48	137.77	122.84
5	2-I	19	ARG	C-N-CA	11.48	137.77	122.84
5	3-I	19	ARG	CA-C-N	11.48	137.77	122.84
5	3-I	19	ARG	C-N-CA	11.48	137.77	122.84
5	1-D	61	MET	N-CA-C	-11.47	87.95	107.80
5	2-D	61	MET	N-CA-C	-11.47	87.95	107.80
5	3-D	61	MET	N-CA-C	-11.47	87.95	107.80
5	1-I	61	MET	N-CA-C	-11.46	87.97	107.80
5	2-I	61	MET	N-CA-C	-11.46	87.97	107.80
5	3-I	61	MET	N-CA-C	-11.46	87.97	107.80
4	1-H	653	GLU	N-CA-C	-11.44	92.68	109.15
4	2-H	653	GLU	N-CA-C	-11.44	92.68	109.15
4	3-H	653	GLU	N-CA-C	-11.44	92.68	109.15
4	1-C	653	GLU	N-CA-C	-11.42	92.71	109.15
4	2-C	653	GLU	N-CA-C	-11.42	92.71	109.15
4	3-C	653	GLU	N-CA-C	-11.42	92.71	109.15
7	1-G	95	MET	N-CA-C	11.39	126.44	112.54
7	2-G	95	MET	N-CA-C	11.39	126.44	112.54
7	3-G	95	MET	N-CA-C	11.39	126.44	112.54
1	1-A	339	ARG	N-CA-C	-11.39	92.10	109.41
1	2-A	339	ARG	N-CA-C	-11.39	92.10	109.41
1	3-A	339	ARG	N-CA-C	-11.39	92.10	109.41
1	1-A	528	ILE	N-CA-C	-11.36	92.71	108.27
1	2-A	528	ILE	N-CA-C	-11.36	92.71	108.27
1	3-A	528	ILE	N-CA-C	-11.36	92.71	108.27
7	1-G	829	LEU	N-CA-C	-11.35	89.91	108.41
7	2-G	829	LEU	N-CA-C	-11.35	89.91	108.41
7	3-G	829	LEU	N-CA-C	-11.35	89.91	108.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	547	ASN	N-CA-C	-11.34	99.79	112.72
1	2-A	547	ASN	N-CA-C	-11.34	99.79	112.72
1	3-A	547	ASN	N-CA-C	-11.34	99.79	112.72
7	1-K	829	LEU	N-CA-C	-11.34	89.93	108.41
7	2-K	829	LEU	N-CA-C	-11.34	89.93	108.41
7	3-K	829	LEU	N-CA-C	-11.34	89.93	108.41
1	1-A	554	THR	N-CA-C	11.32	127.06	108.26
1	2-A	554	THR	N-CA-C	11.32	127.06	108.26
1	3-A	554	THR	N-CA-C	11.32	127.06	108.26
5	1-D	14	LYS	CA-C-N	11.32	138.14	121.72
5	1-D	14	LYS	C-N-CA	11.32	138.14	121.72
5	2-D	14	LYS	CA-C-N	11.32	138.14	121.72
5	2-D	14	LYS	C-N-CA	11.32	138.14	121.72
5	3-D	14	LYS	CA-C-N	11.32	138.14	121.72
5	3-D	14	LYS	C-N-CA	11.32	138.14	121.72
5	1-I	14	LYS	CA-C-N	11.32	138.13	121.72
5	1-I	14	LYS	C-N-CA	11.32	138.13	121.72
5	2-I	14	LYS	CA-C-N	11.32	138.13	121.72
5	2-I	14	LYS	C-N-CA	11.32	138.13	121.72
5	3-I	14	LYS	CA-C-N	11.32	138.13	121.72
5	3-I	14	LYS	C-N-CA	11.32	138.13	121.72
5	1-D	56	TYR	N-CA-C	-11.31	89.64	108.76
5	2-D	56	TYR	N-CA-C	-11.31	89.64	108.76
5	3-D	56	TYR	N-CA-C	-11.31	89.64	108.76
5	1-I	56	TYR	N-CA-C	-11.28	89.69	108.76
5	2-I	56	TYR	N-CA-C	-11.28	89.69	108.76
5	3-I	56	TYR	N-CA-C	-11.28	89.69	108.76
7	1-K	131	ILE	N-CA-C	11.25	125.16	111.09
7	2-K	131	ILE	N-CA-C	11.25	125.16	111.09
7	3-K	131	ILE	N-CA-C	11.25	125.16	111.09
4	1-C	113	PHE	N-CA-C	11.22	127.80	109.95
4	2-C	113	PHE	N-CA-C	11.22	127.80	109.95
4	3-C	113	PHE	N-CA-C	11.22	127.80	109.95
4	1-H	113	PHE	N-CA-C	11.22	127.78	109.95
4	2-H	113	PHE	N-CA-C	11.22	127.78	109.95
4	3-H	113	PHE	N-CA-C	11.22	127.78	109.95
5	1-D	36	PHE	CA-C-N	11.15	130.56	118.97
5	1-D	36	PHE	C-N-CA	11.15	130.56	118.97
5	2-D	36	PHE	CA-C-N	11.15	130.56	118.97
5	2-D	36	PHE	C-N-CA	11.15	130.56	118.97
5	3-D	36	PHE	CA-C-N	11.15	130.56	118.97
5	3-D	36	PHE	C-N-CA	11.15	130.56	118.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1-I	36	PHE	CA-C-N	11.10	130.52	118.97
5	1-I	36	PHE	C-N-CA	11.10	130.52	118.97
5	2-I	36	PHE	CA-C-N	11.10	130.52	118.97
5	2-I	36	PHE	C-N-CA	11.10	130.52	118.97
5	3-I	36	PHE	CA-C-N	11.10	130.52	118.97
5	3-I	36	PHE	C-N-CA	11.10	130.52	118.97
7	1-G	117	GLU	N-CA-C	-11.08	90.90	108.63
7	2-G	117	GLU	N-CA-C	-11.08	90.90	108.63
7	3-G	117	GLU	N-CA-C	-11.08	90.90	108.63
3	1-B	749	VAL	N-CA-C	-11.08	91.38	107.77
3	2-B	749	VAL	N-CA-C	-11.08	91.38	107.77
3	3-B	749	VAL	N-CA-C	-11.08	91.38	107.77
8	1-L	14	LYS	N-CA-C	-11.07	97.89	111.40
8	2-L	14	LYS	N-CA-C	-11.07	97.89	111.40
8	3-L	14	LYS	N-CA-C	-11.07	97.89	111.40
1	1-A	207	GLY	N-CA-C	-11.04	101.47	111.95
1	2-A	207	GLY	N-CA-C	-11.04	101.47	111.95
1	3-A	207	GLY	N-CA-C	-11.04	101.47	111.95
7	1-G	141	GLU	N-CA-C	10.98	124.61	111.33
7	2-G	141	GLU	N-CA-C	10.98	124.61	111.33
7	3-G	141	GLU	N-CA-C	10.98	124.61	111.33
1	1-A	302	ASN	N-CA-C	-10.97	100.39	113.88
1	2-A	302	ASN	N-CA-C	-10.97	100.39	113.88
1	3-A	302	ASN	N-CA-C	-10.97	100.39	113.88
6	1-F	59	LYS	CA-C-N	10.95	142.44	121.54
6	1-F	59	LYS	C-N-CA	10.95	142.44	121.54
6	2-F	59	LYS	CA-C-N	10.95	142.44	121.54
6	2-F	59	LYS	C-N-CA	10.95	142.44	121.54
6	3-F	59	LYS	CA-C-N	10.95	142.44	121.54
6	3-F	59	LYS	C-N-CA	10.95	142.44	121.54
3	1-B	234	PHE	CA-C-N	10.93	130.41	119.92
3	1-B	234	PHE	C-N-CA	10.93	130.41	119.92
3	2-B	234	PHE	CA-C-N	10.93	130.41	119.92
3	2-B	234	PHE	C-N-CA	10.93	130.41	119.92
3	3-B	234	PHE	CA-C-N	10.93	130.41	119.92
3	3-B	234	PHE	C-N-CA	10.93	130.41	119.92
3	1-N	234	PHE	CA-C-N	10.92	130.40	119.92
3	1-N	234	PHE	C-N-CA	10.92	130.40	119.92
3	2-N	234	PHE	CA-C-N	10.92	130.40	119.92
3	2-N	234	PHE	C-N-CA	10.92	130.40	119.92
3	3-N	234	PHE	CA-C-N	10.92	130.40	119.92
3	3-N	234	PHE	C-N-CA	10.92	130.40	119.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	321	ARG	N-CA-C	-10.91	90.50	108.49
3	1-B	750	ASN	N-CA-C	-10.91	90.45	108.34
1	2-A	321	ARG	N-CA-C	-10.91	90.50	108.49
3	2-B	750	ASN	N-CA-C	-10.91	90.45	108.34
1	3-A	321	ARG	N-CA-C	-10.91	90.50	108.49
3	3-B	750	ASN	N-CA-C	-10.91	90.45	108.34
1	1-A	86	LEU	N-CA-C	10.87	122.70	111.07
1	2-A	86	LEU	N-CA-C	10.87	122.70	111.07
1	3-A	86	LEU	N-CA-C	10.87	122.70	111.07
5	1-D	118	ALA	N-CA-C	-10.84	90.86	108.52
5	2-D	118	ALA	N-CA-C	-10.84	90.86	108.52
5	3-D	118	ALA	N-CA-C	-10.84	90.86	108.52
3	1-B	905	PHE	CA-C-N	10.81	136.96	121.50
3	1-B	905	PHE	C-N-CA	10.81	136.96	121.50
3	2-B	905	PHE	CA-C-N	10.81	136.96	121.50
3	2-B	905	PHE	C-N-CA	10.81	136.96	121.50
3	3-B	905	PHE	CA-C-N	10.81	136.96	121.50
3	3-B	905	PHE	C-N-CA	10.81	136.96	121.50
5	1-I	118	ALA	N-CA-C	-10.80	90.92	108.52
5	2-I	118	ALA	N-CA-C	-10.80	90.92	108.52
5	3-I	118	ALA	N-CA-C	-10.80	90.92	108.52
6	1-R	122	LEU	N-CA-C	-10.77	88.93	107.99
6	2-R	122	LEU	N-CA-C	-10.77	88.93	107.99
6	3-R	122	LEU	N-CA-C	-10.77	88.93	107.99
1	1-A	491	VAL	CA-C-N	10.76	142.09	121.54
1	1-A	491	VAL	C-N-CA	10.76	142.09	121.54
1	2-A	491	VAL	CA-C-N	10.76	142.09	121.54
1	2-A	491	VAL	C-N-CA	10.76	142.09	121.54
1	3-A	491	VAL	CA-C-N	10.76	142.09	121.54
1	3-A	491	VAL	C-N-CA	10.76	142.09	121.54
6	1-M	62	SER	CA-C-N	10.74	137.33	122.19
6	1-M	62	SER	C-N-CA	10.74	137.33	122.19
6	2-M	62	SER	CA-C-N	10.74	137.33	122.19
6	2-M	62	SER	C-N-CA	10.74	137.33	122.19
6	3-M	62	SER	CA-C-N	10.74	137.33	122.19
6	3-M	62	SER	C-N-CA	10.74	137.33	122.19
1	1-A	802	MET	CA-C-N	10.71	133.23	119.84
1	1-A	802	MET	C-N-CA	10.71	133.23	119.84
1	2-A	802	MET	CA-C-N	10.71	133.23	119.84
1	2-A	802	MET	C-N-CA	10.71	133.23	119.84
1	3-A	802	MET	CA-C-N	10.71	133.23	119.84
1	3-A	802	MET	C-N-CA	10.71	133.23	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	693	VAL	N-CA-C	10.71	118.75	108.15
7	2-G	693	VAL	N-CA-C	10.71	118.75	108.15
7	3-G	693	VAL	N-CA-C	10.71	118.75	108.15
3	1-B	894	THR	O-C-N	10.68	129.32	121.85
3	2-B	894	THR	O-C-N	10.68	129.32	121.85
3	3-B	894	THR	O-C-N	10.68	129.32	121.85
4	1-C	176	SER	N-CA-C	-10.67	98.57	108.07
4	2-C	176	SER	N-CA-C	-10.67	98.57	108.07
4	3-C	176	SER	N-CA-C	-10.67	98.57	108.07
7	1-K	120	TYR	CA-C-N	10.66	134.29	120.44
7	1-K	120	TYR	C-N-CA	10.66	134.29	120.44
7	2-K	120	TYR	CA-C-N	10.66	134.29	120.44
7	2-K	120	TYR	C-N-CA	10.66	134.29	120.44
7	3-K	120	TYR	CA-C-N	10.66	134.29	120.44
7	3-K	120	TYR	C-N-CA	10.66	134.29	120.44
3	1-B	256	GLU	N-CA-C	10.65	125.78	113.01
4	1-H	176	SER	N-CA-C	-10.65	98.59	108.07
3	2-B	256	GLU	N-CA-C	10.65	125.78	113.01
4	2-H	176	SER	N-CA-C	-10.65	98.59	108.07
3	3-B	256	GLU	N-CA-C	10.65	125.78	113.01
4	3-H	176	SER	N-CA-C	-10.65	98.59	108.07
6	1-R	78	TRP	N-CA-C	-10.64	99.22	111.03
6	2-R	78	TRP	N-CA-C	-10.64	99.22	111.03
6	3-R	78	TRP	N-CA-C	-10.64	99.22	111.03
3	1-N	256	GLU	N-CA-C	10.63	125.77	113.01
3	2-N	256	GLU	N-CA-C	10.63	125.77	113.01
3	3-N	256	GLU	N-CA-C	10.63	125.77	113.01
7	1-G	815	ARG	N-CA-C	-10.60	97.42	111.74
7	2-G	815	ARG	N-CA-C	-10.60	97.42	111.74
7	3-G	815	ARG	N-CA-C	-10.60	97.42	111.74
1	1-A	656	GLY	N-CA-C	-10.58	99.66	115.32
1	2-A	656	GLY	N-CA-C	-10.58	99.66	115.32
1	3-A	656	GLY	N-CA-C	-10.58	99.66	115.32
7	1-K	838	HIS	CA-C-N	10.55	137.50	120.94
7	1-K	838	HIS	C-N-CA	10.55	137.50	120.94
7	2-K	838	HIS	CA-C-N	10.55	137.50	120.94
7	2-K	838	HIS	C-N-CA	10.55	137.50	120.94
7	3-K	838	HIS	CA-C-N	10.55	137.50	120.94
7	3-K	838	HIS	C-N-CA	10.55	137.50	120.94
7	1-K	814	GLU	N-CA-C	-10.55	96.48	111.56
7	2-K	814	GLU	N-CA-C	-10.55	96.48	111.56
7	3-K	814	GLU	N-CA-C	-10.55	96.48	111.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	838	HIS	CA-C-N	10.54	137.48	120.94
7	1-G	838	HIS	C-N-CA	10.54	137.48	120.94
7	2-G	838	HIS	CA-C-N	10.54	137.48	120.94
7	2-G	838	HIS	C-N-CA	10.54	137.48	120.94
7	3-G	838	HIS	CA-C-N	10.54	137.48	120.94
7	3-G	838	HIS	C-N-CA	10.54	137.48	120.94
3	1-N	444	GLN	N-CA-C	10.53	122.76	111.28
3	2-N	444	GLN	N-CA-C	10.53	122.76	111.28
3	3-N	444	GLN	N-CA-C	10.53	122.76	111.28
3	1-B	444	GLN	N-CA-C	10.53	122.75	111.28
3	2-B	444	GLN	N-CA-C	10.53	122.75	111.28
3	3-B	444	GLN	N-CA-C	10.53	122.75	111.28
7	1-G	813	CYS	N-CA-C	10.51	122.11	108.24
7	2-G	813	CYS	N-CA-C	10.51	122.11	108.24
7	3-G	813	CYS	N-CA-C	10.51	122.11	108.24
7	1-G	435	GLY	CA-C-N	10.49	134.34	120.28
7	1-G	435	GLY	C-N-CA	10.49	134.34	120.28
7	2-G	435	GLY	CA-C-N	10.49	134.34	120.28
7	2-G	435	GLY	C-N-CA	10.49	134.34	120.28
7	3-G	435	GLY	CA-C-N	10.49	134.34	120.28
7	3-G	435	GLY	C-N-CA	10.49	134.34	120.28
7	1-G	207	ASP	N-CA-C	10.48	127.34	108.48
7	2-G	207	ASP	N-CA-C	10.48	127.34	108.48
7	3-G	207	ASP	N-CA-C	10.48	127.34	108.48
7	1-G	535	LEU	CA-C-N	10.46	134.04	120.44
7	1-G	535	LEU	C-N-CA	10.46	134.04	120.44
7	2-G	535	LEU	CA-C-N	10.46	134.04	120.44
7	2-G	535	LEU	C-N-CA	10.46	134.04	120.44
7	3-G	535	LEU	CA-C-N	10.46	134.04	120.44
7	3-G	535	LEU	C-N-CA	10.46	134.04	120.44
6	1-M	155	ILE	N-CA-C	-10.46	93.52	108.17
6	2-M	155	ILE	N-CA-C	-10.46	93.52	108.17
6	3-M	155	ILE	N-CA-C	-10.46	93.52	108.17
7	1-K	152	VAL	N-CA-C	-10.45	98.05	107.56
7	2-K	152	VAL	N-CA-C	-10.45	98.05	107.56
7	3-K	152	VAL	N-CA-C	-10.45	98.05	107.56
1	1-A	243	ASP	N-CA-C	-10.38	92.48	109.40
1	2-A	243	ASP	N-CA-C	-10.38	92.48	109.40
1	3-A	243	ASP	N-CA-C	-10.38	92.48	109.40
6	1-M	41	GLU	CA-C-N	10.37	140.63	121.97
6	1-M	41	GLU	C-N-CA	10.37	140.63	121.97
6	2-M	41	GLU	CA-C-N	10.37	140.63	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	2-M	41	GLU	C-N-CA	10.37	140.63	121.97
6	3-M	41	GLU	CA-C-N	10.37	140.63	121.97
6	3-M	41	GLU	C-N-CA	10.37	140.63	121.97
4	1-C	567	ILE	N-CA-C	-10.36	97.29	107.55
4	2-C	567	ILE	N-CA-C	-10.36	97.29	107.55
4	3-C	567	ILE	N-CA-C	-10.36	97.29	107.55
1	1-A	216	THR	N-CA-C	-10.34	100.66	113.38
1	2-A	216	THR	N-CA-C	-10.34	100.66	113.38
1	3-A	216	THR	N-CA-C	-10.34	100.66	113.38
4	1-H	567	ILE	N-CA-C	-10.32	97.33	107.55
4	2-H	567	ILE	N-CA-C	-10.32	97.33	107.55
4	3-H	567	ILE	N-CA-C	-10.32	97.33	107.55
1	1-A	631	LYS	N-CA-C	-10.30	88.86	110.80
1	2-A	631	LYS	N-CA-C	-10.30	88.86	110.80
1	3-A	631	LYS	N-CA-C	-10.30	88.86	110.80
6	1-J	24	GLY	N-CA-C	-10.27	101.57	112.04
6	2-J	24	GLY	N-CA-C	-10.27	101.57	112.04
6	3-J	24	GLY	N-CA-C	-10.27	101.57	112.04
6	1-F	24	GLY	N-CA-C	-10.26	101.58	112.04
6	2-F	24	GLY	N-CA-C	-10.26	101.58	112.04
6	3-F	24	GLY	N-CA-C	-10.26	101.58	112.04
8	1-L	61	LEU	CA-C-N	-10.25	106.95	122.74
8	1-L	61	LEU	C-N-CA	-10.25	106.95	122.74
8	2-L	61	LEU	CA-C-N	-10.25	106.95	122.74
8	2-L	61	LEU	C-N-CA	-10.25	106.95	122.74
8	3-L	61	LEU	CA-C-N	-10.25	106.95	122.74
8	3-L	61	LEU	C-N-CA	-10.25	106.95	122.74
3	1-B	754	ILE	N-CA-C	-10.25	93.70	108.36
3	2-B	754	ILE	N-CA-C	-10.25	93.70	108.36
3	3-B	754	ILE	N-CA-C	-10.25	93.70	108.36
3	1-B	928	LYS	CA-C-N	10.24	132.64	119.84
3	1-B	928	LYS	C-N-CA	10.24	132.64	119.84
3	2-B	928	LYS	CA-C-N	10.24	132.64	119.84
3	2-B	928	LYS	C-N-CA	10.24	132.64	119.84
3	3-B	928	LYS	CA-C-N	10.24	132.64	119.84
3	3-B	928	LYS	C-N-CA	10.24	132.64	119.84
1	1-A	589	VAL	N-CA-C	-10.23	93.69	108.53
1	2-A	589	VAL	N-CA-C	-10.23	93.69	108.53
1	3-A	589	VAL	N-CA-C	-10.23	93.69	108.53
1	1-A	317	PHE	CA-C-N	10.19	137.71	122.93
1	1-A	317	PHE	C-N-CA	10.19	137.71	122.93
1	2-A	317	PHE	CA-C-N	10.19	137.71	122.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	317	PHE	C-N-CA	10.19	137.71	122.93
1	3-A	317	PHE	CA-C-N	10.19	137.71	122.93
1	3-A	317	PHE	C-N-CA	10.19	137.71	122.93
7	1-K	283	LYS	CA-C-N	10.14	133.86	120.28
7	1-K	283	LYS	C-N-CA	10.14	133.86	120.28
7	2-K	283	LYS	CA-C-N	10.14	133.86	120.28
7	2-K	283	LYS	C-N-CA	10.14	133.86	120.28
7	3-K	283	LYS	CA-C-N	10.14	133.86	120.28
7	3-K	283	LYS	C-N-CA	10.14	133.86	120.28
1	1-A	104	GLU	N-CA-C	-10.13	99.78	111.03
4	1-C	4	ARG	N-CA-C	-10.13	98.89	112.26
1	2-A	104	GLU	N-CA-C	-10.13	99.78	111.03
4	2-C	4	ARG	N-CA-C	-10.13	98.89	112.26
1	3-A	104	GLU	N-CA-C	-10.13	99.78	111.03
4	3-C	4	ARG	N-CA-C	-10.13	98.89	112.26
4	1-H	4	ARG	N-CA-C	-10.11	98.92	112.26
4	2-H	4	ARG	N-CA-C	-10.11	98.92	112.26
4	3-H	4	ARG	N-CA-C	-10.11	98.92	112.26
1	1-A	36	TRP	N-CA-C	-10.09	92.38	109.24
1	2-A	36	TRP	N-CA-C	-10.09	92.38	109.24
1	3-A	36	TRP	N-CA-C	-10.09	92.38	109.24
6	1-M	72	ASP	N-CA-C	10.06	123.19	111.11
6	2-M	72	ASP	N-CA-C	10.06	123.19	111.11
6	3-M	72	ASP	N-CA-C	10.06	123.19	111.11
7	1-G	828	LEU	N-CA-C	-9.98	93.00	109.07
7	2-G	828	LEU	N-CA-C	-9.98	93.00	109.07
7	3-G	828	LEU	N-CA-C	-9.98	93.00	109.07
3	1-B	811	ASN	N-CA-C	-9.97	92.10	109.06
3	2-B	811	ASN	N-CA-C	-9.97	92.10	109.06
3	3-B	811	ASN	N-CA-C	-9.97	92.10	109.06
7	1-K	828	LEU	N-CA-C	-9.96	93.04	109.07
7	2-K	828	LEU	N-CA-C	-9.96	93.04	109.07
7	3-K	828	LEU	N-CA-C	-9.96	93.04	109.07
6	1-M	63	PHE	N-CA-C	9.94	125.97	109.46
6	2-M	63	PHE	N-CA-C	9.94	125.97	109.46
6	3-M	63	PHE	N-CA-C	9.94	125.97	109.46
4	1-C	204	SER	CA-C-N	-9.92	115.34	122.18
4	1-C	204	SER	C-N-CA	-9.92	115.34	122.18
4	2-C	204	SER	CA-C-N	-9.92	115.34	122.18
4	2-C	204	SER	C-N-CA	-9.92	115.34	122.18
4	3-C	204	SER	CA-C-N	-9.92	115.34	122.18
4	3-C	204	SER	C-N-CA	-9.92	115.34	122.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	396	TRP	N-CA-C	-9.92	94.55	110.32
4	2-C	396	TRP	N-CA-C	-9.92	94.55	110.32
4	3-C	396	TRP	N-CA-C	-9.92	94.55	110.32
4	1-H	396	TRP	N-CA-C	-9.91	94.56	110.32
4	2-H	396	TRP	N-CA-C	-9.91	94.56	110.32
4	3-H	396	TRP	N-CA-C	-9.91	94.56	110.32
4	1-C	379	THR	N-CA-C	-9.91	93.20	108.96
4	2-C	379	THR	N-CA-C	-9.91	93.20	108.96
4	3-C	379	THR	N-CA-C	-9.91	93.20	108.96
1	1-A	59	PHE	CA-C-N	9.91	133.32	120.44
1	1-A	59	PHE	C-N-CA	9.91	133.32	120.44
3	1-B	483	THR	N-CA-C	-9.91	99.56	112.24
1	2-A	59	PHE	CA-C-N	9.91	133.32	120.44
1	2-A	59	PHE	C-N-CA	9.91	133.32	120.44
3	2-B	483	THR	N-CA-C	-9.91	99.56	112.24
1	3-A	59	PHE	CA-C-N	9.91	133.32	120.44
1	3-A	59	PHE	C-N-CA	9.91	133.32	120.44
3	3-B	483	THR	N-CA-C	-9.91	99.56	112.24
4	1-C	221	CYS	N-CA-C	-9.90	91.26	108.20
4	2-C	221	CYS	N-CA-C	-9.90	91.26	108.20
4	3-C	221	CYS	N-CA-C	-9.90	91.26	108.20
6	1-R	30	LYS	CA-C-N	9.90	133.55	120.28
6	1-R	30	LYS	C-N-CA	9.90	133.55	120.28
6	2-R	30	LYS	CA-C-N	9.90	133.55	120.28
6	2-R	30	LYS	C-N-CA	9.90	133.55	120.28
6	3-R	30	LYS	CA-C-N	9.90	133.55	120.28
6	3-R	30	LYS	C-N-CA	9.90	133.55	120.28
3	1-N	483	THR	N-CA-C	-9.90	99.57	112.24
3	2-N	483	THR	N-CA-C	-9.90	99.57	112.24
3	3-N	483	THR	N-CA-C	-9.90	99.57	112.24
4	1-H	379	THR	N-CA-C	-9.89	93.23	108.96
4	2-H	379	THR	N-CA-C	-9.89	93.23	108.96
4	3-H	379	THR	N-CA-C	-9.89	93.23	108.96
1	1-A	430	ASP	N-CA-C	-9.88	92.80	108.90
1	2-A	430	ASP	N-CA-C	-9.88	92.80	108.90
1	3-A	430	ASP	N-CA-C	-9.88	92.80	108.90
3	1-N	255	SER	CA-C-N	9.87	140.72	121.18
3	1-N	255	SER	C-N-CA	9.87	140.72	121.18
3	2-N	255	SER	CA-C-N	9.87	140.72	121.18
3	2-N	255	SER	C-N-CA	9.87	140.72	121.18
3	3-N	255	SER	CA-C-N	9.87	140.72	121.18
3	3-N	255	SER	C-N-CA	9.87	140.72	121.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-K	129	CYS	N-CA-C	9.86	123.25	111.82
4	1-H	204	SER	CA-C-N	-9.86	115.38	122.18
4	1-H	204	SER	C-N-CA	-9.86	115.38	122.18
4	1-H	221	CYS	N-CA-C	-9.86	91.34	108.20
7	2-K	129	CYS	N-CA-C	9.86	123.25	111.82
4	2-H	204	SER	CA-C-N	-9.86	115.38	122.18
4	2-H	204	SER	C-N-CA	-9.86	115.38	122.18
4	2-H	221	CYS	N-CA-C	-9.86	91.34	108.20
7	3-K	129	CYS	N-CA-C	9.86	123.25	111.82
4	3-H	204	SER	CA-C-N	-9.86	115.38	122.18
4	3-H	204	SER	C-N-CA	-9.86	115.38	122.18
4	3-H	221	CYS	N-CA-C	-9.86	91.34	108.20
3	1-B	255	SER	CA-C-N	9.85	140.68	121.18
3	1-B	255	SER	C-N-CA	9.85	140.68	121.18
3	2-B	255	SER	CA-C-N	9.85	140.68	121.18
3	2-B	255	SER	C-N-CA	9.85	140.68	121.18
3	3-B	255	SER	CA-C-N	9.85	140.68	121.18
3	3-B	255	SER	C-N-CA	9.85	140.68	121.18
7	1-G	536	GLU	N-CA-C	-9.82	100.56	111.07
7	2-G	536	GLU	N-CA-C	-9.82	100.56	111.07
7	3-G	536	GLU	N-CA-C	-9.82	100.56	111.07
1	1-A	301	PRO	N-CA-C	-9.81	102.13	114.68
1	2-A	301	PRO	N-CA-C	-9.81	102.13	114.68
1	3-A	301	PRO	N-CA-C	-9.81	102.13	114.68
4	1-C	151	ASN	N-CA-C	-9.80	94.92	109.42
4	2-C	151	ASN	N-CA-C	-9.80	94.92	109.42
4	3-C	151	ASN	N-CA-C	-9.80	94.92	109.42
1	1-A	272	SER	N-CA-C	9.79	125.32	109.85
1	2-A	272	SER	N-CA-C	9.79	125.32	109.85
1	3-A	272	SER	N-CA-C	9.79	125.32	109.85
7	1-G	693	VAL	CA-C-O	-9.79	114.22	120.88
7	2-G	693	VAL	CA-C-O	-9.79	114.22	120.88
7	3-G	693	VAL	CA-C-O	-9.79	114.22	120.88
3	1-N	369	GLU	CA-C-N	9.76	133.36	120.28
3	1-N	369	GLU	C-N-CA	9.76	133.36	120.28
3	2-N	369	GLU	CA-C-N	9.76	133.36	120.28
3	2-N	369	GLU	C-N-CA	9.76	133.36	120.28
3	3-N	369	GLU	CA-C-N	9.76	133.36	120.28
3	3-N	369	GLU	C-N-CA	9.76	133.36	120.28
4	1-H	151	ASN	N-CA-C	-9.74	95.00	109.42
4	2-H	151	ASN	N-CA-C	-9.74	95.00	109.42
4	3-H	151	ASN	N-CA-C	-9.74	95.00	109.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-B	369	GLU	CA-C-N	9.74	133.33	120.28
3	1-B	369	GLU	C-N-CA	9.74	133.33	120.28
3	2-B	369	GLU	CA-C-N	9.74	133.33	120.28
3	2-B	369	GLU	C-N-CA	9.74	133.33	120.28
3	3-B	369	GLU	CA-C-N	9.74	133.33	120.28
3	3-B	369	GLU	C-N-CA	9.74	133.33	120.28
3	1-N	120	TYR	CA-C-N	9.73	133.32	120.28
3	1-N	120	TYR	C-N-CA	9.73	133.32	120.28
4	1-H	92	VAL	N-CA-C	9.73	119.68	110.53
3	2-N	120	TYR	CA-C-N	9.73	133.32	120.28
3	2-N	120	TYR	C-N-CA	9.73	133.32	120.28
4	2-H	92	VAL	N-CA-C	9.73	119.68	110.53
3	3-N	120	TYR	CA-C-N	9.73	133.32	120.28
3	3-N	120	TYR	C-N-CA	9.73	133.32	120.28
4	3-H	92	VAL	N-CA-C	9.73	119.68	110.53
4	1-C	315	ILE	N-CA-C	-9.73	94.55	108.17
4	2-C	315	ILE	N-CA-C	-9.73	94.55	108.17
4	3-C	315	ILE	N-CA-C	-9.73	94.55	108.17
4	1-C	92	VAL	N-CA-C	9.72	119.67	110.53
4	2-C	92	VAL	N-CA-C	9.72	119.67	110.53
4	3-C	92	VAL	N-CA-C	9.72	119.67	110.53
3	1-B	120	TYR	CA-C-N	9.70	133.28	120.28
3	1-B	120	TYR	C-N-CA	9.70	133.28	120.28
3	2-B	120	TYR	CA-C-N	9.70	133.28	120.28
3	2-B	120	TYR	C-N-CA	9.70	133.28	120.28
3	3-B	120	TYR	CA-C-N	9.70	133.28	120.28
3	3-B	120	TYR	C-N-CA	9.70	133.28	120.28
4	1-H	269	TYR	N-CA-C	-9.70	98.20	111.87
4	2-H	269	TYR	N-CA-C	-9.70	98.20	111.87
4	3-H	269	TYR	N-CA-C	-9.70	98.20	111.87
4	1-H	315	ILE	N-CA-C	-9.69	94.60	108.17
4	2-H	315	ILE	N-CA-C	-9.69	94.60	108.17
4	3-H	315	ILE	N-CA-C	-9.69	94.60	108.17
4	1-C	269	TYR	N-CA-C	-9.66	98.25	111.87
4	2-C	269	TYR	N-CA-C	-9.66	98.25	111.87
4	3-C	269	TYR	N-CA-C	-9.66	98.25	111.87
4	1-C	311	ASN	N-CA-C	-9.63	100.74	111.14
4	2-C	311	ASN	N-CA-C	-9.63	100.74	111.14
4	3-C	311	ASN	N-CA-C	-9.63	100.74	111.14
7	1-G	498	PHE	N-CA-C	9.62	121.77	111.28
7	2-G	498	PHE	N-CA-C	9.62	121.77	111.28
7	3-G	498	PHE	N-CA-C	9.62	121.77	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	311	ASN	N-CA-C	-9.62	100.75	111.14
4	2-H	311	ASN	N-CA-C	-9.62	100.75	111.14
4	3-H	311	ASN	N-CA-C	-9.62	100.75	111.14
1	1-A	519	ASP	N-CA-C	-9.59	91.64	108.13
1	2-A	519	ASP	N-CA-C	-9.59	91.64	108.13
1	3-A	519	ASP	N-CA-C	-9.59	91.64	108.13
4	1-C	551	ILE	N-CA-C	-9.59	94.69	108.11
4	2-C	551	ILE	N-CA-C	-9.59	94.69	108.11
4	3-C	551	ILE	N-CA-C	-9.59	94.69	108.11
6	1-F	166	LEU	CA-C-N	9.58	134.88	120.31
6	1-F	166	LEU	C-N-CA	9.58	134.88	120.31
6	2-F	166	LEU	CA-C-N	9.58	134.88	120.31
6	2-F	166	LEU	C-N-CA	9.58	134.88	120.31
6	3-F	166	LEU	CA-C-N	9.58	134.88	120.31
6	3-F	166	LEU	C-N-CA	9.58	134.88	120.31
6	1-F	95	ASN	N-CA-C	-9.58	101.71	113.97
6	2-F	95	ASN	N-CA-C	-9.58	101.71	113.97
6	3-F	95	ASN	N-CA-C	-9.58	101.71	113.97
1	1-A	241	GLU	CA-C-N	9.57	130.64	121.65
1	1-A	241	GLU	C-N-CA	9.57	130.64	121.65
1	2-A	241	GLU	CA-C-N	9.57	130.64	121.65
1	2-A	241	GLU	C-N-CA	9.57	130.64	121.65
1	3-A	241	GLU	CA-C-N	9.57	130.64	121.65
1	3-A	241	GLU	C-N-CA	9.57	130.64	121.65
6	1-J	166	LEU	CA-C-N	9.55	134.83	120.31
6	1-J	166	LEU	C-N-CA	9.55	134.83	120.31
6	2-J	166	LEU	CA-C-N	9.55	134.83	120.31
6	2-J	166	LEU	C-N-CA	9.55	134.83	120.31
6	3-J	166	LEU	CA-C-N	9.55	134.83	120.31
6	3-J	166	LEU	C-N-CA	9.55	134.83	120.31
4	1-H	551	ILE	N-CA-C	-9.54	94.75	108.11
4	2-H	551	ILE	N-CA-C	-9.54	94.75	108.11
4	3-H	551	ILE	N-CA-C	-9.54	94.75	108.11
6	1-J	95	ASN	N-CA-C	-9.53	101.78	113.97
6	2-J	95	ASN	N-CA-C	-9.53	101.78	113.97
6	3-J	95	ASN	N-CA-C	-9.53	101.78	113.97
5	1-D	235	VAL	CA-C-N	9.51	132.80	120.44
5	1-D	235	VAL	C-N-CA	9.51	132.80	120.44
5	2-D	235	VAL	CA-C-N	9.51	132.80	120.44
5	2-D	235	VAL	C-N-CA	9.51	132.80	120.44
5	3-D	235	VAL	CA-C-N	9.51	132.80	120.44
5	3-D	235	VAL	C-N-CA	9.51	132.80	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1-I	235	VAL	CA-C-N	9.50	132.79	120.44
5	1-I	235	VAL	C-N-CA	9.50	132.79	120.44
5	2-I	235	VAL	CA-C-N	9.50	132.79	120.44
5	2-I	235	VAL	C-N-CA	9.50	132.79	120.44
5	3-I	235	VAL	CA-C-N	9.50	132.79	120.44
5	3-I	235	VAL	C-N-CA	9.50	132.79	120.44
1	1-A	337	LYS	N-CA-C	9.48	123.98	110.23
1	2-A	337	LYS	N-CA-C	9.48	123.98	110.23
1	3-A	337	LYS	N-CA-C	9.48	123.98	110.23
1	1-A	803	PRO	N-CA-C	9.48	132.00	112.47
1	2-A	803	PRO	N-CA-C	9.48	132.00	112.47
1	3-A	803	PRO	N-CA-C	9.48	132.00	112.47
7	1-G	274	ILE	N-CA-C	9.47	125.52	111.89
7	2-G	274	ILE	N-CA-C	9.47	125.52	111.89
7	3-G	274	ILE	N-CA-C	9.47	125.52	111.89
6	1-J	97	ARG	N-CA-C	-9.45	90.68	110.80
6	2-J	97	ARG	N-CA-C	-9.45	90.68	110.80
6	3-J	97	ARG	N-CA-C	-9.45	90.68	110.80
4	1-C	245	ILE	N-CA-C	-9.44	94.89	108.11
4	2-C	245	ILE	N-CA-C	-9.44	94.89	108.11
4	3-C	245	ILE	N-CA-C	-9.44	94.89	108.11
6	1-F	97	ARG	N-CA-C	-9.43	90.72	110.80
6	2-F	97	ARG	N-CA-C	-9.43	90.72	110.80
6	3-F	97	ARG	N-CA-C	-9.43	90.72	110.80
6	1-M	130	LEU	N-CA-C	-9.42	97.79	109.65
6	2-M	130	LEU	N-CA-C	-9.42	97.79	109.65
6	3-M	130	LEU	N-CA-C	-9.42	97.79	109.65
4	1-H	245	ILE	N-CA-C	-9.41	94.93	108.11
4	2-H	245	ILE	N-CA-C	-9.41	94.93	108.11
4	3-H	245	ILE	N-CA-C	-9.41	94.93	108.11
5	1-I	89	VAL	N-CA-C	9.41	119.38	110.53
5	2-I	89	VAL	N-CA-C	9.41	119.38	110.53
5	3-I	89	VAL	N-CA-C	9.41	119.38	110.53
5	1-D	89	VAL	N-CA-C	9.40	119.37	110.53
5	2-D	89	VAL	N-CA-C	9.40	119.37	110.53
5	3-D	89	VAL	N-CA-C	9.40	119.37	110.53
4	1-C	808	GLU	N-CA-C	9.35	121.08	111.07
4	2-C	808	GLU	N-CA-C	9.35	121.08	111.07
4	3-C	808	GLU	N-CA-C	9.35	121.08	111.07
4	1-H	554	ILE	N-CA-C	-9.34	101.75	110.53
4	2-H	554	ILE	N-CA-C	-9.34	101.75	110.53
4	3-H	554	ILE	N-CA-C	-9.34	101.75	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	198	LYS	N-CA-C	-9.32	90.94	110.80
1	2-A	198	LYS	N-CA-C	-9.32	90.94	110.80
1	3-A	198	LYS	N-CA-C	-9.32	90.94	110.80
4	1-H	412	VAL	N-CA-C	9.32	121.19	108.89
4	2-H	412	VAL	N-CA-C	9.32	121.19	108.89
4	3-H	412	VAL	N-CA-C	9.32	121.19	108.89
4	1-C	554	ILE	N-CA-C	-9.32	101.77	110.53
4	2-C	554	ILE	N-CA-C	-9.32	101.77	110.53
4	3-C	554	ILE	N-CA-C	-9.32	101.77	110.53
4	1-C	412	VAL	N-CA-C	9.31	121.18	108.89
4	2-C	412	VAL	N-CA-C	9.31	121.18	108.89
4	3-C	412	VAL	N-CA-C	9.31	121.18	108.89
7	1-G	201	TYR	N-CA-C	-9.30	100.83	110.97
7	2-G	201	TYR	N-CA-C	-9.30	100.83	110.97
7	3-G	201	TYR	N-CA-C	-9.30	100.83	110.97
3	1-B	414	ALA	O-C-N	9.28	131.74	122.09
3	1-B	821	ASP	N-CA-C	9.28	124.44	108.76
3	2-B	414	ALA	O-C-N	9.28	131.74	122.09
3	2-B	821	ASP	N-CA-C	9.28	124.44	108.76
3	3-B	414	ALA	O-C-N	9.28	131.74	122.09
3	3-B	821	ASP	N-CA-C	9.28	124.44	108.76
1	1-A	429	LEU	N-CA-C	-9.27	95.25	109.24
1	2-A	429	LEU	N-CA-C	-9.27	95.25	109.24
1	3-A	429	LEU	N-CA-C	-9.27	95.25	109.24
1	1-A	625	ILE	N-CA-C	-9.25	103.67	112.83
1	2-A	625	ILE	N-CA-C	-9.25	103.67	112.83
1	3-A	625	ILE	N-CA-C	-9.25	103.67	112.83
8	1-Z	62	LEU	N-CA-C	-9.25	93.33	109.06
8	2-Z	62	LEU	N-CA-C	-9.25	93.33	109.06
8	3-Z	62	LEU	N-CA-C	-9.25	93.33	109.06
6	1-M	53	VAL	N-CA-C	-9.25	94.81	108.12
6	2-M	53	VAL	N-CA-C	-9.25	94.81	108.12
6	3-M	53	VAL	N-CA-C	-9.25	94.81	108.12
1	1-A	108	ILE	N-CA-C	9.23	122.21	108.46
1	2-A	108	ILE	N-CA-C	9.23	122.21	108.46
1	3-A	108	ILE	N-CA-C	9.23	122.21	108.46
1	1-A	599	PHE	CA-C-O	-9.20	111.16	120.82
1	2-A	599	PHE	CA-C-O	-9.20	111.16	120.82
1	3-A	599	PHE	CA-C-O	-9.20	111.16	120.82
1	1-A	496	TRP	N-CA-C	-9.19	95.33	109.85
1	2-A	496	TRP	N-CA-C	-9.19	95.33	109.85
1	3-A	496	TRP	N-CA-C	-9.19	95.33	109.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	600	LYS	N-CA-C	-9.16	101.87	113.23
1	2-A	600	LYS	N-CA-C	-9.16	101.87	113.23
1	3-A	600	LYS	N-CA-C	-9.16	101.87	113.23
1	1-A	588	ARG	N-CA-C	9.16	123.43	109.23
1	2-A	588	ARG	N-CA-C	9.16	123.43	109.23
1	3-A	588	ARG	N-CA-C	9.16	123.43	109.23
5	1-D	136	MET	N-CA-C	-9.16	91.29	110.80
5	2-D	136	MET	N-CA-C	-9.16	91.29	110.80
5	3-D	136	MET	N-CA-C	-9.16	91.29	110.80
5	1-I	136	MET	N-CA-C	-9.14	91.32	110.80
5	2-I	136	MET	N-CA-C	-9.14	91.32	110.80
5	3-I	136	MET	N-CA-C	-9.14	91.32	110.80
1	1-A	453	CYS	N-CA-C	-9.13	101.03	112.72
1	2-A	453	CYS	N-CA-C	-9.13	101.03	112.72
1	3-A	453	CYS	N-CA-C	-9.13	101.03	112.72
7	1-G	523	GLU	N-CA-C	-9.12	100.95	112.90
3	1-N	216	ASP	CA-C-N	9.12	132.50	120.28
3	1-N	216	ASP	C-N-CA	9.12	132.50	120.28
7	2-G	523	GLU	N-CA-C	-9.12	100.95	112.90
3	2-N	216	ASP	CA-C-N	9.12	132.50	120.28
3	2-N	216	ASP	C-N-CA	9.12	132.50	120.28
7	3-G	523	GLU	N-CA-C	-9.12	100.95	112.90
3	3-N	216	ASP	CA-C-N	9.12	132.50	120.28
3	3-N	216	ASP	C-N-CA	9.12	132.50	120.28
3	1-N	414	ALA	O-C-N	9.09	131.76	122.12
3	2-N	414	ALA	O-C-N	9.09	131.76	122.12
3	3-N	414	ALA	O-C-N	9.09	131.76	122.12
1	1-A	467	ARG	N-CA-C	-9.08	98.06	110.68
1	2-A	467	ARG	N-CA-C	-9.08	98.06	110.68
1	3-A	467	ARG	N-CA-C	-9.08	98.06	110.68
1	1-A	598	LYS	N-CA-C	-9.08	101.39	111.28
1	2-A	598	LYS	N-CA-C	-9.08	101.39	111.28
1	3-A	598	LYS	N-CA-C	-9.08	101.39	111.28
3	1-B	216	ASP	CA-C-N	9.07	132.44	120.28
3	1-B	216	ASP	C-N-CA	9.07	132.44	120.28
3	2-B	216	ASP	CA-C-N	9.07	132.44	120.28
3	2-B	216	ASP	C-N-CA	9.07	132.44	120.28
3	3-B	216	ASP	CA-C-N	9.07	132.44	120.28
3	3-B	216	ASP	C-N-CA	9.07	132.44	120.28
1	1-A	240	TRP	CA-C-N	9.07	138.86	121.54
1	1-A	240	TRP	C-N-CA	9.07	138.86	121.54
1	2-A	240	TRP	CA-C-N	9.07	138.86	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	240	TRP	C-N-CA	9.07	138.86	121.54
1	3-A	240	TRP	CA-C-N	9.07	138.86	121.54
1	3-A	240	TRP	C-N-CA	9.07	138.86	121.54
4	1-C	85	ASN	N-CA-C	-9.06	94.42	109.46
4	1-H	85	ASN	N-CA-C	-9.06	94.42	109.46
4	2-C	85	ASN	N-CA-C	-9.06	94.42	109.46
4	2-H	85	ASN	N-CA-C	-9.06	94.42	109.46
4	3-C	85	ASN	N-CA-C	-9.06	94.42	109.46
4	3-H	85	ASN	N-CA-C	-9.06	94.42	109.46
7	1-G	736	ASP	N-CA-C	-9.04	94.93	109.40
7	1-K	736	ASP	N-CA-C	-9.04	94.93	109.40
7	2-G	736	ASP	N-CA-C	-9.04	94.93	109.40
7	2-K	736	ASP	N-CA-C	-9.04	94.93	109.40
7	3-G	736	ASP	N-CA-C	-9.04	94.93	109.40
7	3-K	736	ASP	N-CA-C	-9.04	94.93	109.40
4	1-H	546	TYR	N-CA-C	-9.04	93.78	108.52
4	2-H	546	TYR	N-CA-C	-9.04	93.78	108.52
4	3-H	546	TYR	N-CA-C	-9.04	93.78	108.52
3	1-B	67	GLY	N-CA-C	-9.02	91.80	113.18
7	1-G	831	ALA	N-CA-C	9.02	123.21	109.23
3	2-B	67	GLY	N-CA-C	-9.02	91.80	113.18
7	2-G	831	ALA	N-CA-C	9.02	123.21	109.23
3	3-B	67	GLY	N-CA-C	-9.02	91.80	113.18
7	3-G	831	ALA	N-CA-C	9.02	123.21	109.23
7	1-K	120	TYR	CA-C-O	9.01	129.97	120.42
7	2-K	120	TYR	CA-C-O	9.01	129.97	120.42
7	3-K	120	TYR	CA-C-O	9.01	129.97	120.42
8	1-L	88	LEU	N-CA-C	9.01	121.10	111.28
8	2-L	88	LEU	N-CA-C	9.01	121.10	111.28
8	3-L	88	LEU	N-CA-C	9.01	121.10	111.28
3	1-B	331	ARG	CA-C-N	9.00	133.22	120.53
3	1-B	331	ARG	C-N-CA	9.00	133.22	120.53
4	1-C	546	TYR	N-CA-C	-9.00	93.85	108.52
6	1-F	106	VAL	CA-C-N	9.00	133.99	120.31
6	1-F	106	VAL	C-N-CA	9.00	133.99	120.31
3	2-B	331	ARG	CA-C-N	9.00	133.22	120.53
3	2-B	331	ARG	C-N-CA	9.00	133.22	120.53
4	2-C	546	TYR	N-CA-C	-9.00	93.85	108.52
6	2-F	106	VAL	CA-C-N	9.00	133.99	120.31
6	2-F	106	VAL	C-N-CA	9.00	133.99	120.31
3	3-B	331	ARG	CA-C-N	9.00	133.22	120.53
3	3-B	331	ARG	C-N-CA	9.00	133.22	120.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	3-C	546	TYR	N-CA-C	-9.00	93.85	108.52
6	3-F	106	VAL	CA-C-N	9.00	133.99	120.31
6	3-F	106	VAL	C-N-CA	9.00	133.99	120.31
3	1-N	67	GLY	N-CA-C	-9.00	91.85	113.18
3	2-N	67	GLY	N-CA-C	-9.00	91.85	113.18
3	3-N	67	GLY	N-CA-C	-9.00	91.85	113.18
7	1-K	831	ALA	N-CA-C	9.00	123.18	109.23
7	2-K	831	ALA	N-CA-C	9.00	123.18	109.23
7	3-K	831	ALA	N-CA-C	9.00	123.18	109.23
3	1-N	331	ARG	CA-C-N	8.99	133.21	120.53
3	1-N	331	ARG	C-N-CA	8.99	133.21	120.53
3	2-N	331	ARG	CA-C-N	8.99	133.21	120.53
3	2-N	331	ARG	C-N-CA	8.99	133.21	120.53
3	3-N	331	ARG	CA-C-N	8.99	133.21	120.53
3	3-N	331	ARG	C-N-CA	8.99	133.21	120.53
7	1-K	749	ASP	N-CA-C	-8.98	95.41	109.07
7	2-K	749	ASP	N-CA-C	-8.98	95.41	109.07
7	3-K	749	ASP	N-CA-C	-8.98	95.41	109.07
6	1-J	106	VAL	CA-C-N	8.97	133.95	120.31
6	1-J	106	VAL	C-N-CA	8.97	133.95	120.31
6	2-J	106	VAL	CA-C-N	8.97	133.95	120.31
6	2-J	106	VAL	C-N-CA	8.97	133.95	120.31
6	3-J	106	VAL	CA-C-N	8.97	133.95	120.31
6	3-J	106	VAL	C-N-CA	8.97	133.95	120.31
1	1-A	714	GLU	N-CA-C	8.97	120.67	111.07
1	2-A	714	GLU	N-CA-C	8.97	120.67	111.07
1	3-A	714	GLU	N-CA-C	8.97	120.67	111.07
1	1-A	511	ILE	N-CA-C	-8.97	94.54	108.44
6	1-R	61	ILE	N-CA-C	-8.97	95.54	108.36
1	2-A	511	ILE	N-CA-C	-8.97	94.54	108.44
6	2-R	61	ILE	N-CA-C	-8.97	95.54	108.36
1	3-A	511	ILE	N-CA-C	-8.97	94.54	108.44
6	3-R	61	ILE	N-CA-C	-8.97	95.54	108.36
4	1-H	170	TRP	CA-C-N	8.96	136.88	122.81
4	1-H	170	TRP	C-N-CA	8.96	136.88	122.81
4	2-H	170	TRP	CA-C-N	8.96	136.88	122.81
4	2-H	170	TRP	C-N-CA	8.96	136.88	122.81
4	3-H	170	TRP	CA-C-N	8.96	136.88	122.81
4	3-H	170	TRP	C-N-CA	8.96	136.88	122.81
7	1-G	749	ASP	N-CA-C	-8.95	95.46	109.07
7	2-G	749	ASP	N-CA-C	-8.95	95.46	109.07
7	3-G	749	ASP	N-CA-C	-8.95	95.46	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	462	GLU	N-CA-C	8.95	120.81	111.14
7	2-G	462	GLU	N-CA-C	8.95	120.81	111.14
7	3-G	462	GLU	N-CA-C	8.95	120.81	111.14
6	1-F	161	THR	N-CA-C	-8.95	100.68	113.21
6	2-F	161	THR	N-CA-C	-8.95	100.68	113.21
6	3-F	161	THR	N-CA-C	-8.95	100.68	113.21
1	1-A	779	ASP	N-CA-C	-8.94	90.06	109.81
1	2-A	779	ASP	N-CA-C	-8.94	90.06	109.81
1	3-A	779	ASP	N-CA-C	-8.94	90.06	109.81
6	1-J	161	THR	N-CA-C	-8.94	100.70	113.21
6	2-J	161	THR	N-CA-C	-8.94	100.70	113.21
6	3-J	161	THR	N-CA-C	-8.94	100.70	113.21
1	1-A	606	ARG	CA-C-N	8.94	133.42	120.82
1	1-A	606	ARG	C-N-CA	8.94	133.42	120.82
1	2-A	606	ARG	CA-C-N	8.94	133.42	120.82
1	2-A	606	ARG	C-N-CA	8.94	133.42	120.82
1	3-A	606	ARG	CA-C-N	8.94	133.42	120.82
1	3-A	606	ARG	C-N-CA	8.94	133.42	120.82
4	1-C	170	TRP	CA-C-N	8.93	136.83	122.81
4	1-C	170	TRP	C-N-CA	8.93	136.83	122.81
4	2-C	170	TRP	CA-C-N	8.93	136.83	122.81
4	2-C	170	TRP	C-N-CA	8.93	136.83	122.81
4	3-C	170	TRP	CA-C-N	8.93	136.83	122.81
4	3-C	170	TRP	C-N-CA	8.93	136.83	122.81
1	1-A	67	VAL	N-CA-C	-8.93	95.62	108.48
1	2-A	67	VAL	N-CA-C	-8.93	95.62	108.48
1	3-A	67	VAL	N-CA-C	-8.93	95.62	108.48
3	1-N	35	PRO	N-CA-C	8.92	121.58	110.70
3	2-N	35	PRO	N-CA-C	8.92	121.58	110.70
3	3-N	35	PRO	N-CA-C	8.92	121.58	110.70
7	1-G	836	GLY	N-CA-C	-8.91	102.86	115.43
7	2-G	836	GLY	N-CA-C	-8.91	102.86	115.43
7	3-G	836	GLY	N-CA-C	-8.91	102.86	115.43
3	1-N	269	GLN	N-CA-C	-8.91	91.82	110.80
3	2-N	269	GLN	N-CA-C	-8.91	91.82	110.80
3	3-N	269	GLN	N-CA-C	-8.91	91.82	110.80
7	1-K	836	GLY	N-CA-C	-8.91	102.87	115.43
6	1-M	79	ARG	N-CA-C	-8.91	101.54	111.07
7	2-K	836	GLY	N-CA-C	-8.91	102.87	115.43
6	2-M	79	ARG	N-CA-C	-8.91	101.54	111.07
7	3-K	836	GLY	N-CA-C	-8.91	102.87	115.43
6	3-M	79	ARG	N-CA-C	-8.91	101.54	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-B	269	GLN	N-CA-C	-8.90	91.84	110.80
3	2-B	269	GLN	N-CA-C	-8.90	91.84	110.80
3	3-B	269	GLN	N-CA-C	-8.90	91.84	110.80
4	1-C	722	ASP	N-CA-C	8.89	121.93	111.71
4	2-C	722	ASP	N-CA-C	8.89	121.93	111.71
4	3-C	722	ASP	N-CA-C	8.89	121.93	111.71
1	1-A	507	ALA	N-CA-C	-8.88	95.57	109.07
1	2-A	507	ALA	N-CA-C	-8.88	95.57	109.07
1	3-A	507	ALA	N-CA-C	-8.88	95.57	109.07
3	1-B	35	PRO	N-CA-C	8.88	121.53	110.70
3	2-B	35	PRO	N-CA-C	8.88	121.53	110.70
3	3-B	35	PRO	N-CA-C	8.88	121.53	110.70
3	1-B	748	HIS	N-CA-C	-8.88	95.47	109.50
3	2-B	748	HIS	N-CA-C	-8.88	95.47	109.50
3	3-B	748	HIS	N-CA-C	-8.88	95.47	109.50
6	1-R	166	LEU	N-CA-C	8.87	120.64	110.97
6	1-J	165	GLY	CA-C-N	8.87	131.97	120.44
6	1-J	165	GLY	C-N-CA	8.87	131.97	120.44
6	2-R	166	LEU	N-CA-C	8.87	120.64	110.97
6	2-J	165	GLY	CA-C-N	8.87	131.97	120.44
6	2-J	165	GLY	C-N-CA	8.87	131.97	120.44
6	3-R	166	LEU	N-CA-C	8.87	120.64	110.97
6	3-J	165	GLY	CA-C-N	8.87	131.97	120.44
6	3-J	165	GLY	C-N-CA	8.87	131.97	120.44
6	1-F	165	GLY	CA-C-N	8.86	131.96	120.44
6	1-F	165	GLY	C-N-CA	8.86	131.96	120.44
6	2-F	165	GLY	CA-C-N	8.86	131.96	120.44
6	2-F	165	GLY	C-N-CA	8.86	131.96	120.44
6	3-F	165	GLY	CA-C-N	8.86	131.96	120.44
6	3-F	165	GLY	C-N-CA	8.86	131.96	120.44
1	1-A	740	GLY	N-CA-C	-8.86	92.19	113.18
7	1-G	731	THR	N-CA-C	-8.86	94.81	109.07
1	2-A	740	GLY	N-CA-C	-8.86	92.19	113.18
7	2-G	731	THR	N-CA-C	-8.86	94.81	109.07
1	3-A	740	GLY	N-CA-C	-8.86	92.19	113.18
7	3-G	731	THR	N-CA-C	-8.86	94.81	109.07
7	1-K	731	THR	N-CA-C	-8.85	94.82	109.07
7	2-K	731	THR	N-CA-C	-8.85	94.82	109.07
7	3-K	731	THR	N-CA-C	-8.85	94.82	109.07
7	1-K	244	ASP	N-CA-C	-8.84	91.96	110.80
7	2-K	244	ASP	N-CA-C	-8.84	91.96	110.80
7	3-K	244	ASP	N-CA-C	-8.84	91.96	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	134	SER	N-CA-C	8.83	120.91	111.28
7	2-G	134	SER	N-CA-C	8.83	120.91	111.28
7	3-G	134	SER	N-CA-C	8.83	120.91	111.28
3	1-N	49	ASP	N-CA-C	-8.82	92.00	110.80
3	2-N	49	ASP	N-CA-C	-8.82	92.00	110.80
3	3-N	49	ASP	N-CA-C	-8.82	92.00	110.80
3	1-B	49	ASP	N-CA-C	-8.82	92.01	110.80
3	2-B	49	ASP	N-CA-C	-8.82	92.01	110.80
3	3-B	49	ASP	N-CA-C	-8.82	92.01	110.80
1	1-A	522	CYS	N-CA-C	-8.80	95.75	108.60
1	2-A	522	CYS	N-CA-C	-8.80	95.75	108.60
1	3-A	522	CYS	N-CA-C	-8.80	95.75	108.60
1	1-A	249	TYR	N-CA-C	-8.79	97.45	110.46
1	2-A	249	TYR	N-CA-C	-8.79	97.45	110.46
1	3-A	249	TYR	N-CA-C	-8.79	97.45	110.46
3	1-B	843	ASP	N-CA-C	8.77	120.46	111.07
3	2-B	843	ASP	N-CA-C	8.77	120.46	111.07
3	3-B	843	ASP	N-CA-C	8.77	120.46	111.07
6	1-M	91	VAL	CA-C-N	8.75	135.10	122.94
6	1-M	91	VAL	C-N-CA	8.75	135.10	122.94
6	2-M	91	VAL	CA-C-N	8.75	135.10	122.94
6	2-M	91	VAL	C-N-CA	8.75	135.10	122.94
6	3-M	91	VAL	CA-C-N	8.75	135.10	122.94
6	3-M	91	VAL	C-N-CA	8.75	135.10	122.94
3	1-B	792	LEU	N-CA-C	-8.72	93.52	109.56
3	2-B	792	LEU	N-CA-C	-8.72	93.52	109.56
3	3-B	792	LEU	N-CA-C	-8.72	93.52	109.56
3	1-B	871	ASN	N-CA-C	-8.71	92.25	110.80
3	2-B	871	ASN	N-CA-C	-8.71	92.25	110.80
3	3-B	871	ASN	N-CA-C	-8.71	92.25	110.80
7	1-K	853	THR	N-CA-C	-8.70	95.75	109.50
7	2-K	853	THR	N-CA-C	-8.70	95.75	109.50
7	3-K	853	THR	N-CA-C	-8.70	95.75	109.50
3	1-B	840	ASP	CA-C-N	8.69	132.76	120.42
3	1-B	840	ASP	C-N-CA	8.69	132.76	120.42
3	2-B	840	ASP	CA-C-N	8.69	132.76	120.42
3	2-B	840	ASP	C-N-CA	8.69	132.76	120.42
3	3-B	840	ASP	CA-C-N	8.69	132.76	120.42
3	3-B	840	ASP	C-N-CA	8.69	132.76	120.42
7	1-G	853	THR	N-CA-C	-8.69	95.78	109.50
7	2-G	853	THR	N-CA-C	-8.69	95.78	109.50
7	3-G	853	THR	N-CA-C	-8.69	95.78	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	202	LEU	N-CA-C	-8.67	96.08	109.52
4	2-H	202	LEU	N-CA-C	-8.67	96.08	109.52
4	3-H	202	LEU	N-CA-C	-8.67	96.08	109.52
1	1-A	587	PRO	N-CA-C	8.65	126.22	111.77
1	2-A	587	PRO	N-CA-C	8.65	126.22	111.77
1	3-A	587	PRO	N-CA-C	8.65	126.22	111.77
6	1-R	161	THR	N-CA-C	-8.65	101.93	111.36
6	2-R	161	THR	N-CA-C	-8.65	101.93	111.36
6	3-R	161	THR	N-CA-C	-8.65	101.93	111.36
4	1-C	202	LEU	N-CA-C	-8.65	96.11	109.52
4	2-C	202	LEU	N-CA-C	-8.65	96.11	109.52
4	3-C	202	LEU	N-CA-C	-8.65	96.11	109.52
8	1-Z	129	VAL	N-CA-C	-8.64	94.69	108.95
8	2-Z	129	VAL	N-CA-C	-8.64	94.69	108.95
8	3-Z	129	VAL	N-CA-C	-8.64	94.69	108.95
1	1-A	77	VAL	N-CA-C	-8.63	95.69	108.12
6	1-R	71	GLN	N-CA-C	-8.63	94.82	108.63
1	2-A	77	VAL	N-CA-C	-8.63	95.69	108.12
6	2-R	71	GLN	N-CA-C	-8.63	94.82	108.63
1	3-A	77	VAL	N-CA-C	-8.63	95.69	108.12
6	3-R	71	GLN	N-CA-C	-8.63	94.82	108.63
6	1-R	99	ARG	N-CA-C	-8.63	102.46	113.16
6	2-R	99	ARG	N-CA-C	-8.63	102.46	113.16
6	3-R	99	ARG	N-CA-C	-8.63	102.46	113.16
8	1-L	60	ALA	CA-C-N	8.62	135.15	122.99
8	1-L	60	ALA	C-N-CA	8.62	135.15	122.99
8	2-L	60	ALA	CA-C-N	8.62	135.15	122.99
8	2-L	60	ALA	C-N-CA	8.62	135.15	122.99
8	3-L	60	ALA	CA-C-N	8.62	135.15	122.99
8	3-L	60	ALA	C-N-CA	8.62	135.15	122.99
3	1-B	804	VAL	N-CA-C	-8.61	95.56	108.99
3	2-B	804	VAL	N-CA-C	-8.61	95.56	108.99
3	3-B	804	VAL	N-CA-C	-8.61	95.56	108.99
1	1-A	406	ASP	N-CA-C	-8.60	99.65	112.04
1	2-A	406	ASP	N-CA-C	-8.60	99.65	112.04
1	3-A	406	ASP	N-CA-C	-8.60	99.65	112.04
7	1-K	609	ARG	CA-C-O	8.59	129.65	120.55
7	2-K	609	ARG	CA-C-O	8.59	129.65	120.55
7	3-K	609	ARG	CA-C-O	8.59	129.65	120.55
7	1-G	640	THR	N-CA-C	-8.59	94.90	109.24
7	2-G	640	THR	N-CA-C	-8.59	94.90	109.24
7	3-G	640	THR	N-CA-C	-8.59	94.90	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-K	640	THR	N-CA-C	-8.58	94.92	109.24
7	2-K	640	THR	N-CA-C	-8.58	94.92	109.24
7	3-K	640	THR	N-CA-C	-8.58	94.92	109.24
3	1-B	893	LEU	N-CA-C	8.57	120.40	111.14
3	2-B	893	LEU	N-CA-C	8.57	120.40	111.14
3	3-B	893	LEU	N-CA-C	8.57	120.40	111.14
7	1-G	609	ARG	CA-C-O	8.56	129.63	120.55
7	2-G	609	ARG	CA-C-O	8.56	129.63	120.55
7	3-G	609	ARG	CA-C-O	8.56	129.63	120.55
1	1-A	647	THR	CA-C-N	8.56	131.75	120.28
1	1-A	647	THR	C-N-CA	8.56	131.75	120.28
1	2-A	647	THR	CA-C-N	8.56	131.75	120.28
1	2-A	647	THR	C-N-CA	8.56	131.75	120.28
1	3-A	647	THR	CA-C-N	8.56	131.75	120.28
1	3-A	647	THR	C-N-CA	8.56	131.75	120.28
6	1-R	150	ASN	CA-C-N	8.54	142.64	121.80
6	1-R	150	ASN	C-N-CA	8.54	142.64	121.80
6	2-R	150	ASN	CA-C-N	8.54	142.64	121.80
6	2-R	150	ASN	C-N-CA	8.54	142.64	121.80
6	3-R	150	ASN	CA-C-N	8.54	142.64	121.80
6	3-R	150	ASN	C-N-CA	8.54	142.64	121.80
1	1-A	371	ASN	N-CA-C	-8.52	90.01	108.93
1	2-A	371	ASN	N-CA-C	-8.52	90.01	108.93
1	3-A	371	ASN	N-CA-C	-8.52	90.01	108.93
1	1-A	236	GLU	N-CA-C	-8.51	92.68	110.80
1	2-A	236	GLU	N-CA-C	-8.51	92.68	110.80
1	3-A	236	GLU	N-CA-C	-8.51	92.68	110.80
1	1-A	509	HIS	N-CA-C	-8.50	95.54	109.40
1	2-A	509	HIS	N-CA-C	-8.50	95.54	109.40
1	3-A	509	HIS	N-CA-C	-8.50	95.54	109.40
1	1-A	105	TYR	CA-C-N	-8.49	109.22	119.84
1	1-A	105	TYR	C-N-CA	-8.49	109.22	119.84
1	2-A	105	TYR	CA-C-N	-8.49	109.22	119.84
1	2-A	105	TYR	C-N-CA	-8.49	109.22	119.84
1	3-A	105	TYR	CA-C-N	-8.49	109.22	119.84
1	3-A	105	TYR	C-N-CA	-8.49	109.22	119.84
3	1-B	837	ILE	N-CA-C	-8.49	91.68	109.34
3	2-B	837	ILE	N-CA-C	-8.49	91.68	109.34
3	3-B	837	ILE	N-CA-C	-8.49	91.68	109.34
3	1-B	850	CYS	N-CA-C	8.47	121.46	108.42
7	1-K	858	ALA	N-CA-C	-8.47	95.10	109.24
3	2-B	850	CYS	N-CA-C	8.47	121.46	108.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-K	858	ALA	N-CA-C	-8.47	95.10	109.24
3	3-B	850	CYS	N-CA-C	8.47	121.46	108.42
7	3-K	858	ALA	N-CA-C	-8.47	95.10	109.24
7	1-G	858	ALA	N-CA-C	-8.45	95.12	109.24
6	1-R	96	ASP	N-CA-C	-8.45	94.95	108.73
7	2-G	858	ALA	N-CA-C	-8.45	95.12	109.24
6	2-R	96	ASP	N-CA-C	-8.45	94.95	108.73
7	3-G	858	ALA	N-CA-C	-8.45	95.12	109.24
6	3-R	96	ASP	N-CA-C	-8.45	94.95	108.73
1	1-A	515	ASN	N-CA-C	-8.45	97.26	110.36
4	1-H	682	GLN	CA-C-N	8.45	131.60	120.28
4	1-H	682	GLN	C-N-CA	8.45	131.60	120.28
1	2-A	515	ASN	N-CA-C	-8.45	97.26	110.36
4	2-H	682	GLN	CA-C-N	8.45	131.60	120.28
4	2-H	682	GLN	C-N-CA	8.45	131.60	120.28
1	3-A	515	ASN	N-CA-C	-8.45	97.26	110.36
4	3-H	682	GLN	CA-C-N	8.45	131.60	120.28
4	3-H	682	GLN	C-N-CA	8.45	131.60	120.28
3	1-B	740	PRO	N-CA-C	-8.44	95.09	112.47
3	2-B	740	PRO	N-CA-C	-8.44	95.09	112.47
3	3-B	740	PRO	N-CA-C	-8.44	95.09	112.47
1	1-A	132	THR	N-CA-C	-8.44	96.22	109.72
1	2-A	132	THR	N-CA-C	-8.44	96.22	109.72
1	3-A	132	THR	N-CA-C	-8.44	96.22	109.72
7	1-G	368	MET	N-CA-C	8.43	120.47	111.28
7	2-G	368	MET	N-CA-C	8.43	120.47	111.28
7	3-G	368	MET	N-CA-C	8.43	120.47	111.28
4	1-H	262	ARG	N-CA-C	-8.43	96.56	109.95
4	2-H	262	ARG	N-CA-C	-8.43	96.56	109.95
4	3-H	262	ARG	N-CA-C	-8.43	96.56	109.95
7	1-K	762	ASP	N-CA-C	-8.40	102.81	113.23
7	2-K	762	ASP	N-CA-C	-8.40	102.81	113.23
7	3-K	762	ASP	N-CA-C	-8.40	102.81	113.23
4	1-C	262	ARG	N-CA-C	-8.40	96.60	109.95
4	2-C	262	ARG	N-CA-C	-8.40	96.60	109.95
4	3-C	262	ARG	N-CA-C	-8.40	96.60	109.95
6	1-R	130	LEU	CA-C-N	8.39	130.33	119.84
6	1-R	130	LEU	C-N-CA	8.39	130.33	119.84
6	2-R	130	LEU	CA-C-N	8.39	130.33	119.84
6	2-R	130	LEU	C-N-CA	8.39	130.33	119.84
6	3-R	130	LEU	CA-C-N	8.39	130.33	119.84
6	3-R	130	LEU	C-N-CA	8.39	130.33	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	807	VAL	N-CA-C	8.38	119.24	111.45
4	2-C	807	VAL	N-CA-C	8.38	119.24	111.45
4	3-C	807	VAL	N-CA-C	8.38	119.24	111.45
5	1-I	131	ARG	CA-C-N	8.37	131.85	120.38
5	1-I	131	ARG	C-N-CA	8.37	131.85	120.38
5	2-I	131	ARG	CA-C-N	8.37	131.85	120.38
5	2-I	131	ARG	C-N-CA	8.37	131.85	120.38
5	3-I	131	ARG	CA-C-N	8.37	131.85	120.38
5	3-I	131	ARG	C-N-CA	8.37	131.85	120.38
6	1-R	42	VAL	CA-C-N	8.37	137.03	121.97
6	1-R	42	VAL	C-N-CA	8.37	137.03	121.97
6	2-R	42	VAL	CA-C-N	8.37	137.03	121.97
6	2-R	42	VAL	C-N-CA	8.37	137.03	121.97
6	3-R	42	VAL	CA-C-N	8.37	137.03	121.97
6	3-R	42	VAL	C-N-CA	8.37	137.03	121.97
3	1-B	800	ILE	N-CA-C	-8.36	96.00	108.46
7	1-G	150	ASP	CA-C-N	8.36	137.51	121.54
7	1-G	150	ASP	C-N-CA	8.36	137.51	121.54
7	1-G	762	ASP	N-CA-C	-8.36	102.86	113.23
3	2-B	800	ILE	N-CA-C	-8.36	96.00	108.46
7	2-G	150	ASP	CA-C-N	8.36	137.51	121.54
7	2-G	150	ASP	C-N-CA	8.36	137.51	121.54
7	2-G	762	ASP	N-CA-C	-8.36	102.86	113.23
3	3-B	800	ILE	N-CA-C	-8.36	96.00	108.46
7	3-G	150	ASP	CA-C-N	8.36	137.51	121.54
7	3-G	150	ASP	C-N-CA	8.36	137.51	121.54
7	3-G	762	ASP	N-CA-C	-8.36	102.86	113.23
3	1-B	554	ARG	CA-C-N	8.35	128.98	120.38
3	1-B	554	ARG	C-N-CA	8.35	128.98	120.38
3	2-B	554	ARG	CA-C-N	8.35	128.98	120.38
3	2-B	554	ARG	C-N-CA	8.35	128.98	120.38
3	3-B	554	ARG	CA-C-N	8.35	128.98	120.38
3	3-B	554	ARG	C-N-CA	8.35	128.98	120.38
3	1-N	103	THR	N-CA-C	-8.35	104.12	112.97
3	2-N	103	THR	N-CA-C	-8.35	104.12	112.97
3	3-N	103	THR	N-CA-C	-8.35	104.12	112.97
4	1-H	446	GLY	N-CA-C	-8.34	98.53	110.96
4	2-H	446	GLY	N-CA-C	-8.34	98.53	110.96
4	3-H	446	GLY	N-CA-C	-8.34	98.53	110.96
8	1-Z	16	ILE	N-CA-C	-8.32	96.14	108.12
3	1-N	554	ARG	CA-C-N	8.32	128.95	120.38
3	1-N	554	ARG	C-N-CA	8.32	128.95	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2-Z	16	ILE	N-CA-C	-8.32	96.14	108.12
3	2-N	554	ARG	CA-C-N	8.32	128.95	120.38
3	2-N	554	ARG	C-N-CA	8.32	128.95	120.38
8	3-Z	16	ILE	N-CA-C	-8.32	96.14	108.12
3	3-N	554	ARG	CA-C-N	8.32	128.95	120.38
3	3-N	554	ARG	C-N-CA	8.32	128.95	120.38
4	1-C	446	GLY	N-CA-C	-8.32	98.57	110.96
4	2-C	446	GLY	N-CA-C	-8.32	98.57	110.96
4	3-C	446	GLY	N-CA-C	-8.32	98.57	110.96
6	1-J	159	CYS	N-CA-C	-8.31	93.09	110.80
6	2-J	159	CYS	N-CA-C	-8.31	93.09	110.80
6	3-J	159	CYS	N-CA-C	-8.31	93.09	110.80
5	1-D	50	GLU	N-CA-C	-8.31	94.72	108.76
5	1-D	131	ARG	CA-C-N	8.31	131.76	120.38
5	1-D	131	ARG	C-N-CA	8.31	131.76	120.38
5	2-D	50	GLU	N-CA-C	-8.31	94.72	108.76
5	2-D	131	ARG	CA-C-N	8.31	131.76	120.38
5	2-D	131	ARG	C-N-CA	8.31	131.76	120.38
5	3-D	50	GLU	N-CA-C	-8.31	94.72	108.76
5	3-D	131	ARG	CA-C-N	8.31	131.76	120.38
5	3-D	131	ARG	C-N-CA	8.31	131.76	120.38
8	1-Z	29	LYS	N-CA-C	-8.31	93.99	108.69
8	2-Z	29	LYS	N-CA-C	-8.31	93.99	108.69
8	3-Z	29	LYS	N-CA-C	-8.31	93.99	108.69
6	1-F	159	CYS	N-CA-C	-8.30	93.12	110.80
6	2-F	159	CYS	N-CA-C	-8.30	93.12	110.80
6	3-F	159	CYS	N-CA-C	-8.30	93.12	110.80
5	1-I	50	GLU	N-CA-C	-8.30	94.74	108.76
5	2-I	50	GLU	N-CA-C	-8.30	94.74	108.76
5	3-I	50	GLU	N-CA-C	-8.30	94.74	108.76
3	1-B	103	THR	N-CA-C	-8.30	104.18	112.97
3	2-B	103	THR	N-CA-C	-8.30	104.18	112.97
3	3-B	103	THR	N-CA-C	-8.30	104.18	112.97
7	1-G	197	LEU	N-CA-C	8.29	120.32	111.28
4	1-H	110	THR	N-CA-C	-8.29	100.93	112.45
7	2-G	197	LEU	N-CA-C	8.29	120.32	111.28
4	2-H	110	THR	N-CA-C	-8.29	100.93	112.45
7	3-G	197	LEU	N-CA-C	8.29	120.32	111.28
4	3-H	110	THR	N-CA-C	-8.29	100.93	112.45
4	1-C	155	ASN	CA-C-N	8.28	137.34	121.54
4	1-C	155	ASN	C-N-CA	8.28	137.34	121.54
6	1-R	106	VAL	N-CA-C	8.28	118.36	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-C	155	ASN	CA-C-N	8.28	137.34	121.54
4	2-C	155	ASN	C-N-CA	8.28	137.34	121.54
6	2-R	106	VAL	N-CA-C	8.28	118.36	110.42
4	3-C	155	ASN	CA-C-N	8.28	137.34	121.54
4	3-C	155	ASN	C-N-CA	8.28	137.34	121.54
6	3-R	106	VAL	N-CA-C	8.28	118.36	110.42
4	1-C	110	THR	N-CA-C	-8.27	100.95	112.45
4	2-C	110	THR	N-CA-C	-8.27	100.95	112.45
4	3-C	110	THR	N-CA-C	-8.27	100.95	112.45
8	1-Z	11	TYR	N-CA-C	-8.27	93.19	110.80
8	2-Z	11	TYR	N-CA-C	-8.27	93.19	110.80
8	3-Z	11	TYR	N-CA-C	-8.27	93.19	110.80
7	1-K	797	LEU	CA-C-N	8.26	131.35	120.28
7	1-K	797	LEU	C-N-CA	8.26	131.35	120.28
8	1-L	48	ILE	N-CA-C	8.26	118.30	110.53
7	2-K	797	LEU	CA-C-N	8.26	131.35	120.28
7	2-K	797	LEU	C-N-CA	8.26	131.35	120.28
8	2-L	48	ILE	N-CA-C	8.26	118.30	110.53
7	3-K	797	LEU	CA-C-N	8.26	131.35	120.28
7	3-K	797	LEU	C-N-CA	8.26	131.35	120.28
8	3-L	48	ILE	N-CA-C	8.26	118.30	110.53
3	1-B	446	PHE	N-CA-C	-8.25	103.35	113.50
3	2-B	446	PHE	N-CA-C	-8.25	103.35	113.50
3	3-B	446	PHE	N-CA-C	-8.25	103.35	113.50
4	1-H	155	ASN	CA-C-N	8.25	137.30	121.54
4	1-H	155	ASN	C-N-CA	8.25	137.30	121.54
4	2-H	155	ASN	CA-C-N	8.25	137.30	121.54
4	2-H	155	ASN	C-N-CA	8.25	137.30	121.54
4	3-H	155	ASN	CA-C-N	8.25	137.30	121.54
4	3-H	155	ASN	C-N-CA	8.25	137.30	121.54
7	1-G	797	LEU	CA-C-N	8.24	131.32	120.28
7	1-G	797	LEU	C-N-CA	8.24	131.32	120.28
7	2-G	797	LEU	CA-C-N	8.24	131.32	120.28
7	2-G	797	LEU	C-N-CA	8.24	131.32	120.28
7	3-G	797	LEU	CA-C-N	8.24	131.32	120.28
7	3-G	797	LEU	C-N-CA	8.24	131.32	120.28
4	1-C	233	SER	N-CA-C	-8.24	102.38	111.36
4	2-C	233	SER	N-CA-C	-8.24	102.38	111.36
4	3-C	233	SER	N-CA-C	-8.24	102.38	111.36
8	1-L	35	TYR	N-CA-C	-8.23	97.68	109.62
8	2-L	35	TYR	N-CA-C	-8.23	97.68	109.62
8	3-L	35	TYR	N-CA-C	-8.23	97.68	109.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	442	ARG	N-CA-C	-8.23	95.82	109.07
4	2-H	442	ARG	N-CA-C	-8.23	95.82	109.07
4	3-H	442	ARG	N-CA-C	-8.23	95.82	109.07
4	1-C	793	GLU	CA-C-N	8.23	131.31	120.28
4	1-C	793	GLU	C-N-CA	8.23	131.31	120.28
4	2-C	793	GLU	CA-C-N	8.23	131.31	120.28
4	2-C	793	GLU	C-N-CA	8.23	131.31	120.28
4	3-C	793	GLU	CA-C-N	8.23	131.31	120.28
4	3-C	793	GLU	C-N-CA	8.23	131.31	120.28
1	1-A	87	PHE	N-CA-C	-8.22	95.78	108.76
6	1-R	58	TYR	N-CA-C	-8.22	94.62	108.26
1	2-A	87	PHE	N-CA-C	-8.22	95.78	108.76
6	2-R	58	TYR	N-CA-C	-8.22	94.62	108.26
1	3-A	87	PHE	N-CA-C	-8.22	95.78	108.76
6	3-R	58	TYR	N-CA-C	-8.22	94.62	108.26
1	1-A	457	PHE	N-CA-C	-8.21	93.31	110.80
1	2-A	457	PHE	N-CA-C	-8.21	93.31	110.80
1	3-A	457	PHE	N-CA-C	-8.21	93.31	110.80
3	1-B	744	GLU	N-CA-C	-8.21	96.53	109.50
3	2-B	744	GLU	N-CA-C	-8.21	96.53	109.50
3	3-B	744	GLU	N-CA-C	-8.21	96.53	109.50
4	1-C	492	SER	N-CA-C	8.21	120.30	111.36
3	1-N	446	PHE	N-CA-C	-8.20	103.41	113.50
4	2-C	492	SER	N-CA-C	8.21	120.30	111.36
3	2-N	446	PHE	N-CA-C	-8.20	103.41	113.50
4	3-C	492	SER	N-CA-C	8.21	120.30	111.36
3	3-N	446	PHE	N-CA-C	-8.20	103.41	113.50
4	1-C	442	ARG	N-CA-C	-8.20	95.86	109.07
7	1-K	667	ASN	N-CA-C	-8.20	93.33	110.80
4	2-C	442	ARG	N-CA-C	-8.20	95.86	109.07
7	2-K	667	ASN	N-CA-C	-8.20	93.33	110.80
4	3-C	442	ARG	N-CA-C	-8.20	95.86	109.07
7	3-K	667	ASN	N-CA-C	-8.20	93.33	110.80
4	1-H	233	SER	N-CA-C	-8.20	102.42	111.36
4	2-H	233	SER	N-CA-C	-8.20	102.42	111.36
4	3-H	233	SER	N-CA-C	-8.20	102.42	111.36
4	1-H	492	SER	N-CA-C	8.19	120.29	111.36
4	2-H	492	SER	N-CA-C	8.19	120.29	111.36
4	3-H	492	SER	N-CA-C	8.19	120.29	111.36
6	1-M	100	ILE	N-CA-C	8.19	118.23	110.53
6	2-M	100	ILE	N-CA-C	8.19	118.23	110.53
6	3-M	100	ILE	N-CA-C	8.19	118.23	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	667	ASN	N-CA-C	-8.19	93.36	110.80
7	2-G	667	ASN	N-CA-C	-8.19	93.36	110.80
7	3-G	667	ASN	N-CA-C	-8.19	93.36	110.80
8	1-Z	22	ASP	N-CA-C	-8.18	103.39	112.72
8	2-Z	22	ASP	N-CA-C	-8.18	103.39	112.72
8	3-Z	22	ASP	N-CA-C	-8.18	103.39	112.72
6	1-R	144	GLY	N-CA-C	-8.18	93.80	113.18
6	2-R	144	GLY	N-CA-C	-8.18	93.80	113.18
6	3-R	144	GLY	N-CA-C	-8.18	93.80	113.18
7	1-K	645	GLU	N-CA-C	-8.18	102.31	111.71
7	2-K	645	GLU	N-CA-C	-8.18	102.31	111.71
7	3-K	645	GLU	N-CA-C	-8.18	102.31	111.71
1	1-A	387	GLU	N-CA-C	-8.17	102.32	111.14
1	2-A	387	GLU	N-CA-C	-8.17	102.32	111.14
1	3-A	387	GLU	N-CA-C	-8.17	102.32	111.14
4	1-C	327	LEU	N-CA-C	-8.17	96.17	108.99
4	2-C	327	LEU	N-CA-C	-8.17	96.17	108.99
4	3-C	327	LEU	N-CA-C	-8.17	96.17	108.99
7	1-K	74	THR	N-CA-C	8.15	120.17	111.28
1	1-A	392	ASP	N-CA-C	-8.15	94.99	108.76
7	1-K	242	GLU	N-CA-C	-8.15	103.35	113.38
7	1-K	695	ALA	N-CA-C	-8.15	95.29	108.41
7	2-K	74	THR	N-CA-C	8.15	120.17	111.28
1	2-A	392	ASP	N-CA-C	-8.15	94.99	108.76
7	2-K	242	GLU	N-CA-C	-8.15	103.35	113.38
7	2-K	695	ALA	N-CA-C	-8.15	95.29	108.41
7	3-K	74	THR	N-CA-C	8.15	120.17	111.28
1	3-A	392	ASP	N-CA-C	-8.15	94.99	108.76
7	3-K	242	GLU	N-CA-C	-8.15	103.35	113.38
7	3-K	695	ALA	N-CA-C	-8.15	95.29	108.41
7	1-G	215	ILE	N-CA-C	-8.14	102.88	110.53
7	1-K	831	ALA	CA-C-N	8.14	133.82	121.04
7	1-K	831	ALA	C-N-CA	8.14	133.82	121.04
4	1-H	327	LEU	N-CA-C	-8.14	96.21	108.99
7	2-G	215	ILE	N-CA-C	-8.14	102.88	110.53
7	2-K	831	ALA	CA-C-N	8.14	133.82	121.04
7	2-K	831	ALA	C-N-CA	8.14	133.82	121.04
4	2-H	327	LEU	N-CA-C	-8.14	96.21	108.99
7	3-G	215	ILE	N-CA-C	-8.14	102.88	110.53
7	3-K	831	ALA	CA-C-N	8.14	133.82	121.04
7	3-K	831	ALA	C-N-CA	8.14	133.82	121.04
4	3-H	327	LEU	N-CA-C	-8.14	96.21	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	522	GLU	CA-C-N	8.13	133.69	123.12
4	1-C	522	GLU	C-N-CA	8.13	133.69	123.12
4	2-C	522	GLU	CA-C-N	8.13	133.69	123.12
4	2-C	522	GLU	C-N-CA	8.13	133.69	123.12
4	3-C	522	GLU	CA-C-N	8.13	133.69	123.12
4	3-C	522	GLU	C-N-CA	8.13	133.69	123.12
1	1-A	436	LEU	N-CA-C	-8.13	97.02	109.95
1	2-A	436	LEU	N-CA-C	-8.13	97.02	109.95
1	3-A	436	LEU	N-CA-C	-8.13	97.02	109.95
3	1-B	795	HIS	CA-C-N	8.12	136.44	122.64
3	1-B	795	HIS	C-N-CA	8.12	136.44	122.64
4	1-H	106	ALA	N-CA-C	-8.12	96.67	109.50
3	2-B	795	HIS	CA-C-N	8.12	136.44	122.64
3	2-B	795	HIS	C-N-CA	8.12	136.44	122.64
4	2-H	106	ALA	N-CA-C	-8.12	96.67	109.50
3	3-B	795	HIS	CA-C-N	8.12	136.44	122.64
3	3-B	795	HIS	C-N-CA	8.12	136.44	122.64
4	3-H	106	ALA	N-CA-C	-8.12	96.67	109.50
7	1-G	831	ALA	CA-C-N	8.11	133.77	121.04
7	1-G	831	ALA	C-N-CA	8.11	133.77	121.04
7	1-K	693	VAL	CA-C-N	8.11	129.97	119.84
7	1-K	693	VAL	C-N-CA	8.11	129.97	119.84
7	2-G	831	ALA	CA-C-N	8.11	133.77	121.04
7	2-G	831	ALA	C-N-CA	8.11	133.77	121.04
7	2-K	693	VAL	CA-C-N	8.11	129.97	119.84
7	2-K	693	VAL	C-N-CA	8.11	129.97	119.84
7	3-G	831	ALA	CA-C-N	8.11	133.77	121.04
7	3-G	831	ALA	C-N-CA	8.11	133.77	121.04
7	3-K	693	VAL	CA-C-N	8.11	129.97	119.84
7	3-K	693	VAL	C-N-CA	8.11	129.97	119.84
1	1-A	493	TYR	CA-C-N	8.10	133.55	123.10
1	1-A	493	TYR	C-N-CA	8.10	133.55	123.10
1	2-A	493	TYR	CA-C-N	8.10	133.55	123.10
1	2-A	493	TYR	C-N-CA	8.10	133.55	123.10
1	3-A	493	TYR	CA-C-N	8.10	133.55	123.10
1	3-A	493	TYR	C-N-CA	8.10	133.55	123.10
1	1-A	409	GLU	N-CA-C	-8.10	102.43	112.88
1	2-A	409	GLU	N-CA-C	-8.10	102.43	112.88
1	3-A	409	GLU	N-CA-C	-8.10	102.43	112.88
7	1-G	298	SER	CA-C-N	8.09	129.96	119.84
7	1-G	298	SER	C-N-CA	8.09	129.96	119.84
7	2-G	298	SER	CA-C-N	8.09	129.96	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-G	298	SER	C-N-CA	8.09	129.96	119.84
7	3-G	298	SER	CA-C-N	8.09	129.96	119.84
7	3-G	298	SER	C-N-CA	8.09	129.96	119.84
4	1-H	522	GLU	CA-C-N	8.09	133.64	123.12
4	1-H	522	GLU	C-N-CA	8.09	133.64	123.12
4	2-H	522	GLU	CA-C-N	8.09	133.64	123.12
4	2-H	522	GLU	C-N-CA	8.09	133.64	123.12
4	3-H	522	GLU	CA-C-N	8.09	133.64	123.12
4	3-H	522	GLU	C-N-CA	8.09	133.64	123.12
8	1-L	30	TYR	N-CA-C	-8.09	94.37	108.20
8	2-L	30	TYR	N-CA-C	-8.09	94.37	108.20
8	3-L	30	TYR	N-CA-C	-8.09	94.37	108.20
4	1-C	106	ALA	N-CA-C	-8.08	96.73	109.50
4	2-C	106	ALA	N-CA-C	-8.08	96.73	109.50
4	3-C	106	ALA	N-CA-C	-8.08	96.73	109.50
1	1-A	329	HIS	N-CA-C	-8.07	96.72	109.23
1	2-A	329	HIS	N-CA-C	-8.07	96.72	109.23
1	3-A	329	HIS	N-CA-C	-8.07	96.72	109.23
7	1-K	96	SER	N-CA-C	8.07	127.98	110.80
7	2-K	96	SER	N-CA-C	8.07	127.98	110.80
7	3-K	96	SER	N-CA-C	8.07	127.98	110.80
7	1-G	845	ARG	N-CA-C	-8.06	95.38	108.52
7	2-G	845	ARG	N-CA-C	-8.06	95.38	108.52
7	3-G	845	ARG	N-CA-C	-8.06	95.38	108.52
1	1-A	596	GLU	N-CA-C	8.06	120.98	111.71
7	1-K	849	LEU	N-CA-C	-8.06	93.63	110.80
1	2-A	596	GLU	N-CA-C	8.06	120.98	111.71
7	2-K	849	LEU	N-CA-C	-8.06	93.63	110.80
1	3-A	596	GLU	N-CA-C	8.06	120.98	111.71
7	3-K	849	LEU	N-CA-C	-8.06	93.63	110.80
7	1-K	845	ARG	N-CA-C	-8.06	95.39	108.52
7	2-K	845	ARG	N-CA-C	-8.06	95.39	108.52
7	3-K	845	ARG	N-CA-C	-8.06	95.39	108.52
1	1-A	413	SER	N-CA-C	-8.04	97.52	108.38
1	2-A	413	SER	N-CA-C	-8.04	97.52	108.38
1	3-A	413	SER	N-CA-C	-8.04	97.52	108.38
7	1-G	849	LEU	N-CA-C	-8.04	93.67	110.80
7	2-G	849	LEU	N-CA-C	-8.04	93.67	110.80
7	3-G	849	LEU	N-CA-C	-8.04	93.67	110.80
1	1-A	664	ALA	CA-C-N	8.04	131.05	120.28
1	1-A	664	ALA	C-N-CA	8.04	131.05	120.28
3	1-B	829	ARG	N-CA-C	-8.04	104.08	114.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1-Z	25	ARG	N-CA-C	-8.04	94.46	108.69
6	1-M	154	PHE	N-CA-C	-8.04	96.06	108.76
1	2-A	664	ALA	CA-C-N	8.04	131.05	120.28
1	2-A	664	ALA	C-N-CA	8.04	131.05	120.28
6	2-M	154	PHE	N-CA-C	-8.04	96.06	108.76
1	3-A	664	ALA	CA-C-N	8.04	131.05	120.28
3	2-B	829	ARG	N-CA-C	-8.04	104.08	114.04
8	2-Z	25	ARG	N-CA-C	-8.04	94.46	108.69
1	3-A	664	ALA	C-N-CA	8.04	131.05	120.28
3	3-B	829	ARG	N-CA-C	-8.04	104.08	114.04
8	3-Z	25	ARG	N-CA-C	-8.04	94.46	108.69
6	3-M	154	PHE	N-CA-C	-8.04	96.06	108.76
1	1-A	636	GLU	N-CA-C	-8.03	102.51	111.82
1	2-A	636	GLU	N-CA-C	-8.03	102.51	111.82
1	3-A	636	GLU	N-CA-C	-8.03	102.51	111.82
7	1-K	817	ASP	CA-C-N	8.01	132.08	120.71
7	1-K	817	ASP	C-N-CA	8.01	132.08	120.71
7	2-K	817	ASP	CA-C-N	8.01	132.08	120.71
7	2-K	817	ASP	C-N-CA	8.01	132.08	120.71
7	3-K	817	ASP	CA-C-N	8.01	132.08	120.71
7	3-K	817	ASP	C-N-CA	8.01	132.08	120.71
7	1-G	510	LEU	N-CA-C	-8.01	102.50	111.07
7	2-G	510	LEU	N-CA-C	-8.01	102.50	111.07
7	3-G	510	LEU	N-CA-C	-8.01	102.50	111.07
7	1-G	817	ASP	CA-C-N	7.99	132.06	120.71
7	1-G	817	ASP	C-N-CA	7.99	132.06	120.71
3	1-N	385	VAL	CA-C-N	7.99	136.80	121.54
3	1-N	385	VAL	C-N-CA	7.99	136.80	121.54
7	2-G	817	ASP	CA-C-N	7.99	132.06	120.71
7	2-G	817	ASP	C-N-CA	7.99	132.06	120.71
3	2-N	385	VAL	CA-C-N	7.99	136.80	121.54
3	2-N	385	VAL	C-N-CA	7.99	136.80	121.54
7	3-G	817	ASP	CA-C-N	7.99	132.06	120.71
7	3-G	817	ASP	C-N-CA	7.99	132.06	120.71
3	3-N	385	VAL	CA-C-N	7.99	136.80	121.54
3	3-N	385	VAL	C-N-CA	7.99	136.80	121.54
4	1-C	530	VAL	N-CA-C	-7.99	95.51	106.85
7	1-G	484	HIS	N-CA-C	-7.99	93.79	110.80
4	2-C	530	VAL	N-CA-C	-7.99	95.51	106.85
7	2-G	484	HIS	N-CA-C	-7.99	93.79	110.80
4	3-C	530	VAL	N-CA-C	-7.99	95.51	106.85
7	3-G	484	HIS	N-CA-C	-7.99	93.79	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	120	TYR	CA-C-N	7.98	130.82	120.44
7	1-G	120	TYR	C-N-CA	7.98	130.82	120.44
7	2-G	120	TYR	CA-C-N	7.98	130.82	120.44
7	2-G	120	TYR	C-N-CA	7.98	130.82	120.44
7	3-G	120	TYR	CA-C-N	7.98	130.82	120.44
7	3-G	120	TYR	C-N-CA	7.98	130.82	120.44
7	1-G	485	GLU	N-CA-C	-7.97	102.54	111.07
7	2-G	485	GLU	N-CA-C	-7.97	102.54	111.07
7	3-G	485	GLU	N-CA-C	-7.97	102.54	111.07
1	1-A	622	GLY	N-CA-C	-7.97	94.30	113.18
1	1-A	655	CYS	N-CA-C	-7.97	101.89	111.69
4	1-H	530	VAL	N-CA-C	-7.97	95.54	106.85
1	2-A	622	GLY	N-CA-C	-7.97	94.30	113.18
1	2-A	655	CYS	N-CA-C	-7.97	101.89	111.69
4	2-H	530	VAL	N-CA-C	-7.97	95.54	106.85
1	3-A	622	GLY	N-CA-C	-7.97	94.30	113.18
1	3-A	655	CYS	N-CA-C	-7.97	101.89	111.69
4	3-H	530	VAL	N-CA-C	-7.97	95.54	106.85
7	1-G	189	ASN	CA-C-N	7.96	130.75	120.56
7	1-G	189	ASN	C-N-CA	7.96	130.75	120.56
7	2-G	189	ASN	CA-C-N	7.96	130.75	120.56
7	2-G	189	ASN	C-N-CA	7.96	130.75	120.56
7	3-G	189	ASN	CA-C-N	7.96	130.75	120.56
7	3-G	189	ASN	C-N-CA	7.96	130.75	120.56
1	1-A	532	SER	CA-C-N	7.96	132.57	121.26
1	1-A	532	SER	C-N-CA	7.96	132.57	121.26
7	1-K	206	ASN	N-CA-C	-7.96	93.98	107.99
1	2-A	532	SER	CA-C-N	7.96	132.57	121.26
1	2-A	532	SER	C-N-CA	7.96	132.57	121.26
7	2-K	206	ASN	N-CA-C	-7.96	93.98	107.99
1	3-A	532	SER	CA-C-N	7.96	132.57	121.26
1	3-A	532	SER	C-N-CA	7.96	132.57	121.26
7	3-K	206	ASN	N-CA-C	-7.96	93.98	107.99
4	1-C	549	GLY	N-CA-C	-7.96	104.58	114.92
4	2-C	549	GLY	N-CA-C	-7.96	104.58	114.92
4	3-C	549	GLY	N-CA-C	-7.96	104.58	114.92
4	1-C	682	GLN	CA-C-N	7.95	131.58	120.29
4	1-C	682	GLN	C-N-CA	7.95	131.58	120.29
4	2-C	682	GLN	CA-C-N	7.95	131.58	120.29
4	2-C	682	GLN	C-N-CA	7.95	131.58	120.29
4	3-C	682	GLN	CA-C-N	7.95	131.58	120.29
4	3-C	682	GLN	C-N-CA	7.95	131.58	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	767	LEU	CA-C-N	7.95	132.39	120.31
1	1-A	767	LEU	C-N-CA	7.95	132.39	120.31
7	1-G	682	GLU	CA-C-N	7.95	130.53	120.51
7	1-G	682	GLU	C-N-CA	7.95	130.53	120.51
1	2-A	767	LEU	CA-C-N	7.95	132.39	120.31
1	2-A	767	LEU	C-N-CA	7.95	132.39	120.31
7	2-G	682	GLU	CA-C-N	7.95	130.53	120.51
7	2-G	682	GLU	C-N-CA	7.95	130.53	120.51
1	3-A	767	LEU	CA-C-N	7.95	132.39	120.31
1	3-A	767	LEU	C-N-CA	7.95	132.39	120.31
7	3-G	682	GLU	CA-C-N	7.95	130.53	120.51
7	3-G	682	GLU	C-N-CA	7.95	130.53	120.51
3	1-B	385	VAL	CA-C-N	7.95	136.72	121.54
3	1-B	385	VAL	C-N-CA	7.95	136.72	121.54
3	2-B	385	VAL	CA-C-N	7.95	136.72	121.54
3	2-B	385	VAL	C-N-CA	7.95	136.72	121.54
3	3-B	385	VAL	CA-C-N	7.95	136.72	121.54
3	3-B	385	VAL	C-N-CA	7.95	136.72	121.54
3	1-B	822	VAL	N-CA-C	-7.94	96.99	108.11
3	2-B	822	VAL	N-CA-C	-7.94	96.99	108.11
3	3-B	822	VAL	N-CA-C	-7.94	96.99	108.11
1	1-A	55	ARG	CA-C-N	-7.94	115.50	121.61
1	1-A	55	ARG	C-N-CA	-7.94	115.50	121.61
6	1-R	30	LYS	CA-C-O	7.94	128.97	120.55
1	2-A	55	ARG	CA-C-N	-7.94	115.50	121.61
1	2-A	55	ARG	C-N-CA	-7.94	115.50	121.61
6	2-R	30	LYS	CA-C-O	7.94	128.97	120.55
1	3-A	55	ARG	CA-C-N	-7.94	115.50	121.61
1	3-A	55	ARG	C-N-CA	-7.94	115.50	121.61
6	3-R	30	LYS	CA-C-O	7.94	128.97	120.55
4	1-C	254	ARG	N-CA-C	-7.92	96.98	109.50
4	2-C	254	ARG	N-CA-C	-7.92	96.98	109.50
4	3-C	254	ARG	N-CA-C	-7.92	96.98	109.50
8	1-Z	30	TYR	N-CA-C	-7.92	94.66	108.20
6	1-M	149	ARG	N-CA-C	-7.92	93.94	110.80
8	2-Z	30	TYR	N-CA-C	-7.92	94.66	108.20
6	2-M	149	ARG	N-CA-C	-7.92	93.94	110.80
8	3-Z	30	TYR	N-CA-C	-7.92	94.66	108.20
6	3-M	149	ARG	N-CA-C	-7.92	93.94	110.80
4	1-C	178	ASN	N-CA-C	-7.91	102.74	111.36
4	2-C	178	ASN	N-CA-C	-7.91	102.74	111.36
4	3-C	178	ASN	N-CA-C	-7.91	102.74	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	553	VAL	CA-C-N	7.91	134.09	122.39
1	1-A	553	VAL	C-N-CA	7.91	134.09	122.39
1	2-A	553	VAL	CA-C-N	7.91	134.09	122.39
1	2-A	553	VAL	C-N-CA	7.91	134.09	122.39
1	3-A	553	VAL	CA-C-N	7.91	134.09	122.39
1	3-A	553	VAL	C-N-CA	7.91	134.09	122.39
3	1-B	816	GLY	N-CA-C	-7.90	97.52	110.95
7	1-K	682	GLU	CA-C-N	7.90	130.47	120.51
7	1-K	682	GLU	C-N-CA	7.90	130.47	120.51
4	1-H	549	GLY	N-CA-C	-7.90	104.65	114.92
3	2-B	816	GLY	N-CA-C	-7.90	97.52	110.95
7	2-K	682	GLU	CA-C-N	7.90	130.47	120.51
7	2-K	682	GLU	C-N-CA	7.90	130.47	120.51
4	2-H	549	GLY	N-CA-C	-7.90	104.65	114.92
3	3-B	816	GLY	N-CA-C	-7.90	97.52	110.95
7	3-K	682	GLU	CA-C-N	7.90	130.47	120.51
7	3-K	682	GLU	C-N-CA	7.90	130.47	120.51
4	3-H	549	GLY	N-CA-C	-7.90	104.65	114.92
4	1-H	178	ASN	N-CA-C	-7.90	102.75	111.36
4	2-H	178	ASN	N-CA-C	-7.90	102.75	111.36
4	3-H	178	ASN	N-CA-C	-7.90	102.75	111.36
4	1-H	348	MET	N-CA-C	-7.89	97.73	108.86
4	1-H	546	TYR	O-C-N	7.89	132.58	123.27
4	2-H	348	MET	N-CA-C	-7.89	97.73	108.86
4	2-H	546	TYR	O-C-N	7.89	132.58	123.27
4	3-H	348	MET	N-CA-C	-7.89	97.73	108.86
4	3-H	546	TYR	O-C-N	7.89	132.58	123.27
4	1-C	546	TYR	O-C-N	7.88	132.57	123.27
4	2-C	546	TYR	O-C-N	7.88	132.57	123.27
4	3-C	546	TYR	O-C-N	7.88	132.57	123.27
4	1-H	103	ARG	N-CA-C	7.88	121.01	111.40
4	2-H	103	ARG	N-CA-C	7.88	121.01	111.40
4	3-H	103	ARG	N-CA-C	7.88	121.01	111.40
4	1-H	517	LEU	N-CA-C	7.87	121.00	111.40
4	2-H	517	LEU	N-CA-C	7.87	121.00	111.40
4	3-H	517	LEU	N-CA-C	7.87	121.00	111.40
4	1-C	348	MET	N-CA-C	-7.87	97.77	108.86
4	2-C	348	MET	N-CA-C	-7.87	97.77	108.86
4	3-C	348	MET	N-CA-C	-7.87	97.77	108.86
4	1-C	103	ARG	N-CA-C	7.86	120.99	111.40
4	2-C	103	ARG	N-CA-C	7.86	120.99	111.40
4	3-C	103	ARG	N-CA-C	7.86	120.99	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	254	ARG	N-CA-C	-7.86	97.08	109.50
4	2-H	254	ARG	N-CA-C	-7.86	97.08	109.50
4	3-H	254	ARG	N-CA-C	-7.86	97.08	109.50
4	1-C	517	LEU	N-CA-C	7.86	120.98	111.40
6	1-F	79	ARG	N-CA-C	7.86	121.96	112.38
4	2-C	517	LEU	N-CA-C	7.86	120.98	111.40
6	2-F	79	ARG	N-CA-C	7.86	121.96	112.38
4	3-C	517	LEU	N-CA-C	7.86	120.98	111.40
6	3-F	79	ARG	N-CA-C	7.86	121.96	112.38
1	1-A	543	TYR	N-CA-C	-7.85	97.39	109.24
1	2-A	543	TYR	N-CA-C	-7.85	97.39	109.24
1	3-A	543	TYR	N-CA-C	-7.85	97.39	109.24
1	1-A	73	TYR	N-CA-C	-7.85	94.08	110.80
1	2-A	73	TYR	N-CA-C	-7.85	94.08	110.80
1	3-A	73	TYR	N-CA-C	-7.85	94.08	110.80
6	1-J	79	ARG	N-CA-C	7.84	121.94	112.38
6	2-J	79	ARG	N-CA-C	7.84	121.94	112.38
6	3-J	79	ARG	N-CA-C	7.84	121.94	112.38
1	1-A	50	HIS	CA-C-N	7.82	131.10	120.54
1	1-A	50	HIS	C-N-CA	7.82	131.10	120.54
1	2-A	50	HIS	CA-C-N	7.82	131.10	120.54
1	2-A	50	HIS	C-N-CA	7.82	131.10	120.54
1	3-A	50	HIS	CA-C-N	7.82	131.10	120.54
1	3-A	50	HIS	C-N-CA	7.82	131.10	120.54
4	1-C	839	ALA	N-CA-C	7.82	119.43	111.07
4	2-C	839	ALA	N-CA-C	7.82	119.43	111.07
4	3-C	839	ALA	N-CA-C	7.82	119.43	111.07
3	1-B	908	ALA	CA-C-N	-7.81	112.22	123.00
3	1-B	908	ALA	C-N-CA	-7.81	112.22	123.00
3	2-B	908	ALA	CA-C-N	-7.81	112.22	123.00
3	2-B	908	ALA	C-N-CA	-7.81	112.22	123.00
3	3-B	908	ALA	CA-C-N	-7.81	112.22	123.00
3	3-B	908	ALA	C-N-CA	-7.81	112.22	123.00
7	1-G	506	LEU	N-CA-C	7.80	127.05	109.81
7	2-G	506	LEU	N-CA-C	7.80	127.05	109.81
7	3-G	506	LEU	N-CA-C	7.80	127.05	109.81
8	1-Z	85	GLU	CA-C-N	7.80	132.93	121.31
8	1-Z	85	GLU	C-N-CA	7.80	132.93	121.31
8	2-Z	85	GLU	CA-C-N	7.80	132.93	121.31
8	2-Z	85	GLU	C-N-CA	7.80	132.93	121.31
8	3-Z	85	GLU	CA-C-N	7.80	132.93	121.31
8	3-Z	85	GLU	C-N-CA	7.80	132.93	121.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	178	VAL	CA-C-O	-7.79	112.95	121.05
7	2-G	178	VAL	CA-C-O	-7.79	112.95	121.05
7	3-G	178	VAL	CA-C-O	-7.79	112.95	121.05
3	1-N	390	ASP	N-CA-C	-7.78	102.84	113.18
3	2-N	390	ASP	N-CA-C	-7.78	102.84	113.18
3	3-N	390	ASP	N-CA-C	-7.78	102.84	113.18
1	1-A	149	LEU	N-CA-C	-7.76	98.11	110.14
1	2-A	149	LEU	N-CA-C	-7.76	98.11	110.14
1	3-A	149	LEU	N-CA-C	-7.76	98.11	110.14
7	1-K	215	ILE	N-CA-C	-7.76	103.23	110.53
7	2-K	215	ILE	N-CA-C	-7.76	103.23	110.53
7	3-K	215	ILE	N-CA-C	-7.76	103.23	110.53
7	1-G	253	ASP	CA-C-N	7.75	130.52	120.44
7	1-G	253	ASP	C-N-CA	7.75	130.52	120.44
3	1-N	550	LYS	N-CA-C	-7.75	103.66	113.43
7	2-G	253	ASP	CA-C-N	7.75	130.52	120.44
7	2-G	253	ASP	C-N-CA	7.75	130.52	120.44
3	2-N	550	LYS	N-CA-C	-7.75	103.66	113.43
7	3-G	253	ASP	CA-C-N	7.75	130.52	120.44
7	3-G	253	ASP	C-N-CA	7.75	130.52	120.44
3	3-N	550	LYS	N-CA-C	-7.75	103.66	113.43
8	1-Z	56	ASP	N-CA-C	-7.75	97.38	108.07
8	2-Z	56	ASP	N-CA-C	-7.75	97.38	108.07
8	3-Z	56	ASP	N-CA-C	-7.75	97.38	108.07
1	1-A	797	PRO	N-CA-C	7.75	120.15	110.70
3	1-B	390	ASP	N-CA-C	-7.75	102.87	113.18
1	2-A	797	PRO	N-CA-C	7.75	120.15	110.70
3	2-B	390	ASP	N-CA-C	-7.75	102.87	113.18
1	3-A	797	PRO	N-CA-C	7.75	120.15	110.70
3	3-B	390	ASP	N-CA-C	-7.75	102.87	113.18
1	1-A	97	ARG	N-CA-C	7.74	121.21	111.69
4	1-H	316	TRP	N-CA-C	-7.74	97.96	109.81
1	2-A	97	ARG	N-CA-C	7.74	121.21	111.69
4	2-H	316	TRP	N-CA-C	-7.74	97.96	109.81
1	3-A	97	ARG	N-CA-C	7.74	121.21	111.69
4	3-H	316	TRP	N-CA-C	-7.74	97.96	109.81
4	1-C	316	TRP	N-CA-C	-7.74	97.97	109.81
3	1-N	370	GLU	N-CA-C	-7.74	102.84	111.28
4	2-C	316	TRP	N-CA-C	-7.74	97.97	109.81
3	2-N	370	GLU	N-CA-C	-7.74	102.84	111.28
4	3-C	316	TRP	N-CA-C	-7.74	97.97	109.81
3	3-N	370	GLU	N-CA-C	-7.74	102.84	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	175	SER	CA-C-N	7.74	133.28	122.06
4	1-C	175	SER	C-N-CA	7.74	133.28	122.06
4	2-C	175	SER	CA-C-N	7.74	133.28	122.06
4	2-C	175	SER	C-N-CA	7.74	133.28	122.06
4	3-C	175	SER	CA-C-N	7.74	133.28	122.06
4	3-C	175	SER	C-N-CA	7.74	133.28	122.06
3	1-B	928	LYS	N-CA-C	7.73	126.90	109.81
3	2-B	928	LYS	N-CA-C	7.73	126.90	109.81
3	3-B	928	LYS	N-CA-C	7.73	126.90	109.81
3	1-B	878	ASN	N-CA-C	-7.73	99.06	111.04
3	2-B	878	ASN	N-CA-C	-7.73	99.06	111.04
3	3-B	878	ASN	N-CA-C	-7.73	99.06	111.04
4	1-H	175	SER	CA-C-N	7.73	133.26	122.06
4	1-H	175	SER	C-N-CA	7.73	133.26	122.06
4	2-H	175	SER	CA-C-N	7.73	133.26	122.06
4	2-H	175	SER	C-N-CA	7.73	133.26	122.06
4	3-H	175	SER	CA-C-N	7.73	133.26	122.06
4	3-H	175	SER	C-N-CA	7.73	133.26	122.06
6	1-M	59	LYS	N-CA-C	-7.72	102.05	113.40
6	2-M	59	LYS	N-CA-C	-7.72	102.05	113.40
6	3-M	59	LYS	N-CA-C	-7.72	102.05	113.40
3	1-B	536	TYR	N-CA-C	-7.72	102.81	111.07
3	2-B	536	TYR	N-CA-C	-7.72	102.81	111.07
3	3-B	536	TYR	N-CA-C	-7.72	102.81	111.07
3	1-B	550	LYS	N-CA-C	-7.71	103.71	113.43
3	2-B	550	LYS	N-CA-C	-7.71	103.71	113.43
3	3-B	550	LYS	N-CA-C	-7.71	103.71	113.43
8	1-L	111	LYS	N-CA-C	-7.70	102.89	111.28
8	2-L	111	LYS	N-CA-C	-7.70	102.89	111.28
8	3-L	111	LYS	N-CA-C	-7.70	102.89	111.28
5	1-D	147	VAL	N-CA-C	7.70	117.81	110.42
5	2-D	147	VAL	N-CA-C	7.70	117.81	110.42
5	3-D	147	VAL	N-CA-C	7.70	117.81	110.42
3	1-B	370	GLU	N-CA-C	-7.69	102.90	111.28
3	2-B	370	GLU	N-CA-C	-7.69	102.90	111.28
3	3-B	370	GLU	N-CA-C	-7.69	102.90	111.28
3	1-B	758	VAL	N-CA-C	-7.69	96.36	108.81
5	1-I	147	VAL	N-CA-C	7.69	117.80	110.42
3	2-B	758	VAL	N-CA-C	-7.69	96.36	108.81
5	2-I	147	VAL	N-CA-C	7.69	117.80	110.42
3	3-B	758	VAL	N-CA-C	-7.69	96.36	108.81
5	3-I	147	VAL	N-CA-C	7.69	117.80	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	27	GLU	N-CA-C	-7.67	92.86	109.81
4	2-H	27	GLU	N-CA-C	-7.67	92.86	109.81
4	3-H	27	GLU	N-CA-C	-7.67	92.86	109.81
3	1-N	536	TYR	N-CA-C	-7.67	102.87	111.07
3	2-N	536	TYR	N-CA-C	-7.67	102.87	111.07
3	3-N	536	TYR	N-CA-C	-7.67	102.87	111.07
4	1-C	27	GLU	N-CA-C	-7.67	92.87	109.81
6	1-F	30	LYS	N-CA-C	-7.67	102.92	111.28
4	2-C	27	GLU	N-CA-C	-7.67	92.87	109.81
6	2-F	30	LYS	N-CA-C	-7.67	102.92	111.28
4	3-C	27	GLU	N-CA-C	-7.67	92.87	109.81
6	3-F	30	LYS	N-CA-C	-7.67	102.92	111.28
4	1-H	538	SER	N-CA-C	-7.66	97.64	109.52
4	2-H	538	SER	N-CA-C	-7.66	97.64	109.52
4	3-H	538	SER	N-CA-C	-7.66	97.64	109.52
4	1-C	574	TYR	N-CA-C	-7.66	96.91	109.40
4	2-C	574	TYR	N-CA-C	-7.66	96.91	109.40
4	3-C	574	TYR	N-CA-C	-7.66	96.91	109.40
6	1-F	96	ASP	N-CA-C	-7.66	97.10	109.96
6	2-F	96	ASP	N-CA-C	-7.66	97.10	109.96
6	3-F	96	ASP	N-CA-C	-7.66	97.10	109.96
6	1-R	41	GLU	CA-C-N	7.65	135.75	121.97
6	1-R	41	GLU	C-N-CA	7.65	135.75	121.97
6	2-R	41	GLU	CA-C-N	7.65	135.75	121.97
6	2-R	41	GLU	C-N-CA	7.65	135.75	121.97
6	3-R	41	GLU	CA-C-N	7.65	135.75	121.97
6	3-R	41	GLU	C-N-CA	7.65	135.75	121.97
4	1-C	538	SER	N-CA-C	-7.65	97.66	109.52
4	2-C	538	SER	N-CA-C	-7.65	97.66	109.52
4	3-C	538	SER	N-CA-C	-7.65	97.66	109.52
1	1-A	78	TRP	N-CA-C	-7.65	96.06	109.06
1	2-A	78	TRP	N-CA-C	-7.65	96.06	109.06
1	3-A	78	TRP	N-CA-C	-7.65	96.06	109.06
1	1-A	562	ARG	N-CA-C	-7.65	97.43	108.60
1	2-A	562	ARG	N-CA-C	-7.65	97.43	108.60
1	3-A	562	ARG	N-CA-C	-7.65	97.43	108.60
4	1-H	574	TYR	N-CA-C	-7.65	96.94	109.40
4	2-H	574	TYR	N-CA-C	-7.65	96.94	109.40
4	3-H	574	TYR	N-CA-C	-7.65	96.94	109.40
7	1-K	63	THR	N-CA-C	7.64	119.25	111.07
7	2-K	63	THR	N-CA-C	7.64	119.25	111.07
7	3-K	63	THR	N-CA-C	7.64	119.25	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	1-J	96	ASP	N-CA-C	-7.64	97.13	109.96
6	2-J	96	ASP	N-CA-C	-7.64	97.13	109.96
6	3-J	96	ASP	N-CA-C	-7.64	97.13	109.96
7	1-K	104	ILE	CA-C-O	7.63	128.89	120.95
7	2-K	104	ILE	CA-C-O	7.63	128.89	120.95
7	3-K	104	ILE	CA-C-O	7.63	128.89	120.95
7	1-G	129	CYS	N-CA-C	7.63	120.49	111.71
7	2-G	129	CYS	N-CA-C	7.63	120.49	111.71
7	3-G	129	CYS	N-CA-C	7.63	120.49	111.71
4	1-C	569	LYS	CA-C-N	7.63	133.46	120.72
4	1-C	569	LYS	C-N-CA	7.63	133.46	120.72
4	2-C	569	LYS	CA-C-N	7.63	133.46	120.72
4	2-C	569	LYS	C-N-CA	7.63	133.46	120.72
4	3-C	569	LYS	CA-C-N	7.63	133.46	120.72
4	3-C	569	LYS	C-N-CA	7.63	133.46	120.72
4	1-H	569	LYS	CA-C-N	7.62	133.45	120.72
4	1-H	569	LYS	C-N-CA	7.62	133.45	120.72
4	2-H	569	LYS	CA-C-N	7.62	133.45	120.72
4	2-H	569	LYS	C-N-CA	7.62	133.45	120.72
4	3-H	569	LYS	CA-C-N	7.62	133.45	120.72
4	3-H	569	LYS	C-N-CA	7.62	133.45	120.72
6	1-J	30	LYS	N-CA-C	-7.62	102.97	111.28
6	2-J	30	LYS	N-CA-C	-7.62	102.97	111.28
6	3-J	30	LYS	N-CA-C	-7.62	102.97	111.28
8	1-Z	86	ASN	CA-C-N	7.61	130.48	120.28
8	1-Z	86	ASN	C-N-CA	7.61	130.48	120.28
8	2-Z	86	ASN	CA-C-N	7.61	130.48	120.28
8	2-Z	86	ASN	C-N-CA	7.61	130.48	120.28
8	3-Z	86	ASN	CA-C-N	7.61	130.48	120.28
8	3-Z	86	ASN	C-N-CA	7.61	130.48	120.28
1	1-A	737	LEU	N-CA-C	7.61	119.65	111.36
1	2-A	737	LEU	N-CA-C	7.61	119.65	111.36
1	3-A	737	LEU	N-CA-C	7.61	119.65	111.36
6	1-M	169	GLY	N-CA-C	-7.60	103.69	112.50
6	2-M	169	GLY	N-CA-C	-7.60	103.69	112.50
6	3-M	169	GLY	N-CA-C	-7.60	103.69	112.50
1	1-A	221	VAL	N-CA-C	-7.60	97.14	108.46
1	2-A	221	VAL	N-CA-C	-7.60	97.14	108.46
1	3-A	221	VAL	N-CA-C	-7.60	97.14	108.46
1	1-A	617	ASN	N-CA-C	7.58	121.96	112.03
7	1-K	777	ASP	CA-C-N	7.58	130.44	120.28
7	1-K	777	ASP	C-N-CA	7.58	130.44	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	617	ASN	N-CA-C	7.58	121.96	112.03
7	2-K	777	ASP	CA-C-N	7.58	130.44	120.28
7	2-K	777	ASP	C-N-CA	7.58	130.44	120.28
1	3-A	617	ASN	N-CA-C	7.58	121.96	112.03
7	3-K	777	ASP	CA-C-N	7.58	130.44	120.28
7	3-K	777	ASP	C-N-CA	7.58	130.44	120.28
7	1-K	772	PHE	CA-C-O	-7.58	112.89	120.70
7	2-K	772	PHE	CA-C-O	-7.58	112.89	120.70
7	3-K	772	PHE	CA-C-O	-7.58	112.89	120.70
1	1-A	200	VAL	N-CA-C	-7.58	97.53	108.36
1	2-A	200	VAL	N-CA-C	-7.58	97.53	108.36
1	3-A	200	VAL	N-CA-C	-7.58	97.53	108.36
4	1-C	472	ASP	N-CA-C	-7.57	96.18	108.52
7	1-G	419	ASP	N-CA-C	7.57	119.17	111.07
4	2-C	472	ASP	N-CA-C	-7.57	96.18	108.52
7	2-G	419	ASP	N-CA-C	7.57	119.17	111.07
4	3-C	472	ASP	N-CA-C	-7.57	96.18	108.52
7	3-G	419	ASP	N-CA-C	7.57	119.17	111.07
7	1-G	218	PHE	N-CA-C	-7.57	102.97	111.07
7	1-K	673	THR	N-CA-C	-7.57	96.20	109.06
7	2-G	218	PHE	N-CA-C	-7.57	102.97	111.07
7	2-K	673	THR	N-CA-C	-7.57	96.20	109.06
7	3-G	218	PHE	N-CA-C	-7.57	102.97	111.07
7	3-K	673	THR	N-CA-C	-7.57	96.20	109.06
4	1-H	237	PHE	N-CA-C	-7.56	96.90	109.46
4	2-H	237	PHE	N-CA-C	-7.56	96.90	109.46
4	3-H	237	PHE	N-CA-C	-7.56	96.90	109.46
4	1-C	8	LYS	N-CA-C	-7.56	97.51	109.23
7	1-G	772	PHE	CA-C-O	-7.56	112.91	120.70
4	2-C	8	LYS	N-CA-C	-7.56	97.51	109.23
7	2-G	772	PHE	CA-C-O	-7.56	112.91	120.70
4	3-C	8	LYS	N-CA-C	-7.56	97.51	109.23
7	3-G	772	PHE	CA-C-O	-7.56	112.91	120.70
7	1-G	498	PHE	CA-C-N	7.56	128.18	119.94
7	1-G	498	PHE	C-N-CA	7.56	128.18	119.94
7	2-G	498	PHE	CA-C-N	7.56	128.18	119.94
7	2-G	498	PHE	C-N-CA	7.56	128.18	119.94
7	3-G	498	PHE	CA-C-N	7.56	128.18	119.94
7	3-G	498	PHE	C-N-CA	7.56	128.18	119.94
4	1-C	237	PHE	N-CA-C	-7.55	96.92	109.46
4	1-H	472	ASP	N-CA-C	-7.55	96.21	108.52
4	2-C	237	PHE	N-CA-C	-7.55	96.92	109.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-H	472	ASP	N-CA-C	-7.55	96.21	108.52
4	3-C	237	PHE	N-CA-C	-7.55	96.92	109.46
4	3-H	472	ASP	N-CA-C	-7.55	96.21	108.52
7	1-G	777	ASP	CA-C-N	7.55	130.40	120.28
7	1-G	777	ASP	C-N-CA	7.55	130.40	120.28
7	2-G	777	ASP	CA-C-N	7.55	130.40	120.28
7	2-G	777	ASP	C-N-CA	7.55	130.40	120.28
7	3-G	777	ASP	CA-C-N	7.55	130.40	120.28
7	3-G	777	ASP	C-N-CA	7.55	130.40	120.28
1	1-A	602	ALA	CA-C-N	7.55	130.39	120.28
1	1-A	602	ALA	C-N-CA	7.55	130.39	120.28
1	2-A	602	ALA	CA-C-N	7.55	130.39	120.28
1	2-A	602	ALA	C-N-CA	7.55	130.39	120.28
1	3-A	602	ALA	CA-C-N	7.55	130.39	120.28
1	3-A	602	ALA	C-N-CA	7.55	130.39	120.28
6	1-M	69	GLY	N-CA-C	-7.55	95.30	113.18
6	2-M	69	GLY	N-CA-C	-7.55	95.30	113.18
6	3-M	69	GLY	N-CA-C	-7.55	95.30	113.18
1	1-A	487	LYS	CA-C-N	7.54	135.55	121.97
1	1-A	487	LYS	C-N-CA	7.54	135.55	121.97
7	1-G	673	THR	N-CA-C	-7.54	96.24	109.06
8	1-L	13	VAL	N-CA-C	-7.54	96.69	108.23
1	2-A	487	LYS	CA-C-N	7.54	135.55	121.97
1	2-A	487	LYS	C-N-CA	7.54	135.55	121.97
7	2-G	673	THR	N-CA-C	-7.54	96.24	109.06
8	2-L	13	VAL	N-CA-C	-7.54	96.69	108.23
1	3-A	487	LYS	CA-C-N	7.54	135.55	121.97
1	3-A	487	LYS	C-N-CA	7.54	135.55	121.97
7	3-G	673	THR	N-CA-C	-7.54	96.24	109.06
8	3-L	13	VAL	N-CA-C	-7.54	96.69	108.23
5	1-D	56	TYR	CA-C-N	-7.54	112.66	123.06
5	1-D	56	TYR	C-N-CA	-7.54	112.66	123.06
5	2-D	56	TYR	CA-C-N	-7.54	112.66	123.06
5	2-D	56	TYR	C-N-CA	-7.54	112.66	123.06
5	3-D	56	TYR	CA-C-N	-7.54	112.66	123.06
5	3-D	56	TYR	C-N-CA	-7.54	112.66	123.06
4	1-H	424	PHE	N-CA-C	-7.53	94.77	110.80
4	2-H	424	PHE	N-CA-C	-7.53	94.77	110.80
4	3-H	424	PHE	N-CA-C	-7.53	94.77	110.80
4	1-H	8	LYS	N-CA-C	-7.52	97.57	109.23
4	2-H	8	LYS	N-CA-C	-7.52	97.57	109.23
4	3-H	8	LYS	N-CA-C	-7.52	97.57	109.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	424	PHE	N-CA-C	-7.52	94.79	110.80
4	2-C	424	PHE	N-CA-C	-7.52	94.79	110.80
4	3-C	424	PHE	N-CA-C	-7.52	94.79	110.80
3	1-B	782	LYS	N-CA-C	-7.51	97.19	108.99
3	2-B	782	LYS	N-CA-C	-7.51	97.19	108.99
3	3-B	782	LYS	N-CA-C	-7.51	97.19	108.99
4	1-C	594	TYR	N-CA-C	-7.51	103.03	111.07
6	1-M	156	GLN	CA-C-N	7.51	131.47	120.95
6	1-M	156	GLN	C-N-CA	7.51	131.47	120.95
5	1-I	24	MET	CA-C-N	7.51	135.89	121.54
5	1-I	24	MET	C-N-CA	7.51	135.89	121.54
4	2-C	594	TYR	N-CA-C	-7.51	103.03	111.07
6	2-M	156	GLN	CA-C-N	7.51	131.47	120.95
6	2-M	156	GLN	C-N-CA	7.51	131.47	120.95
5	2-I	24	MET	CA-C-N	7.51	135.89	121.54
5	2-I	24	MET	C-N-CA	7.51	135.89	121.54
4	3-C	594	TYR	N-CA-C	-7.51	103.03	111.07
6	3-M	156	GLN	CA-C-N	7.51	131.47	120.95
6	3-M	156	GLN	C-N-CA	7.51	131.47	120.95
5	3-I	24	MET	CA-C-N	7.51	135.89	121.54
5	3-I	24	MET	C-N-CA	7.51	135.89	121.54
1	1-A	540	VAL	CA-C-N	-7.51	112.54	123.05
1	1-A	540	VAL	C-N-CA	-7.51	112.54	123.05
5	1-I	56	TYR	CA-C-N	-7.51	112.70	123.06
5	1-I	56	TYR	C-N-CA	-7.51	112.70	123.06
5	1-I	77	LEU	CA-C-N	7.51	130.20	120.44
5	1-I	77	LEU	C-N-CA	7.51	130.20	120.44
1	2-A	540	VAL	CA-C-N	-7.51	112.54	123.05
1	2-A	540	VAL	C-N-CA	-7.51	112.54	123.05
5	2-I	56	TYR	CA-C-N	-7.51	112.70	123.06
5	2-I	56	TYR	C-N-CA	-7.51	112.70	123.06
5	2-I	77	LEU	CA-C-N	7.51	130.20	120.44
5	2-I	77	LEU	C-N-CA	7.51	130.20	120.44
1	3-A	540	VAL	CA-C-N	-7.51	112.54	123.05
1	3-A	540	VAL	C-N-CA	-7.51	112.54	123.05
5	3-I	56	TYR	CA-C-N	-7.51	112.70	123.06
5	3-I	56	TYR	C-N-CA	-7.51	112.70	123.06
5	3-I	77	LEU	CA-C-N	7.51	130.20	120.44
5	3-I	77	LEU	C-N-CA	7.51	130.20	120.44
7	1-G	54	LEU	CA-C-N	7.51	131.08	120.42
7	1-G	54	LEU	C-N-CA	7.51	131.08	120.42
7	2-G	54	LEU	CA-C-N	7.51	131.08	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-G	54	LEU	C-N-CA	7.51	131.08	120.42
7	3-G	54	LEU	CA-C-N	7.51	131.08	120.42
7	3-G	54	LEU	C-N-CA	7.51	131.08	120.42
8	1-Z	69	TYR	N-CA-C	-7.50	97.67	109.07
8	2-Z	69	TYR	N-CA-C	-7.50	97.67	109.07
8	3-Z	69	TYR	N-CA-C	-7.50	97.67	109.07
4	1-H	594	TYR	N-CA-C	-7.49	103.05	111.07
4	2-H	594	TYR	N-CA-C	-7.49	103.05	111.07
4	3-H	594	TYR	N-CA-C	-7.49	103.05	111.07
7	1-K	132	THR	N-CA-C	7.49	121.48	110.17
7	2-K	132	THR	N-CA-C	7.49	121.48	110.17
7	3-K	132	THR	N-CA-C	7.49	121.48	110.17
3	1-B	927	GLU	N-CA-C	7.49	123.65	111.37
3	2-B	927	GLU	N-CA-C	7.49	123.65	111.37
3	3-B	927	GLU	N-CA-C	7.49	123.65	111.37
3	1-B	48	GLY	N-CA-C	-7.49	95.43	113.18
3	1-B	414	ALA	CA-C-O	-7.49	112.89	120.90
3	2-B	48	GLY	N-CA-C	-7.49	95.43	113.18
3	2-B	414	ALA	CA-C-O	-7.49	112.89	120.90
3	3-B	48	GLY	N-CA-C	-7.49	95.43	113.18
3	3-B	414	ALA	CA-C-O	-7.49	112.89	120.90
5	1-D	24	MET	CA-C-N	7.49	135.84	121.54
5	1-D	24	MET	C-N-CA	7.49	135.84	121.54
5	1-D	77	LEU	CA-C-N	7.49	130.17	120.44
5	1-D	77	LEU	C-N-CA	7.49	130.17	120.44
5	2-D	24	MET	CA-C-N	7.49	135.84	121.54
5	2-D	24	MET	C-N-CA	7.49	135.84	121.54
5	2-D	77	LEU	CA-C-N	7.49	130.17	120.44
5	2-D	77	LEU	C-N-CA	7.49	130.17	120.44
5	3-D	24	MET	CA-C-N	7.49	135.84	121.54
5	3-D	24	MET	C-N-CA	7.49	135.84	121.54
5	3-D	77	LEU	CA-C-N	7.49	130.17	120.44
5	3-D	77	LEU	C-N-CA	7.49	130.17	120.44
7	1-G	433	GLU	CA-C-N	7.49	130.17	120.44
7	1-G	433	GLU	C-N-CA	7.49	130.17	120.44
7	2-G	433	GLU	CA-C-N	7.49	130.17	120.44
7	2-G	433	GLU	C-N-CA	7.49	130.17	120.44
7	3-G	433	GLU	CA-C-N	7.49	130.17	120.44
7	3-G	433	GLU	C-N-CA	7.49	130.17	120.44
7	1-G	39	ILE	N-CA-C	-7.48	97.13	107.75
7	2-G	39	ILE	N-CA-C	-7.48	97.13	107.75
7	3-G	39	ILE	N-CA-C	-7.48	97.13	107.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	1-F	35	TYR	CA-C-N	7.48	130.16	120.44
6	1-F	35	TYR	C-N-CA	7.48	130.16	120.44
6	2-F	35	TYR	CA-C-N	7.48	130.16	120.44
6	2-F	35	TYR	C-N-CA	7.48	130.16	120.44
6	3-F	35	TYR	CA-C-N	7.48	130.16	120.44
6	3-F	35	TYR	C-N-CA	7.48	130.16	120.44
4	1-C	456	GLU	CA-C-N	-7.48	112.47	122.42
4	1-C	456	GLU	C-N-CA	-7.48	112.47	122.42
4	2-C	456	GLU	CA-C-N	-7.48	112.47	122.42
4	2-C	456	GLU	C-N-CA	-7.48	112.47	122.42
4	3-C	456	GLU	CA-C-N	-7.48	112.47	122.42
4	3-C	456	GLU	C-N-CA	-7.48	112.47	122.42
1	1-A	325	ALA	N-CA-C	7.47	126.71	110.80
3	1-B	504	VAL	N-CA-C	7.47	124.87	109.34
3	1-N	48	GLY	N-CA-C	-7.47	95.48	113.18
1	2-A	325	ALA	N-CA-C	7.47	126.71	110.80
3	2-B	504	VAL	N-CA-C	7.47	124.87	109.34
3	2-N	48	GLY	N-CA-C	-7.47	95.48	113.18
1	3-A	325	ALA	N-CA-C	7.47	126.71	110.80
3	3-B	504	VAL	N-CA-C	7.47	124.87	109.34
3	3-N	48	GLY	N-CA-C	-7.47	95.48	113.18
5	1-D	29	ILE	N-CA-C	-7.46	93.81	109.34
7	1-K	80	ASN	N-CA-C	-7.46	94.90	110.80
5	2-D	29	ILE	N-CA-C	-7.46	93.81	109.34
7	2-K	80	ASN	N-CA-C	-7.46	94.90	110.80
5	3-D	29	ILE	N-CA-C	-7.46	93.81	109.34
7	3-K	80	ASN	N-CA-C	-7.46	94.90	110.80
4	1-C	174	SER	N-CA-C	-7.46	94.91	110.80
4	2-C	174	SER	N-CA-C	-7.46	94.91	110.80
4	3-C	174	SER	N-CA-C	-7.46	94.91	110.80
1	1-A	245	CYS	N-CA-C	-7.46	97.08	109.24
1	2-A	245	CYS	N-CA-C	-7.46	97.08	109.24
1	3-A	245	CYS	N-CA-C	-7.46	97.08	109.24
1	1-A	557	ASP	N-CA-C	7.46	121.98	110.42
4	1-H	58	LEU	N-CA-C	-7.46	100.00	110.29
4	1-H	174	SER	N-CA-C	-7.46	94.91	110.80
1	2-A	557	ASP	N-CA-C	7.46	121.98	110.42
4	2-H	58	LEU	N-CA-C	-7.46	100.00	110.29
4	2-H	174	SER	N-CA-C	-7.46	94.91	110.80
1	3-A	557	ASP	N-CA-C	7.46	121.98	110.42
4	3-H	58	LEU	N-CA-C	-7.46	100.00	110.29
4	3-H	174	SER	N-CA-C	-7.46	94.91	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	456	GLU	CA-C-N	-7.45	112.51	122.42
4	1-H	456	GLU	C-N-CA	-7.45	112.51	122.42
4	2-H	456	GLU	CA-C-N	-7.45	112.51	122.42
4	2-H	456	GLU	C-N-CA	-7.45	112.51	122.42
4	3-H	456	GLU	CA-C-N	-7.45	112.51	122.42
4	3-H	456	GLU	C-N-CA	-7.45	112.51	122.42
5	1-I	29	ILE	N-CA-C	-7.45	93.85	109.34
5	2-I	29	ILE	N-CA-C	-7.45	93.85	109.34
5	3-I	29	ILE	N-CA-C	-7.45	93.85	109.34
1	1-A	437	ILE	N-CA-C	-7.45	97.57	108.89
1	2-A	437	ILE	N-CA-C	-7.45	97.57	108.89
1	3-A	437	ILE	N-CA-C	-7.45	97.57	108.89
4	1-C	58	LEU	N-CA-C	-7.44	100.03	110.29
4	1-H	78	ASP	N-CA-C	-7.44	103.94	113.16
4	2-C	58	LEU	N-CA-C	-7.44	100.03	110.29
4	2-H	78	ASP	N-CA-C	-7.44	103.94	113.16
4	3-C	58	LEU	N-CA-C	-7.44	100.03	110.29
4	3-H	78	ASP	N-CA-C	-7.44	103.94	113.16
3	1-N	410	PRO	N-CA-C	-7.44	97.15	112.47
3	2-N	410	PRO	N-CA-C	-7.44	97.15	112.47
3	3-N	410	PRO	N-CA-C	-7.44	97.15	112.47
4	1-H	7	ILE	N-CA-C	-7.43	97.32	108.17
4	2-H	7	ILE	N-CA-C	-7.43	97.32	108.17
4	3-H	7	ILE	N-CA-C	-7.43	97.32	108.17
3	1-N	504	VAL	N-CA-C	7.43	124.80	109.34
3	2-N	504	VAL	N-CA-C	7.43	124.80	109.34
3	3-N	504	VAL	N-CA-C	7.43	124.80	109.34
3	1-B	410	PRO	N-CA-C	-7.43	97.16	112.47
5	1-I	76	ILE	N-CA-C	7.43	117.55	110.42
3	2-B	410	PRO	N-CA-C	-7.43	97.16	112.47
5	2-I	76	ILE	N-CA-C	7.43	117.55	110.42
3	3-B	410	PRO	N-CA-C	-7.43	97.16	112.47
5	3-I	76	ILE	N-CA-C	7.43	117.55	110.42
1	1-A	324	PRO	CA-C-N	7.43	135.73	121.54
1	1-A	324	PRO	C-N-CA	7.43	135.73	121.54
1	2-A	324	PRO	CA-C-N	7.43	135.73	121.54
1	2-A	324	PRO	C-N-CA	7.43	135.73	121.54
1	3-A	324	PRO	CA-C-N	7.43	135.73	121.54
1	3-A	324	PRO	C-N-CA	7.43	135.73	121.54
7	1-G	319	PRO	CA-C-N	7.43	130.23	120.28
7	1-G	319	PRO	C-N-CA	7.43	130.23	120.28
4	1-H	368	VAL	N-CA-C	-7.43	97.71	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-G	319	PRO	CA-C-N	7.43	130.23	120.28
7	2-G	319	PRO	C-N-CA	7.43	130.23	120.28
4	2-H	368	VAL	N-CA-C	-7.43	97.71	108.11
7	3-G	319	PRO	CA-C-N	7.43	130.23	120.28
7	3-G	319	PRO	C-N-CA	7.43	130.23	120.28
4	3-H	368	VAL	N-CA-C	-7.43	97.71	108.11
4	1-C	290	TYR	N-CA-C	-7.42	98.13	109.41
4	2-C	290	TYR	N-CA-C	-7.42	98.13	109.41
4	3-C	290	TYR	N-CA-C	-7.42	98.13	109.41
7	1-G	414	LYS	CA-C-N	7.42	130.08	120.44
7	1-G	414	LYS	C-N-CA	7.42	130.08	120.44
7	2-G	414	LYS	CA-C-N	7.42	130.08	120.44
7	2-G	414	LYS	C-N-CA	7.42	130.08	120.44
7	3-G	414	LYS	CA-C-N	7.42	130.08	120.44
7	3-G	414	LYS	C-N-CA	7.42	130.08	120.44
4	1-H	407	GLU	N-CA-C	-7.42	98.53	110.32
4	2-H	407	GLU	N-CA-C	-7.42	98.53	110.32
4	3-H	407	GLU	N-CA-C	-7.42	98.53	110.32
4	1-C	368	VAL	N-CA-C	-7.42	97.73	108.11
4	2-C	368	VAL	N-CA-C	-7.42	97.73	108.11
4	3-C	368	VAL	N-CA-C	-7.42	97.73	108.11
6	1-J	35	TYR	CA-C-N	7.41	130.07	120.44
6	1-J	35	TYR	C-N-CA	7.41	130.07	120.44
6	2-J	35	TYR	CA-C-N	7.41	130.07	120.44
6	2-J	35	TYR	C-N-CA	7.41	130.07	120.44
6	3-J	35	TYR	CA-C-N	7.41	130.07	120.44
6	3-J	35	TYR	C-N-CA	7.41	130.07	120.44
4	1-C	7	ILE	N-CA-C	-7.40	97.36	108.17
4	2-C	7	ILE	N-CA-C	-7.40	97.36	108.17
4	3-C	7	ILE	N-CA-C	-7.40	97.36	108.17
4	1-C	88	THR	N-CA-C	-7.40	95.04	110.80
6	1-R	151	ARG	N-CA-C	7.40	126.16	109.81
4	2-C	88	THR	N-CA-C	-7.40	95.04	110.80
6	2-R	151	ARG	N-CA-C	7.40	126.16	109.81
4	3-C	88	THR	N-CA-C	-7.40	95.04	110.80
6	3-R	151	ARG	N-CA-C	7.40	126.16	109.81
7	1-G	525	ARG	CA-C-N	7.39	130.19	120.28
7	1-G	525	ARG	C-N-CA	7.39	130.19	120.28
7	2-G	525	ARG	CA-C-N	7.39	130.19	120.28
7	2-G	525	ARG	C-N-CA	7.39	130.19	120.28
7	3-G	525	ARG	CA-C-N	7.39	130.19	120.28
7	3-G	525	ARG	C-N-CA	7.39	130.19	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-B	833	VAL	N-CA-C	-7.39	97.76	108.11
3	1-B	851	THR	CA-C-N	7.39	130.19	120.28
3	1-B	851	THR	C-N-CA	7.39	130.19	120.28
4	1-C	78	ASP	N-CA-C	-7.39	103.99	113.16
7	1-G	683	PRO	N-CA-C	7.39	125.61	112.01
6	1-R	146	HIS	N-CA-C	-7.39	104.23	113.18
3	2-B	833	VAL	N-CA-C	-7.39	97.76	108.11
3	2-B	851	THR	CA-C-N	7.39	130.19	120.28
3	2-B	851	THR	C-N-CA	7.39	130.19	120.28
4	2-C	78	ASP	N-CA-C	-7.39	103.99	113.16
7	2-G	683	PRO	N-CA-C	7.39	125.61	112.01
6	2-R	146	HIS	N-CA-C	-7.39	104.23	113.18
3	3-B	833	VAL	N-CA-C	-7.39	97.76	108.11
3	3-B	851	THR	CA-C-N	7.39	130.19	120.28
3	3-B	851	THR	C-N-CA	7.39	130.19	120.28
4	3-C	78	ASP	N-CA-C	-7.39	103.99	113.16
7	3-G	683	PRO	N-CA-C	7.39	125.61	112.01
6	3-R	146	HIS	N-CA-C	-7.39	104.23	113.18
4	1-C	407	GLU	N-CA-C	-7.39	98.58	110.32
4	1-C	526	THR	N-CA-C	-7.39	97.95	108.96
4	2-C	407	GLU	N-CA-C	-7.39	98.58	110.32
4	2-C	526	THR	N-CA-C	-7.39	97.95	108.96
4	3-C	407	GLU	N-CA-C	-7.39	98.58	110.32
4	3-C	526	THR	N-CA-C	-7.39	97.95	108.96
4	1-H	88	THR	N-CA-C	-7.38	95.07	110.80
4	2-H	88	THR	N-CA-C	-7.38	95.07	110.80
4	3-H	88	THR	N-CA-C	-7.38	95.07	110.80
7	1-G	800	ALA	CA-C-N	7.38	130.57	120.46
7	1-G	800	ALA	C-N-CA	7.38	130.57	120.46
4	1-H	683	PHE	N-CA-C	7.38	119.32	111.28
7	2-G	800	ALA	CA-C-N	7.38	130.57	120.46
7	2-G	800	ALA	C-N-CA	7.38	130.57	120.46
4	2-H	683	PHE	N-CA-C	7.38	119.32	111.28
7	3-G	800	ALA	CA-C-N	7.38	130.57	120.46
7	3-G	800	ALA	C-N-CA	7.38	130.57	120.46
4	3-H	683	PHE	N-CA-C	7.38	119.32	111.28
4	1-H	526	THR	N-CA-C	-7.38	97.97	108.96
4	2-H	526	THR	N-CA-C	-7.38	97.97	108.96
4	3-H	526	THR	N-CA-C	-7.38	97.97	108.96
7	1-G	616	GLN	CA-C-N	7.37	130.16	120.28
7	1-G	616	GLN	C-N-CA	7.37	130.16	120.28
7	2-G	616	GLN	CA-C-N	7.37	130.16	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-G	616	GLN	C-N-CA	7.37	130.16	120.28
7	3-G	616	GLN	CA-C-N	7.37	130.16	120.28
7	3-G	616	GLN	C-N-CA	7.37	130.16	120.28
7	1-K	616	GLN	CA-C-N	7.37	130.16	120.28
7	1-K	616	GLN	C-N-CA	7.37	130.16	120.28
7	2-K	616	GLN	CA-C-N	7.37	130.16	120.28
7	2-K	616	GLN	C-N-CA	7.37	130.16	120.28
7	3-K	616	GLN	CA-C-N	7.37	130.16	120.28
7	3-K	616	GLN	C-N-CA	7.37	130.16	120.28
1	1-A	423	ARG	CA-C-N	7.37	135.61	121.54
1	1-A	423	ARG	C-N-CA	7.37	135.61	121.54
1	2-A	423	ARG	CA-C-N	7.37	135.61	121.54
1	2-A	423	ARG	C-N-CA	7.37	135.61	121.54
1	3-A	423	ARG	CA-C-N	7.37	135.61	121.54
1	3-A	423	ARG	C-N-CA	7.37	135.61	121.54
7	1-K	683	PRO	N-CA-C	7.36	125.55	112.01
4	1-H	290	TYR	N-CA-C	-7.36	98.22	109.41
7	2-K	683	PRO	N-CA-C	7.36	125.55	112.01
4	2-H	290	TYR	N-CA-C	-7.36	98.22	109.41
7	3-K	683	PRO	N-CA-C	7.36	125.55	112.01
4	3-H	290	TYR	N-CA-C	-7.36	98.22	109.41
1	1-A	105	TYR	N-CA-C	-7.35	93.45	109.11
1	2-A	105	TYR	N-CA-C	-7.35	93.45	109.11
1	3-A	105	TYR	N-CA-C	-7.35	93.45	109.11
4	1-C	661	ALA	N-CA-C	-7.35	103.21	111.07
7	1-G	494	ALA	CA-C-O	7.35	128.34	120.55
4	2-C	661	ALA	N-CA-C	-7.35	103.21	111.07
7	2-G	494	ALA	CA-C-O	7.35	128.34	120.55
4	3-C	661	ALA	N-CA-C	-7.35	103.21	111.07
7	3-G	494	ALA	CA-C-O	7.35	128.34	120.55
8	1-L	18	ILE	O-C-N	7.34	130.82	123.18
8	2-L	18	ILE	O-C-N	7.34	130.82	123.18
8	3-L	18	ILE	O-C-N	7.34	130.82	123.18
5	1-D	76	ILE	N-CA-C	7.34	117.47	110.42
4	1-H	218	ASN	N-CA-C	-7.34	102.44	111.40
5	2-D	76	ILE	N-CA-C	7.34	117.47	110.42
4	2-H	218	ASN	N-CA-C	-7.34	102.44	111.40
5	3-D	76	ILE	N-CA-C	7.34	117.47	110.42
4	3-H	218	ASN	N-CA-C	-7.34	102.44	111.40
1	1-A	280	LYS	N-CA-C	-7.34	103.30	114.16
1	2-A	280	LYS	N-CA-C	-7.34	103.30	114.16
1	3-A	280	LYS	N-CA-C	-7.34	103.30	114.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-K	800	ALA	CA-C-N	7.33	130.51	120.46
7	1-K	800	ALA	C-N-CA	7.33	130.51	120.46
7	2-K	800	ALA	CA-C-N	7.33	130.51	120.46
7	2-K	800	ALA	C-N-CA	7.33	130.51	120.46
7	3-K	800	ALA	CA-C-N	7.33	130.51	120.46
7	3-K	800	ALA	C-N-CA	7.33	130.51	120.46
4	1-C	314	ILE	N-CA-C	-7.33	97.29	107.99
4	2-C	314	ILE	N-CA-C	-7.33	97.29	107.99
4	3-C	314	ILE	N-CA-C	-7.33	97.29	107.99
1	1-A	155	LEU	N-CA-C	-7.33	104.37	112.72
1	2-A	155	LEU	N-CA-C	-7.33	104.37	112.72
1	3-A	155	LEU	N-CA-C	-7.33	104.37	112.72
4	1-C	218	ASN	N-CA-C	-7.33	102.46	111.40
4	2-C	218	ASN	N-CA-C	-7.33	102.46	111.40
4	3-C	218	ASN	N-CA-C	-7.33	102.46	111.40
4	1-H	661	ALA	N-CA-C	-7.32	103.24	111.07
4	2-H	661	ALA	N-CA-C	-7.32	103.24	111.07
4	3-H	661	ALA	N-CA-C	-7.32	103.24	111.07
4	1-C	575	LEU	N-CA-C	-7.32	98.29	109.85
4	2-C	575	LEU	N-CA-C	-7.32	98.29	109.85
4	3-C	575	LEU	N-CA-C	-7.32	98.29	109.85
4	1-H	314	ILE	N-CA-C	-7.31	97.31	107.99
4	1-H	575	LEU	N-CA-C	-7.31	98.29	109.85
4	2-H	314	ILE	N-CA-C	-7.31	97.31	107.99
4	2-H	575	LEU	N-CA-C	-7.31	98.29	109.85
4	3-H	314	ILE	N-CA-C	-7.31	97.31	107.99
4	3-H	575	LEU	N-CA-C	-7.31	98.29	109.85
7	1-K	37	THR	CA-C-N	7.31	128.98	119.84
7	1-K	37	THR	C-N-CA	7.31	128.98	119.84
7	2-K	37	THR	CA-C-N	7.31	128.98	119.84
7	2-K	37	THR	C-N-CA	7.31	128.98	119.84
7	3-K	37	THR	CA-C-N	7.31	128.98	119.84
7	3-K	37	THR	C-N-CA	7.31	128.98	119.84
1	1-A	386	LEU	N-CA-C	-7.30	98.77	108.19
6	1-M	148	ILE	CA-C-N	7.30	135.49	121.54
6	1-M	148	ILE	C-N-CA	7.30	135.49	121.54
1	2-A	386	LEU	N-CA-C	-7.30	98.77	108.19
6	2-M	148	ILE	CA-C-N	7.30	135.49	121.54
6	2-M	148	ILE	C-N-CA	7.30	135.49	121.54
1	3-A	386	LEU	N-CA-C	-7.30	98.77	108.19
6	3-M	148	ILE	CA-C-N	7.30	135.49	121.54
6	3-M	148	ILE	C-N-CA	7.30	135.49	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	300	LYS	N-CA-C	-7.30	95.25	110.80
7	2-G	300	LYS	N-CA-C	-7.30	95.25	110.80
7	3-G	300	LYS	N-CA-C	-7.30	95.25	110.80
1	1-A	188	ASP	CA-C-N	7.30	133.21	120.87
1	1-A	188	ASP	C-N-CA	7.30	133.21	120.87
1	1-A	426	PHE	N-CA-C	-7.30	99.11	110.42
1	2-A	188	ASP	CA-C-N	7.30	133.21	120.87
1	2-A	188	ASP	C-N-CA	7.30	133.21	120.87
1	2-A	426	PHE	N-CA-C	-7.30	99.11	110.42
1	3-A	188	ASP	CA-C-N	7.30	133.21	120.87
1	3-A	188	ASP	C-N-CA	7.30	133.21	120.87
1	3-A	426	PHE	N-CA-C	-7.30	99.11	110.42
4	1-C	545	TYR	N-CA-C	-7.28	97.94	109.23
4	2-C	545	TYR	N-CA-C	-7.28	97.94	109.23
4	3-C	545	TYR	N-CA-C	-7.28	97.94	109.23
1	1-A	89	LEU	N-CA-C	-7.28	97.56	108.99
4	1-C	630	PHE	N-CA-C	-7.28	99.45	109.71
8	1-L	102	SER	CA-C-N	7.28	130.03	120.28
8	1-L	102	SER	C-N-CA	7.28	130.03	120.28
1	2-A	89	LEU	N-CA-C	-7.28	97.56	108.99
4	2-C	630	PHE	N-CA-C	-7.28	99.45	109.71
8	2-L	102	SER	CA-C-N	7.28	130.03	120.28
8	2-L	102	SER	C-N-CA	7.28	130.03	120.28
1	3-A	89	LEU	N-CA-C	-7.28	97.56	108.99
4	3-C	630	PHE	N-CA-C	-7.28	99.45	109.71
8	3-L	102	SER	CA-C-N	7.28	130.03	120.28
8	3-L	102	SER	C-N-CA	7.28	130.03	120.28
4	1-C	683	PHE	N-CA-C	7.27	119.29	111.36
4	2-C	683	PHE	N-CA-C	7.27	119.29	111.36
4	3-C	683	PHE	N-CA-C	7.27	119.29	111.36
1	1-A	332	MET	CA-C-N	7.27	132.85	122.09
1	1-A	332	MET	C-N-CA	7.27	132.85	122.09
4	1-H	36	ASN	N-CA-C	-7.27	101.57	112.04
1	2-A	332	MET	CA-C-N	7.27	132.85	122.09
1	2-A	332	MET	C-N-CA	7.27	132.85	122.09
4	2-H	36	ASN	N-CA-C	-7.27	101.57	112.04
1	3-A	332	MET	CA-C-N	7.27	132.85	122.09
1	3-A	332	MET	C-N-CA	7.27	132.85	122.09
4	3-H	36	ASN	N-CA-C	-7.27	101.57	112.04
4	1-H	545	TYR	N-CA-C	-7.27	97.96	109.23
4	2-H	545	TYR	N-CA-C	-7.27	97.96	109.23
4	3-H	545	TYR	N-CA-C	-7.27	97.96	109.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	630	PHE	N-CA-C	-7.27	99.47	109.71
4	2-H	630	PHE	N-CA-C	-7.27	99.47	109.71
4	3-H	630	PHE	N-CA-C	-7.27	99.47	109.71
4	1-H	469	PHE	N-CA-C	-7.26	97.11	109.24
4	2-H	469	PHE	N-CA-C	-7.26	97.11	109.24
4	3-H	469	PHE	N-CA-C	-7.26	97.11	109.24
7	1-G	107	SER	CA-C-N	7.26	130.01	120.28
7	1-G	107	SER	C-N-CA	7.26	130.01	120.28
7	2-G	107	SER	CA-C-N	7.26	130.01	120.28
7	2-G	107	SER	C-N-CA	7.26	130.01	120.28
7	3-G	107	SER	CA-C-N	7.26	130.01	120.28
7	3-G	107	SER	C-N-CA	7.26	130.01	120.28
7	1-G	844	SER	N-CA-C	-7.26	96.44	108.34
7	2-G	844	SER	N-CA-C	-7.26	96.44	108.34
7	3-G	844	SER	N-CA-C	-7.26	96.44	108.34
3	1-B	807	ALA	N-CA-C	-7.25	103.62	114.64
3	2-B	807	ALA	N-CA-C	-7.25	103.62	114.64
3	3-B	807	ALA	N-CA-C	-7.25	103.62	114.64
7	1-G	851	THR	N-CA-C	-7.25	101.18	110.53
7	2-G	851	THR	N-CA-C	-7.25	101.18	110.53
7	3-G	851	THR	N-CA-C	-7.25	101.18	110.53
7	1-K	796	THR	CA-C-N	7.24	130.58	120.29
7	1-K	796	THR	C-N-CA	7.24	130.58	120.29
7	2-K	796	THR	CA-C-N	7.24	130.58	120.29
7	2-K	796	THR	C-N-CA	7.24	130.58	120.29
7	3-K	796	THR	CA-C-N	7.24	130.58	120.29
7	3-K	796	THR	C-N-CA	7.24	130.58	120.29
6	1-M	159	CYS	N-CA-C	-7.24	97.60	109.40
6	2-M	159	CYS	N-CA-C	-7.24	97.60	109.40
6	3-M	159	CYS	N-CA-C	-7.24	97.60	109.40
4	1-C	726	ASN	N-CA-C	7.24	119.17	111.28
4	2-C	726	ASN	N-CA-C	7.24	119.17	111.28
4	3-C	726	ASN	N-CA-C	7.24	119.17	111.28
4	1-C	36	ASN	N-CA-C	-7.24	101.62	112.04
4	2-C	36	ASN	N-CA-C	-7.24	101.62	112.04
4	3-C	36	ASN	N-CA-C	-7.24	101.62	112.04
6	1-M	26	ASP	N-CA-C	-7.23	100.30	110.50
6	2-M	26	ASP	N-CA-C	-7.23	100.30	110.50
6	3-M	26	ASP	N-CA-C	-7.23	100.30	110.50
7	1-G	529	THR	CA-C-N	7.23	130.56	120.29
7	1-G	529	THR	C-N-CA	7.23	130.56	120.29
7	2-G	529	THR	CA-C-N	7.23	130.56	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-G	529	THR	C-N-CA	7.23	130.56	120.29
7	3-G	529	THR	CA-C-N	7.23	130.56	120.29
7	3-G	529	THR	C-N-CA	7.23	130.56	120.29
7	1-G	796	THR	CA-C-N	7.23	130.56	120.29
7	1-G	796	THR	C-N-CA	7.23	130.56	120.29
7	2-G	796	THR	CA-C-N	7.23	130.56	120.29
7	2-G	796	THR	C-N-CA	7.23	130.56	120.29
7	3-G	796	THR	CA-C-N	7.23	130.56	120.29
7	3-G	796	THR	C-N-CA	7.23	130.56	120.29
4	1-C	469	PHE	N-CA-C	-7.23	97.17	109.24
4	2-C	469	PHE	N-CA-C	-7.23	97.17	109.24
4	3-C	469	PHE	N-CA-C	-7.23	97.17	109.24
1	1-A	548	HIS	N-CA-C	-7.22	98.08	109.50
1	2-A	548	HIS	N-CA-C	-7.22	98.08	109.50
1	3-A	548	HIS	N-CA-C	-7.22	98.08	109.50
4	1-C	56	CYS	N-CA-C	-7.22	97.70	107.88
4	2-C	56	CYS	N-CA-C	-7.22	97.70	107.88
4	3-C	56	CYS	N-CA-C	-7.22	97.70	107.88
1	1-A	516	ARG	CA-C-N	7.22	135.32	121.54
1	1-A	516	ARG	C-N-CA	7.22	135.32	121.54
4	1-C	244	ILE	N-CA-C	-7.22	97.71	108.46
1	2-A	516	ARG	CA-C-N	7.22	135.32	121.54
1	2-A	516	ARG	C-N-CA	7.22	135.32	121.54
4	2-C	244	ILE	N-CA-C	-7.22	97.71	108.46
1	3-A	516	ARG	CA-C-N	7.22	135.32	121.54
1	3-A	516	ARG	C-N-CA	7.22	135.32	121.54
4	3-C	244	ILE	N-CA-C	-7.22	97.71	108.46
4	1-H	244	ILE	N-CA-C	-7.21	97.71	108.46
4	2-H	244	ILE	N-CA-C	-7.21	97.71	108.46
4	3-H	244	ILE	N-CA-C	-7.21	97.71	108.46
1	1-A	636	GLU	CA-C-N	7.21	130.66	120.42
1	1-A	636	GLU	C-N-CA	7.21	130.66	120.42
4	1-C	651	LEU	N-CA-C	7.21	119.22	111.36
7	1-K	851	THR	N-CA-C	-7.21	101.23	110.53
3	1-N	414	ALA	CA-C-O	-7.21	112.84	120.63
5	1-I	98	GLU	N-CA-C	-7.21	95.44	110.80
1	2-A	636	GLU	CA-C-N	7.21	130.66	120.42
1	2-A	636	GLU	C-N-CA	7.21	130.66	120.42
4	2-C	651	LEU	N-CA-C	7.21	119.22	111.36
7	2-K	851	THR	N-CA-C	-7.21	101.23	110.53
3	2-N	414	ALA	CA-C-O	-7.21	112.84	120.63
5	2-I	98	GLU	N-CA-C	-7.21	95.44	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3-A	636	GLU	CA-C-N	7.21	130.66	120.42
1	3-A	636	GLU	C-N-CA	7.21	130.66	120.42
4	3-C	651	LEU	N-CA-C	7.21	119.22	111.36
7	3-K	851	THR	N-CA-C	-7.21	101.23	110.53
3	3-N	414	ALA	CA-C-O	-7.21	112.84	120.63
5	3-I	98	GLU	N-CA-C	-7.21	95.44	110.80
7	1-K	844	SER	N-CA-C	-7.21	96.52	108.34
7	2-K	844	SER	N-CA-C	-7.21	96.52	108.34
7	3-K	844	SER	N-CA-C	-7.21	96.52	108.34
4	1-C	397	ALA	N-CA-C	-7.20	97.50	108.67
4	2-C	397	ALA	N-CA-C	-7.20	97.50	108.67
4	3-C	397	ALA	N-CA-C	-7.20	97.50	108.67
4	1-H	397	ALA	N-CA-C	-7.20	97.51	108.67
4	2-H	397	ALA	N-CA-C	-7.20	97.51	108.67
4	3-H	397	ALA	N-CA-C	-7.20	97.51	108.67
4	1-H	651	LEU	N-CA-C	7.20	119.21	111.36
4	2-H	651	LEU	N-CA-C	7.20	119.21	111.36
4	3-H	651	LEU	N-CA-C	7.20	119.21	111.36
4	1-H	56	CYS	N-CA-C	-7.20	97.73	107.88
4	2-H	56	CYS	N-CA-C	-7.20	97.73	107.88
4	3-H	56	CYS	N-CA-C	-7.20	97.73	107.88
5	1-D	98	GLU	N-CA-C	-7.19	95.48	110.80
5	2-D	98	GLU	N-CA-C	-7.19	95.48	110.80
5	3-D	98	GLU	N-CA-C	-7.19	95.48	110.80
1	1-A	393	LEU	N-CA-C	-7.19	98.01	109.59
1	2-A	393	LEU	N-CA-C	-7.19	98.01	109.59
1	3-A	393	LEU	N-CA-C	-7.19	98.01	109.59
8	1-L	127	GLU	N-CA-C	7.18	119.19	111.36
8	2-L	127	GLU	N-CA-C	7.18	119.19	111.36
8	3-L	127	GLU	N-CA-C	7.18	119.19	111.36
7	1-G	80	ASN	N-CA-C	-7.18	103.83	112.59
7	2-G	80	ASN	N-CA-C	-7.18	103.83	112.59
7	3-G	80	ASN	N-CA-C	-7.18	103.83	112.59
4	1-H	507	GLU	N-CA-C	-7.18	103.53	111.36
4	2-H	507	GLU	N-CA-C	-7.18	103.53	111.36
4	3-H	507	GLU	N-CA-C	-7.18	103.53	111.36
7	1-K	859	ARG	N-CA-C	-7.18	98.10	109.23
7	2-K	859	ARG	N-CA-C	-7.18	98.10	109.23
7	3-K	859	ARG	N-CA-C	-7.18	98.10	109.23
7	1-K	263	HIS	CA-C-N	7.17	129.89	120.28
7	1-K	263	HIS	C-N-CA	7.17	129.89	120.28
7	2-K	263	HIS	CA-C-N	7.17	129.89	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-K	263	HIS	C-N-CA	7.17	129.89	120.28
7	3-K	263	HIS	CA-C-N	7.17	129.89	120.28
7	3-K	263	HIS	C-N-CA	7.17	129.89	120.28
4	1-C	507	GLU	N-CA-C	-7.16	103.55	111.36
5	1-D	233	LYS	CA-C-N	7.16	129.75	120.44
5	1-D	233	LYS	C-N-CA	7.16	129.75	120.44
4	2-C	507	GLU	N-CA-C	-7.16	103.55	111.36
5	2-D	233	LYS	CA-C-N	7.16	129.75	120.44
5	2-D	233	LYS	C-N-CA	7.16	129.75	120.44
4	3-C	507	GLU	N-CA-C	-7.16	103.55	111.36
5	3-D	233	LYS	CA-C-N	7.16	129.75	120.44
5	3-D	233	LYS	C-N-CA	7.16	129.75	120.44
6	1-R	25	LEU	N-CA-C	7.16	119.81	110.43
5	1-I	233	LYS	CA-C-N	7.16	129.75	120.44
5	1-I	233	LYS	C-N-CA	7.16	129.75	120.44
6	2-R	25	LEU	N-CA-C	7.16	119.81	110.43
5	2-I	233	LYS	CA-C-N	7.16	129.75	120.44
5	2-I	233	LYS	C-N-CA	7.16	129.75	120.44
6	3-R	25	LEU	N-CA-C	7.16	119.81	110.43
5	3-I	233	LYS	CA-C-N	7.16	129.75	120.44
5	3-I	233	LYS	C-N-CA	7.16	129.75	120.44
7	1-G	859	ARG	N-CA-C	-7.16	98.14	109.23
7	2-G	859	ARG	N-CA-C	-7.16	98.14	109.23
7	3-G	859	ARG	N-CA-C	-7.16	98.14	109.23
4	1-C	774	ARG	N-CA-C	-7.15	103.48	111.28
4	2-C	774	ARG	N-CA-C	-7.15	103.48	111.28
4	3-C	774	ARG	N-CA-C	-7.15	103.48	111.28
6	1-M	64	THR	N-CA-C	7.15	120.38	108.73
3	1-N	249	VAL	N-CA-C	7.15	117.91	110.62
6	2-M	64	THR	N-CA-C	7.15	120.38	108.73
3	2-N	249	VAL	N-CA-C	7.15	117.91	110.62
6	3-M	64	THR	N-CA-C	7.15	120.38	108.73
3	3-N	249	VAL	N-CA-C	7.15	117.91	110.62
6	1-R	93	ASP	N-CA-C	7.14	119.91	108.41
6	2-R	93	ASP	N-CA-C	7.14	119.91	108.41
6	3-R	93	ASP	N-CA-C	7.14	119.91	108.41
1	1-A	31	GLY	N-CA-C	-7.14	105.21	115.64
1	2-A	31	GLY	N-CA-C	-7.14	105.21	115.64
1	3-A	31	GLY	N-CA-C	-7.14	105.21	115.64
3	1-B	821	ASP	CA-C-N	7.14	132.49	123.14
3	1-B	821	ASP	C-N-CA	7.14	132.49	123.14
3	2-B	821	ASP	CA-C-N	7.14	132.49	123.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2-B	821	ASP	C-N-CA	7.14	132.49	123.14
3	3-B	821	ASP	CA-C-N	7.14	132.49	123.14
3	3-B	821	ASP	C-N-CA	7.14	132.49	123.14
1	1-A	395	THR	CA-C-N	7.13	124.73	120.24
1	1-A	395	THR	C-N-CA	7.13	124.73	120.24
1	2-A	395	THR	CA-C-N	7.13	124.73	120.24
1	2-A	395	THR	C-N-CA	7.13	124.73	120.24
1	3-A	395	THR	CA-C-N	7.13	124.73	120.24
1	3-A	395	THR	C-N-CA	7.13	124.73	120.24
4	1-C	686	ALA	CA-C-N	7.13	129.84	120.28
4	1-C	686	ALA	C-N-CA	7.13	129.84	120.28
7	1-G	431	SER	N-CA-C	-7.13	103.02	112.72
4	2-C	686	ALA	CA-C-N	7.13	129.84	120.28
4	2-C	686	ALA	C-N-CA	7.13	129.84	120.28
7	2-G	431	SER	N-CA-C	-7.13	103.02	112.72
4	3-C	686	ALA	CA-C-N	7.13	129.84	120.28
4	3-C	686	ALA	C-N-CA	7.13	129.84	120.28
7	3-G	431	SER	N-CA-C	-7.13	103.02	112.72
4	1-H	686	ALA	CA-C-N	7.12	129.81	120.28
4	1-H	686	ALA	C-N-CA	7.12	129.81	120.28
4	2-H	686	ALA	CA-C-N	7.12	129.81	120.28
4	2-H	686	ALA	C-N-CA	7.12	129.81	120.28
4	3-H	686	ALA	CA-C-N	7.12	129.81	120.28
4	3-H	686	ALA	C-N-CA	7.12	129.81	120.28
7	1-K	177	TRP	N-CA-C	7.11	121.66	113.19
7	2-K	177	TRP	N-CA-C	7.11	121.66	113.19
7	3-K	177	TRP	N-CA-C	7.11	121.66	113.19
3	1-B	853	ALA	CA-C-N	7.10	131.10	120.31
3	1-B	853	ALA	C-N-CA	7.10	131.10	120.31
3	2-B	853	ALA	CA-C-N	7.10	131.10	120.31
3	2-B	853	ALA	C-N-CA	7.10	131.10	120.31
3	3-B	853	ALA	CA-C-N	7.10	131.10	120.31
3	3-B	853	ALA	C-N-CA	7.10	131.10	120.31
7	1-K	704	GLY	N-CA-C	-7.09	97.35	110.97
4	1-H	693	ALA	CA-C-N	7.09	132.22	122.07
4	1-H	693	ALA	C-N-CA	7.09	132.22	122.07
7	2-K	704	GLY	N-CA-C	-7.09	97.35	110.97
4	2-H	693	ALA	CA-C-N	7.09	132.22	122.07
4	2-H	693	ALA	C-N-CA	7.09	132.22	122.07
7	3-K	704	GLY	N-CA-C	-7.09	97.35	110.97
4	3-H	693	ALA	CA-C-N	7.09	132.22	122.07
4	3-H	693	ALA	C-N-CA	7.09	132.22	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	768	MET	N-CA-C	-7.09	98.29	109.50
7	2-G	768	MET	N-CA-C	-7.09	98.29	109.50
7	3-G	768	MET	N-CA-C	-7.09	98.29	109.50
7	1-K	248	ASP	CA-C-N	-7.09	110.99	119.78
7	1-K	248	ASP	C-N-CA	-7.09	110.99	119.78
7	2-K	248	ASP	CA-C-N	-7.09	110.99	119.78
7	2-K	248	ASP	C-N-CA	-7.09	110.99	119.78
7	3-K	248	ASP	CA-C-N	-7.09	110.99	119.78
7	3-K	248	ASP	C-N-CA	-7.09	110.99	119.78
1	1-A	766	GLY	N-CA-C	-7.08	96.39	113.18
1	2-A	766	GLY	N-CA-C	-7.08	96.39	113.18
1	3-A	766	GLY	N-CA-C	-7.08	96.39	113.18
7	1-K	670	ASN	N-CA-C	-7.08	104.61	113.18
4	1-H	365	ARG	N-CA-C	7.08	125.88	110.80
7	2-K	670	ASN	N-CA-C	-7.08	104.61	113.18
4	2-H	365	ARG	N-CA-C	7.08	125.88	110.80
7	3-K	670	ASN	N-CA-C	-7.08	104.61	113.18
4	3-H	365	ARG	N-CA-C	7.08	125.88	110.80
7	1-G	670	ASN	N-CA-C	-7.08	104.62	113.18
7	2-G	670	ASN	N-CA-C	-7.08	104.62	113.18
7	3-G	670	ASN	N-CA-C	-7.08	104.62	113.18
7	1-G	132	THR	N-CA-C	7.07	125.86	110.80
7	1-G	706	CYS	N-CA-C	-7.07	98.56	109.24
7	2-G	132	THR	N-CA-C	7.07	125.86	110.80
7	2-G	706	CYS	N-CA-C	-7.07	98.56	109.24
7	3-G	132	THR	N-CA-C	7.07	125.86	110.80
7	3-G	706	CYS	N-CA-C	-7.07	98.56	109.24
7	1-G	704	GLY	N-CA-C	-7.07	97.41	110.97
7	2-G	704	GLY	N-CA-C	-7.07	97.41	110.97
7	3-G	704	GLY	N-CA-C	-7.07	97.41	110.97
3	1-N	251	HIS	N-CA-C	-7.06	103.66	111.36
3	2-N	251	HIS	N-CA-C	-7.06	103.66	111.36
3	3-N	251	HIS	N-CA-C	-7.06	103.66	111.36
7	1-G	242	GLU	N-CA-C	-7.06	104.81	113.50
7	2-G	242	GLU	N-CA-C	-7.06	104.81	113.50
7	3-G	242	GLU	N-CA-C	-7.06	104.81	113.50
4	1-C	693	ALA	CA-C-N	7.06	132.16	122.07
4	1-C	693	ALA	C-N-CA	7.06	132.16	122.07
4	2-C	693	ALA	CA-C-N	7.06	132.16	122.07
4	2-C	693	ALA	C-N-CA	7.06	132.16	122.07
4	3-C	693	ALA	CA-C-N	7.06	132.16	122.07
4	3-C	693	ALA	C-N-CA	7.06	132.16	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	568	ILE	N-CA-C	-7.05	97.51	108.44
4	1-H	293	GLY	N-CA-C	-7.05	100.77	111.42
1	2-A	568	ILE	N-CA-C	-7.05	97.51	108.44
4	2-H	293	GLY	N-CA-C	-7.05	100.77	111.42
1	3-A	568	ILE	N-CA-C	-7.05	97.51	108.44
4	3-H	293	GLY	N-CA-C	-7.05	100.77	111.42
4	1-C	365	ARG	N-CA-C	7.05	125.82	110.80
4	2-C	365	ARG	N-CA-C	7.05	125.82	110.80
4	3-C	365	ARG	N-CA-C	7.05	125.82	110.80
3	1-N	479	GLU	N-CA-C	7.05	118.61	111.07
3	2-N	479	GLU	N-CA-C	7.05	118.61	111.07
3	3-N	479	GLU	N-CA-C	7.05	118.61	111.07
1	1-A	570	VAL	O-C-N	-7.04	114.94	122.83
1	2-A	570	VAL	O-C-N	-7.04	114.94	122.83
1	3-A	570	VAL	O-C-N	-7.04	114.94	122.83
3	1-B	806	VAL	N-CA-C	7.04	123.99	109.34
3	2-B	806	VAL	N-CA-C	7.04	123.99	109.34
3	3-B	806	VAL	N-CA-C	7.04	123.99	109.34
3	1-B	249	VAL	N-CA-C	7.04	117.80	110.62
3	2-B	249	VAL	N-CA-C	7.04	117.80	110.62
3	3-B	249	VAL	N-CA-C	7.04	117.80	110.62
4	1-C	293	GLY	N-CA-C	-7.04	100.80	111.42
8	1-Z	15	ALA	N-CA-C	-7.04	97.58	108.42
4	2-C	293	GLY	N-CA-C	-7.04	100.80	111.42
8	2-Z	15	ALA	N-CA-C	-7.04	97.58	108.42
4	3-C	293	GLY	N-CA-C	-7.04	100.80	111.42
8	3-Z	15	ALA	N-CA-C	-7.04	97.58	108.42
7	1-G	721	ALA	N-CA-C	-7.03	97.75	109.07
7	2-G	721	ALA	N-CA-C	-7.03	97.75	109.07
7	3-G	721	ALA	N-CA-C	-7.03	97.75	109.07
3	1-B	479	GLU	N-CA-C	7.03	118.59	111.07
3	2-B	479	GLU	N-CA-C	7.03	118.59	111.07
3	3-B	479	GLU	N-CA-C	7.03	118.59	111.07
1	1-A	391	TYR	N-CA-C	-7.03	97.50	109.24
1	2-A	391	TYR	N-CA-C	-7.03	97.50	109.24
1	3-A	391	TYR	N-CA-C	-7.03	97.50	109.24
4	1-C	698	GLY	CA-C-N	7.03	129.70	120.28
4	1-C	698	GLY	C-N-CA	7.03	129.70	120.28
7	1-K	846	LEU	N-CA-C	-7.03	97.78	109.24
4	2-C	698	GLY	CA-C-N	7.03	129.70	120.28
4	2-C	698	GLY	C-N-CA	7.03	129.70	120.28
7	2-K	846	LEU	N-CA-C	-7.03	97.78	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	3-C	698	GLY	CA-C-N	7.03	129.70	120.28
4	3-C	698	GLY	C-N-CA	7.03	129.70	120.28
7	3-K	846	LEU	N-CA-C	-7.03	97.78	109.24
1	1-A	724	GLU	N-CA-C	-7.03	103.55	111.07
7	1-G	116	LYS	N-CA-C	7.03	125.77	110.80
4	1-H	213	ILE	CA-C-N	-7.03	111.35	122.73
4	1-H	213	ILE	C-N-CA	-7.03	111.35	122.73
1	2-A	724	GLU	N-CA-C	-7.03	103.55	111.07
7	2-G	116	LYS	N-CA-C	7.03	125.77	110.80
4	2-H	213	ILE	CA-C-N	-7.03	111.35	122.73
4	2-H	213	ILE	C-N-CA	-7.03	111.35	122.73
1	3-A	724	GLU	N-CA-C	-7.03	103.55	111.07
7	3-G	116	LYS	N-CA-C	7.03	125.77	110.80
4	3-H	213	ILE	CA-C-N	-7.03	111.35	122.73
4	3-H	213	ILE	C-N-CA	-7.03	111.35	122.73
4	1-H	540	VAL	N-CA-C	-7.02	105.88	112.83
4	2-H	540	VAL	N-CA-C	-7.02	105.88	112.83
4	3-H	540	VAL	N-CA-C	-7.02	105.88	112.83
7	1-K	768	MET	N-CA-C	-7.02	98.41	109.50
7	2-K	768	MET	N-CA-C	-7.02	98.41	109.50
7	3-K	768	MET	N-CA-C	-7.02	98.41	109.50
4	1-C	213	ILE	CA-C-N	-7.02	111.36	122.73
4	1-C	213	ILE	C-N-CA	-7.02	111.36	122.73
4	2-C	213	ILE	CA-C-N	-7.02	111.36	122.73
4	2-C	213	ILE	C-N-CA	-7.02	111.36	122.73
4	3-C	213	ILE	CA-C-N	-7.02	111.36	122.73
4	3-C	213	ILE	C-N-CA	-7.02	111.36	122.73
6	1-J	40	GLY	N-CA-C	-7.01	106.34	114.69
6	2-J	40	GLY	N-CA-C	-7.01	106.34	114.69
6	3-J	40	GLY	N-CA-C	-7.01	106.34	114.69
3	1-B	251	HIS	N-CA-C	-7.01	103.72	111.36
3	1-B	763	GLN	CA-C-N	7.01	134.94	121.54
3	1-B	763	GLN	C-N-CA	7.01	134.94	121.54
7	1-K	721	ALA	N-CA-C	-7.01	97.78	109.07
3	2-B	251	HIS	N-CA-C	-7.01	103.72	111.36
3	2-B	763	GLN	CA-C-N	7.01	134.94	121.54
3	2-B	763	GLN	C-N-CA	7.01	134.94	121.54
7	2-K	721	ALA	N-CA-C	-7.01	97.78	109.07
3	3-B	251	HIS	N-CA-C	-7.01	103.72	111.36
3	3-B	763	GLN	CA-C-N	7.01	134.94	121.54
3	3-B	763	GLN	C-N-CA	7.01	134.94	121.54
7	3-K	721	ALA	N-CA-C	-7.01	97.78	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-B	526	VAL	CA-C-N	7.01	129.67	120.28
3	1-B	526	VAL	C-N-CA	7.01	129.67	120.28
3	2-B	526	VAL	CA-C-N	7.01	129.67	120.28
3	2-B	526	VAL	C-N-CA	7.01	129.67	120.28
3	3-B	526	VAL	CA-C-N	7.01	129.67	120.28
3	3-B	526	VAL	C-N-CA	7.01	129.67	120.28
7	1-K	706	CYS	N-CA-C	-7.00	98.67	109.24
7	2-K	706	CYS	N-CA-C	-7.00	98.67	109.24
7	3-K	706	CYS	N-CA-C	-7.00	98.67	109.24
8	1-L	29	LYS	N-CA-C	-7.00	96.30	108.69
8	2-L	29	LYS	N-CA-C	-7.00	96.30	108.69
8	3-L	29	LYS	N-CA-C	-7.00	96.30	108.69
4	1-H	698	GLY	CA-C-N	7.00	129.66	120.28
4	1-H	698	GLY	C-N-CA	7.00	129.66	120.28
4	2-H	698	GLY	CA-C-N	7.00	129.66	120.28
4	2-H	698	GLY	C-N-CA	7.00	129.66	120.28
4	3-H	698	GLY	CA-C-N	7.00	129.66	120.28
4	3-H	698	GLY	C-N-CA	7.00	129.66	120.28
6	1-F	154	PHE	N-CA-C	-7.00	99.58	110.42
6	2-F	154	PHE	N-CA-C	-7.00	99.58	110.42
6	3-F	154	PHE	N-CA-C	-7.00	99.58	110.42
3	1-B	405	CYS	CA-C-N	6.99	129.65	120.28
3	1-B	405	CYS	C-N-CA	6.99	129.65	120.28
6	1-F	40	GLY	N-CA-C	-6.99	106.37	114.69
3	2-B	405	CYS	CA-C-N	6.99	129.65	120.28
3	2-B	405	CYS	C-N-CA	6.99	129.65	120.28
6	2-F	40	GLY	N-CA-C	-6.99	106.37	114.69
3	3-B	405	CYS	CA-C-N	6.99	129.65	120.28
3	3-B	405	CYS	C-N-CA	6.99	129.65	120.28
6	3-F	40	GLY	N-CA-C	-6.99	106.37	114.69
1	1-A	428	VAL	N-CA-C	-6.99	97.47	108.86
7	1-G	846	LEU	N-CA-C	-6.99	97.85	109.24
1	2-A	428	VAL	N-CA-C	-6.99	97.47	108.86
7	2-G	846	LEU	N-CA-C	-6.99	97.85	109.24
1	3-A	428	VAL	N-CA-C	-6.99	97.47	108.86
7	3-G	846	LEU	N-CA-C	-6.99	97.85	109.24
1	1-A	340	PHE	CA-C-N	6.98	134.88	121.54
1	1-A	340	PHE	C-N-CA	6.98	134.88	121.54
7	1-K	258	CYS	CA-C-N	6.98	129.52	120.44
7	1-K	258	CYS	C-N-CA	6.98	129.52	120.44
1	2-A	340	PHE	CA-C-N	6.98	134.88	121.54
1	2-A	340	PHE	C-N-CA	6.98	134.88	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-K	258	CYS	CA-C-N	6.98	129.52	120.44
7	2-K	258	CYS	C-N-CA	6.98	129.52	120.44
1	3-A	340	PHE	CA-C-N	6.98	134.88	121.54
1	3-A	340	PHE	C-N-CA	6.98	134.88	121.54
7	3-K	258	CYS	CA-C-N	6.98	129.52	120.44
7	3-K	258	CYS	C-N-CA	6.98	129.52	120.44
1	1-A	178	GLU	N-CA-C	-6.98	99.11	108.74
3	1-B	819	VAL	CA-C-N	6.98	134.04	122.73
3	1-B	819	VAL	C-N-CA	6.98	134.04	122.73
1	2-A	178	GLU	N-CA-C	-6.98	99.11	108.74
3	2-B	819	VAL	CA-C-N	6.98	134.04	122.73
3	2-B	819	VAL	C-N-CA	6.98	134.04	122.73
1	3-A	178	GLU	N-CA-C	-6.98	99.11	108.74
3	3-B	819	VAL	CA-C-N	6.98	134.04	122.73
3	3-B	819	VAL	C-N-CA	6.98	134.04	122.73
6	1-J	154	PHE	N-CA-C	-6.98	99.61	110.42
6	2-J	154	PHE	N-CA-C	-6.98	99.61	110.42
6	3-J	154	PHE	N-CA-C	-6.98	99.61	110.42
4	1-C	546	TYR	CA-C-N	6.97	133.36	122.70
4	1-C	546	TYR	C-N-CA	6.97	133.36	122.70
3	1-N	526	VAL	CA-C-N	6.97	129.62	120.28
3	1-N	526	VAL	C-N-CA	6.97	129.62	120.28
4	2-C	546	TYR	CA-C-N	6.97	133.36	122.70
4	2-C	546	TYR	C-N-CA	6.97	133.36	122.70
3	2-N	526	VAL	CA-C-N	6.97	129.62	120.28
3	2-N	526	VAL	C-N-CA	6.97	129.62	120.28
4	3-C	546	TYR	CA-C-N	6.97	133.36	122.70
4	3-C	546	TYR	C-N-CA	6.97	133.36	122.70
3	3-N	526	VAL	CA-C-N	6.97	129.62	120.28
3	3-N	526	VAL	C-N-CA	6.97	129.62	120.28
3	1-B	742	TYR	N-CA-C	-6.97	97.61	109.24
3	2-B	742	TYR	N-CA-C	-6.97	97.61	109.24
3	3-B	742	TYR	N-CA-C	-6.97	97.61	109.24
1	1-A	444	ILE	N-CA-C	-6.96	96.50	107.15
1	2-A	444	ILE	N-CA-C	-6.96	96.50	107.15
1	3-A	444	ILE	N-CA-C	-6.96	96.50	107.15
4	1-C	788	LEU	N-CA-C	6.96	121.01	108.48
4	2-C	788	LEU	N-CA-C	6.96	121.01	108.48
4	3-C	788	LEU	N-CA-C	6.96	121.01	108.48
4	1-C	540	VAL	N-CA-C	-6.96	105.94	112.83
4	2-C	540	VAL	N-CA-C	-6.96	105.94	112.83
4	3-C	540	VAL	N-CA-C	-6.96	105.94	112.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-N	482	SER	N-CA-C	6.96	125.62	110.80
3	2-N	482	SER	N-CA-C	6.96	125.62	110.80
3	3-N	482	SER	N-CA-C	6.96	125.62	110.80
8	1-L	136	GLU	N-CA-C	6.96	119.71	110.53
8	2-L	136	GLU	N-CA-C	6.96	119.71	110.53
8	3-L	136	GLU	N-CA-C	6.96	119.71	110.53
7	1-G	794	ILE	N-CA-C	-6.96	99.17	108.35
7	2-G	794	ILE	N-CA-C	-6.96	99.17	108.35
7	3-G	794	ILE	N-CA-C	-6.96	99.17	108.35
1	1-A	383	ALA	CA-C-N	6.95	134.81	121.54
1	1-A	383	ALA	C-N-CA	6.95	134.81	121.54
1	2-A	383	ALA	CA-C-N	6.95	134.81	121.54
1	2-A	383	ALA	C-N-CA	6.95	134.81	121.54
1	3-A	383	ALA	CA-C-N	6.95	134.81	121.54
1	3-A	383	ALA	C-N-CA	6.95	134.81	121.54
3	1-B	482	SER	N-CA-C	6.95	125.60	110.80
3	2-B	482	SER	N-CA-C	6.95	125.60	110.80
3	3-B	482	SER	N-CA-C	6.95	125.60	110.80
8	1-Z	65	LEU	N-CA-C	-6.95	98.61	109.72
8	2-Z	65	LEU	N-CA-C	-6.95	98.61	109.72
8	3-Z	65	LEU	N-CA-C	-6.95	98.61	109.72
7	1-K	794	ILE	N-CA-C	-6.93	99.20	108.35
7	2-K	794	ILE	N-CA-C	-6.93	99.20	108.35
7	3-K	794	ILE	N-CA-C	-6.93	99.20	108.35
4	1-H	546	TYR	CA-C-N	6.93	133.30	122.70
4	1-H	546	TYR	C-N-CA	6.93	133.30	122.70
4	2-H	546	TYR	CA-C-N	6.93	133.30	122.70
4	2-H	546	TYR	C-N-CA	6.93	133.30	122.70
4	3-H	546	TYR	CA-C-N	6.93	133.30	122.70
4	3-H	546	TYR	C-N-CA	6.93	133.30	122.70
3	1-B	428	ASN	N-CA-C	6.92	118.91	111.36
3	2-B	428	ASN	N-CA-C	6.92	118.91	111.36
3	3-B	428	ASN	N-CA-C	6.92	118.91	111.36
6	1-M	147	SER	N-CA-C	-6.92	104.81	113.18
4	1-H	213	ILE	CA-C-O	-6.92	112.83	120.72
6	2-M	147	SER	N-CA-C	-6.92	104.81	113.18
4	2-H	213	ILE	CA-C-O	-6.92	112.83	120.72
6	3-M	147	SER	N-CA-C	-6.92	104.81	113.18
4	3-H	213	ILE	CA-C-O	-6.92	112.83	120.72
1	1-A	76	LYS	N-CA-C	-6.92	98.57	109.50
1	1-A	464	LEU	N-CA-C	-6.92	101.85	112.99
7	1-K	210	ALA	CA-C-N	6.92	129.94	120.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-K	210	ALA	C-N-CA	6.92	129.94	120.46
1	2-A	76	LYS	N-CA-C	-6.92	98.57	109.50
1	2-A	464	LEU	N-CA-C	-6.92	101.85	112.99
7	2-K	210	ALA	CA-C-N	6.92	129.94	120.46
7	2-K	210	ALA	C-N-CA	6.92	129.94	120.46
1	3-A	76	LYS	N-CA-C	-6.92	98.57	109.50
1	3-A	464	LEU	N-CA-C	-6.92	101.85	112.99
7	3-K	210	ALA	CA-C-N	6.92	129.94	120.46
7	3-K	210	ALA	C-N-CA	6.92	129.94	120.46
7	1-G	240	LEU	N-CA-C	6.91	119.66	111.71
3	1-N	63	MET	CA-C-N	6.91	130.24	120.42
3	1-N	63	MET	C-N-CA	6.91	130.24	120.42
7	2-G	240	LEU	N-CA-C	6.91	119.66	111.71
3	2-N	63	MET	CA-C-N	6.91	130.24	120.42
3	2-N	63	MET	C-N-CA	6.91	130.24	120.42
7	3-G	240	LEU	N-CA-C	6.91	119.66	111.71
3	3-N	63	MET	CA-C-N	6.91	130.24	120.42
3	3-N	63	MET	C-N-CA	6.91	130.24	120.42
4	1-C	593	GLU	CA-C-N	6.91	129.43	120.44
4	1-C	593	GLU	C-N-CA	6.91	129.43	120.44
4	2-C	593	GLU	CA-C-N	6.91	129.43	120.44
4	2-C	593	GLU	C-N-CA	6.91	129.43	120.44
4	3-C	593	GLU	CA-C-N	6.91	129.43	120.44
4	3-C	593	GLU	C-N-CA	6.91	129.43	120.44
4	1-C	397	ALA	CA-C-N	6.91	130.47	120.38
4	1-C	397	ALA	C-N-CA	6.91	130.47	120.38
4	1-H	397	ALA	CA-C-N	6.91	130.47	120.38
4	1-H	397	ALA	C-N-CA	6.91	130.47	120.38
4	2-C	397	ALA	CA-C-N	6.91	130.47	120.38
4	2-C	397	ALA	C-N-CA	6.91	130.47	120.38
4	2-H	397	ALA	CA-C-N	6.91	130.47	120.38
4	2-H	397	ALA	C-N-CA	6.91	130.47	120.38
4	3-C	397	ALA	CA-C-N	6.91	130.47	120.38
4	3-C	397	ALA	C-N-CA	6.91	130.47	120.38
4	3-H	397	ALA	CA-C-N	6.91	130.47	120.38
4	3-H	397	ALA	C-N-CA	6.91	130.47	120.38
7	1-G	539	GLN	N-CA-C	-6.91	99.67	109.96
7	2-G	539	GLN	N-CA-C	-6.91	99.67	109.96
7	3-G	539	GLN	N-CA-C	-6.91	99.67	109.96
4	1-C	213	ILE	CA-C-O	-6.91	112.85	120.72
4	2-C	213	ILE	CA-C-O	-6.91	112.85	120.72
4	3-C	213	ILE	CA-C-O	-6.91	112.85	120.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	1178	ARG	CA-C-N	6.90	128.77	120.14
1	1-A	1178	ARG	C-N-CA	6.90	128.77	120.14
8	1-L	80	ILE	CA-C-N	6.90	134.94	121.41
8	1-L	80	ILE	C-N-CA	6.90	134.94	121.41
1	2-A	1178	ARG	CA-C-N	6.90	128.77	120.14
1	2-A	1178	ARG	C-N-CA	6.90	128.77	120.14
8	2-L	80	ILE	CA-C-N	6.90	134.94	121.41
8	2-L	80	ILE	C-N-CA	6.90	134.94	121.41
1	3-A	1178	ARG	CA-C-N	6.90	128.77	120.14
1	3-A	1178	ARG	C-N-CA	6.90	128.77	120.14
8	3-L	80	ILE	CA-C-N	6.90	134.94	121.41
8	3-L	80	ILE	C-N-CA	6.90	134.94	121.41
4	1-C	535	ILE	N-CA-C	-6.89	98.50	108.36
4	2-C	535	ILE	N-CA-C	-6.89	98.50	108.36
4	3-C	535	ILE	N-CA-C	-6.89	98.50	108.36
6	1-F	29	GLY	N-CA-C	-6.89	105.36	115.63
6	2-F	29	GLY	N-CA-C	-6.89	105.36	115.63
6	3-F	29	GLY	N-CA-C	-6.89	105.36	115.63
7	1-G	23	GLU	CA-C-N	6.89	130.07	120.29
7	1-G	23	GLU	C-N-CA	6.89	130.07	120.29
7	2-G	23	GLU	CA-C-N	6.89	130.07	120.29
7	2-G	23	GLU	C-N-CA	6.89	130.07	120.29
7	3-G	23	GLU	CA-C-N	6.89	130.07	120.29
7	3-G	23	GLU	C-N-CA	6.89	130.07	120.29
6	1-J	26	ASP	N-CA-C	6.88	121.42	112.89
6	2-J	26	ASP	N-CA-C	6.88	121.42	112.89
6	3-J	26	ASP	N-CA-C	6.88	121.42	112.89
4	1-H	593	GLU	CA-C-N	6.88	129.39	120.44
4	1-H	593	GLU	C-N-CA	6.88	129.39	120.44
4	2-H	593	GLU	CA-C-N	6.88	129.39	120.44
4	2-H	593	GLU	C-N-CA	6.88	129.39	120.44
4	3-H	593	GLU	CA-C-N	6.88	129.39	120.44
4	3-H	593	GLU	C-N-CA	6.88	129.39	120.44
1	1-A	799	ALA	CA-C-O	-6.88	113.30	120.87
3	1-B	828	ASP	N-CA-C	-6.88	96.15	110.80
1	2-A	799	ALA	CA-C-O	-6.88	113.30	120.87
3	2-B	828	ASP	N-CA-C	-6.88	96.15	110.80
1	3-A	799	ALA	CA-C-O	-6.88	113.30	120.87
3	3-B	828	ASP	N-CA-C	-6.88	96.15	110.80
1	1-A	312	GLY	N-CA-C	-6.88	106.13	114.66
6	1-F	26	ASP	N-CA-C	6.88	121.42	112.89
3	1-N	428	ASN	N-CA-C	6.88	118.86	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	535	ILE	N-CA-C	-6.88	98.53	108.36
1	2-A	312	GLY	N-CA-C	-6.88	106.13	114.66
6	2-F	26	ASP	N-CA-C	6.88	121.42	112.89
3	2-N	428	ASN	N-CA-C	6.88	118.86	111.36
4	2-H	535	ILE	N-CA-C	-6.88	98.53	108.36
1	3-A	312	GLY	N-CA-C	-6.88	106.13	114.66
6	3-F	26	ASP	N-CA-C	6.88	121.42	112.89
3	3-N	428	ASN	N-CA-C	6.88	118.86	111.36
4	3-H	535	ILE	N-CA-C	-6.88	98.53	108.36
4	1-H	89	LEU	N-CA-C	-6.88	96.16	110.80
4	2-H	89	LEU	N-CA-C	-6.88	96.16	110.80
4	3-H	89	LEU	N-CA-C	-6.88	96.16	110.80
3	1-B	63	MET	CA-C-N	6.87	130.18	120.42
3	1-B	63	MET	C-N-CA	6.87	130.18	120.42
3	2-B	63	MET	CA-C-N	6.87	130.18	120.42
3	2-B	63	MET	C-N-CA	6.87	130.18	120.42
3	3-B	63	MET	CA-C-N	6.87	130.18	120.42
3	3-B	63	MET	C-N-CA	6.87	130.18	120.42
3	1-B	250	CYS	N-CA-C	6.87	119.61	111.71
3	2-B	250	CYS	N-CA-C	6.87	119.61	111.71
3	3-B	250	CYS	N-CA-C	6.87	119.61	111.71
4	1-H	246	THR	N-CA-C	-6.87	98.65	109.50
4	2-H	246	THR	N-CA-C	-6.87	98.65	109.50
4	3-H	246	THR	N-CA-C	-6.87	98.65	109.50
1	1-A	597	PHE	CA-C-N	6.86	129.48	120.28
1	1-A	597	PHE	C-N-CA	6.86	129.48	120.28
1	2-A	597	PHE	CA-C-N	6.86	129.48	120.28
1	2-A	597	PHE	C-N-CA	6.86	129.48	120.28
1	3-A	597	PHE	CA-C-N	6.86	129.48	120.28
1	3-A	597	PHE	C-N-CA	6.86	129.48	120.28
4	1-H	377	ILE	CA-C-N	-6.86	112.04	122.81
4	1-H	377	ILE	C-N-CA	-6.86	112.04	122.81
4	2-H	377	ILE	CA-C-N	-6.86	112.04	122.81
4	2-H	377	ILE	C-N-CA	-6.86	112.04	122.81
4	3-H	377	ILE	CA-C-N	-6.86	112.04	122.81
4	3-H	377	ILE	C-N-CA	-6.86	112.04	122.81
4	1-C	377	ILE	CA-C-N	-6.86	112.04	122.81
4	1-C	377	ILE	C-N-CA	-6.86	112.04	122.81
7	1-K	865	PRO	N-CA-C	6.86	122.91	113.65
4	2-C	377	ILE	CA-C-N	-6.86	112.04	122.81
4	2-C	377	ILE	C-N-CA	-6.86	112.04	122.81
7	2-K	865	PRO	N-CA-C	6.86	122.91	113.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	3-C	377	ILE	CA-C-N	-6.86	112.04	122.81
4	3-C	377	ILE	C-N-CA	-6.86	112.04	122.81
7	3-K	865	PRO	N-CA-C	6.86	122.91	113.65
6	1-J	29	GLY	N-CA-C	-6.86	105.41	115.63
6	2-J	29	GLY	N-CA-C	-6.86	105.41	115.63
6	3-J	29	GLY	N-CA-C	-6.86	105.41	115.63
4	1-C	89	LEU	N-CA-C	-6.86	96.19	110.80
4	1-C	322	VAL	N-CA-C	-6.86	102.46	110.21
7	1-G	865	PRO	N-CA-C	6.86	122.91	113.65
4	2-C	89	LEU	N-CA-C	-6.86	96.19	110.80
4	2-C	322	VAL	N-CA-C	-6.86	102.46	110.21
7	2-G	865	PRO	N-CA-C	6.86	122.91	113.65
4	3-C	89	LEU	N-CA-C	-6.86	96.19	110.80
4	3-C	322	VAL	N-CA-C	-6.86	102.46	110.21
7	3-G	865	PRO	N-CA-C	6.86	122.91	113.65
7	1-G	703	PRO	CA-C-N	6.86	133.06	121.47
7	1-G	703	PRO	C-N-CA	6.86	133.06	121.47
7	2-G	703	PRO	CA-C-N	6.86	133.06	121.47
7	2-G	703	PRO	C-N-CA	6.86	133.06	121.47
7	3-G	703	PRO	CA-C-N	6.86	133.06	121.47
7	3-G	703	PRO	C-N-CA	6.86	133.06	121.47
8	1-L	37	SER	CA-C-N	6.85	130.15	120.42
8	1-L	37	SER	C-N-CA	6.85	130.15	120.42
8	2-L	37	SER	CA-C-N	6.85	130.15	120.42
8	2-L	37	SER	C-N-CA	6.85	130.15	120.42
8	3-L	37	SER	CA-C-N	6.85	130.15	120.42
8	3-L	37	SER	C-N-CA	6.85	130.15	120.42
4	1-C	246	THR	N-CA-C	-6.85	98.68	109.50
6	1-R	91	VAL	CA-C-N	6.85	132.46	122.94
6	1-R	91	VAL	C-N-CA	6.85	132.46	122.94
8	1-Z	139	PRO	N-CA-C	6.85	122.54	113.57
4	2-C	246	THR	N-CA-C	-6.85	98.68	109.50
6	2-R	91	VAL	CA-C-N	6.85	132.46	122.94
6	2-R	91	VAL	C-N-CA	6.85	132.46	122.94
8	2-Z	139	PRO	N-CA-C	6.85	122.54	113.57
4	3-C	246	THR	N-CA-C	-6.85	98.68	109.50
6	3-R	91	VAL	CA-C-N	6.85	132.46	122.94
6	3-R	91	VAL	C-N-CA	6.85	132.46	122.94
8	3-Z	139	PRO	N-CA-C	6.85	122.54	113.57
4	1-C	282	GLY	N-CA-C	-6.84	104.85	115.73
4	2-C	282	GLY	N-CA-C	-6.84	104.85	115.73
4	3-C	282	GLY	N-CA-C	-6.84	104.85	115.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	301	ARG	N-CA-C	-6.84	99.84	110.17
4	2-C	301	ARG	N-CA-C	-6.84	99.84	110.17
4	3-C	301	ARG	N-CA-C	-6.84	99.84	110.17
4	1-C	474	GLY	CA-C-N	6.84	134.60	121.54
4	1-C	474	GLY	C-N-CA	6.84	134.60	121.54
6	1-R	146	HIS	CA-C-N	6.84	134.60	121.54
6	1-R	146	HIS	C-N-CA	6.84	134.60	121.54
3	1-N	407	VAL	N-CA-C	-6.84	103.85	110.42
4	2-C	474	GLY	CA-C-N	6.84	134.60	121.54
4	2-C	474	GLY	C-N-CA	6.84	134.60	121.54
6	2-R	146	HIS	CA-C-N	6.84	134.60	121.54
6	2-R	146	HIS	C-N-CA	6.84	134.60	121.54
3	2-N	407	VAL	N-CA-C	-6.84	103.85	110.42
4	3-C	474	GLY	CA-C-N	6.84	134.60	121.54
4	3-C	474	GLY	C-N-CA	6.84	134.60	121.54
6	3-R	146	HIS	CA-C-N	6.84	134.60	121.54
6	3-R	146	HIS	C-N-CA	6.84	134.60	121.54
3	3-N	407	VAL	N-CA-C	-6.84	103.85	110.42
3	1-B	407	VAL	N-CA-C	-6.84	103.86	110.42
4	1-C	747	ARG	N-CA-C	6.84	118.39	111.07
3	2-B	407	VAL	N-CA-C	-6.84	103.86	110.42
4	2-C	747	ARG	N-CA-C	6.84	118.39	111.07
3	3-B	407	VAL	N-CA-C	-6.84	103.86	110.42
4	3-C	747	ARG	N-CA-C	6.84	118.39	111.07
4	1-C	9	ARG	N-CA-C	-6.83	95.96	107.99
4	2-C	9	ARG	N-CA-C	-6.83	95.96	107.99
4	3-C	9	ARG	N-CA-C	-6.83	95.96	107.99
4	1-C	795	GLU	N-CA-C	-6.83	98.93	109.52
4	1-H	474	GLY	CA-C-N	6.83	134.59	121.54
4	1-H	474	GLY	C-N-CA	6.83	134.59	121.54
4	2-C	795	GLU	N-CA-C	-6.83	98.93	109.52
4	2-H	474	GLY	CA-C-N	6.83	134.59	121.54
4	2-H	474	GLY	C-N-CA	6.83	134.59	121.54
4	3-C	795	GLU	N-CA-C	-6.83	98.93	109.52
4	3-H	474	GLY	CA-C-N	6.83	134.59	121.54
4	3-H	474	GLY	C-N-CA	6.83	134.59	121.54
7	1-G	838	HIS	CA-C-O	6.83	128.77	120.92
4	1-H	394	PHE	N-CA-C	6.83	119.81	109.23
4	1-H	509	GLY	N-CA-C	-6.83	99.85	112.62
7	2-G	838	HIS	CA-C-O	6.83	128.77	120.92
4	2-H	394	PHE	N-CA-C	6.83	119.81	109.23
4	2-H	509	GLY	N-CA-C	-6.83	99.85	112.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	3-G	838	HIS	CA-C-O	6.83	128.77	120.92
4	3-H	394	PHE	N-CA-C	6.83	119.81	109.23
4	3-H	509	GLY	N-CA-C	-6.83	99.85	112.62
3	1-N	250	CYS	N-CA-C	6.83	119.56	111.71
3	2-N	250	CYS	N-CA-C	6.83	119.56	111.71
3	3-N	250	CYS	N-CA-C	6.83	119.56	111.71
4	1-C	383	LEU	N-CA-C	-6.82	102.78	111.92
4	2-C	383	LEU	N-CA-C	-6.82	102.78	111.92
4	3-C	383	LEU	N-CA-C	-6.82	102.78	111.92
6	1-R	25	LEU	CA-C-N	6.82	131.61	121.72
6	1-R	25	LEU	C-N-CA	6.82	131.61	121.72
4	1-H	9	ARG	N-CA-C	-6.82	95.98	107.99
6	2-R	25	LEU	CA-C-N	6.82	131.61	121.72
6	2-R	25	LEU	C-N-CA	6.82	131.61	121.72
4	2-H	9	ARG	N-CA-C	-6.82	95.98	107.99
6	3-R	25	LEU	CA-C-N	6.82	131.61	121.72
6	3-R	25	LEU	C-N-CA	6.82	131.61	121.72
4	3-H	9	ARG	N-CA-C	-6.82	95.98	107.99
3	1-B	788	SER	N-CA-C	6.82	122.02	112.75
4	1-C	509	GLY	N-CA-C	-6.82	99.87	112.62
3	2-B	788	SER	N-CA-C	6.82	122.02	112.75
4	2-C	509	GLY	N-CA-C	-6.82	99.87	112.62
3	3-B	788	SER	N-CA-C	6.82	122.02	112.75
4	3-C	509	GLY	N-CA-C	-6.82	99.87	112.62
4	1-C	394	PHE	N-CA-C	6.81	119.79	109.23
4	2-C	394	PHE	N-CA-C	6.81	119.79	109.23
4	3-C	394	PHE	N-CA-C	6.81	119.79	109.23
7	1-K	703	PRO	CA-C-N	6.81	132.98	121.47
7	1-K	703	PRO	C-N-CA	6.81	132.98	121.47
7	2-K	703	PRO	CA-C-N	6.81	132.98	121.47
7	2-K	703	PRO	C-N-CA	6.81	132.98	121.47
7	3-K	703	PRO	CA-C-N	6.81	132.98	121.47
7	3-K	703	PRO	C-N-CA	6.81	132.98	121.47
3	1-N	259	ARG	N-CA-C	-6.81	103.86	111.28
3	2-N	259	ARG	N-CA-C	-6.81	103.86	111.28
3	3-N	259	ARG	N-CA-C	-6.81	103.86	111.28
1	1-A	189	LEU	N-CA-C	6.80	119.34	110.43
7	1-K	838	HIS	CA-C-O	6.80	128.74	120.92
1	2-A	189	LEU	N-CA-C	6.80	119.34	110.43
7	2-K	838	HIS	CA-C-O	6.80	128.74	120.92
1	3-A	189	LEU	N-CA-C	6.80	119.34	110.43
7	3-K	838	HIS	CA-C-O	6.80	128.74	120.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	1-R	46	ILE	CA-C-N	6.79	128.33	119.84
6	1-R	46	ILE	C-N-CA	6.79	128.33	119.84
4	1-H	301	ARG	N-CA-C	-6.79	99.91	110.17
4	1-H	383	LEU	N-CA-C	-6.79	102.82	111.92
6	2-R	46	ILE	CA-C-N	6.79	128.33	119.84
6	2-R	46	ILE	C-N-CA	6.79	128.33	119.84
4	2-H	301	ARG	N-CA-C	-6.79	99.91	110.17
4	2-H	383	LEU	N-CA-C	-6.79	102.82	111.92
6	3-R	46	ILE	CA-C-N	6.79	128.33	119.84
6	3-R	46	ILE	C-N-CA	6.79	128.33	119.84
4	3-H	301	ARG	N-CA-C	-6.79	99.91	110.17
4	3-H	383	LEU	N-CA-C	-6.79	102.82	111.92
7	1-G	292	LEU	N-CA-C	6.79	118.33	111.07
7	2-G	292	LEU	N-CA-C	6.79	118.33	111.07
7	3-G	292	LEU	N-CA-C	6.79	118.33	111.07
1	1-A	370	TYR	N-CA-C	-6.79	100.44	110.48
1	2-A	370	TYR	N-CA-C	-6.79	100.44	110.48
1	3-A	370	TYR	N-CA-C	-6.79	100.44	110.48
7	1-G	686	ALA	N-CA-C	6.78	125.25	110.80
7	2-G	686	ALA	N-CA-C	6.78	125.25	110.80
7	3-G	686	ALA	N-CA-C	6.78	125.25	110.80
4	1-H	282	GLY	N-CA-C	-6.78	104.95	115.73
4	2-H	282	GLY	N-CA-C	-6.78	104.95	115.73
4	3-H	282	GLY	N-CA-C	-6.78	104.95	115.73
3	1-B	259	ARG	N-CA-C	-6.78	103.89	111.28
3	2-B	259	ARG	N-CA-C	-6.78	103.89	111.28
3	3-B	259	ARG	N-CA-C	-6.78	103.89	111.28
3	1-B	939	THR	N-CA-C	-6.78	96.37	110.80
3	2-B	939	THR	N-CA-C	-6.78	96.37	110.80
3	3-B	939	THR	N-CA-C	-6.78	96.37	110.80
4	1-H	322	VAL	N-CA-C	-6.77	102.56	110.21
4	2-H	322	VAL	N-CA-C	-6.77	102.56	110.21
4	3-H	322	VAL	N-CA-C	-6.77	102.56	110.21
3	1-B	936	ALA	N-CA-C	-6.77	102.09	112.99
3	2-B	936	ALA	N-CA-C	-6.77	102.09	112.99
3	3-B	936	ALA	N-CA-C	-6.77	102.09	112.99
7	1-K	686	ALA	N-CA-C	6.76	125.20	110.80
7	2-K	686	ALA	N-CA-C	6.76	125.20	110.80
7	3-K	686	ALA	N-CA-C	6.76	125.20	110.80
7	1-G	296	CYS	CA-C-N	6.76	134.45	121.54
7	1-G	296	CYS	C-N-CA	6.76	134.45	121.54
7	2-G	296	CYS	CA-C-N	6.76	134.45	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-G	296	CYS	C-N-CA	6.76	134.45	121.54
7	3-G	296	CYS	CA-C-N	6.76	134.45	121.54
7	3-G	296	CYS	C-N-CA	6.76	134.45	121.54
1	1-A	747	ARG	CA-C-N	6.76	129.72	120.46
1	1-A	747	ARG	C-N-CA	6.76	129.72	120.46
6	1-R	37	LEU	N-CA-C	6.76	118.30	111.07
1	2-A	747	ARG	CA-C-N	6.76	129.72	120.46
1	2-A	747	ARG	C-N-CA	6.76	129.72	120.46
6	2-R	37	LEU	N-CA-C	6.76	118.30	111.07
1	3-A	747	ARG	CA-C-N	6.76	129.72	120.46
1	3-A	747	ARG	C-N-CA	6.76	129.72	120.46
6	3-R	37	LEU	N-CA-C	6.76	118.30	111.07
6	1-F	46	ILE	CA-C-N	6.76	128.29	119.84
6	1-F	46	ILE	C-N-CA	6.76	128.29	119.84
6	1-R	92	VAL	N-CA-C	6.76	118.53	108.46
6	2-F	46	ILE	CA-C-N	6.76	128.29	119.84
6	2-F	46	ILE	C-N-CA	6.76	128.29	119.84
6	2-R	92	VAL	N-CA-C	6.76	118.53	108.46
6	3-F	46	ILE	CA-C-N	6.76	128.29	119.84
6	3-F	46	ILE	C-N-CA	6.76	128.29	119.84
6	3-R	92	VAL	N-CA-C	6.76	118.53	108.46
4	1-C	323	GLN	CA-C-N	6.75	131.40	120.60
4	1-C	323	GLN	C-N-CA	6.75	131.40	120.60
4	2-C	323	GLN	CA-C-N	6.75	131.40	120.60
4	2-C	323	GLN	C-N-CA	6.75	131.40	120.60
4	3-C	323	GLN	CA-C-N	6.75	131.40	120.60
4	3-C	323	GLN	C-N-CA	6.75	131.40	120.60
1	1-A	687	HIS	N-CA-C	-6.75	104.94	113.72
1	2-A	687	HIS	N-CA-C	-6.75	104.94	113.72
1	3-A	687	HIS	N-CA-C	-6.75	104.94	113.72
6	1-F	58	TYR	N-CA-C	6.75	119.46	108.26
6	2-F	58	TYR	N-CA-C	6.75	119.46	108.26
6	3-F	58	TYR	N-CA-C	6.75	119.46	108.26
7	1-K	834	PHE	CA-C-N	6.73	130.27	120.71
7	1-K	834	PHE	C-N-CA	6.73	130.27	120.71
7	2-K	834	PHE	CA-C-N	6.73	130.27	120.71
7	2-K	834	PHE	C-N-CA	6.73	130.27	120.71
7	3-K	834	PHE	CA-C-N	6.73	130.27	120.71
7	3-K	834	PHE	C-N-CA	6.73	130.27	120.71
3	1-B	857	GLN	N-CA-C	-6.73	103.94	111.28
3	2-B	857	GLN	N-CA-C	-6.73	103.94	111.28
3	3-B	857	GLN	N-CA-C	-6.73	103.94	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1-I	57	VAL	N-CA-C	-6.73	98.79	108.48
5	2-I	57	VAL	N-CA-C	-6.73	98.79	108.48
5	3-I	57	VAL	N-CA-C	-6.73	98.79	108.48
3	1-B	757	ASP	N-CA-C	-6.73	98.66	109.96
6	1-R	171	GLU	N-CA-C	6.73	118.50	111.03
3	2-B	757	ASP	N-CA-C	-6.73	98.66	109.96
6	2-R	171	GLU	N-CA-C	6.73	118.50	111.03
3	3-B	757	ASP	N-CA-C	-6.73	98.66	109.96
6	3-R	171	GLU	N-CA-C	6.73	118.50	111.03
6	1-J	58	TYR	N-CA-C	6.72	119.42	108.26
6	2-J	58	TYR	N-CA-C	6.72	119.42	108.26
6	3-J	58	TYR	N-CA-C	6.72	119.42	108.26
4	1-H	323	GLN	CA-C-N	6.72	131.35	120.60
4	1-H	323	GLN	C-N-CA	6.72	131.35	120.60
4	2-H	323	GLN	CA-C-N	6.72	131.35	120.60
4	2-H	323	GLN	C-N-CA	6.72	131.35	120.60
4	3-H	323	GLN	CA-C-N	6.72	131.35	120.60
4	3-H	323	GLN	C-N-CA	6.72	131.35	120.60
7	1-G	136	MET	N-CA-C	-6.71	104.56	112.89
7	2-G	136	MET	N-CA-C	-6.71	104.56	112.89
7	3-G	136	MET	N-CA-C	-6.71	104.56	112.89
7	1-G	382	ALA	CA-C-N	6.71	129.65	120.46
7	1-G	382	ALA	C-N-CA	6.71	129.65	120.46
7	2-G	382	ALA	CA-C-N	6.71	129.65	120.46
7	2-G	382	ALA	C-N-CA	6.71	129.65	120.46
7	3-G	382	ALA	CA-C-N	6.71	129.65	120.46
7	3-G	382	ALA	C-N-CA	6.71	129.65	120.46
4	1-C	65	PHE	N-CA-C	-6.71	98.79	109.59
5	1-D	57	VAL	N-CA-C	-6.71	98.82	108.48
6	1-J	46	ILE	CA-C-N	6.71	128.23	119.84
6	1-J	46	ILE	C-N-CA	6.71	128.23	119.84
4	2-C	65	PHE	N-CA-C	-6.71	98.79	109.59
5	2-D	57	VAL	N-CA-C	-6.71	98.82	108.48
6	2-J	46	ILE	CA-C-N	6.71	128.23	119.84
6	2-J	46	ILE	C-N-CA	6.71	128.23	119.84
4	3-C	65	PHE	N-CA-C	-6.71	98.79	109.59
5	3-D	57	VAL	N-CA-C	-6.71	98.82	108.48
6	3-J	46	ILE	CA-C-N	6.71	128.23	119.84
6	3-J	46	ILE	C-N-CA	6.71	128.23	119.84
7	1-K	220	ARG	N-CA-C	-6.70	99.00	109.25
7	2-K	220	ARG	N-CA-C	-6.70	99.00	109.25
7	3-K	220	ARG	N-CA-C	-6.70	99.00	109.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	661	ALA	O-C-N	6.70	128.97	122.07
4	1-H	661	ALA	O-C-N	6.70	128.97	122.07
4	2-C	661	ALA	O-C-N	6.70	128.97	122.07
4	2-H	661	ALA	O-C-N	6.70	128.97	122.07
4	3-C	661	ALA	O-C-N	6.70	128.97	122.07
4	3-H	661	ALA	O-C-N	6.70	128.97	122.07
8	1-Z	18	ILE	CA-C-O	6.70	127.04	120.27
8	2-Z	18	ILE	CA-C-O	6.70	127.04	120.27
8	3-Z	18	ILE	CA-C-O	6.70	127.04	120.27
7	1-K	297	SER	N-CA-C	6.70	125.07	110.80
7	2-K	297	SER	N-CA-C	6.70	125.07	110.80
7	3-K	297	SER	N-CA-C	6.70	125.07	110.80
7	1-G	61	LEU	CA-C-N	6.70	126.70	120.34
7	1-G	61	LEU	C-N-CA	6.70	126.70	120.34
7	2-G	61	LEU	CA-C-N	6.70	126.70	120.34
7	2-G	61	LEU	C-N-CA	6.70	126.70	120.34
7	3-G	61	LEU	CA-C-N	6.70	126.70	120.34
7	3-G	61	LEU	C-N-CA	6.70	126.70	120.34
1	1-A	793	LYS	N-CA-C	6.70	119.19	108.41
7	1-G	25	SER	N-CA-C	6.70	118.58	111.28
1	2-A	793	LYS	N-CA-C	6.70	119.19	108.41
7	2-G	25	SER	N-CA-C	6.70	118.58	111.28
1	3-A	793	LYS	N-CA-C	6.70	119.19	108.41
7	3-G	25	SER	N-CA-C	6.70	118.58	111.28
8	1-Z	140	GLN	N-CA-C	6.69	118.65	111.36
8	2-Z	140	GLN	N-CA-C	6.69	118.65	111.36
8	3-Z	140	GLN	N-CA-C	6.69	118.65	111.36
4	1-C	111	GLN	CA-C-N	6.68	128.19	119.84
4	1-C	111	GLN	C-N-CA	6.68	128.19	119.84
7	1-G	118	ASP	CA-C-O	6.68	127.50	120.42
4	2-C	111	GLN	CA-C-N	6.68	128.19	119.84
4	2-C	111	GLN	C-N-CA	6.68	128.19	119.84
7	2-G	118	ASP	CA-C-O	6.68	127.50	120.42
4	3-C	111	GLN	CA-C-N	6.68	128.19	119.84
4	3-C	111	GLN	C-N-CA	6.68	128.19	119.84
7	3-G	118	ASP	CA-C-O	6.68	127.50	120.42
4	1-C	650	GLN	CA-C-N	6.67	129.77	120.29
4	1-C	650	GLN	C-N-CA	6.67	129.77	120.29
4	2-C	650	GLN	CA-C-N	6.67	129.77	120.29
4	2-C	650	GLN	C-N-CA	6.67	129.77	120.29
4	3-C	650	GLN	CA-C-N	6.67	129.77	120.29
4	3-C	650	GLN	C-N-CA	6.67	129.77	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	65	PHE	N-CA-C	-6.67	98.85	109.59
4	2-H	65	PHE	N-CA-C	-6.67	98.85	109.59
4	3-H	65	PHE	N-CA-C	-6.67	98.85	109.59
7	1-G	54	LEU	N-CA-C	-6.67	104.09	111.36
7	2-G	54	LEU	N-CA-C	-6.67	104.09	111.36
7	3-G	54	LEU	N-CA-C	-6.67	104.09	111.36
7	1-G	834	PHE	CA-C-N	6.66	130.17	120.71
7	1-G	834	PHE	C-N-CA	6.66	130.17	120.71
7	2-G	834	PHE	CA-C-N	6.66	130.17	120.71
7	2-G	834	PHE	C-N-CA	6.66	130.17	120.71
7	3-G	834	PHE	CA-C-N	6.66	130.17	120.71
7	3-G	834	PHE	C-N-CA	6.66	130.17	120.71
3	1-B	323	LEU	CA-C-N	6.66	129.87	120.28
3	1-B	323	LEU	C-N-CA	6.66	129.87	120.28
7	1-G	264	GLU	N-CA-C	6.66	118.54	111.28
3	2-B	323	LEU	CA-C-N	6.66	129.87	120.28
3	2-B	323	LEU	C-N-CA	6.66	129.87	120.28
7	2-G	264	GLU	N-CA-C	6.66	118.54	111.28
3	3-B	323	LEU	CA-C-N	6.66	129.87	120.28
3	3-B	323	LEU	C-N-CA	6.66	129.87	120.28
7	3-G	264	GLU	N-CA-C	6.66	118.54	111.28
1	1-A	760	LEU	CA-C-N	6.66	129.50	120.44
1	1-A	760	LEU	C-N-CA	6.66	129.50	120.44
3	1-B	917	GLY	N-CA-C	6.66	124.22	115.36
7	1-K	78	GLN	N-CA-C	-6.66	103.62	113.61
1	2-A	760	LEU	CA-C-N	6.66	129.50	120.44
1	2-A	760	LEU	C-N-CA	6.66	129.50	120.44
3	2-B	917	GLY	N-CA-C	6.66	124.22	115.36
7	2-K	78	GLN	N-CA-C	-6.66	103.62	113.61
1	3-A	760	LEU	CA-C-N	6.66	129.50	120.44
1	3-A	760	LEU	C-N-CA	6.66	129.50	120.44
3	3-B	917	GLY	N-CA-C	6.66	124.22	115.36
7	3-K	78	GLN	N-CA-C	-6.66	103.62	113.61
7	1-G	533	ASN	CA-C-N	6.66	129.87	120.42
7	1-G	533	ASN	C-N-CA	6.66	129.87	120.42
7	2-G	533	ASN	CA-C-N	6.66	129.87	120.42
7	2-G	533	ASN	C-N-CA	6.66	129.87	120.42
7	3-G	533	ASN	CA-C-N	6.66	129.87	120.42
7	3-G	533	ASN	C-N-CA	6.66	129.87	120.42
4	1-H	650	GLN	CA-C-N	6.65	129.74	120.29
4	1-H	650	GLN	C-N-CA	6.65	129.74	120.29
4	2-H	650	GLN	CA-C-N	6.65	129.74	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-H	650	GLN	C-N-CA	6.65	129.74	120.29
4	3-H	650	GLN	CA-C-N	6.65	129.74	120.29
4	3-H	650	GLN	C-N-CA	6.65	129.74	120.29
3	1-N	323	LEU	CA-C-N	6.65	129.86	120.28
3	1-N	323	LEU	C-N-CA	6.65	129.86	120.28
3	2-N	323	LEU	CA-C-N	6.65	129.86	120.28
3	2-N	323	LEU	C-N-CA	6.65	129.86	120.28
3	3-N	323	LEU	CA-C-N	6.65	129.86	120.28
3	3-N	323	LEU	C-N-CA	6.65	129.86	120.28
7	1-K	283	LYS	N-CA-C	6.65	119.13	111.02
7	2-K	283	LYS	N-CA-C	6.65	119.13	111.02
7	3-K	283	LYS	N-CA-C	6.65	119.13	111.02
7	1-G	542	LEU	CA-C-N	6.65	129.08	120.44
7	1-G	542	LEU	C-N-CA	6.65	129.08	120.44
4	1-H	150	ILE	N-CA-C	-6.65	98.81	108.71
7	2-G	542	LEU	CA-C-N	6.65	129.08	120.44
7	2-G	542	LEU	C-N-CA	6.65	129.08	120.44
4	2-H	150	ILE	N-CA-C	-6.65	98.81	108.71
7	3-G	542	LEU	CA-C-N	6.65	129.08	120.44
7	3-G	542	LEU	C-N-CA	6.65	129.08	120.44
4	3-H	150	ILE	N-CA-C	-6.65	98.81	108.71
7	1-G	119	ASN	CA-C-N	6.65	129.73	120.29
7	1-G	119	ASN	C-N-CA	6.65	129.73	120.29
7	2-G	119	ASN	CA-C-N	6.65	129.73	120.29
7	2-G	119	ASN	C-N-CA	6.65	129.73	120.29
7	3-G	119	ASN	CA-C-N	6.65	129.73	120.29
7	3-G	119	ASN	C-N-CA	6.65	129.73	120.29
7	1-K	812	PRO	CA-C-O	-6.64	113.34	121.31
7	2-K	812	PRO	CA-C-O	-6.64	113.34	121.31
7	3-K	812	PRO	CA-C-O	-6.64	113.34	121.31
4	1-H	711	MET	N-CA-C	-6.64	104.04	111.28
4	2-H	711	MET	N-CA-C	-6.64	104.04	111.28
4	3-H	711	MET	N-CA-C	-6.64	104.04	111.28
4	1-C	150	ILE	N-CA-C	-6.64	98.82	108.71
4	2-C	150	ILE	N-CA-C	-6.64	98.82	108.71
4	3-C	150	ILE	N-CA-C	-6.64	98.82	108.71
4	1-H	111	GLN	CA-C-N	6.63	128.13	119.84
4	1-H	111	GLN	C-N-CA	6.63	128.13	119.84
4	2-H	111	GLN	CA-C-N	6.63	128.13	119.84
4	2-H	111	GLN	C-N-CA	6.63	128.13	119.84
4	3-H	111	GLN	CA-C-N	6.63	128.13	119.84
4	3-H	111	GLN	C-N-CA	6.63	128.13	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	96	ILE	N-CA-C	6.62	117.38	107.51
7	1-G	812	PRO	CA-C-O	-6.62	113.36	121.31
1	2-A	96	ILE	N-CA-C	6.62	117.38	107.51
7	2-G	812	PRO	CA-C-O	-6.62	113.36	121.31
1	3-A	96	ILE	N-CA-C	6.62	117.38	107.51
7	3-G	812	PRO	CA-C-O	-6.62	113.36	121.31
6	1-R	42	VAL	N-CA-C	6.62	123.11	109.34
6	2-R	42	VAL	N-CA-C	6.62	123.11	109.34
6	3-R	42	VAL	N-CA-C	6.62	123.11	109.34
1	1-A	25	LEU	N-CA-C	-6.62	98.94	109.59
1	2-A	25	LEU	N-CA-C	-6.62	98.94	109.59
1	3-A	25	LEU	N-CA-C	-6.62	98.94	109.59
7	1-G	871	ALA	CA-C-N	6.62	129.15	120.28
7	1-G	871	ALA	C-N-CA	6.62	129.15	120.28
7	1-K	150	ASP	CA-C-N	6.62	134.18	121.54
7	1-K	150	ASP	C-N-CA	6.62	134.18	121.54
7	2-G	871	ALA	CA-C-N	6.62	129.15	120.28
7	2-G	871	ALA	C-N-CA	6.62	129.15	120.28
7	2-K	150	ASP	CA-C-N	6.62	134.18	121.54
7	2-K	150	ASP	C-N-CA	6.62	134.18	121.54
7	3-G	871	ALA	CA-C-N	6.62	129.15	120.28
7	3-G	871	ALA	C-N-CA	6.62	129.15	120.28
7	3-K	150	ASP	CA-C-N	6.62	134.18	121.54
7	3-K	150	ASP	C-N-CA	6.62	134.18	121.54
1	1-A	28	LEU	N-CA-C	-6.61	99.89	110.14
4	1-C	711	MET	N-CA-C	-6.61	104.07	111.28
4	1-H	715	LEU	CA-C-N	6.61	129.14	120.28
4	1-H	715	LEU	C-N-CA	6.61	129.14	120.28
1	2-A	28	LEU	N-CA-C	-6.61	99.89	110.14
4	2-C	711	MET	N-CA-C	-6.61	104.07	111.28
4	2-H	715	LEU	CA-C-N	6.61	129.14	120.28
4	2-H	715	LEU	C-N-CA	6.61	129.14	120.28
1	3-A	28	LEU	N-CA-C	-6.61	99.89	110.14
4	3-C	711	MET	N-CA-C	-6.61	104.07	111.28
4	3-H	715	LEU	CA-C-N	6.61	129.14	120.28
4	3-H	715	LEU	C-N-CA	6.61	129.14	120.28
7	1-K	740	GLY	N-CA-C	6.61	123.16	111.73
7	2-K	740	GLY	N-CA-C	6.61	123.16	111.73
7	3-K	740	GLY	N-CA-C	6.61	123.16	111.73
3	1-N	524	GLY	CA-C-N	6.61	126.85	119.32
3	1-N	524	GLY	C-N-CA	6.61	126.85	119.32
6	1-J	45	THR	N-CA-C	-6.61	98.68	108.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2-N	524	GLY	CA-C-N	6.61	126.85	119.32
3	2-N	524	GLY	C-N-CA	6.61	126.85	119.32
6	2-J	45	THR	N-CA-C	-6.61	98.68	108.79
3	3-N	524	GLY	CA-C-N	6.61	126.85	119.32
3	3-N	524	GLY	C-N-CA	6.61	126.85	119.32
6	3-J	45	THR	N-CA-C	-6.61	98.68	108.79
4	1-C	715	LEU	CA-C-N	6.60	129.12	120.28
4	1-C	715	LEU	C-N-CA	6.60	129.12	120.28
7	1-G	700	TYR	N-CA-C	6.60	119.86	109.96
4	2-C	715	LEU	CA-C-N	6.60	129.12	120.28
4	2-C	715	LEU	C-N-CA	6.60	129.12	120.28
7	2-G	700	TYR	N-CA-C	6.60	119.86	109.96
4	3-C	715	LEU	CA-C-N	6.60	129.12	120.28
4	3-C	715	LEU	C-N-CA	6.60	129.12	120.28
7	3-G	700	TYR	N-CA-C	6.60	119.86	109.96
1	1-A	273	ILE	O-C-N	-6.59	116.14	123.26
1	2-A	273	ILE	O-C-N	-6.59	116.14	123.26
1	3-A	273	ILE	O-C-N	-6.59	116.14	123.26
3	1-B	755	VAL	N-CA-C	-6.59	98.14	108.81
7	1-G	250	PRO	CA-C-N	6.59	129.01	120.44
7	1-G	250	PRO	C-N-CA	6.59	129.01	120.44
7	1-G	740	GLY	N-CA-C	6.59	123.13	111.73
3	2-B	755	VAL	N-CA-C	-6.59	98.14	108.81
7	2-G	250	PRO	CA-C-N	6.59	129.01	120.44
7	2-G	250	PRO	C-N-CA	6.59	129.01	120.44
7	2-G	740	GLY	N-CA-C	6.59	123.13	111.73
3	3-B	755	VAL	N-CA-C	-6.59	98.14	108.81
7	3-G	250	PRO	CA-C-N	6.59	129.01	120.44
7	3-G	250	PRO	C-N-CA	6.59	129.01	120.44
7	3-G	740	GLY	N-CA-C	6.59	123.13	111.73
8	1-L	62	LEU	CA-C-N	6.59	134.12	121.54
8	1-L	62	LEU	C-N-CA	6.59	134.12	121.54
8	2-L	62	LEU	CA-C-N	6.59	134.12	121.54
8	2-L	62	LEU	C-N-CA	6.59	134.12	121.54
8	3-L	62	LEU	CA-C-N	6.59	134.12	121.54
8	3-L	62	LEU	C-N-CA	6.59	134.12	121.54
1	1-A	71	ASP	CA-C-N	6.58	129.00	120.44
1	1-A	71	ASP	C-N-CA	6.58	129.00	120.44
3	1-B	524	GLY	CA-C-N	6.58	126.83	119.32
3	1-B	524	GLY	C-N-CA	6.58	126.83	119.32
4	1-C	697	GLY	N-CA-C	6.58	120.14	112.50
1	2-A	71	ASP	CA-C-N	6.58	129.00	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	71	ASP	C-N-CA	6.58	129.00	120.44
3	2-B	524	GLY	CA-C-N	6.58	126.83	119.32
3	2-B	524	GLY	C-N-CA	6.58	126.83	119.32
4	2-C	697	GLY	N-CA-C	6.58	120.14	112.50
1	3-A	71	ASP	CA-C-N	6.58	129.00	120.44
1	3-A	71	ASP	C-N-CA	6.58	129.00	120.44
3	3-B	524	GLY	CA-C-N	6.58	126.83	119.32
3	3-B	524	GLY	C-N-CA	6.58	126.83	119.32
4	3-C	697	GLY	N-CA-C	6.58	120.14	112.50
4	1-C	426	PRO	N-CA-C	-6.58	102.01	111.22
5	1-D	83	LEU	CA-C-N	6.58	129.10	120.28
5	1-D	83	LEU	C-N-CA	6.58	129.10	120.28
6	1-F	45	THR	N-CA-C	-6.58	98.72	108.79
4	2-C	426	PRO	N-CA-C	-6.58	102.01	111.22
5	2-D	83	LEU	CA-C-N	6.58	129.10	120.28
5	2-D	83	LEU	C-N-CA	6.58	129.10	120.28
6	2-F	45	THR	N-CA-C	-6.58	98.72	108.79
4	3-C	426	PRO	N-CA-C	-6.58	102.01	111.22
5	3-D	83	LEU	CA-C-N	6.58	129.10	120.28
5	3-D	83	LEU	C-N-CA	6.58	129.10	120.28
6	3-F	45	THR	N-CA-C	-6.58	98.72	108.79
1	1-A	595	THR	CA-C-N	6.58	129.75	120.28
1	1-A	595	THR	C-N-CA	6.58	129.75	120.28
4	1-C	335	ILE	CA-C-N	6.58	130.69	120.75
4	1-C	335	ILE	C-N-CA	6.58	130.69	120.75
7	1-G	494	ALA	CA-C-N	6.58	129.10	120.28
7	1-G	494	ALA	C-N-CA	6.58	129.10	120.28
1	2-A	595	THR	CA-C-N	6.58	129.75	120.28
1	2-A	595	THR	C-N-CA	6.58	129.75	120.28
4	2-C	335	ILE	CA-C-N	6.58	130.69	120.75
4	2-C	335	ILE	C-N-CA	6.58	130.69	120.75
7	2-G	494	ALA	CA-C-N	6.58	129.10	120.28
7	2-G	494	ALA	C-N-CA	6.58	129.10	120.28
1	3-A	595	THR	CA-C-N	6.58	129.75	120.28
1	3-A	595	THR	C-N-CA	6.58	129.75	120.28
4	3-C	335	ILE	CA-C-N	6.58	130.69	120.75
4	3-C	335	ILE	C-N-CA	6.58	130.69	120.75
7	3-G	494	ALA	CA-C-N	6.58	129.10	120.28
7	3-G	494	ALA	C-N-CA	6.58	129.10	120.28
7	1-K	871	ALA	CA-C-N	6.58	129.09	120.28
7	1-K	871	ALA	C-N-CA	6.58	129.09	120.28
7	2-K	871	ALA	CA-C-N	6.58	129.09	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-K	871	ALA	C-N-CA	6.58	129.09	120.28
7	3-K	871	ALA	CA-C-N	6.58	129.09	120.28
7	3-K	871	ALA	C-N-CA	6.58	129.09	120.28
3	1-B	863	GLU	CA-C-N	6.58	129.09	120.28
3	1-B	863	GLU	C-N-CA	6.58	129.09	120.28
3	2-B	863	GLU	CA-C-N	6.58	129.09	120.28
3	2-B	863	GLU	C-N-CA	6.58	129.09	120.28
3	3-B	863	GLU	CA-C-N	6.58	129.09	120.28
3	3-B	863	GLU	C-N-CA	6.58	129.09	120.28
4	1-H	426	PRO	N-CA-C	-6.57	102.02	111.22
4	2-H	426	PRO	N-CA-C	-6.57	102.02	111.22
4	3-H	426	PRO	N-CA-C	-6.57	102.02	111.22
4	1-C	640	ASP	O-C-N	-6.57	117.25	121.85
7	1-G	756	LEU	N-CA-C	-6.57	98.69	109.40
4	2-C	640	ASP	O-C-N	-6.57	117.25	121.85
7	2-G	756	LEU	N-CA-C	-6.57	98.69	109.40
4	3-C	640	ASP	O-C-N	-6.57	117.25	121.85
7	3-G	756	LEU	N-CA-C	-6.57	98.69	109.40
4	1-C	708	ASN	CA-C-N	6.57	129.08	120.28
4	1-C	708	ASN	C-N-CA	6.57	129.08	120.28
7	1-K	168	LYS	N-CA-C	-6.57	103.81	110.97
4	2-C	708	ASN	CA-C-N	6.57	129.08	120.28
4	2-C	708	ASN	C-N-CA	6.57	129.08	120.28
7	2-K	168	LYS	N-CA-C	-6.57	103.81	110.97
4	3-C	708	ASN	CA-C-N	6.57	129.08	120.28
4	3-C	708	ASN	C-N-CA	6.57	129.08	120.28
7	3-K	168	LYS	N-CA-C	-6.57	103.81	110.97
4	1-C	736	GLY	N-CA-C	-6.57	97.61	113.18
7	1-K	756	LEU	N-CA-C	-6.57	98.69	109.40
4	2-C	736	GLY	N-CA-C	-6.57	97.61	113.18
7	2-K	756	LEU	N-CA-C	-6.57	98.69	109.40
4	3-C	736	GLY	N-CA-C	-6.57	97.61	113.18
7	3-K	756	LEU	N-CA-C	-6.57	98.69	109.40
3	1-B	753	ASP	CA-C-O	6.56	127.58	120.43
3	2-B	753	ASP	CA-C-O	6.56	127.58	120.43
3	3-B	753	ASP	CA-C-O	6.56	127.58	120.43
7	1-G	263	HIS	CA-C-N	6.56	129.07	120.28
7	1-G	263	HIS	C-N-CA	6.56	129.07	120.28
7	2-G	263	HIS	CA-C-N	6.56	129.07	120.28
7	2-G	263	HIS	C-N-CA	6.56	129.07	120.28
7	3-G	263	HIS	CA-C-N	6.56	129.07	120.28
7	3-G	263	HIS	C-N-CA	6.56	129.07	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	724	LYS	N-CA-C	-6.56	98.29	109.24
6	1-F	82	TYR	N-CA-C	-6.56	98.54	108.96
7	1-G	247	ARG	N-CA-C	-6.56	105.00	112.87
4	2-C	724	LYS	N-CA-C	-6.56	98.29	109.24
6	2-F	82	TYR	N-CA-C	-6.56	98.54	108.96
7	2-G	247	ARG	N-CA-C	-6.56	105.00	112.87
4	3-C	724	LYS	N-CA-C	-6.56	98.29	109.24
6	3-F	82	TYR	N-CA-C	-6.56	98.54	108.96
7	3-G	247	ARG	N-CA-C	-6.56	105.00	112.87
4	1-C	419	LYS	N-CA-C	-6.55	98.29	109.24
5	1-I	83	LEU	CA-C-N	6.55	129.06	120.28
5	1-I	83	LEU	C-N-CA	6.55	129.06	120.28
4	2-C	419	LYS	N-CA-C	-6.55	98.29	109.24
5	2-I	83	LEU	CA-C-N	6.55	129.06	120.28
5	2-I	83	LEU	C-N-CA	6.55	129.06	120.28
4	3-C	419	LYS	N-CA-C	-6.55	98.29	109.24
5	3-I	83	LEU	CA-C-N	6.55	129.06	120.28
5	3-I	83	LEU	C-N-CA	6.55	129.06	120.28
4	1-H	419	LYS	N-CA-C	-6.55	98.30	109.24
4	2-H	419	LYS	N-CA-C	-6.55	98.30	109.24
4	3-H	419	LYS	N-CA-C	-6.55	98.30	109.24
4	1-C	802	LYS	N-CA-C	6.55	124.75	110.80
4	2-C	802	LYS	N-CA-C	6.55	124.75	110.80
4	3-C	802	LYS	N-CA-C	6.55	124.75	110.80
4	1-C	411	ILE	N-CA-C	-6.55	95.72	109.34
4	2-C	411	ILE	N-CA-C	-6.55	95.72	109.34
4	3-C	411	ILE	N-CA-C	-6.55	95.72	109.34
4	1-H	697	GLY	N-CA-C	6.54	120.09	112.50
4	2-H	697	GLY	N-CA-C	6.54	120.09	112.50
4	3-H	697	GLY	N-CA-C	6.54	120.09	112.50
6	1-J	82	TYR	N-CA-C	-6.54	98.56	108.96
6	2-J	82	TYR	N-CA-C	-6.54	98.56	108.96
6	3-J	82	TYR	N-CA-C	-6.54	98.56	108.96
7	1-G	318	HIS	N-CA-C	6.54	121.64	112.75
4	1-H	640	ASP	O-C-N	-6.54	117.27	121.85
7	2-G	318	HIS	N-CA-C	6.54	121.64	112.75
4	2-H	640	ASP	O-C-N	-6.54	117.27	121.85
7	3-G	318	HIS	N-CA-C	6.54	121.64	112.75
4	3-H	640	ASP	O-C-N	-6.54	117.27	121.85
4	1-H	335	ILE	CA-C-N	6.54	130.62	120.75
4	1-H	335	ILE	C-N-CA	6.54	130.62	120.75
4	2-H	335	ILE	CA-C-N	6.54	130.62	120.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-H	335	ILE	C-N-CA	6.54	130.62	120.75
4	3-H	335	ILE	CA-C-N	6.54	130.62	120.75
4	3-H	335	ILE	C-N-CA	6.54	130.62	120.75
6	1-R	41	GLU	N-CA-C	-6.54	100.61	110.28
6	2-R	41	GLU	N-CA-C	-6.54	100.61	110.28
6	3-R	41	GLU	N-CA-C	-6.54	100.61	110.28
7	1-K	220	ARG	CA-C-N	6.53	134.02	121.54
7	1-K	220	ARG	C-N-CA	6.53	134.02	121.54
7	2-K	220	ARG	CA-C-N	6.53	134.02	121.54
7	2-K	220	ARG	C-N-CA	6.53	134.02	121.54
7	3-K	220	ARG	CA-C-N	6.53	134.02	121.54
7	3-K	220	ARG	C-N-CA	6.53	134.02	121.54
4	1-C	803	GLU	N-CA-C	6.53	124.71	110.80
7	1-G	217	LYS	N-CA-C	-6.53	103.99	112.68
4	2-C	803	GLU	N-CA-C	6.53	124.71	110.80
7	2-G	217	LYS	N-CA-C	-6.53	103.99	112.68
4	3-C	803	GLU	N-CA-C	6.53	124.71	110.80
7	3-G	217	LYS	N-CA-C	-6.53	103.99	112.68
6	1-R	155	ILE	N-CA-C	-6.52	99.04	108.17
6	2-R	155	ILE	N-CA-C	-6.52	99.04	108.17
6	3-R	155	ILE	N-CA-C	-6.52	99.04	108.17
8	1-L	110	GLU	CA-C-N	6.51	129.01	120.28
8	1-L	110	GLU	C-N-CA	6.51	129.01	120.28
8	2-L	110	GLU	CA-C-N	6.51	129.01	120.28
8	2-L	110	GLU	C-N-CA	6.51	129.01	120.28
8	3-L	110	GLU	CA-C-N	6.51	129.01	120.28
8	3-L	110	GLU	C-N-CA	6.51	129.01	120.28
5	1-D	53	SER	N-CA-C	-6.51	104.64	112.58
5	2-D	53	SER	N-CA-C	-6.51	104.64	112.58
5	3-D	53	SER	N-CA-C	-6.51	104.64	112.58
7	1-K	785	LYS	N-CA-C	-6.51	99.41	109.24
7	2-K	785	LYS	N-CA-C	-6.51	99.41	109.24
7	3-K	785	LYS	N-CA-C	-6.51	99.41	109.24
4	1-H	411	ILE	N-CA-C	-6.50	95.81	109.34
4	2-H	411	ILE	N-CA-C	-6.50	95.81	109.34
4	3-H	411	ILE	N-CA-C	-6.50	95.81	109.34
7	1-K	178	VAL	CA-C-O	6.50	127.72	120.64
7	2-K	178	VAL	CA-C-O	6.50	127.72	120.64
7	3-K	178	VAL	CA-C-O	6.50	127.72	120.64
4	1-C	696	TYR	N-CA-C	6.50	118.36	111.28
3	1-N	405	CYS	CA-C-N	6.50	129.64	120.28
3	1-N	405	CYS	C-N-CA	6.50	129.64	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-C	696	TYR	N-CA-C	6.50	118.36	111.28
3	2-N	405	CYS	CA-C-N	6.50	129.64	120.28
3	2-N	405	CYS	C-N-CA	6.50	129.64	120.28
4	3-C	696	TYR	N-CA-C	6.50	118.36	111.28
3	3-N	405	CYS	CA-C-N	6.50	129.64	120.28
3	3-N	405	CYS	C-N-CA	6.50	129.64	120.28
7	1-G	785	LYS	N-CA-C	-6.50	99.43	109.24
7	2-G	785	LYS	N-CA-C	-6.50	99.43	109.24
7	3-G	785	LYS	N-CA-C	-6.50	99.43	109.24
4	1-C	202	LEU	O-C-N	6.49	131.59	123.15
4	2-C	202	LEU	O-C-N	6.49	131.59	123.15
4	3-C	202	LEU	O-C-N	6.49	131.59	123.15
4	1-H	185	GLU	N-CA-C	-6.49	103.98	112.41
4	2-H	185	GLU	N-CA-C	-6.49	103.98	112.41
4	3-H	185	GLU	N-CA-C	-6.49	103.98	112.41
1	1-A	731	GLY	CA-C-N	6.48	131.55	120.72
1	1-A	731	GLY	C-N-CA	6.48	131.55	120.72
1	2-A	731	GLY	CA-C-N	6.48	131.55	120.72
1	2-A	731	GLY	C-N-CA	6.48	131.55	120.72
1	3-A	731	GLY	CA-C-N	6.48	131.55	120.72
1	3-A	731	GLY	C-N-CA	6.48	131.55	120.72
4	1-H	708	ASN	CA-C-N	6.48	128.97	120.28
4	1-H	708	ASN	C-N-CA	6.48	128.97	120.28
4	2-H	708	ASN	CA-C-N	6.48	128.97	120.28
4	2-H	708	ASN	C-N-CA	6.48	128.97	120.28
4	3-H	708	ASN	CA-C-N	6.48	128.97	120.28
4	3-H	708	ASN	C-N-CA	6.48	128.97	120.28
4	1-C	185	GLU	N-CA-C	-6.48	103.99	112.41
4	2-C	185	GLU	N-CA-C	-6.48	103.99	112.41
4	3-C	185	GLU	N-CA-C	-6.48	103.99	112.41
7	1-K	813	CYS	N-CA-C	6.47	124.59	110.80
7	2-K	813	CYS	N-CA-C	6.47	124.59	110.80
7	3-K	813	CYS	N-CA-C	6.47	124.59	110.80
7	1-G	670	ASN	CA-C-N	6.47	129.28	120.54
7	1-G	670	ASN	C-N-CA	6.47	129.28	120.54
7	2-G	670	ASN	CA-C-N	6.47	129.28	120.54
7	2-G	670	ASN	C-N-CA	6.47	129.28	120.54
7	3-G	670	ASN	CA-C-N	6.47	129.28	120.54
7	3-G	670	ASN	C-N-CA	6.47	129.28	120.54
7	1-K	40	ASN	N-CA-C	-6.46	95.53	109.81
7	2-K	40	ASN	N-CA-C	-6.46	95.53	109.81
7	3-K	40	ASN	N-CA-C	-6.46	95.53	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	144	HIS	CA-C-N	6.46	127.92	119.84
1	1-A	144	HIS	C-N-CA	6.46	127.92	119.84
7	1-K	670	ASN	CA-C-N	6.46	129.26	120.54
7	1-K	670	ASN	C-N-CA	6.46	129.26	120.54
1	2-A	144	HIS	CA-C-N	6.46	127.92	119.84
1	2-A	144	HIS	C-N-CA	6.46	127.92	119.84
7	2-K	670	ASN	CA-C-N	6.46	129.26	120.54
7	2-K	670	ASN	C-N-CA	6.46	129.26	120.54
1	3-A	144	HIS	CA-C-N	6.46	127.92	119.84
1	3-A	144	HIS	C-N-CA	6.46	127.92	119.84
7	3-K	670	ASN	CA-C-N	6.46	129.26	120.54
7	3-K	670	ASN	C-N-CA	6.46	129.26	120.54
7	1-K	288	ALA	CA-C-N	6.46	128.70	120.56
7	1-K	288	ALA	C-N-CA	6.46	128.70	120.56
7	2-K	288	ALA	CA-C-N	6.46	128.70	120.56
7	2-K	288	ALA	C-N-CA	6.46	128.70	120.56
7	3-K	288	ALA	CA-C-N	6.46	128.70	120.56
7	3-K	288	ALA	C-N-CA	6.46	128.70	120.56
7	1-G	161	VAL	CA-C-O	6.45	127.47	120.57
6	1-M	22	MET	CA-C-N	-6.45	113.63	122.92
6	1-M	22	MET	C-N-CA	-6.45	113.63	122.92
4	1-H	696	TYR	N-CA-C	6.45	118.31	111.28
7	2-G	161	VAL	CA-C-O	6.45	127.47	120.57
6	2-M	22	MET	CA-C-N	-6.45	113.63	122.92
6	2-M	22	MET	C-N-CA	-6.45	113.63	122.92
4	2-H	696	TYR	N-CA-C	6.45	118.31	111.28
7	3-G	161	VAL	CA-C-O	6.45	127.47	120.57
6	3-M	22	MET	CA-C-N	-6.45	113.63	122.92
6	3-M	22	MET	C-N-CA	-6.45	113.63	122.92
4	3-H	696	TYR	N-CA-C	6.45	118.31	111.28
5	1-I	53	SER	N-CA-C	-6.45	104.71	112.58
5	2-I	53	SER	N-CA-C	-6.45	104.71	112.58
5	3-I	53	SER	N-CA-C	-6.45	104.71	112.58
1	1-A	402	SER	N-CA-C	-6.45	96.87	108.48
4	1-C	602	ASP	CA-C-N	6.45	128.82	120.44
4	1-C	602	ASP	C-N-CA	6.45	128.82	120.44
7	1-G	111	LYS	N-CA-C	-6.45	104.25	111.28
3	1-N	364	SER	N-CA-C	-6.45	102.52	111.81
4	1-H	133	SER	CA-C-O	-6.45	114.53	121.56
4	1-H	588	LEU	N-CA-C	-6.45	97.06	110.80
1	2-A	402	SER	N-CA-C	-6.45	96.87	108.48
4	2-C	602	ASP	CA-C-N	6.45	128.82	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-C	602	ASP	C-N-CA	6.45	128.82	120.44
7	2-G	111	LYS	N-CA-C	-6.45	104.25	111.28
3	2-N	364	SER	N-CA-C	-6.45	102.52	111.81
4	2-H	133	SER	CA-C-O	-6.45	114.53	121.56
4	2-H	588	LEU	N-CA-C	-6.45	97.06	110.80
1	3-A	402	SER	N-CA-C	-6.45	96.87	108.48
4	3-C	602	ASP	CA-C-N	6.45	128.82	120.44
4	3-C	602	ASP	C-N-CA	6.45	128.82	120.44
7	3-G	111	LYS	N-CA-C	-6.45	104.25	111.28
3	3-N	364	SER	N-CA-C	-6.45	102.52	111.81
4	3-H	133	SER	CA-C-O	-6.45	114.53	121.56
4	3-H	588	LEU	N-CA-C	-6.45	97.06	110.80
3	1-B	364	SER	N-CA-C	-6.45	102.53	111.81
3	2-B	364	SER	N-CA-C	-6.45	102.53	111.81
3	3-B	364	SER	N-CA-C	-6.45	102.53	111.81
4	1-C	105	ILE	N-CA-C	-6.44	98.87	108.46
4	2-C	105	ILE	N-CA-C	-6.44	98.87	108.46
4	3-C	105	ILE	N-CA-C	-6.44	98.87	108.46
3	1-B	803	ASN	N-CA-C	-6.44	100.95	110.48
8	1-L	85	GLU	CA-C-N	6.44	133.83	121.54
8	1-L	85	GLU	C-N-CA	6.44	133.83	121.54
3	2-B	803	ASN	N-CA-C	-6.44	100.95	110.48
8	2-L	85	GLU	CA-C-N	6.44	133.83	121.54
8	2-L	85	GLU	C-N-CA	6.44	133.83	121.54
3	3-B	803	ASN	N-CA-C	-6.44	100.95	110.48
8	3-L	85	GLU	CA-C-N	6.44	133.83	121.54
8	3-L	85	GLU	C-N-CA	6.44	133.83	121.54
1	1-A	621	VAL	CA-C-N	6.43	134.02	121.41
1	1-A	621	VAL	C-N-CA	6.43	134.02	121.41
1	2-A	621	VAL	CA-C-N	6.43	134.02	121.41
1	2-A	621	VAL	C-N-CA	6.43	134.02	121.41
1	3-A	621	VAL	CA-C-N	6.43	134.02	121.41
1	3-A	621	VAL	C-N-CA	6.43	134.02	121.41
4	1-C	111	GLN	N-CA-C	-6.43	100.61	110.32
4	1-C	615	LYS	CA-C-N	6.43	128.90	120.28
4	1-C	615	LYS	C-N-CA	6.43	128.90	120.28
7	1-K	273	ALA	N-CA-C	6.43	118.37	111.36
4	2-C	111	GLN	N-CA-C	-6.43	100.61	110.32
4	2-C	615	LYS	CA-C-N	6.43	128.90	120.28
4	2-C	615	LYS	C-N-CA	6.43	128.90	120.28
7	2-K	273	ALA	N-CA-C	6.43	118.37	111.36
4	3-C	111	GLN	N-CA-C	-6.43	100.61	110.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	3-C	615	LYS	CA-C-N	6.43	128.90	120.28
4	3-C	615	LYS	C-N-CA	6.43	128.90	120.28
7	3-K	273	ALA	N-CA-C	6.43	118.37	111.36
4	1-C	661	ALA	CA-C-N	6.43	133.54	121.97
4	1-C	661	ALA	C-N-CA	6.43	133.54	121.97
4	2-C	661	ALA	CA-C-N	6.43	133.54	121.97
4	2-C	661	ALA	C-N-CA	6.43	133.54	121.97
4	3-C	661	ALA	CA-C-N	6.43	133.54	121.97
4	3-C	661	ALA	C-N-CA	6.43	133.54	121.97
4	1-H	602	ASP	CA-C-N	6.42	128.79	120.44
4	1-H	602	ASP	C-N-CA	6.42	128.79	120.44
4	2-H	602	ASP	CA-C-N	6.42	128.79	120.44
4	2-H	602	ASP	C-N-CA	6.42	128.79	120.44
4	3-H	602	ASP	CA-C-N	6.42	128.79	120.44
4	3-H	602	ASP	C-N-CA	6.42	128.79	120.44
4	1-C	588	LEU	N-CA-C	-6.42	97.12	110.80
4	2-C	588	LEU	N-CA-C	-6.42	97.12	110.80
4	3-C	588	LEU	N-CA-C	-6.42	97.12	110.80
1	1-A	758	ALA	CA-C-O	-6.42	113.75	120.55
4	1-H	202	LEU	O-C-N	6.42	131.49	123.15
1	2-A	758	ALA	CA-C-O	-6.42	113.75	120.55
4	2-H	202	LEU	O-C-N	6.42	131.49	123.15
1	3-A	758	ALA	CA-C-O	-6.42	113.75	120.55
4	3-H	202	LEU	O-C-N	6.42	131.49	123.15
3	1-B	528	LYS	CA-C-N	6.42	128.88	120.28
3	1-B	528	LYS	C-N-CA	6.42	128.88	120.28
4	1-C	176	SER	O-C-N	-6.42	115.21	121.56
3	2-B	528	LYS	CA-C-N	6.42	128.88	120.28
3	2-B	528	LYS	C-N-CA	6.42	128.88	120.28
4	2-C	176	SER	O-C-N	-6.42	115.21	121.56
3	3-B	528	LYS	CA-C-N	6.42	128.88	120.28
3	3-B	528	LYS	C-N-CA	6.42	128.88	120.28
4	3-C	176	SER	O-C-N	-6.42	115.21	121.56
4	1-C	662	VAL	N-CA-C	-6.41	96.00	109.34
4	2-C	662	VAL	N-CA-C	-6.41	96.00	109.34
4	3-C	662	VAL	N-CA-C	-6.41	96.00	109.34
3	1-B	935	ASP	N-CA-C	6.41	124.45	110.80
3	2-B	935	ASP	N-CA-C	6.41	124.45	110.80
3	3-B	935	ASP	N-CA-C	6.41	124.45	110.80
7	1-K	183	GLU	CA-C-O	6.41	127.21	120.42
7	2-K	183	GLU	CA-C-O	6.41	127.21	120.42
7	3-K	183	GLU	CA-C-O	6.41	127.21	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	732	HIS	CA-C-N	6.41	128.87	120.28
1	1-A	732	HIS	C-N-CA	6.41	128.87	120.28
4	1-H	105	ILE	N-CA-C	-6.41	98.91	108.46
1	2-A	732	HIS	CA-C-N	6.41	128.87	120.28
1	2-A	732	HIS	C-N-CA	6.41	128.87	120.28
4	2-H	105	ILE	N-CA-C	-6.41	98.91	108.46
1	3-A	732	HIS	CA-C-N	6.41	128.87	120.28
1	3-A	732	HIS	C-N-CA	6.41	128.87	120.28
4	3-H	105	ILE	N-CA-C	-6.41	98.91	108.46
1	1-A	629	LEU	N-CA-C	-6.41	104.62	112.88
4	1-H	615	LYS	CA-C-N	6.41	128.86	120.28
4	1-H	615	LYS	C-N-CA	6.41	128.86	120.28
1	2-A	629	LEU	N-CA-C	-6.41	104.62	112.88
4	2-H	615	LYS	CA-C-N	6.41	128.86	120.28
4	2-H	615	LYS	C-N-CA	6.41	128.86	120.28
1	3-A	629	LEU	N-CA-C	-6.41	104.62	112.88
4	3-H	615	LYS	CA-C-N	6.41	128.86	120.28
4	3-H	615	LYS	C-N-CA	6.41	128.86	120.28
3	1-N	528	LYS	CA-C-N	6.40	128.86	120.28
3	1-N	528	LYS	C-N-CA	6.40	128.86	120.28
3	2-N	528	LYS	CA-C-N	6.40	128.86	120.28
3	2-N	528	LYS	C-N-CA	6.40	128.86	120.28
3	3-N	528	LYS	CA-C-N	6.40	128.86	120.28
3	3-N	528	LYS	C-N-CA	6.40	128.86	120.28
4	1-C	133	SER	CA-C-O	-6.40	114.58	121.56
4	1-H	111	GLN	N-CA-C	-6.40	100.65	110.32
4	2-C	133	SER	CA-C-O	-6.40	114.58	121.56
4	2-H	111	GLN	N-CA-C	-6.40	100.65	110.32
4	3-C	133	SER	CA-C-O	-6.40	114.58	121.56
4	3-H	111	GLN	N-CA-C	-6.40	100.65	110.32
1	1-A	424	ASN	N-CA-C	6.40	124.43	110.80
4	1-H	176	SER	O-C-N	-6.40	115.22	121.56
4	1-H	184	HIS	N-CA-C	6.40	118.82	110.43
1	2-A	424	ASN	N-CA-C	6.40	124.43	110.80
4	2-H	176	SER	O-C-N	-6.40	115.22	121.56
4	2-H	184	HIS	N-CA-C	6.40	118.82	110.43
1	3-A	424	ASN	N-CA-C	6.40	124.43	110.80
4	3-H	176	SER	O-C-N	-6.40	115.22	121.56
4	3-H	184	HIS	N-CA-C	6.40	118.82	110.43
8	1-L	141	GLN	CA-C-N	6.39	128.62	120.56
8	1-L	141	GLN	C-N-CA	6.39	128.62	120.56
6	1-M	62	SER	N-CA-C	6.39	119.64	107.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	661	ALA	CA-C-N	6.39	133.48	121.97
4	1-H	661	ALA	C-N-CA	6.39	133.48	121.97
8	2-L	141	GLN	CA-C-N	6.39	128.62	120.56
8	2-L	141	GLN	C-N-CA	6.39	128.62	120.56
6	2-M	62	SER	N-CA-C	6.39	119.64	107.75
4	2-H	661	ALA	CA-C-N	6.39	133.48	121.97
4	2-H	661	ALA	C-N-CA	6.39	133.48	121.97
8	3-L	141	GLN	CA-C-N	6.39	128.62	120.56
8	3-L	141	GLN	C-N-CA	6.39	128.62	120.56
6	3-M	62	SER	N-CA-C	6.39	119.64	107.75
4	3-H	661	ALA	CA-C-N	6.39	133.48	121.97
4	3-H	661	ALA	C-N-CA	6.39	133.48	121.97
4	1-H	662	VAL	N-CA-C	-6.39	96.05	109.34
4	2-H	662	VAL	N-CA-C	-6.39	96.05	109.34
4	3-H	662	VAL	N-CA-C	-6.39	96.05	109.34
3	1-B	849	THR	N-CA-C	6.38	119.11	109.41
3	2-B	849	THR	N-CA-C	6.38	119.11	109.41
3	3-B	849	THR	N-CA-C	6.38	119.11	109.41
6	1-F	32	THR	CA-C-N	6.38	128.83	120.60
6	1-F	32	THR	C-N-CA	6.38	128.83	120.60
6	2-F	32	THR	CA-C-N	6.38	128.83	120.60
6	2-F	32	THR	C-N-CA	6.38	128.83	120.60
6	3-F	32	THR	CA-C-N	6.38	128.83	120.60
6	3-F	32	THR	C-N-CA	6.38	128.83	120.60
1	1-A	400	ALA	CA-C-N	6.38	128.83	120.28
1	1-A	400	ALA	C-N-CA	6.38	128.83	120.28
1	1-A	574	LYS	CA-C-N	6.38	133.91	121.41
1	1-A	574	LYS	C-N-CA	6.38	133.91	121.41
4	1-C	100	ASP	CA-C-N	6.38	133.00	121.97
4	1-C	100	ASP	C-N-CA	6.38	133.00	121.97
1	2-A	400	ALA	CA-C-N	6.38	128.83	120.28
1	2-A	400	ALA	C-N-CA	6.38	128.83	120.28
1	2-A	574	LYS	CA-C-N	6.38	133.91	121.41
1	2-A	574	LYS	C-N-CA	6.38	133.91	121.41
4	2-C	100	ASP	CA-C-N	6.38	133.00	121.97
4	2-C	100	ASP	C-N-CA	6.38	133.00	121.97
1	3-A	400	ALA	CA-C-N	6.38	128.83	120.28
1	3-A	400	ALA	C-N-CA	6.38	128.83	120.28
1	3-A	574	LYS	CA-C-N	6.38	133.91	121.41
1	3-A	574	LYS	C-N-CA	6.38	133.91	121.41
4	3-C	100	ASP	CA-C-N	6.38	133.00	121.97
4	3-C	100	ASP	C-N-CA	6.38	133.00	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	488	LEU	N-CA-C	6.37	119.91	109.85
4	2-H	488	LEU	N-CA-C	6.37	119.91	109.85
4	3-H	488	LEU	N-CA-C	6.37	119.91	109.85
3	1-N	236	ASP	N-CA-C	6.37	118.22	111.28
3	2-N	236	ASP	N-CA-C	6.37	118.22	111.28
3	3-N	236	ASP	N-CA-C	6.37	118.22	111.28
1	1-A	173	SER	N-CA-C	6.37	113.95	108.22
7	1-K	189	ASN	N-CA-C	-6.37	98.61	109.24
1	2-A	173	SER	N-CA-C	6.37	113.95	108.22
7	2-K	189	ASN	N-CA-C	-6.37	98.61	109.24
1	3-A	173	SER	N-CA-C	6.37	113.95	108.22
7	3-K	189	ASN	N-CA-C	-6.37	98.61	109.24
3	1-B	914	SER	CA-C-N	6.36	131.20	120.64
3	1-B	914	SER	C-N-CA	6.36	131.20	120.64
7	1-G	104	ILE	CA-C-O	6.36	127.57	120.95
3	2-B	914	SER	CA-C-N	6.36	131.20	120.64
3	2-B	914	SER	C-N-CA	6.36	131.20	120.64
7	2-G	104	ILE	CA-C-O	6.36	127.57	120.95
3	3-B	914	SER	CA-C-N	6.36	131.20	120.64
3	3-B	914	SER	C-N-CA	6.36	131.20	120.64
7	3-G	104	ILE	CA-C-O	6.36	127.57	120.95
7	1-G	355	SER	CA-C-N	6.36	128.71	120.44
7	1-G	355	SER	C-N-CA	6.36	128.71	120.44
7	2-G	355	SER	CA-C-N	6.36	128.71	120.44
7	2-G	355	SER	C-N-CA	6.36	128.71	120.44
7	3-G	355	SER	CA-C-N	6.36	128.71	120.44
7	3-G	355	SER	C-N-CA	6.36	128.71	120.44
1	1-A	611	VAL	CA-C-N	6.36	128.80	120.28
1	1-A	611	VAL	C-N-CA	6.36	128.80	120.28
4	1-H	100	ASP	CA-C-N	6.36	132.97	121.97
4	1-H	100	ASP	C-N-CA	6.36	132.97	121.97
1	2-A	611	VAL	CA-C-N	6.36	128.80	120.28
1	2-A	611	VAL	C-N-CA	6.36	128.80	120.28
4	2-H	100	ASP	CA-C-N	6.36	132.97	121.97
4	2-H	100	ASP	C-N-CA	6.36	132.97	121.97
1	3-A	611	VAL	CA-C-N	6.36	128.80	120.28
1	3-A	611	VAL	C-N-CA	6.36	128.80	120.28
4	3-H	100	ASP	CA-C-N	6.36	132.97	121.97
4	3-H	100	ASP	C-N-CA	6.36	132.97	121.97
4	1-C	524	VAL	CA-C-N	-6.35	111.80	120.44
4	1-C	524	VAL	C-N-CA	-6.35	111.80	120.44
4	2-C	524	VAL	CA-C-N	-6.35	111.80	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-C	524	VAL	C-N-CA	-6.35	111.80	120.44
4	3-C	524	VAL	CA-C-N	-6.35	111.80	120.44
4	3-C	524	VAL	C-N-CA	-6.35	111.80	120.44
4	1-C	488	LEU	N-CA-C	6.35	119.88	109.85
4	2-C	488	LEU	N-CA-C	6.35	119.88	109.85
4	3-C	488	LEU	N-CA-C	6.35	119.88	109.85
4	1-C	184	HIS	N-CA-C	6.35	118.75	110.43
4	2-C	184	HIS	N-CA-C	6.35	118.75	110.43
4	3-C	184	HIS	N-CA-C	6.35	118.75	110.43
7	1-G	811	HIS	CA-C-N	6.35	126.11	119.76
7	1-G	811	HIS	C-N-CA	6.35	126.11	119.76
4	1-H	524	VAL	CA-C-N	-6.35	111.81	120.44
4	1-H	524	VAL	C-N-CA	-6.35	111.81	120.44
7	2-G	811	HIS	CA-C-N	6.35	126.11	119.76
7	2-G	811	HIS	C-N-CA	6.35	126.11	119.76
4	2-H	524	VAL	CA-C-N	-6.35	111.81	120.44
4	2-H	524	VAL	C-N-CA	-6.35	111.81	120.44
7	3-G	811	HIS	CA-C-N	6.35	126.11	119.76
7	3-G	811	HIS	C-N-CA	6.35	126.11	119.76
4	3-H	524	VAL	CA-C-N	-6.35	111.81	120.44
4	3-H	524	VAL	C-N-CA	-6.35	111.81	120.44
1	1-A	677	LEU	N-CA-C	6.34	118.27	111.36
6	1-J	32	THR	CA-C-N	6.34	128.78	120.60
6	1-J	32	THR	C-N-CA	6.34	128.78	120.60
1	2-A	677	LEU	N-CA-C	6.34	118.27	111.36
6	2-J	32	THR	CA-C-N	6.34	128.78	120.60
6	2-J	32	THR	C-N-CA	6.34	128.78	120.60
1	3-A	677	LEU	N-CA-C	6.34	118.27	111.36
6	3-J	32	THR	CA-C-N	6.34	128.78	120.60
6	3-J	32	THR	C-N-CA	6.34	128.78	120.60
3	1-N	557	LEU	N-CA-C	-6.34	104.37	111.28
3	2-N	557	LEU	N-CA-C	-6.34	104.37	111.28
3	3-N	557	LEU	N-CA-C	-6.34	104.37	111.28
5	1-D	123	GLU	N-CA-C	6.33	117.98	111.14
5	2-D	123	GLU	N-CA-C	6.33	117.98	111.14
5	3-D	123	GLU	N-CA-C	6.33	117.98	111.14
3	1-B	64	ILE	CA-C-N	6.33	128.76	120.28
3	1-B	64	ILE	C-N-CA	6.33	128.76	120.28
3	2-B	64	ILE	CA-C-N	6.33	128.76	120.28
3	2-B	64	ILE	C-N-CA	6.33	128.76	120.28
3	3-B	64	ILE	CA-C-N	6.33	128.76	120.28
3	3-B	64	ILE	C-N-CA	6.33	128.76	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	20	LYS	N-CA-C	-6.33	106.19	114.04
4	1-H	151	ASN	CA-C-O	-6.33	114.59	119.46
1	2-A	20	LYS	N-CA-C	-6.33	106.19	114.04
4	2-H	151	ASN	CA-C-O	-6.33	114.59	119.46
1	3-A	20	LYS	N-CA-C	-6.33	106.19	114.04
4	3-H	151	ASN	CA-C-O	-6.33	114.59	119.46
1	1-A	116	THR	CA-C-N	6.33	131.78	122.99
1	1-A	116	THR	C-N-CA	6.33	131.78	122.99
1	2-A	116	THR	CA-C-N	6.33	131.78	122.99
1	2-A	116	THR	C-N-CA	6.33	131.78	122.99
1	3-A	116	THR	CA-C-N	6.33	131.78	122.99
1	3-A	116	THR	C-N-CA	6.33	131.78	122.99
7	1-K	811	HIS	CA-C-N	6.32	126.08	119.76
7	1-K	811	HIS	C-N-CA	6.32	126.08	119.76
7	2-K	811	HIS	CA-C-N	6.32	126.08	119.76
7	2-K	811	HIS	C-N-CA	6.32	126.08	119.76
7	3-K	811	HIS	CA-C-N	6.32	126.08	119.76
7	3-K	811	HIS	C-N-CA	6.32	126.08	119.76
3	1-N	64	ILE	CA-C-N	6.32	128.75	120.28
3	1-N	64	ILE	C-N-CA	6.32	128.75	120.28
5	1-I	54	VAL	CA-C-N	6.32	130.46	121.42
5	1-I	54	VAL	C-N-CA	6.32	130.46	121.42
3	2-N	64	ILE	CA-C-N	6.32	128.75	120.28
3	2-N	64	ILE	C-N-CA	6.32	128.75	120.28
5	2-I	54	VAL	CA-C-N	6.32	130.46	121.42
5	2-I	54	VAL	C-N-CA	6.32	130.46	121.42
3	3-N	64	ILE	CA-C-N	6.32	128.75	120.28
3	3-N	64	ILE	C-N-CA	6.32	128.75	120.28
5	3-I	54	VAL	CA-C-N	6.32	130.46	121.42
5	3-I	54	VAL	C-N-CA	6.32	130.46	121.42
4	1-H	43	ASN	CA-C-N	6.32	129.38	120.28
4	1-H	43	ASN	C-N-CA	6.32	129.38	120.28
4	2-H	43	ASN	CA-C-N	6.32	129.38	120.28
4	2-H	43	ASN	C-N-CA	6.32	129.38	120.28
4	3-H	43	ASN	CA-C-N	6.32	129.38	120.28
4	3-H	43	ASN	C-N-CA	6.32	129.38	120.28
4	1-C	629	GLY	N-CA-C	-6.32	105.97	115.32
4	2-C	629	GLY	N-CA-C	-6.32	105.97	115.32
4	3-C	629	GLY	N-CA-C	-6.32	105.97	115.32
1	1-A	487	LYS	O-C-N	6.31	130.41	123.22
7	1-G	484	HIS	CA-C-N	6.31	128.64	120.44
7	1-G	484	HIS	C-N-CA	6.31	128.64	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	367	VAL	CA-C-N	-6.31	114.88	123.14
4	1-H	367	VAL	C-N-CA	-6.31	114.88	123.14
4	1-H	414	ILE	CA-C-O	-6.31	113.60	120.67
1	2-A	487	LYS	O-C-N	6.31	130.41	123.22
7	2-G	484	HIS	CA-C-N	6.31	128.64	120.44
7	2-G	484	HIS	C-N-CA	6.31	128.64	120.44
4	2-H	367	VAL	CA-C-N	-6.31	114.88	123.14
4	2-H	367	VAL	C-N-CA	-6.31	114.88	123.14
4	2-H	414	ILE	CA-C-O	-6.31	113.60	120.67
1	3-A	487	LYS	O-C-N	6.31	130.41	123.22
7	3-G	484	HIS	CA-C-N	6.31	128.64	120.44
7	3-G	484	HIS	C-N-CA	6.31	128.64	120.44
4	3-H	367	VAL	CA-C-N	-6.31	114.88	123.14
4	3-H	367	VAL	C-N-CA	-6.31	114.88	123.14
4	3-H	414	ILE	CA-C-O	-6.31	113.60	120.67
3	1-B	896	GLU	N-CA-C	-6.31	98.10	108.76
4	1-C	414	ILE	CA-C-O	-6.31	113.61	120.67
7	1-K	156	SER	N-CA-C	-6.31	104.41	111.28
3	2-B	896	GLU	N-CA-C	-6.31	98.10	108.76
4	2-C	414	ILE	CA-C-O	-6.31	113.61	120.67
7	2-K	156	SER	N-CA-C	-6.31	104.41	111.28
3	3-B	896	GLU	N-CA-C	-6.31	98.10	108.76
4	3-C	414	ILE	CA-C-O	-6.31	113.61	120.67
7	3-K	156	SER	N-CA-C	-6.31	104.41	111.28
7	1-G	509	ILE	CA-C-N	6.31	128.64	120.44
7	1-G	509	ILE	C-N-CA	6.31	128.64	120.44
7	2-G	509	ILE	CA-C-N	6.31	128.64	120.44
7	2-G	509	ILE	C-N-CA	6.31	128.64	120.44
7	3-G	509	ILE	CA-C-N	6.31	128.64	120.44
7	3-G	509	ILE	C-N-CA	6.31	128.64	120.44
7	1-G	537	GLN	CA-C-O	-6.30	113.74	120.42
4	1-H	504	GLY	N-CA-C	6.30	128.12	113.18
7	2-G	537	GLN	CA-C-O	-6.30	113.74	120.42
4	2-H	504	GLY	N-CA-C	6.30	128.12	113.18
7	3-G	537	GLN	CA-C-O	-6.30	113.74	120.42
4	3-H	504	GLY	N-CA-C	6.30	128.12	113.18
7	1-G	130	GLN	N-CA-C	-6.30	104.49	111.36
7	2-G	130	GLN	N-CA-C	-6.30	104.49	111.36
7	3-G	130	GLN	N-CA-C	-6.30	104.49	111.36
4	1-H	629	GLY	N-CA-C	-6.30	106.00	115.32
4	2-H	629	GLY	N-CA-C	-6.30	106.00	115.32
4	3-H	629	GLY	N-CA-C	-6.30	106.00	115.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-K	222	GLY	N-CA-C	-6.30	98.26	113.18
7	2-K	222	GLY	N-CA-C	-6.30	98.26	113.18
7	3-K	222	GLY	N-CA-C	-6.30	98.26	113.18
1	1-A	604	ILE	N-CA-C	-6.29	104.36	110.72
3	1-B	557	LEU	N-CA-C	-6.29	104.42	111.28
5	1-D	54	VAL	CA-C-N	6.29	130.42	121.42
5	1-D	54	VAL	C-N-CA	6.29	130.42	121.42
1	2-A	604	ILE	N-CA-C	-6.29	104.36	110.72
3	2-B	557	LEU	N-CA-C	-6.29	104.42	111.28
5	2-D	54	VAL	CA-C-N	6.29	130.42	121.42
5	2-D	54	VAL	C-N-CA	6.29	130.42	121.42
1	3-A	604	ILE	N-CA-C	-6.29	104.36	110.72
3	3-B	557	LEU	N-CA-C	-6.29	104.42	111.28
5	3-D	54	VAL	CA-C-N	6.29	130.42	121.42
5	3-D	54	VAL	C-N-CA	6.29	130.42	121.42
3	1-B	236	ASP	N-CA-C	6.29	118.13	111.28
4	1-C	153	LYS	N-CA-C	-6.29	104.34	111.07
3	2-B	236	ASP	N-CA-C	6.29	118.13	111.28
4	2-C	153	LYS	N-CA-C	-6.29	104.34	111.07
3	3-B	236	ASP	N-CA-C	6.29	118.13	111.28
4	3-C	153	LYS	N-CA-C	-6.29	104.34	111.07
4	1-C	43	ASN	CA-C-N	6.29	129.33	120.28
4	1-C	43	ASN	C-N-CA	6.29	129.33	120.28
4	2-C	43	ASN	CA-C-N	6.29	129.33	120.28
4	2-C	43	ASN	C-N-CA	6.29	129.33	120.28
4	3-C	43	ASN	CA-C-N	6.29	129.33	120.28
4	3-C	43	ASN	C-N-CA	6.29	129.33	120.28
1	1-A	80	TYR	N-CA-C	-6.28	104.06	111.03
8	1-Z	141	GLN	CA-C-N	6.28	128.48	120.56
8	1-Z	141	GLN	C-N-CA	6.28	128.48	120.56
7	1-K	292	LEU	N-CA-C	6.28	118.93	111.33
1	2-A	80	TYR	N-CA-C	-6.28	104.06	111.03
8	2-Z	141	GLN	CA-C-N	6.28	128.48	120.56
8	2-Z	141	GLN	C-N-CA	6.28	128.48	120.56
7	2-K	292	LEU	N-CA-C	6.28	118.93	111.33
1	3-A	80	TYR	N-CA-C	-6.28	104.06	111.03
8	3-Z	141	GLN	CA-C-N	6.28	128.48	120.56
8	3-Z	141	GLN	C-N-CA	6.28	128.48	120.56
7	3-K	292	LEU	N-CA-C	6.28	118.93	111.33
1	1-A	804	LEU	CA-C-N	6.28	133.54	121.54
1	1-A	804	LEU	C-N-CA	6.28	133.54	121.54
1	2-A	804	LEU	CA-C-N	6.28	133.54	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	804	LEU	C-N-CA	6.28	133.54	121.54
1	3-A	804	LEU	CA-C-N	6.28	133.54	121.54
1	3-A	804	LEU	C-N-CA	6.28	133.54	121.54
1	1-A	519	ASP	CA-C-N	-6.28	114.07	122.42
1	1-A	519	ASP	C-N-CA	-6.28	114.07	122.42
1	2-A	519	ASP	CA-C-N	-6.28	114.07	122.42
1	2-A	519	ASP	C-N-CA	-6.28	114.07	122.42
1	3-A	519	ASP	CA-C-N	-6.28	114.07	122.42
1	3-A	519	ASP	C-N-CA	-6.28	114.07	122.42
4	1-C	367	VAL	CA-C-N	-6.28	114.92	123.14
4	1-C	367	VAL	C-N-CA	-6.28	114.92	123.14
8	1-L	21	ASN	N-CA-C	-6.28	104.54	111.82
5	1-I	123	GLU	N-CA-C	6.28	117.92	111.14
4	2-C	367	VAL	CA-C-N	-6.28	114.92	123.14
4	2-C	367	VAL	C-N-CA	-6.28	114.92	123.14
8	2-L	21	ASN	N-CA-C	-6.28	104.54	111.82
5	2-I	123	GLU	N-CA-C	6.28	117.92	111.14
4	3-C	367	VAL	CA-C-N	-6.28	114.92	123.14
4	3-C	367	VAL	C-N-CA	-6.28	114.92	123.14
8	3-L	21	ASN	N-CA-C	-6.28	104.54	111.82
5	3-I	123	GLU	N-CA-C	6.28	117.92	111.14
1	1-A	158	THR	CA-C-N	6.27	131.66	122.94
1	1-A	158	THR	C-N-CA	6.27	131.66	122.94
1	2-A	158	THR	CA-C-N	6.27	131.66	122.94
1	2-A	158	THR	C-N-CA	6.27	131.66	122.94
1	3-A	158	THR	CA-C-N	6.27	131.66	122.94
1	3-A	158	THR	C-N-CA	6.27	131.66	122.94
1	1-A	578	VAL	CA-C-O	-6.27	114.52	121.23
1	2-A	578	VAL	CA-C-O	-6.27	114.52	121.23
1	3-A	578	VAL	CA-C-O	-6.27	114.52	121.23
7	1-G	279	GLY	N-CA-C	-6.26	103.13	114.46
3	1-N	110	LEU	N-CA-C	-6.26	104.56	111.82
3	1-N	532	GLU	N-CA-C	6.26	117.77	111.07
7	2-G	279	GLY	N-CA-C	-6.26	103.13	114.46
3	2-N	110	LEU	N-CA-C	-6.26	104.56	111.82
3	2-N	532	GLU	N-CA-C	6.26	117.77	111.07
7	3-G	279	GLY	N-CA-C	-6.26	103.13	114.46
3	3-N	110	LEU	N-CA-C	-6.26	104.56	111.82
3	3-N	532	GLU	N-CA-C	6.26	117.77	111.07
4	1-C	164	ASP	N-CA-C	-6.26	105.63	113.20
4	2-C	164	ASP	N-CA-C	-6.26	105.63	113.20
4	3-C	164	ASP	N-CA-C	-6.26	105.63	113.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-B	894	THR	CA-C-N	6.26	127.48	120.66
3	1-B	894	THR	C-N-CA	6.26	127.48	120.66
4	1-C	504	GLY	N-CA-C	6.26	128.01	113.18
4	1-C	567	ILE	CA-C-O	6.26	124.01	119.25
3	2-B	894	THR	CA-C-N	6.26	127.48	120.66
3	2-B	894	THR	C-N-CA	6.26	127.48	120.66
4	2-C	504	GLY	N-CA-C	6.26	128.01	113.18
4	2-C	567	ILE	CA-C-O	6.26	124.01	119.25
3	3-B	894	THR	CA-C-N	6.26	127.48	120.66
3	3-B	894	THR	C-N-CA	6.26	127.48	120.66
4	3-C	504	GLY	N-CA-C	6.26	128.01	113.18
4	3-C	567	ILE	CA-C-O	6.26	124.01	119.25
4	1-C	835	VAL	CA-C-N	6.25	128.57	120.44
4	1-C	835	VAL	C-N-CA	6.25	128.57	120.44
4	2-C	835	VAL	CA-C-N	6.25	128.57	120.44
4	2-C	835	VAL	C-N-CA	6.25	128.57	120.44
4	3-C	835	VAL	CA-C-N	6.25	128.57	120.44
4	3-C	835	VAL	C-N-CA	6.25	128.57	120.44
4	1-H	569	LYS	N-CA-C	-6.25	104.38	111.07
4	2-H	569	LYS	N-CA-C	-6.25	104.38	111.07
4	3-H	569	LYS	N-CA-C	-6.25	104.38	111.07
8	1-Z	141	GLN	N-CA-C	-6.25	104.38	111.07
8	2-Z	141	GLN	N-CA-C	-6.25	104.38	111.07
8	3-Z	141	GLN	N-CA-C	-6.25	104.38	111.07
3	1-B	110	LEU	N-CA-C	-6.25	104.57	111.82
3	1-B	842	MET	CA-C-N	6.25	128.56	120.44
3	1-B	842	MET	C-N-CA	6.25	128.56	120.44
3	2-B	110	LEU	N-CA-C	-6.25	104.57	111.82
3	2-B	842	MET	CA-C-N	6.25	128.56	120.44
3	2-B	842	MET	C-N-CA	6.25	128.56	120.44
3	3-B	110	LEU	N-CA-C	-6.25	104.57	111.82
3	3-B	842	MET	CA-C-N	6.25	128.56	120.44
3	3-B	842	MET	C-N-CA	6.25	128.56	120.44
7	1-K	871	ALA	N-CA-C	6.25	117.89	111.14
7	2-K	871	ALA	N-CA-C	6.25	117.89	111.14
7	3-K	871	ALA	N-CA-C	6.25	117.89	111.14
6	1-M	48	THR	CA-C-O	6.24	128.17	121.55
6	2-M	48	THR	CA-C-O	6.24	128.17	121.55
6	3-M	48	THR	CA-C-O	6.24	128.17	121.55
1	1-A	800	PRO	CA-C-N	6.24	133.20	121.97
1	1-A	800	PRO	C-N-CA	6.24	133.20	121.97
4	1-C	151	ASN	CA-C-O	-6.24	114.66	119.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	800	PRO	CA-C-N	6.24	133.20	121.97
1	2-A	800	PRO	C-N-CA	6.24	133.20	121.97
4	2-C	151	ASN	CA-C-O	-6.24	114.66	119.46
1	3-A	800	PRO	CA-C-N	6.24	133.20	121.97
1	3-A	800	PRO	C-N-CA	6.24	133.20	121.97
4	3-C	151	ASN	CA-C-O	-6.24	114.66	119.46
6	1-M	68	VAL	N-CA-C	6.24	117.10	107.99
4	1-H	153	LYS	N-CA-C	-6.24	104.39	111.07
6	2-M	68	VAL	N-CA-C	6.24	117.10	107.99
4	2-H	153	LYS	N-CA-C	-6.24	104.39	111.07
6	3-M	68	VAL	N-CA-C	6.24	117.10	107.99
4	3-H	153	LYS	N-CA-C	-6.24	104.39	111.07
1	1-A	42	THR	CA-C-N	6.23	129.67	120.95
1	1-A	42	THR	C-N-CA	6.23	129.67	120.95
3	1-B	532	GLU	N-CA-C	6.23	117.73	111.07
7	1-K	750	GLU	N-CA-C	-6.23	99.58	109.23
1	2-A	42	THR	CA-C-N	6.23	129.67	120.95
1	2-A	42	THR	C-N-CA	6.23	129.67	120.95
3	2-B	532	GLU	N-CA-C	6.23	117.73	111.07
7	2-K	750	GLU	N-CA-C	-6.23	99.58	109.23
1	3-A	42	THR	CA-C-N	6.23	129.67	120.95
1	3-A	42	THR	C-N-CA	6.23	129.67	120.95
3	3-B	532	GLU	N-CA-C	6.23	117.73	111.07
7	3-K	750	GLU	N-CA-C	-6.23	99.58	109.23
1	1-A	297	LEU	N-CA-C	-6.23	99.84	109.24
1	2-A	297	LEU	N-CA-C	-6.23	99.84	109.24
1	3-A	297	LEU	N-CA-C	-6.23	99.84	109.24
1	1-A	239	ALA	CA-C-N	6.22	133.42	121.54
1	1-A	239	ALA	C-N-CA	6.22	133.42	121.54
7	1-G	226	PRO	CA-C-N	6.22	128.53	120.44
7	1-G	226	PRO	C-N-CA	6.22	128.53	120.44
1	2-A	239	ALA	CA-C-N	6.22	133.42	121.54
1	2-A	239	ALA	C-N-CA	6.22	133.42	121.54
7	2-G	226	PRO	CA-C-N	6.22	128.53	120.44
7	2-G	226	PRO	C-N-CA	6.22	128.53	120.44
1	3-A	239	ALA	CA-C-N	6.22	133.42	121.54
1	3-A	239	ALA	C-N-CA	6.22	133.42	121.54
7	3-G	226	PRO	CA-C-N	6.22	128.53	120.44
7	3-G	226	PRO	C-N-CA	6.22	128.53	120.44
3	1-B	743	ALA	N-CA-C	-6.22	98.85	109.24
3	2-B	743	ALA	N-CA-C	-6.22	98.85	109.24
3	3-B	743	ALA	N-CA-C	-6.22	98.85	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	569	LYS	N-CA-C	-6.21	104.42	111.07
4	2-C	569	LYS	N-CA-C	-6.21	104.42	111.07
4	3-C	569	LYS	N-CA-C	-6.21	104.42	111.07
3	1-B	262	ARG	N-CA-C	-6.21	104.42	111.07
4	1-H	164	ASP	N-CA-C	-6.21	105.69	113.20
3	2-B	262	ARG	N-CA-C	-6.21	104.42	111.07
4	2-H	164	ASP	N-CA-C	-6.21	105.69	113.20
3	3-B	262	ARG	N-CA-C	-6.21	104.42	111.07
4	3-H	164	ASP	N-CA-C	-6.21	105.69	113.20
8	1-L	38	VAL	CA-C-N	6.21	128.51	120.44
8	1-L	38	VAL	C-N-CA	6.21	128.51	120.44
8	2-L	38	VAL	CA-C-N	6.21	128.51	120.44
8	2-L	38	VAL	C-N-CA	6.21	128.51	120.44
8	3-L	38	VAL	CA-C-N	6.21	128.51	120.44
8	3-L	38	VAL	C-N-CA	6.21	128.51	120.44
7	1-G	871	ALA	N-CA-C	6.20	117.84	111.14
7	2-G	871	ALA	N-CA-C	6.20	117.84	111.14
7	3-G	871	ALA	N-CA-C	6.20	117.84	111.14
3	1-B	460	VAL	CA-C-N	6.20	128.50	120.44
3	1-B	460	VAL	C-N-CA	6.20	128.50	120.44
3	2-B	460	VAL	CA-C-N	6.20	128.50	120.44
3	2-B	460	VAL	C-N-CA	6.20	128.50	120.44
3	3-B	460	VAL	CA-C-N	6.20	128.50	120.44
3	3-B	460	VAL	C-N-CA	6.20	128.50	120.44
7	1-K	169	CYS	N-CA-C	-6.20	104.44	111.07
7	2-K	169	CYS	N-CA-C	-6.20	104.44	111.07
7	3-K	169	CYS	N-CA-C	-6.20	104.44	111.07
6	1-R	52	ASN	N-CA-C	6.20	118.39	107.61
6	2-R	52	ASN	N-CA-C	6.20	118.39	107.61
6	3-R	52	ASN	N-CA-C	6.20	118.39	107.61
4	1-H	602	ASP	N-CA-C	-6.20	100.23	109.83
4	2-H	602	ASP	N-CA-C	-6.20	100.23	109.83
4	3-H	602	ASP	N-CA-C	-6.20	100.23	109.83
7	1-K	308	VAL	CA-C-N	-6.19	114.26	122.99
7	1-K	308	VAL	C-N-CA	-6.19	114.26	122.99
7	1-K	624	GLN	N-CA-C	-6.19	100.23	109.83
7	2-K	308	VAL	CA-C-N	-6.19	114.26	122.99
7	2-K	308	VAL	C-N-CA	-6.19	114.26	122.99
7	2-K	624	GLN	N-CA-C	-6.19	100.23	109.83
7	3-K	308	VAL	CA-C-N	-6.19	114.26	122.99
7	3-K	308	VAL	C-N-CA	-6.19	114.26	122.99
7	3-K	624	GLN	N-CA-C	-6.19	100.23	109.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	718	GLY	CA-C-N	6.19	128.58	120.28
4	1-H	718	GLY	C-N-CA	6.19	128.58	120.28
4	2-H	718	GLY	CA-C-N	6.19	128.58	120.28
4	2-H	718	GLY	C-N-CA	6.19	128.58	120.28
4	3-H	718	GLY	CA-C-N	6.19	128.58	120.28
4	3-H	718	GLY	C-N-CA	6.19	128.58	120.28
1	1-A	249	TYR	CA-C-N	6.19	133.35	121.54
1	1-A	249	TYR	C-N-CA	6.19	133.35	121.54
8	1-L	115	LEU	CA-C-N	6.19	128.57	120.28
8	1-L	115	LEU	C-N-CA	6.19	128.57	120.28
1	2-A	249	TYR	CA-C-N	6.19	133.35	121.54
1	2-A	249	TYR	C-N-CA	6.19	133.35	121.54
8	2-L	115	LEU	CA-C-N	6.19	128.57	120.28
8	2-L	115	LEU	C-N-CA	6.19	128.57	120.28
1	3-A	249	TYR	CA-C-N	6.19	133.35	121.54
1	3-A	249	TYR	C-N-CA	6.19	133.35	121.54
8	3-L	115	LEU	CA-C-N	6.19	128.57	120.28
8	3-L	115	LEU	C-N-CA	6.19	128.57	120.28
1	1-A	662	LEU	CA-C-N	6.18	129.07	120.29
1	1-A	662	LEU	C-N-CA	6.18	129.07	120.29
7	1-G	750	GLU	N-CA-C	-6.18	99.65	109.23
5	1-I	101	GLU	CA-C-N	6.18	128.93	120.46
5	1-I	101	GLU	C-N-CA	6.18	128.93	120.46
1	2-A	662	LEU	CA-C-N	6.18	129.07	120.29
1	2-A	662	LEU	C-N-CA	6.18	129.07	120.29
7	2-G	750	GLU	N-CA-C	-6.18	99.65	109.23
5	2-I	101	GLU	CA-C-N	6.18	128.93	120.46
5	2-I	101	GLU	C-N-CA	6.18	128.93	120.46
1	3-A	662	LEU	CA-C-N	6.18	129.07	120.29
1	3-A	662	LEU	C-N-CA	6.18	129.07	120.29
7	3-G	750	GLU	N-CA-C	-6.18	99.65	109.23
5	3-I	101	GLU	CA-C-N	6.18	128.93	120.46
5	3-I	101	GLU	C-N-CA	6.18	128.93	120.46
8	1-L	38	VAL	N-CA-C	-6.18	104.48	110.72
8	2-L	38	VAL	N-CA-C	-6.18	104.48	110.72
8	3-L	38	VAL	N-CA-C	-6.18	104.48	110.72
3	1-B	321	VAL	N-CA-C	-6.18	104.32	110.62
4	1-C	145	VAL	CA-C-N	6.18	129.06	120.29
4	1-C	145	VAL	C-N-CA	6.18	129.06	120.29
4	1-C	602	ASP	N-CA-C	-6.18	100.25	109.83
7	1-G	369	SER	N-CA-C	6.18	118.82	111.71
3	2-B	321	VAL	N-CA-C	-6.18	104.32	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-C	145	VAL	CA-C-N	6.18	129.06	120.29
4	2-C	145	VAL	C-N-CA	6.18	129.06	120.29
4	2-C	602	ASP	N-CA-C	-6.18	100.25	109.83
7	2-G	369	SER	N-CA-C	6.18	118.82	111.71
3	3-B	321	VAL	N-CA-C	-6.18	104.32	110.62
4	3-C	145	VAL	CA-C-N	6.18	129.06	120.29
4	3-C	145	VAL	C-N-CA	6.18	129.06	120.29
4	3-C	602	ASP	N-CA-C	-6.18	100.25	109.83
7	3-G	369	SER	N-CA-C	6.18	118.82	111.71
3	1-N	321	VAL	N-CA-C	-6.18	104.32	110.62
3	2-N	321	VAL	N-CA-C	-6.18	104.32	110.62
3	3-N	321	VAL	N-CA-C	-6.18	104.32	110.62
1	1-A	438	LYS	N-CA-C	-6.18	98.32	108.76
1	1-A	1189	GLY	N-CA-C	-6.18	106.80	115.32
4	1-C	727	VAL	CA-C-N	6.18	128.56	120.28
4	1-C	727	VAL	C-N-CA	6.18	128.56	120.28
1	2-A	438	LYS	N-CA-C	-6.18	98.32	108.76
1	2-A	1189	GLY	N-CA-C	-6.18	106.80	115.32
4	2-C	727	VAL	CA-C-N	6.18	128.56	120.28
4	2-C	727	VAL	C-N-CA	6.18	128.56	120.28
1	3-A	438	LYS	N-CA-C	-6.18	98.32	108.76
1	3-A	1189	GLY	N-CA-C	-6.18	106.80	115.32
4	3-C	727	VAL	CA-C-N	6.18	128.56	120.28
4	3-C	727	VAL	C-N-CA	6.18	128.56	120.28
4	1-C	718	GLY	CA-C-N	6.17	128.55	120.28
4	1-C	718	GLY	C-N-CA	6.17	128.55	120.28
4	2-C	718	GLY	CA-C-N	6.17	128.55	120.28
4	2-C	718	GLY	C-N-CA	6.17	128.55	120.28
4	3-C	718	GLY	CA-C-N	6.17	128.55	120.28
4	3-C	718	GLY	C-N-CA	6.17	128.55	120.28
3	1-B	412	MET	N-CA-C	6.17	115.58	108.49
3	2-B	412	MET	N-CA-C	6.17	115.58	108.49
3	3-B	412	MET	N-CA-C	6.17	115.58	108.49
4	1-H	145	VAL	CA-C-N	6.17	129.04	120.29
4	1-H	145	VAL	C-N-CA	6.17	129.04	120.29
4	2-H	145	VAL	CA-C-N	6.17	129.04	120.29
4	2-H	145	VAL	C-N-CA	6.17	129.04	120.29
4	3-H	145	VAL	CA-C-N	6.17	129.04	120.29
4	3-H	145	VAL	C-N-CA	6.17	129.04	120.29
7	1-K	746	GLY	CA-C-O	-6.16	115.07	121.91
4	1-H	567	ILE	CA-C-O	6.16	123.93	119.25
7	2-K	746	GLY	CA-C-O	-6.16	115.07	121.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-H	567	ILE	CA-C-O	6.16	123.93	119.25
7	3-K	746	GLY	CA-C-O	-6.16	115.07	121.91
4	3-H	567	ILE	CA-C-O	6.16	123.93	119.25
1	1-A	666	LYS	N-CA-C	-6.16	104.56	111.28
3	1-N	349	LEU	CA-C-N	6.16	128.53	120.28
3	1-N	349	LEU	C-N-CA	6.16	128.53	120.28
1	2-A	666	LYS	N-CA-C	-6.16	104.56	111.28
3	2-N	349	LEU	CA-C-N	6.16	128.53	120.28
3	2-N	349	LEU	C-N-CA	6.16	128.53	120.28
1	3-A	666	LYS	N-CA-C	-6.16	104.56	111.28
3	3-N	349	LEU	CA-C-N	6.16	128.53	120.28
3	3-N	349	LEU	C-N-CA	6.16	128.53	120.28
7	1-K	169	CYS	O-C-N	6.16	128.41	122.07
8	1-L	46	LYS	CA-C-N	-6.16	112.52	120.65
8	1-L	46	LYS	C-N-CA	-6.16	112.52	120.65
3	1-N	412	MET	N-CA-C	6.16	115.57	108.49
7	2-K	169	CYS	O-C-N	6.16	128.41	122.07
8	2-L	46	LYS	CA-C-N	-6.16	112.52	120.65
8	2-L	46	LYS	C-N-CA	-6.16	112.52	120.65
3	2-N	412	MET	N-CA-C	6.16	115.57	108.49
7	3-K	169	CYS	O-C-N	6.16	128.41	122.07
8	3-L	46	LYS	CA-C-N	-6.16	112.52	120.65
8	3-L	46	LYS	C-N-CA	-6.16	112.52	120.65
3	3-N	412	MET	N-CA-C	6.16	115.57	108.49
5	1-D	101	GLU	CA-C-N	6.16	128.90	120.46
5	1-D	101	GLU	C-N-CA	6.16	128.90	120.46
3	1-N	460	VAL	CA-C-N	6.16	128.44	120.44
3	1-N	460	VAL	C-N-CA	6.16	128.44	120.44
5	2-D	101	GLU	CA-C-N	6.16	128.90	120.46
5	2-D	101	GLU	C-N-CA	6.16	128.90	120.46
3	2-N	460	VAL	CA-C-N	6.16	128.44	120.44
3	2-N	460	VAL	C-N-CA	6.16	128.44	120.44
5	3-D	101	GLU	CA-C-N	6.16	128.90	120.46
5	3-D	101	GLU	C-N-CA	6.16	128.90	120.46
3	3-N	460	VAL	CA-C-N	6.16	128.44	120.44
3	3-N	460	VAL	C-N-CA	6.16	128.44	120.44
1	1-A	78	TRP	CA-C-N	6.16	130.87	122.19
1	1-A	78	TRP	C-N-CA	6.16	130.87	122.19
1	2-A	78	TRP	CA-C-N	6.16	130.87	122.19
1	2-A	78	TRP	C-N-CA	6.16	130.87	122.19
1	3-A	78	TRP	CA-C-N	6.16	130.87	122.19
1	3-A	78	TRP	C-N-CA	6.16	130.87	122.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-N	262	ARG	N-CA-C	-6.15	104.48	111.07
4	1-H	572	ARG	N-CA-C	-6.15	99.95	109.24
3	2-N	262	ARG	N-CA-C	-6.15	104.48	111.07
4	2-H	572	ARG	N-CA-C	-6.15	99.95	109.24
3	3-N	262	ARG	N-CA-C	-6.15	104.48	111.07
4	3-H	572	ARG	N-CA-C	-6.15	99.95	109.24
4	1-C	378	TYR	O-C-N	6.15	131.19	123.19
4	2-C	378	TYR	O-C-N	6.15	131.19	123.19
4	3-C	378	TYR	O-C-N	6.15	131.19	123.19
4	1-C	824	TYR	CA-C-O	-6.15	111.74	120.16
3	1-N	433	ALA	CA-C-N	6.15	128.43	120.44
3	1-N	433	ALA	C-N-CA	6.15	128.43	120.44
4	2-C	824	TYR	CA-C-O	-6.15	111.74	120.16
3	2-N	433	ALA	CA-C-N	6.15	128.43	120.44
3	2-N	433	ALA	C-N-CA	6.15	128.43	120.44
4	3-C	824	TYR	CA-C-O	-6.15	111.74	120.16
3	3-N	433	ALA	CA-C-N	6.15	128.43	120.44
3	3-N	433	ALA	C-N-CA	6.15	128.43	120.44
6	1-R	57	GLN	N-CA-C	-6.15	99.19	108.96
6	2-R	57	GLN	N-CA-C	-6.15	99.19	108.96
6	3-R	57	GLN	N-CA-C	-6.15	99.19	108.96
7	1-K	646	TYR	N-CA-C	-6.14	99.71	109.23
7	2-K	646	TYR	N-CA-C	-6.14	99.71	109.23
7	3-K	646	TYR	N-CA-C	-6.14	99.71	109.23
4	1-C	716	ALA	N-CA-C	-6.14	104.58	111.28
7	1-G	624	GLN	N-CA-C	-6.14	100.31	109.83
4	2-C	716	ALA	N-CA-C	-6.14	104.58	111.28
7	2-G	624	GLN	N-CA-C	-6.14	100.31	109.83
4	3-C	716	ALA	N-CA-C	-6.14	104.58	111.28
7	3-G	624	GLN	N-CA-C	-6.14	100.31	109.83
4	1-C	84	PHE	N-CA-C	-6.14	100.00	109.52
4	2-C	84	PHE	N-CA-C	-6.14	100.00	109.52
4	3-C	84	PHE	N-CA-C	-6.14	100.00	109.52
7	1-K	208	ARG	CA-C-O	6.14	127.02	120.70
7	2-K	208	ARG	CA-C-O	6.14	127.02	120.70
7	3-K	208	ARG	CA-C-O	6.14	127.02	120.70
6	1-M	171	GLU	CA-C-N	6.14	128.79	120.38
6	1-M	171	GLU	C-N-CA	6.14	128.79	120.38
3	1-N	49	ASP	CA-C-N	6.14	128.87	120.46
3	1-N	49	ASP	C-N-CA	6.14	128.87	120.46
6	2-M	171	GLU	CA-C-N	6.14	128.79	120.38
6	2-M	171	GLU	C-N-CA	6.14	128.79	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2-N	49	ASP	CA-C-N	6.14	128.87	120.46
3	2-N	49	ASP	C-N-CA	6.14	128.87	120.46
6	3-M	171	GLU	CA-C-N	6.14	128.79	120.38
6	3-M	171	GLU	C-N-CA	6.14	128.79	120.38
3	3-N	49	ASP	CA-C-N	6.14	128.87	120.46
3	3-N	49	ASP	C-N-CA	6.14	128.87	120.46
1	1-A	611	VAL	O-C-N	6.13	128.15	121.83
3	1-B	349	LEU	CA-C-N	6.13	128.50	120.28
3	1-B	349	LEU	C-N-CA	6.13	128.50	120.28
4	1-H	378	TYR	O-C-N	6.13	131.16	123.19
1	2-A	611	VAL	O-C-N	6.13	128.15	121.83
3	2-B	349	LEU	CA-C-N	6.13	128.50	120.28
3	2-B	349	LEU	C-N-CA	6.13	128.50	120.28
4	2-H	378	TYR	O-C-N	6.13	131.16	123.19
1	3-A	611	VAL	O-C-N	6.13	128.15	121.83
3	3-B	349	LEU	CA-C-N	6.13	128.50	120.28
3	3-B	349	LEU	C-N-CA	6.13	128.50	120.28
4	3-H	378	TYR	O-C-N	6.13	131.16	123.19
8	1-Z	19	LEU	N-CA-C	-6.13	99.92	109.72
8	2-Z	19	LEU	N-CA-C	-6.13	99.92	109.72
8	3-Z	19	LEU	N-CA-C	-6.13	99.92	109.72
3	1-B	784	VAL	CA-C-O	-6.12	113.12	120.78
3	2-B	784	VAL	CA-C-O	-6.12	113.12	120.78
3	3-B	784	VAL	CA-C-O	-6.12	113.12	120.78
3	1-B	434	ASP	CA-C-N	6.12	128.28	120.56
3	1-B	434	ASP	C-N-CA	6.12	128.28	120.56
3	2-B	434	ASP	CA-C-N	6.12	128.28	120.56
3	2-B	434	ASP	C-N-CA	6.12	128.28	120.56
3	3-B	434	ASP	CA-C-N	6.12	128.28	120.56
3	3-B	434	ASP	C-N-CA	6.12	128.28	120.56
1	1-A	35	LEU	N-CA-C	-6.12	98.93	108.90
1	1-A	458	TYR	N-CA-C	-6.12	100.22	109.95
1	2-A	35	LEU	N-CA-C	-6.12	98.93	108.90
1	2-A	458	TYR	N-CA-C	-6.12	100.22	109.95
1	3-A	35	LEU	N-CA-C	-6.12	98.93	108.90
1	3-A	458	TYR	N-CA-C	-6.12	100.22	109.95
1	1-A	533	GLY	N-CA-C	-6.12	99.59	111.03
4	1-C	572	ARG	N-CA-C	-6.12	100.00	109.24
8	1-Z	32	ASP	N-CA-C	-6.12	99.93	109.72
4	1-H	84	PHE	N-CA-C	-6.12	100.04	109.52
1	2-A	533	GLY	N-CA-C	-6.12	99.59	111.03
4	2-C	572	ARG	N-CA-C	-6.12	100.00	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2-Z	32	ASP	N-CA-C	-6.12	99.93	109.72
4	2-H	84	PHE	N-CA-C	-6.12	100.04	109.52
1	3-A	533	GLY	N-CA-C	-6.12	99.59	111.03
4	3-C	572	ARG	N-CA-C	-6.12	100.00	109.24
8	3-Z	32	ASP	N-CA-C	-6.12	99.93	109.72
4	3-H	84	PHE	N-CA-C	-6.12	100.04	109.52
3	1-B	49	ASP	CA-C-N	6.12	128.84	120.46
3	1-B	49	ASP	C-N-CA	6.12	128.84	120.46
7	1-G	679	VAL	N-CA-C	6.12	116.68	107.75
3	2-B	49	ASP	CA-C-N	6.12	128.84	120.46
3	2-B	49	ASP	C-N-CA	6.12	128.84	120.46
7	2-G	679	VAL	N-CA-C	6.12	116.68	107.75
3	3-B	49	ASP	CA-C-N	6.12	128.84	120.46
3	3-B	49	ASP	C-N-CA	6.12	128.84	120.46
7	3-G	679	VAL	N-CA-C	6.12	116.68	107.75
3	1-B	433	ALA	CA-C-N	6.11	128.38	120.44
3	1-B	433	ALA	C-N-CA	6.11	128.38	120.44
3	2-B	433	ALA	CA-C-N	6.11	128.38	120.44
3	2-B	433	ALA	C-N-CA	6.11	128.38	120.44
3	3-B	433	ALA	CA-C-N	6.11	128.38	120.44
3	3-B	433	ALA	C-N-CA	6.11	128.38	120.44
4	1-C	626	GLU	N-CA-C	-6.11	104.62	111.28
4	1-H	716	ALA	N-CA-C	-6.11	104.62	111.28
4	2-C	626	GLU	N-CA-C	-6.11	104.62	111.28
4	2-H	716	ALA	N-CA-C	-6.11	104.62	111.28
4	3-C	626	GLU	N-CA-C	-6.11	104.62	111.28
4	3-H	716	ALA	N-CA-C	-6.11	104.62	111.28
5	1-D	55	ARG	N-CA-C	-6.11	100.55	110.20
8	1-Z	18	ILE	N-CA-C	-6.11	98.73	107.77
8	1-L	34	THR	N-CA-C	-6.11	107.66	114.62
5	2-D	55	ARG	N-CA-C	-6.11	100.55	110.20
8	2-Z	18	ILE	N-CA-C	-6.11	98.73	107.77
8	2-L	34	THR	N-CA-C	-6.11	107.66	114.62
5	3-D	55	ARG	N-CA-C	-6.11	100.55	110.20
8	3-Z	18	ILE	N-CA-C	-6.11	98.73	107.77
8	3-L	34	THR	N-CA-C	-6.11	107.66	114.62
3	1-B	258	ALA	N-CA-C	6.10	117.93	111.28
3	2-B	258	ALA	N-CA-C	6.10	117.93	111.28
3	3-B	258	ALA	N-CA-C	6.10	117.93	111.28
8	1-Z	31	TYR	N-CA-C	-6.10	104.55	111.14
8	1-Z	67	VAL	N-CA-C	-6.10	98.85	107.75
8	2-Z	31	TYR	N-CA-C	-6.10	104.55	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2-Z	67	VAL	N-CA-C	-6.10	98.85	107.75
8	3-Z	31	TYR	N-CA-C	-6.10	104.55	111.14
8	3-Z	67	VAL	N-CA-C	-6.10	98.85	107.75
3	1-B	90	LYS	N-CA-C	-6.10	104.71	111.36
7	1-G	746	GLY	CA-C-O	-6.10	115.14	121.91
3	2-B	90	LYS	N-CA-C	-6.10	104.71	111.36
7	2-G	746	GLY	CA-C-O	-6.10	115.14	121.91
3	3-B	90	LYS	N-CA-C	-6.10	104.71	111.36
7	3-G	746	GLY	CA-C-O	-6.10	115.14	121.91
3	1-B	412	MET	CA-C-O	6.10	124.58	120.19
3	2-B	412	MET	CA-C-O	6.10	124.58	120.19
3	3-B	412	MET	CA-C-O	6.10	124.58	120.19
3	1-N	434	ASP	CA-C-N	6.09	128.24	120.56
3	1-N	434	ASP	C-N-CA	6.09	128.24	120.56
5	1-I	55	ARG	N-CA-C	-6.09	100.57	110.20
3	2-N	434	ASP	CA-C-N	6.09	128.24	120.56
3	2-N	434	ASP	C-N-CA	6.09	128.24	120.56
5	2-I	55	ARG	N-CA-C	-6.09	100.57	110.20
3	3-N	434	ASP	CA-C-N	6.09	128.24	120.56
3	3-N	434	ASP	C-N-CA	6.09	128.24	120.56
5	3-I	55	ARG	N-CA-C	-6.09	100.57	110.20
7	1-K	679	VAL	N-CA-C	6.09	116.64	107.75
7	2-K	679	VAL	N-CA-C	6.09	116.64	107.75
7	3-K	679	VAL	N-CA-C	6.09	116.64	107.75
1	1-A	18	HIS	CA-C-N	6.09	125.79	119.82
1	1-A	18	HIS	C-N-CA	6.09	125.79	119.82
3	1-N	258	ALA	N-CA-C	6.09	117.92	111.28
1	2-A	18	HIS	CA-C-N	6.09	125.79	119.82
1	2-A	18	HIS	C-N-CA	6.09	125.79	119.82
3	2-N	258	ALA	N-CA-C	6.09	117.92	111.28
1	3-A	18	HIS	CA-C-N	6.09	125.79	119.82
1	3-A	18	HIS	C-N-CA	6.09	125.79	119.82
3	3-N	258	ALA	N-CA-C	6.09	117.92	111.28
7	1-K	732	VAL	N-CA-C	-6.09	99.65	108.17
7	2-K	732	VAL	N-CA-C	-6.09	99.65	108.17
7	3-K	732	VAL	N-CA-C	-6.09	99.65	108.17
6	1-F	52	ASN	N-CA-C	-6.09	99.48	109.40
7	1-K	261	ASN	N-CA-C	6.09	118.63	110.35
6	2-F	52	ASN	N-CA-C	-6.09	99.48	109.40
7	2-K	261	ASN	N-CA-C	6.09	118.63	110.35
6	3-F	52	ASN	N-CA-C	-6.09	99.48	109.40
7	3-K	261	ASN	N-CA-C	6.09	118.63	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-B	456	LYS	CA-C-N	6.08	128.43	120.28
3	1-B	456	LYS	C-N-CA	6.08	128.43	120.28
3	2-B	456	LYS	CA-C-N	6.08	128.43	120.28
3	2-B	456	LYS	C-N-CA	6.08	128.43	120.28
3	3-B	456	LYS	CA-C-N	6.08	128.43	120.28
3	3-B	456	LYS	C-N-CA	6.08	128.43	120.28
6	1-R	45	THR	N-CA-C	-6.08	106.21	113.21
6	2-R	45	THR	N-CA-C	-6.08	106.21	113.21
6	3-R	45	THR	N-CA-C	-6.08	106.21	113.21
1	1-A	267	ASN	N-CA-C	-6.08	99.44	108.99
7	1-G	732	VAL	N-CA-C	-6.08	99.66	108.17
1	2-A	267	ASN	N-CA-C	-6.08	99.44	108.99
7	2-G	732	VAL	N-CA-C	-6.08	99.66	108.17
1	3-A	267	ASN	N-CA-C	-6.08	99.44	108.99
7	3-G	732	VAL	N-CA-C	-6.08	99.66	108.17
1	1-A	635	PRO	N-CA-C	-6.08	99.95	112.47
4	1-C	738	LEU	CA-C-N	6.08	128.34	120.44
4	1-C	738	LEU	C-N-CA	6.08	128.34	120.44
1	2-A	635	PRO	N-CA-C	-6.08	99.95	112.47
4	2-C	738	LEU	CA-C-N	6.08	128.34	120.44
4	2-C	738	LEU	C-N-CA	6.08	128.34	120.44
1	3-A	635	PRO	N-CA-C	-6.08	99.95	112.47
4	3-C	738	LEU	CA-C-N	6.08	128.34	120.44
4	3-C	738	LEU	C-N-CA	6.08	128.34	120.44
7	1-G	175	LYS	CA-C-N	6.07	129.03	120.28
7	1-G	175	LYS	C-N-CA	6.07	129.03	120.28
7	1-K	782	GLU	N-CA-C	-6.07	104.01	112.45
3	1-N	412	MET	CA-C-O	6.07	124.56	120.19
7	2-G	175	LYS	CA-C-N	6.07	129.03	120.28
7	2-G	175	LYS	C-N-CA	6.07	129.03	120.28
7	2-K	782	GLU	N-CA-C	-6.07	104.01	112.45
3	2-N	412	MET	CA-C-O	6.07	124.56	120.19
7	3-G	175	LYS	CA-C-N	6.07	129.03	120.28
7	3-G	175	LYS	C-N-CA	6.07	129.03	120.28
7	3-K	782	GLU	N-CA-C	-6.07	104.01	112.45
3	3-N	412	MET	CA-C-O	6.07	124.56	120.19
1	1-A	156	ASP	N-CA-C	-6.07	104.38	112.94
5	1-D	62	GLU	CA-C-N	6.07	133.13	121.54
5	1-D	62	GLU	C-N-CA	6.07	133.13	121.54
4	1-H	626	GLU	N-CA-C	-6.07	104.66	111.28
1	2-A	156	ASP	N-CA-C	-6.07	104.38	112.94
5	2-D	62	GLU	CA-C-N	6.07	133.13	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	2-D	62	GLU	C-N-CA	6.07	133.13	121.54
4	2-H	626	GLU	N-CA-C	-6.07	104.66	111.28
1	3-A	156	ASP	N-CA-C	-6.07	104.38	112.94
5	3-D	62	GLU	CA-C-N	6.07	133.13	121.54
5	3-D	62	GLU	C-N-CA	6.07	133.13	121.54
4	3-H	626	GLU	N-CA-C	-6.07	104.66	111.28
4	1-H	278	ALA	N-CA-C	-6.07	99.46	108.99
4	2-H	278	ALA	N-CA-C	-6.07	99.46	108.99
4	3-H	278	ALA	N-CA-C	-6.07	99.46	108.99
4	1-C	361	ASN	N-CA-C	-6.06	101.30	110.39
7	1-G	782	GLU	N-CA-C	-6.06	104.03	112.45
4	2-C	361	ASN	N-CA-C	-6.06	101.30	110.39
7	2-G	782	GLU	N-CA-C	-6.06	104.03	112.45
4	3-C	361	ASN	N-CA-C	-6.06	101.30	110.39
7	3-G	782	GLU	N-CA-C	-6.06	104.03	112.45
1	1-A	30	ASN	N-CA-C	-6.05	105.75	113.01
3	1-B	815	PHE	CA-C-N	6.05	127.26	120.42
3	1-B	815	PHE	C-N-CA	6.05	127.26	120.42
7	1-G	685	GLU	N-CA-C	-6.05	98.41	108.34
8	1-Z	36	PRO	CA-C-N	6.05	133.10	121.54
8	1-Z	36	PRO	C-N-CA	6.05	133.10	121.54
1	2-A	30	ASN	N-CA-C	-6.05	105.75	113.01
3	2-B	815	PHE	CA-C-N	6.05	127.26	120.42
3	2-B	815	PHE	C-N-CA	6.05	127.26	120.42
7	2-G	685	GLU	N-CA-C	-6.05	98.41	108.34
8	2-Z	36	PRO	CA-C-N	6.05	133.10	121.54
8	2-Z	36	PRO	C-N-CA	6.05	133.10	121.54
1	3-A	30	ASN	N-CA-C	-6.05	105.75	113.01
3	3-B	815	PHE	CA-C-N	6.05	127.26	120.42
3	3-B	815	PHE	C-N-CA	6.05	127.26	120.42
7	3-G	685	GLU	N-CA-C	-6.05	98.41	108.34
8	3-Z	36	PRO	CA-C-N	6.05	133.10	121.54
8	3-Z	36	PRO	C-N-CA	6.05	133.10	121.54
6	1-J	132	GLU	CA-C-N	6.05	132.15	121.80
6	1-J	132	GLU	C-N-CA	6.05	132.15	121.80
6	2-J	132	GLU	CA-C-N	6.05	132.15	121.80
6	2-J	132	GLU	C-N-CA	6.05	132.15	121.80
6	3-J	132	GLU	CA-C-N	6.05	132.15	121.80
6	3-J	132	GLU	C-N-CA	6.05	132.15	121.80
3	1-N	90	LYS	N-CA-C	-6.05	104.76	111.36
3	1-N	460	VAL	O-C-N	6.05	127.84	121.91
3	2-N	90	LYS	N-CA-C	-6.05	104.76	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2-N	460	VAL	O-C-N	6.05	127.84	121.91
3	3-N	90	LYS	N-CA-C	-6.05	104.76	111.36
3	3-N	460	VAL	O-C-N	6.05	127.84	121.91
4	1-H	573	LEU	CA-C-N	6.05	132.01	122.94
4	1-H	573	LEU	C-N-CA	6.05	132.01	122.94
6	1-J	52	ASN	N-CA-C	-6.05	99.54	109.40
4	2-H	573	LEU	CA-C-N	6.05	132.01	122.94
4	2-H	573	LEU	C-N-CA	6.05	132.01	122.94
6	2-J	52	ASN	N-CA-C	-6.05	99.54	109.40
4	3-H	573	LEU	CA-C-N	6.05	132.01	122.94
4	3-H	573	LEU	C-N-CA	6.05	132.01	122.94
6	3-J	52	ASN	N-CA-C	-6.05	99.54	109.40
1	1-A	376	ALA	CA-C-N	6.05	131.42	122.71
1	1-A	376	ALA	C-N-CA	6.05	131.42	122.71
3	1-B	231	VAL	CA-C-N	6.05	128.99	120.28
3	1-B	231	VAL	C-N-CA	6.05	128.99	120.28
6	1-M	90	PHE	CA-C-N	-6.05	114.57	122.37
6	1-M	90	PHE	C-N-CA	-6.05	114.57	122.37
4	1-H	361	ASN	N-CA-C	-6.05	101.32	110.39
1	2-A	376	ALA	CA-C-N	6.05	131.42	122.71
1	2-A	376	ALA	C-N-CA	6.05	131.42	122.71
3	2-B	231	VAL	CA-C-N	6.05	128.99	120.28
3	2-B	231	VAL	C-N-CA	6.05	128.99	120.28
6	2-M	90	PHE	CA-C-N	-6.05	114.57	122.37
6	2-M	90	PHE	C-N-CA	-6.05	114.57	122.37
4	2-H	361	ASN	N-CA-C	-6.05	101.32	110.39
1	3-A	376	ALA	CA-C-N	6.05	131.42	122.71
1	3-A	376	ALA	C-N-CA	6.05	131.42	122.71
3	3-B	231	VAL	CA-C-N	6.05	128.99	120.28
3	3-B	231	VAL	C-N-CA	6.05	128.99	120.28
6	3-M	90	PHE	CA-C-N	-6.05	114.57	122.37
6	3-M	90	PHE	C-N-CA	-6.05	114.57	122.37
4	3-H	361	ASN	N-CA-C	-6.05	101.32	110.39
1	1-A	79	ASN	CA-C-O	-6.05	113.71	120.54
1	2-A	79	ASN	CA-C-O	-6.05	113.71	120.54
1	3-A	79	ASN	CA-C-O	-6.05	113.71	120.54
3	1-N	73	LEU	CA-C-N	6.04	128.66	120.38
3	1-N	73	LEU	C-N-CA	6.04	128.66	120.38
3	2-N	73	LEU	CA-C-N	6.04	128.66	120.38
3	2-N	73	LEU	C-N-CA	6.04	128.66	120.38
3	3-N	73	LEU	CA-C-N	6.04	128.66	120.38
3	3-N	73	LEU	C-N-CA	6.04	128.66	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	278	ALA	N-CA-C	-6.04	99.50	108.99
6	1-F	81	TYR	N-CA-C	-6.04	105.56	113.17
7	1-G	372	SER	CA-C-N	6.04	133.08	121.54
7	1-G	372	SER	C-N-CA	6.04	133.08	121.54
5	1-I	62	GLU	CA-C-N	6.04	133.08	121.54
5	1-I	62	GLU	C-N-CA	6.04	133.08	121.54
4	2-C	278	ALA	N-CA-C	-6.04	99.50	108.99
6	2-F	81	TYR	N-CA-C	-6.04	105.56	113.17
7	2-G	372	SER	CA-C-N	6.04	133.08	121.54
7	2-G	372	SER	C-N-CA	6.04	133.08	121.54
5	2-I	62	GLU	CA-C-N	6.04	133.08	121.54
5	2-I	62	GLU	C-N-CA	6.04	133.08	121.54
4	3-C	278	ALA	N-CA-C	-6.04	99.50	108.99
6	3-F	81	TYR	N-CA-C	-6.04	105.56	113.17
7	3-G	372	SER	CA-C-N	6.04	133.08	121.54
7	3-G	372	SER	C-N-CA	6.04	133.08	121.54
5	3-I	62	GLU	CA-C-N	6.04	133.08	121.54
5	3-I	62	GLU	C-N-CA	6.04	133.08	121.54
1	1-A	765	HIS	N-CA-C	-6.04	105.87	113.18
4	1-C	573	LEU	CA-C-N	6.04	132.00	122.94
4	1-C	573	LEU	C-N-CA	6.04	132.00	122.94
1	2-A	765	HIS	N-CA-C	-6.04	105.87	113.18
4	2-C	573	LEU	CA-C-N	6.04	132.00	122.94
4	2-C	573	LEU	C-N-CA	6.04	132.00	122.94
1	3-A	765	HIS	N-CA-C	-6.04	105.87	113.18
4	3-C	573	LEU	CA-C-N	6.04	132.00	122.94
4	3-C	573	LEU	C-N-CA	6.04	132.00	122.94
6	1-F	106	VAL	N-CA-C	6.04	116.78	110.62
6	2-F	106	VAL	N-CA-C	6.04	116.78	110.62
6	3-F	106	VAL	N-CA-C	6.04	116.78	110.62
3	1-B	73	LEU	CA-C-N	6.04	128.65	120.38
3	1-B	73	LEU	C-N-CA	6.04	128.65	120.38
3	2-B	73	LEU	CA-C-N	6.04	128.65	120.38
3	2-B	73	LEU	C-N-CA	6.04	128.65	120.38
3	3-B	73	LEU	CA-C-N	6.04	128.65	120.38
3	3-B	73	LEU	C-N-CA	6.04	128.65	120.38
7	1-K	685	GLU	N-CA-C	-6.04	98.44	108.34
3	1-N	456	LYS	CA-C-N	6.04	128.37	120.28
3	1-N	456	LYS	C-N-CA	6.04	128.37	120.28
5	1-I	26	ARG	CA-C-N	6.04	130.25	120.60
5	1-I	26	ARG	C-N-CA	6.04	130.25	120.60
6	1-J	81	TYR	N-CA-C	-6.04	105.57	113.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-K	685	GLU	N-CA-C	-6.04	98.44	108.34
3	2-N	456	LYS	CA-C-N	6.04	128.37	120.28
3	2-N	456	LYS	C-N-CA	6.04	128.37	120.28
5	2-I	26	ARG	CA-C-N	6.04	130.25	120.60
5	2-I	26	ARG	C-N-CA	6.04	130.25	120.60
6	2-J	81	TYR	N-CA-C	-6.04	105.57	113.17
7	3-K	685	GLU	N-CA-C	-6.04	98.44	108.34
3	3-N	456	LYS	CA-C-N	6.04	128.37	120.28
3	3-N	456	LYS	C-N-CA	6.04	128.37	120.28
5	3-I	26	ARG	CA-C-N	6.04	130.25	120.60
5	3-I	26	ARG	C-N-CA	6.04	130.25	120.60
6	3-J	81	TYR	N-CA-C	-6.04	105.57	113.17
1	1-A	251	ASN	CA-C-N	6.03	132.83	121.97
1	1-A	251	ASN	C-N-CA	6.03	132.83	121.97
1	1-A	806	THR	N-CA-C	-6.03	104.27	111.69
1	2-A	251	ASN	CA-C-N	6.03	132.83	121.97
1	2-A	251	ASN	C-N-CA	6.03	132.83	121.97
1	2-A	806	THR	N-CA-C	-6.03	104.27	111.69
1	3-A	251	ASN	CA-C-N	6.03	132.83	121.97
1	3-A	251	ASN	C-N-CA	6.03	132.83	121.97
1	3-A	806	THR	N-CA-C	-6.03	104.27	111.69
4	1-C	352	GLU	N-CA-C	-6.03	97.95	110.80
4	2-C	352	GLU	N-CA-C	-6.03	97.95	110.80
4	3-C	352	GLU	N-CA-C	-6.03	97.95	110.80
4	1-H	381	MET	CA-C-N	6.03	128.85	120.29
4	1-H	381	MET	C-N-CA	6.03	128.85	120.29
4	2-H	381	MET	CA-C-N	6.03	128.85	120.29
4	2-H	381	MET	C-N-CA	6.03	128.85	120.29
4	3-H	381	MET	CA-C-N	6.03	128.85	120.29
4	3-H	381	MET	C-N-CA	6.03	128.85	120.29
4	1-C	381	MET	CA-C-N	6.03	128.85	120.29
4	1-C	381	MET	C-N-CA	6.03	128.85	120.29
4	2-C	381	MET	CA-C-N	6.03	128.85	120.29
4	2-C	381	MET	C-N-CA	6.03	128.85	120.29
4	3-C	381	MET	CA-C-N	6.03	128.85	120.29
4	3-C	381	MET	C-N-CA	6.03	128.85	120.29
3	1-B	460	VAL	O-C-N	6.03	127.82	121.91
3	2-B	460	VAL	O-C-N	6.03	127.82	121.91
3	3-B	460	VAL	O-C-N	6.03	127.82	121.91
3	1-N	132	ARG	CA-C-N	6.02	126.67	119.98
3	1-N	132	ARG	C-N-CA	6.02	126.67	119.98
4	1-H	352	GLU	N-CA-C	-6.02	97.97	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2-N	132	ARG	CA-C-N	6.02	126.67	119.98
3	2-N	132	ARG	C-N-CA	6.02	126.67	119.98
4	2-H	352	GLU	N-CA-C	-6.02	97.97	110.80
3	3-N	132	ARG	CA-C-N	6.02	126.67	119.98
3	3-N	132	ARG	C-N-CA	6.02	126.67	119.98
4	3-H	352	GLU	N-CA-C	-6.02	97.97	110.80
7	1-K	54	LEU	N-CA-C	-6.02	104.80	111.36
7	2-K	54	LEU	N-CA-C	-6.02	104.80	111.36
7	3-K	54	LEU	N-CA-C	-6.02	104.80	111.36
1	1-A	720	MET	N-CA-C	-6.02	104.80	111.36
7	1-G	224	LYS	N-CA-C	6.02	120.71	112.04
1	2-A	720	MET	N-CA-C	-6.02	104.80	111.36
7	2-G	224	LYS	N-CA-C	6.02	120.71	112.04
1	3-A	720	MET	N-CA-C	-6.02	104.80	111.36
7	3-G	224	LYS	N-CA-C	6.02	120.71	112.04
7	1-K	68	GLU	N-CA-C	-6.02	104.72	111.28
3	1-N	231	VAL	CA-C-N	6.02	128.95	120.28
3	1-N	231	VAL	C-N-CA	6.02	128.95	120.28
7	2-K	68	GLU	N-CA-C	-6.02	104.72	111.28
3	2-N	231	VAL	CA-C-N	6.02	128.95	120.28
3	2-N	231	VAL	C-N-CA	6.02	128.95	120.28
7	3-K	68	GLU	N-CA-C	-6.02	104.72	111.28
3	3-N	231	VAL	CA-C-N	6.02	128.95	120.28
3	3-N	231	VAL	C-N-CA	6.02	128.95	120.28
3	1-B	256	GLU	CA-C-O	6.02	126.87	119.05
3	2-B	256	GLU	CA-C-O	6.02	126.87	119.05
3	3-B	256	GLU	CA-C-O	6.02	126.87	119.05
5	1-D	26	ARG	CA-C-N	6.01	130.22	120.60
5	1-D	26	ARG	C-N-CA	6.01	130.22	120.60
7	1-G	396	VAL	N-CA-C	-6.01	104.64	110.72
3	1-N	436	LEU	N-CA-C	-6.01	104.64	111.07
5	2-D	26	ARG	CA-C-N	6.01	130.22	120.60
5	2-D	26	ARG	C-N-CA	6.01	130.22	120.60
7	2-G	396	VAL	N-CA-C	-6.01	104.64	110.72
3	2-N	436	LEU	N-CA-C	-6.01	104.64	111.07
5	3-D	26	ARG	CA-C-N	6.01	130.22	120.60
5	3-D	26	ARG	C-N-CA	6.01	130.22	120.60
7	3-G	396	VAL	N-CA-C	-6.01	104.64	110.72
3	3-N	436	LEU	N-CA-C	-6.01	104.64	111.07
4	1-C	277	VAL	N-CA-C	-6.01	99.12	108.44
4	1-H	402	GLU	N-CA-C	-6.01	100.00	108.96
4	2-C	277	VAL	N-CA-C	-6.01	99.12	108.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-H	402	GLU	N-CA-C	-6.01	100.00	108.96
4	3-C	277	VAL	N-CA-C	-6.01	99.12	108.44
4	3-H	402	GLU	N-CA-C	-6.01	100.00	108.96
3	1-B	132	ARG	CA-C-N	6.01	126.65	119.98
3	1-B	132	ARG	C-N-CA	6.01	126.65	119.98
3	1-N	256	GLU	CA-C-O	6.01	126.86	119.05
3	2-B	132	ARG	CA-C-N	6.01	126.65	119.98
3	2-B	132	ARG	C-N-CA	6.01	126.65	119.98
3	2-N	256	GLU	CA-C-O	6.01	126.86	119.05
3	3-B	132	ARG	CA-C-N	6.01	126.65	119.98
3	3-B	132	ARG	C-N-CA	6.01	126.65	119.98
3	3-N	256	GLU	CA-C-O	6.01	126.86	119.05
1	1-A	607	LYS	CA-C-N	6.00	131.27	122.08
1	1-A	607	LYS	C-N-CA	6.00	131.27	122.08
1	2-A	607	LYS	CA-C-N	6.00	131.27	122.08
1	2-A	607	LYS	C-N-CA	6.00	131.27	122.08
1	3-A	607	LYS	CA-C-N	6.00	131.27	122.08
1	3-A	607	LYS	C-N-CA	6.00	131.27	122.08
7	1-G	805	VAL	O-C-N	6.00	127.79	121.91
7	1-K	805	VAL	O-C-N	6.00	127.79	121.91
7	2-G	805	VAL	O-C-N	6.00	127.79	121.91
7	2-K	805	VAL	O-C-N	6.00	127.79	121.91
7	3-G	805	VAL	O-C-N	6.00	127.79	121.91
7	3-K	805	VAL	O-C-N	6.00	127.79	121.91
7	1-G	208	ARG	N-CA-C	6.00	119.07	111.69
7	2-G	208	ARG	N-CA-C	6.00	119.07	111.69
7	3-G	208	ARG	N-CA-C	6.00	119.07	111.69
6	1-F	132	GLU	CA-C-N	6.00	132.06	121.80
6	1-F	132	GLU	C-N-CA	6.00	132.06	121.80
6	2-F	132	GLU	CA-C-N	6.00	132.06	121.80
6	2-F	132	GLU	C-N-CA	6.00	132.06	121.80
6	3-F	132	GLU	CA-C-N	6.00	132.06	121.80
6	3-F	132	GLU	C-N-CA	6.00	132.06	121.80
8	1-Z	76	TYR	CA-C-O	6.00	126.84	120.36
8	2-Z	76	TYR	CA-C-O	6.00	126.84	120.36
8	3-Z	76	TYR	CA-C-O	6.00	126.84	120.36
4	1-C	573	LEU	N-CA-C	-6.00	99.94	109.59
4	2-C	573	LEU	N-CA-C	-6.00	99.94	109.59
4	3-C	573	LEU	N-CA-C	-6.00	99.94	109.59
6	1-J	106	VAL	N-CA-C	6.00	116.73	110.62
6	2-J	106	VAL	N-CA-C	6.00	116.73	110.62
6	3-J	106	VAL	N-CA-C	6.00	116.73	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	1-R	54	GLU	N-CA-C	-5.99	99.94	109.23
4	1-H	573	LEU	N-CA-C	-5.99	99.94	109.59
6	2-R	54	GLU	N-CA-C	-5.99	99.94	109.23
4	2-H	573	LEU	N-CA-C	-5.99	99.94	109.59
6	3-R	54	GLU	N-CA-C	-5.99	99.94	109.23
4	3-H	573	LEU	N-CA-C	-5.99	99.94	109.59
5	1-I	60	PRO	N-CA-C	-5.99	101.08	111.32
5	2-I	60	PRO	N-CA-C	-5.99	101.08	111.32
5	3-I	60	PRO	N-CA-C	-5.99	101.08	111.32
4	1-C	402	GLU	N-CA-C	-5.99	100.04	108.96
4	2-C	402	GLU	N-CA-C	-5.99	100.04	108.96
4	3-C	402	GLU	N-CA-C	-5.99	100.04	108.96
3	1-B	436	LEU	N-CA-C	-5.98	104.67	111.07
3	2-B	436	LEU	N-CA-C	-5.98	104.67	111.07
3	3-B	436	LEU	N-CA-C	-5.98	104.67	111.07
5	1-D	11	LYS	N-CA-C	5.98	119.41	111.75
5	2-D	11	LYS	N-CA-C	5.98	119.41	111.75
5	3-D	11	LYS	N-CA-C	5.98	119.41	111.75
1	1-A	599	PHE	N-CA-C	5.98	117.47	111.07
1	1-A	789	ASP	N-CA-C	-5.98	89.68	107.37
3	1-N	181	PHE	CA-C-N	5.98	132.96	121.54
3	1-N	181	PHE	C-N-CA	5.98	132.96	121.54
1	2-A	599	PHE	N-CA-C	5.98	117.47	111.07
1	2-A	789	ASP	N-CA-C	-5.98	89.68	107.37
3	2-N	181	PHE	CA-C-N	5.98	132.96	121.54
3	2-N	181	PHE	C-N-CA	5.98	132.96	121.54
1	3-A	599	PHE	N-CA-C	5.98	117.47	111.07
1	3-A	789	ASP	N-CA-C	-5.98	89.68	107.37
3	3-N	181	PHE	CA-C-N	5.98	132.96	121.54
3	3-N	181	PHE	C-N-CA	5.98	132.96	121.54
8	1-L	129	VAL	N-CA-C	-5.98	99.56	108.46
8	2-L	129	VAL	N-CA-C	-5.98	99.56	108.46
8	3-L	129	VAL	N-CA-C	-5.98	99.56	108.46
4	1-C	154	ASP	N-CA-C	-5.97	93.80	107.48
4	2-C	154	ASP	N-CA-C	-5.97	93.80	107.48
4	3-C	154	ASP	N-CA-C	-5.97	93.80	107.48
5	1-I	11	LYS	N-CA-C	5.97	119.39	111.75
5	2-I	11	LYS	N-CA-C	5.97	119.39	111.75
5	3-I	11	LYS	N-CA-C	5.97	119.39	111.75
1	1-A	729	MET	N-CA-C	-5.97	107.23	114.75
1	2-A	729	MET	N-CA-C	-5.97	107.23	114.75
1	3-A	729	MET	N-CA-C	-5.97	107.23	114.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	744	GLU	N-CA-C	-5.97	104.85	111.71
3	1-B	150	PRO	N-CA-C	-5.97	104.60	114.75
7	1-G	531	TYR	N-CA-C	-5.97	104.85	111.36
7	1-K	118	ASP	CA-C-O	5.97	126.75	120.42
1	2-A	744	GLU	N-CA-C	-5.97	104.85	111.71
3	2-B	150	PRO	N-CA-C	-5.97	104.60	114.75
7	2-G	531	TYR	N-CA-C	-5.97	104.85	111.36
7	2-K	118	ASP	CA-C-O	5.97	126.75	120.42
1	3-A	744	GLU	N-CA-C	-5.97	104.85	111.71
3	3-B	150	PRO	N-CA-C	-5.97	104.60	114.75
7	3-G	531	TYR	N-CA-C	-5.97	104.85	111.36
7	3-K	118	ASP	CA-C-O	5.97	126.75	120.42
4	1-C	143	HIS	CA-C-N	5.97	129.31	120.90
4	1-C	143	HIS	C-N-CA	5.97	129.31	120.90
4	2-C	143	HIS	CA-C-N	5.97	129.31	120.90
4	2-C	143	HIS	C-N-CA	5.97	129.31	120.90
4	3-C	143	HIS	CA-C-N	5.97	129.31	120.90
4	3-C	143	HIS	C-N-CA	5.97	129.31	120.90
5	1-D	60	PRO	N-CA-C	-5.96	101.12	111.32
5	1-I	68	LEU	CA-C-N	-5.96	113.75	122.58
5	1-I	68	LEU	C-N-CA	-5.96	113.75	122.58
5	2-D	60	PRO	N-CA-C	-5.96	101.12	111.32
5	2-I	68	LEU	CA-C-N	-5.96	113.75	122.58
5	2-I	68	LEU	C-N-CA	-5.96	113.75	122.58
5	3-D	60	PRO	N-CA-C	-5.96	101.12	111.32
5	3-I	68	LEU	CA-C-N	-5.96	113.75	122.58
5	3-I	68	LEU	C-N-CA	-5.96	113.75	122.58
4	1-H	277	VAL	N-CA-C	-5.96	99.20	108.44
4	2-H	277	VAL	N-CA-C	-5.96	99.20	108.44
4	3-H	277	VAL	N-CA-C	-5.96	99.20	108.44
4	1-H	154	ASP	N-CA-C	-5.96	93.83	107.48
4	2-H	154	ASP	N-CA-C	-5.96	93.83	107.48
4	3-H	154	ASP	N-CA-C	-5.96	93.83	107.48
7	1-G	181	ALA	N-CA-C	5.96	117.45	111.07
7	2-G	181	ALA	N-CA-C	5.96	117.45	111.07
7	3-G	181	ALA	N-CA-C	5.96	117.45	111.07
1	1-A	310	HIS	CA-C-N	5.96	128.54	120.44
1	1-A	310	HIS	C-N-CA	5.96	128.54	120.44
4	1-C	410	SER	N-CA-C	-5.96	98.11	110.80
7	1-G	120	TYR	CA-C-O	5.96	126.73	120.42
7	1-G	371	ILE	N-CA-C	-5.96	99.58	108.46
1	2-A	310	HIS	CA-C-N	5.96	128.54	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	310	HIS	C-N-CA	5.96	128.54	120.44
4	2-C	410	SER	N-CA-C	-5.96	98.11	110.80
7	2-G	120	TYR	CA-C-O	5.96	126.73	120.42
7	2-G	371	ILE	N-CA-C	-5.96	99.58	108.46
1	3-A	310	HIS	CA-C-N	5.96	128.54	120.44
1	3-A	310	HIS	C-N-CA	5.96	128.54	120.44
4	3-C	410	SER	N-CA-C	-5.96	98.11	110.80
7	3-G	120	TYR	CA-C-O	5.96	126.73	120.42
7	3-G	371	ILE	N-CA-C	-5.96	99.58	108.46
3	1-B	181	PHE	CA-C-N	5.96	132.91	121.54
3	1-B	181	PHE	C-N-CA	5.96	132.91	121.54
3	2-B	181	PHE	CA-C-N	5.96	132.91	121.54
3	2-B	181	PHE	C-N-CA	5.96	132.91	121.54
3	3-B	181	PHE	CA-C-N	5.96	132.91	121.54
3	3-B	181	PHE	C-N-CA	5.96	132.91	121.54
5	1-D	68	LEU	CA-C-N	-5.95	113.77	122.58
5	1-D	68	LEU	C-N-CA	-5.95	113.77	122.58
7	1-G	711	ALA	N-CA-C	-5.95	100.48	109.95
3	1-N	150	PRO	N-CA-C	-5.95	104.63	114.75
5	2-D	68	LEU	CA-C-N	-5.95	113.77	122.58
5	2-D	68	LEU	C-N-CA	-5.95	113.77	122.58
7	2-G	711	ALA	N-CA-C	-5.95	100.48	109.95
3	2-N	150	PRO	N-CA-C	-5.95	104.63	114.75
5	3-D	68	LEU	CA-C-N	-5.95	113.77	122.58
5	3-D	68	LEU	C-N-CA	-5.95	113.77	122.58
7	3-G	711	ALA	N-CA-C	-5.95	100.48	109.95
3	3-N	150	PRO	N-CA-C	-5.95	104.63	114.75
1	1-A	29	HIS	N-CA-C	-5.95	105.94	112.72
3	1-B	448	ASN	CA-C-N	5.95	128.53	120.38
3	1-B	448	ASN	C-N-CA	5.95	128.53	120.38
4	1-C	812	LYS	CA-C-N	5.95	128.25	120.28
4	1-C	812	LYS	C-N-CA	5.95	128.25	120.28
4	1-H	707	GLY	CA-C-O	-5.95	117.24	121.88
1	2-A	29	HIS	N-CA-C	-5.95	105.94	112.72
3	2-B	448	ASN	CA-C-N	5.95	128.53	120.38
3	2-B	448	ASN	C-N-CA	5.95	128.53	120.38
4	2-C	812	LYS	CA-C-N	5.95	128.25	120.28
4	2-C	812	LYS	C-N-CA	5.95	128.25	120.28
4	2-H	707	GLY	CA-C-O	-5.95	117.24	121.88
1	3-A	29	HIS	N-CA-C	-5.95	105.94	112.72
3	3-B	448	ASN	CA-C-N	5.95	128.53	120.38
3	3-B	448	ASN	C-N-CA	5.95	128.53	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	3-C	812	LYS	CA-C-N	5.95	128.25	120.28
4	3-C	812	LYS	C-N-CA	5.95	128.25	120.28
4	3-H	707	GLY	CA-C-O	-5.95	117.24	121.88
3	1-N	258	ALA	CA-C-N	5.95	128.25	120.28
3	1-N	258	ALA	C-N-CA	5.95	128.25	120.28
3	2-N	258	ALA	CA-C-N	5.95	128.25	120.28
3	2-N	258	ALA	C-N-CA	5.95	128.25	120.28
3	3-N	258	ALA	CA-C-N	5.95	128.25	120.28
3	3-N	258	ALA	C-N-CA	5.95	128.25	120.28
3	1-N	428	ASN	CA-C-N	5.95	128.53	120.38
3	1-N	428	ASN	C-N-CA	5.95	128.53	120.38
4	1-H	90	GLU	N-CA-C	-5.95	99.55	109.24
3	2-N	428	ASN	CA-C-N	5.95	128.53	120.38
3	2-N	428	ASN	C-N-CA	5.95	128.53	120.38
4	2-H	90	GLU	N-CA-C	-5.95	99.55	109.24
3	3-N	428	ASN	CA-C-N	5.95	128.53	120.38
3	3-N	428	ASN	C-N-CA	5.95	128.53	120.38
4	3-H	90	GLU	N-CA-C	-5.95	99.55	109.24
3	1-N	448	ASN	CA-C-N	5.94	128.52	120.38
3	1-N	448	ASN	C-N-CA	5.94	128.52	120.38
3	2-N	448	ASN	CA-C-N	5.94	128.52	120.38
3	2-N	448	ASN	C-N-CA	5.94	128.52	120.38
3	3-N	448	ASN	CA-C-N	5.94	128.52	120.38
3	3-N	448	ASN	C-N-CA	5.94	128.52	120.38
7	1-G	207	ASP	CA-C-N	5.94	130.74	120.58
7	1-G	207	ASP	C-N-CA	5.94	130.74	120.58
7	2-G	207	ASP	CA-C-N	5.94	130.74	120.58
7	2-G	207	ASP	C-N-CA	5.94	130.74	120.58
7	3-G	207	ASP	CA-C-N	5.94	130.74	120.58
7	3-G	207	ASP	C-N-CA	5.94	130.74	120.58
6	1-J	144	GLY	CA-C-N	5.93	128.82	120.28
6	1-J	144	GLY	C-N-CA	5.93	128.82	120.28
6	2-J	144	GLY	CA-C-N	5.93	128.82	120.28
6	2-J	144	GLY	C-N-CA	5.93	128.82	120.28
6	3-J	144	GLY	CA-C-N	5.93	128.82	120.28
6	3-J	144	GLY	C-N-CA	5.93	128.82	120.28
1	1-A	75	ILE	N-CA-C	-5.93	99.20	107.80
4	1-C	90	GLU	N-CA-C	-5.93	99.57	109.24
1	2-A	75	ILE	N-CA-C	-5.93	99.20	107.80
4	2-C	90	GLU	N-CA-C	-5.93	99.57	109.24
1	3-A	75	ILE	N-CA-C	-5.93	99.20	107.80
4	3-C	90	GLU	N-CA-C	-5.93	99.57	109.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-B	360	LEU	CA-C-N	5.93	128.82	120.28
3	1-B	360	LEU	C-N-CA	5.93	128.82	120.28
4	1-H	410	SER	N-CA-C	-5.93	98.17	110.80
3	2-B	360	LEU	CA-C-N	5.93	128.82	120.28
3	2-B	360	LEU	C-N-CA	5.93	128.82	120.28
4	2-H	410	SER	N-CA-C	-5.93	98.17	110.80
3	3-B	360	LEU	CA-C-N	5.93	128.82	120.28
3	3-B	360	LEU	C-N-CA	5.93	128.82	120.28
4	3-H	410	SER	N-CA-C	-5.93	98.17	110.80
7	1-G	434	THR	N-CA-C	5.93	117.41	111.07
6	1-M	80	HIS	N-CA-C	5.93	123.42	110.80
7	2-G	434	THR	N-CA-C	5.93	117.41	111.07
6	2-M	80	HIS	N-CA-C	5.93	123.42	110.80
7	3-G	434	THR	N-CA-C	5.93	117.41	111.07
6	3-M	80	HIS	N-CA-C	5.93	123.42	110.80
8	1-Z	80	ILE	O-C-N	5.92	129.58	123.18
8	2-Z	80	ILE	O-C-N	5.92	129.58	123.18
8	3-Z	80	ILE	O-C-N	5.92	129.58	123.18
4	1-C	707	GLY	CA-C-O	-5.92	117.26	121.88
7	1-K	54	LEU	CA-C-N	5.92	128.14	120.56
7	1-K	54	LEU	C-N-CA	5.92	128.14	120.56
7	1-K	255	ILE	N-CA-C	5.92	116.10	110.42
4	2-C	707	GLY	CA-C-O	-5.92	117.26	121.88
7	2-K	54	LEU	CA-C-N	5.92	128.14	120.56
7	2-K	54	LEU	C-N-CA	5.92	128.14	120.56
7	2-K	255	ILE	N-CA-C	5.92	116.10	110.42
4	3-C	707	GLY	CA-C-O	-5.92	117.26	121.88
7	3-K	54	LEU	CA-C-N	5.92	128.14	120.56
7	3-K	54	LEU	C-N-CA	5.92	128.14	120.56
7	3-K	255	ILE	N-CA-C	5.92	116.10	110.42
4	1-C	134	CYS	N-CA-C	-5.92	97.57	107.99
4	1-H	143	HIS	CA-C-N	5.92	129.25	120.90
4	1-H	143	HIS	C-N-CA	5.92	129.25	120.90
4	2-C	134	CYS	N-CA-C	-5.92	97.57	107.99
4	2-H	143	HIS	CA-C-N	5.92	129.25	120.90
4	2-H	143	HIS	C-N-CA	5.92	129.25	120.90
4	3-C	134	CYS	N-CA-C	-5.92	97.57	107.99
4	3-H	143	HIS	CA-C-N	5.92	129.25	120.90
4	3-H	143	HIS	C-N-CA	5.92	129.25	120.90
8	1-L	143	VAL	N-CA-C	-5.92	104.74	110.42
8	2-L	143	VAL	N-CA-C	-5.92	104.74	110.42
8	3-L	143	VAL	N-CA-C	-5.92	104.74	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	135	THR	CA-C-O	5.91	126.81	120.55
6	1-R	113	GLU	N-CA-C	-5.91	100.86	110.20
7	1-K	686	ALA	CA-C-N	5.91	132.83	121.54
7	1-K	686	ALA	C-N-CA	5.91	132.83	121.54
4	1-H	134	CYS	N-CA-C	-5.91	97.59	107.99
7	2-G	135	THR	CA-C-O	5.91	126.81	120.55
6	2-R	113	GLU	N-CA-C	-5.91	100.86	110.20
7	2-K	686	ALA	CA-C-N	5.91	132.83	121.54
7	2-K	686	ALA	C-N-CA	5.91	132.83	121.54
4	2-H	134	CYS	N-CA-C	-5.91	97.59	107.99
7	3-G	135	THR	CA-C-O	5.91	126.81	120.55
6	3-R	113	GLU	N-CA-C	-5.91	100.86	110.20
7	3-K	686	ALA	CA-C-N	5.91	132.83	121.54
7	3-K	686	ALA	C-N-CA	5.91	132.83	121.54
4	3-H	134	CYS	N-CA-C	-5.91	97.59	107.99
3	1-B	559	GLY	N-CA-C	5.91	119.36	112.50
3	2-B	559	GLY	N-CA-C	5.91	119.36	112.50
3	3-B	559	GLY	N-CA-C	5.91	119.36	112.50
3	1-B	428	ASN	CA-C-N	5.91	128.47	120.38
3	1-B	428	ASN	C-N-CA	5.91	128.47	120.38
3	1-N	306	LYS	CA-C-N	5.91	129.50	120.82
3	1-N	306	LYS	C-N-CA	5.91	129.50	120.82
3	2-B	428	ASN	CA-C-N	5.91	128.47	120.38
3	2-B	428	ASN	C-N-CA	5.91	128.47	120.38
3	2-N	306	LYS	CA-C-N	5.91	129.50	120.82
3	2-N	306	LYS	C-N-CA	5.91	129.50	120.82
3	3-B	428	ASN	CA-C-N	5.91	128.47	120.38
3	3-B	428	ASN	C-N-CA	5.91	128.47	120.38
3	3-N	306	LYS	CA-C-N	5.91	129.50	120.82
3	3-N	306	LYS	C-N-CA	5.91	129.50	120.82
3	1-B	258	ALA	CA-C-N	5.90	128.19	120.28
3	1-B	258	ALA	C-N-CA	5.90	128.19	120.28
3	2-B	258	ALA	CA-C-N	5.90	128.19	120.28
3	2-B	258	ALA	C-N-CA	5.90	128.19	120.28
3	3-B	258	ALA	CA-C-N	5.90	128.19	120.28
3	3-B	258	ALA	C-N-CA	5.90	128.19	120.28
6	1-F	144	GLY	CA-C-N	5.90	128.78	120.28
6	1-F	144	GLY	C-N-CA	5.90	128.78	120.28
6	2-F	144	GLY	CA-C-N	5.90	128.78	120.28
6	2-F	144	GLY	C-N-CA	5.90	128.78	120.28
6	3-F	144	GLY	CA-C-N	5.90	128.78	120.28
6	3-F	144	GLY	C-N-CA	5.90	128.78	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-B	889	ASN	N-CA-C	-5.90	103.32	111.28
3	2-B	889	ASN	N-CA-C	-5.90	103.32	111.28
3	3-B	889	ASN	N-CA-C	-5.90	103.32	111.28
4	1-C	476	LEU	N-CA-C	-5.89	100.09	109.76
7	1-K	154	SER	CA-C-N	5.89	128.79	120.42
7	1-K	154	SER	C-N-CA	5.89	128.79	120.42
4	2-C	476	LEU	N-CA-C	-5.89	100.09	109.76
7	2-K	154	SER	CA-C-N	5.89	128.79	120.42
7	2-K	154	SER	C-N-CA	5.89	128.79	120.42
4	3-C	476	LEU	N-CA-C	-5.89	100.09	109.76
7	3-K	154	SER	CA-C-N	5.89	128.79	120.42
7	3-K	154	SER	C-N-CA	5.89	128.79	120.42
7	1-G	62	GLY	CA-C-N	5.89	128.18	120.28
7	1-G	62	GLY	C-N-CA	5.89	128.18	120.28
7	2-G	62	GLY	CA-C-N	5.89	128.18	120.28
7	2-G	62	GLY	C-N-CA	5.89	128.18	120.28
7	3-G	62	GLY	CA-C-N	5.89	128.18	120.28
7	3-G	62	GLY	C-N-CA	5.89	128.18	120.28
1	1-A	744	GLU	CA-C-N	5.89	128.17	120.28
1	1-A	744	GLU	C-N-CA	5.89	128.17	120.28
6	1-F	55	THR	N-CA-C	-5.89	100.11	109.59
1	2-A	744	GLU	CA-C-N	5.89	128.17	120.28
1	2-A	744	GLU	C-N-CA	5.89	128.17	120.28
6	2-F	55	THR	N-CA-C	-5.89	100.11	109.59
1	3-A	744	GLU	CA-C-N	5.89	128.17	120.28
1	3-A	744	GLU	C-N-CA	5.89	128.17	120.28
6	3-F	55	THR	N-CA-C	-5.89	100.11	109.59
7	1-G	686	ALA	CA-C-N	5.89	132.79	121.54
7	1-G	686	ALA	C-N-CA	5.89	132.79	121.54
7	2-G	686	ALA	CA-C-N	5.89	132.79	121.54
7	2-G	686	ALA	C-N-CA	5.89	132.79	121.54
7	3-G	686	ALA	CA-C-N	5.89	132.79	121.54
7	3-G	686	ALA	C-N-CA	5.89	132.79	121.54
7	1-K	661	PHE	N-CA-C	-5.89	98.93	108.52
7	2-K	661	PHE	N-CA-C	-5.89	98.93	108.52
7	3-K	661	PHE	N-CA-C	-5.89	98.93	108.52
7	1-K	861	SER	N-CA-C	-5.88	105.29	112.88
8	1-L	126	ASP	CA-C-N	-5.88	111.93	120.29
8	1-L	126	ASP	C-N-CA	-5.88	111.93	120.29
6	1-J	115	GLU	CA-C-N	5.88	132.68	122.32
6	1-J	115	GLU	C-N-CA	5.88	132.68	122.32
7	2-K	861	SER	N-CA-C	-5.88	105.29	112.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2-L	126	ASP	CA-C-N	-5.88	111.93	120.29
8	2-L	126	ASP	C-N-CA	-5.88	111.93	120.29
6	2-J	115	GLU	CA-C-N	5.88	132.68	122.32
6	2-J	115	GLU	C-N-CA	5.88	132.68	122.32
7	3-K	861	SER	N-CA-C	-5.88	105.29	112.88
8	3-L	126	ASP	CA-C-N	-5.88	111.93	120.29
8	3-L	126	ASP	C-N-CA	-5.88	111.93	120.29
6	3-J	115	GLU	CA-C-N	5.88	132.68	122.32
6	3-J	115	GLU	C-N-CA	5.88	132.68	122.32
1	1-A	330	GLY	CA-C-N	5.88	130.73	122.08
1	1-A	330	GLY	C-N-CA	5.88	130.73	122.08
1	2-A	330	GLY	CA-C-N	5.88	130.73	122.08
1	2-A	330	GLY	C-N-CA	5.88	130.73	122.08
1	3-A	330	GLY	CA-C-N	5.88	130.73	122.08
1	3-A	330	GLY	C-N-CA	5.88	130.73	122.08
1	1-A	335	TYR	N-CA-C	-5.88	100.36	109.24
8	1-Z	71	SER	N-CA-C	-5.88	100.38	109.14
4	1-H	476	LEU	N-CA-C	-5.88	100.11	109.76
6	1-J	130	LEU	O-C-N	5.88	126.65	121.18
1	2-A	335	TYR	N-CA-C	-5.88	100.36	109.24
8	2-Z	71	SER	N-CA-C	-5.88	100.38	109.14
4	2-H	476	LEU	N-CA-C	-5.88	100.11	109.76
6	2-J	130	LEU	O-C-N	5.88	126.65	121.18
1	3-A	335	TYR	N-CA-C	-5.88	100.36	109.24
8	3-Z	71	SER	N-CA-C	-5.88	100.38	109.14
4	3-H	476	LEU	N-CA-C	-5.88	100.11	109.76
6	3-J	130	LEU	O-C-N	5.88	126.65	121.18
6	1-R	122	LEU	CA-C-O	5.88	126.75	120.46
3	1-N	559	GLY	N-CA-C	5.88	119.32	112.50
6	2-R	122	LEU	CA-C-O	5.88	126.75	120.46
3	2-N	559	GLY	N-CA-C	5.88	119.32	112.50
6	3-R	122	LEU	CA-C-O	5.88	126.75	120.46
3	3-N	559	GLY	N-CA-C	5.88	119.32	112.50
7	1-G	861	SER	N-CA-C	-5.88	105.30	112.88
3	1-N	421	MET	CA-C-N	5.88	128.08	120.44
3	1-N	421	MET	C-N-CA	5.88	128.08	120.44
7	2-G	861	SER	N-CA-C	-5.88	105.30	112.88
3	2-N	421	MET	CA-C-N	5.88	128.08	120.44
3	2-N	421	MET	C-N-CA	5.88	128.08	120.44
7	3-G	861	SER	N-CA-C	-5.88	105.30	112.88
3	3-N	421	MET	CA-C-N	5.88	128.08	120.44
3	3-N	421	MET	C-N-CA	5.88	128.08	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	179	ASN	CA-C-O	5.88	126.99	120.82
7	2-G	179	ASN	CA-C-O	5.88	126.99	120.82
7	3-G	179	ASN	CA-C-O	5.88	126.99	120.82
4	1-C	154	ASP	CA-C-N	5.88	130.53	121.19
4	1-C	154	ASP	C-N-CA	5.88	130.53	121.19
4	1-C	782	GLN	N-CA-C	-5.88	98.29	110.80
4	2-C	154	ASP	CA-C-N	5.88	130.53	121.19
4	2-C	154	ASP	C-N-CA	5.88	130.53	121.19
4	2-C	782	GLN	N-CA-C	-5.88	98.29	110.80
4	3-C	154	ASP	CA-C-N	5.88	130.53	121.19
4	3-C	154	ASP	C-N-CA	5.88	130.53	121.19
4	3-C	782	GLN	N-CA-C	-5.88	98.29	110.80
3	1-B	401	THR	CA-C-N	5.87	128.15	120.28
3	1-B	401	THR	C-N-CA	5.87	128.15	120.28
4	1-C	721	ARG	N-CA-C	5.87	117.68	111.28
3	1-N	360	LEU	CA-C-N	5.87	128.74	120.28
3	1-N	360	LEU	C-N-CA	5.87	128.74	120.28
3	2-B	401	THR	CA-C-N	5.87	128.15	120.28
3	2-B	401	THR	C-N-CA	5.87	128.15	120.28
4	2-C	721	ARG	N-CA-C	5.87	117.68	111.28
3	2-N	360	LEU	CA-C-N	5.87	128.74	120.28
3	2-N	360	LEU	C-N-CA	5.87	128.74	120.28
3	3-B	401	THR	CA-C-N	5.87	128.15	120.28
3	3-B	401	THR	C-N-CA	5.87	128.15	120.28
4	3-C	721	ARG	N-CA-C	5.87	117.68	111.28
3	3-N	360	LEU	CA-C-N	5.87	128.74	120.28
3	3-N	360	LEU	C-N-CA	5.87	128.74	120.28
4	1-C	44	HIS	CA-C-N	5.87	128.42	120.38
4	1-C	44	HIS	C-N-CA	5.87	128.42	120.38
7	1-G	283	LYS	CA-C-N	5.87	128.15	120.28
7	1-G	283	LYS	C-N-CA	5.87	128.15	120.28
4	2-C	44	HIS	CA-C-N	5.87	128.42	120.38
4	2-C	44	HIS	C-N-CA	5.87	128.42	120.38
7	2-G	283	LYS	CA-C-N	5.87	128.15	120.28
7	2-G	283	LYS	C-N-CA	5.87	128.15	120.28
4	3-C	44	HIS	CA-C-N	5.87	128.42	120.38
4	3-C	44	HIS	C-N-CA	5.87	128.42	120.38
7	3-G	283	LYS	CA-C-N	5.87	128.15	120.28
7	3-G	283	LYS	C-N-CA	5.87	128.15	120.28
3	1-B	306	LYS	CA-C-N	5.87	129.45	120.82
3	1-B	306	LYS	C-N-CA	5.87	129.45	120.82
6	1-J	55	THR	N-CA-C	-5.87	100.14	109.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2-B	306	LYS	CA-C-N	5.87	129.45	120.82
3	2-B	306	LYS	C-N-CA	5.87	129.45	120.82
6	2-J	55	THR	N-CA-C	-5.87	100.14	109.59
3	3-B	306	LYS	CA-C-N	5.87	129.45	120.82
3	3-B	306	LYS	C-N-CA	5.87	129.45	120.82
6	3-J	55	THR	N-CA-C	-5.87	100.14	109.59
4	1-H	44	HIS	CA-C-N	5.87	128.42	120.38
4	1-H	44	HIS	C-N-CA	5.87	128.42	120.38
4	2-H	44	HIS	CA-C-N	5.87	128.42	120.38
4	2-H	44	HIS	C-N-CA	5.87	128.42	120.38
4	3-H	44	HIS	CA-C-N	5.87	128.42	120.38
4	3-H	44	HIS	C-N-CA	5.87	128.42	120.38
7	1-G	168	LYS	N-CA-C	-5.87	103.86	111.02
7	2-G	168	LYS	N-CA-C	-5.87	103.86	111.02
7	3-G	168	LYS	N-CA-C	-5.87	103.86	111.02
7	1-K	631	LYS	N-CA-C	-5.87	99.22	108.14
7	2-K	631	LYS	N-CA-C	-5.87	99.22	108.14
7	3-K	631	LYS	N-CA-C	-5.87	99.22	108.14
6	1-F	115	GLU	CA-C-N	5.86	132.64	122.32
6	1-F	115	GLU	C-N-CA	5.86	132.64	122.32
6	2-F	115	GLU	CA-C-N	5.86	132.64	122.32
6	2-F	115	GLU	C-N-CA	5.86	132.64	122.32
6	3-F	115	GLU	CA-C-N	5.86	132.64	122.32
6	3-F	115	GLU	C-N-CA	5.86	132.64	122.32
6	1-J	116	LEU	CA-C-N	5.86	132.74	121.54
6	1-J	116	LEU	C-N-CA	5.86	132.74	121.54
6	2-J	116	LEU	CA-C-N	5.86	132.74	121.54
6	2-J	116	LEU	C-N-CA	5.86	132.74	121.54
6	3-J	116	LEU	CA-C-N	5.86	132.74	121.54
6	3-J	116	LEU	C-N-CA	5.86	132.74	121.54
5	1-I	115	GLU	N-CA-C	-5.86	104.81	111.14
5	2-I	115	GLU	N-CA-C	-5.86	104.81	111.14
5	3-I	115	GLU	N-CA-C	-5.86	104.81	111.14
7	1-K	279	GLY	N-CA-C	-5.86	99.29	113.18
7	2-K	279	GLY	N-CA-C	-5.86	99.29	113.18
7	3-K	279	GLY	N-CA-C	-5.86	99.29	113.18
2	1-E	266	PRO	O-C-N	5.86	123.90	121.15
3	1-B	421	MET	CA-C-N	5.86	128.05	120.44
3	1-B	421	MET	C-N-CA	5.86	128.05	120.44
6	1-F	130	LEU	O-C-N	5.86	126.63	121.18
7	1-G	661	PHE	N-CA-C	-5.86	98.98	108.52
4	1-H	154	ASP	CA-C-N	5.86	130.50	121.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	154	ASP	C-N-CA	5.86	130.50	121.19
2	2-E	266	PRO	O-C-N	5.86	123.90	121.15
3	2-B	421	MET	CA-C-N	5.86	128.05	120.44
3	2-B	421	MET	C-N-CA	5.86	128.05	120.44
6	2-F	130	LEU	O-C-N	5.86	126.63	121.18
7	2-G	661	PHE	N-CA-C	-5.86	98.98	108.52
4	2-H	154	ASP	CA-C-N	5.86	130.50	121.19
4	2-H	154	ASP	C-N-CA	5.86	130.50	121.19
2	3-E	266	PRO	O-C-N	5.86	123.90	121.15
3	3-B	421	MET	CA-C-N	5.86	128.05	120.44
3	3-B	421	MET	C-N-CA	5.86	128.05	120.44
6	3-F	130	LEU	O-C-N	5.86	126.63	121.18
7	3-G	661	PHE	N-CA-C	-5.86	98.98	108.52
4	3-H	154	ASP	CA-C-N	5.86	130.50	121.19
4	3-H	154	ASP	C-N-CA	5.86	130.50	121.19
3	1-B	369	GLU	N-CA-C	5.85	117.74	111.36
3	2-B	369	GLU	N-CA-C	5.85	117.74	111.36
3	3-B	369	GLU	N-CA-C	5.85	117.74	111.36
6	1-R	83	ARG	CA-C-N	5.85	132.71	121.54
6	1-R	83	ARG	C-N-CA	5.85	132.71	121.54
6	2-R	83	ARG	CA-C-N	5.85	132.71	121.54
6	2-R	83	ARG	C-N-CA	5.85	132.71	121.54
6	3-R	83	ARG	CA-C-N	5.85	132.71	121.54
6	3-R	83	ARG	C-N-CA	5.85	132.71	121.54
3	1-N	401	THR	CA-C-N	5.85	128.12	120.28
3	1-N	401	THR	C-N-CA	5.85	128.12	120.28
3	2-N	401	THR	CA-C-N	5.85	128.12	120.28
3	2-N	401	THR	C-N-CA	5.85	128.12	120.28
3	3-N	401	THR	CA-C-N	5.85	128.12	120.28
3	3-N	401	THR	C-N-CA	5.85	128.12	120.28
6	1-R	23	VAL	N-CA-C	-5.85	100.27	108.80
6	2-R	23	VAL	N-CA-C	-5.85	100.27	108.80
6	3-R	23	VAL	N-CA-C	-5.85	100.27	108.80
8	1-Z	118	MET	N-CA-C	5.84	119.59	112.23
8	1-Z	140	GLN	CA-C-N	5.84	128.04	120.44
8	1-Z	140	GLN	C-N-CA	5.84	128.04	120.44
8	2-Z	118	MET	N-CA-C	5.84	119.59	112.23
8	2-Z	140	GLN	CA-C-N	5.84	128.04	120.44
8	2-Z	140	GLN	C-N-CA	5.84	128.04	120.44
8	3-Z	118	MET	N-CA-C	5.84	119.59	112.23
8	3-Z	140	GLN	CA-C-N	5.84	128.04	120.44
8	3-Z	140	GLN	C-N-CA	5.84	128.04	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1-D	115	GLU	N-CA-C	-5.84	104.83	111.14
7	1-K	263	HIS	N-CA-C	-5.84	97.67	108.24
4	1-H	152	PRO	CA-C-N	5.84	128.04	120.44
4	1-H	152	PRO	C-N-CA	5.84	128.04	120.44
5	2-D	115	GLU	N-CA-C	-5.84	104.83	111.14
7	2-K	263	HIS	N-CA-C	-5.84	97.67	108.24
4	2-H	152	PRO	CA-C-N	5.84	128.04	120.44
4	2-H	152	PRO	C-N-CA	5.84	128.04	120.44
5	3-D	115	GLU	N-CA-C	-5.84	104.83	111.14
7	3-K	263	HIS	N-CA-C	-5.84	97.67	108.24
4	3-H	152	PRO	CA-C-N	5.84	128.04	120.44
4	3-H	152	PRO	C-N-CA	5.84	128.04	120.44
7	1-G	631	LYS	N-CA-C	-5.84	99.27	108.14
7	1-K	95	MET	N-CA-C	5.84	119.66	112.54
7	2-G	631	LYS	N-CA-C	-5.84	99.27	108.14
7	2-K	95	MET	N-CA-C	5.84	119.66	112.54
7	3-G	631	LYS	N-CA-C	-5.84	99.27	108.14
7	3-K	95	MET	N-CA-C	5.84	119.66	112.54
6	1-F	116	LEU	CA-C-N	5.84	132.69	121.54
6	1-F	116	LEU	C-N-CA	5.84	132.69	121.54
6	2-F	116	LEU	CA-C-N	5.84	132.69	121.54
6	2-F	116	LEU	C-N-CA	5.84	132.69	121.54
6	3-F	116	LEU	CA-C-N	5.84	132.69	121.54
6	3-F	116	LEU	C-N-CA	5.84	132.69	121.54
7	1-G	29	GLN	CA-C-N	5.84	129.94	120.60
7	1-G	29	GLN	C-N-CA	5.84	129.94	120.60
3	1-N	369	GLU	N-CA-C	5.84	117.72	111.36
7	2-G	29	GLN	CA-C-N	5.84	129.94	120.60
7	2-G	29	GLN	C-N-CA	5.84	129.94	120.60
3	2-N	369	GLU	N-CA-C	5.84	117.72	111.36
7	3-G	29	GLN	CA-C-N	5.84	129.94	120.60
7	3-G	29	GLN	C-N-CA	5.84	129.94	120.60
3	3-N	369	GLU	N-CA-C	5.84	117.72	111.36
6	1-J	121	TRP	CA-C-N	5.83	131.23	123.00
6	1-J	121	TRP	C-N-CA	5.83	131.23	123.00
6	2-J	121	TRP	CA-C-N	5.83	131.23	123.00
6	2-J	121	TRP	C-N-CA	5.83	131.23	123.00
6	3-J	121	TRP	CA-C-N	5.83	131.23	123.00
6	3-J	121	TRP	C-N-CA	5.83	131.23	123.00
6	1-F	121	TRP	CA-C-N	5.83	131.22	123.00
6	1-F	121	TRP	C-N-CA	5.83	131.22	123.00
7	1-G	293	GLN	CA-C-N	5.83	128.02	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	293	GLN	C-N-CA	5.83	128.02	120.44
6	2-F	121	TRP	CA-C-N	5.83	131.22	123.00
6	2-F	121	TRP	C-N-CA	5.83	131.22	123.00
7	2-G	293	GLN	CA-C-N	5.83	128.02	120.44
7	2-G	293	GLN	C-N-CA	5.83	128.02	120.44
6	3-F	121	TRP	CA-C-N	5.83	131.22	123.00
6	3-F	121	TRP	C-N-CA	5.83	131.22	123.00
7	3-G	293	GLN	CA-C-N	5.83	128.02	120.44
7	3-G	293	GLN	C-N-CA	5.83	128.02	120.44
3	1-B	129	GLU	N-CA-C	5.83	117.71	111.36
7	1-K	221	HIS	CA-C-N	5.83	132.83	121.41
7	1-K	221	HIS	C-N-CA	5.83	132.83	121.41
3	2-B	129	GLU	N-CA-C	5.83	117.71	111.36
7	2-K	221	HIS	CA-C-N	5.83	132.83	121.41
7	2-K	221	HIS	C-N-CA	5.83	132.83	121.41
3	3-B	129	GLU	N-CA-C	5.83	117.71	111.36
7	3-K	221	HIS	CA-C-N	5.83	132.83	121.41
7	3-K	221	HIS	C-N-CA	5.83	132.83	121.41
4	1-H	571	ASN	CA-C-N	-5.83	112.77	122.21
4	1-H	571	ASN	C-N-CA	-5.83	112.77	122.21
4	2-H	571	ASN	CA-C-N	-5.83	112.77	122.21
4	2-H	571	ASN	C-N-CA	-5.83	112.77	122.21
4	3-H	571	ASN	CA-C-N	-5.83	112.77	122.21
4	3-H	571	ASN	C-N-CA	-5.83	112.77	122.21
1	1-A	65	LEU	N-CA-C	-5.82	99.88	108.79
1	2-A	65	LEU	N-CA-C	-5.82	99.88	108.79
1	3-A	65	LEU	N-CA-C	-5.82	99.88	108.79
1	1-A	934	GLY	N-CA-C	-5.82	107.06	115.27
1	2-A	934	GLY	N-CA-C	-5.82	107.06	115.27
1	3-A	934	GLY	N-CA-C	-5.82	107.06	115.27
1	1-A	47	PHE	N-CA-C	-5.82	99.16	109.06
4	1-H	82	ARG	N-CA-C	-5.82	100.30	109.50
1	2-A	47	PHE	N-CA-C	-5.82	99.16	109.06
4	2-H	82	ARG	N-CA-C	-5.82	100.30	109.50
1	3-A	47	PHE	N-CA-C	-5.82	99.16	109.06
4	3-H	82	ARG	N-CA-C	-5.82	100.30	109.50
3	1-B	923	ASN	N-CA-C	-5.82	98.80	108.34
4	1-C	571	ASN	CA-C-N	-5.82	112.78	122.21
4	1-C	571	ASN	C-N-CA	-5.82	112.78	122.21
8	1-L	27	PHE	N-CA-C	-5.82	98.80	108.75
3	2-B	923	ASN	N-CA-C	-5.82	98.80	108.34
4	2-C	571	ASN	CA-C-N	-5.82	112.78	122.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-C	571	ASN	C-N-CA	-5.82	112.78	122.21
8	2-L	27	PHE	N-CA-C	-5.82	98.80	108.75
3	3-B	923	ASN	N-CA-C	-5.82	98.80	108.34
4	3-C	571	ASN	CA-C-N	-5.82	112.78	122.21
4	3-C	571	ASN	C-N-CA	-5.82	112.78	122.21
8	3-L	27	PHE	N-CA-C	-5.82	98.80	108.75
7	1-G	608	THR	CA-C-N	5.81	128.07	120.28
7	1-G	608	THR	C-N-CA	5.81	128.07	120.28
7	2-G	608	THR	CA-C-N	5.81	128.07	120.28
7	2-G	608	THR	C-N-CA	5.81	128.07	120.28
7	3-G	608	THR	CA-C-N	5.81	128.07	120.28
7	3-G	608	THR	C-N-CA	5.81	128.07	120.28
6	1-J	160	ALA	N-CA-C	-5.81	103.64	112.99
6	2-J	160	ALA	N-CA-C	-5.81	103.64	112.99
6	3-J	160	ALA	N-CA-C	-5.81	103.64	112.99
6	1-J	20	ILE	N-CA-C	-5.81	100.12	108.48
6	2-J	20	ILE	N-CA-C	-5.81	100.12	108.48
6	3-J	20	ILE	N-CA-C	-5.81	100.12	108.48
1	1-A	531	LYS	CA-C-N	5.80	131.72	121.80
1	1-A	531	LYS	C-N-CA	5.80	131.72	121.80
4	1-C	82	ARG	N-CA-C	-5.80	100.33	109.50
4	1-C	152	PRO	CA-C-N	5.80	127.98	120.44
4	1-C	152	PRO	C-N-CA	5.80	127.98	120.44
1	2-A	531	LYS	CA-C-N	5.80	131.72	121.80
1	2-A	531	LYS	C-N-CA	5.80	131.72	121.80
4	2-C	82	ARG	N-CA-C	-5.80	100.33	109.50
4	2-C	152	PRO	CA-C-N	5.80	127.98	120.44
4	2-C	152	PRO	C-N-CA	5.80	127.98	120.44
1	3-A	531	LYS	CA-C-N	5.80	131.72	121.80
1	3-A	531	LYS	C-N-CA	5.80	131.72	121.80
4	3-C	82	ARG	N-CA-C	-5.80	100.33	109.50
4	3-C	152	PRO	CA-C-N	5.80	127.98	120.44
4	3-C	152	PRO	C-N-CA	5.80	127.98	120.44
1	1-A	577	ASN	N-CA-C	-5.80	98.44	110.80
6	1-F	160	ALA	N-CA-C	-5.80	103.65	112.99
6	1-F	169	GLY	N-CA-C	-5.80	105.77	112.50
1	2-A	577	ASN	N-CA-C	-5.80	98.44	110.80
6	2-F	160	ALA	N-CA-C	-5.80	103.65	112.99
6	2-F	169	GLY	N-CA-C	-5.80	105.77	112.50
1	3-A	577	ASN	N-CA-C	-5.80	98.44	110.80
6	3-F	160	ALA	N-CA-C	-5.80	103.65	112.99
6	3-F	169	GLY	N-CA-C	-5.80	105.77	112.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-N	384	ASN	N-CA-C	5.80	123.15	110.80
3	2-N	384	ASN	N-CA-C	5.80	123.15	110.80
3	3-N	384	ASN	N-CA-C	5.80	123.15	110.80
6	1-J	169	GLY	N-CA-C	-5.80	105.78	112.50
6	2-J	169	GLY	N-CA-C	-5.80	105.78	112.50
6	3-J	169	GLY	N-CA-C	-5.80	105.78	112.50
4	1-C	533	CYS	CA-C-N	-5.79	114.94	123.05
4	1-C	533	CYS	C-N-CA	-5.79	114.94	123.05
6	1-F	20	ILE	N-CA-C	-5.79	100.14	108.48
7	1-G	843	ARG	N-CA-C	-5.79	98.97	108.76
7	1-K	608	THR	CA-C-N	5.79	128.04	120.28
7	1-K	608	THR	C-N-CA	5.79	128.04	120.28
4	2-C	533	CYS	CA-C-N	-5.79	114.94	123.05
4	2-C	533	CYS	C-N-CA	-5.79	114.94	123.05
6	2-F	20	ILE	N-CA-C	-5.79	100.14	108.48
7	2-G	843	ARG	N-CA-C	-5.79	98.97	108.76
7	2-K	608	THR	CA-C-N	5.79	128.04	120.28
7	2-K	608	THR	C-N-CA	5.79	128.04	120.28
4	3-C	533	CYS	CA-C-N	-5.79	114.94	123.05
4	3-C	533	CYS	C-N-CA	-5.79	114.94	123.05
6	3-F	20	ILE	N-CA-C	-5.79	100.14	108.48
7	3-G	843	ARG	N-CA-C	-5.79	98.97	108.76
7	3-K	608	THR	CA-C-N	5.79	128.04	120.28
7	3-K	608	THR	C-N-CA	5.79	128.04	120.28
1	1-A	181	VAL	N-CA-C	-5.79	104.71	110.62
1	1-A	670	ASP	N-CA-C	-5.79	106.03	112.57
1	2-A	181	VAL	N-CA-C	-5.79	104.71	110.62
1	2-A	670	ASP	N-CA-C	-5.79	106.03	112.57
1	3-A	181	VAL	N-CA-C	-5.79	104.71	110.62
1	3-A	670	ASP	N-CA-C	-5.79	106.03	112.57
4	1-C	256	TRP	N-CA-C	-5.79	100.46	109.72
4	2-C	256	TRP	N-CA-C	-5.79	100.46	109.72
4	3-C	256	TRP	N-CA-C	-5.79	100.46	109.72
1	1-A	258	HIS	CA-C-N	5.78	127.07	119.84
1	1-A	258	HIS	C-N-CA	5.78	127.07	119.84
1	2-A	258	HIS	CA-C-N	5.78	127.07	119.84
1	2-A	258	HIS	C-N-CA	5.78	127.07	119.84
1	3-A	258	HIS	CA-C-N	5.78	127.07	119.84
1	3-A	258	HIS	C-N-CA	5.78	127.07	119.84
7	1-G	867	ASP	CA-C-N	5.78	127.84	120.56
7	1-G	867	ASP	C-N-CA	5.78	127.84	120.56
4	1-H	300	GLY	N-CA-C	5.78	121.62	111.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-G	867	ASP	CA-C-N	5.78	127.84	120.56
7	2-G	867	ASP	C-N-CA	5.78	127.84	120.56
4	2-H	300	GLY	N-CA-C	5.78	121.62	111.57
7	3-G	867	ASP	CA-C-N	5.78	127.84	120.56
7	3-G	867	ASP	C-N-CA	5.78	127.84	120.56
4	3-H	300	GLY	N-CA-C	5.78	121.62	111.57
1	1-A	374	GLU	N-CA-C	-5.78	106.62	113.38
3	1-B	384	ASN	N-CA-C	5.78	123.10	110.80
1	2-A	374	GLU	N-CA-C	-5.78	106.62	113.38
3	2-B	384	ASN	N-CA-C	5.78	123.10	110.80
1	3-A	374	GLU	N-CA-C	-5.78	106.62	113.38
3	3-B	384	ASN	N-CA-C	5.78	123.10	110.80
4	1-H	256	TRP	N-CA-C	-5.77	100.49	109.72
4	2-H	256	TRP	N-CA-C	-5.77	100.49	109.72
4	3-H	256	TRP	N-CA-C	-5.77	100.49	109.72
4	1-C	508	ASP	N-CA-C	-5.77	105.90	113.17
4	1-H	375	TYR	N-CA-C	5.77	117.92	108.52
4	2-C	508	ASP	N-CA-C	-5.77	105.90	113.17
4	2-H	375	TYR	N-CA-C	5.77	117.92	108.52
4	3-C	508	ASP	N-CA-C	-5.77	105.90	113.17
4	3-H	375	TYR	N-CA-C	5.77	117.92	108.52
6	1-R	62	SER	CA-C-N	5.77	130.32	122.19
6	1-R	62	SER	C-N-CA	5.77	130.32	122.19
6	2-R	62	SER	CA-C-N	5.77	130.32	122.19
6	2-R	62	SER	C-N-CA	5.77	130.32	122.19
6	3-R	62	SER	CA-C-N	5.77	130.32	122.19
6	3-R	62	SER	C-N-CA	5.77	130.32	122.19
8	1-L	104	MET	N-CA-C	-5.76	104.90	111.07
8	2-L	104	MET	N-CA-C	-5.76	104.90	111.07
8	3-L	104	MET	N-CA-C	-5.76	104.90	111.07
1	1-A	248	HIS	N-CA-C	-5.76	98.53	110.80
3	1-B	916	PHE	N-CA-C	-5.76	104.92	112.41
6	1-R	117	ARG	N-CA-C	-5.76	105.51	112.54
7	1-K	843	ARG	N-CA-C	-5.76	99.02	108.76
1	2-A	248	HIS	N-CA-C	-5.76	98.53	110.80
3	2-B	916	PHE	N-CA-C	-5.76	104.92	112.41
6	2-R	117	ARG	N-CA-C	-5.76	105.51	112.54
7	2-K	843	ARG	N-CA-C	-5.76	99.02	108.76
1	3-A	248	HIS	N-CA-C	-5.76	98.53	110.80
3	3-B	916	PHE	N-CA-C	-5.76	104.92	112.41
6	3-R	117	ARG	N-CA-C	-5.76	105.51	112.54
7	3-K	843	ARG	N-CA-C	-5.76	99.02	108.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	784	THR	N-CA-C	-5.76	99.98	108.79
4	1-C	300	GLY	N-CA-C	5.76	121.59	111.57
7	1-G	675	GLU	N-CA-C	-5.76	100.54	109.24
1	2-A	784	THR	N-CA-C	-5.76	99.98	108.79
4	2-C	300	GLY	N-CA-C	5.76	121.59	111.57
7	2-G	675	GLU	N-CA-C	-5.76	100.54	109.24
1	3-A	784	THR	N-CA-C	-5.76	99.98	108.79
4	3-C	300	GLY	N-CA-C	5.76	121.59	111.57
7	3-G	675	GLU	N-CA-C	-5.76	100.54	109.24
3	1-B	770	ASN	CA-C-N	5.76	132.54	121.54
3	1-B	770	ASN	C-N-CA	5.76	132.54	121.54
3	2-B	770	ASN	CA-C-N	5.76	132.54	121.54
3	2-B	770	ASN	C-N-CA	5.76	132.54	121.54
3	3-B	770	ASN	CA-C-N	5.76	132.54	121.54
3	3-B	770	ASN	C-N-CA	5.76	132.54	121.54
7	1-G	104	ILE	N-CA-C	5.76	116.49	110.62
6	1-M	30	LYS	CA-C-N	5.76	127.99	120.28
6	1-M	30	LYS	C-N-CA	5.76	127.99	120.28
7	2-G	104	ILE	N-CA-C	5.76	116.49	110.62
6	2-M	30	LYS	CA-C-N	5.76	127.99	120.28
6	2-M	30	LYS	C-N-CA	5.76	127.99	120.28
7	3-G	104	ILE	N-CA-C	5.76	116.49	110.62
6	3-M	30	LYS	CA-C-N	5.76	127.99	120.28
6	3-M	30	LYS	C-N-CA	5.76	127.99	120.28
1	1-A	120	TRP	N-CA-C	5.75	118.78	109.40
1	2-A	120	TRP	N-CA-C	5.75	118.78	109.40
1	3-A	120	TRP	N-CA-C	5.75	118.78	109.40
4	1-C	801	LEU	CA-C-O	-5.75	114.85	122.44
7	1-K	26	ALA	CA-C-N	5.75	128.34	120.46
7	1-K	26	ALA	C-N-CA	5.75	128.34	120.46
8	1-L	110	GLU	N-CA-C	-5.75	100.81	108.34
4	2-C	801	LEU	CA-C-O	-5.75	114.85	122.44
7	2-K	26	ALA	CA-C-N	5.75	128.34	120.46
7	2-K	26	ALA	C-N-CA	5.75	128.34	120.46
8	2-L	110	GLU	N-CA-C	-5.75	100.81	108.34
4	3-C	801	LEU	CA-C-O	-5.75	114.85	122.44
7	3-K	26	ALA	CA-C-N	5.75	128.34	120.46
7	3-K	26	ALA	C-N-CA	5.75	128.34	120.46
8	3-L	110	GLU	N-CA-C	-5.75	100.81	108.34
3	1-B	849	THR	CA-C-O	-5.75	114.91	121.58
4	1-C	228	HIS	N-CA-C	5.75	123.05	110.80
3	2-B	849	THR	CA-C-O	-5.75	114.91	121.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-C	228	HIS	N-CA-C	5.75	123.05	110.80
3	3-B	849	THR	CA-C-O	-5.75	114.91	121.58
4	3-C	228	HIS	N-CA-C	5.75	123.05	110.80
3	1-B	512	ALA	N-CA-C	5.75	117.22	111.07
4	1-C	375	TYR	N-CA-C	5.75	117.89	108.52
7	1-G	428	ASN	CA-C-N	5.75	129.27	120.82
7	1-G	428	ASN	C-N-CA	5.75	129.27	120.82
3	2-B	512	ALA	N-CA-C	5.75	117.22	111.07
4	2-C	375	TYR	N-CA-C	5.75	117.89	108.52
7	2-G	428	ASN	CA-C-N	5.75	129.27	120.82
7	2-G	428	ASN	C-N-CA	5.75	129.27	120.82
3	3-B	512	ALA	N-CA-C	5.75	117.22	111.07
4	3-C	375	TYR	N-CA-C	5.75	117.89	108.52
7	3-G	428	ASN	CA-C-N	5.75	129.27	120.82
7	3-G	428	ASN	C-N-CA	5.75	129.27	120.82
6	1-R	26	ASP	N-CA-C	-5.74	100.46	109.25
4	1-H	228	HIS	N-CA-C	5.74	123.03	110.80
6	2-R	26	ASP	N-CA-C	-5.74	100.46	109.25
4	2-H	228	HIS	N-CA-C	5.74	123.03	110.80
6	3-R	26	ASP	N-CA-C	-5.74	100.46	109.25
4	3-H	228	HIS	N-CA-C	5.74	123.03	110.80
3	1-N	129	GLU	N-CA-C	5.74	117.62	111.36
3	2-N	129	GLU	N-CA-C	5.74	117.62	111.36
3	3-N	129	GLU	N-CA-C	5.74	117.62	111.36
7	1-G	373	ASP	N-CA-C	-5.74	98.58	110.80
4	1-H	533	CYS	CA-C-N	-5.74	115.01	123.05
4	1-H	533	CYS	C-N-CA	-5.74	115.01	123.05
7	2-G	373	ASP	N-CA-C	-5.74	98.58	110.80
4	2-H	533	CYS	CA-C-N	-5.74	115.01	123.05
4	2-H	533	CYS	C-N-CA	-5.74	115.01	123.05
7	3-G	373	ASP	N-CA-C	-5.74	98.58	110.80
4	3-H	533	CYS	CA-C-N	-5.74	115.01	123.05
4	3-H	533	CYS	C-N-CA	-5.74	115.01	123.05
1	1-A	796	GLN	CA-C-N	-5.74	114.47	120.38
1	1-A	796	GLN	C-N-CA	-5.74	114.47	120.38
1	2-A	796	GLN	CA-C-N	-5.74	114.47	120.38
1	2-A	796	GLN	C-N-CA	-5.74	114.47	120.38
1	3-A	796	GLN	CA-C-N	-5.74	114.47	120.38
1	3-A	796	GLN	C-N-CA	-5.74	114.47	120.38
7	1-K	306	ALA	N-CA-C	-5.74	105.11	111.36
7	2-K	306	ALA	N-CA-C	-5.74	105.11	111.36
7	3-K	306	ALA	N-CA-C	-5.74	105.11	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	261	TYR	N-CA-C	-5.73	105.58	112.58
4	2-H	261	TYR	N-CA-C	-5.73	105.58	112.58
4	3-H	261	TYR	N-CA-C	-5.73	105.58	112.58
1	1-A	549	ILE	CA-C-O	-5.73	114.43	120.39
1	1-A	638	ALA	N-CA-C	-5.73	105.03	111.28
3	1-B	130	PHE	CA-C-N	5.73	127.78	120.56
3	1-B	130	PHE	C-N-CA	5.73	127.78	120.56
3	1-N	110	LEU	CA-C-N	5.73	132.49	121.54
3	1-N	110	LEU	C-N-CA	5.73	132.49	121.54
1	2-A	549	ILE	CA-C-O	-5.73	114.43	120.39
1	2-A	638	ALA	N-CA-C	-5.73	105.03	111.28
3	2-B	130	PHE	CA-C-N	5.73	127.78	120.56
3	2-B	130	PHE	C-N-CA	5.73	127.78	120.56
3	2-N	110	LEU	CA-C-N	5.73	132.49	121.54
3	2-N	110	LEU	C-N-CA	5.73	132.49	121.54
1	3-A	549	ILE	CA-C-O	-5.73	114.43	120.39
1	3-A	638	ALA	N-CA-C	-5.73	105.03	111.28
3	3-B	130	PHE	CA-C-N	5.73	127.78	120.56
3	3-B	130	PHE	C-N-CA	5.73	127.78	120.56
3	3-N	110	LEU	CA-C-N	5.73	132.49	121.54
3	3-N	110	LEU	C-N-CA	5.73	132.49	121.54
4	1-C	261	TYR	N-CA-C	-5.73	105.59	112.58
4	1-H	368	VAL	CA-C-O	5.73	126.41	120.39
4	2-C	261	TYR	N-CA-C	-5.73	105.59	112.58
4	2-H	368	VAL	CA-C-O	5.73	126.41	120.39
4	3-C	261	TYR	N-CA-C	-5.73	105.59	112.58
4	3-H	368	VAL	CA-C-O	5.73	126.41	120.39
3	1-B	937	ALA	N-CA-C	-5.73	98.60	110.80
7	1-K	867	ASP	CA-C-N	5.73	127.78	120.56
7	1-K	867	ASP	C-N-CA	5.73	127.78	120.56
3	2-B	937	ALA	N-CA-C	-5.73	98.60	110.80
7	2-K	867	ASP	CA-C-N	5.73	127.78	120.56
7	2-K	867	ASP	C-N-CA	5.73	127.78	120.56
3	3-B	937	ALA	N-CA-C	-5.73	98.60	110.80
7	3-K	867	ASP	CA-C-N	5.73	127.78	120.56
7	3-K	867	ASP	C-N-CA	5.73	127.78	120.56
4	1-C	504	GLY	CA-C-N	5.73	130.29	123.19
4	1-C	504	GLY	C-N-CA	5.73	130.29	123.19
4	2-C	504	GLY	CA-C-N	5.73	130.29	123.19
4	2-C	504	GLY	C-N-CA	5.73	130.29	123.19
4	3-C	504	GLY	CA-C-N	5.73	130.29	123.19
4	3-C	504	GLY	C-N-CA	5.73	130.29	123.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	567	ILE	CA-C-N	5.72	125.57	119.28
4	1-H	567	ILE	C-N-CA	5.72	125.57	119.28
4	2-H	567	ILE	CA-C-N	5.72	125.57	119.28
4	2-H	567	ILE	C-N-CA	5.72	125.57	119.28
4	3-H	567	ILE	CA-C-N	5.72	125.57	119.28
4	3-H	567	ILE	C-N-CA	5.72	125.57	119.28
4	1-C	529	TRP	N-CA-C	-5.72	99.92	109.24
4	1-H	504	GLY	CA-C-N	5.72	130.28	123.19
4	1-H	504	GLY	C-N-CA	5.72	130.28	123.19
4	2-C	529	TRP	N-CA-C	-5.72	99.92	109.24
4	2-H	504	GLY	CA-C-N	5.72	130.28	123.19
4	2-H	504	GLY	C-N-CA	5.72	130.28	123.19
4	3-C	529	TRP	N-CA-C	-5.72	99.92	109.24
4	3-H	504	GLY	CA-C-N	5.72	130.28	123.19
4	3-H	504	GLY	C-N-CA	5.72	130.28	123.19
7	1-G	103	ILE	N-CA-C	5.72	119.06	111.17
7	2-G	103	ILE	N-CA-C	5.72	119.06	111.17
7	3-G	103	ILE	N-CA-C	5.72	119.06	111.17
4	1-H	456	GLU	CA-C-O	-5.71	113.69	120.43
4	2-H	456	GLU	CA-C-O	-5.71	113.69	120.43
4	3-H	456	GLU	CA-C-O	-5.71	113.69	120.43
7	1-K	208	ARG	N-CA-C	5.71	117.31	111.14
7	2-K	208	ARG	N-CA-C	5.71	117.31	111.14
7	3-K	208	ARG	N-CA-C	5.71	117.31	111.14
4	1-H	508	ASP	N-CA-C	-5.71	105.98	113.17
4	2-H	508	ASP	N-CA-C	-5.71	105.98	113.17
4	3-H	508	ASP	N-CA-C	-5.71	105.98	113.17
1	1-A	681	ALA	N-CA-C	-5.71	104.96	111.07
3	1-N	512	ALA	N-CA-C	5.71	117.17	111.07
1	2-A	681	ALA	N-CA-C	-5.71	104.96	111.07
3	2-N	512	ALA	N-CA-C	5.71	117.17	111.07
1	3-A	681	ALA	N-CA-C	-5.71	104.96	111.07
3	3-N	512	ALA	N-CA-C	5.71	117.17	111.07
1	1-A	554	THR	CA-C-N	5.70	132.44	121.54
1	1-A	554	THR	C-N-CA	5.70	132.44	121.54
4	1-C	368	VAL	CA-C-O	5.70	126.38	120.39
1	2-A	554	THR	CA-C-N	5.70	132.44	121.54
1	2-A	554	THR	C-N-CA	5.70	132.44	121.54
4	2-C	368	VAL	CA-C-O	5.70	126.38	120.39
1	3-A	554	THR	CA-C-N	5.70	132.44	121.54
1	3-A	554	THR	C-N-CA	5.70	132.44	121.54
4	3-C	368	VAL	CA-C-O	5.70	126.38	120.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	456	GLU	CA-C-O	-5.70	113.70	120.43
7	1-G	692	TYR	CA-C-N	-5.70	116.98	123.25
7	1-G	692	TYR	C-N-CA	-5.70	116.98	123.25
4	2-C	456	GLU	CA-C-O	-5.70	113.70	120.43
7	2-G	692	TYR	CA-C-N	-5.70	116.98	123.25
7	2-G	692	TYR	C-N-CA	-5.70	116.98	123.25
4	3-C	456	GLU	CA-C-O	-5.70	113.70	120.43
7	3-G	692	TYR	CA-C-N	-5.70	116.98	123.25
7	3-G	692	TYR	C-N-CA	-5.70	116.98	123.25
3	1-N	130	PHE	CA-C-N	5.70	127.74	120.56
3	1-N	130	PHE	C-N-CA	5.70	127.74	120.56
3	2-N	130	PHE	CA-C-N	5.70	127.74	120.56
3	2-N	130	PHE	C-N-CA	5.70	127.74	120.56
3	3-N	130	PHE	CA-C-N	5.70	127.74	120.56
3	3-N	130	PHE	C-N-CA	5.70	127.74	120.56
7	1-K	675	GLU	N-CA-C	-5.70	100.64	109.24
7	2-K	675	GLU	N-CA-C	-5.70	100.64	109.24
7	3-K	675	GLU	N-CA-C	-5.70	100.64	109.24
1	1-A	106	PRO	CA-C-N	5.69	132.32	122.64
1	1-A	106	PRO	C-N-CA	5.69	132.32	122.64
1	2-A	106	PRO	CA-C-N	5.69	132.32	122.64
1	2-A	106	PRO	C-N-CA	5.69	132.32	122.64
1	3-A	106	PRO	CA-C-N	5.69	132.32	122.64
1	3-A	106	PRO	C-N-CA	5.69	132.32	122.64
4	1-C	567	ILE	CA-C-N	5.69	125.54	119.28
4	1-C	567	ILE	C-N-CA	5.69	125.54	119.28
4	1-C	784	ALA	N-CA-C	-5.69	105.08	111.28
4	2-C	567	ILE	CA-C-N	5.69	125.54	119.28
4	2-C	567	ILE	C-N-CA	5.69	125.54	119.28
4	2-C	784	ALA	N-CA-C	-5.69	105.08	111.28
4	3-C	567	ILE	CA-C-N	5.69	125.54	119.28
4	3-C	567	ILE	C-N-CA	5.69	125.54	119.28
4	3-C	784	ALA	N-CA-C	-5.69	105.08	111.28
3	1-B	110	LEU	CA-C-N	5.69	132.41	121.54
3	1-B	110	LEU	C-N-CA	5.69	132.41	121.54
7	1-K	135	THR	N-CA-C	5.69	122.92	110.80
3	2-B	110	LEU	CA-C-N	5.69	132.41	121.54
3	2-B	110	LEU	C-N-CA	5.69	132.41	121.54
7	2-K	135	THR	N-CA-C	5.69	122.92	110.80
3	3-B	110	LEU	CA-C-N	5.69	132.41	121.54
3	3-B	110	LEU	C-N-CA	5.69	132.41	121.54
7	3-K	135	THR	N-CA-C	5.69	122.92	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-B	799	ASN	CA-C-N	-5.69	115.03	122.94
3	1-B	799	ASN	C-N-CA	-5.69	115.03	122.94
3	2-B	799	ASN	CA-C-N	-5.69	115.03	122.94
3	2-B	799	ASN	C-N-CA	-5.69	115.03	122.94
3	3-B	799	ASN	CA-C-N	-5.69	115.03	122.94
3	3-B	799	ASN	C-N-CA	-5.69	115.03	122.94
3	1-B	447	ASP	N-CA-C	5.69	122.92	110.80
4	1-C	522	GLU	N-CA-C	5.69	118.05	109.23
3	2-B	447	ASP	N-CA-C	5.69	122.92	110.80
4	2-C	522	GLU	N-CA-C	5.69	118.05	109.23
3	3-B	447	ASP	N-CA-C	5.69	122.92	110.80
4	3-C	522	GLU	N-CA-C	5.69	118.05	109.23
7	1-K	830	LEU	N-CA-C	5.69	118.48	109.50
7	2-K	830	LEU	N-CA-C	5.69	118.48	109.50
7	3-K	830	LEU	N-CA-C	5.69	118.48	109.50
3	1-B	127	PRO	CA-C-N	5.68	132.40	121.54
3	1-B	127	PRO	C-N-CA	5.68	132.40	121.54
3	2-B	127	PRO	CA-C-N	5.68	132.40	121.54
3	2-B	127	PRO	C-N-CA	5.68	132.40	121.54
3	3-B	127	PRO	CA-C-N	5.68	132.40	121.54
3	3-B	127	PRO	C-N-CA	5.68	132.40	121.54
1	1-A	450	VAL	CA-C-N	5.68	126.01	119.93
1	1-A	450	VAL	C-N-CA	5.68	126.01	119.93
3	1-B	412	MET	O-C-N	-5.68	118.85	123.11
1	2-A	450	VAL	CA-C-N	5.68	126.01	119.93
1	2-A	450	VAL	C-N-CA	5.68	126.01	119.93
3	2-B	412	MET	O-C-N	-5.68	118.85	123.11
1	3-A	450	VAL	CA-C-N	5.68	126.01	119.93
1	3-A	450	VAL	C-N-CA	5.68	126.01	119.93
3	3-B	412	MET	O-C-N	-5.68	118.85	123.11
8	1-Z	83	SER	N-CA-C	-5.68	98.46	108.23
8	2-Z	83	SER	N-CA-C	-5.68	98.46	108.23
8	3-Z	83	SER	N-CA-C	-5.68	98.46	108.23
4	1-H	529	TRP	N-CA-C	-5.68	99.98	109.24
4	2-H	529	TRP	N-CA-C	-5.68	99.98	109.24
4	3-H	529	TRP	N-CA-C	-5.68	99.98	109.24
4	1-H	268	ASN	N-CA-C	5.68	117.96	108.02
4	2-H	268	ASN	N-CA-C	5.68	117.96	108.02
4	3-H	268	ASN	N-CA-C	5.68	117.96	108.02
3	1-B	327	PRO	N-CA-C	-5.67	106.61	114.27
3	1-N	327	PRO	N-CA-C	-5.67	106.61	114.27
5	1-I	49	VAL	N-CA-C	-5.67	100.31	108.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2-B	327	PRO	N-CA-C	-5.67	106.61	114.27
3	2-N	327	PRO	N-CA-C	-5.67	106.61	114.27
5	2-I	49	VAL	N-CA-C	-5.67	100.31	108.42
3	3-B	327	PRO	N-CA-C	-5.67	106.61	114.27
3	3-N	327	PRO	N-CA-C	-5.67	106.61	114.27
5	3-I	49	VAL	N-CA-C	-5.67	100.31	108.42
4	1-C	227	GLY	CA-C-N	5.67	132.37	121.54
4	1-C	227	GLY	C-N-CA	5.67	132.37	121.54
4	1-H	522	GLU	N-CA-C	5.67	118.02	109.23
4	2-C	227	GLY	CA-C-N	5.67	132.37	121.54
4	2-C	227	GLY	C-N-CA	5.67	132.37	121.54
4	2-H	522	GLU	N-CA-C	5.67	118.02	109.23
4	3-C	227	GLY	CA-C-N	5.67	132.37	121.54
4	3-C	227	GLY	C-N-CA	5.67	132.37	121.54
4	3-H	522	GLU	N-CA-C	5.67	118.02	109.23
1	1-A	245	CYS	O-C-N	5.67	129.67	123.27
1	2-A	245	CYS	O-C-N	5.67	129.67	123.27
1	3-A	245	CYS	O-C-N	5.67	129.67	123.27
1	1-A	180	ASP	N-CA-C	-5.66	106.72	113.97
3	1-B	809	THR	CA-C-N	-5.66	113.71	122.09
3	1-B	809	THR	C-N-CA	-5.66	113.71	122.09
4	1-C	768	ARG	N-CA-C	5.66	117.13	111.07
1	2-A	180	ASP	N-CA-C	-5.66	106.72	113.97
3	2-B	809	THR	CA-C-N	-5.66	113.71	122.09
3	2-B	809	THR	C-N-CA	-5.66	113.71	122.09
4	2-C	768	ARG	N-CA-C	5.66	117.13	111.07
1	3-A	180	ASP	N-CA-C	-5.66	106.72	113.97
3	3-B	809	THR	CA-C-N	-5.66	113.71	122.09
3	3-B	809	THR	C-N-CA	-5.66	113.71	122.09
4	3-C	768	ARG	N-CA-C	5.66	117.13	111.07
3	1-B	926	ILE	O-C-N	-5.66	117.09	123.20
7	1-G	325	CYS	N-CA-C	5.66	117.45	111.28
3	1-N	127	PRO	CA-C-N	5.66	132.35	121.54
3	1-N	127	PRO	C-N-CA	5.66	132.35	121.54
3	2-B	926	ILE	O-C-N	-5.66	117.09	123.20
7	2-G	325	CYS	N-CA-C	5.66	117.45	111.28
3	2-N	127	PRO	CA-C-N	5.66	132.35	121.54
3	2-N	127	PRO	C-N-CA	5.66	132.35	121.54
3	3-B	926	ILE	O-C-N	-5.66	117.09	123.20
7	3-G	325	CYS	N-CA-C	5.66	117.45	111.28
3	3-N	127	PRO	CA-C-N	5.66	132.35	121.54
3	3-N	127	PRO	C-N-CA	5.66	132.35	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-N	447	ASP	N-CA-C	5.66	122.85	110.80
3	2-N	447	ASP	N-CA-C	5.66	122.85	110.80
3	3-N	447	ASP	N-CA-C	5.66	122.85	110.80
7	1-K	290	SER	CA-C-O	5.66	126.76	120.82
7	2-K	290	SER	CA-C-O	5.66	126.76	120.82
7	3-K	290	SER	CA-C-O	5.66	126.76	120.82
4	1-C	433	ILE	N-CA-C	-5.66	100.03	108.46
7	1-K	711	ALA	N-CA-C	-5.66	100.49	109.59
4	2-C	433	ILE	N-CA-C	-5.66	100.03	108.46
7	2-K	711	ALA	N-CA-C	-5.66	100.49	109.59
4	3-C	433	ILE	N-CA-C	-5.66	100.03	108.46
7	3-K	711	ALA	N-CA-C	-5.66	100.49	109.59
1	1-A	12	VAL	N-CA-C	5.65	115.74	107.37
1	1-A	803	PRO	CA-C-N	5.65	132.34	121.54
1	1-A	803	PRO	C-N-CA	5.65	132.34	121.54
5	1-D	49	VAL	N-CA-C	-5.65	100.34	108.42
1	2-A	12	VAL	N-CA-C	5.65	115.74	107.37
1	2-A	803	PRO	CA-C-N	5.65	132.34	121.54
1	2-A	803	PRO	C-N-CA	5.65	132.34	121.54
5	2-D	49	VAL	N-CA-C	-5.65	100.34	108.42
1	3-A	12	VAL	N-CA-C	5.65	115.74	107.37
1	3-A	803	PRO	CA-C-N	5.65	132.34	121.54
1	3-A	803	PRO	C-N-CA	5.65	132.34	121.54
5	3-D	49	VAL	N-CA-C	-5.65	100.34	108.42
8	1-L	19	LEU	CA-C-O	-5.65	114.72	121.11
8	2-L	19	LEU	CA-C-O	-5.65	114.72	121.11
8	3-L	19	LEU	CA-C-O	-5.65	114.72	121.11
7	1-G	830	LEU	N-CA-C	5.64	118.42	109.50
3	1-N	254	PRO	CA-C-N	5.64	132.32	121.54
3	1-N	254	PRO	C-N-CA	5.64	132.32	121.54
7	2-G	830	LEU	N-CA-C	5.64	118.42	109.50
3	2-N	254	PRO	CA-C-N	5.64	132.32	121.54
3	2-N	254	PRO	C-N-CA	5.64	132.32	121.54
7	3-G	830	LEU	N-CA-C	5.64	118.42	109.50
3	3-N	254	PRO	CA-C-N	5.64	132.32	121.54
3	3-N	254	PRO	C-N-CA	5.64	132.32	121.54
3	1-N	474	LEU	N-CA-C	5.64	117.11	111.07
3	2-N	474	LEU	N-CA-C	5.64	117.11	111.07
3	3-N	474	LEU	N-CA-C	5.64	117.11	111.07
1	1-A	650	SER	CA-C-N	5.64	127.84	120.28
1	1-A	650	SER	C-N-CA	5.64	127.84	120.28
4	1-C	268	ASN	N-CA-C	5.64	117.89	108.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	120	TYR	N-CA-C	5.64	117.51	111.36
4	1-H	227	GLY	CA-C-N	5.64	132.31	121.54
4	1-H	227	GLY	C-N-CA	5.64	132.31	121.54
1	2-A	650	SER	CA-C-N	5.64	127.84	120.28
1	2-A	650	SER	C-N-CA	5.64	127.84	120.28
4	2-C	268	ASN	N-CA-C	5.64	117.89	108.02
7	2-G	120	TYR	N-CA-C	5.64	117.51	111.36
4	2-H	227	GLY	CA-C-N	5.64	132.31	121.54
4	2-H	227	GLY	C-N-CA	5.64	132.31	121.54
1	3-A	650	SER	CA-C-N	5.64	127.84	120.28
1	3-A	650	SER	C-N-CA	5.64	127.84	120.28
4	3-C	268	ASN	N-CA-C	5.64	117.89	108.02
7	3-G	120	TYR	N-CA-C	5.64	117.51	111.36
4	3-H	227	GLY	CA-C-N	5.64	132.31	121.54
4	3-H	227	GLY	C-N-CA	5.64	132.31	121.54
4	1-H	252	THR	N-CA-C	-5.64	100.52	109.59
4	2-H	252	THR	N-CA-C	-5.64	100.52	109.59
4	3-H	252	THR	N-CA-C	-5.64	100.52	109.59
1	1-A	38	TYR	N-CA-C	5.63	118.19	111.71
4	1-C	840	LYS	CA-C-N	5.63	126.35	119.99
4	1-C	840	LYS	C-N-CA	5.63	126.35	119.99
6	1-M	124	PHE	CA-C-N	5.63	129.91	122.42
6	1-M	124	PHE	C-N-CA	5.63	129.91	122.42
3	1-N	412	MET	O-C-N	-5.63	118.89	123.11
1	2-A	38	TYR	N-CA-C	5.63	118.19	111.71
4	2-C	840	LYS	CA-C-N	5.63	126.35	119.99
4	2-C	840	LYS	C-N-CA	5.63	126.35	119.99
6	2-M	124	PHE	CA-C-N	5.63	129.91	122.42
6	2-M	124	PHE	C-N-CA	5.63	129.91	122.42
3	2-N	412	MET	O-C-N	-5.63	118.89	123.11
1	3-A	38	TYR	N-CA-C	5.63	118.19	111.71
4	3-C	840	LYS	CA-C-N	5.63	126.35	119.99
4	3-C	840	LYS	C-N-CA	5.63	126.35	119.99
6	3-M	124	PHE	CA-C-N	5.63	129.91	122.42
6	3-M	124	PHE	C-N-CA	5.63	129.91	122.42
3	3-N	412	MET	O-C-N	-5.63	118.89	123.11
5	1-I	66	MET	N-CA-C	-5.63	100.53	109.59
5	2-I	66	MET	N-CA-C	-5.63	100.53	109.59
5	3-I	66	MET	N-CA-C	-5.63	100.53	109.59
1	1-A	586	ARG	O-C-N	5.63	127.79	121.32
1	2-A	586	ARG	O-C-N	5.63	127.79	121.32
1	3-A	586	ARG	O-C-N	5.63	127.79	121.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	1-R	46	ILE	N-CA-C	-5.62	103.79	109.02
6	2-R	46	ILE	N-CA-C	-5.62	103.79	109.02
6	3-R	46	ILE	N-CA-C	-5.62	103.79	109.02
5	1-I	111	PHE	N-CA-C	-5.62	105.15	111.28
5	2-I	111	PHE	N-CA-C	-5.62	105.15	111.28
5	3-I	111	PHE	N-CA-C	-5.62	105.15	111.28
3	1-B	254	PRO	CA-C-N	5.62	132.28	121.54
3	1-B	254	PRO	C-N-CA	5.62	132.28	121.54
7	1-K	827	THR	CA-C-N	-5.62	115.24	123.00
7	1-K	827	THR	C-N-CA	-5.62	115.24	123.00
3	2-B	254	PRO	CA-C-N	5.62	132.28	121.54
3	2-B	254	PRO	C-N-CA	5.62	132.28	121.54
7	2-K	827	THR	CA-C-N	-5.62	115.24	123.00
7	2-K	827	THR	C-N-CA	-5.62	115.24	123.00
3	3-B	254	PRO	CA-C-N	5.62	132.28	121.54
3	3-B	254	PRO	C-N-CA	5.62	132.28	121.54
7	3-K	827	THR	CA-C-N	-5.62	115.24	123.00
7	3-K	827	THR	C-N-CA	-5.62	115.24	123.00
1	1-A	478	GLN	CA-C-N	5.62	132.28	121.54
1	1-A	478	GLN	C-N-CA	5.62	132.28	121.54
3	1-B	865	GLU	N-CA-C	5.62	122.77	110.80
1	2-A	478	GLN	CA-C-N	5.62	132.28	121.54
1	2-A	478	GLN	C-N-CA	5.62	132.28	121.54
3	2-B	865	GLU	N-CA-C	5.62	122.77	110.80
1	3-A	478	GLN	CA-C-N	5.62	132.28	121.54
1	3-A	478	GLN	C-N-CA	5.62	132.28	121.54
3	3-B	865	GLU	N-CA-C	5.62	122.77	110.80
4	1-H	433	ILE	N-CA-C	-5.62	100.09	108.46
4	2-H	433	ILE	N-CA-C	-5.62	100.09	108.46
4	3-H	433	ILE	N-CA-C	-5.62	100.09	108.46
5	1-I	12	ALA	N-CA-C	5.61	122.75	110.80
5	2-I	12	ALA	N-CA-C	5.61	122.75	110.80
5	3-I	12	ALA	N-CA-C	5.61	122.75	110.80
8	1-L	68	VAL	N-CA-C	5.61	117.49	108.85
8	2-L	68	VAL	N-CA-C	5.61	117.49	108.85
8	3-L	68	VAL	N-CA-C	5.61	117.49	108.85
1	1-A	37	ASP	N-CA-C	-5.61	97.31	107.75
1	2-A	37	ASP	N-CA-C	-5.61	97.31	107.75
1	3-A	37	ASP	N-CA-C	-5.61	97.31	107.75
4	1-C	252	THR	N-CA-C	-5.61	100.56	109.59
4	2-C	252	THR	N-CA-C	-5.61	100.56	109.59
4	3-C	252	THR	N-CA-C	-5.61	100.56	109.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1-L	84	TYR	N-CA-C	-5.61	98.86	110.80
8	2-L	84	TYR	N-CA-C	-5.61	98.86	110.80
8	3-L	84	TYR	N-CA-C	-5.61	98.86	110.80
4	1-C	828	THR	CA-C-N	5.61	126.39	120.11
4	1-C	828	THR	C-N-CA	5.61	126.39	120.11
7	1-G	312	ASN	CA-C-N	5.61	129.74	120.94
7	1-G	312	ASN	C-N-CA	5.61	129.74	120.94
7	1-G	379	VAL	CA-C-O	-5.61	115.12	120.95
4	1-H	412	VAL	CA-C-O	-5.61	114.46	120.85
4	2-C	828	THR	CA-C-N	5.61	126.39	120.11
4	2-C	828	THR	C-N-CA	5.61	126.39	120.11
7	2-G	312	ASN	CA-C-N	5.61	129.74	120.94
7	2-G	312	ASN	C-N-CA	5.61	129.74	120.94
7	2-G	379	VAL	CA-C-O	-5.61	115.12	120.95
4	2-H	412	VAL	CA-C-O	-5.61	114.46	120.85
4	3-C	828	THR	CA-C-N	5.61	126.39	120.11
4	3-C	828	THR	C-N-CA	5.61	126.39	120.11
7	3-G	312	ASN	CA-C-N	5.61	129.74	120.94
7	3-G	312	ASN	C-N-CA	5.61	129.74	120.94
7	3-G	379	VAL	CA-C-O	-5.61	115.12	120.95
4	3-H	412	VAL	CA-C-O	-5.61	114.46	120.85
4	1-C	367	VAL	N-CA-C	-5.60	100.37	108.89
4	2-C	367	VAL	N-CA-C	-5.60	100.37	108.89
4	3-C	367	VAL	N-CA-C	-5.60	100.37	108.89
3	1-B	791	THR	N-CA-C	-5.60	100.83	109.52
6	1-J	34	LEU	N-CA-C	5.60	117.39	111.28
3	2-B	791	THR	N-CA-C	-5.60	100.83	109.52
6	2-J	34	LEU	N-CA-C	5.60	117.39	111.28
3	3-B	791	THR	N-CA-C	-5.60	100.83	109.52
6	3-J	34	LEU	N-CA-C	5.60	117.39	111.28
1	1-A	173	SER	CA-C-O	-5.60	114.94	120.26
3	1-B	474	LEU	N-CA-C	5.60	117.06	111.07
7	1-G	506	LEU	CA-C-O	-5.60	112.49	120.16
1	2-A	173	SER	CA-C-O	-5.60	114.94	120.26
3	2-B	474	LEU	N-CA-C	5.60	117.06	111.07
7	2-G	506	LEU	CA-C-O	-5.60	112.49	120.16
1	3-A	173	SER	CA-C-O	-5.60	114.94	120.26
3	3-B	474	LEU	N-CA-C	5.60	117.06	111.07
7	3-G	506	LEU	CA-C-O	-5.60	112.49	120.16
1	1-A	146	SER	N-CA-C	-5.60	101.36	109.59
4	1-C	412	VAL	CA-C-O	-5.60	114.47	120.85
4	1-C	461	ILE	CA-C-N	5.60	132.23	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	461	ILE	C-N-CA	5.60	132.23	121.54
1	2-A	146	SER	N-CA-C	-5.60	101.36	109.59
4	2-C	412	VAL	CA-C-O	-5.60	114.47	120.85
4	2-C	461	ILE	CA-C-N	5.60	132.23	121.54
4	2-C	461	ILE	C-N-CA	5.60	132.23	121.54
1	3-A	146	SER	N-CA-C	-5.60	101.36	109.59
4	3-C	412	VAL	CA-C-O	-5.60	114.47	120.85
4	3-C	461	ILE	CA-C-N	5.60	132.23	121.54
4	3-C	461	ILE	C-N-CA	5.60	132.23	121.54
7	1-K	81	ASP	CA-C-N	5.59	125.25	119.05
7	1-K	81	ASP	C-N-CA	5.59	125.25	119.05
7	2-K	81	ASP	CA-C-N	5.59	125.25	119.05
7	2-K	81	ASP	C-N-CA	5.59	125.25	119.05
7	3-K	81	ASP	CA-C-N	5.59	125.25	119.05
7	3-K	81	ASP	C-N-CA	5.59	125.25	119.05
7	1-G	358	ASP	CA-C-N	5.59	127.70	120.44
7	1-G	358	ASP	C-N-CA	5.59	127.70	120.44
7	2-G	358	ASP	CA-C-N	5.59	127.70	120.44
7	2-G	358	ASP	C-N-CA	5.59	127.70	120.44
7	3-G	358	ASP	CA-C-N	5.59	127.70	120.44
7	3-G	358	ASP	C-N-CA	5.59	127.70	120.44
1	1-A	107	TRP	N-CA-C	5.59	119.17	110.17
1	1-A	184	ILE	CA-C-N	5.59	132.21	121.54
1	1-A	184	ILE	C-N-CA	5.59	132.21	121.54
5	1-D	66	MET	N-CA-C	-5.59	100.59	109.59
6	1-F	34	LEU	N-CA-C	5.59	117.37	111.28
7	1-G	765	GLN	N-CA-C	-5.59	100.07	109.07
4	1-H	187	GLY	N-CA-C	-5.59	102.11	110.38
1	2-A	107	TRP	N-CA-C	5.59	119.17	110.17
1	2-A	184	ILE	CA-C-N	5.59	132.21	121.54
1	2-A	184	ILE	C-N-CA	5.59	132.21	121.54
5	2-D	66	MET	N-CA-C	-5.59	100.59	109.59
6	2-F	34	LEU	N-CA-C	5.59	117.37	111.28
7	2-G	765	GLN	N-CA-C	-5.59	100.07	109.07
4	2-H	187	GLY	N-CA-C	-5.59	102.11	110.38
1	3-A	107	TRP	N-CA-C	5.59	119.17	110.17
1	3-A	184	ILE	CA-C-N	5.59	132.21	121.54
1	3-A	184	ILE	C-N-CA	5.59	132.21	121.54
5	3-D	66	MET	N-CA-C	-5.59	100.59	109.59
6	3-F	34	LEU	N-CA-C	5.59	117.37	111.28
7	3-G	765	GLN	N-CA-C	-5.59	100.07	109.07
4	3-H	187	GLY	N-CA-C	-5.59	102.11	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-K	765	GLN	N-CA-C	-5.58	100.08	109.07
7	2-K	765	GLN	N-CA-C	-5.58	100.08	109.07
7	3-K	765	GLN	N-CA-C	-5.58	100.08	109.07
4	1-H	238	HIS	CA-C-O	-5.58	114.79	119.76
4	2-H	238	HIS	CA-C-O	-5.58	114.79	119.76
4	3-H	238	HIS	CA-C-O	-5.58	114.79	119.76
4	1-H	367	VAL	N-CA-C	-5.58	100.41	108.89
4	2-H	367	VAL	N-CA-C	-5.58	100.41	108.89
4	3-H	367	VAL	N-CA-C	-5.58	100.41	108.89
5	1-D	12	ALA	N-CA-C	5.58	122.68	110.80
5	2-D	12	ALA	N-CA-C	5.58	122.68	110.80
5	3-D	12	ALA	N-CA-C	5.58	122.68	110.80
3	1-B	437	GLU	CA-C-N	5.58	128.07	120.54
3	1-B	437	GLU	C-N-CA	5.58	128.07	120.54
7	1-G	612	ILE	N-CA-C	-5.58	104.93	110.62
3	2-B	437	GLU	CA-C-N	5.58	128.07	120.54
3	2-B	437	GLU	C-N-CA	5.58	128.07	120.54
7	2-G	612	ILE	N-CA-C	-5.58	104.93	110.62
3	3-B	437	GLU	CA-C-N	5.58	128.07	120.54
3	3-B	437	GLU	C-N-CA	5.58	128.07	120.54
7	3-G	612	ILE	N-CA-C	-5.58	104.93	110.62
1	1-A	372	PRO	CA-C-O	-5.57	115.24	121.32
3	1-B	324	LYS	CA-C-N	5.57	130.46	122.21
3	1-B	324	LYS	C-N-CA	5.57	130.46	122.21
1	2-A	372	PRO	CA-C-O	-5.57	115.24	121.32
3	2-B	324	LYS	CA-C-N	5.57	130.46	122.21
3	2-B	324	LYS	C-N-CA	5.57	130.46	122.21
1	3-A	372	PRO	CA-C-O	-5.57	115.24	121.32
3	3-B	324	LYS	CA-C-N	5.57	130.46	122.21
3	3-B	324	LYS	C-N-CA	5.57	130.46	122.21
7	1-K	176	ARG	CA-C-N	5.57	134.56	121.52
7	1-K	176	ARG	C-N-CA	5.57	134.56	121.52
7	2-K	176	ARG	CA-C-N	5.57	134.56	121.52
7	2-K	176	ARG	C-N-CA	5.57	134.56	121.52
7	3-K	176	ARG	CA-C-N	5.57	134.56	121.52
7	3-K	176	ARG	C-N-CA	5.57	134.56	121.52
3	1-B	515	LEU	N-CA-C	-5.57	101.04	108.34
5	1-D	111	PHE	N-CA-C	-5.57	105.21	111.28
3	2-B	515	LEU	N-CA-C	-5.57	101.04	108.34
5	2-D	111	PHE	N-CA-C	-5.57	105.21	111.28
3	3-B	515	LEU	N-CA-C	-5.57	101.04	108.34
5	3-D	111	PHE	N-CA-C	-5.57	105.21	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	139	ALA	N-CA-C	5.57	122.66	110.80
7	2-G	139	ALA	N-CA-C	5.57	122.66	110.80
7	3-G	139	ALA	N-CA-C	5.57	122.66	110.80
1	1-A	124	SER	CA-C-N	5.57	132.17	121.54
1	1-A	124	SER	C-N-CA	5.57	132.17	121.54
4	1-C	444	VAL	CA-C-N	5.57	130.31	122.46
4	1-C	444	VAL	C-N-CA	5.57	130.31	122.46
7	1-K	647	VAL	N-CA-C	5.57	115.88	107.75
3	1-N	515	LEU	N-CA-C	-5.57	101.05	108.34
4	1-H	461	ILE	CA-C-N	5.57	132.18	121.54
4	1-H	461	ILE	C-N-CA	5.57	132.18	121.54
1	2-A	124	SER	CA-C-N	5.57	132.17	121.54
1	2-A	124	SER	C-N-CA	5.57	132.17	121.54
4	2-C	444	VAL	CA-C-N	5.57	130.31	122.46
4	2-C	444	VAL	C-N-CA	5.57	130.31	122.46
7	2-K	647	VAL	N-CA-C	5.57	115.88	107.75
3	2-N	515	LEU	N-CA-C	-5.57	101.05	108.34
4	2-H	461	ILE	CA-C-N	5.57	132.18	121.54
4	2-H	461	ILE	C-N-CA	5.57	132.18	121.54
1	3-A	124	SER	CA-C-N	5.57	132.17	121.54
1	3-A	124	SER	C-N-CA	5.57	132.17	121.54
4	3-C	444	VAL	CA-C-N	5.57	130.31	122.46
4	3-C	444	VAL	C-N-CA	5.57	130.31	122.46
7	3-K	647	VAL	N-CA-C	5.57	115.88	107.75
3	3-N	515	LEU	N-CA-C	-5.57	101.05	108.34
4	3-H	461	ILE	CA-C-N	5.57	132.18	121.54
4	3-H	461	ILE	C-N-CA	5.57	132.18	121.54
1	1-A	274	ARG	N-CA-C	-5.57	100.81	109.72
7	1-G	610	GLN	N-CA-C	-5.57	105.21	111.28
1	2-A	274	ARG	N-CA-C	-5.57	100.81	109.72
7	2-G	610	GLN	N-CA-C	-5.57	105.21	111.28
1	3-A	274	ARG	N-CA-C	-5.57	100.81	109.72
7	3-G	610	GLN	N-CA-C	-5.57	105.21	111.28
3	1-B	448	ASN	CA-C-O	5.56	126.43	120.70
3	2-B	448	ASN	CA-C-O	5.56	126.43	120.70
3	3-B	448	ASN	CA-C-O	5.56	126.43	120.70
4	1-C	818	LEU	CA-C-O	-5.56	114.52	120.42
4	2-C	818	LEU	CA-C-O	-5.56	114.52	120.42
4	3-C	818	LEU	CA-C-O	-5.56	114.52	120.42
1	1-A	611	VAL	CA-C-O	5.56	126.74	120.85
3	1-B	535	THR	CA-C-N	5.56	127.66	120.44
3	1-B	535	THR	C-N-CA	5.56	127.66	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-K	190	ILE	N-CA-C	5.56	115.75	110.53
1	2-A	611	VAL	CA-C-O	5.56	126.74	120.85
3	2-B	535	THR	CA-C-N	5.56	127.66	120.44
3	2-B	535	THR	C-N-CA	5.56	127.66	120.44
7	2-K	190	ILE	N-CA-C	5.56	115.75	110.53
1	3-A	611	VAL	CA-C-O	5.56	126.74	120.85
3	3-B	535	THR	CA-C-N	5.56	127.66	120.44
3	3-B	535	THR	C-N-CA	5.56	127.66	120.44
7	3-K	190	ILE	N-CA-C	5.56	115.75	110.53
3	1-N	324	LYS	CA-C-N	5.55	130.43	122.21
3	1-N	324	LYS	C-N-CA	5.55	130.43	122.21
3	2-N	324	LYS	CA-C-N	5.55	130.43	122.21
3	2-N	324	LYS	C-N-CA	5.55	130.43	122.21
3	3-N	324	LYS	CA-C-N	5.55	130.43	122.21
3	3-N	324	LYS	C-N-CA	5.55	130.43	122.21
7	1-G	382	ALA	N-CA-C	-5.55	105.13	111.07
7	2-G	382	ALA	N-CA-C	-5.55	105.13	111.07
7	3-G	382	ALA	N-CA-C	-5.55	105.13	111.07
1	1-A	769	GLU	N-CA-C	5.55	117.01	111.07
8	1-L	61	LEU	CA-C-O	-5.55	114.37	120.36
1	2-A	769	GLU	N-CA-C	5.55	117.01	111.07
8	2-L	61	LEU	CA-C-O	-5.55	114.37	120.36
1	3-A	769	GLU	N-CA-C	5.55	117.01	111.07
8	3-L	61	LEU	CA-C-O	-5.55	114.37	120.36
7	1-G	118	ASP	CA-C-N	5.54	127.65	120.44
7	1-G	118	ASP	C-N-CA	5.54	127.65	120.44
7	2-G	118	ASP	CA-C-N	5.54	127.65	120.44
7	2-G	118	ASP	C-N-CA	5.54	127.65	120.44
7	3-G	118	ASP	CA-C-N	5.54	127.65	120.44
7	3-G	118	ASP	C-N-CA	5.54	127.65	120.44
7	1-G	457	HIS	N-CA-C	-5.54	105.14	111.07
6	1-R	35	TYR	N-CA-C	5.54	119.76	112.89
7	2-G	457	HIS	N-CA-C	-5.54	105.14	111.07
6	2-R	35	TYR	N-CA-C	5.54	119.76	112.89
7	3-G	457	HIS	N-CA-C	-5.54	105.14	111.07
6	3-R	35	TYR	N-CA-C	5.54	119.76	112.89
4	1-C	534	PHE	CA-C-O	5.54	126.42	120.32
7	1-G	827	THR	CA-C-N	-5.54	115.35	123.00
7	1-G	827	THR	C-N-CA	-5.54	115.35	123.00
4	2-C	534	PHE	CA-C-O	5.54	126.42	120.32
7	2-G	827	THR	CA-C-N	-5.54	115.35	123.00
7	2-G	827	THR	C-N-CA	-5.54	115.35	123.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	3-C	534	PHE	CA-C-O	5.54	126.42	120.32
7	3-G	827	THR	CA-C-N	-5.54	115.35	123.00
7	3-G	827	THR	C-N-CA	-5.54	115.35	123.00
1	1-A	452	ASN	N-CA-C	-5.54	99.00	110.80
4	1-C	432	SER	N-CA-C	-5.54	100.90	108.38
7	1-K	193	GLN	N-CA-C	-5.54	105.24	111.28
5	1-I	13	GLY	N-CA-C	-5.54	107.99	115.36
1	2-A	452	ASN	N-CA-C	-5.54	99.00	110.80
4	2-C	432	SER	N-CA-C	-5.54	100.90	108.38
7	2-K	193	GLN	N-CA-C	-5.54	105.24	111.28
5	2-I	13	GLY	N-CA-C	-5.54	107.99	115.36
1	3-A	452	ASN	N-CA-C	-5.54	99.00	110.80
4	3-C	432	SER	N-CA-C	-5.54	100.90	108.38
7	3-K	193	GLN	N-CA-C	-5.54	105.24	111.28
5	3-I	13	GLY	N-CA-C	-5.54	107.99	115.36
1	1-A	33	ILE	N-CA-C	-5.54	100.50	108.48
7	1-G	546	TYR	N-CA-C	5.54	117.00	111.07
1	2-A	33	ILE	N-CA-C	-5.54	100.50	108.48
7	2-G	546	TYR	N-CA-C	5.54	117.00	111.07
1	3-A	33	ILE	N-CA-C	-5.54	100.50	108.48
7	3-G	546	TYR	N-CA-C	5.54	117.00	111.07
4	1-H	100	ASP	N-CA-C	-5.54	100.99	109.41
4	2-H	100	ASP	N-CA-C	-5.54	100.99	109.41
4	3-H	100	ASP	N-CA-C	-5.54	100.99	109.41
3	1-B	103	THR	CA-C-N	5.54	135.31	121.80
3	1-B	103	THR	C-N-CA	5.54	135.31	121.80
6	1-R	100	ILE	N-CA-C	-5.54	105.33	110.53
3	1-N	448	ASN	CA-C-O	5.54	126.40	120.70
3	2-B	103	THR	CA-C-N	5.54	135.31	121.80
3	2-B	103	THR	C-N-CA	5.54	135.31	121.80
6	2-R	100	ILE	N-CA-C	-5.54	105.33	110.53
3	2-N	448	ASN	CA-C-O	5.54	126.40	120.70
3	3-B	103	THR	CA-C-N	5.54	135.31	121.80
3	3-B	103	THR	C-N-CA	5.54	135.31	121.80
6	3-R	100	ILE	N-CA-C	-5.54	105.33	110.53
3	3-N	448	ASN	CA-C-O	5.54	126.40	120.70
3	1-B	121	ARG	N-CA-C	-5.53	105.25	111.28
3	1-B	842	MET	CA-C-O	5.53	126.42	120.55
4	1-H	663	GLU	N-CA-C	-5.53	101.46	109.59
3	2-B	121	ARG	N-CA-C	-5.53	105.25	111.28
3	2-B	842	MET	CA-C-O	5.53	126.42	120.55
4	2-H	663	GLU	N-CA-C	-5.53	101.46	109.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3-B	121	ARG	N-CA-C	-5.53	105.25	111.28
3	3-B	842	MET	CA-C-O	5.53	126.42	120.55
4	3-H	663	GLU	N-CA-C	-5.53	101.46	109.59
4	1-C	187	GLY	N-CA-C	-5.53	102.19	110.38
8	1-Z	70	LYS	CA-C-N	5.53	131.21	122.36
8	1-Z	70	LYS	C-N-CA	5.53	131.21	122.36
4	2-C	187	GLY	N-CA-C	-5.53	102.19	110.38
8	2-Z	70	LYS	CA-C-N	5.53	131.21	122.36
8	2-Z	70	LYS	C-N-CA	5.53	131.21	122.36
4	3-C	187	GLY	N-CA-C	-5.53	102.19	110.38
8	3-Z	70	LYS	CA-C-N	5.53	131.21	122.36
8	3-Z	70	LYS	C-N-CA	5.53	131.21	122.36
7	1-K	610	GLN	N-CA-C	-5.53	105.25	111.28
3	1-N	437	GLU	CA-C-N	5.53	128.01	120.54
3	1-N	437	GLU	C-N-CA	5.53	128.01	120.54
7	2-K	610	GLN	N-CA-C	-5.53	105.25	111.28
3	2-N	437	GLU	CA-C-N	5.53	128.01	120.54
3	2-N	437	GLU	C-N-CA	5.53	128.01	120.54
7	3-K	610	GLN	N-CA-C	-5.53	105.25	111.28
3	3-N	437	GLU	CA-C-N	5.53	128.01	120.54
3	3-N	437	GLU	C-N-CA	5.53	128.01	120.54
1	1-A	180	ASP	CA-C-N	5.53	128.03	120.46
1	1-A	180	ASP	C-N-CA	5.53	128.03	120.46
1	1-A	713	LEU	N-CA-C	5.53	120.52	113.55
3	1-B	954	SER	N-CA-C	-5.53	105.25	111.28
4	1-C	203	ILE	N-CA-C	-5.53	99.85	108.86
7	1-G	400	PHE	CA-C-N	5.53	127.69	120.28
7	1-G	400	PHE	C-N-CA	5.53	127.69	120.28
3	1-N	121	ARG	N-CA-C	-5.53	105.25	111.28
3	1-N	535	THR	CA-C-N	5.53	127.63	120.44
3	1-N	535	THR	C-N-CA	5.53	127.63	120.44
4	1-H	432	SER	N-CA-C	-5.53	100.92	108.38
1	2-A	180	ASP	CA-C-N	5.53	128.03	120.46
1	2-A	180	ASP	C-N-CA	5.53	128.03	120.46
1	2-A	713	LEU	N-CA-C	5.53	120.52	113.55
3	2-B	954	SER	N-CA-C	-5.53	105.25	111.28
4	2-C	203	ILE	N-CA-C	-5.53	99.85	108.86
7	2-G	400	PHE	CA-C-N	5.53	127.69	120.28
7	2-G	400	PHE	C-N-CA	5.53	127.69	120.28
3	2-N	121	ARG	N-CA-C	-5.53	105.25	111.28
3	2-N	535	THR	CA-C-N	5.53	127.63	120.44
3	2-N	535	THR	C-N-CA	5.53	127.63	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-H	432	SER	N-CA-C	-5.53	100.92	108.38
1	3-A	180	ASP	CA-C-N	5.53	128.03	120.46
1	3-A	180	ASP	C-N-CA	5.53	128.03	120.46
1	3-A	713	LEU	N-CA-C	5.53	120.52	113.55
3	3-B	954	SER	N-CA-C	-5.53	105.25	111.28
4	3-C	203	ILE	N-CA-C	-5.53	99.85	108.86
7	3-G	400	PHE	CA-C-N	5.53	127.69	120.28
7	3-G	400	PHE	C-N-CA	5.53	127.69	120.28
3	3-N	121	ARG	N-CA-C	-5.53	105.25	111.28
3	3-N	535	THR	CA-C-N	5.53	127.63	120.44
3	3-N	535	THR	C-N-CA	5.53	127.63	120.44
4	3-H	432	SER	N-CA-C	-5.53	100.92	108.38
1	1-A	44	ILE	N-CA-C	-5.53	105.46	110.82
8	1-Z	20	ASP	N-CA-C	-5.53	103.61	110.41
4	1-H	444	VAL	CA-C-N	5.53	130.25	122.46
4	1-H	444	VAL	C-N-CA	5.53	130.25	122.46
1	2-A	44	ILE	N-CA-C	-5.53	105.46	110.82
8	2-Z	20	ASP	N-CA-C	-5.53	103.61	110.41
4	2-H	444	VAL	CA-C-N	5.53	130.25	122.46
4	2-H	444	VAL	C-N-CA	5.53	130.25	122.46
1	3-A	44	ILE	N-CA-C	-5.53	105.46	110.82
8	3-Z	20	ASP	N-CA-C	-5.53	103.61	110.41
4	3-H	444	VAL	CA-C-N	5.53	130.25	122.46
4	3-H	444	VAL	C-N-CA	5.53	130.25	122.46
7	1-G	259	LEU	CA-C-O	-5.53	115.02	120.82
7	2-G	259	LEU	CA-C-O	-5.53	115.02	120.82
7	3-G	259	LEU	CA-C-O	-5.53	115.02	120.82
3	1-B	826	ALA	CA-C-N	5.52	132.09	121.54
3	1-B	826	ALA	C-N-CA	5.52	132.09	121.54
3	2-B	826	ALA	CA-C-N	5.52	132.09	121.54
3	2-B	826	ALA	C-N-CA	5.52	132.09	121.54
3	3-B	826	ALA	CA-C-N	5.52	132.09	121.54
3	3-B	826	ALA	C-N-CA	5.52	132.09	121.54
3	1-N	103	THR	CA-C-N	5.52	135.28	121.80
3	1-N	103	THR	C-N-CA	5.52	135.28	121.80
3	2-N	103	THR	CA-C-N	5.52	135.28	121.80
3	2-N	103	THR	C-N-CA	5.52	135.28	121.80
3	3-N	103	THR	CA-C-N	5.52	135.28	121.80
3	3-N	103	THR	C-N-CA	5.52	135.28	121.80
3	1-B	834	LEU	CA-C-N	5.52	131.76	122.87
3	1-B	834	LEU	C-N-CA	5.52	131.76	122.87
5	1-D	13	GLY	N-CA-C	-5.52	108.02	115.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2-B	834	LEU	CA-C-N	5.52	131.76	122.87
3	2-B	834	LEU	C-N-CA	5.52	131.76	122.87
5	2-D	13	GLY	N-CA-C	-5.52	108.02	115.36
3	3-B	834	LEU	CA-C-N	5.52	131.76	122.87
3	3-B	834	LEU	C-N-CA	5.52	131.76	122.87
5	3-D	13	GLY	N-CA-C	-5.52	108.02	115.36
5	1-D	21	PHE	N-CA-C	-5.52	104.67	111.40
7	1-G	251	LEU	N-CA-C	-5.52	105.17	111.07
8	1-Z	80	ILE	CA-C-N	5.52	132.23	121.41
8	1-Z	80	ILE	C-N-CA	5.52	132.23	121.41
5	2-D	21	PHE	N-CA-C	-5.52	104.67	111.40
7	2-G	251	LEU	N-CA-C	-5.52	105.17	111.07
8	2-Z	80	ILE	CA-C-N	5.52	132.23	121.41
8	2-Z	80	ILE	C-N-CA	5.52	132.23	121.41
5	3-D	21	PHE	N-CA-C	-5.52	104.67	111.40
7	3-G	251	LEU	N-CA-C	-5.52	105.17	111.07
8	3-Z	80	ILE	CA-C-N	5.52	132.23	121.41
8	3-Z	80	ILE	C-N-CA	5.52	132.23	121.41
7	1-G	499	GLY	N-CA-C	-5.52	105.82	112.49
7	2-G	499	GLY	N-CA-C	-5.52	105.82	112.49
7	3-G	499	GLY	N-CA-C	-5.52	105.82	112.49
3	1-B	868	VAL	N-CA-C	-5.51	100.34	108.23
3	2-B	868	VAL	N-CA-C	-5.51	100.34	108.23
3	3-B	868	VAL	N-CA-C	-5.51	100.34	108.23
1	1-A	103	HIS	N-CA-C	5.51	122.53	110.80
4	1-C	100	ASP	N-CA-C	-5.51	101.04	109.41
1	2-A	103	HIS	N-CA-C	5.51	122.53	110.80
4	2-C	100	ASP	N-CA-C	-5.51	101.04	109.41
1	3-A	103	HIS	N-CA-C	5.51	122.53	110.80
4	3-C	100	ASP	N-CA-C	-5.51	101.04	109.41
4	1-H	534	PHE	CA-C-O	5.51	126.38	120.32
4	2-H	534	PHE	CA-C-O	5.51	126.38	120.32
4	3-H	534	PHE	CA-C-O	5.51	126.38	120.32
6	1-F	71	GLN	N-CA-C	-5.51	103.43	110.53
6	2-F	71	GLN	N-CA-C	-5.51	103.43	110.53
6	3-F	71	GLN	N-CA-C	-5.51	103.43	110.53
1	1-A	763	ALA	N-CA-C	5.50	117.28	111.28
1	2-A	763	ALA	N-CA-C	5.50	117.28	111.28
1	3-A	763	ALA	N-CA-C	5.50	117.28	111.28
1	1-A	167	LEU	N-CA-C	-5.50	99.08	110.80
7	1-G	547	ILE	CA-C-N	5.50	127.65	120.28
7	1-G	547	ILE	C-N-CA	5.50	127.65	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-K	719	ALA	N-CA-C	5.50	120.92	113.21
4	1-H	222	VAL	CA-C-N	-5.50	112.39	121.80
4	1-H	222	VAL	C-N-CA	-5.50	112.39	121.80
1	2-A	167	LEU	N-CA-C	-5.50	99.08	110.80
7	2-G	547	ILE	CA-C-N	5.50	127.65	120.28
7	2-G	547	ILE	C-N-CA	5.50	127.65	120.28
7	2-K	719	ALA	N-CA-C	5.50	120.92	113.21
4	2-H	222	VAL	CA-C-N	-5.50	112.39	121.80
4	2-H	222	VAL	C-N-CA	-5.50	112.39	121.80
1	3-A	167	LEU	N-CA-C	-5.50	99.08	110.80
7	3-G	547	ILE	CA-C-N	5.50	127.65	120.28
7	3-G	547	ILE	C-N-CA	5.50	127.65	120.28
7	3-K	719	ALA	N-CA-C	5.50	120.92	113.21
4	3-H	222	VAL	CA-C-N	-5.50	112.39	121.80
4	3-H	222	VAL	C-N-CA	-5.50	112.39	121.80
7	1-K	790	THR	CA-C-N	5.50	130.50	122.85
7	1-K	790	THR	C-N-CA	5.50	130.50	122.85
7	2-K	790	THR	CA-C-N	5.50	130.50	122.85
7	2-K	790	THR	C-N-CA	5.50	130.50	122.85
7	3-K	790	THR	CA-C-N	5.50	130.50	122.85
7	3-K	790	THR	C-N-CA	5.50	130.50	122.85
1	1-A	223	GLY	N-CA-C	-5.50	100.73	111.12
1	2-A	223	GLY	N-CA-C	-5.50	100.73	111.12
1	3-A	223	GLY	N-CA-C	-5.50	100.73	111.12
3	1-B	745	ALA	N-CA-C	-5.50	100.38	108.79
7	1-K	234	ARG	CA-C-O	5.50	126.38	120.55
3	1-N	360	LEU	CA-C-O	5.50	126.31	120.10
3	2-B	745	ALA	N-CA-C	-5.50	100.38	108.79
7	2-K	234	ARG	CA-C-O	5.50	126.38	120.55
3	2-N	360	LEU	CA-C-O	5.50	126.31	120.10
3	3-B	745	ALA	N-CA-C	-5.50	100.38	108.79
7	3-K	234	ARG	CA-C-O	5.50	126.38	120.55
3	3-N	360	LEU	CA-C-O	5.50	126.31	120.10
8	1-Z	70	LYS	N-CA-C	-5.50	101.16	108.74
8	2-Z	70	LYS	N-CA-C	-5.50	101.16	108.74
8	3-Z	70	LYS	N-CA-C	-5.50	101.16	108.74
4	1-C	222	VAL	CA-C-N	-5.49	112.41	121.80
4	1-C	222	VAL	C-N-CA	-5.49	112.41	121.80
7	1-G	443	ILE	N-CA-C	-5.49	104.59	110.36
4	1-H	203	ILE	N-CA-C	-5.49	99.91	108.86
4	2-C	222	VAL	CA-C-N	-5.49	112.41	121.80
4	2-C	222	VAL	C-N-CA	-5.49	112.41	121.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-G	443	ILE	N-CA-C	-5.49	104.59	110.36
4	2-H	203	ILE	N-CA-C	-5.49	99.91	108.86
4	3-C	222	VAL	CA-C-N	-5.49	112.41	121.80
4	3-C	222	VAL	C-N-CA	-5.49	112.41	121.80
7	3-G	443	ILE	N-CA-C	-5.49	104.59	110.36
4	3-H	203	ILE	N-CA-C	-5.49	99.91	108.86
4	1-H	452	TRP	N-CA-C	-5.49	105.58	114.09
4	2-H	452	TRP	N-CA-C	-5.49	105.58	114.09
4	3-H	452	TRP	N-CA-C	-5.49	105.58	114.09
4	1-C	238	HIS	CA-C-O	-5.49	114.87	119.76
4	1-C	663	GLU	N-CA-C	-5.49	101.52	109.59
4	1-H	572	ARG	O-C-N	5.49	129.81	123.17
5	1-I	21	PHE	N-CA-C	-5.49	104.70	111.40
4	2-C	238	HIS	CA-C-O	-5.49	114.87	119.76
4	2-C	663	GLU	N-CA-C	-5.49	101.52	109.59
4	2-H	572	ARG	O-C-N	5.49	129.81	123.17
5	2-I	21	PHE	N-CA-C	-5.49	104.70	111.40
4	3-C	238	HIS	CA-C-O	-5.49	114.87	119.76
4	3-C	663	GLU	N-CA-C	-5.49	101.52	109.59
4	3-H	572	ARG	O-C-N	5.49	129.81	123.17
5	3-I	21	PHE	N-CA-C	-5.49	104.70	111.40
7	1-K	612	ILE	N-CA-C	-5.49	105.02	110.62
7	2-K	612	ILE	N-CA-C	-5.49	105.02	110.62
7	3-K	612	ILE	N-CA-C	-5.49	105.02	110.62
7	1-G	296	CYS	O-C-N	5.49	127.94	122.12
7	2-G	296	CYS	O-C-N	5.49	127.94	122.12
7	3-G	296	CYS	O-C-N	5.49	127.94	122.12
1	1-A	261	GLN	CA-C-N	5.49	132.02	121.54
1	1-A	261	GLN	C-N-CA	5.49	132.02	121.54
7	1-G	463	GLY	N-CA-C	5.49	123.53	112.34
1	2-A	261	GLN	CA-C-N	5.49	132.02	121.54
1	2-A	261	GLN	C-N-CA	5.49	132.02	121.54
7	2-G	463	GLY	N-CA-C	5.49	123.53	112.34
1	3-A	261	GLN	CA-C-N	5.49	132.02	121.54
1	3-A	261	GLN	C-N-CA	5.49	132.02	121.54
7	3-G	463	GLY	N-CA-C	5.49	123.53	112.34
7	1-G	790	THR	CA-C-N	5.48	130.47	122.85
7	1-G	790	THR	C-N-CA	5.48	130.47	122.85
7	1-G	811	HIS	CA-C-O	-5.48	113.47	119.61
7	2-G	790	THR	CA-C-N	5.48	130.47	122.85
7	2-G	790	THR	C-N-CA	5.48	130.47	122.85
7	2-G	811	HIS	CA-C-O	-5.48	113.47	119.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	3-G	790	THR	CA-C-N	5.48	130.47	122.85
7	3-G	790	THR	C-N-CA	5.48	130.47	122.85
7	3-G	811	HIS	CA-C-O	-5.48	113.47	119.61
7	1-G	825	THR	CA-C-O	-5.48	115.05	121.46
7	1-K	771	ASN	CA-C-N	-5.48	112.99	120.44
7	1-K	771	ASN	C-N-CA	-5.48	112.99	120.44
7	2-G	825	THR	CA-C-O	-5.48	115.05	121.46
7	2-K	771	ASN	CA-C-N	-5.48	112.99	120.44
7	2-K	771	ASN	C-N-CA	-5.48	112.99	120.44
7	3-G	825	THR	CA-C-O	-5.48	115.05	121.46
7	3-K	771	ASN	CA-C-N	-5.48	112.99	120.44
7	3-K	771	ASN	C-N-CA	-5.48	112.99	120.44
7	1-K	149	VAL	CA-C-N	-5.48	114.47	122.19
7	1-K	149	VAL	C-N-CA	-5.48	114.47	122.19
6	1-J	71	GLN	N-CA-C	-5.48	103.46	110.53
7	2-K	149	VAL	CA-C-N	-5.48	114.47	122.19
7	2-K	149	VAL	C-N-CA	-5.48	114.47	122.19
6	2-J	71	GLN	N-CA-C	-5.48	103.46	110.53
7	3-K	149	VAL	CA-C-N	-5.48	114.47	122.19
7	3-K	149	VAL	C-N-CA	-5.48	114.47	122.19
6	3-J	71	GLN	N-CA-C	-5.48	103.46	110.53
6	1-J	130	LEU	N-CA-C	-5.47	99.53	109.44
6	2-J	130	LEU	N-CA-C	-5.47	99.53	109.44
6	3-J	130	LEU	N-CA-C	-5.47	99.53	109.44
1	1-A	483	LEU	N-CA-C	-5.47	105.23	111.14
3	1-B	360	LEU	CA-C-O	5.47	126.28	120.10
3	1-B	952	ALA	N-CA-C	5.47	117.25	111.28
7	1-G	142	ARG	N-CA-C	-5.47	105.23	111.14
3	1-N	128	ASN	CA-C-N	5.47	128.06	120.29
3	1-N	128	ASN	C-N-CA	5.47	128.06	120.29
1	2-A	483	LEU	N-CA-C	-5.47	105.23	111.14
3	2-B	360	LEU	CA-C-O	5.47	126.28	120.10
3	2-B	952	ALA	N-CA-C	5.47	117.25	111.28
7	2-G	142	ARG	N-CA-C	-5.47	105.23	111.14
3	2-N	128	ASN	CA-C-N	5.47	128.06	120.29
3	2-N	128	ASN	C-N-CA	5.47	128.06	120.29
1	3-A	483	LEU	N-CA-C	-5.47	105.23	111.14
3	3-B	360	LEU	CA-C-O	5.47	126.28	120.10
3	3-B	952	ALA	N-CA-C	5.47	117.25	111.28
7	3-G	142	ARG	N-CA-C	-5.47	105.23	111.14
3	3-N	128	ASN	CA-C-N	5.47	128.06	120.29
3	3-N	128	ASN	C-N-CA	5.47	128.06	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-K	825	THR	CA-C-O	-5.47	115.06	121.46
7	2-K	825	THR	CA-C-O	-5.47	115.06	121.46
7	3-K	825	THR	CA-C-O	-5.47	115.06	121.46
8	1-L	76	TYR	CA-C-O	5.46	126.94	120.66
8	2-L	76	TYR	CA-C-O	5.46	126.94	120.66
8	3-L	76	TYR	CA-C-O	5.46	126.94	120.66
1	1-A	599	PHE	CA-C-N	-5.46	112.05	121.66
1	1-A	599	PHE	C-N-CA	-5.46	112.05	121.66
3	1-B	309	ASP	CA-C-O	5.46	128.32	120.51
4	1-C	452	TRP	N-CA-C	-5.46	105.62	114.09
1	2-A	599	PHE	CA-C-N	-5.46	112.05	121.66
1	2-A	599	PHE	C-N-CA	-5.46	112.05	121.66
3	2-B	309	ASP	CA-C-O	5.46	128.32	120.51
4	2-C	452	TRP	N-CA-C	-5.46	105.62	114.09
1	3-A	599	PHE	CA-C-N	-5.46	112.05	121.66
1	3-A	599	PHE	C-N-CA	-5.46	112.05	121.66
3	3-B	309	ASP	CA-C-O	5.46	128.32	120.51
4	3-C	452	TRP	N-CA-C	-5.46	105.62	114.09
6	1-R	175	ASN	N-CA-C	5.46	122.43	110.80
8	1-L	26	LEU	CA-C-N	-5.46	112.33	121.94
8	1-L	26	LEU	C-N-CA	-5.46	112.33	121.94
6	2-R	175	ASN	N-CA-C	5.46	122.43	110.80
8	2-L	26	LEU	CA-C-N	-5.46	112.33	121.94
8	2-L	26	LEU	C-N-CA	-5.46	112.33	121.94
6	3-R	175	ASN	N-CA-C	5.46	122.43	110.80
8	3-L	26	LEU	CA-C-N	-5.46	112.33	121.94
8	3-L	26	LEU	C-N-CA	-5.46	112.33	121.94
3	1-B	128	ASN	CA-C-N	5.46	128.04	120.29
3	1-B	128	ASN	C-N-CA	5.46	128.04	120.29
3	2-B	128	ASN	CA-C-N	5.46	128.04	120.29
3	2-B	128	ASN	C-N-CA	5.46	128.04	120.29
3	3-B	128	ASN	CA-C-N	5.46	128.04	120.29
3	3-B	128	ASN	C-N-CA	5.46	128.04	120.29
6	1-F	130	LEU	N-CA-C	-5.46	99.56	109.44
6	1-M	21	LEU	CA-C-N	5.46	130.69	123.05
6	1-M	21	LEU	C-N-CA	5.46	130.69	123.05
4	1-H	385	ASN	N-CA-C	-5.46	101.57	109.59
6	2-F	130	LEU	N-CA-C	-5.46	99.56	109.44
6	2-M	21	LEU	CA-C-N	5.46	130.69	123.05
6	2-M	21	LEU	C-N-CA	5.46	130.69	123.05
4	2-H	385	ASN	N-CA-C	-5.46	101.57	109.59
6	3-F	130	LEU	N-CA-C	-5.46	99.56	109.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	3-M	21	LEU	CA-C-N	5.46	130.69	123.05
6	3-M	21	LEU	C-N-CA	5.46	130.69	123.05
4	3-H	385	ASN	N-CA-C	-5.46	101.57	109.59
4	1-H	25	PRO	CA-C-N	5.46	131.96	121.54
4	1-H	25	PRO	C-N-CA	5.46	131.96	121.54
4	2-H	25	PRO	CA-C-N	5.46	131.96	121.54
4	2-H	25	PRO	C-N-CA	5.46	131.96	121.54
4	3-H	25	PRO	CA-C-N	5.46	131.96	121.54
4	3-H	25	PRO	C-N-CA	5.46	131.96	121.54
7	1-G	719	ALA	N-CA-C	5.45	120.84	113.21
7	2-G	719	ALA	N-CA-C	5.45	120.84	113.21
7	3-G	719	ALA	N-CA-C	5.45	120.84	113.21
8	1-L	146	VAL	N-CA-C	-5.45	101.55	109.29
8	2-L	146	VAL	N-CA-C	-5.45	101.55	109.29
8	3-L	146	VAL	N-CA-C	-5.45	101.55	109.29
1	1-A	947	VAL	N-CA-C	-5.45	101.22	108.96
3	1-B	320	LEU	CA-C-N	5.45	127.92	120.46
3	1-B	320	LEU	C-N-CA	5.45	127.92	120.46
4	1-C	18	VAL	N-CA-C	-5.45	99.31	107.37
4	1-H	18	VAL	N-CA-C	-5.45	99.31	107.37
1	2-A	947	VAL	N-CA-C	-5.45	101.22	108.96
3	2-B	320	LEU	CA-C-N	5.45	127.92	120.46
3	2-B	320	LEU	C-N-CA	5.45	127.92	120.46
4	2-C	18	VAL	N-CA-C	-5.45	99.31	107.37
4	2-H	18	VAL	N-CA-C	-5.45	99.31	107.37
1	3-A	947	VAL	N-CA-C	-5.45	101.22	108.96
3	3-B	320	LEU	CA-C-N	5.45	127.92	120.46
3	3-B	320	LEU	C-N-CA	5.45	127.92	120.46
4	3-C	18	VAL	N-CA-C	-5.45	99.31	107.37
4	3-H	18	VAL	N-CA-C	-5.45	99.31	107.37
7	1-K	117	GLU	CA-C-O	5.45	128.19	121.87
7	2-K	117	GLU	CA-C-O	5.45	128.19	121.87
7	3-K	117	GLU	CA-C-O	5.45	128.19	121.87
3	1-B	808	SER	N-CA-C	5.44	122.39	110.80
3	2-B	808	SER	N-CA-C	5.44	122.39	110.80
3	3-B	808	SER	N-CA-C	5.44	122.39	110.80
6	1-M	123	VAL	CA-C-N	5.44	129.92	122.84
6	1-M	123	VAL	C-N-CA	5.44	129.92	122.84
6	2-M	123	VAL	CA-C-N	5.44	129.92	122.84
6	2-M	123	VAL	C-N-CA	5.44	129.92	122.84
6	3-M	123	VAL	CA-C-N	5.44	129.92	122.84
6	3-M	123	VAL	C-N-CA	5.44	129.92	122.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-B	328	ALA	CA-C-N	5.44	131.93	121.54
3	1-B	328	ALA	C-N-CA	5.44	131.93	121.54
7	1-G	406	ARG	CA-C-N	5.44	127.51	120.44
7	1-G	406	ARG	C-N-CA	5.44	127.51	120.44
3	2-B	328	ALA	CA-C-N	5.44	131.93	121.54
3	2-B	328	ALA	C-N-CA	5.44	131.93	121.54
7	2-G	406	ARG	CA-C-N	5.44	127.51	120.44
7	2-G	406	ARG	C-N-CA	5.44	127.51	120.44
3	3-B	328	ALA	CA-C-N	5.44	131.93	121.54
3	3-B	328	ALA	C-N-CA	5.44	131.93	121.54
7	3-G	406	ARG	CA-C-N	5.44	127.51	120.44
7	3-G	406	ARG	C-N-CA	5.44	127.51	120.44
7	1-K	267	VAL	N-CA-C	-5.44	105.20	110.42
7	2-K	267	VAL	N-CA-C	-5.44	105.20	110.42
7	3-K	267	VAL	N-CA-C	-5.44	105.20	110.42
7	1-K	852	VAL	N-CA-C	-5.44	100.61	108.71
4	1-H	260	THR	N-CA-C	-5.44	104.21	112.04
7	2-K	852	VAL	N-CA-C	-5.44	100.61	108.71
4	2-H	260	THR	N-CA-C	-5.44	104.21	112.04
7	3-K	852	VAL	N-CA-C	-5.44	100.61	108.71
4	3-H	260	THR	N-CA-C	-5.44	104.21	112.04
7	1-G	771	ASN	CA-C-N	-5.44	113.05	120.44
7	1-G	771	ASN	C-N-CA	-5.44	113.05	120.44
7	2-G	771	ASN	CA-C-N	-5.44	113.05	120.44
7	2-G	771	ASN	C-N-CA	-5.44	113.05	120.44
7	3-G	771	ASN	CA-C-N	-5.44	113.05	120.44
7	3-G	771	ASN	C-N-CA	-5.44	113.05	120.44
1	1-A	205	ASP	N-CA-C	-5.43	99.22	110.80
1	2-A	205	ASP	N-CA-C	-5.43	99.22	110.80
1	3-A	205	ASP	N-CA-C	-5.43	99.22	110.80
8	1-Z	77	PHE	N-CA-C	-5.43	100.84	109.59
8	2-Z	77	PHE	N-CA-C	-5.43	100.84	109.59
8	3-Z	77	PHE	N-CA-C	-5.43	100.84	109.59
4	1-C	417	ASN	CA-C-N	5.43	130.28	122.35
4	1-C	417	ASN	C-N-CA	5.43	130.28	122.35
4	2-C	417	ASN	CA-C-N	5.43	130.28	122.35
4	2-C	417	ASN	C-N-CA	5.43	130.28	122.35
4	3-C	417	ASN	CA-C-N	5.43	130.28	122.35
4	3-C	417	ASN	C-N-CA	5.43	130.28	122.35
7	1-G	503	GLU	CA-C-N	5.43	131.91	121.54
7	1-G	503	GLU	C-N-CA	5.43	131.91	121.54
4	1-H	479	ILE	CA-C-N	5.43	130.21	122.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	479	ILE	C-N-CA	5.43	130.21	122.72
4	1-H	697	GLY	CA-C-N	5.43	125.97	120.00
4	1-H	697	GLY	C-N-CA	5.43	125.97	120.00
7	2-G	503	GLU	CA-C-N	5.43	131.91	121.54
7	2-G	503	GLU	C-N-CA	5.43	131.91	121.54
4	2-H	479	ILE	CA-C-N	5.43	130.21	122.72
4	2-H	479	ILE	C-N-CA	5.43	130.21	122.72
4	2-H	697	GLY	CA-C-N	5.43	125.97	120.00
4	2-H	697	GLY	C-N-CA	5.43	125.97	120.00
7	3-G	503	GLU	CA-C-N	5.43	131.91	121.54
7	3-G	503	GLU	C-N-CA	5.43	131.91	121.54
4	3-H	479	ILE	CA-C-N	5.43	130.21	122.72
4	3-H	479	ILE	C-N-CA	5.43	130.21	122.72
4	3-H	697	GLY	CA-C-N	5.43	125.97	120.00
4	3-H	697	GLY	C-N-CA	5.43	125.97	120.00
7	1-K	51	ILE	CA-C-N	5.43	127.55	120.28
7	1-K	51	ILE	C-N-CA	5.43	127.55	120.28
7	1-K	811	HIS	CA-C-O	-5.43	113.53	119.61
3	1-N	328	ALA	CA-C-N	5.43	131.91	121.54
3	1-N	328	ALA	C-N-CA	5.43	131.91	121.54
7	2-K	51	ILE	CA-C-N	5.43	127.55	120.28
7	2-K	51	ILE	C-N-CA	5.43	127.55	120.28
7	2-K	811	HIS	CA-C-O	-5.43	113.53	119.61
3	2-N	328	ALA	CA-C-N	5.43	131.91	121.54
3	2-N	328	ALA	C-N-CA	5.43	131.91	121.54
7	3-K	51	ILE	CA-C-N	5.43	127.55	120.28
7	3-K	51	ILE	C-N-CA	5.43	127.55	120.28
7	3-K	811	HIS	CA-C-O	-5.43	113.53	119.61
3	3-N	328	ALA	CA-C-N	5.43	131.91	121.54
3	3-N	328	ALA	C-N-CA	5.43	131.91	121.54
1	1-A	966	GLY	CA-C-N	-5.43	114.15	122.62
1	1-A	966	GLY	C-N-CA	-5.43	114.15	122.62
1	2-A	966	GLY	CA-C-N	-5.43	114.15	122.62
1	2-A	966	GLY	C-N-CA	-5.43	114.15	122.62
1	3-A	966	GLY	CA-C-N	-5.43	114.15	122.62
1	3-A	966	GLY	C-N-CA	-5.43	114.15	122.62
4	1-C	625	LEU	CA-C-N	5.42	127.55	120.28
4	1-C	625	LEU	C-N-CA	5.42	127.55	120.28
7	1-K	284	GLU	CA-C-N	5.42	127.55	120.28
7	1-K	284	GLU	C-N-CA	5.42	127.55	120.28
4	2-C	625	LEU	CA-C-N	5.42	127.55	120.28
4	2-C	625	LEU	C-N-CA	5.42	127.55	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-K	284	GLU	CA-C-N	5.42	127.55	120.28
7	2-K	284	GLU	C-N-CA	5.42	127.55	120.28
4	3-C	625	LEU	CA-C-N	5.42	127.55	120.28
4	3-C	625	LEU	C-N-CA	5.42	127.55	120.28
7	3-K	284	GLU	CA-C-N	5.42	127.55	120.28
7	3-K	284	GLU	C-N-CA	5.42	127.55	120.28
4	1-C	366	PHE	CA-C-N	-5.42	114.55	122.68
4	1-C	366	PHE	C-N-CA	-5.42	114.55	122.68
4	2-C	366	PHE	CA-C-N	-5.42	114.55	122.68
4	2-C	366	PHE	C-N-CA	-5.42	114.55	122.68
4	3-C	366	PHE	CA-C-N	-5.42	114.55	122.68
4	3-C	366	PHE	C-N-CA	-5.42	114.55	122.68
4	1-C	260	THR	N-CA-C	-5.42	104.23	112.04
4	1-H	417	ASN	CA-C-N	5.42	130.26	122.35
4	1-H	417	ASN	C-N-CA	5.42	130.26	122.35
4	2-C	260	THR	N-CA-C	-5.42	104.23	112.04
4	2-H	417	ASN	CA-C-N	5.42	130.26	122.35
4	2-H	417	ASN	C-N-CA	5.42	130.26	122.35
4	3-C	260	THR	N-CA-C	-5.42	104.23	112.04
4	3-H	417	ASN	CA-C-N	5.42	130.26	122.35
4	3-H	417	ASN	C-N-CA	5.42	130.26	122.35
4	1-C	385	ASN	N-CA-C	-5.42	101.62	109.59
4	2-C	385	ASN	N-CA-C	-5.42	101.62	109.59
4	3-C	385	ASN	N-CA-C	-5.42	101.62	109.59
4	1-C	25	PRO	CA-C-N	5.42	131.89	121.54
4	1-C	25	PRO	C-N-CA	5.42	131.89	121.54
4	1-C	572	ARG	CA-C-N	5.42	130.78	122.93
4	1-C	572	ARG	C-N-CA	5.42	130.78	122.93
4	2-C	25	PRO	CA-C-N	5.42	131.89	121.54
4	2-C	25	PRO	C-N-CA	5.42	131.89	121.54
4	2-C	572	ARG	CA-C-N	5.42	130.78	122.93
4	2-C	572	ARG	C-N-CA	5.42	130.78	122.93
4	3-C	25	PRO	CA-C-N	5.42	131.89	121.54
4	3-C	25	PRO	C-N-CA	5.42	131.89	121.54
4	3-C	572	ARG	CA-C-N	5.42	130.78	122.93
4	3-C	572	ARG	C-N-CA	5.42	130.78	122.93
4	1-C	572	ARG	O-C-N	5.42	129.72	123.17
4	2-C	572	ARG	O-C-N	5.42	129.72	123.17
4	3-C	572	ARG	O-C-N	5.42	129.72	123.17
7	1-G	757	GLU	N-CA-C	-5.41	100.58	109.40
7	2-G	757	GLU	N-CA-C	-5.41	100.58	109.40
7	3-G	757	GLU	N-CA-C	-5.41	100.58	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	688	GLN	N-CA-C	-5.41	105.28	111.07
4	1-C	479	ILE	CA-C-N	5.41	130.19	122.72
4	1-C	479	ILE	C-N-CA	5.41	130.19	122.72
7	1-G	325	CYS	CA-C-N	5.41	127.47	120.44
7	1-G	325	CYS	C-N-CA	5.41	127.47	120.44
7	1-K	757	GLU	N-CA-C	-5.41	100.58	109.40
1	2-A	688	GLN	N-CA-C	-5.41	105.28	111.07
4	2-C	479	ILE	CA-C-N	5.41	130.19	122.72
4	2-C	479	ILE	C-N-CA	5.41	130.19	122.72
7	2-G	325	CYS	CA-C-N	5.41	127.47	120.44
7	2-G	325	CYS	C-N-CA	5.41	127.47	120.44
7	2-K	757	GLU	N-CA-C	-5.41	100.58	109.40
1	3-A	688	GLN	N-CA-C	-5.41	105.28	111.07
4	3-C	479	ILE	CA-C-N	5.41	130.19	122.72
4	3-C	479	ILE	C-N-CA	5.41	130.19	122.72
7	3-G	325	CYS	CA-C-N	5.41	127.47	120.44
7	3-G	325	CYS	C-N-CA	5.41	127.47	120.44
7	3-K	757	GLU	N-CA-C	-5.41	100.58	109.40
7	1-G	852	VAL	N-CA-C	-5.41	100.65	108.71
7	1-K	213	LYS	CA-C-N	5.41	127.53	120.28
7	1-K	213	LYS	C-N-CA	5.41	127.53	120.28
7	2-G	852	VAL	N-CA-C	-5.41	100.65	108.71
7	2-K	213	LYS	CA-C-N	5.41	127.53	120.28
7	2-K	213	LYS	C-N-CA	5.41	127.53	120.28
7	3-G	852	VAL	N-CA-C	-5.41	100.65	108.71
7	3-K	213	LYS	CA-C-N	5.41	127.53	120.28
7	3-K	213	LYS	C-N-CA	5.41	127.53	120.28
6	1-F	102	GLU	CA-C-N	5.41	127.47	120.44
6	1-F	102	GLU	C-N-CA	5.41	127.47	120.44
4	1-H	604	SER	CA-C-N	5.41	127.52	120.28
4	1-H	604	SER	C-N-CA	5.41	127.52	120.28
6	2-F	102	GLU	CA-C-N	5.41	127.47	120.44
6	2-F	102	GLU	C-N-CA	5.41	127.47	120.44
4	2-H	604	SER	CA-C-N	5.41	127.52	120.28
4	2-H	604	SER	C-N-CA	5.41	127.52	120.28
6	3-F	102	GLU	CA-C-N	5.41	127.47	120.44
6	3-F	102	GLU	C-N-CA	5.41	127.47	120.44
4	3-H	604	SER	CA-C-N	5.41	127.52	120.28
4	3-H	604	SER	C-N-CA	5.41	127.52	120.28
1	1-A	76	LYS	CA-C-N	-5.40	115.48	122.99
1	1-A	76	LYS	C-N-CA	-5.40	115.48	122.99
1	2-A	76	LYS	CA-C-N	-5.40	115.48	122.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	76	LYS	C-N-CA	-5.40	115.48	122.99
1	3-A	76	LYS	CA-C-N	-5.40	115.48	122.99
1	3-A	76	LYS	C-N-CA	-5.40	115.48	122.99
4	1-C	307	SER	N-CA-C	-5.40	100.51	108.99
4	1-H	265	SER	N-CA-C	5.40	117.06	108.79
5	1-I	235	VAL	O-C-N	5.40	127.20	121.91
4	2-C	307	SER	N-CA-C	-5.40	100.51	108.99
4	2-H	265	SER	N-CA-C	5.40	117.06	108.79
5	2-I	235	VAL	O-C-N	5.40	127.20	121.91
4	3-C	307	SER	N-CA-C	-5.40	100.51	108.99
4	3-H	265	SER	N-CA-C	5.40	117.06	108.79
5	3-I	235	VAL	O-C-N	5.40	127.20	121.91
1	1-A	723	ALA	CA-C-N	5.40	127.46	120.44
1	1-A	723	ALA	C-N-CA	5.40	127.46	120.44
1	1-A	743	SER	CA-C-N	5.40	128.06	120.28
1	1-A	743	SER	C-N-CA	5.40	128.06	120.28
7	1-K	296	CYS	CA-C-N	5.40	131.85	121.54
7	1-K	296	CYS	C-N-CA	5.40	131.85	121.54
7	1-K	632	SER	N-CA-C	-5.40	101.15	109.52
4	1-H	366	PHE	CA-C-N	-5.40	114.58	122.68
4	1-H	366	PHE	C-N-CA	-5.40	114.58	122.68
1	2-A	723	ALA	CA-C-N	5.40	127.46	120.44
1	2-A	723	ALA	C-N-CA	5.40	127.46	120.44
1	2-A	743	SER	CA-C-N	5.40	128.06	120.28
1	2-A	743	SER	C-N-CA	5.40	128.06	120.28
7	2-K	296	CYS	CA-C-N	5.40	131.85	121.54
7	2-K	296	CYS	C-N-CA	5.40	131.85	121.54
7	2-K	632	SER	N-CA-C	-5.40	101.15	109.52
4	2-H	366	PHE	CA-C-N	-5.40	114.58	122.68
4	2-H	366	PHE	C-N-CA	-5.40	114.58	122.68
1	3-A	723	ALA	CA-C-N	5.40	127.46	120.44
1	3-A	723	ALA	C-N-CA	5.40	127.46	120.44
1	3-A	743	SER	CA-C-N	5.40	128.06	120.28
1	3-A	743	SER	C-N-CA	5.40	128.06	120.28
7	3-K	296	CYS	CA-C-N	5.40	131.85	121.54
7	3-K	296	CYS	C-N-CA	5.40	131.85	121.54
7	3-K	632	SER	N-CA-C	-5.40	101.15	109.52
4	3-H	366	PHE	CA-C-N	-5.40	114.58	122.68
4	3-H	366	PHE	C-N-CA	-5.40	114.58	122.68
3	1-B	934	PRO	N-CA-C	5.40	123.59	112.47
7	1-K	178	VAL	CA-C-N	5.40	127.51	120.28
7	1-K	178	VAL	C-N-CA	5.40	127.51	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	2-B	934	PRO	N-CA-C	5.40	123.59	112.47
7	2-K	178	VAL	CA-C-N	5.40	127.51	120.28
7	2-K	178	VAL	C-N-CA	5.40	127.51	120.28
3	3-B	934	PRO	N-CA-C	5.40	123.59	112.47
7	3-K	178	VAL	CA-C-N	5.40	127.51	120.28
7	3-K	178	VAL	C-N-CA	5.40	127.51	120.28
7	1-G	169	CYS	N-CA-C	-5.40	105.09	110.97
7	2-G	169	CYS	N-CA-C	-5.40	105.09	110.97
7	3-G	169	CYS	N-CA-C	-5.40	105.09	110.97
3	1-B	938	VAL	N-CA-C	-5.39	98.12	109.34
3	2-B	938	VAL	N-CA-C	-5.39	98.12	109.34
3	3-B	938	VAL	N-CA-C	-5.39	98.12	109.34
1	1-A	219	LEU	N-CA-C	-5.39	102.90	110.50
8	1-Z	86	ASN	N-CA-C	5.39	117.90	110.35
6	1-J	102	GLU	CA-C-N	5.39	127.45	120.44
6	1-J	102	GLU	C-N-CA	5.39	127.45	120.44
1	2-A	219	LEU	N-CA-C	-5.39	102.90	110.50
8	2-Z	86	ASN	N-CA-C	5.39	117.90	110.35
6	2-J	102	GLU	CA-C-N	5.39	127.45	120.44
6	2-J	102	GLU	C-N-CA	5.39	127.45	120.44
1	3-A	219	LEU	N-CA-C	-5.39	102.90	110.50
8	3-Z	86	ASN	N-CA-C	5.39	117.90	110.35
6	3-J	102	GLU	CA-C-N	5.39	127.45	120.44
6	3-J	102	GLU	C-N-CA	5.39	127.45	120.44
4	1-C	506	THR	N-CA-C	-5.39	106.18	114.16
3	1-N	529	LEU	CA-C-N	5.39	127.35	120.56
3	1-N	529	LEU	C-N-CA	5.39	127.35	120.56
4	2-C	506	THR	N-CA-C	-5.39	106.18	114.16
3	2-N	529	LEU	CA-C-N	5.39	127.35	120.56
3	2-N	529	LEU	C-N-CA	5.39	127.35	120.56
4	3-C	506	THR	N-CA-C	-5.39	106.18	114.16
3	3-N	529	LEU	CA-C-N	5.39	127.35	120.56
3	3-N	529	LEU	C-N-CA	5.39	127.35	120.56
6	1-J	122	LEU	N-CA-C	5.39	117.19	108.41
6	2-J	122	LEU	N-CA-C	5.39	117.19	108.41
6	3-J	122	LEU	N-CA-C	5.39	117.19	108.41
6	1-F	113	GLU	CA-C-N	5.39	130.70	122.24
6	1-F	113	GLU	C-N-CA	5.39	130.70	122.24
7	1-K	83	THR	N-CA-C	-5.39	105.57	111.82
6	2-F	113	GLU	CA-C-N	5.39	130.70	122.24
6	2-F	113	GLU	C-N-CA	5.39	130.70	122.24
7	2-K	83	THR	N-CA-C	-5.39	105.57	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	3-F	113	GLU	CA-C-N	5.39	130.70	122.24
6	3-F	113	GLU	C-N-CA	5.39	130.70	122.24
7	3-K	83	THR	N-CA-C	-5.39	105.57	111.82
4	1-C	265	SER	N-CA-C	5.38	117.03	108.79
4	1-C	604	SER	CA-C-N	5.38	127.50	120.28
4	1-C	604	SER	C-N-CA	5.38	127.50	120.28
4	1-H	572	ARG	CA-C-N	5.38	130.74	122.93
4	1-H	572	ARG	C-N-CA	5.38	130.74	122.93
4	2-C	265	SER	N-CA-C	5.38	117.03	108.79
4	2-C	604	SER	CA-C-N	5.38	127.50	120.28
4	2-C	604	SER	C-N-CA	5.38	127.50	120.28
4	2-H	572	ARG	CA-C-N	5.38	130.74	122.93
4	2-H	572	ARG	C-N-CA	5.38	130.74	122.93
4	3-C	265	SER	N-CA-C	5.38	117.03	108.79
4	3-C	604	SER	CA-C-N	5.38	127.50	120.28
4	3-C	604	SER	C-N-CA	5.38	127.50	120.28
4	3-H	572	ARG	CA-C-N	5.38	130.74	122.93
4	3-H	572	ARG	C-N-CA	5.38	130.74	122.93
4	1-H	625	LEU	CA-C-N	5.38	127.49	120.28
4	1-H	625	LEU	C-N-CA	5.38	127.49	120.28
6	1-J	113	GLU	CA-C-N	5.38	130.69	122.24
6	1-J	113	GLU	C-N-CA	5.38	130.69	122.24
4	2-H	625	LEU	CA-C-N	5.38	127.49	120.28
4	2-H	625	LEU	C-N-CA	5.38	127.49	120.28
6	2-J	113	GLU	CA-C-N	5.38	130.69	122.24
6	2-J	113	GLU	C-N-CA	5.38	130.69	122.24
4	3-H	625	LEU	CA-C-N	5.38	127.49	120.28
4	3-H	625	LEU	C-N-CA	5.38	127.49	120.28
6	3-J	113	GLU	CA-C-N	5.38	130.69	122.24
6	3-J	113	GLU	C-N-CA	5.38	130.69	122.24
3	1-N	309	ASP	CA-C-O	5.38	128.21	120.51
3	2-N	309	ASP	CA-C-O	5.38	128.21	120.51
3	3-N	309	ASP	CA-C-O	5.38	128.21	120.51
5	1-D	124	ASN	CA-C-N	5.38	131.65	121.97
5	1-D	124	ASN	C-N-CA	5.38	131.65	121.97
6	1-M	42	VAL	CA-C-N	5.38	131.65	121.97
6	1-M	42	VAL	C-N-CA	5.38	131.65	121.97
5	2-D	124	ASN	CA-C-N	5.38	131.65	121.97
5	2-D	124	ASN	C-N-CA	5.38	131.65	121.97
6	2-M	42	VAL	CA-C-N	5.38	131.65	121.97
6	2-M	42	VAL	C-N-CA	5.38	131.65	121.97
5	3-D	124	ASN	CA-C-N	5.38	131.65	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	3-D	124	ASN	C-N-CA	5.38	131.65	121.97
6	3-M	42	VAL	CA-C-N	5.38	131.65	121.97
6	3-M	42	VAL	C-N-CA	5.38	131.65	121.97
1	1-A	149	LEU	CA-C-N	-5.38	115.47	122.51
1	1-A	149	LEU	C-N-CA	-5.38	115.47	122.51
5	1-D	235	VAL	O-C-N	5.38	127.18	121.91
7	1-G	632	SER	N-CA-C	-5.38	101.18	109.52
6	1-R	29	GLY	N-CA-C	-5.38	100.43	113.18
3	1-N	320	LEU	CA-C-N	5.38	127.83	120.46
3	1-N	320	LEU	C-N-CA	5.38	127.83	120.46
1	2-A	149	LEU	CA-C-N	-5.38	115.47	122.51
1	2-A	149	LEU	C-N-CA	-5.38	115.47	122.51
5	2-D	235	VAL	O-C-N	5.38	127.18	121.91
7	2-G	632	SER	N-CA-C	-5.38	101.18	109.52
6	2-R	29	GLY	N-CA-C	-5.38	100.43	113.18
3	2-N	320	LEU	CA-C-N	5.38	127.83	120.46
3	2-N	320	LEU	C-N-CA	5.38	127.83	120.46
1	3-A	149	LEU	CA-C-N	-5.38	115.47	122.51
1	3-A	149	LEU	C-N-CA	-5.38	115.47	122.51
5	3-D	235	VAL	O-C-N	5.38	127.18	121.91
7	3-G	632	SER	N-CA-C	-5.38	101.18	109.52
6	3-R	29	GLY	N-CA-C	-5.38	100.43	113.18
3	3-N	320	LEU	CA-C-N	5.38	127.83	120.46
3	3-N	320	LEU	C-N-CA	5.38	127.83	120.46
4	1-H	307	SER	N-CA-C	-5.38	100.55	108.99
4	1-H	652	GLY	N-CA-C	5.38	123.18	114.90
4	2-H	307	SER	N-CA-C	-5.38	100.55	108.99
4	2-H	652	GLY	N-CA-C	5.38	123.18	114.90
4	3-H	307	SER	N-CA-C	-5.38	100.55	108.99
4	3-H	652	GLY	N-CA-C	5.38	123.18	114.90
5	1-I	124	ASN	CA-C-N	5.37	131.64	121.97
5	1-I	124	ASN	C-N-CA	5.37	131.64	121.97
5	2-I	124	ASN	CA-C-N	5.37	131.64	121.97
5	2-I	124	ASN	C-N-CA	5.37	131.64	121.97
5	3-I	124	ASN	CA-C-N	5.37	131.64	121.97
5	3-I	124	ASN	C-N-CA	5.37	131.64	121.97
1	1-A	568	ILE	CA-C-N	5.37	131.43	122.73
1	1-A	568	ILE	C-N-CA	5.37	131.43	122.73
4	1-C	11	LEU	N-CA-C	-5.37	100.27	108.76
4	1-C	524	VAL	N-CA-C	5.37	115.82	107.28
4	1-H	506	THR	N-CA-C	-5.37	106.21	114.16
1	2-A	568	ILE	CA-C-N	5.37	131.43	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	568	ILE	C-N-CA	5.37	131.43	122.73
4	2-C	11	LEU	N-CA-C	-5.37	100.27	108.76
4	2-C	524	VAL	N-CA-C	5.37	115.82	107.28
4	2-H	506	THR	N-CA-C	-5.37	106.21	114.16
1	3-A	568	ILE	CA-C-N	5.37	131.43	122.73
1	3-A	568	ILE	C-N-CA	5.37	131.43	122.73
4	3-C	11	LEU	N-CA-C	-5.37	100.27	108.76
4	3-C	524	VAL	N-CA-C	5.37	115.82	107.28
4	3-H	506	THR	N-CA-C	-5.37	106.21	114.16
4	1-C	652	GLY	N-CA-C	5.37	123.16	114.90
4	2-C	652	GLY	N-CA-C	5.37	123.16	114.90
4	3-C	652	GLY	N-CA-C	5.37	123.16	114.90
4	1-C	692	HIS	N-CA-C	-5.36	105.43	111.28
4	2-C	692	HIS	N-CA-C	-5.36	105.43	111.28
4	3-C	692	HIS	N-CA-C	-5.36	105.43	111.28
4	1-C	421	LYS	CA-C-O	5.36	126.19	120.46
4	2-C	421	LYS	CA-C-O	5.36	126.19	120.46
4	3-C	421	LYS	CA-C-O	5.36	126.19	120.46
1	1-A	569	TYR	CA-C-N	-5.36	114.30	121.80
1	1-A	569	TYR	C-N-CA	-5.36	114.30	121.80
4	1-C	759	ARG	N-CA-C	5.36	116.92	111.14
7	1-G	514	LYS	CA-C-N	5.36	127.89	120.29
7	1-G	514	LYS	C-N-CA	5.36	127.89	120.29
1	2-A	569	TYR	CA-C-N	-5.36	114.30	121.80
1	2-A	569	TYR	C-N-CA	-5.36	114.30	121.80
4	2-C	759	ARG	N-CA-C	5.36	116.92	111.14
7	2-G	514	LYS	CA-C-N	5.36	127.89	120.29
7	2-G	514	LYS	C-N-CA	5.36	127.89	120.29
1	3-A	569	TYR	CA-C-N	-5.36	114.30	121.80
1	3-A	569	TYR	C-N-CA	-5.36	114.30	121.80
4	3-C	759	ARG	N-CA-C	5.36	116.92	111.14
7	3-G	514	LYS	CA-C-N	5.36	127.89	120.29
7	3-G	514	LYS	C-N-CA	5.36	127.89	120.29
1	1-A	810	LEU	CA-C-N	5.35	131.76	121.54
1	1-A	810	LEU	C-N-CA	5.35	131.76	121.54
4	1-H	431	GLU	N-CA-C	-5.35	99.40	110.80
6	1-J	94	SER	N-CA-C	-5.35	106.94	112.93
1	2-A	810	LEU	CA-C-N	5.35	131.76	121.54
1	2-A	810	LEU	C-N-CA	5.35	131.76	121.54
4	2-H	431	GLU	N-CA-C	-5.35	99.40	110.80
6	2-J	94	SER	N-CA-C	-5.35	106.94	112.93
1	3-A	810	LEU	CA-C-N	5.35	131.76	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3-A	810	LEU	C-N-CA	5.35	131.76	121.54
4	3-H	431	GLU	N-CA-C	-5.35	99.40	110.80
6	3-J	94	SER	N-CA-C	-5.35	106.94	112.93
4	1-C	431	GLU	N-CA-C	-5.35	99.40	110.80
8	1-Z	68	VAL	N-CA-C	-5.35	100.62	108.11
4	2-C	431	GLU	N-CA-C	-5.35	99.40	110.80
8	2-Z	68	VAL	N-CA-C	-5.35	100.62	108.11
4	3-C	431	GLU	N-CA-C	-5.35	99.40	110.80
8	3-Z	68	VAL	N-CA-C	-5.35	100.62	108.11
4	1-C	697	GLY	CA-C-N	5.35	125.88	120.00
4	1-C	697	GLY	C-N-CA	5.35	125.88	120.00
7	1-G	209	LEU	CA-C-O	5.35	126.22	120.55
4	1-H	692	HIS	N-CA-C	-5.35	105.45	111.28
4	2-C	697	GLY	CA-C-N	5.35	125.88	120.00
4	2-C	697	GLY	C-N-CA	5.35	125.88	120.00
7	2-G	209	LEU	CA-C-O	5.35	126.22	120.55
4	2-H	692	HIS	N-CA-C	-5.35	105.45	111.28
4	3-C	697	GLY	CA-C-N	5.35	125.88	120.00
4	3-C	697	GLY	C-N-CA	5.35	125.88	120.00
7	3-G	209	LEU	CA-C-O	5.35	126.22	120.55
4	3-H	692	HIS	N-CA-C	-5.35	105.45	111.28
4	1-H	22	ASP	N-CA-C	-5.35	100.59	108.99
4	1-H	65	PHE	CA-C-O	-5.35	115.04	120.71
4	2-H	22	ASP	N-CA-C	-5.35	100.59	108.99
4	2-H	65	PHE	CA-C-O	-5.35	115.04	120.71
4	3-H	22	ASP	N-CA-C	-5.35	100.59	108.99
4	3-H	65	PHE	CA-C-O	-5.35	115.04	120.71
1	1-A	377	VAL	N-CA-C	5.35	116.36	108.45
6	1-F	122	LEU	N-CA-C	5.35	117.12	108.41
1	2-A	377	VAL	N-CA-C	5.35	116.36	108.45
6	2-F	122	LEU	N-CA-C	5.35	117.12	108.41
1	3-A	377	VAL	N-CA-C	5.35	116.36	108.45
6	3-F	122	LEU	N-CA-C	5.35	117.12	108.41
4	1-H	524	VAL	N-CA-C	5.34	115.78	107.28
4	2-H	524	VAL	N-CA-C	5.34	115.78	107.28
4	3-H	524	VAL	N-CA-C	5.34	115.78	107.28
7	1-G	177	TRP	CA-C-N	5.34	128.06	120.53
7	1-G	177	TRP	C-N-CA	5.34	128.06	120.53
8	1-Z	44	PHE	N-CA-C	-5.34	105.54	111.36
7	1-K	220	ARG	CA-C-O	-5.34	114.30	120.49
7	2-G	177	TRP	CA-C-N	5.34	128.06	120.53
7	2-G	177	TRP	C-N-CA	5.34	128.06	120.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2-Z	44	PHE	N-CA-C	-5.34	105.54	111.36
7	2-K	220	ARG	CA-C-O	-5.34	114.30	120.49
7	3-G	177	TRP	CA-C-N	5.34	128.06	120.53
7	3-G	177	TRP	C-N-CA	5.34	128.06	120.53
8	3-Z	44	PHE	N-CA-C	-5.34	105.54	111.36
7	3-K	220	ARG	CA-C-O	-5.34	114.30	120.49
6	1-M	97	ARG	N-CA-C	-5.34	106.45	113.17
6	2-M	97	ARG	N-CA-C	-5.34	106.45	113.17
6	3-M	97	ARG	N-CA-C	-5.34	106.45	113.17
5	1-D	55	ARG	CA-C-N	-5.33	114.53	122.74
5	1-D	55	ARG	C-N-CA	-5.33	114.53	122.74
5	2-D	55	ARG	CA-C-N	-5.33	114.53	122.74
5	2-D	55	ARG	C-N-CA	-5.33	114.53	122.74
5	3-D	55	ARG	CA-C-N	-5.33	114.53	122.74
5	3-D	55	ARG	C-N-CA	-5.33	114.53	122.74
6	1-F	94	SER	N-CA-C	-5.33	106.96	112.93
6	2-F	94	SER	N-CA-C	-5.33	106.96	112.93
6	3-F	94	SER	N-CA-C	-5.33	106.96	112.93
1	1-A	222	SER	N-CA-C	5.33	117.49	109.23
4	1-C	314	ILE	CA-C-N	-5.33	116.58	123.19
4	1-C	314	ILE	C-N-CA	-5.33	116.58	123.19
1	2-A	222	SER	N-CA-C	5.33	117.49	109.23
4	2-C	314	ILE	CA-C-N	-5.33	116.58	123.19
4	2-C	314	ILE	C-N-CA	-5.33	116.58	123.19
1	3-A	222	SER	N-CA-C	5.33	117.49	109.23
4	3-C	314	ILE	CA-C-N	-5.33	116.58	123.19
4	3-C	314	ILE	C-N-CA	-5.33	116.58	123.19
3	1-B	529	LEU	CA-C-N	5.33	127.27	120.56
3	1-B	529	LEU	C-N-CA	5.33	127.27	120.56
3	1-B	794	PRO	CA-C-O	-5.33	115.53	121.23
7	1-G	148	ILE	N-CA-C	-5.33	105.19	110.62
3	2-B	529	LEU	CA-C-N	5.33	127.27	120.56
3	2-B	529	LEU	C-N-CA	5.33	127.27	120.56
3	2-B	794	PRO	CA-C-O	-5.33	115.53	121.23
7	2-G	148	ILE	N-CA-C	-5.33	105.19	110.62
3	3-B	529	LEU	CA-C-N	5.33	127.27	120.56
3	3-B	529	LEU	C-N-CA	5.33	127.27	120.56
3	3-B	794	PRO	CA-C-O	-5.33	115.53	121.23
7	3-G	148	ILE	N-CA-C	-5.33	105.19	110.62
3	1-B	794	PRO	N-CA-C	5.32	119.22	111.03
6	1-M	19	ARG	N-CA-C	-5.32	99.84	108.41
3	2-B	794	PRO	N-CA-C	5.32	119.22	111.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	2-M	19	ARG	N-CA-C	-5.32	99.84	108.41
3	3-B	794	PRO	N-CA-C	5.32	119.22	111.03
6	3-M	19	ARG	N-CA-C	-5.32	99.84	108.41
7	1-K	122	GLY	CA-C-N	5.32	124.95	119.05
7	1-K	122	GLY	C-N-CA	5.32	124.95	119.05
5	1-I	55	ARG	CA-C-N	-5.32	114.55	122.74
5	1-I	55	ARG	C-N-CA	-5.32	114.55	122.74
7	2-K	122	GLY	CA-C-N	5.32	124.95	119.05
7	2-K	122	GLY	C-N-CA	5.32	124.95	119.05
5	2-I	55	ARG	CA-C-N	-5.32	114.55	122.74
5	2-I	55	ARG	C-N-CA	-5.32	114.55	122.74
7	3-K	122	GLY	CA-C-N	5.32	124.95	119.05
7	3-K	122	GLY	C-N-CA	5.32	124.95	119.05
5	3-I	55	ARG	CA-C-N	-5.32	114.55	122.74
5	3-I	55	ARG	C-N-CA	-5.32	114.55	122.74
1	1-A	220	ILE	N-CA-C	-5.32	100.19	108.86
3	1-B	538	THR	CA-C-N	5.32	127.41	120.28
3	1-B	538	THR	C-N-CA	5.32	127.41	120.28
5	1-D	53	SER	CA-C-N	-5.32	115.60	122.99
5	1-D	53	SER	C-N-CA	-5.32	115.60	122.99
7	1-K	663	PHE	CA-C-N	5.32	130.06	122.72
7	1-K	663	PHE	C-N-CA	5.32	130.06	122.72
4	1-H	386	LYS	CA-C-O	-5.32	115.22	120.70
1	2-A	220	ILE	N-CA-C	-5.32	100.19	108.86
3	2-B	538	THR	CA-C-N	5.32	127.41	120.28
3	2-B	538	THR	C-N-CA	5.32	127.41	120.28
5	2-D	53	SER	CA-C-N	-5.32	115.60	122.99
5	2-D	53	SER	C-N-CA	-5.32	115.60	122.99
7	2-K	663	PHE	CA-C-N	5.32	130.06	122.72
7	2-K	663	PHE	C-N-CA	5.32	130.06	122.72
4	2-H	386	LYS	CA-C-O	-5.32	115.22	120.70
1	3-A	220	ILE	N-CA-C	-5.32	100.19	108.86
3	3-B	538	THR	CA-C-N	5.32	127.41	120.28
3	3-B	538	THR	C-N-CA	5.32	127.41	120.28
5	3-D	53	SER	CA-C-N	-5.32	115.60	122.99
5	3-D	53	SER	C-N-CA	-5.32	115.60	122.99
7	3-K	663	PHE	CA-C-N	5.32	130.06	122.72
7	3-K	663	PHE	C-N-CA	5.32	130.06	122.72
4	3-H	386	LYS	CA-C-O	-5.32	115.22	120.70
1	1-A	494	VAL	N-CA-C	-5.32	100.82	108.53
7	1-G	99	ALA	CA-C-N	5.32	131.69	121.54
7	1-G	99	ALA	C-N-CA	5.32	131.69	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	494	VAL	N-CA-C	-5.32	100.82	108.53
7	2-G	99	ALA	CA-C-N	5.32	131.69	121.54
7	2-G	99	ALA	C-N-CA	5.32	131.69	121.54
1	3-A	494	VAL	N-CA-C	-5.32	100.82	108.53
7	3-G	99	ALA	CA-C-N	5.32	131.69	121.54
7	3-G	99	ALA	C-N-CA	5.32	131.69	121.54
4	1-H	11	LEU	N-CA-C	-5.31	100.36	108.76
4	2-H	11	LEU	N-CA-C	-5.31	100.36	108.76
4	3-H	11	LEU	N-CA-C	-5.31	100.36	108.76
7	1-G	412	GLU	CA-C-N	5.31	127.40	120.28
7	1-G	412	GLU	C-N-CA	5.31	127.40	120.28
4	1-H	314	ILE	CA-C-N	-5.31	116.60	123.19
4	1-H	314	ILE	C-N-CA	-5.31	116.60	123.19
7	2-G	412	GLU	CA-C-N	5.31	127.40	120.28
7	2-G	412	GLU	C-N-CA	5.31	127.40	120.28
4	2-H	314	ILE	CA-C-N	-5.31	116.60	123.19
4	2-H	314	ILE	C-N-CA	-5.31	116.60	123.19
7	3-G	412	GLU	CA-C-N	5.31	127.40	120.28
7	3-G	412	GLU	C-N-CA	5.31	127.40	120.28
4	3-H	314	ILE	CA-C-N	-5.31	116.60	123.19
4	3-H	314	ILE	C-N-CA	-5.31	116.60	123.19
4	1-C	22	ASP	N-CA-C	-5.31	100.65	108.99
4	2-C	22	ASP	N-CA-C	-5.31	100.65	108.99
4	3-C	22	ASP	N-CA-C	-5.31	100.65	108.99
1	1-A	403	GLN	CA-C-N	5.31	128.42	120.83
1	1-A	403	GLN	C-N-CA	5.31	128.42	120.83
1	1-A	764	THR	N-CA-C	5.31	119.02	112.54
1	2-A	403	GLN	CA-C-N	5.31	128.42	120.83
1	2-A	403	GLN	C-N-CA	5.31	128.42	120.83
1	2-A	764	THR	N-CA-C	5.31	119.02	112.54
1	3-A	403	GLN	CA-C-N	5.31	128.42	120.83
1	3-A	403	GLN	C-N-CA	5.31	128.42	120.83
1	3-A	764	THR	N-CA-C	5.31	119.02	112.54
1	1-A	86	LEU	CA-C-N	5.31	131.82	121.63
1	1-A	86	LEU	C-N-CA	5.31	131.82	121.63
5	1-D	6	ALA	N-CA-C	-5.31	100.25	108.90
8	1-L	79	VAL	CA-C-O	-5.31	114.73	120.67
5	1-I	6	ALA	N-CA-C	-5.31	100.25	108.90
1	2-A	86	LEU	CA-C-N	5.31	131.82	121.63
1	2-A	86	LEU	C-N-CA	5.31	131.82	121.63
5	2-D	6	ALA	N-CA-C	-5.31	100.25	108.90
8	2-L	79	VAL	CA-C-O	-5.31	114.73	120.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	2-I	6	ALA	N-CA-C	-5.31	100.25	108.90
1	3-A	86	LEU	CA-C-N	5.31	131.82	121.63
1	3-A	86	LEU	C-N-CA	5.31	131.82	121.63
5	3-D	6	ALA	N-CA-C	-5.31	100.25	108.90
8	3-L	79	VAL	CA-C-O	-5.31	114.73	120.67
5	3-I	6	ALA	N-CA-C	-5.31	100.25	108.90
3	1-B	836	ASP	N-CA-C	-5.31	102.61	110.46
4	1-H	476	LEU	CA-C-N	-5.31	114.30	122.68
4	1-H	476	LEU	C-N-CA	-5.31	114.30	122.68
4	1-H	542	ARG	N-CA-C	-5.31	101.05	109.59
5	1-I	51	THR	CA-C-N	5.31	129.90	122.36
5	1-I	51	THR	C-N-CA	5.31	129.90	122.36
3	2-B	836	ASP	N-CA-C	-5.31	102.61	110.46
4	2-H	476	LEU	CA-C-N	-5.31	114.30	122.68
4	2-H	476	LEU	C-N-CA	-5.31	114.30	122.68
4	2-H	542	ARG	N-CA-C	-5.31	101.05	109.59
5	2-I	51	THR	CA-C-N	5.31	129.90	122.36
5	2-I	51	THR	C-N-CA	5.31	129.90	122.36
3	3-B	836	ASP	N-CA-C	-5.31	102.61	110.46
4	3-H	476	LEU	CA-C-N	-5.31	114.30	122.68
4	3-H	476	LEU	C-N-CA	-5.31	114.30	122.68
4	3-H	542	ARG	N-CA-C	-5.31	101.05	109.59
5	3-I	51	THR	CA-C-N	5.31	129.90	122.36
5	3-I	51	THR	C-N-CA	5.31	129.90	122.36
7	1-G	222	GLY	N-CA-C	-5.30	104.33	111.54
7	2-G	222	GLY	N-CA-C	-5.30	104.33	111.54
7	3-G	222	GLY	N-CA-C	-5.30	104.33	111.54
3	1-B	825	ALA	N-CA-C	5.30	122.10	110.80
3	2-B	825	ALA	N-CA-C	5.30	122.10	110.80
3	3-B	825	ALA	N-CA-C	5.30	122.10	110.80
6	1-F	115	GLU	O-C-N	5.30	127.74	122.12
7	1-K	147	ALA	CA-C-N	5.30	127.72	120.46
7	1-K	147	ALA	C-N-CA	5.30	127.72	120.46
6	2-F	115	GLU	O-C-N	5.30	127.74	122.12
7	2-K	147	ALA	CA-C-N	5.30	127.72	120.46
7	2-K	147	ALA	C-N-CA	5.30	127.72	120.46
6	3-F	115	GLU	O-C-N	5.30	127.74	122.12
7	3-K	147	ALA	CA-C-N	5.30	127.72	120.46
7	3-K	147	ALA	C-N-CA	5.30	127.72	120.46
4	1-C	231	ASN	CA-C-N	-5.30	115.75	122.37
4	1-C	231	ASN	C-N-CA	-5.30	115.75	122.37
7	1-G	242	GLU	CA-C-N	5.30	131.66	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	242	GLU	C-N-CA	5.30	131.66	121.54
7	1-G	288	ALA	CA-C-N	5.30	127.24	120.56
7	1-G	288	ALA	C-N-CA	5.30	127.24	120.56
3	1-N	538	THR	CA-C-N	5.30	127.38	120.28
3	1-N	538	THR	C-N-CA	5.30	127.38	120.28
4	2-C	231	ASN	CA-C-N	-5.30	115.75	122.37
4	2-C	231	ASN	C-N-CA	-5.30	115.75	122.37
7	2-G	242	GLU	CA-C-N	5.30	131.66	121.54
7	2-G	242	GLU	C-N-CA	5.30	131.66	121.54
7	2-G	288	ALA	CA-C-N	5.30	127.24	120.56
7	2-G	288	ALA	C-N-CA	5.30	127.24	120.56
3	2-N	538	THR	CA-C-N	5.30	127.38	120.28
3	2-N	538	THR	C-N-CA	5.30	127.38	120.28
4	3-C	231	ASN	CA-C-N	-5.30	115.75	122.37
4	3-C	231	ASN	C-N-CA	-5.30	115.75	122.37
7	3-G	242	GLU	CA-C-N	5.30	131.66	121.54
7	3-G	242	GLU	C-N-CA	5.30	131.66	121.54
7	3-G	288	ALA	CA-C-N	5.30	127.24	120.56
7	3-G	288	ALA	C-N-CA	5.30	127.24	120.56
3	3-N	538	THR	CA-C-N	5.30	127.38	120.28
3	3-N	538	THR	C-N-CA	5.30	127.38	120.28
1	1-A	623	GLN	N-CA-C	-5.30	101.23	108.38
4	1-C	386	LYS	CA-C-O	-5.30	115.24	120.70
1	2-A	623	GLN	N-CA-C	-5.30	101.23	108.38
4	2-C	386	LYS	CA-C-O	-5.30	115.24	120.70
1	3-A	623	GLN	N-CA-C	-5.30	101.23	108.38
4	3-C	386	LYS	CA-C-O	-5.30	115.24	120.70
7	1-G	403	THR	O-C-N	5.30	127.73	122.12
7	2-G	403	THR	O-C-N	5.30	127.73	122.12
7	3-G	403	THR	O-C-N	5.30	127.73	122.12
4	1-H	421	LYS	CA-C-O	5.29	126.12	120.46
4	2-H	421	LYS	CA-C-O	5.29	126.12	120.46
4	3-H	421	LYS	CA-C-O	5.29	126.12	120.46
4	1-C	299	LEU	N-CA-C	5.29	119.29	112.41
6	1-F	110	MET	N-CA-C	-5.29	105.59	111.36
4	2-C	299	LEU	N-CA-C	5.29	119.29	112.41
6	2-F	110	MET	N-CA-C	-5.29	105.59	111.36
4	3-C	299	LEU	N-CA-C	5.29	119.29	112.41
6	3-F	110	MET	N-CA-C	-5.29	105.59	111.36
1	1-A	779	ASP	CA-C-N	5.29	125.58	119.92
1	1-A	779	ASP	C-N-CA	5.29	125.58	119.92
4	1-H	299	LEU	N-CA-C	5.29	119.28	112.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	779	ASP	CA-C-N	5.29	125.58	119.92
1	2-A	779	ASP	C-N-CA	5.29	125.58	119.92
4	2-H	299	LEU	N-CA-C	5.29	119.28	112.41
1	3-A	779	ASP	CA-C-N	5.29	125.58	119.92
1	3-A	779	ASP	C-N-CA	5.29	125.58	119.92
4	3-H	299	LEU	N-CA-C	5.29	119.28	112.41
4	1-C	542	ARG	N-CA-C	-5.29	101.08	109.59
4	2-C	542	ARG	N-CA-C	-5.29	101.08	109.59
4	3-C	542	ARG	N-CA-C	-5.29	101.08	109.59
7	1-G	56	ASN	N-CA-C	-5.29	105.52	111.28
7	2-G	56	ASN	N-CA-C	-5.29	105.52	111.28
7	3-G	56	ASN	N-CA-C	-5.29	105.52	111.28
7	1-G	209	LEU	CA-C-N	5.28	127.36	120.28
7	1-G	209	LEU	C-N-CA	5.28	127.36	120.28
6	1-J	101	GLY	CA-C-O	5.28	126.19	120.75
6	1-J	115	GLU	O-C-N	5.28	127.72	122.12
7	2-G	209	LEU	CA-C-N	5.28	127.36	120.28
7	2-G	209	LEU	C-N-CA	5.28	127.36	120.28
6	2-J	101	GLY	CA-C-O	5.28	126.19	120.75
6	2-J	115	GLU	O-C-N	5.28	127.72	122.12
7	3-G	209	LEU	CA-C-N	5.28	127.36	120.28
7	3-G	209	LEU	C-N-CA	5.28	127.36	120.28
6	3-J	101	GLY	CA-C-O	5.28	126.19	120.75
6	3-J	115	GLU	O-C-N	5.28	127.72	122.12
7	1-K	740	GLY	CA-C-N	5.28	131.62	121.54
7	1-K	740	GLY	C-N-CA	5.28	131.62	121.54
7	2-K	740	GLY	CA-C-N	5.28	131.62	121.54
7	2-K	740	GLY	C-N-CA	5.28	131.62	121.54
7	3-K	740	GLY	CA-C-N	5.28	131.62	121.54
7	3-K	740	GLY	C-N-CA	5.28	131.62	121.54
4	1-C	503	GLU	CA-C-N	5.28	131.75	121.41
4	1-C	503	GLU	C-N-CA	5.28	131.75	121.41
6	1-R	22	MET	N-CA-C	-5.28	99.92	108.52
8	1-Z	106	ARG	N-CA-C	-5.28	102.22	113.20
4	2-C	503	GLU	CA-C-N	5.28	131.75	121.41
4	2-C	503	GLU	C-N-CA	5.28	131.75	121.41
6	2-R	22	MET	N-CA-C	-5.28	99.92	108.52
8	2-Z	106	ARG	N-CA-C	-5.28	102.22	113.20
4	3-C	503	GLU	CA-C-N	5.28	131.75	121.41
4	3-C	503	GLU	C-N-CA	5.28	131.75	121.41
6	3-R	22	MET	N-CA-C	-5.28	99.92	108.52
8	3-Z	106	ARG	N-CA-C	-5.28	102.22	113.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	476	LEU	CA-C-N	-5.28	114.34	122.68
4	1-C	476	LEU	C-N-CA	-5.28	114.34	122.68
5	1-D	51	THR	CA-C-N	5.28	129.85	122.36
5	1-D	51	THR	C-N-CA	5.28	129.85	122.36
6	1-F	133	ALA	CA-C-N	5.28	131.99	122.02
6	1-F	133	ALA	C-N-CA	5.28	131.99	122.02
4	2-C	476	LEU	CA-C-N	-5.28	114.34	122.68
4	2-C	476	LEU	C-N-CA	-5.28	114.34	122.68
5	2-D	51	THR	CA-C-N	5.28	129.85	122.36
5	2-D	51	THR	C-N-CA	5.28	129.85	122.36
6	2-F	133	ALA	CA-C-N	5.28	131.99	122.02
6	2-F	133	ALA	C-N-CA	5.28	131.99	122.02
4	3-C	476	LEU	CA-C-N	-5.28	114.34	122.68
4	3-C	476	LEU	C-N-CA	-5.28	114.34	122.68
5	3-D	51	THR	CA-C-N	5.28	129.85	122.36
5	3-D	51	THR	C-N-CA	5.28	129.85	122.36
6	3-F	133	ALA	CA-C-N	5.28	131.99	122.02
6	3-F	133	ALA	C-N-CA	5.28	131.99	122.02
4	1-H	717	GLU	CA-C-N	5.27	125.83	119.98
4	1-H	717	GLU	C-N-CA	5.27	125.83	119.98
4	2-H	717	GLU	CA-C-N	5.27	125.83	119.98
4	2-H	717	GLU	C-N-CA	5.27	125.83	119.98
4	3-H	717	GLU	CA-C-N	5.27	125.83	119.98
4	3-H	717	GLU	C-N-CA	5.27	125.83	119.98
7	1-G	410	GLY	N-CA-C	-5.27	100.68	113.18
6	1-M	139	ILE	N-CA-C	5.27	116.00	110.62
7	2-G	410	GLY	N-CA-C	-5.27	100.68	113.18
6	2-M	139	ILE	N-CA-C	5.27	116.00	110.62
7	3-G	410	GLY	N-CA-C	-5.27	100.68	113.18
6	3-M	139	ILE	N-CA-C	5.27	116.00	110.62
6	1-J	133	ALA	CA-C-N	5.27	131.98	122.02
6	1-J	133	ALA	C-N-CA	5.27	131.98	122.02
6	2-J	133	ALA	CA-C-N	5.27	131.98	122.02
6	2-J	133	ALA	C-N-CA	5.27	131.98	122.02
6	3-J	133	ALA	CA-C-N	5.27	131.98	122.02
6	3-J	133	ALA	C-N-CA	5.27	131.98	122.02
1	1-A	487	LYS	N-CA-C	-5.27	100.14	108.73
1	2-A	487	LYS	N-CA-C	-5.27	100.14	108.73
1	3-A	487	LYS	N-CA-C	-5.27	100.14	108.73
4	1-C	790	ASP	CA-C-O	-5.27	112.94	120.16
6	1-F	115	GLU	N-CA-C	-5.27	105.54	111.28
4	2-C	790	ASP	CA-C-O	-5.27	112.94	120.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	2-F	115	GLU	N-CA-C	-5.27	105.54	111.28
4	3-C	790	ASP	CA-C-O	-5.27	112.94	120.16
6	3-F	115	GLU	N-CA-C	-5.27	105.54	111.28
3	1-B	906	MET	N-CA-C	5.26	118.13	109.76
3	2-B	906	MET	N-CA-C	5.26	118.13	109.76
3	3-B	906	MET	N-CA-C	5.26	118.13	109.76
3	1-B	750	ASN	CA-C-N	5.26	131.59	121.54
3	1-B	750	ASN	C-N-CA	5.26	131.59	121.54
6	1-J	115	GLU	N-CA-C	-5.26	105.54	111.28
3	2-B	750	ASN	CA-C-N	5.26	131.59	121.54
3	2-B	750	ASN	C-N-CA	5.26	131.59	121.54
6	2-J	115	GLU	N-CA-C	-5.26	105.54	111.28
3	3-B	750	ASN	CA-C-N	5.26	131.59	121.54
3	3-B	750	ASN	C-N-CA	5.26	131.59	121.54
6	3-J	115	GLU	N-CA-C	-5.26	105.54	111.28
1	1-A	495	ILE	CA-C-O	5.26	125.92	120.39
6	1-F	101	GLY	CA-C-O	5.26	126.17	120.75
6	1-R	65	VAL	CA-C-N	5.26	129.68	122.84
6	1-R	65	VAL	C-N-CA	5.26	129.68	122.84
3	1-N	387	GLU	N-CA-C	-5.26	99.30	109.24
1	2-A	495	ILE	CA-C-O	5.26	125.92	120.39
6	2-F	101	GLY	CA-C-O	5.26	126.17	120.75
6	2-R	65	VAL	CA-C-N	5.26	129.68	122.84
6	2-R	65	VAL	C-N-CA	5.26	129.68	122.84
3	2-N	387	GLU	N-CA-C	-5.26	99.30	109.24
1	3-A	495	ILE	CA-C-O	5.26	125.92	120.39
6	3-F	101	GLY	CA-C-O	5.26	126.17	120.75
6	3-R	65	VAL	CA-C-N	5.26	129.68	122.84
6	3-R	65	VAL	C-N-CA	5.26	129.68	122.84
3	3-N	387	GLU	N-CA-C	-5.26	99.30	109.24
1	1-A	811	LEU	CA-C-N	5.26	127.33	120.28
1	1-A	811	LEU	C-N-CA	5.26	127.33	120.28
7	1-G	740	GLY	CA-C-N	5.26	131.58	121.54
7	1-G	740	GLY	C-N-CA	5.26	131.58	121.54
1	2-A	811	LEU	CA-C-N	5.26	127.33	120.28
1	2-A	811	LEU	C-N-CA	5.26	127.33	120.28
7	2-G	740	GLY	CA-C-N	5.26	131.58	121.54
7	2-G	740	GLY	C-N-CA	5.26	131.58	121.54
1	3-A	811	LEU	CA-C-N	5.26	127.33	120.28
1	3-A	811	LEU	C-N-CA	5.26	127.33	120.28
7	3-G	740	GLY	CA-C-N	5.26	131.58	121.54
7	3-G	740	GLY	C-N-CA	5.26	131.58	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1-A	566	LEU	N-CA-C	-5.26	98.19	109.81
1	2-A	566	LEU	N-CA-C	-5.26	98.19	109.81
1	3-A	566	LEU	N-CA-C	-5.26	98.19	109.81
1	1-A	461	THR	CA-C-N	5.25	129.37	120.86
1	1-A	461	THR	C-N-CA	5.25	129.37	120.86
1	2-A	461	THR	CA-C-N	5.25	129.37	120.86
1	2-A	461	THR	C-N-CA	5.25	129.37	120.86
1	3-A	461	THR	CA-C-N	5.25	129.37	120.86
1	3-A	461	THR	C-N-CA	5.25	129.37	120.86
1	1-A	513	ILE	CA-C-O	5.25	126.05	120.48
4	1-C	712	VAL	CA-C-O	-5.25	115.49	120.95
7	1-G	527	ARG	N-CA-C	-5.25	105.45	111.07
6	1-R	145	LEU	N-CA-C	5.25	121.99	110.80
1	2-A	513	ILE	CA-C-O	5.25	126.05	120.48
4	2-C	712	VAL	CA-C-O	-5.25	115.49	120.95
7	2-G	527	ARG	N-CA-C	-5.25	105.45	111.07
6	2-R	145	LEU	N-CA-C	5.25	121.99	110.80
1	3-A	513	ILE	CA-C-O	5.25	126.05	120.48
4	3-C	712	VAL	CA-C-O	-5.25	115.49	120.95
7	3-G	527	ARG	N-CA-C	-5.25	105.45	111.07
6	3-R	145	LEU	N-CA-C	5.25	121.99	110.80
5	1-I	53	SER	CA-C-N	-5.25	115.69	122.99
5	1-I	53	SER	C-N-CA	-5.25	115.69	122.99
5	2-I	53	SER	CA-C-N	-5.25	115.69	122.99
5	2-I	53	SER	C-N-CA	-5.25	115.69	122.99
5	3-I	53	SER	CA-C-N	-5.25	115.69	122.99
5	3-I	53	SER	C-N-CA	-5.25	115.69	122.99
8	1-L	11	TYR	CA-C-N	5.25	131.56	121.54
8	1-L	11	TYR	C-N-CA	5.25	131.56	121.54
4	1-H	672	GLN	CA-C-O	5.25	126.11	120.55
8	2-L	11	TYR	CA-C-N	5.25	131.56	121.54
8	2-L	11	TYR	C-N-CA	5.25	131.56	121.54
4	2-H	672	GLN	CA-C-O	5.25	126.11	120.55
8	3-L	11	TYR	CA-C-N	5.25	131.56	121.54
8	3-L	11	TYR	C-N-CA	5.25	131.56	121.54
4	3-H	672	GLN	CA-C-O	5.25	126.11	120.55
3	1-B	778	LEU	CA-C-N	5.25	131.69	121.41
3	1-B	778	LEU	C-N-CA	5.25	131.69	121.41
7	1-G	223	LEU	N-CA-C	5.25	118.22	110.46
3	2-B	778	LEU	CA-C-N	5.25	131.69	121.41
3	2-B	778	LEU	C-N-CA	5.25	131.69	121.41
7	2-G	223	LEU	N-CA-C	5.25	118.22	110.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3-B	778	LEU	CA-C-N	5.25	131.69	121.41
3	3-B	778	LEU	C-N-CA	5.25	131.69	121.41
7	3-G	223	LEU	N-CA-C	5.25	118.22	110.46
4	1-C	672	GLN	CA-C-O	5.24	126.11	120.55
7	1-K	62	GLY	CA-C-N	5.24	127.26	120.44
7	1-K	62	GLY	C-N-CA	5.24	127.26	120.44
4	2-C	672	GLN	CA-C-O	5.24	126.11	120.55
7	2-K	62	GLY	CA-C-N	5.24	127.26	120.44
7	2-K	62	GLY	C-N-CA	5.24	127.26	120.44
4	3-C	672	GLN	CA-C-O	5.24	126.11	120.55
7	3-K	62	GLY	CA-C-N	5.24	127.26	120.44
7	3-K	62	GLY	C-N-CA	5.24	127.26	120.44
4	1-C	717	GLU	CA-C-N	5.24	125.80	119.98
4	1-C	717	GLU	C-N-CA	5.24	125.80	119.98
7	1-K	615	GLU	CA-C-N	5.24	127.30	120.28
7	1-K	615	GLU	C-N-CA	5.24	127.30	120.28
4	2-C	717	GLU	CA-C-N	5.24	125.80	119.98
4	2-C	717	GLU	C-N-CA	5.24	125.80	119.98
7	2-K	615	GLU	CA-C-N	5.24	127.30	120.28
7	2-K	615	GLU	C-N-CA	5.24	127.30	120.28
4	3-C	717	GLU	CA-C-N	5.24	125.80	119.98
4	3-C	717	GLU	C-N-CA	5.24	125.80	119.98
7	3-K	615	GLU	CA-C-N	5.24	127.30	120.28
7	3-K	615	GLU	C-N-CA	5.24	127.30	120.28
3	1-B	387	GLU	N-CA-C	-5.24	99.34	109.24
3	2-B	387	GLU	N-CA-C	-5.24	99.34	109.24
3	3-B	387	GLU	N-CA-C	-5.24	99.34	109.24
1	1-A	191	GLY	N-CA-C	-5.24	100.77	113.18
3	1-B	453	ILE	CA-C-N	5.24	127.64	120.46
3	1-B	453	ILE	C-N-CA	5.24	127.64	120.46
5	1-I	67	VAL	CA-C-O	5.24	126.54	120.67
1	2-A	191	GLY	N-CA-C	-5.24	100.77	113.18
3	2-B	453	ILE	CA-C-N	5.24	127.64	120.46
3	2-B	453	ILE	C-N-CA	5.24	127.64	120.46
5	2-I	67	VAL	CA-C-O	5.24	126.54	120.67
1	3-A	191	GLY	N-CA-C	-5.24	100.77	113.18
3	3-B	453	ILE	CA-C-N	5.24	127.64	120.46
3	3-B	453	ILE	C-N-CA	5.24	127.64	120.46
5	3-I	67	VAL	CA-C-O	5.24	126.54	120.67
5	1-D	67	VAL	CA-C-O	5.24	126.53	120.67
6	1-J	110	MET	N-CA-C	-5.24	105.65	111.36
5	2-D	67	VAL	CA-C-O	5.24	126.53	120.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	2-J	110	MET	N-CA-C	-5.24	105.65	111.36
5	3-D	67	VAL	CA-C-O	5.24	126.53	120.67
6	3-J	110	MET	N-CA-C	-5.24	105.65	111.36
4	1-C	65	PHE	CA-C-O	-5.23	115.16	120.71
4	2-C	65	PHE	CA-C-O	-5.23	115.16	120.71
4	3-C	65	PHE	CA-C-O	-5.23	115.16	120.71
4	1-H	712	VAL	CA-C-O	-5.23	115.51	120.95
4	2-H	712	VAL	CA-C-O	-5.23	115.51	120.95
4	3-H	712	VAL	CA-C-O	-5.23	115.51	120.95
1	1-A	710	THR	N-CA-C	5.23	119.37	112.89
1	2-A	710	THR	N-CA-C	5.23	119.37	112.89
1	3-A	710	THR	N-CA-C	5.23	119.37	112.89
7	1-K	702	GLN	N-CA-C	5.23	121.36	109.81
4	1-H	503	GLU	CA-C-N	5.23	131.66	121.41
4	1-H	503	GLU	C-N-CA	5.23	131.66	121.41
5	1-I	51	THR	N-CA-C	-5.23	101.13	109.23
7	2-K	702	GLN	N-CA-C	5.23	121.36	109.81
4	2-H	503	GLU	CA-C-N	5.23	131.66	121.41
4	2-H	503	GLU	C-N-CA	5.23	131.66	121.41
5	2-I	51	THR	N-CA-C	-5.23	101.13	109.23
7	3-K	702	GLN	N-CA-C	5.23	121.36	109.81
4	3-H	503	GLU	CA-C-N	5.23	131.66	121.41
4	3-H	503	GLU	C-N-CA	5.23	131.66	121.41
5	3-I	51	THR	N-CA-C	-5.23	101.13	109.23
6	1-F	23	VAL	O-C-N	5.23	128.75	123.00
6	1-R	105	GLU	CA-C-N	-5.23	113.97	120.56
6	1-R	105	GLU	C-N-CA	-5.23	113.97	120.56
6	2-F	23	VAL	O-C-N	5.23	128.75	123.00
6	2-R	105	GLU	CA-C-N	-5.23	113.97	120.56
6	2-R	105	GLU	C-N-CA	-5.23	113.97	120.56
6	3-F	23	VAL	O-C-N	5.23	128.75	123.00
6	3-R	105	GLU	CA-C-N	-5.23	113.97	120.56
6	3-R	105	GLU	C-N-CA	-5.23	113.97	120.56
7	1-G	663	PHE	CA-C-N	5.22	129.93	122.72
7	1-G	663	PHE	C-N-CA	5.22	129.93	122.72
7	2-G	663	PHE	CA-C-N	5.22	129.93	122.72
7	2-G	663	PHE	C-N-CA	5.22	129.93	122.72
7	3-G	663	PHE	CA-C-N	5.22	129.93	122.72
7	3-G	663	PHE	C-N-CA	5.22	129.93	122.72
4	1-C	763	PRO	CA-C-N	5.22	130.76	122.61
4	1-C	763	PRO	C-N-CA	5.22	130.76	122.61
7	1-G	615	GLU	CA-C-N	5.22	127.28	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-G	615	GLU	C-N-CA	5.22	127.28	120.28
3	1-N	453	ILE	CA-C-N	5.22	127.62	120.46
3	1-N	453	ILE	C-N-CA	5.22	127.62	120.46
4	1-H	637	VAL	O-C-N	5.22	127.21	121.83
4	2-C	763	PRO	CA-C-N	5.22	130.76	122.61
4	2-C	763	PRO	C-N-CA	5.22	130.76	122.61
7	2-G	615	GLU	CA-C-N	5.22	127.28	120.28
7	2-G	615	GLU	C-N-CA	5.22	127.28	120.28
3	2-N	453	ILE	CA-C-N	5.22	127.62	120.46
3	2-N	453	ILE	C-N-CA	5.22	127.62	120.46
4	2-H	637	VAL	O-C-N	5.22	127.21	121.83
4	3-C	763	PRO	CA-C-N	5.22	130.76	122.61
4	3-C	763	PRO	C-N-CA	5.22	130.76	122.61
7	3-G	615	GLU	CA-C-N	5.22	127.28	120.28
7	3-G	615	GLU	C-N-CA	5.22	127.28	120.28
3	3-N	453	ILE	CA-C-N	5.22	127.62	120.46
3	3-N	453	ILE	C-N-CA	5.22	127.62	120.46
4	3-H	637	VAL	O-C-N	5.22	127.21	121.83
6	1-M	89	ILE	CA-C-N	-5.22	115.70	123.11
6	1-M	89	ILE	C-N-CA	-5.22	115.70	123.11
4	1-H	231	ASN	CA-C-N	-5.22	115.84	122.37
4	1-H	231	ASN	C-N-CA	-5.22	115.84	122.37
6	2-M	89	ILE	CA-C-N	-5.22	115.70	123.11
6	2-M	89	ILE	C-N-CA	-5.22	115.70	123.11
4	2-H	231	ASN	CA-C-N	-5.22	115.84	122.37
4	2-H	231	ASN	C-N-CA	-5.22	115.84	122.37
6	3-M	89	ILE	CA-C-N	-5.22	115.70	123.11
6	3-M	89	ILE	C-N-CA	-5.22	115.70	123.11
4	3-H	231	ASN	CA-C-N	-5.22	115.84	122.37
4	3-H	231	ASN	C-N-CA	-5.22	115.84	122.37
6	1-R	142	LYS	N-CA-C	-5.22	105.67	111.36
6	2-R	142	LYS	N-CA-C	-5.22	105.67	111.36
6	3-R	142	LYS	N-CA-C	-5.22	105.67	111.36
1	1-A	358	ARG	N-CA-C	-5.21	104.26	110.41
1	1-A	662	LEU	CA-C-O	5.21	126.08	120.55
4	1-C	459	ARG	N-CA-C	-5.21	100.39	108.42
4	1-C	637	VAL	O-C-N	5.21	127.20	121.83
1	2-A	358	ARG	N-CA-C	-5.21	104.26	110.41
1	2-A	662	LEU	CA-C-O	5.21	126.08	120.55
4	2-C	459	ARG	N-CA-C	-5.21	100.39	108.42
4	2-C	637	VAL	O-C-N	5.21	127.20	121.83
1	3-A	358	ARG	N-CA-C	-5.21	104.26	110.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3-A	662	LEU	CA-C-O	5.21	126.08	120.55
4	3-C	459	ARG	N-CA-C	-5.21	100.39	108.42
4	3-C	637	VAL	O-C-N	5.21	127.20	121.83
6	1-F	102	GLU	N-CA-C	-5.21	105.68	111.36
6	2-F	102	GLU	N-CA-C	-5.21	105.68	111.36
6	3-F	102	GLU	N-CA-C	-5.21	105.68	111.36
6	1-J	23	VAL	O-C-N	5.21	128.73	123.00
6	2-J	23	VAL	O-C-N	5.21	128.73	123.00
6	3-J	23	VAL	O-C-N	5.21	128.73	123.00
5	1-D	51	THR	N-CA-C	-5.21	101.16	109.23
5	2-D	51	THR	N-CA-C	-5.21	101.16	109.23
5	3-D	51	THR	N-CA-C	-5.21	101.16	109.23
1	1-A	230	LYS	N-CA-C	-5.21	100.91	109.40
1	2-A	230	LYS	N-CA-C	-5.21	100.91	109.40
1	3-A	230	LYS	N-CA-C	-5.21	100.91	109.40
8	1-Z	114	LEU	N-CA-C	-5.20	105.50	111.07
8	2-Z	114	LEU	N-CA-C	-5.20	105.50	111.07
8	3-Z	114	LEU	N-CA-C	-5.20	105.50	111.07
1	1-A	635	PRO	CA-C-N	5.20	128.21	120.31
1	1-A	635	PRO	C-N-CA	5.20	128.21	120.31
1	2-A	635	PRO	CA-C-N	5.20	128.21	120.31
1	2-A	635	PRO	C-N-CA	5.20	128.21	120.31
1	3-A	635	PRO	CA-C-N	5.20	128.21	120.31
1	3-A	635	PRO	C-N-CA	5.20	128.21	120.31
6	1-J	129	ASP	N-CA-C	-5.20	105.61	111.28
6	2-J	129	ASP	N-CA-C	-5.20	105.61	111.28
6	3-J	129	ASP	N-CA-C	-5.20	105.61	111.28
7	1-G	446	CYS	CA-C-N	5.20	131.47	121.54
7	1-G	446	CYS	C-N-CA	5.20	131.47	121.54
7	2-G	446	CYS	CA-C-N	5.20	131.47	121.54
7	2-G	446	CYS	C-N-CA	5.20	131.47	121.54
7	3-G	446	CYS	CA-C-N	5.20	131.47	121.54
7	3-G	446	CYS	C-N-CA	5.20	131.47	121.54
1	1-A	364	PRO	CA-C-N	5.20	128.83	121.66
1	1-A	364	PRO	C-N-CA	5.20	128.83	121.66
7	1-G	141	GLU	CA-C-O	-5.20	115.02	120.63
1	2-A	364	PRO	CA-C-N	5.20	128.83	121.66
1	2-A	364	PRO	C-N-CA	5.20	128.83	121.66
7	2-G	141	GLU	CA-C-O	-5.20	115.02	120.63
1	3-A	364	PRO	CA-C-N	5.20	128.83	121.66
1	3-A	364	PRO	C-N-CA	5.20	128.83	121.66
7	3-G	141	GLU	CA-C-O	-5.20	115.02	120.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-H	459	ARG	N-CA-C	-5.19	100.42	108.42
4	2-H	459	ARG	N-CA-C	-5.19	100.42	108.42
4	3-H	459	ARG	N-CA-C	-5.19	100.42	108.42
4	1-C	633	GLN	N-CA-C	-5.19	105.70	111.36
4	2-C	633	GLN	N-CA-C	-5.19	105.70	111.36
4	3-C	633	GLN	N-CA-C	-5.19	105.70	111.36
7	1-K	150	ASP	N-CA-C	5.19	118.08	109.46
7	2-K	150	ASP	N-CA-C	5.19	118.08	109.46
7	3-K	150	ASP	N-CA-C	5.19	118.08	109.46
7	1-G	859	ARG	O-C-N	-5.19	117.25	123.27
7	2-G	859	ARG	O-C-N	-5.19	117.25	123.27
7	3-G	859	ARG	O-C-N	-5.19	117.25	123.27
6	1-J	102	GLU	N-CA-C	-5.18	105.71	111.36
6	2-J	102	GLU	N-CA-C	-5.18	105.71	111.36
6	3-J	102	GLU	N-CA-C	-5.18	105.71	111.36
3	1-B	390	ASP	CA-C-O	5.18	126.41	119.47
5	1-D	67	VAL	CA-C-N	5.18	130.71	122.62
5	1-D	67	VAL	C-N-CA	5.18	130.71	122.62
7	1-K	609	ARG	N-CA-C	-5.18	105.63	111.28
3	2-B	390	ASP	CA-C-O	5.18	126.41	119.47
5	2-D	67	VAL	CA-C-N	5.18	130.71	122.62
5	2-D	67	VAL	C-N-CA	5.18	130.71	122.62
7	2-K	609	ARG	N-CA-C	-5.18	105.63	111.28
3	3-B	390	ASP	CA-C-O	5.18	126.41	119.47
5	3-D	67	VAL	CA-C-N	5.18	130.71	122.62
5	3-D	67	VAL	C-N-CA	5.18	130.71	122.62
7	3-K	609	ARG	N-CA-C	-5.18	105.63	111.28
1	1-A	761	SER	CA-C-N	5.17	127.17	120.44
1	1-A	761	SER	C-N-CA	5.17	127.17	120.44
4	1-C	391	ALA	O-C-N	5.17	128.76	122.14
1	2-A	761	SER	CA-C-N	5.17	127.17	120.44
1	2-A	761	SER	C-N-CA	5.17	127.17	120.44
4	2-C	391	ALA	O-C-N	5.17	128.76	122.14
1	3-A	761	SER	CA-C-N	5.17	127.17	120.44
1	3-A	761	SER	C-N-CA	5.17	127.17	120.44
4	3-C	391	ALA	O-C-N	5.17	128.76	122.14
1	1-A	762	ALA	N-CA-C	5.17	116.60	111.07
7	1-K	859	ARG	O-C-N	-5.17	117.27	123.27
1	2-A	762	ALA	N-CA-C	5.17	116.60	111.07
7	2-K	859	ARG	O-C-N	-5.17	117.27	123.27
1	3-A	762	ALA	N-CA-C	5.17	116.60	111.07
7	3-K	859	ARG	O-C-N	-5.17	117.27	123.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	634	ALA	N-CA-C	-5.17	105.65	111.28
7	1-G	86	ARG	N-CA-C	5.17	116.60	111.07
7	1-K	607	ALA	CA-C-N	5.17	131.41	121.54
7	1-K	607	ALA	C-N-CA	5.17	131.41	121.54
6	1-M	99	ARG	CA-C-O	5.17	125.40	119.35
4	2-C	634	ALA	N-CA-C	-5.17	105.65	111.28
7	2-G	86	ARG	N-CA-C	5.17	116.60	111.07
7	2-K	607	ALA	CA-C-N	5.17	131.41	121.54
7	2-K	607	ALA	C-N-CA	5.17	131.41	121.54
6	2-M	99	ARG	CA-C-O	5.17	125.40	119.35
4	3-C	634	ALA	N-CA-C	-5.17	105.65	111.28
7	3-G	86	ARG	N-CA-C	5.17	116.60	111.07
7	3-K	607	ALA	CA-C-N	5.17	131.41	121.54
7	3-K	607	ALA	C-N-CA	5.17	131.41	121.54
6	3-M	99	ARG	CA-C-O	5.17	125.40	119.35
6	1-M	22	MET	N-CA-C	-5.17	100.10	108.52
6	2-M	22	MET	N-CA-C	-5.17	100.10	108.52
6	3-M	22	MET	N-CA-C	-5.17	100.10	108.52
6	1-F	126	ASN	N-CA-C	-5.16	102.51	109.95
7	1-K	118	ASP	N-CA-C	-5.16	105.73	111.36
6	2-F	126	ASN	N-CA-C	-5.16	102.51	109.95
7	2-K	118	ASP	N-CA-C	-5.16	105.73	111.36
6	3-F	126	ASN	N-CA-C	-5.16	102.51	109.95
7	3-K	118	ASP	N-CA-C	-5.16	105.73	111.36
7	1-G	609	ARG	N-CA-C	-5.16	105.65	111.28
7	2-G	609	ARG	N-CA-C	-5.16	105.65	111.28
7	3-G	609	ARG	N-CA-C	-5.16	105.65	111.28
1	1-A	280	LYS	CA-C-N	5.16	131.40	121.54
1	1-A	280	LYS	C-N-CA	5.16	131.40	121.54
1	1-A	742	VAL	CA-C-N	5.16	130.47	122.26
1	1-A	742	VAL	C-N-CA	5.16	130.47	122.26
4	1-C	555	ALA	N-CA-C	-5.16	100.47	108.42
7	1-G	815	ARG	CA-C-N	-5.16	113.89	122.92
7	1-G	815	ARG	C-N-CA	-5.16	113.89	122.92
7	1-K	127	ALA	CA-C-O	5.16	125.89	120.42
4	1-H	58	LEU	CA-C-N	5.16	125.16	119.90
4	1-H	58	LEU	C-N-CA	5.16	125.16	119.90
1	2-A	280	LYS	CA-C-N	5.16	131.40	121.54
1	2-A	280	LYS	C-N-CA	5.16	131.40	121.54
1	2-A	742	VAL	CA-C-N	5.16	130.47	122.26
1	2-A	742	VAL	C-N-CA	5.16	130.47	122.26
4	2-C	555	ALA	N-CA-C	-5.16	100.47	108.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	2-G	815	ARG	CA-C-N	-5.16	113.89	122.92
7	2-G	815	ARG	C-N-CA	-5.16	113.89	122.92
7	2-K	127	ALA	CA-C-O	5.16	125.89	120.42
4	2-H	58	LEU	CA-C-N	5.16	125.16	119.90
4	2-H	58	LEU	C-N-CA	5.16	125.16	119.90
1	3-A	280	LYS	CA-C-N	5.16	131.40	121.54
1	3-A	280	LYS	C-N-CA	5.16	131.40	121.54
1	3-A	742	VAL	CA-C-N	5.16	130.47	122.26
1	3-A	742	VAL	C-N-CA	5.16	130.47	122.26
4	3-C	555	ALA	N-CA-C	-5.16	100.47	108.42
7	3-G	815	ARG	CA-C-N	-5.16	113.89	122.92
7	3-G	815	ARG	C-N-CA	-5.16	113.89	122.92
7	3-K	127	ALA	CA-C-O	5.16	125.89	120.42
4	3-H	58	LEU	CA-C-N	5.16	125.16	119.90
4	3-H	58	LEU	C-N-CA	5.16	125.16	119.90
4	1-C	828	THR	N-CA-C	-5.16	98.41	109.81
6	1-F	129	ASP	N-CA-C	-5.16	105.66	111.28
6	1-R	102	GLU	CA-C-O	5.16	125.89	120.42
4	1-H	405	ILE	CA-C-N	5.16	130.27	123.05
4	1-H	405	ILE	C-N-CA	5.16	130.27	123.05
4	2-C	828	THR	N-CA-C	-5.16	98.41	109.81
6	2-F	129	ASP	N-CA-C	-5.16	105.66	111.28
6	2-R	102	GLU	CA-C-O	5.16	125.89	120.42
4	2-H	405	ILE	CA-C-N	5.16	130.27	123.05
4	2-H	405	ILE	C-N-CA	5.16	130.27	123.05
4	3-C	828	THR	N-CA-C	-5.16	98.41	109.81
6	3-F	129	ASP	N-CA-C	-5.16	105.66	111.28
6	3-R	102	GLU	CA-C-O	5.16	125.89	120.42
4	3-H	405	ILE	CA-C-N	5.16	130.27	123.05
4	3-H	405	ILE	C-N-CA	5.16	130.27	123.05
4	1-C	827	VAL	CA-C-N	5.16	134.38	121.80
4	1-C	827	VAL	C-N-CA	5.16	134.38	121.80
4	2-C	827	VAL	CA-C-N	5.16	134.38	121.80
4	2-C	827	VAL	C-N-CA	5.16	134.38	121.80
4	3-C	827	VAL	CA-C-N	5.16	134.38	121.80
4	3-C	827	VAL	C-N-CA	5.16	134.38	121.80
1	1-A	308	ALA	CA-C-N	5.16	127.36	122.36
1	1-A	308	ALA	C-N-CA	5.16	127.36	122.36
3	1-B	38	GLU	N-CA-C	-5.16	105.66	111.28
7	1-K	153	PRO	CA-C-N	5.16	127.14	120.44
7	1-K	153	PRO	C-N-CA	5.16	127.14	120.44
8	1-L	80	ILE	O-C-N	5.16	128.75	123.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2-A	308	ALA	CA-C-N	5.16	127.36	122.36
1	2-A	308	ALA	C-N-CA	5.16	127.36	122.36
3	2-B	38	GLU	N-CA-C	-5.16	105.66	111.28
7	2-K	153	PRO	CA-C-N	5.16	127.14	120.44
7	2-K	153	PRO	C-N-CA	5.16	127.14	120.44
8	2-L	80	ILE	O-C-N	5.16	128.75	123.18
1	3-A	308	ALA	CA-C-N	5.16	127.36	122.36
1	3-A	308	ALA	C-N-CA	5.16	127.36	122.36
3	3-B	38	GLU	N-CA-C	-5.16	105.66	111.28
7	3-K	153	PRO	CA-C-N	5.16	127.14	120.44
7	3-K	153	PRO	C-N-CA	5.16	127.14	120.44
8	3-L	80	ILE	O-C-N	5.16	128.75	123.18
5	1-I	67	VAL	CA-C-N	5.15	130.66	122.62
5	1-I	67	VAL	C-N-CA	5.15	130.66	122.62
5	2-I	67	VAL	CA-C-N	5.15	130.66	122.62
5	2-I	67	VAL	C-N-CA	5.15	130.66	122.62
5	3-I	67	VAL	CA-C-N	5.15	130.66	122.62
5	3-I	67	VAL	C-N-CA	5.15	130.66	122.62
4	1-H	633	GLN	N-CA-C	-5.15	105.74	111.36
4	2-H	633	GLN	N-CA-C	-5.15	105.74	111.36
4	3-H	633	GLN	N-CA-C	-5.15	105.74	111.36
7	1-K	114	THR	N-CA-C	-5.15	106.51	112.89
7	2-K	114	THR	N-CA-C	-5.15	106.51	112.89
7	3-K	114	THR	N-CA-C	-5.15	106.51	112.89
7	1-G	96	SER	O-C-N	-5.15	115.75	122.59
6	1-J	120	ALA	N-CA-C	-5.15	99.40	108.20
7	2-G	96	SER	O-C-N	-5.15	115.75	122.59
6	2-J	120	ALA	N-CA-C	-5.15	99.40	108.20
7	3-G	96	SER	O-C-N	-5.15	115.75	122.59
6	3-J	120	ALA	N-CA-C	-5.15	99.40	108.20
7	1-G	802	GLY	N-CA-C	-5.14	106.19	112.77
8	1-Z	117	ASN	CA-C-N	5.14	129.43	120.68
8	1-Z	117	ASN	C-N-CA	5.14	129.43	120.68
7	1-K	309	ARG	CA-C-N	5.14	131.37	121.54
7	1-K	309	ARG	C-N-CA	5.14	131.37	121.54
4	1-H	391	ALA	O-C-N	5.14	128.72	122.14
7	2-G	802	GLY	N-CA-C	-5.14	106.19	112.77
8	2-Z	117	ASN	CA-C-N	5.14	129.43	120.68
8	2-Z	117	ASN	C-N-CA	5.14	129.43	120.68
7	2-K	309	ARG	CA-C-N	5.14	131.37	121.54
7	2-K	309	ARG	C-N-CA	5.14	131.37	121.54
4	2-H	391	ALA	O-C-N	5.14	128.72	122.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	3-G	802	GLY	N-CA-C	-5.14	106.19	112.77
8	3-Z	117	ASN	CA-C-N	5.14	129.43	120.68
8	3-Z	117	ASN	C-N-CA	5.14	129.43	120.68
7	3-K	309	ARG	CA-C-N	5.14	131.37	121.54
7	3-K	309	ARG	C-N-CA	5.14	131.37	121.54
4	3-H	391	ALA	O-C-N	5.14	128.72	122.14
7	1-G	607	ALA	CA-C-N	5.14	131.36	121.54
7	1-G	607	ALA	C-N-CA	5.14	131.36	121.54
7	1-G	647	VAL	N-CA-C	5.14	115.87	108.93
4	1-H	634	ALA	N-CA-C	-5.14	105.67	111.28
6	1-J	126	ASN	N-CA-C	-5.14	102.55	109.95
7	2-G	607	ALA	CA-C-N	5.14	131.36	121.54
7	2-G	607	ALA	C-N-CA	5.14	131.36	121.54
7	2-G	647	VAL	N-CA-C	5.14	115.87	108.93
4	2-H	634	ALA	N-CA-C	-5.14	105.67	111.28
6	2-J	126	ASN	N-CA-C	-5.14	102.55	109.95
7	3-G	607	ALA	CA-C-N	5.14	131.36	121.54
7	3-G	607	ALA	C-N-CA	5.14	131.36	121.54
7	3-G	647	VAL	N-CA-C	5.14	115.87	108.93
4	3-H	634	ALA	N-CA-C	-5.14	105.67	111.28
6	3-J	126	ASN	N-CA-C	-5.14	102.55	109.95
6	1-M	78	TRP	CA-C-O	5.14	125.71	119.49
6	2-M	78	TRP	CA-C-O	5.14	125.71	119.49
6	3-M	78	TRP	CA-C-O	5.14	125.71	119.49
7	1-K	802	GLY	N-CA-C	-5.14	106.19	112.77
6	1-M	41	GLU	O-C-N	5.14	129.42	123.30
7	2-K	802	GLY	N-CA-C	-5.14	106.19	112.77
6	2-M	41	GLU	O-C-N	5.14	129.42	123.30
7	3-K	802	GLY	N-CA-C	-5.14	106.19	112.77
6	3-M	41	GLU	O-C-N	5.14	129.42	123.30
7	1-K	758	VAL	CA-C-N	5.14	132.36	122.03
7	1-K	758	VAL	C-N-CA	5.14	132.36	122.03
7	2-K	758	VAL	CA-C-N	5.14	132.36	122.03
7	2-K	758	VAL	C-N-CA	5.14	132.36	122.03
7	3-K	758	VAL	CA-C-N	5.14	132.36	122.03
7	3-K	758	VAL	C-N-CA	5.14	132.36	122.03
7	1-K	664	ASP	O-C-N	-5.14	117.47	123.27
3	1-N	333	LEU	N-CA-C	-5.14	105.76	111.36
7	2-K	664	ASP	O-C-N	-5.14	117.47	123.27
3	2-N	333	LEU	N-CA-C	-5.14	105.76	111.36
7	3-K	664	ASP	O-C-N	-5.14	117.47	123.27
3	3-N	333	LEU	N-CA-C	-5.14	105.76	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	1-F	120	ALA	N-CA-C	-5.13	99.42	108.20
6	2-F	120	ALA	N-CA-C	-5.13	99.42	108.20
6	3-F	120	ALA	N-CA-C	-5.13	99.42	108.20
3	1-N	464	ILE	CA-C-N	5.13	131.01	121.62
3	1-N	464	ILE	C-N-CA	5.13	131.01	121.62
3	2-N	464	ILE	CA-C-N	5.13	131.01	121.62
3	2-N	464	ILE	C-N-CA	5.13	131.01	121.62
3	3-N	464	ILE	CA-C-N	5.13	131.01	121.62
3	3-N	464	ILE	C-N-CA	5.13	131.01	121.62
7	1-G	758	VAL	CA-C-N	5.13	132.34	122.03
7	1-G	758	VAL	C-N-CA	5.13	132.34	122.03
7	2-G	758	VAL	CA-C-N	5.13	132.34	122.03
7	2-G	758	VAL	C-N-CA	5.13	132.34	122.03
7	3-G	758	VAL	CA-C-N	5.13	132.34	122.03
7	3-G	758	VAL	C-N-CA	5.13	132.34	122.03
4	1-C	241	LEU	N-CA-C	-5.13	98.48	109.81
5	1-D	81	GLU	N-CA-C	-5.13	105.69	111.28
7	1-G	790	THR	N-CA-C	-5.13	100.05	108.41
4	1-H	171	GLN	N-CA-C	-5.13	101.51	109.72
4	1-H	555	ALA	N-CA-C	-5.13	100.52	108.42
4	2-C	241	LEU	N-CA-C	-5.13	98.48	109.81
5	2-D	81	GLU	N-CA-C	-5.13	105.69	111.28
7	2-G	790	THR	N-CA-C	-5.13	100.05	108.41
4	2-H	171	GLN	N-CA-C	-5.13	101.51	109.72
4	2-H	555	ALA	N-CA-C	-5.13	100.52	108.42
4	3-C	241	LEU	N-CA-C	-5.13	98.48	109.81
5	3-D	81	GLU	N-CA-C	-5.13	105.69	111.28
7	3-G	790	THR	N-CA-C	-5.13	100.05	108.41
4	3-H	171	GLN	N-CA-C	-5.13	101.51	109.72
4	3-H	555	ALA	N-CA-C	-5.13	100.52	108.42
3	1-B	464	ILE	CA-C-N	5.13	131.00	121.62
3	1-B	464	ILE	C-N-CA	5.13	131.00	121.62
6	1-F	173	LEU	N-CA-C	5.13	116.56	111.07
3	2-B	464	ILE	CA-C-N	5.13	131.00	121.62
3	2-B	464	ILE	C-N-CA	5.13	131.00	121.62
6	2-F	173	LEU	N-CA-C	5.13	116.56	111.07
3	3-B	464	ILE	CA-C-N	5.13	131.00	121.62
3	3-B	464	ILE	C-N-CA	5.13	131.00	121.62
6	3-F	173	LEU	N-CA-C	5.13	116.56	111.07
6	1-R	97	ARG	N-CA-C	-5.12	106.44	113.30
5	1-I	81	GLU	N-CA-C	-5.12	105.70	111.28
6	2-R	97	ARG	N-CA-C	-5.12	106.44	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	2-I	81	GLU	N-CA-C	-5.12	105.70	111.28
6	3-R	97	ARG	N-CA-C	-5.12	106.44	113.30
5	3-I	81	GLU	N-CA-C	-5.12	105.70	111.28
1	1-A	578	VAL	CA-C-N	-5.12	115.26	122.94
1	1-A	578	VAL	C-N-CA	-5.12	115.26	122.94
7	1-G	317	LYS	N-CA-C	-5.12	101.29	109.23
1	2-A	578	VAL	CA-C-N	-5.12	115.26	122.94
1	2-A	578	VAL	C-N-CA	-5.12	115.26	122.94
7	2-G	317	LYS	N-CA-C	-5.12	101.29	109.23
1	3-A	578	VAL	CA-C-N	-5.12	115.26	122.94
1	3-A	578	VAL	C-N-CA	-5.12	115.26	122.94
7	3-G	317	LYS	N-CA-C	-5.12	101.29	109.23
7	1-G	213	LYS	N-CA-C	-5.12	105.88	111.82
7	2-G	213	LYS	N-CA-C	-5.12	105.88	111.82
7	3-G	213	LYS	N-CA-C	-5.12	105.88	111.82
4	1-H	241	LEU	N-CA-C	-5.12	98.50	109.81
6	1-J	173	LEU	N-CA-C	5.12	116.54	111.07
4	2-H	241	LEU	N-CA-C	-5.12	98.50	109.81
6	2-J	173	LEU	N-CA-C	5.12	116.54	111.07
4	3-H	241	LEU	N-CA-C	-5.12	98.50	109.81
6	3-J	173	LEU	N-CA-C	5.12	116.54	111.07
1	1-A	456	ILE	CA-C-N	5.11	131.31	121.54
1	1-A	456	ILE	C-N-CA	5.11	131.31	121.54
1	1-A	578	VAL	N-CA-C	5.11	116.18	109.58
7	1-K	257	SER	CA-C-N	5.11	127.13	120.28
7	1-K	257	SER	C-N-CA	5.11	127.13	120.28
1	2-A	456	ILE	CA-C-N	5.11	131.31	121.54
1	2-A	456	ILE	C-N-CA	5.11	131.31	121.54
1	2-A	578	VAL	N-CA-C	5.11	116.18	109.58
7	2-K	257	SER	CA-C-N	5.11	127.13	120.28
7	2-K	257	SER	C-N-CA	5.11	127.13	120.28
1	3-A	456	ILE	CA-C-N	5.11	131.31	121.54
1	3-A	456	ILE	C-N-CA	5.11	131.31	121.54
1	3-A	578	VAL	N-CA-C	5.11	116.18	109.58
7	3-K	257	SER	CA-C-N	5.11	127.13	120.28
7	3-K	257	SER	C-N-CA	5.11	127.13	120.28
8	1-L	37	SER	CA-C-O	5.11	127.82	120.51
3	1-N	38	GLU	N-CA-C	-5.11	105.71	111.28
8	2-L	37	SER	CA-C-O	5.11	127.82	120.51
3	2-N	38	GLU	N-CA-C	-5.11	105.71	111.28
8	3-L	37	SER	CA-C-O	5.11	127.82	120.51
3	3-N	38	GLU	N-CA-C	-5.11	105.71	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-N	390	ASP	CA-C-O	5.11	126.32	119.47
3	2-N	390	ASP	CA-C-O	5.11	126.32	119.47
3	3-N	390	ASP	CA-C-O	5.11	126.32	119.47
4	1-C	58	LEU	CA-C-N	5.11	125.11	119.90
4	1-C	58	LEU	C-N-CA	5.11	125.11	119.90
7	1-K	236	ALA	CA-C-O	5.11	125.84	119.97
8	1-L	45	GLU	N-CA-C	-5.11	105.71	111.28
4	2-C	58	LEU	CA-C-N	5.11	125.11	119.90
4	2-C	58	LEU	C-N-CA	5.11	125.11	119.90
7	2-K	236	ALA	CA-C-O	5.11	125.84	119.97
8	2-L	45	GLU	N-CA-C	-5.11	105.71	111.28
4	3-C	58	LEU	CA-C-N	5.11	125.11	119.90
4	3-C	58	LEU	C-N-CA	5.11	125.11	119.90
7	3-K	236	ALA	CA-C-O	5.11	125.84	119.97
8	3-L	45	GLU	N-CA-C	-5.11	105.71	111.28
6	1-R	133	ALA	N-CA-C	-5.11	99.93	110.80
6	2-R	133	ALA	N-CA-C	-5.11	99.93	110.80
6	3-R	133	ALA	N-CA-C	-5.11	99.93	110.80
1	1-A	787	ASP	CA-C-N	5.10	131.16	121.97
1	1-A	787	ASP	C-N-CA	5.10	131.16	121.97
1	2-A	787	ASP	CA-C-N	5.10	131.16	121.97
1	2-A	787	ASP	C-N-CA	5.10	131.16	121.97
1	3-A	787	ASP	CA-C-N	5.10	131.16	121.97
1	3-A	787	ASP	C-N-CA	5.10	131.16	121.97
1	1-A	652	ALA	N-CA-C	-5.10	105.72	111.28
7	1-K	64	THR	CA-C-O	5.10	126.18	120.82
1	2-A	652	ALA	N-CA-C	-5.10	105.72	111.28
7	2-K	64	THR	CA-C-O	5.10	126.18	120.82
1	3-A	652	ALA	N-CA-C	-5.10	105.72	111.28
7	3-K	64	THR	CA-C-O	5.10	126.18	120.82
1	1-A	427	ALA	N-CA-C	-5.10	101.16	108.60
1	2-A	427	ALA	N-CA-C	-5.10	101.16	108.60
1	3-A	427	ALA	N-CA-C	-5.10	101.16	108.60
3	1-B	333	LEU	N-CA-C	-5.10	105.80	111.36
3	2-B	333	LEU	N-CA-C	-5.10	105.80	111.36
3	3-B	333	LEU	N-CA-C	-5.10	105.80	111.36
4	1-C	405	ILE	CA-C-N	5.09	130.18	123.05
4	1-C	405	ILE	C-N-CA	5.09	130.18	123.05
8	1-Z	90	LEU	CA-C-N	5.09	127.10	120.28
8	1-Z	90	LEU	C-N-CA	5.09	127.10	120.28
7	1-K	38	PRO	N-CA-C	5.09	122.96	112.47
4	2-C	405	ILE	CA-C-N	5.09	130.18	123.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-C	405	ILE	C-N-CA	5.09	130.18	123.05
8	2-Z	90	LEU	CA-C-N	5.09	127.10	120.28
8	2-Z	90	LEU	C-N-CA	5.09	127.10	120.28
7	2-K	38	PRO	N-CA-C	5.09	122.96	112.47
4	3-C	405	ILE	CA-C-N	5.09	130.18	123.05
4	3-C	405	ILE	C-N-CA	5.09	130.18	123.05
8	3-Z	90	LEU	CA-C-N	5.09	127.10	120.28
8	3-Z	90	LEU	C-N-CA	5.09	127.10	120.28
7	3-K	38	PRO	N-CA-C	5.09	122.96	112.47
7	1-K	307	ALA	N-CA-C	-5.09	105.63	111.07
3	1-N	234	PHE	N-CA-C	5.09	118.31	110.42
7	2-K	307	ALA	N-CA-C	-5.09	105.63	111.07
3	2-N	234	PHE	N-CA-C	5.09	118.31	110.42
7	3-K	307	ALA	N-CA-C	-5.09	105.63	111.07
3	3-N	234	PHE	N-CA-C	5.09	118.31	110.42
1	1-A	602	ALA	N-CA-C	-5.09	105.65	111.14
1	1-A	700	PHE	CA-C-N	5.09	127.09	120.28
1	1-A	700	PHE	C-N-CA	5.09	127.09	120.28
1	2-A	602	ALA	N-CA-C	-5.09	105.65	111.14
1	2-A	700	PHE	CA-C-N	5.09	127.09	120.28
1	2-A	700	PHE	C-N-CA	5.09	127.09	120.28
1	3-A	602	ALA	N-CA-C	-5.09	105.65	111.14
1	3-A	700	PHE	CA-C-N	5.09	127.09	120.28
1	3-A	700	PHE	C-N-CA	5.09	127.09	120.28
7	1-K	148	ILE	N-CA-C	-5.08	105.44	110.62
7	2-K	148	ILE	N-CA-C	-5.08	105.44	110.62
7	3-K	148	ILE	N-CA-C	-5.08	105.44	110.62
3	1-N	179	ARG	N-CA-C	5.08	116.63	111.14
3	2-N	179	ARG	N-CA-C	5.08	116.63	111.14
3	3-N	179	ARG	N-CA-C	5.08	116.63	111.14
7	1-K	792	SER	N-CA-C	5.08	120.11	113.30
7	2-K	792	SER	N-CA-C	5.08	120.11	113.30
7	3-K	792	SER	N-CA-C	5.08	120.11	113.30
5	1-D	26	ARG	N-CA-C	-5.08	101.70	108.86
5	2-D	26	ARG	N-CA-C	-5.08	101.70	108.86
5	3-D	26	ARG	N-CA-C	-5.08	101.70	108.86
4	1-C	171	GLN	N-CA-C	-5.08	101.60	109.72
7	1-G	23	GLU	N-CA-C	-5.08	99.99	110.80
4	2-C	171	GLN	N-CA-C	-5.08	101.60	109.72
7	2-G	23	GLU	N-CA-C	-5.08	99.99	110.80
4	3-C	171	GLN	N-CA-C	-5.08	101.60	109.72
7	3-G	23	GLU	N-CA-C	-5.08	99.99	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1-B	777	THR	N-CA-C	-5.08	102.87	110.23
3	2-B	777	THR	N-CA-C	-5.08	102.87	110.23
3	3-B	777	THR	N-CA-C	-5.08	102.87	110.23
3	1-B	107	GLY	N-CA-C	-5.07	101.16	113.18
3	1-B	346	THR	N-CA-C	-5.07	98.60	109.81
3	2-B	107	GLY	N-CA-C	-5.07	101.16	113.18
3	2-B	346	THR	N-CA-C	-5.07	98.60	109.81
3	3-B	107	GLY	N-CA-C	-5.07	101.16	113.18
3	3-B	346	THR	N-CA-C	-5.07	98.60	109.81
3	1-B	188	ALA	N-CA-C	5.07	119.84	113.25
3	1-B	440	ARG	CA-C-N	5.07	127.08	120.28
3	1-B	440	ARG	C-N-CA	5.07	127.08	120.28
3	1-B	445	ARG	N-CA-C	5.07	121.60	110.80
3	1-B	776	ALA	CA-C-N	5.07	127.91	120.71
3	1-B	776	ALA	C-N-CA	5.07	127.91	120.71
8	1-L	78	TYR	N-CA-C	5.07	117.68	109.06
3	2-B	188	ALA	N-CA-C	5.07	119.84	113.25
3	2-B	440	ARG	CA-C-N	5.07	127.08	120.28
3	2-B	440	ARG	C-N-CA	5.07	127.08	120.28
3	2-B	445	ARG	N-CA-C	5.07	121.60	110.80
3	2-B	776	ALA	CA-C-N	5.07	127.91	120.71
3	2-B	776	ALA	C-N-CA	5.07	127.91	120.71
8	2-L	78	TYR	N-CA-C	5.07	117.68	109.06
3	3-B	188	ALA	N-CA-C	5.07	119.84	113.25
3	3-B	440	ARG	CA-C-N	5.07	127.08	120.28
3	3-B	440	ARG	C-N-CA	5.07	127.08	120.28
3	3-B	445	ARG	N-CA-C	5.07	121.60	110.80
3	3-B	776	ALA	CA-C-N	5.07	127.91	120.71
3	3-B	776	ALA	C-N-CA	5.07	127.91	120.71
8	3-L	78	TYR	N-CA-C	5.07	117.68	109.06
4	1-C	336	LYS	N-CA-C	5.07	117.25	110.35
8	1-Z	52	THR	CA-C-N	5.07	131.22	121.54
8	1-Z	52	THR	C-N-CA	5.07	131.22	121.54
6	1-M	51	PHE	N-CA-C	5.07	121.60	110.80
4	2-C	336	LYS	N-CA-C	5.07	117.25	110.35
8	2-Z	52	THR	CA-C-N	5.07	131.22	121.54
8	2-Z	52	THR	C-N-CA	5.07	131.22	121.54
6	2-M	51	PHE	N-CA-C	5.07	121.60	110.80
4	3-C	336	LYS	N-CA-C	5.07	117.25	110.35
8	3-Z	52	THR	CA-C-N	5.07	131.22	121.54
8	3-Z	52	THR	C-N-CA	5.07	131.22	121.54
6	3-M	51	PHE	N-CA-C	5.07	121.60	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1-I	26	ARG	N-CA-C	-5.07	101.71	108.86
5	2-I	26	ARG	N-CA-C	-5.07	101.71	108.86
5	3-I	26	ARG	N-CA-C	-5.07	101.71	108.86
7	1-G	247	ARG	CA-C-N	-5.07	111.87	121.54
7	1-G	247	ARG	C-N-CA	-5.07	111.87	121.54
7	1-G	364	ILE	CA-C-N	5.07	127.57	120.28
7	1-G	364	ILE	C-N-CA	5.07	127.57	120.28
3	1-N	346	THR	N-CA-C	-5.07	98.61	109.81
7	2-G	247	ARG	CA-C-N	-5.07	111.87	121.54
7	2-G	247	ARG	C-N-CA	-5.07	111.87	121.54
7	2-G	364	ILE	CA-C-N	5.07	127.57	120.28
7	2-G	364	ILE	C-N-CA	5.07	127.57	120.28
3	2-N	346	THR	N-CA-C	-5.07	98.61	109.81
7	3-G	247	ARG	CA-C-N	-5.07	111.87	121.54
7	3-G	247	ARG	C-N-CA	-5.07	111.87	121.54
7	3-G	364	ILE	CA-C-N	5.07	127.57	120.28
7	3-G	364	ILE	C-N-CA	5.07	127.57	120.28
3	3-N	346	THR	N-CA-C	-5.07	98.61	109.81
4	1-H	336	LYS	N-CA-C	5.06	117.24	110.35
5	1-I	137	ASP	N-CA-C	-5.06	102.67	108.49
6	1-J	50	GLY	CA-C-N	5.06	127.96	120.82
6	1-J	50	GLY	C-N-CA	5.06	127.96	120.82
4	2-H	336	LYS	N-CA-C	5.06	117.24	110.35
5	2-I	137	ASP	N-CA-C	-5.06	102.67	108.49
6	2-J	50	GLY	CA-C-N	5.06	127.96	120.82
6	2-J	50	GLY	C-N-CA	5.06	127.96	120.82
4	3-H	336	LYS	N-CA-C	5.06	117.24	110.35
5	3-I	137	ASP	N-CA-C	-5.06	102.67	108.49
6	3-J	50	GLY	CA-C-N	5.06	127.96	120.82
6	3-J	50	GLY	C-N-CA	5.06	127.96	120.82
7	1-G	792	SER	N-CA-C	5.06	120.08	113.30
8	1-Z	140	GLN	CA-C-O	5.06	125.79	120.42
7	2-G	792	SER	N-CA-C	5.06	120.08	113.30
8	2-Z	140	GLN	CA-C-O	5.06	125.79	120.42
7	3-G	792	SER	N-CA-C	5.06	120.08	113.30
8	3-Z	140	GLN	CA-C-O	5.06	125.79	120.42
3	1-B	424	LEU	CA-C-N	5.06	131.21	121.54
3	1-B	424	LEU	C-N-CA	5.06	131.21	121.54
4	1-C	835	VAL	N-CA-C	5.06	115.67	110.36
7	1-G	332	LEU	N-CA-C	-5.06	105.76	111.28
3	2-B	424	LEU	CA-C-N	5.06	131.21	121.54
3	2-B	424	LEU	C-N-CA	5.06	131.21	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-C	835	VAL	N-CA-C	5.06	115.67	110.36
7	2-G	332	LEU	N-CA-C	-5.06	105.76	111.28
3	3-B	424	LEU	CA-C-N	5.06	131.21	121.54
3	3-B	424	LEU	C-N-CA	5.06	131.21	121.54
4	3-C	835	VAL	N-CA-C	5.06	115.67	110.36
7	3-G	332	LEU	N-CA-C	-5.06	105.76	111.28
7	1-K	72	ALA	N-CA-C	5.06	116.48	111.07
7	2-K	72	ALA	N-CA-C	5.06	116.48	111.07
7	3-K	72	ALA	N-CA-C	5.06	116.48	111.07
5	1-D	78	GLU	CA-C-O	5.06	126.13	120.82
5	2-D	78	GLU	CA-C-O	5.06	126.13	120.82
5	3-D	78	GLU	CA-C-O	5.06	126.13	120.82
8	1-Z	38	VAL	N-CA-C	-5.05	105.61	110.72
8	2-Z	38	VAL	N-CA-C	-5.05	105.61	110.72
8	3-Z	38	VAL	N-CA-C	-5.05	105.61	110.72
1	1-A	1076	GLU	N-CA-C	5.05	116.47	111.07
3	1-N	424	LEU	CA-C-N	5.05	131.19	121.54
3	1-N	424	LEU	C-N-CA	5.05	131.19	121.54
3	1-N	445	ARG	N-CA-C	5.05	121.56	110.80
5	1-I	129	GLN	N-CA-C	-5.05	105.77	111.28
1	2-A	1076	GLU	N-CA-C	5.05	116.47	111.07
3	2-N	424	LEU	CA-C-N	5.05	131.19	121.54
3	2-N	424	LEU	C-N-CA	5.05	131.19	121.54
3	2-N	445	ARG	N-CA-C	5.05	121.56	110.80
5	2-I	129	GLN	N-CA-C	-5.05	105.77	111.28
1	3-A	1076	GLU	N-CA-C	5.05	116.47	111.07
3	3-N	424	LEU	CA-C-N	5.05	131.19	121.54
3	3-N	424	LEU	C-N-CA	5.05	131.19	121.54
3	3-N	445	ARG	N-CA-C	5.05	121.56	110.80
5	3-I	129	GLN	N-CA-C	-5.05	105.77	111.28
8	1-Z	14	LYS	N-CA-C	-5.05	105.24	111.40
7	1-K	167	LEU	CA-C-N	5.05	127.32	120.65
7	1-K	167	LEU	C-N-CA	5.05	127.32	120.65
3	1-N	107	GLY	N-CA-C	-5.05	101.21	113.18
8	2-Z	14	LYS	N-CA-C	-5.05	105.24	111.40
7	2-K	167	LEU	CA-C-N	5.05	127.32	120.65
7	2-K	167	LEU	C-N-CA	5.05	127.32	120.65
3	2-N	107	GLY	N-CA-C	-5.05	101.21	113.18
8	3-Z	14	LYS	N-CA-C	-5.05	105.24	111.40
7	3-K	167	LEU	CA-C-N	5.05	127.32	120.65
7	3-K	167	LEU	C-N-CA	5.05	127.32	120.65
3	3-N	107	GLY	N-CA-C	-5.05	101.21	113.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1-K	151	LYS	CA-C-N	-5.05	119.17	122.60
7	1-K	151	LYS	C-N-CA	-5.05	119.17	122.60
7	1-K	212	SER	N-CA-C	-5.05	105.67	111.07
7	2-K	151	LYS	CA-C-N	-5.05	119.17	122.60
7	2-K	151	LYS	C-N-CA	-5.05	119.17	122.60
7	2-K	212	SER	N-CA-C	-5.05	105.67	111.07
7	3-K	151	LYS	CA-C-N	-5.05	119.17	122.60
7	3-K	151	LYS	C-N-CA	-5.05	119.17	122.60
7	3-K	212	SER	N-CA-C	-5.05	105.67	111.07
4	1-C	808	GLU	CA-C-N	5.05	127.04	120.28
4	1-C	808	GLU	C-N-CA	5.05	127.04	120.28
8	1-Z	45	GLU	N-CA-C	-5.05	105.86	111.36
3	1-N	546	ARG	N-CA-C	5.05	118.04	109.06
4	1-H	684	SER	CA-C-O	5.05	126.12	120.82
4	2-C	808	GLU	CA-C-N	5.05	127.04	120.28
4	2-C	808	GLU	C-N-CA	5.05	127.04	120.28
8	2-Z	45	GLU	N-CA-C	-5.05	105.86	111.36
3	2-N	546	ARG	N-CA-C	5.05	118.04	109.06
4	2-H	684	SER	CA-C-O	5.05	126.12	120.82
4	3-C	808	GLU	CA-C-N	5.05	127.04	120.28
4	3-C	808	GLU	C-N-CA	5.05	127.04	120.28
8	3-Z	45	GLU	N-CA-C	-5.05	105.86	111.36
3	3-N	546	ARG	N-CA-C	5.05	118.04	109.06
4	3-H	684	SER	CA-C-O	5.05	126.12	120.82
3	1-N	440	ARG	CA-C-N	5.04	127.04	120.28
3	1-N	440	ARG	C-N-CA	5.04	127.04	120.28
3	2-N	440	ARG	CA-C-N	5.04	127.04	120.28
3	2-N	440	ARG	C-N-CA	5.04	127.04	120.28
3	3-N	440	ARG	CA-C-N	5.04	127.04	120.28
3	3-N	440	ARG	C-N-CA	5.04	127.04	120.28
1	1-A	778	PHE	O-C-N	5.04	127.33	122.09
4	1-C	203	ILE	CA-C-N	5.04	130.61	122.29
4	1-C	203	ILE	C-N-CA	5.04	130.61	122.29
4	1-C	588	LEU	CA-C-N	5.04	127.37	120.46
4	1-C	588	LEU	C-N-CA	5.04	127.37	120.46
4	1-C	777	LEU	CA-C-N	5.04	127.04	120.28
4	1-C	777	LEU	C-N-CA	5.04	127.04	120.28
4	1-H	203	ILE	CA-C-N	5.04	130.61	122.29
4	1-H	203	ILE	C-N-CA	5.04	130.61	122.29
1	2-A	778	PHE	O-C-N	5.04	127.33	122.09
4	2-C	203	ILE	CA-C-N	5.04	130.61	122.29
4	2-C	203	ILE	C-N-CA	5.04	130.61	122.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-C	588	LEU	CA-C-N	5.04	127.37	120.46
4	2-C	588	LEU	C-N-CA	5.04	127.37	120.46
4	2-C	777	LEU	CA-C-N	5.04	127.04	120.28
4	2-C	777	LEU	C-N-CA	5.04	127.04	120.28
4	2-H	203	ILE	CA-C-N	5.04	130.61	122.29
4	2-H	203	ILE	C-N-CA	5.04	130.61	122.29
1	3-A	778	PHE	O-C-N	5.04	127.33	122.09
4	3-C	203	ILE	CA-C-N	5.04	130.61	122.29
4	3-C	203	ILE	C-N-CA	5.04	130.61	122.29
4	3-C	588	LEU	CA-C-N	5.04	127.37	120.46
4	3-C	588	LEU	C-N-CA	5.04	127.37	120.46
4	3-C	777	LEU	CA-C-N	5.04	127.04	120.28
4	3-C	777	LEU	C-N-CA	5.04	127.04	120.28
4	3-H	203	ILE	CA-C-N	5.04	130.61	122.29
4	3-H	203	ILE	C-N-CA	5.04	130.61	122.29
7	1-K	790	THR	N-CA-C	-5.04	100.19	108.41
7	2-K	790	THR	N-CA-C	-5.04	100.19	108.41
7	3-K	790	THR	N-CA-C	-5.04	100.19	108.41
3	1-N	188	ALA	N-CA-C	5.04	119.80	113.25
3	2-N	188	ALA	N-CA-C	5.04	119.80	113.25
3	3-N	188	ALA	N-CA-C	5.04	119.80	113.25
1	1-A	732	HIS	CA-C-O	5.04	125.58	119.38
1	2-A	732	HIS	CA-C-O	5.04	125.58	119.38
1	3-A	732	HIS	CA-C-O	5.04	125.58	119.38
4	1-C	790	ASP	O-C-N	-5.04	115.53	121.32
4	2-C	790	ASP	O-C-N	-5.04	115.53	121.32
4	3-C	790	ASP	O-C-N	-5.04	115.53	121.32
1	1-A	462	GLY	CA-C-O	-5.04	116.85	121.63
7	1-G	742	ILE	N-CA-C	-5.04	100.28	107.78
1	2-A	462	GLY	CA-C-O	-5.04	116.85	121.63
7	2-G	742	ILE	N-CA-C	-5.04	100.28	107.78
1	3-A	462	GLY	CA-C-O	-5.04	116.85	121.63
7	3-G	742	ILE	N-CA-C	-5.04	100.28	107.78
7	1-K	862	GLU	CA-C-N	5.03	127.44	120.29
7	1-K	862	GLU	C-N-CA	5.03	127.44	120.29
8	1-L	89	MET	CA-C-O	5.03	125.76	120.42
7	2-K	862	GLU	CA-C-N	5.03	127.44	120.29
7	2-K	862	GLU	C-N-CA	5.03	127.44	120.29
8	2-L	89	MET	CA-C-O	5.03	125.76	120.42
7	3-K	862	GLU	CA-C-N	5.03	127.44	120.29
7	3-K	862	GLU	C-N-CA	5.03	127.44	120.29
8	3-L	89	MET	CA-C-O	5.03	125.76	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	765	GLN	N-CA-C	-5.03	106.40	112.54
4	2-C	765	GLN	N-CA-C	-5.03	106.40	112.54
4	3-C	765	GLN	N-CA-C	-5.03	106.40	112.54
1	1-A	431	ARG	N-CA-C	-5.03	102.03	109.83
1	1-A	1078	LEU	N-CA-C	-5.03	105.80	111.28
7	1-G	87	MET	CA-C-N	5.03	127.02	120.28
7	1-G	87	MET	C-N-CA	5.03	127.02	120.28
6	1-M	157	ALA	N-CA-C	5.03	117.50	109.96
1	2-A	431	ARG	N-CA-C	-5.03	102.03	109.83
1	2-A	1078	LEU	N-CA-C	-5.03	105.80	111.28
7	2-G	87	MET	CA-C-N	5.03	127.02	120.28
7	2-G	87	MET	C-N-CA	5.03	127.02	120.28
6	2-M	157	ALA	N-CA-C	5.03	117.50	109.96
1	3-A	431	ARG	N-CA-C	-5.03	102.03	109.83
1	3-A	1078	LEU	N-CA-C	-5.03	105.80	111.28
7	3-G	87	MET	CA-C-N	5.03	127.02	120.28
7	3-G	87	MET	C-N-CA	5.03	127.02	120.28
6	3-M	157	ALA	N-CA-C	5.03	117.50	109.96
3	1-B	182	GLU	CA-C-N	5.03	131.14	121.54
3	1-B	182	GLU	C-N-CA	5.03	131.14	121.54
5	1-D	98	GLU	CA-C-N	5.03	127.02	120.28
5	1-D	98	GLU	C-N-CA	5.03	127.02	120.28
5	1-D	129	GLN	N-CA-C	-5.03	105.80	111.28
4	1-H	588	LEU	CA-C-N	5.03	127.35	120.46
4	1-H	588	LEU	C-N-CA	5.03	127.35	120.46
3	2-B	182	GLU	CA-C-N	5.03	131.14	121.54
3	2-B	182	GLU	C-N-CA	5.03	131.14	121.54
5	2-D	98	GLU	CA-C-N	5.03	127.02	120.28
5	2-D	98	GLU	C-N-CA	5.03	127.02	120.28
5	2-D	129	GLN	N-CA-C	-5.03	105.80	111.28
4	2-H	588	LEU	CA-C-N	5.03	127.35	120.46
4	2-H	588	LEU	C-N-CA	5.03	127.35	120.46
3	3-B	182	GLU	CA-C-N	5.03	131.14	121.54
3	3-B	182	GLU	C-N-CA	5.03	131.14	121.54
5	3-D	98	GLU	CA-C-N	5.03	127.02	120.28
5	3-D	98	GLU	C-N-CA	5.03	127.02	120.28
5	3-D	129	GLN	N-CA-C	-5.03	105.80	111.28
4	3-H	588	LEU	CA-C-N	5.03	127.35	120.46
4	3-H	588	LEU	C-N-CA	5.03	127.35	120.46
6	1-F	50	GLY	CA-C-N	5.03	127.91	120.82
6	1-F	50	GLY	C-N-CA	5.03	127.91	120.82
6	2-F	50	GLY	CA-C-N	5.03	127.91	120.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	2-F	50	GLY	C-N-CA	5.03	127.91	120.82
6	3-F	50	GLY	CA-C-N	5.03	127.91	120.82
6	3-F	50	GLY	C-N-CA	5.03	127.91	120.82
4	1-C	168	LYS	N-CA-C	-5.02	100.71	108.90
4	1-C	817	ASP	N-CA-C	-5.02	105.25	111.33
6	1-R	73	ARG	N-CA-C	-5.02	105.89	111.36
4	2-C	168	LYS	N-CA-C	-5.02	100.71	108.90
4	2-C	817	ASP	N-CA-C	-5.02	105.25	111.33
6	2-R	73	ARG	N-CA-C	-5.02	105.89	111.36
4	3-C	168	LYS	N-CA-C	-5.02	100.71	108.90
4	3-C	817	ASP	N-CA-C	-5.02	105.25	111.33
6	3-R	73	ARG	N-CA-C	-5.02	105.89	111.36
7	1-G	66	ALA	CA-C-N	5.02	127.01	120.28
7	1-G	66	ALA	C-N-CA	5.02	127.01	120.28
7	1-G	121	ARG	N-CA-C	-5.02	105.70	111.07
3	1-N	182	GLU	CA-C-N	5.02	131.13	121.54
3	1-N	182	GLU	C-N-CA	5.02	131.13	121.54
7	2-G	66	ALA	CA-C-N	5.02	127.01	120.28
7	2-G	66	ALA	C-N-CA	5.02	127.01	120.28
7	2-G	121	ARG	N-CA-C	-5.02	105.70	111.07
3	2-N	182	GLU	CA-C-N	5.02	131.13	121.54
3	2-N	182	GLU	C-N-CA	5.02	131.13	121.54
7	3-G	66	ALA	CA-C-N	5.02	127.01	120.28
7	3-G	66	ALA	C-N-CA	5.02	127.01	120.28
7	3-G	121	ARG	N-CA-C	-5.02	105.70	111.07
3	3-N	182	GLU	CA-C-N	5.02	131.13	121.54
3	3-N	182	GLU	C-N-CA	5.02	131.13	121.54
3	1-B	179	ARG	N-CA-C	5.02	116.56	111.14
3	1-B	234	PHE	N-CA-C	5.02	118.20	110.42
3	1-B	546	ARG	N-CA-C	5.02	117.99	109.06
6	1-R	66	TRP	N-CA-C	5.02	116.78	108.20
4	1-H	312	GLY	N-CA-C	-5.02	101.29	113.18
4	1-H	719	ALA	N-CA-C	-5.02	105.81	111.28
5	1-I	98	GLU	CA-C-N	5.02	127.00	120.28
5	1-I	98	GLU	C-N-CA	5.02	127.00	120.28
3	2-B	179	ARG	N-CA-C	5.02	116.56	111.14
3	2-B	234	PHE	N-CA-C	5.02	118.20	110.42
3	2-B	546	ARG	N-CA-C	5.02	117.99	109.06
6	2-R	66	TRP	N-CA-C	5.02	116.78	108.20
4	2-H	312	GLY	N-CA-C	-5.02	101.29	113.18
4	2-H	719	ALA	N-CA-C	-5.02	105.81	111.28
5	2-I	98	GLU	CA-C-N	5.02	127.00	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	2-I	98	GLU	C-N-CA	5.02	127.00	120.28
3	3-B	179	ARG	N-CA-C	5.02	116.56	111.14
3	3-B	234	PHE	N-CA-C	5.02	118.20	110.42
3	3-B	546	ARG	N-CA-C	5.02	117.99	109.06
6	3-R	66	TRP	N-CA-C	5.02	116.78	108.20
4	3-H	312	GLY	N-CA-C	-5.02	101.29	113.18
4	3-H	719	ALA	N-CA-C	-5.02	105.81	111.28
5	3-I	98	GLU	CA-C-N	5.02	127.00	120.28
5	3-I	98	GLU	C-N-CA	5.02	127.00	120.28
7	1-K	742	ILE	N-CA-C	-5.02	100.31	107.78
4	1-H	404	ALA	CA-C-O	-5.02	115.44	121.11
5	1-I	78	GLU	CA-C-O	5.02	126.09	120.82
7	2-K	742	ILE	N-CA-C	-5.02	100.31	107.78
4	2-H	404	ALA	CA-C-O	-5.02	115.44	121.11
5	2-I	78	GLU	CA-C-O	5.02	126.09	120.82
7	3-K	742	ILE	N-CA-C	-5.02	100.31	107.78
4	3-H	404	ALA	CA-C-O	-5.02	115.44	121.11
5	3-I	78	GLU	CA-C-O	5.02	126.09	120.82
1	1-A	142	GLN	CA-C-N	5.01	129.71	121.39
1	1-A	142	GLN	C-N-CA	5.01	129.71	121.39
1	1-A	438	LYS	O-C-N	-5.01	117.44	123.31
1	1-A	679	GLU	N-CA-C	-5.01	105.72	111.14
4	1-C	528	LEU	N-CA-C	5.01	116.86	108.99
4	1-H	565	GLY	CA-C-N	-5.01	116.03	123.05
4	1-H	565	GLY	C-N-CA	-5.01	116.03	123.05
1	2-A	142	GLN	CA-C-N	5.01	129.71	121.39
1	2-A	142	GLN	C-N-CA	5.01	129.71	121.39
1	2-A	438	LYS	O-C-N	-5.01	117.44	123.31
1	2-A	679	GLU	N-CA-C	-5.01	105.72	111.14
4	2-C	528	LEU	N-CA-C	5.01	116.86	108.99
4	2-H	565	GLY	CA-C-N	-5.01	116.03	123.05
4	2-H	565	GLY	C-N-CA	-5.01	116.03	123.05
1	3-A	142	GLN	CA-C-N	5.01	129.71	121.39
1	3-A	142	GLN	C-N-CA	5.01	129.71	121.39
1	3-A	438	LYS	O-C-N	-5.01	117.44	123.31
1	3-A	679	GLU	N-CA-C	-5.01	105.72	111.14
4	3-C	528	LEU	N-CA-C	5.01	116.86	108.99
4	3-H	565	GLY	CA-C-N	-5.01	116.03	123.05
4	3-H	565	GLY	C-N-CA	-5.01	116.03	123.05
1	1-A	924	SER	CA-C-N	5.01	129.20	120.68
1	1-A	924	SER	C-N-CA	5.01	129.20	120.68
4	1-C	404	ALA	CA-C-O	-5.01	115.45	121.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	1-C	684	SER	CA-C-O	5.01	126.08	120.82
5	1-D	137	ASP	N-CA-C	-5.01	102.73	108.49
1	2-A	924	SER	CA-C-N	5.01	129.20	120.68
1	2-A	924	SER	C-N-CA	5.01	129.20	120.68
4	2-C	404	ALA	CA-C-O	-5.01	115.45	121.11
4	2-C	684	SER	CA-C-O	5.01	126.08	120.82
5	2-D	137	ASP	N-CA-C	-5.01	102.73	108.49
1	3-A	924	SER	CA-C-N	5.01	129.20	120.68
1	3-A	924	SER	C-N-CA	5.01	129.20	120.68
4	3-C	404	ALA	CA-C-O	-5.01	115.45	121.11
4	3-C	684	SER	CA-C-O	5.01	126.08	120.82
5	3-D	137	ASP	N-CA-C	-5.01	102.73	108.49
4	1-C	312	GLY	N-CA-C	-5.01	101.31	113.18
7	1-K	93	LYS	N-CA-C	-5.01	105.82	111.28
4	2-C	312	GLY	N-CA-C	-5.01	101.31	113.18
7	2-K	93	LYS	N-CA-C	-5.01	105.82	111.28
4	3-C	312	GLY	N-CA-C	-5.01	101.31	113.18
7	3-K	93	LYS	N-CA-C	-5.01	105.82	111.28
1	1-A	443	GLU	N-CA-C	-5.01	105.88	112.94
4	1-H	168	LYS	N-CA-C	-5.01	100.74	108.90
1	2-A	443	GLU	N-CA-C	-5.01	105.88	112.94
4	2-H	168	LYS	N-CA-C	-5.01	100.74	108.90
1	3-A	443	GLU	N-CA-C	-5.01	105.88	112.94
4	3-H	168	LYS	N-CA-C	-5.01	100.74	108.90
1	1-A	244	THR	N-CA-C	-5.00	100.75	108.90
2	1-E	228	ALA	N-CA-C	-5.00	105.83	111.28
4	1-C	362	PRO	CA-C-N	5.00	131.10	121.54
4	1-C	362	PRO	C-N-CA	5.00	131.10	121.54
7	1-K	182	GLN	N-CA-C	5.00	116.73	111.28
1	2-A	244	THR	N-CA-C	-5.00	100.75	108.90
2	2-E	228	ALA	N-CA-C	-5.00	105.83	111.28
4	2-C	362	PRO	CA-C-N	5.00	131.10	121.54
4	2-C	362	PRO	C-N-CA	5.00	131.10	121.54
7	2-K	182	GLN	N-CA-C	5.00	116.73	111.28
1	3-A	244	THR	N-CA-C	-5.00	100.75	108.90
2	3-E	228	ALA	N-CA-C	-5.00	105.83	111.28
4	3-C	362	PRO	CA-C-N	5.00	131.10	121.54
4	3-C	362	PRO	C-N-CA	5.00	131.10	121.54
7	3-K	182	GLN	N-CA-C	5.00	116.73	111.28
4	1-H	16	ASP	CA-C-N	5.00	130.27	122.17
4	1-H	16	ASP	C-N-CA	5.00	130.27	122.17
4	2-H	16	ASP	CA-C-N	5.00	130.27	122.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2-H	16	ASP	C-N-CA	5.00	130.27	122.17
4	3-H	16	ASP	CA-C-N	5.00	130.27	122.17
4	3-H	16	ASP	C-N-CA	5.00	130.27	122.17

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	1-B	898	ALA	Peptide
3	1-B	903	CYS	Peptide
3	1-B	938	VAL	Mainchain
3	2-B	898	ALA	Peptide
3	2-B	903	CYS	Peptide
3	2-B	938	VAL	Mainchain
7	2-G	849	LEU	Mainchain
7	2-K	849	LEU	Mainchain
3	3-B	898	ALA	Peptide
3	3-B	903	CYS	Peptide
3	3-B	938	VAL	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	4503	0	1194	42	0
1	2-A	4503	0	1194	40	0
1	3-A	4503	0	1194	42	0
2	1-E	1169	0	303	0	0
2	2-E	1169	0	303	0	0
2	3-E	1169	0	303	0	0
3	1-B	3198	0	810	59	0
3	1-N	2279	0	568	21	0
3	2-B	3198	0	810	59	0
3	2-N	2279	0	568	21	0
3	3-B	3198	0	810	60	0
3	3-N	2279	0	568	21	0
4	1-C	3371	0	919	30	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1-H	2884	0	794	32	0
4	2-C	3371	0	919	28	0
4	2-H	2884	0	794	32	0
4	3-C	3371	0	919	28	0
4	3-H	2884	0	794	30	0
5	1-D	706	0	182	9	0
5	1-I	706	0	182	9	0
5	2-D	706	0	182	9	0
5	2-I	706	0	182	9	0
5	3-D	706	0	182	9	0
5	3-I	706	0	182	9	0
6	1-F	635	0	181	3	0
6	1-J	635	0	181	3	0
6	1-M	635	0	181	21	0
6	1-R	635	0	181	40	0
6	2-F	635	0	181	4	0
6	2-J	635	0	181	4	0
6	2-M	635	0	181	21	0
6	2-R	635	0	181	39	0
6	3-F	635	0	181	4	0
6	3-J	635	0	181	3	0
6	3-M	635	0	181	20	0
6	3-R	635	0	181	39	0
7	1-G	3190	0	822	75	0
7	1-K	2239	0	572	43	0
7	2-G	3190	0	822	74	0
7	2-K	2239	0	572	43	0
7	3-G	3190	0	822	73	0
7	3-K	2239	0	572	43	0
8	1-L	555	0	148	3	0
8	1-Z	555	0	147	14	0
8	2-L	555	0	148	4	0
8	2-Z	555	0	147	15	0
8	3-L	555	0	148	3	0
8	3-Z	555	0	147	14	0
All	All	83685	0	22095	1115	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 11.

All (1115) 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)
7:G:107:SER:H	6:R:50:GLY:CA	1.31	1.43
7:K:107:SER:N	6:M:50:GLY:HA3	1.28	1.42
7:G:107:SER:N	6:R:50:GLY:HA3	1.16	1.42
7:G:107:SER:H	6:R:50:GLY:CA	1.31	1.42
7:G:107:SER:N	6:R:50:GLY:HA3	1.16	1.42
7:G:107:SER:H	6:R:50:GLY:CA	1.31	1.41
7:K:107:SER:N	6:M:50:GLY:HA3	1.28	1.39
7:G:107:SER:N	6:R:50:GLY:HA3	1.16	1.39
7:K:107:SER:N	6:M:50:GLY:HA3	1.28	1.37
7:K:167:LEU:CA	7:K:170:SER:O	1.73	1.36
7:K:167:LEU:CA	7:K:170:SER:O	1.73	1.35
7:K:167:LEU:CA	7:K:170:SER:O	1.73	1.34
1:A:145:PRO:CA	1:A:215:PRO:O	1.80	1.28
6:R:143:LEU:C	6:R:145:LEU:H	1.23	1.28
1:A:145:PRO:CA	1:A:215:PRO:O	1.80	1.27
1:A:145:PRO:CA	1:A:215:PRO:O	1.80	1.27
1:A:503:VAL:O	1:A:514:CYS:O	1.53	1.26
6:R:143:LEU:C	6:R:145:LEU:H	1.23	1.25
4:H:269:TYR:O	4:H:271:MET:N	1.69	1.25
4:C:269:TYR:O	4:C:271:MET:N	1.69	1.25
4:C:269:TYR:O	4:C:271:MET:N	1.69	1.24
4:H:269:TYR:O	4:H:271:MET:N	1.69	1.24
1:A:503:VAL:O	1:A:514:CYS:O	1.53	1.24
4:C:269:TYR:O	4:C:271:MET:N	1.68	1.24
4:H:269:TYR:O	4:H:271:MET:N	1.68	1.23
1:A:503:VAL:O	1:A:514:CYS:O	1.53	1.23
7:K:107:SER:H	6:M:50:GLY:CA	1.53	1.21
7:K:107:SER:H	6:M:50:GLY:CA	1.53	1.21
7:K:107:SER:H	6:M:50:GLY:CA	1.53	1.21
3:B:778:LEU:O	3:B:809:THR:O	1.58	1.21
3:B:778:LEU:O	3:B:809:THR:O	1.58	1.20
6:R:71:GLN:O	6:R:74:ILE:N	1.73	1.19
6:R:143:LEU:C	6:R:145:LEU:H	1.23	1.19
6:R:71:GLN:O	6:R:74:ILE:N	1.74	1.19
6:R:71:GLN:O	6:R:74:ILE:N	1.74	1.19
3:B:778:LEU:O	3:B:809:THR:O	1.58	1.19
5:D:13:GLY:HA2	5:D:38:LYS:CA	1.74	1.17
5:D:13:GLY:HA2	5:D:38:LYS:CA	1.74	1.17
5:D:13:GLY:HA2	5:D:38:LYS:CA	1.75	1.15
5:I:13:GLY:HA2	5:I:38:LYS:CA	1.74	1.15
5:I:13:GLY:HA2	5:I:38:LYS:CA	1.74	1.15
5:I:13:GLY:HA2	5:I:38:LYS:CA	1.74	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:190:ILE:CA	7:K:225:SER:CA	2.26	1.14
7:K:190:ILE:CA	7:K:225:SER:CA	2.26	1.14
3:B:778:LEU:O	3:B:809:THR:C	1.91	1.13
3:B:778:LEU:O	3:B:809:THR:C	1.91	1.13
7:G:167:LEU:CA	7:G:170:SER:O	1.95	1.13
7:G:167:LEU:CA	7:G:170:SER:O	1.95	1.13
7:K:190:ILE:CA	7:K:225:SER:CA	2.26	1.13
3:B:778:LEU:O	3:B:809:THR:C	1.91	1.12
7:G:167:LEU:CA	7:G:170:SER:O	1.95	1.12
6:R:143:LEU:C	6:R:145:LEU:N	1.99	1.10
7:G:179:ASN:N	4:H:350:SER:O	1.86	1.08
7:G:179:ASN:N	4:H:350:SER:O	1.86	1.08
8:Z:11:TYR:CA	8:Z:132:GLY:HA3	1.84	1.07
3:B:781:LEU:O	3:B:808:SER:O	1.63	1.07
7:G:179:ASN:N	4:H:350:SER:O	1.86	1.07
8:L:31:TYR:CA	8:L:131:GLY:O	2.03	1.07
8:L:31:TYR:CA	8:L:131:GLY:O	2.03	1.07
8:L:31:TYR:CA	8:L:131:GLY:O	2.03	1.07
6:R:159:CYS:O	6:R:162:SER:N	1.88	1.07
8:Z:11:TYR:CA	8:Z:132:GLY:HA3	1.84	1.07
6:R:143:LEU:C	6:R:145:LEU:N	1.99	1.07
8:Z:11:TYR:CA	8:Z:132:GLY:HA3	1.84	1.06
6:R:159:CYS:O	6:R:162:SER:N	1.88	1.06
6:R:143:LEU:C	6:R:145:LEU:N	1.99	1.05
3:N:526:VAL:CA	3:N:597:VAL:CA	2.35	1.05
6:R:159:CYS:O	6:R:162:SER:N	1.88	1.04
7:G:276:ASN:O	7:G:281:SER:O	1.75	1.04
3:B:526:VAL:CA	3:B:597:VAL:CA	2.35	1.04
3:B:781:LEU:O	3:B:808:SER:O	1.63	1.04
3:B:526:VAL:CA	3:B:597:VAL:CA	2.35	1.04
3:N:526:VAL:CA	3:N:597:VAL:CA	2.35	1.04
3:B:526:VAL:CA	3:B:597:VAL:CA	2.35	1.04
7:G:276:ASN:O	7:G:281:SER:O	1.75	1.03
3:N:526:VAL:CA	3:N:597:VAL:CA	2.35	1.03
7:G:276:ASN:O	7:G:281:SER:O	1.75	1.02
8:Z:12:THR:H	8:Z:132:GLY:CA	1.72	1.02
7:K:167:LEU:C	7:K:170:SER:O	2.03	1.02
8:Z:12:THR:H	8:Z:132:GLY:CA	1.72	1.01
7:K:167:LEU:C	7:K:170:SER:O	2.03	1.01
8:Z:12:THR:H	8:Z:132:GLY:CA	1.72	1.01
3:B:778:LEU:C	3:B:809:THR:O	2.04	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:130:LEU:O	6:R:132:GLU:N	1.92	1.01
7:K:167:LEU:C	7:K:170:SER:O	2.03	1.00
6:R:130:LEU:O	6:R:132:GLU:N	1.92	1.00
6:R:130:LEU:O	6:R:132:GLU:N	1.92	1.00
7:K:190:ILE:C	7:K:225:SER:CA	2.34	1.00
3:B:781:LEU:O	3:B:808:SER:O	1.63	1.00
7:K:190:ILE:C	7:K:225:SER:CA	2.34	1.00
3:B:778:LEU:C	3:B:809:THR:O	2.04	1.00
3:B:778:LEU:C	3:B:809:THR:O	2.04	1.00
7:K:190:ILE:C	7:K:225:SER:CA	2.34	0.99
7:K:677:VAL:O	7:K:694:PRO:CA	2.11	0.99
6:R:126:ASN:CA	6:R:158:THR:O	2.10	0.99
6:R:126:ASN:CA	6:R:158:THR:O	2.10	0.99
8:Z:11:TYR:CA	8:Z:132:GLY:CA	2.41	0.99
7:K:677:VAL:O	7:K:694:PRO:CA	2.11	0.99
8:Z:11:TYR:CA	8:Z:132:GLY:CA	2.41	0.99
7:K:677:VAL:O	7:K:694:PRO:CA	2.11	0.98
6:R:126:ASN:CA	6:R:158:THR:O	2.10	0.98
8:Z:11:TYR:CA	8:Z:132:GLY:CA	2.41	0.97
7:G:107:SER:N	6:R:50:GLY:CA	2.05	0.96
7:G:107:SER:N	6:R:50:GLY:CA	2.05	0.96
3:B:541:ALA:CA	3:B:624:ASP:N	2.29	0.96
3:B:541:ALA:CA	3:B:624:ASP:N	2.29	0.96
3:N:541:ALA:CA	3:N:624:ASP:N	2.29	0.96
3:B:541:ALA:CA	3:B:624:ASP:N	2.29	0.95
1:A:105:TYR:O	1:A:106:PRO:C	2.08	0.95
3:N:541:ALA:CA	3:N:624:ASP:N	2.29	0.95
8:Z:12:THR:N	8:Z:132:GLY:CA	2.30	0.95
3:N:541:ALA:CA	3:N:624:ASP:N	2.29	0.95
3:B:766:ASP:O	3:B:768:LEU:N	1.99	0.94
1:A:105:TYR:O	1:A:106:PRO:C	2.08	0.94
1:A:105:TYR:O	1:A:106:PRO:C	2.08	0.94
8:Z:12:THR:N	8:Z:132:GLY:CA	2.30	0.94
8:Z:12:THR:N	8:Z:132:GLY:O	2.02	0.93
8:Z:12:THR:N	8:Z:132:GLY:O	2.02	0.93
3:B:766:ASP:O	3:B:768:LEU:N	1.99	0.93
3:B:766:ASP:O	3:B:768:LEU:N	1.99	0.93
3:B:824:GLY:CA	3:B:830:ASN:O	2.16	0.93
3:B:824:GLY:CA	3:B:830:ASN:O	2.16	0.93
8:Z:12:THR:N	8:Z:132:GLY:CA	2.30	0.93
3:B:824:GLY:CA	3:B:830:ASN:O	2.16	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:12:THR:N	8:Z:132:GLY:O	2.02	0.92
1:A:495:ILE:O	1:A:502:HIS:O	1.87	0.91
7:K:107:SER:CA	6:M:50:GLY:HA3	2.00	0.91
1:A:495:ILE:O	1:A:502:HIS:O	1.87	0.91
6:R:125:ALA:O	6:R:158:THR:O	1.89	0.90
1:A:495:ILE:O	1:A:502:HIS:O	1.87	0.90
7:K:107:SER:CA	6:M:50:GLY:HA3	2.00	0.90
7:K:107:SER:CA	6:M:50:GLY:HA3	2.00	0.90
7:G:107:SER:N	6:R:50:GLY:CA	2.05	0.90
7:G:107:SER:H	6:R:50:GLY:C	1.79	0.90
7:G:107:SER:H	6:R:50:GLY:C	1.79	0.90
1:A:503:VAL:O	1:A:514:CYS:C	2.15	0.90
7:G:179:ASN:C	4:H:352:GLU:CA	2.45	0.89
3:B:767:THR:CA	3:B:792:LEU:H	1.85	0.89
3:B:767:THR:CA	3:B:792:LEU:H	1.85	0.89
6:R:125:ALA:O	6:R:158:THR:O	1.89	0.89
7:G:301:ALA:C	7:G:303:LEU:H	1.79	0.89
1:A:503:VAL:O	1:A:514:CYS:C	2.15	0.89
1:A:503:VAL:O	1:A:514:CYS:C	2.15	0.89
7:G:106:THR:C	6:R:50:GLY:HA3	1.98	0.89
1:A:105:TYR:O	1:A:107:TRP:N	2.06	0.89
7:G:106:THR:C	6:R:50:GLY:HA3	1.98	0.89
1:A:105:TYR:O	1:A:107:TRP:N	2.06	0.89
7:G:179:ASN:C	4:H:352:GLU:CA	2.45	0.89
7:G:107:SER:H	6:R:50:GLY:C	1.79	0.88
3:B:767:THR:CA	3:B:792:LEU:H	1.85	0.88
6:R:125:ALA:O	6:R:158:THR:O	1.89	0.88
3:B:781:LEU:CA	3:B:805:LYS:O	2.22	0.88
7:K:167:LEU:O	7:K:170:SER:O	1.92	0.88
3:B:781:LEU:CA	3:B:805:LYS:O	2.22	0.88
6:R:130:LEU:C	6:R:132:GLU:H	1.82	0.88
1:A:105:TYR:O	1:A:107:TRP:N	2.06	0.87
6:R:130:LEU:C	6:R:132:GLU:H	1.82	0.87
7:G:106:THR:C	6:R:50:GLY:HA3	1.98	0.87
7:G:301:ALA:C	7:G:303:LEU:H	1.79	0.87
7:G:198:GLY:O	7:G:201:TYR:N	2.07	0.87
7:G:179:ASN:C	4:H:352:GLU:CA	2.45	0.87
1:A:671:LYS:O	1:A:674:TRP:N	2.08	0.87
7:K:167:LEU:O	7:K:170:SER:O	1.92	0.87
6:R:130:LEU:C	6:R:132:GLU:H	1.82	0.87
3:B:483:THR:O	3:B:484:LYS:C	2.18	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:781:LEU:CA	3:B:805:LYS:O	2.22	0.87
1:A:671:LYS:O	1:A:674:TRP:N	2.08	0.86
7:G:198:GLY:O	7:G:201:TYR:N	2.07	0.86
7:K:190:ILE:O	7:K:225:SER:CA	2.23	0.86
7:K:190:ILE:O	7:K:225:SER:CA	2.23	0.86
7:K:167:LEU:O	7:K:170:SER:O	1.92	0.86
3:B:483:THR:O	3:B:484:LYS:C	2.18	0.86
3:B:767:THR:C	3:B:792:LEU:H	1.84	0.86
7:G:198:GLY:O	7:G:201:TYR:N	2.07	0.86
3:N:483:THR:O	3:N:484:LYS:C	2.18	0.86
7:G:301:ALA:C	7:G:303:LEU:H	1.79	0.86
3:N:483:THR:O	3:N:487:ILE:N	2.09	0.86
3:B:483:THR:O	3:B:484:LYS:C	2.18	0.86
3:N:483:THR:O	3:N:484:LYS:C	2.18	0.86
7:K:190:ILE:O	7:K:225:SER:CA	2.23	0.85
3:N:483:THR:O	3:N:484:LYS:C	2.18	0.85
6:R:78:TRP:O	6:R:81:TYR:O	1.95	0.85
7:K:107:SER:N	6:M:50:GLY:CA	2.24	0.85
1:A:671:LYS:O	1:A:674:TRP:N	2.08	0.85
6:R:78:TRP:O	6:R:81:TYR:O	1.95	0.85
3:N:483:THR:O	3:N:487:ILE:N	2.09	0.85
7:K:190:ILE:CA	7:K:225:SER:N	2.40	0.85
6:R:78:TRP:O	6:R:81:TYR:O	1.95	0.85
3:B:767:THR:C	3:B:792:LEU:H	1.84	0.85
8:Z:11:TYR:C	8:Z:132:GLY:HA3	2.02	0.85
3:N:483:THR:O	3:N:487:ILE:N	2.09	0.85
7:K:190:ILE:CA	7:K:225:SER:N	2.40	0.85
3:B:767:THR:C	3:B:792:LEU:H	1.84	0.85
7:K:190:ILE:CA	7:K:225:SER:N	2.40	0.84
7:K:107:SER:N	6:M:50:GLY:CA	2.24	0.84
8:Z:11:TYR:C	8:Z:132:GLY:HA3	2.02	0.84
8:Z:12:THR:H	8:Z:132:GLY:C	1.86	0.84
3:B:483:THR:O	3:B:487:ILE:N	2.09	0.84
8:Z:11:TYR:C	8:Z:132:GLY:HA3	2.02	0.84
3:B:483:THR:O	3:B:487:ILE:N	2.09	0.84
8:Z:12:THR:H	8:Z:132:GLY:C	1.86	0.84
8:Z:12:THR:H	8:Z:132:GLY:C	1.86	0.84
3:B:483:THR:O	3:B:487:ILE:N	2.09	0.83
3:B:739:ASP:O	3:B:740:PRO:O	1.96	0.83
3:B:824:GLY:HA2	3:B:830:ASN:O	1.78	0.83
1:A:214:HIS:O	1:A:217:MET:N	2.10	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:LYS:O	1:A:673:CYS:N	2.11	0.83
1:A:671:LYS:O	1:A:673:CYS:N	2.11	0.83
1:A:214:HIS:O	1:A:217:MET:N	2.10	0.83
3:B:740:PRO:O	3:B:741:VAL:C	2.18	0.83
7:G:179:ASN:O	4:H:352:GLU:CA	2.26	0.83
7:K:107:SER:N	6:M:50:GLY:CA	2.24	0.83
5:I:41:ASN:O	5:I:43:GLY:N	2.12	0.83
5:I:41:ASN:O	5:I:43:GLY:N	2.12	0.83
1:A:214:HIS:O	1:A:217:MET:N	2.10	0.82
1:A:671:LYS:O	1:A:673:CYS:N	2.11	0.82
7:G:179:ASN:O	4:H:352:GLU:CA	2.26	0.82
5:I:41:ASN:O	5:I:43:GLY:N	2.12	0.82
3:B:824:GLY:HA2	3:B:830:ASN:O	1.78	0.82
3:B:739:ASP:O	3:B:740:PRO:O	1.96	0.82
5:D:41:ASN:O	5:D:43:GLY:N	2.12	0.82
7:G:179:ASN:O	4:H:352:GLU:CA	2.26	0.82
3:B:824:GLY:HA2	3:B:830:ASN:O	1.78	0.82
5:D:41:ASN:O	5:D:43:GLY:N	2.12	0.82
3:B:739:ASP:O	3:B:740:PRO:O	1.96	0.81
3:B:766:ASP:C	3:B:768:LEU:H	1.89	0.81
5:D:41:ASN:O	5:D:43:GLY:N	2.12	0.81
6:M:79:ARG:O	6:M:81:TYR:N	2.13	0.81
8:Z:13:VAL:H	8:Z:132:GLY:HA2	1.46	0.81
6:M:79:ARG:O	6:M:81:TYR:N	2.13	0.81
8:Z:13:VAL:H	8:Z:132:GLY:HA2	1.46	0.81
3:B:766:ASP:C	3:B:768:LEU:H	1.89	0.81
6:M:79:ARG:O	6:M:81:TYR:N	2.13	0.81
3:B:740:PRO:O	3:B:741:VAL:C	2.18	0.81
1:A:496:TRP:CA	1:A:502:HIS:CA	2.59	0.81
8:Z:13:VAL:H	8:Z:132:GLY:HA2	1.46	0.81
3:B:766:ASP:C	3:B:768:LEU:H	1.89	0.81
1:A:496:TRP:CA	1:A:502:HIS:CA	2.59	0.81
1:A:496:TRP:CA	1:A:502:HIS:CA	2.59	0.80
3:B:740:PRO:O	3:B:741:VAL:C	2.18	0.79
1:A:749:LEU:O	1:A:753:GLY:N	2.15	0.79
5:I:13:GLY:CA	5:I:38:LYS:CA	2.60	0.79
1:A:749:LEU:O	1:A:753:GLY:N	2.15	0.79
5:D:13:GLY:CA	5:D:38:LYS:CA	2.60	0.79
7:G:179:ASN:N	4:H:350:SER:C	2.41	0.79
7:G:247:ARG:O	7:G:248:ASP:C	2.24	0.79
5:I:13:GLY:CA	5:I:38:LYS:CA	2.60	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:483:THR:O	3:B:486:ASP:N	2.17	0.78
3:B:483:THR:O	3:B:486:ASP:N	2.17	0.78
5:I:13:GLY:CA	5:I:38:LYS:CA	2.60	0.78
1:A:749:LEU:O	1:A:753:GLY:N	2.15	0.78
7:G:179:ASN:N	4:H:350:SER:C	2.41	0.78
1:A:671:LYS:O	1:A:672:ASN:C	2.26	0.78
7:G:301:ALA:C	7:G:303:LEU:N	2.41	0.78
3:N:483:THR:O	3:N:486:ASP:N	2.17	0.78
5:D:13:GLY:CA	5:D:38:LYS:CA	2.60	0.77
3:N:483:THR:O	3:N:486:ASP:N	2.17	0.77
3:N:483:THR:O	3:N:486:ASP:N	2.17	0.77
7:G:277:LEU:O	7:G:280:CYS:N	2.16	0.77
7:G:105:VAL:O	7:G:107:SER:N	2.17	0.77
3:B:483:THR:O	3:B:486:ASP:N	2.17	0.77
7:G:179:ASN:N	4:H:350:SER:C	2.41	0.77
7:G:277:LEU:O	7:G:280:CYS:N	2.16	0.77
7:G:277:LEU:O	7:G:280:CYS:N	2.16	0.77
7:G:301:ALA:C	7:G:303:LEU:N	2.41	0.77
1:A:671:LYS:C	1:A:673:CYS:N	2.39	0.76
4:H:637:VAL:O	4:H:638:SER:O	2.03	0.76
4:H:637:VAL:O	4:H:638:SER:O	2.03	0.76
4:C:269:TYR:C	4:C:271:MET:N	2.44	0.76
4:H:637:VAL:O	4:H:638:SER:O	2.03	0.76
4:H:269:TYR:C	4:H:271:MET:N	2.44	0.76
4:C:637:VAL:O	4:C:638:SER:O	2.03	0.76
5:D:13:GLY:CA	5:D:38:LYS:CA	2.60	0.76
7:G:301:ALA:C	7:G:303:LEU:N	2.41	0.76
8:Z:12:THR:N	8:Z:132:GLY:C	2.44	0.76
7:G:247:ARG:O	7:G:248:ASP:C	2.24	0.76
4:C:637:VAL:O	4:C:638:SER:O	2.03	0.76
7:G:105:VAL:O	7:G:107:SER:N	2.17	0.76
8:Z:12:THR:N	8:Z:132:GLY:C	2.44	0.76
8:Z:12:THR:N	8:Z:132:GLY:C	2.44	0.75
4:C:637:VAL:O	4:C:638:SER:O	2.03	0.75
1:A:671:LYS:O	1:A:672:ASN:C	2.26	0.75
8:Z:12:THR:N	8:Z:132:GLY:HA3	2.00	0.75
8:Z:12:THR:H	8:Z:132:GLY:HA2	1.51	0.75
1:A:671:LYS:C	1:A:673:CYS:N	2.39	0.75
7:G:167:LEU:C	7:G:170:SER:O	2.30	0.75
3:N:563:ASP:C	3:N:577:THR:C	2.55	0.75
1:A:800:PRO:O	4:C:805:PHE:O	2.05	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:LYS:O	1:A:672:ASN:C	2.26	0.75
1:A:800:PRO:O	4:C:805:PHE:O	2.05	0.75
1:A:800:PRO:O	4:C:805:PHE:O	2.05	0.75
8:Z:12:THR:N	8:Z:132:GLY:HA3	2.00	0.74
5:I:41:ASN:C	5:I:43:GLY:H	1.95	0.74
3:N:563:ASP:C	3:N:577:THR:C	2.55	0.74
5:D:41:ASN:C	5:D:43:GLY:H	1.95	0.74
7:G:167:LEU:C	7:G:170:SER:O	2.30	0.74
8:Z:12:THR:H	8:Z:132:GLY:HA2	1.51	0.74
8:Z:12:THR:H	8:Z:132:GLY:HA2	1.51	0.74
3:B:563:ASP:C	3:B:577:THR:C	2.55	0.74
5:D:41:ASN:C	5:D:43:GLY:H	1.95	0.74
5:I:41:ASN:C	5:I:43:GLY:H	1.95	0.74
7:G:178:VAL:C	4:H:350:SER:O	2.30	0.74
7:G:178:VAL:C	4:H:350:SER:O	2.30	0.74
7:G:178:VAL:C	4:H:350:SER:O	2.30	0.74
7:G:167:LEU:C	7:G:170:SER:O	2.30	0.74
6:M:77:LEU:O	6:M:80:HIS:N	2.20	0.74
5:I:41:ASN:C	5:I:43:GLY:H	1.95	0.74
3:B:563:ASP:C	3:B:577:THR:C	2.55	0.74
6:M:77:LEU:O	6:M:80:HIS:N	2.20	0.74
6:M:77:LEU:O	6:M:80:HIS:N	2.21	0.74
3:B:563:ASP:C	3:B:577:THR:C	2.55	0.73
6:R:174:SER:O	6:R:176:SER:N	2.21	0.73
4:H:269:TYR:C	4:H:271:MET:N	2.44	0.73
3:N:563:ASP:C	3:N:577:THR:C	2.55	0.73
5:D:41:ASN:C	5:D:43:GLY:H	1.95	0.73
7:G:105:VAL:O	7:G:107:SER:N	2.17	0.73
7:G:215:ILE:O	7:G:219:THR:N	2.22	0.73
7:G:215:ILE:O	7:G:219:THR:N	2.22	0.73
6:R:143:LEU:O	6:R:145:LEU:N	2.22	0.73
8:Z:10:LEU:O	8:Z:11:TYR:C	2.32	0.73
6:R:143:LEU:O	6:R:145:LEU:N	2.22	0.72
4:C:269:TYR:C	4:C:271:MET:N	2.44	0.72
6:R:174:SER:O	6:R:176:SER:N	2.21	0.72
4:H:269:TYR:C	4:H:271:MET:N	2.44	0.72
6:R:143:LEU:O	6:R:145:LEU:N	2.22	0.72
6:R:174:SER:O	6:R:176:SER:N	2.21	0.72
8:Z:10:LEU:O	8:Z:11:TYR:C	2.32	0.72
8:Z:10:LEU:O	8:Z:11:TYR:C	2.32	0.72
8:Z:12:THR:N	8:Z:132:GLY:HA3	2.00	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:928:LYS:O	3:B:934:PRO:O	2.08	0.71
6:J:29:GLY:HA2	6:J:32:THR:H	1.56	0.71
6:J:29:GLY:HA2	6:J:32:THR:H	1.56	0.71
6:J:29:GLY:HA2	6:J:32:THR:H	1.56	0.71
3:B:766:ASP:C	3:B:768:LEU:N	2.45	0.71
6:F:29:GLY:HA2	6:F:32:THR:H	1.56	0.71
7:G:215:ILE:O	7:G:219:THR:N	2.22	0.71
3:B:928:LYS:O	3:B:934:PRO:O	2.08	0.71
3:B:928:LYS:O	3:B:934:PRO:O	2.08	0.70
6:F:29:GLY:HA2	6:F:32:THR:H	1.56	0.70
1:A:801:ILE:O	4:C:805:PHE:N	2.24	0.70
1:A:496:TRP:CA	1:A:502:HIS:N	2.54	0.70
6:F:29:GLY:HA2	6:F:32:THR:H	1.56	0.70
1:A:496:TRP:CA	1:A:502:HIS:N	2.54	0.70
6:R:71:GLN:C	6:R:74:ILE:H	2.00	0.70
1:A:496:TRP:CA	1:A:502:HIS:N	2.54	0.70
7:K:135:THR:C	7:K:137:LEU:H	2.00	0.70
5:I:39:LEU:C	5:I:41:ASN:H	2.00	0.70
7:G:215:ILE:O	7:G:217:LYS:N	2.24	0.70
5:D:39:LEU:C	5:D:41:ASN:H	2.00	0.70
5:D:39:LEU:C	5:D:41:ASN:H	2.00	0.70
1:A:801:ILE:O	4:C:805:PHE:N	2.24	0.70
6:R:71:GLN:C	6:R:74:ILE:H	2.00	0.70
1:A:801:ILE:O	4:C:805:PHE:N	2.24	0.70
7:G:215:ILE:O	7:G:217:LYS:N	2.25	0.70
7:K:133:ASP:O	7:K:134:SER:O	2.10	0.70
5:I:39:LEU:C	5:I:41:ASN:H	2.00	0.70
3:B:766:ASP:C	3:B:768:LEU:N	2.45	0.70
7:G:247:ARG:O	7:G:248:ASP:C	2.24	0.70
6:R:71:GLN:C	6:R:74:ILE:H	2.00	0.70
7:K:133:ASP:O	7:K:134:SER:O	2.10	0.70
7:G:337:ASN:O	7:G:340:ILE:N	2.25	0.69
7:K:135:THR:C	7:K:137:LEU:H	2.00	0.69
1:A:214:HIS:O	1:A:217:MET:CA	2.40	0.69
7:G:337:ASN:O	7:G:340:ILE:N	2.25	0.69
7:K:133:ASP:O	7:K:134:SER:O	2.10	0.69
7:G:215:ILE:O	7:G:217:LYS:N	2.25	0.69
1:A:671:LYS:C	1:A:673:CYS:N	2.39	0.69
5:D:39:LEU:C	5:D:41:ASN:H	2.00	0.69
7:K:135:THR:C	7:K:137:LEU:H	2.00	0.69
7:G:337:ASN:O	7:G:340:ILE:N	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:HIS:O	1:A:217:MET:CA	2.40	0.69
7:G:172:ASP:O	7:G:175:LYS:N	2.26	0.69
3:B:766:ASP:C	3:B:768:LEU:N	2.45	0.68
1:A:214:HIS:O	1:A:217:MET:CA	2.40	0.68
5:I:39:LEU:C	5:I:41:ASN:H	2.00	0.68
7:G:172:ASP:O	7:G:175:LYS:N	2.26	0.68
7:G:172:ASP:O	7:G:175:LYS:N	2.26	0.68
7:G:247:ARG:O	7:G:248:ASP:O	2.12	0.68
1:A:754:GLN:C	1:A:756:SER:H	2.02	0.68
4:H:269:TYR:C	4:H:271:MET:H	2.02	0.67
7:K:107:SER:CA	6:M:50:GLY:O	2.43	0.67
1:A:754:GLN:C	1:A:756:SER:H	2.02	0.67
7:K:107:SER:CA	6:M:50:GLY:O	2.43	0.67
8:Z:10:LEU:O	8:Z:11:TYR:O	2.13	0.67
8:Z:10:LEU:O	8:Z:11:TYR:O	2.13	0.67
4:H:269:TYR:C	4:H:271:MET:H	2.02	0.67
1:A:754:GLN:C	1:A:756:SER:H	2.02	0.67
7:G:247:ARG:O	7:G:248:ASP:O	2.12	0.67
8:Z:10:LEU:O	8:Z:11:TYR:O	2.13	0.67
7:G:247:ARG:O	7:G:248:ASP:O	2.12	0.67
7:K:107:SER:CA	6:M:50:GLY:O	2.43	0.67
7:G:277:LEU:CA	7:G:280:CYS:CA	2.73	0.67
3:B:779:GLY:O	3:B:808:SER:O	2.14	0.66
3:B:779:GLY:O	3:B:808:SER:O	2.14	0.66
3:B:779:GLY:O	3:B:808:SER:O	2.14	0.66
4:C:269:TYR:C	4:C:271:MET:N	2.43	0.66
3:B:929:PRO:CA	3:B:935:ASP:O	2.44	0.66
7:G:277:LEU:CA	7:G:280:CYS:CA	2.74	0.66
4:H:269:TYR:C	4:H:271:MET:H	2.03	0.66
7:G:277:LEU:CA	7:G:280:CYS:CA	2.73	0.66
1:A:749:LEU:O	1:A:753:GLY:CA	2.44	0.66
1:A:749:LEU:O	1:A:753:GLY:CA	2.44	0.66
6:R:71:GLN:O	6:R:72:ASP:C	2.39	0.66
1:A:214:HIS:O	1:A:217:MET:O	2.14	0.66
1:A:749:LEU:O	1:A:753:GLY:CA	2.44	0.66
6:R:71:GLN:O	6:R:74:ILE:CA	2.44	0.66
3:B:824:GLY:HA3	3:B:830:ASN:O	1.96	0.66
3:B:929:PRO:CA	3:B:935:ASP:O	2.44	0.66
6:R:71:GLN:O	6:R:74:ILE:CA	2.44	0.66
3:B:929:PRO:CA	3:B:935:ASP:O	2.44	0.66
6:R:69:GLY:C	6:R:71:GLN:H	2.04	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:71:GLN:O	6:R:74:ILE:CA	2.44	0.65
7:G:167:LEU:O	7:G:170:SER:O	2.15	0.65
1:A:214:HIS:O	1:A:217:MET:C	2.40	0.65
6:R:69:GLY:C	6:R:71:GLN:H	2.04	0.65
7:G:167:LEU:O	7:G:170:SER:O	2.15	0.65
6:R:71:GLN:O	6:R:72:ASP:C	2.39	0.65
7:G:167:LEU:O	7:G:170:SER:O	2.15	0.65
3:B:824:GLY:HA3	3:B:830:ASN:O	1.96	0.65
1:A:214:HIS:O	1:A:217:MET:O	2.14	0.65
1:A:214:HIS:O	1:A:217:MET:C	2.40	0.65
1:A:214:HIS:O	1:A:217:MET:C	2.40	0.65
3:B:824:GLY:HA3	3:B:830:ASN:O	1.96	0.65
4:C:269:TYR:C	4:C:271:MET:H	2.02	0.65
6:R:69:GLY:C	6:R:71:GLN:H	2.04	0.65
7:G:215:ILE:C	7:G:217:LYS:H	2.05	0.65
7:G:215:ILE:C	7:G:217:LYS:H	2.05	0.65
6:R:71:GLN:O	6:R:72:ASP:C	2.39	0.65
3:B:557:LEU:O	3:B:558:ARG:C	2.41	0.64
7:G:172:ASP:O	7:G:173:VAL:C	2.36	0.64
3:N:563:ASP:C	3:N:577:THR:CA	2.71	0.64
4:C:269:TYR:C	4:C:271:MET:H	2.02	0.64
3:N:563:ASP:C	3:N:577:THR:CA	2.71	0.64
3:B:557:LEU:O	3:B:558:ARG:C	2.41	0.64
3:B:112:GLU:O	3:B:114:ILE:N	2.30	0.64
3:B:563:ASP:C	3:B:577:THR:CA	2.71	0.64
3:N:563:ASP:C	3:N:577:THR:CA	2.71	0.64
3:B:563:ASP:C	3:B:577:THR:CA	2.71	0.64
7:K:243:GLU:O	7:K:245:GLY:N	2.31	0.64
7:G:215:ILE:C	7:G:217:LYS:H	2.05	0.64
3:B:112:GLU:O	3:B:114:ILE:N	2.30	0.64
3:N:112:GLU:O	3:N:114:ILE:N	2.30	0.64
4:C:269:TYR:C	4:C:271:MET:H	2.02	0.64
7:G:215:ILE:C	7:G:217:LYS:N	2.55	0.64
7:G:215:ILE:C	7:G:217:LYS:N	2.55	0.64
7:G:215:ILE:C	7:G:217:LYS:N	2.55	0.64
1:A:671:LYS:C	1:A:673:CYS:H	2.06	0.64
3:N:112:GLU:O	3:N:114:ILE:N	2.30	0.64
1:A:214:HIS:O	1:A:217:MET:O	2.14	0.64
3:B:112:GLU:O	3:B:114:ILE:N	2.30	0.64
3:B:563:ASP:C	3:B:577:THR:CA	2.71	0.64
3:B:766:ASP:O	3:B:792:LEU:O	2.16	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:82:TYR:O	6:R:83:ARG:C	2.39	0.64
3:N:112:GLU:O	3:N:114:ILE:N	2.30	0.64
7:G:172:ASP:O	7:G:173:VAL:C	2.36	0.63
7:G:337:ASN:O	7:G:338:ARG:C	2.39	0.63
6:M:116:LEU:O	6:M:118:ASN:N	2.32	0.63
3:B:739:ASP:O	3:B:740:PRO:C	2.38	0.63
6:R:82:TYR:O	6:R:83:ARG:C	2.39	0.63
3:B:766:ASP:O	3:B:792:LEU:O	2.16	0.63
6:M:116:LEU:O	6:M:118:ASN:N	2.32	0.63
7:G:172:ASP:O	7:G:173:VAL:C	2.36	0.63
7:K:243:GLU:O	7:K:245:GLY:N	2.31	0.63
6:M:116:LEU:O	6:M:118:ASN:N	2.32	0.63
7:K:243:GLU:O	7:K:245:GLY:N	2.31	0.63
3:B:766:ASP:O	3:B:792:LEU:O	2.16	0.63
6:M:24:GLY:O	6:M:68:VAL:O	2.17	0.63
7:G:198:GLY:C	7:G:201:TYR:H	2.07	0.63
3:B:739:ASP:O	3:B:740:PRO:C	2.38	0.62
7:G:277:LEU:CA	7:G:280:CYS:C	2.72	0.62
7:G:277:LEU:CA	7:G:280:CYS:C	2.72	0.62
6:R:82:TYR:O	6:R:83:ARG:C	2.39	0.62
6:M:24:GLY:O	6:M:68:VAL:O	2.17	0.62
3:N:557:LEU:O	3:N:558:ARG:C	2.41	0.62
1:A:671:LYS:C	1:A:673:CYS:H	2.06	0.62
1:A:227:ARG:O	1:A:245:CYS:O	2.17	0.62
7:G:198:GLY:C	7:G:201:TYR:H	2.07	0.62
3:N:557:LEU:O	3:N:558:ARG:C	2.41	0.62
3:N:563:ASP:C	3:N:577:THR:O	2.43	0.62
1:A:227:ARG:O	1:A:245:CYS:O	2.18	0.62
1:A:227:ARG:O	1:A:245:CYS:O	2.17	0.62
7:G:277:LEU:CA	7:G:280:CYS:C	2.72	0.62
3:N:563:ASP:C	3:N:577:THR:O	2.43	0.62
1:A:671:LYS:C	1:A:673:CYS:H	2.06	0.62
7:G:337:ASN:O	7:G:338:ARG:C	2.39	0.62
8:Z:11:TYR:C	8:Z:132:GLY:CA	2.69	0.62
6:M:24:GLY:O	6:M:68:VAL:O	2.17	0.61
1:A:803:PRO:N	4:C:803:GLU:H	1.97	0.61
1:A:803:PRO:N	4:C:803:GLU:H	1.97	0.61
3:B:563:ASP:C	3:B:577:THR:O	2.43	0.61
3:B:739:ASP:O	3:B:740:PRO:C	2.38	0.61
3:B:563:ASP:C	3:B:577:THR:O	2.43	0.61
7:G:337:ASN:O	7:G:338:ARG:C	2.39	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:PRO:N	4:C:803:GLU:H	1.97	0.61
3:N:563:ASP:C	3:N:577:THR:O	2.43	0.61
3:B:899:LEU:O	3:B:900:SER:C	2.43	0.61
4:C:269:TYR:O	4:C:271:MET:CA	2.49	0.61
1:A:205:ASP:H	1:A:207:GLY:H	1.49	0.61
3:B:563:ASP:C	3:B:577:THR:O	2.43	0.61
3:B:899:LEU:O	3:B:900:SER:C	2.44	0.61
3:N:557:LEU:O	3:N:558:ARG:C	2.41	0.60
7:K:135:THR:O	7:K:137:LEU:N	2.35	0.60
1:A:205:ASP:H	1:A:207:GLY:H	1.49	0.60
3:B:899:LEU:O	3:B:900:SER:C	2.44	0.60
1:A:205:ASP:H	1:A:207:GLY:H	1.49	0.60
4:H:506:THR:C	4:H:509:GLY:H	2.10	0.60
7:K:135:THR:O	7:K:137:LEU:N	2.34	0.60
4:C:269:TYR:O	4:C:271:MET:CA	2.49	0.60
3:B:557:LEU:O	3:B:558:ARG:C	2.41	0.60
4:H:506:THR:C	4:H:509:GLY:H	2.10	0.60
4:C:506:THR:C	4:C:509:GLY:H	2.10	0.60
7:K:135:THR:O	7:K:137:LEU:N	2.35	0.60
3:B:740:PRO:O	3:B:742:TYR:N	2.35	0.60
4:C:506:THR:C	4:C:509:GLY:H	2.10	0.60
7:G:215:ILE:O	7:G:218:PHE:N	2.36	0.59
7:G:215:ILE:O	7:G:218:PHE:N	2.36	0.59
7:K:107:SER:CA	6:M:50:GLY:CA	2.75	0.59
4:C:269:TYR:O	4:C:271:MET:CA	2.49	0.59
3:B:740:PRO:O	3:B:742:TYR:N	2.35	0.59
6:M:128:GLN:H	6:M:159:CYS:CA	2.16	0.59
3:B:740:PRO:O	3:B:742:TYR:N	2.35	0.59
3:N:102:LYS:C	3:N:104:THR:H	2.09	0.59
6:M:128:GLN:H	6:M:159:CYS:CA	2.16	0.59
4:C:506:THR:C	4:C:509:GLY:H	2.10	0.59
7:G:215:ILE:O	7:G:218:PHE:N	2.36	0.59
4:H:506:THR:C	4:H:509:GLY:H	2.10	0.59
7:G:179:ASN:H	4:H:350:SER:C	2.11	0.59
4:H:269:TYR:O	4:H:271:MET:CA	2.49	0.59
7:K:107:SER:CA	6:M:50:GLY:CA	2.75	0.58
4:C:174:SER:C	4:C:176:SER:H	2.12	0.58
7:G:198:GLY:C	7:G:200:LEU:N	2.58	0.58
6:R:159:CYS:O	6:R:162:SER:CA	2.50	0.58
7:G:198:GLY:C	7:G:200:LEU:N	2.58	0.58
3:B:102:LYS:C	3:B:104:THR:H	2.09	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:159:CYS:O	6:R:162:SER:CA	2.50	0.58
6:M:128:GLN:H	6:M:159:CYS:CA	2.16	0.58
3:B:504:VAL:O	3:B:507:GLU:N	2.37	0.58
6:M:47:PRO:C	6:M:69:GLY:HA3	2.29	0.58
3:B:102:LYS:C	3:B:104:THR:H	2.09	0.58
6:R:159:CYS:O	6:R:162:SER:CA	2.50	0.58
4:H:269:TYR:O	4:H:271:MET:CA	2.49	0.58
3:N:112:GLU:C	3:N:114:ILE:H	2.12	0.58
3:N:526:VAL:CA	3:N:597:VAL:N	2.67	0.58
6:R:71:GLN:C	6:R:73:ARG:N	2.60	0.58
3:N:112:GLU:C	3:N:114:ILE:H	2.12	0.58
3:B:112:GLU:C	3:B:114:ILE:H	2.12	0.58
3:B:526:VAL:CA	3:B:597:VAL:N	2.67	0.58
6:M:47:PRO:C	6:M:69:GLY:HA3	2.29	0.58
6:R:71:GLN:C	6:R:73:ARG:N	2.60	0.58
3:N:526:VAL:CA	3:N:597:VAL:N	2.67	0.58
7:G:179:ASN:H	4:H:350:SER:C	2.11	0.58
6:M:47:PRO:C	6:M:69:GLY:HA3	2.29	0.58
3:B:112:GLU:C	3:B:114:ILE:H	2.12	0.58
6:M:25:LEU:C	6:M:69:GLY:HA2	2.29	0.57
7:G:387:CYS:O	7:G:391:PRO:CA	2.53	0.57
6:R:71:GLN:C	6:R:73:ARG:N	2.60	0.57
3:B:102:LYS:C	3:B:104:THR:H	2.09	0.57
4:H:174:SER:C	4:H:176:SER:H	2.12	0.57
3:B:526:VAL:CA	3:B:597:VAL:N	2.67	0.57
5:I:41:ASN:C	5:I:43:GLY:N	2.60	0.57
1:A:754:GLN:O	1:A:756:SER:N	2.38	0.57
4:H:269:TYR:O	4:H:271:MET:CA	2.49	0.57
3:B:526:VAL:CA	3:B:597:VAL:N	2.67	0.57
3:N:102:LYS:C	3:N:104:THR:H	2.09	0.57
7:K:107:SER:CA	6:M:50:GLY:CA	2.75	0.57
3:N:102:LYS:C	3:N:104:THR:H	2.09	0.57
7:G:387:CYS:O	7:G:391:PRO:CA	2.53	0.57
6:M:25:LEU:C	6:M:69:GLY:HA2	2.29	0.57
7:G:274:ILE:O	7:G:275:VAL:C	2.48	0.57
3:N:112:GLU:C	3:N:114:ILE:H	2.12	0.57
7:G:274:ILE:O	7:G:275:VAL:C	2.48	0.57
3:N:526:VAL:CA	3:N:597:VAL:N	2.67	0.57
6:M:25:LEU:C	6:M:69:GLY:HA2	2.29	0.57
7:G:274:ILE:O	7:G:275:VAL:C	2.48	0.57
6:R:69:GLY:O	6:R:71:GLN:N	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:135:THR:C	7:K:137:LEU:N	2.58	0.57
7:G:198:GLY:C	7:G:200:LEU:N	2.58	0.57
3:B:112:GLU:C	3:B:114:ILE:H	2.12	0.57
7:K:135:THR:C	7:K:137:LEU:N	2.58	0.57
1:A:754:GLN:O	1:A:756:SER:N	2.38	0.57
7:G:387:CYS:O	7:G:391:PRO:CA	2.53	0.56
3:N:541:ALA:N	3:N:624:ASP:N	2.53	0.56
3:N:504:VAL:O	3:N:507:GLU:N	2.37	0.56
3:N:541:ALA:N	3:N:624:ASP:N	2.53	0.56
7:G:179:ASN:H	4:H:350:SER:C	2.11	0.56
7:G:198:GLY:O	7:G:199:LEU:C	2.49	0.56
3:B:504:VAL:O	3:B:507:GLU:N	2.37	0.56
3:B:767:THR:CA	3:B:792:LEU:N	2.65	0.56
7:G:198:GLY:O	7:G:199:LEU:C	2.49	0.56
4:C:174:SER:C	4:C:176:SER:H	2.12	0.56
1:A:754:GLN:C	1:A:756:SER:N	2.62	0.56
3:B:779:GLY:HA2	3:B:811:ASN:H	1.70	0.56
1:A:495:ILE:O	1:A:502:HIS:C	2.49	0.56
7:G:172:ASP:C	7:G:175:LYS:H	2.14	0.56
7:G:198:GLY:O	7:G:199:LEU:C	2.49	0.56
3:B:541:ALA:N	3:B:624:ASP:N	2.53	0.56
4:C:174:SER:C	4:C:176:SER:H	2.12	0.56
1:A:754:GLN:O	1:A:756:SER:N	2.38	0.56
4:H:174:SER:C	4:H:176:SER:H	2.12	0.56
3:B:767:THR:O	3:B:768:LEU:C	2.49	0.56
3:N:504:VAL:O	3:N:507:GLU:N	2.37	0.56
5:I:41:ASN:C	5:I:43:GLY:N	2.60	0.56
3:B:767:THR:O	3:B:768:LEU:C	2.49	0.56
7:G:172:ASP:C	7:G:175:LYS:H	2.14	0.56
7:G:277:LEU:CA	7:G:280:CYS:N	2.69	0.56
7:K:274:ILE:O	7:K:276:ASN:N	2.39	0.56
7:G:179:ASN:CA	4:H:350:SER:O	2.53	0.56
7:G:179:ASN:CA	4:H:350:SER:O	2.54	0.56
7:G:198:GLY:C	7:G:201:TYR:H	2.07	0.56
7:G:277:LEU:CA	7:G:280:CYS:N	2.69	0.56
3:N:504:VAL:O	3:N:507:GLU:N	2.37	0.56
7:G:172:ASP:C	7:G:175:LYS:H	2.14	0.55
7:G:179:ASN:CA	4:H:350:SER:O	2.53	0.55
3:N:541:ALA:N	3:N:624:ASP:N	2.53	0.55
4:H:174:SER:C	4:H:176:SER:H	2.12	0.55
3:B:779:GLY:HA2	3:B:811:ASN:H	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:41:ASN:C	5:D:43:GLY:N	2.60	0.55
3:N:324:LYS:C	3:N:326:HIS:H	2.15	0.55
3:B:767:THR:CA	3:B:792:LEU:N	2.65	0.55
1:A:495:ILE:O	1:A:502:HIS:C	2.49	0.55
7:G:106:THR:CA	6:R:50:GLY:HA3	2.37	0.55
6:M:78:TRP:O	6:M:79:ARG:C	2.46	0.55
6:R:135:SER:O	6:R:136:ALA:C	2.48	0.55
3:B:541:ALA:N	3:B:624:ASP:N	2.53	0.55
7:G:277:LEU:CA	7:G:280:CYS:N	2.69	0.55
7:G:666:THR:O	7:G:667:ASN:C	2.49	0.55
3:N:324:LYS:C	3:N:326:HIS:H	2.15	0.55
3:B:324:LYS:C	3:B:326:HIS:H	2.15	0.55
3:B:767:THR:O	3:B:768:LEU:C	2.49	0.55
7:K:135:THR:C	7:K:137:LEU:N	2.58	0.55
7:K:274:ILE:O	7:K:276:ASN:N	2.39	0.55
6:R:69:GLY:C	6:R:71:GLN:N	2.65	0.55
6:R:135:SER:O	6:R:136:ALA:C	2.48	0.55
3:B:324:LYS:C	3:B:326:HIS:H	2.15	0.55
3:B:541:ALA:N	3:B:624:ASP:N	2.53	0.55
1:A:495:ILE:O	1:A:502:HIS:C	2.49	0.55
4:C:269:TYR:O	4:C:270:GLY:C	2.48	0.55
3:B:767:THR:CA	3:B:792:LEU:N	2.65	0.55
3:B:779:GLY:HA2	3:B:811:ASN:H	1.70	0.55
4:C:375:TYR:O	4:C:388:PHE:CA	2.55	0.55
3:B:324:LYS:C	3:B:326:HIS:H	2.15	0.54
4:C:375:TYR:O	4:C:388:PHE:CA	2.55	0.54
7:G:106:THR:CA	6:R:50:GLY:HA3	2.36	0.54
4:H:375:TYR:O	4:H:388:PHE:CA	2.56	0.54
3:N:324:LYS:C	3:N:326:HIS:H	2.15	0.54
7:G:666:THR:O	7:G:667:ASN:C	2.49	0.54
7:G:726:CYS:O	7:G:753:LEU:O	2.25	0.54
4:C:375:TYR:O	4:C:388:PHE:CA	2.55	0.54
5:D:42:THR:O	5:D:43:GLY:C	2.50	0.54
6:R:135:SER:O	6:R:136:ALA:C	2.48	0.54
8:Z:11:TYR:C	8:Z:132:GLY:CA	2.69	0.54
1:A:496:TRP:CA	1:A:502:HIS:H	2.21	0.54
4:H:375:TYR:O	4:H:388:PHE:CA	2.56	0.54
5:D:42:THR:O	5:D:43:GLY:C	2.50	0.54
4:C:269:TYR:O	4:C:270:GLY:C	2.48	0.54
6:R:69:GLY:C	6:R:71:GLN:N	2.65	0.54
6:M:173:LEU:C	6:M:175:ASN:H	2.15	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:149:ARG:C	6:F:151:ARG:H	2.16	0.54
7:G:106:THR:CA	6:R:50:GLY:HA3	2.36	0.54
6:R:69:GLY:O	6:R:71:GLN:N	2.34	0.54
7:K:274:ILE:O	7:K:276:ASN:N	2.39	0.54
7:K:665:CYS:O	7:K:703:PRO:CA	2.55	0.54
5:I:42:THR:O	5:I:43:GLY:C	2.50	0.54
7:G:726:CYS:O	7:G:753:LEU:O	2.25	0.54
3:B:928:LYS:C	3:B:934:PRO:O	2.51	0.54
3:B:928:LYS:C	3:B:934:PRO:O	2.51	0.54
6:M:173:LEU:C	6:M:175:ASN:H	2.15	0.54
4:H:568:PRO:C	4:H:571:ASN:H	2.16	0.54
4:H:568:PRO:C	4:H:571:ASN:H	2.16	0.54
1:A:343:GLN:CA	1:A:354:VAL:H	2.21	0.54
7:G:277:LEU:C	7:G:280:CYS:N	2.66	0.54
7:K:665:CYS:O	7:K:703:PRO:CA	2.56	0.54
4:H:568:PRO:C	4:H:571:ASN:H	2.16	0.54
1:A:754:GLN:C	1:A:756:SER:N	2.62	0.54
4:C:568:PRO:C	4:C:571:ASN:H	2.16	0.54
4:H:375:TYR:O	4:H:388:PHE:CA	2.56	0.54
5:D:39:LEU:C	5:D:41:ASN:N	2.66	0.54
4:C:568:PRO:C	4:C:571:ASN:H	2.16	0.54
7:G:726:CYS:O	7:G:753:LEU:O	2.25	0.54
1:A:343:GLN:CA	1:A:354:VAL:H	2.21	0.54
5:D:42:THR:O	5:D:43:GLY:C	2.50	0.54
1:A:496:TRP:CA	1:A:502:HIS:H	2.21	0.53
5:D:39:LEU:C	5:D:41:ASN:N	2.66	0.53
3:B:928:LYS:C	3:B:934:PRO:O	2.51	0.53
6:M:173:LEU:C	6:M:175:ASN:H	2.15	0.53
6:F:149:ARG:C	6:F:151:ARG:H	2.16	0.53
7:K:665:CYS:O	7:K:703:PRO:CA	2.55	0.53
6:M:78:TRP:O	6:M:79:ARG:C	2.46	0.53
1:A:343:GLN:N	1:A:354:VAL:H	2.07	0.53
1:A:321:ARG:H	1:A:338:ASP:CA	2.22	0.53
1:A:343:GLN:CA	1:A:354:VAL:H	2.21	0.53
4:H:269:TYR:O	4:H:270:GLY:C	2.48	0.53
4:C:568:PRO:C	4:C:571:ASN:H	2.16	0.53
6:M:78:TRP:O	6:M:79:ARG:C	2.46	0.53
5:I:41:ASN:C	5:I:43:GLY:N	2.61	0.53
1:A:321:ARG:H	1:A:338:ASP:CA	2.22	0.53
5:I:42:THR:O	5:I:43:GLY:C	2.50	0.53
1:A:321:ARG:H	1:A:338:ASP:CA	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:69:GLY:O	6:R:71:GLN:N	2.34	0.53
7:K:274:ILE:O	7:K:275:VAL:C	2.52	0.53
1:A:496:TRP:CA	1:A:502:HIS:H	2.21	0.53
1:A:754:GLN:C	1:A:756:SER:N	2.62	0.53
7:G:666:THR:O	7:G:667:ASN:C	2.49	0.53
7:G:246:SER:C	7:G:248:ASP:N	2.66	0.53
7:K:274:ILE:O	7:K:275:VAL:C	2.52	0.53
1:A:343:GLN:N	1:A:354:VAL:H	2.07	0.53
7:G:277:LEU:C	7:G:280:CYS:N	2.66	0.52
7:G:247:ARG:O	7:G:251:LEU:N	2.37	0.52
1:A:343:GLN:N	1:A:354:VAL:H	2.07	0.52
8:Z:11:TYR:C	8:Z:132:GLY:CA	2.69	0.52
7:G:277:LEU:C	7:G:280:CYS:N	2.66	0.52
7:G:665:CYS:O	7:G:703:PRO:CA	2.57	0.52
7:G:666:THR:O	7:G:668:THR:N	2.43	0.52
3:B:767:THR:CA	3:B:792:LEU:C	2.83	0.52
7:G:246:SER:C	7:G:248:ASP:N	2.66	0.52
7:G:247:ARG:O	7:G:251:LEU:N	2.37	0.52
6:M:173:LEU:C	6:M:175:ASN:N	2.68	0.52
5:I:42:THR:O	5:I:43:GLY:C	2.50	0.52
1:A:802:MET:O	4:C:804:ALA:CA	2.58	0.52
3:B:767:THR:CA	3:B:793:ALA:N	2.73	0.52
6:J:149:ARG:C	6:J:151:ARG:H	2.16	0.52
4:H:637:VAL:O	4:H:638:SER:C	2.52	0.52
7:G:665:CYS:O	7:G:703:PRO:CA	2.57	0.52
4:H:375:TYR:N	4:H:389:GLY:O	2.41	0.52
4:C:637:VAL:O	4:C:638:SER:C	2.53	0.52
7:G:665:CYS:O	7:G:703:PRO:CA	2.57	0.52
7:G:666:THR:O	7:G:668:THR:N	2.43	0.52
4:H:637:VAL:O	4:H:638:SER:C	2.52	0.52
3:B:767:THR:CA	3:B:792:LEU:C	2.83	0.52
7:G:247:ARG:O	7:G:251:LEU:N	2.37	0.52
6:M:173:LEU:C	6:M:175:ASN:N	2.68	0.52
3:N:483:THR:O	3:N:484:LYS:O	2.28	0.52
6:F:149:ARG:C	6:F:151:ARG:H	2.16	0.52
7:G:666:THR:O	7:G:668:THR:N	2.43	0.52
4:H:637:VAL:O	4:H:638:SER:C	2.52	0.52
3:B:767:THR:CA	3:B:793:ALA:N	2.73	0.52
3:B:767:THR:CA	3:B:793:ALA:N	2.73	0.51
6:R:71:GLN:O	6:R:73:ARG:N	2.43	0.51
6:J:149:ARG:C	6:J:151:ARG:H	2.16	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:767:THR:CA	3:B:792:LEU:C	2.83	0.51
4:C:637:VAL:O	4:C:638:SER:C	2.52	0.51
7:G:246:SER:C	7:G:248:ASP:N	2.66	0.51
1:A:802:MET:O	4:C:804:ALA:CA	2.58	0.51
6:M:77:LEU:O	6:M:80:HIS:CA	2.59	0.51
3:B:483:THR:O	3:B:484:LYS:O	2.28	0.51
6:R:71:GLN:O	6:R:73:ARG:N	2.43	0.51
6:M:173:LEU:C	6:M:175:ASN:N	2.68	0.51
1:A:802:MET:O	4:C:804:ALA:CA	2.58	0.51
4:C:86:TYR:C	4:C:88:THR:H	2.19	0.51
3:B:483:THR:O	3:B:484:LYS:O	2.28	0.51
4:C:637:VAL:O	4:C:638:SER:C	2.52	0.51
6:R:127:LYS:H	6:R:159:CYS:CA	2.24	0.51
6:R:71:GLN:O	6:R:73:ARG:N	2.43	0.51
6:J:149:ARG:C	6:J:151:ARG:H	2.16	0.51
7:K:244:ASP:O	7:K:245:GLY:C	2.54	0.51
3:N:483:THR:O	3:N:484:LYS:O	2.28	0.51
4:C:86:TYR:C	4:C:88:THR:H	2.19	0.50
7:K:274:ILE:O	7:K:275:VAL:C	2.52	0.50
4:H:86:TYR:C	4:H:88:THR:H	2.19	0.50
7:K:665:CYS:O	7:K:702:GLN:C	2.54	0.50
7:K:244:ASP:O	7:K:245:GLY:C	2.54	0.50
4:C:86:TYR:C	4:C:88:THR:H	2.19	0.50
7:K:243:GLU:C	7:K:245:GLY:N	2.69	0.50
7:K:665:CYS:O	7:K:702:GLN:C	2.54	0.50
4:H:86:TYR:C	4:H:88:THR:H	2.19	0.50
4:H:269:TYR:O	4:H:270:GLY:C	2.48	0.50
4:C:269:TYR:O	4:C:270:GLY:C	2.48	0.50
7:G:211:VAL:O	7:G:215:ILE:N	2.45	0.50
3:B:483:THR:O	3:B:484:LYS:O	2.28	0.50
7:K:133:ASP:O	7:K:134:SER:C	2.53	0.50
6:R:127:LYS:H	6:R:159:CYS:CA	2.24	0.50
6:R:127:LYS:H	6:R:159:CYS:CA	2.24	0.50
7:K:243:GLU:C	7:K:245:GLY:N	2.69	0.50
3:B:751:GLN:C	3:B:753:ASP:H	2.20	0.50
6:R:130:LEU:C	6:R:132:GLU:N	2.51	0.50
7:K:695:ALA:O	7:K:696:ARG:C	2.55	0.50
4:H:459:ARG:CA	4:H:509:GLY:HA3	2.42	0.50
3:B:751:GLN:C	3:B:753:ASP:H	2.19	0.50
4:C:375:TYR:N	4:C:389:GLY:O	2.41	0.50
4:C:459:ARG:CA	4:C:509:GLY:HA3	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:375:TYR:N	4:H:389:GLY:O	2.41	0.50
7:K:133:ASP:O	7:K:134:SER:C	2.53	0.50
6:M:77:LEU:O	6:M:80:HIS:CA	2.59	0.50
4:C:459:ARG:CA	4:C:509:GLY:HA3	2.42	0.50
7:K:133:ASP:O	7:K:134:SER:C	2.53	0.50
7:K:665:CYS:O	7:K:702:GLN:C	2.54	0.50
5:I:39:LEU:C	5:I:41:ASN:N	2.66	0.50
7:G:211:VAL:O	7:G:215:ILE:N	2.45	0.50
7:K:244:ASP:O	7:K:245:GLY:C	2.54	0.50
4:H:459:ARG:CA	4:H:509:GLY:HA3	2.42	0.49
6:M:77:LEU:O	6:M:80:HIS:CA	2.59	0.49
7:G:172:ASP:C	7:G:174:VAL:N	2.66	0.49
4:H:86:TYR:C	4:H:88:THR:H	2.19	0.49
3:N:483:THR:O	3:N:484:LYS:O	2.28	0.49
7:K:243:GLU:C	7:K:245:GLY:N	2.69	0.49
5:I:39:LEU:C	5:I:41:ASN:N	2.66	0.49
4:C:459:ARG:CA	4:C:509:GLY:HA3	2.42	0.49
7:G:211:VAL:O	7:G:215:ILE:N	2.45	0.49
7:G:277:LEU:CA	7:G:280:CYS:H	2.26	0.49
4:H:459:ARG:CA	4:H:509:GLY:HA3	2.42	0.49
7:K:273:ALA:C	7:K:275:VAL:H	2.21	0.49
5:D:41:ASN:C	5:D:43:GLY:N	2.60	0.49
6:R:159:CYS:C	6:R:161:THR:N	2.68	0.49
6:R:69:GLY:C	6:R:71:GLN:N	2.65	0.49
7:K:273:ALA:C	7:K:275:VAL:H	2.21	0.49
6:R:159:CYS:C	6:R:161:THR:N	2.68	0.49
7:K:666:THR:O	7:K:667:ASN:C	2.53	0.49
4:C:375:TYR:N	4:C:389:GLY:O	2.41	0.49
7:K:172:ASP:O	7:K:175:LYS:N	2.46	0.49
7:G:172:ASP:C	7:G:174:VAL:N	2.66	0.48
7:K:666:THR:O	7:K:667:ASN:C	2.54	0.48
5:I:39:LEU:C	5:I:41:ASN:N	2.66	0.48
7:G:107:SER:CA	6:R:50:GLY:HA3	2.24	0.48
7:G:176:ARG:C	7:G:178:VAL:H	2.21	0.48
7:K:135:THR:O	7:K:136:MET:C	2.54	0.48
7:K:695:ALA:O	7:K:696:ARG:C	2.55	0.48
7:G:277:LEU:CA	7:G:280:CYS:H	2.26	0.48
7:G:176:ARG:C	7:G:178:VAL:H	2.21	0.48
7:G:277:LEU:CA	7:G:280:CYS:H	2.26	0.48
3:B:762:ASN:C	3:B:764:THR:H	2.18	0.48
7:K:172:ASP:O	7:K:175:LYS:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:504:VAL:O	3:B:507:GLU:N	2.37	0.48
3:B:751:GLN:C	3:B:753:ASP:H	2.20	0.48
4:C:375:TYR:N	4:C:389:GLY:O	2.41	0.47
7:K:666:THR:O	7:K:668:THR:N	2.47	0.47
6:J:29:GLY:CA	6:J:32:THR:H	2.26	0.47
7:G:301:ALA:O	7:G:303:LEU:N	2.48	0.47
7:G:441:GLU:O	7:G:444:GLU:O	2.32	0.47
7:G:176:ARG:C	7:G:178:VAL:H	2.21	0.47
7:G:460:GLY:HA2	7:G:494:ALA:CA	2.44	0.47
7:K:666:THR:O	7:K:668:THR:N	2.47	0.47
7:G:665:CYS:O	7:G:703:PRO:N	2.48	0.47
7:K:172:ASP:O	7:K:175:LYS:N	2.46	0.47
3:B:762:ASN:C	3:B:764:THR:H	2.18	0.47
7:K:135:THR:O	7:K:136:MET:C	2.54	0.47
7:K:273:ALA:C	7:K:275:VAL:H	2.21	0.47
7:K:666:THR:O	7:K:667:ASN:C	2.54	0.47
6:F:29:GLY:CA	6:F:32:THR:H	2.26	0.47
7:G:116:LYS:O	7:G:118:ASP:N	2.48	0.47
7:G:460:GLY:HA2	7:G:494:ALA:CA	2.44	0.47
3:N:482:SER:C	3:N:484:LYS:N	2.71	0.47
3:B:779:GLY:O	3:B:808:SER:C	2.58	0.47
7:G:460:GLY:HA2	7:G:494:ALA:CA	2.44	0.47
7:K:666:THR:O	7:K:668:THR:N	2.47	0.47
7:G:116:LYS:O	7:G:118:ASP:N	2.48	0.47
7:G:665:CYS:O	7:G:703:PRO:N	2.48	0.47
6:J:29:GLY:CA	6:J:32:THR:H	2.26	0.47
7:G:116:LYS:O	7:G:118:ASP:N	2.48	0.47
7:K:695:ALA:O	7:K:696:ARG:C	2.55	0.47
7:G:276:ASN:O	7:G:281:SER:C	2.56	0.47
7:G:441:GLU:O	7:G:444:GLU:O	2.32	0.47
7:G:301:ALA:O	7:G:303:LEU:N	2.48	0.47
7:G:665:CYS:O	7:G:703:PRO:N	2.48	0.47
4:H:233:SER:H	4:H:248:SER:CA	2.28	0.47
3:B:779:GLY:O	3:B:808:SER:C	2.58	0.46
6:R:109:ARG:C	6:R:112:ASN:H	2.23	0.46
3:B:112:GLU:C	3:B:114:ILE:N	2.73	0.46
7:G:726:CYS:O	7:G:753:LEU:N	2.44	0.46
7:G:172:ASP:C	7:G:174:VAL:N	2.66	0.46
7:G:726:CYS:O	7:G:753:LEU:N	2.44	0.46
6:J:29:GLY:CA	6:J:32:THR:H	2.26	0.46
3:B:267:LEU:C	3:B:269:GLN:H	2.24	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:267:LEU:C	3:N:269:GLN:H	2.24	0.46
6:R:109:ARG:C	6:R:112:ASN:H	2.23	0.46
5:I:62:GLU:C	5:I:64:LEU:H	2.23	0.46
3:B:779:GLY:O	3:B:808:SER:C	2.58	0.46
4:H:233:SER:H	4:H:248:SER:CA	2.28	0.46
3:B:112:GLU:C	3:B:114:ILE:N	2.73	0.46
3:B:842:MET:O	3:B:888:THR:O	2.34	0.46
5:D:62:GLU:C	5:D:64:LEU:H	2.23	0.46
7:G:441:GLU:O	7:G:444:GLU:O	2.32	0.46
6:R:130:LEU:C	6:R:132:GLU:N	2.51	0.46
3:N:267:LEU:C	3:N:269:GLN:H	2.24	0.46
7:K:665:CYS:O	7:K:702:GLN:O	2.34	0.46
3:B:842:MET:O	3:B:888:THR:O	2.34	0.46
5:D:62:GLU:C	5:D:64:LEU:H	2.24	0.46
7:G:726:CYS:O	7:G:753:LEU:N	2.44	0.46
5:I:62:GLU:C	5:I:64:LEU:H	2.23	0.46
3:B:482:SER:C	3:B:484:LYS:N	2.71	0.46
7:K:665:CYS:O	7:K:702:GLN:O	2.34	0.46
6:F:29:GLY:CA	6:F:32:THR:H	2.26	0.46
5:I:62:GLU:C	5:I:64:LEU:H	2.23	0.46
3:N:267:LEU:C	3:N:269:GLN:H	2.24	0.46
3:B:267:LEU:C	3:B:269:GLN:H	2.24	0.46
6:F:29:GLY:CA	6:F:32:THR:H	2.26	0.46
7:G:107:SER:N	6:R:50:GLY:C	2.59	0.46
4:H:233:SER:H	4:H:248:SER:CA	2.28	0.46
7:G:179:ASN:CA	4:H:350:SER:C	2.89	0.46
3:B:842:MET:O	3:B:888:THR:O	2.34	0.46
5:D:62:GLU:C	5:D:64:LEU:H	2.23	0.46
6:R:109:ARG:C	6:R:112:ASN:H	2.23	0.46
4:C:233:SER:H	4:C:248:SER:CA	2.28	0.45
7:G:179:ASN:CA	4:H:350:SER:C	2.88	0.45
7:G:215:ILE:O	7:G:216:SER:C	2.60	0.45
6:R:160:ALA:C	6:R:163:GLY:H	2.25	0.45
7:K:135:THR:O	7:K:136:MET:C	2.54	0.45
7:G:301:ALA:O	7:G:303:LEU:N	2.48	0.45
7:K:665:CYS:O	7:K:702:GLN:O	2.34	0.45
3:B:482:SER:C	3:B:484:LYS:N	2.71	0.45
4:C:233:SER:H	4:C:248:SER:CA	2.29	0.45
7:G:215:ILE:O	7:G:216:SER:C	2.60	0.45
7:G:298:SER:O	7:G:300:LYS:N	2.50	0.45
6:R:159:CYS:C	6:R:161:THR:N	2.68	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:112:GLU:C	3:N:114:ILE:N	2.73	0.45
5:D:41:ASN:C	5:D:43:GLY:N	2.60	0.45
6:R:160:ALA:C	6:R:163:GLY:H	2.25	0.45
6:R:25:LEU:C	6:R:70:GLY:H	2.24	0.45
7:G:276:ASN:O	7:G:281:SER:C	2.56	0.45
6:R:25:LEU:C	6:R:70:GLY:H	2.24	0.45
7:G:298:SER:O	7:G:300:LYS:N	2.50	0.45
7:G:702:GLN:O	7:G:703:PRO:C	2.60	0.45
7:G:179:ASN:CA	4:H:350:SER:C	2.88	0.45
3:B:267:LEU:C	3:B:269:GLN:H	2.24	0.45
7:G:298:SER:O	7:G:300:LYS:N	2.50	0.45
7:G:215:ILE:O	7:G:216:SER:C	2.60	0.45
7:K:107:SER:H	6:M:50:GLY:HA3	0.67	0.45
4:H:375:TYR:N	4:H:389:GLY:O	2.41	0.45
5:D:39:LEU:C	5:D:41:ASN:N	2.66	0.45
6:R:25:LEU:C	6:R:70:GLY:H	2.24	0.45
7:G:276:ASN:O	7:G:281:SER:C	2.56	0.45
6:R:160:ALA:C	6:R:163:GLY:H	2.24	0.45
7:G:702:GLN:O	7:G:703:PRO:C	2.60	0.45
7:G:277:LEU:C	7:G:280:CYS:H	2.24	0.45
1:A:321:ARG:N	1:A:338:ASP:O	2.50	0.45
3:B:762:ASN:C	3:B:764:THR:H	2.18	0.45
3:N:482:SER:C	3:N:484:LYS:N	2.71	0.44
3:N:112:GLU:C	3:N:114:ILE:N	2.72	0.44
7:K:107:SER:CA	6:M:50:GLY:C	2.91	0.44
4:C:233:SER:H	4:C:248:SER:CA	2.29	0.44
7:G:702:GLN:O	7:G:703:PRO:C	2.60	0.44
7:K:107:SER:CA	6:M:50:GLY:C	2.91	0.44
3:B:767:THR:C	3:B:792:LEU:N	2.65	0.44
4:H:715:LEU:O	4:H:719:ALA:N	2.51	0.44
3:B:482:SER:C	3:B:484:LYS:N	2.71	0.44
4:H:715:LEU:O	4:H:719:ALA:N	2.51	0.44
7:K:107:SER:CA	6:M:50:GLY:C	2.91	0.44
7:K:181:ALA:O	7:K:185:ALA:N	2.51	0.44
4:H:715:LEU:O	4:H:719:ALA:N	2.51	0.44
7:G:430:GLU:C	7:G:432:LYS:H	2.26	0.44
8:Z:12:THR:N	8:Z:132:GLY:HA2	2.20	0.44
7:K:181:ALA:O	7:K:185:ALA:N	2.51	0.44
7:K:107:SER:H	6:M:50:GLY:HA3	0.67	0.44
4:C:257:HIS:C	4:C:259:SER:H	2.26	0.43
4:C:715:LEU:O	4:C:719:ALA:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:715:LEU:O	4:C:719:ALA:N	2.51	0.43
8:L:49:PHE:O	8:L:53:HIS:N	2.52	0.43
4:H:257:HIS:C	4:H:259:SER:H	2.26	0.43
1:A:9:SER:C	1:A:313:GLY:HA2	2.43	0.43
7:G:430:GLU:C	7:G:432:LYS:H	2.26	0.43
1:A:321:ARG:N	1:A:338:ASP:O	2.50	0.43
4:H:280:LEU:C	4:H:283:SER:H	2.27	0.43
4:H:484:SER:CA	4:H:522:GLU:H	2.32	0.43
7:G:277:LEU:C	7:G:280:CYS:H	2.24	0.43
4:C:280:LEU:C	4:C:283:SER:H	2.27	0.43
4:C:715:LEU:O	4:C:719:ALA:N	2.51	0.43
1:A:9:SER:C	1:A:313:GLY:HA2	2.43	0.43
7:G:277:LEU:C	7:G:280:CYS:H	2.24	0.43
4:C:257:HIS:C	4:C:259:SER:H	2.26	0.43
3:N:482:SER:C	3:N:484:LYS:N	2.71	0.43
4:H:280:LEU:C	4:H:283:SER:H	2.27	0.43
7:G:529:THR:O	7:G:533:ASN:N	2.52	0.43
4:H:257:HIS:C	4:H:259:SER:H	2.26	0.43
1:A:321:ARG:N	1:A:338:ASP:O	2.50	0.43
4:H:257:HIS:C	4:H:259:SER:H	2.26	0.43
4:H:484:SER:CA	4:H:522:GLU:H	2.32	0.43
6:R:125:ALA:C	6:R:158:THR:O	2.60	0.43
4:C:484:SER:CA	4:C:522:GLU:H	2.32	0.43
1:A:9:SER:C	1:A:313:GLY:HA2	2.43	0.43
3:B:767:THR:C	3:B:792:LEU:N	2.65	0.43
4:H:510:ILE:C	4:H:512:ASP:H	2.27	0.43
7:G:107:SER:N	6:R:50:GLY:C	2.59	0.43
7:G:107:SER:CA	6:R:50:GLY:HA3	2.24	0.43
7:K:181:ALA:O	7:K:185:ALA:N	2.51	0.43
7:G:107:SER:CA	6:R:50:GLY:CA	2.92	0.43
7:K:171:PHE:O	7:K:174:VAL:N	2.52	0.43
6:R:70:GLY:O	6:R:72:ASP:N	2.52	0.43
4:H:280:LEU:C	4:H:283:SER:H	2.27	0.43
7:G:529:THR:O	7:G:533:ASN:N	2.52	0.43
6:R:70:GLY:O	6:R:72:ASP:N	2.52	0.43
4:C:842:PHE:O	4:C:843:GLN:C	2.62	0.43
7:G:529:THR:O	7:G:533:ASN:N	2.52	0.43
4:C:280:LEU:C	4:C:283:SER:H	2.27	0.43
1:A:373:ALA:C	1:A:375:ASN:N	2.75	0.43
4:C:257:HIS:C	4:C:259:SER:H	2.26	0.43
4:C:280:LEU:C	4:C:283:SER:H	2.27	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:49:PHE:O	8:L:53:HIS:N	2.52	0.43
4:H:484:SER:CA	4:H:522:GLU:H	2.32	0.43
7:K:166:LEU:O	7:K:170:SER:N	2.42	0.42
4:C:842:PHE:O	4:C:843:GLN:C	2.62	0.42
4:H:510:ILE:C	4:H:512:ASP:H	2.27	0.42
1:A:373:ALA:C	1:A:375:ASN:N	2.75	0.42
1:A:502:HIS:C	1:A:504:ALA:H	2.27	0.42
7:K:226:PRO:O	7:K:229:TYR:N	2.51	0.42
4:H:510:ILE:C	4:H:512:ASP:H	2.27	0.42
1:A:749:LEU:O	1:A:753:GLY:HA2	2.18	0.42
3:B:778:LEU:O	3:B:809:THR:CA	2.65	0.42
7:G:274:ILE:O	7:G:275:VAL:O	2.37	0.42
1:A:749:LEU:O	1:A:753:GLY:HA2	2.18	0.42
3:B:780:ASP:C	3:B:808:SER:N	2.78	0.42
4:C:484:SER:CA	4:C:522:GLU:H	2.32	0.42
7:G:246:SER:C	7:G:248:ASP:H	2.27	0.42
1:A:502:HIS:C	1:A:504:ALA:H	2.27	0.42
7:G:274:ILE:O	7:G:275:VAL:O	2.37	0.42
7:K:226:PRO:O	7:K:229:TYR:N	2.51	0.42
1:A:749:LEU:O	1:A:753:GLY:HA2	2.18	0.42
4:C:842:PHE:O	4:C:843:GLN:C	2.62	0.42
7:G:274:ILE:O	7:G:275:VAL:O	2.37	0.42
4:C:690:LEU:O	4:C:694:GLN:N	2.53	0.42
6:R:70:GLY:O	6:R:72:ASP:N	2.52	0.42
8:L:49:PHE:O	8:L:53:HIS:N	2.51	0.42
7:K:171:PHE:O	7:K:174:VAL:N	2.51	0.42
1:A:373:ALA:C	1:A:375:ASN:N	2.75	0.42
6:R:125:ALA:C	6:R:158:THR:O	2.60	0.42
3:B:779:GLY:N	3:B:809:THR:O	2.22	0.42
6:R:82:TYR:C	6:R:83:ARG:O	2.61	0.42
7:K:171:PHE:O	7:K:174:VAL:N	2.52	0.42
3:B:780:ASP:C	3:B:808:SER:N	2.78	0.42
4:C:690:LEU:O	4:C:694:GLN:N	2.53	0.42
7:G:107:SER:CA	6:R:50:GLY:CA	2.93	0.42
1:A:502:HIS:C	1:A:504:ALA:H	2.27	0.42
4:C:510:ILE:C	4:C:512:ASP:H	2.27	0.42
7:K:226:PRO:O	7:K:229:TYR:N	2.51	0.42
3:B:780:ASP:C	3:B:808:SER:N	2.78	0.42
4:C:163:LEU:C	4:C:165:ARG:N	2.78	0.42
4:C:484:SER:CA	4:C:522:GLU:H	2.32	0.42
6:R:130:LEU:C	6:R:132:GLU:N	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:166:LEU:O	7:K:170:SER:N	2.42	0.42
7:G:107:SER:CA	6:R:50:GLY:CA	2.92	0.42
6:M:27:GLY:C	6:M:45:THR:O	2.63	0.42
6:M:27:GLY:C	6:M:45:THR:O	2.63	0.42
7:G:522:ASN:C	7:G:525:ARG:H	2.28	0.41
7:K:107:SER:H	6:M:50:GLY:HA3	0.67	0.41
3:B:778:LEU:O	3:B:809:THR:CA	2.65	0.41
3:B:866:ASN:O	3:B:944:ILE:O	2.39	0.41
3:B:135:THR:O	3:B:139:LEU:N	2.52	0.41
4:C:690:LEU:O	4:C:694:GLN:N	2.53	0.41
4:H:690:LEU:O	4:H:694:GLN:N	2.53	0.41
3:B:767:THR:C	3:B:768:LEU:O	2.64	0.41
7:G:246:SER:C	7:G:248:ASP:H	2.27	0.41
3:B:866:ASN:O	3:B:944:ILE:O	2.39	0.41
7:K:182:GLN:C	7:K:185:ALA:H	2.29	0.41
3:N:135:THR:O	3:N:139:LEU:N	2.52	0.41
4:C:510:ILE:C	4:C:512:ASP:H	2.27	0.41
7:G:107:SER:N	6:R:50:GLY:O	2.52	0.41
3:B:866:ASN:O	3:B:944:ILE:O	2.39	0.41
7:K:182:GLN:C	7:K:185:ALA:H	2.29	0.41
7:G:522:ASN:C	7:G:525:ARG:H	2.28	0.41
4:H:690:LEU:O	4:H:694:GLN:N	2.53	0.41
3:B:767:THR:CA	3:B:793:ALA:CA	2.99	0.41
4:H:690:LEU:O	4:H:694:GLN:N	2.53	0.41
4:C:510:ILE:C	4:C:512:ASP:H	2.27	0.41
6:M:27:GLY:C	6:M:45:THR:O	2.63	0.41
4:H:269:TYR:O	4:H:270:GLY:C	2.48	0.41
3:B:767:THR:CA	3:B:793:ALA:CA	2.99	0.41
7:K:182:GLN:C	7:K:185:ALA:H	2.29	0.41
7:K:200:LEU:O	7:K:201:TYR:C	2.59	0.41
7:K:232:MET:O	7:K:236:ALA:N	2.53	0.41
8:L:46:LYS:O	8:L:47:ASN:C	2.59	0.41
6:M:27:GLY:H	6:M:46:ILE:CA	2.34	0.41
3:B:135:THR:O	3:B:139:LEU:N	2.52	0.41
7:G:522:ASN:C	7:G:525:ARG:H	2.28	0.41
3:B:778:LEU:O	3:B:809:THR:CA	2.65	0.41
7:K:200:LEU:O	7:K:201:TYR:C	2.60	0.41
7:K:214:MET:C	7:K:217:LYS:H	2.29	0.41
4:C:637:VAL:C	4:C:638:SER:O	2.64	0.41
6:F:93:ASP:C	6:F:95:ASN:H	2.29	0.41
7:K:214:MET:C	7:K:217:LYS:H	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:644:THR:C	7:K:646:TYR:N	2.78	0.41
4:H:637:VAL:C	4:H:638:SER:O	2.64	0.41
1:A:9:SER:N	1:A:313:GLY:HA3	2.36	0.41
7:K:644:THR:C	7:K:646:TYR:N	2.78	0.41
1:A:9:SER:N	1:A:313:GLY:HA3	2.36	0.41
7:G:105:VAL:C	7:G:107:SER:N	2.79	0.41
7:G:430:GLU:C	7:G:432:LYS:H	2.26	0.41
3:N:122:LYS:O	3:N:126:HIS:N	2.54	0.41
3:B:122:LYS:O	3:B:126:HIS:N	2.54	0.41
7:G:105:VAL:C	7:G:107:SER:N	2.79	0.41
7:K:200:LEU:O	7:K:201:TYR:C	2.60	0.41
3:B:767:THR:C	3:B:768:LEU:O	2.64	0.41
3:N:122:LYS:O	3:N:126:HIS:N	2.54	0.41
1:A:300:HIS:C	1:A:303:LEU:H	2.30	0.40
1:A:576:ASN:O	1:A:578:VAL:N	2.55	0.40
7:G:107:SER:N	6:R:50:GLY:O	2.52	0.40
8:L:46:LYS:O	8:L:47:ASN:C	2.59	0.40
6:M:27:GLY:H	6:M:46:ILE:CA	2.34	0.40
4:H:163:LEU:C	4:H:165:ARG:N	2.78	0.40
1:A:576:ASN:O	1:A:578:VAL:N	2.55	0.40
3:B:767:THR:C	3:B:792:LEU:N	2.65	0.40
3:B:767:THR:CA	3:B:793:ALA:CA	2.99	0.40
1:A:9:SER:N	1:A:313:GLY:HA3	2.36	0.40
7:G:246:SER:C	7:G:248:ASP:H	2.27	0.40
7:K:214:MET:C	7:K:217:LYS:H	2.29	0.40
3:N:135:THR:O	3:N:139:LEU:N	2.52	0.40
4:H:371:GLY:C	4:H:373:GLY:H	2.29	0.40
1:A:300:HIS:C	1:A:303:LEU:H	2.30	0.40
6:J:93:ASP:C	6:J:95:ASN:H	2.29	0.40
1:A:300:HIS:C	1:A:303:LEU:H	2.30	0.40
1:A:598:LYS:O	1:A:602:ALA:N	2.54	0.40
4:C:566:TYR:CA	4:C:572:ARG:O	2.69	0.40
6:F:93:ASP:C	6:F:95:ASN:H	2.29	0.40
4:H:213:ILE:O	4:H:222:VAL:N	2.54	0.40
4:C:163:LEU:C	4:C:165:ARG:N	2.78	0.40
4:H:566:TYR:CA	4:H:572:ARG:O	2.69	0.40
3:B:122:LYS:O	3:B:126:HIS:N	2.54	0.40
1:A:765:HIS:C	4:C:824:TYR:O	2.65	0.40
4:C:566:TYR:CA	4:C:572:ARG:O	2.69	0.40
7:G:107:SER:N	6:R:50:GLY:C	2.59	0.40
4:H:163:LEU:C	4:H:165:ARG:N	2.78	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:925:SER:O	3:B:940:GLY:CA	2.70	0.40
4:C:566:TYR:CA	4:C:572:ARG:O	2.69	0.40
8:L:142:VAL:C	8:L:145:ARG:H	2.30	0.40
4:C:15:SER:H	4:C:293:GLY:HA2	1.86	0.40
7:K:166:LEU:O	7:K:170:SER:N	2.42	0.40
8:L:142:VAL:C	8:L:145:ARG:H	2.30	0.40
4:H:637:VAL:C	4:H:638:SER:O	2.64	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 PDB entries followed by that with respect to all EM entries.

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	1-A	1122/1262 (89%)	891 (79%)	119 (11%)	112 (10%)	0 7
1	2-A	1122/1262 (89%)	891 (79%)	120 (11%)	111 (10%)	0 7
1	3-A	1122/1262 (89%)	891 (79%)	119 (11%)	112 (10%)	0 7
2	1-E	290/308 (94%)	276 (95%)	9 (3%)	5 (2%)	7 36
2	2-E	290/308 (94%)	276 (95%)	9 (3%)	5 (2%)	7 36
2	3-E	290/308 (94%)	276 (95%)	10 (3%)	4 (1%)	9 40
3	1-B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	0 8
3	1-N	562/968 (58%)	478 (85%)	40 (7%)	44 (8%)	1 10
3	2-B	790/968 (82%)	648 (82%)	69 (9%)	73 (9%)	0 8
3	2-N	562/968 (58%)	478 (85%)	40 (7%)	44 (8%)	1 10
3	3-B	790/968 (82%)	648 (82%)	68 (9%)	74 (9%)	0 8
3	3-N	562/968 (58%)	478 (85%)	40 (7%)	44 (8%)	1 10
4	1-C	841/905 (93%)	681 (81%)	91 (11%)	69 (8%)	0 9
4	1-H	719/905 (79%)	587 (82%)	77 (11%)	55 (8%)	1 10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	2-C	841/905 (93%)	682 (81%)	90 (11%)	69 (8%)	0 9
4	2-H	719/905 (79%)	588 (82%)	76 (11%)	55 (8%)	1 10
4	3-C	841/905 (93%)	680 (81%)	92 (11%)	69 (8%)	0 9
4	3-H	719/905 (79%)	587 (82%)	77 (11%)	55 (8%)	1 10
5	1-D	173/511 (34%)	144 (83%)	16 (9%)	13 (8%)	1 10
5	1-I	173/511 (34%)	144 (83%)	16 (9%)	13 (8%)	1 10
5	2-D	173/511 (34%)	144 (83%)	16 (9%)	13 (8%)	1 10
5	2-I	173/511 (34%)	144 (83%)	16 (9%)	13 (8%)	1 10
5	3-D	173/511 (34%)	144 (83%)	16 (9%)	13 (8%)	1 10
5	3-I	173/511 (34%)	144 (83%)	16 (9%)	13 (8%)	1 10
6	1-F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1 14
6	1-J	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1 14
6	1-M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0 5
6	1-R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0 4
6	2-F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1 14
6	2-J	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1 14
6	2-M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0 5
6	2-R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0 4
6	3-F	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1 14
6	3-J	157/181 (87%)	134 (85%)	14 (9%)	9 (6%)	1 14
6	3-M	157/181 (87%)	126 (80%)	13 (8%)	18 (12%)	0 5
6	3-R	157/181 (87%)	120 (76%)	17 (11%)	20 (13%)	0 4
7	1-G	794/874 (91%)	678 (85%)	61 (8%)	55 (7%)	1 11
7	1-K	556/874 (64%)	475 (85%)	42 (8%)	39 (7%)	1 11
7	2-G	794/874 (91%)	678 (85%)	61 (8%)	55 (7%)	1 11
7	2-K	542/874 (62%)	467 (86%)	37 (7%)	38 (7%)	1 11
7	3-G	794/874 (91%)	678 (85%)	61 (8%)	55 (7%)	1 11
7	3-K	556/874 (64%)	475 (85%)	43 (8%)	38 (7%)	1 11
8	1-L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1 12
8	1-Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	1 15
8	2-L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1 12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	2-Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	1 15
8	3-L	137/177 (77%)	117 (85%)	11 (8%)	9 (7%)	1 12
8	3-Z	137/177 (77%)	119 (87%)	11 (8%)	7 (5%)	1 15
All	All	20752/27492 (76%)	17249 (83%)	1855 (9%)	1648 (8%)	1 10

All (1648) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	63	GLN
1	1-A	64	PRO
1	1-A	92	HIS
1	1-A	106	PRO
1	1-A	125	ARG
1	1-A	169	LYS
1	1-A	174	PRO
1	1-A	187	VAL
1	1-A	215	PRO
1	1-A	237	SER
1	1-A	250	ASN
1	1-A	252	VAL
1	1-A	271	LYS
1	1-A	278	MET
1	1-A	281	ARG
1	1-A	324	PRO
1	1-A	325	ALA
1	1-A	341	LEU
1	1-A	343	GLN
1	1-A	384	SER
1	1-A	454	ASP
1	1-A	457	PHE
1	1-A	466	LEU
1	1-A	479	GLN
1	1-A	492	LYS
1	1-A	566	LEU
1	1-A	583	ARG
1	1-A	584	GLU
1	1-A	592	ILE
1	1-A	593	ASP
1	1-A	619	LYS
1	1-A	642	VAL
1	1-A	671	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-A	728	ASP
1	1-A	779	ASP
1	1-A	788	ILE
1	1-A	796	GLN
1	1-A	797	PRO
1	1-A	798	PRO
1	1-A	803	PRO
1	1-A	805	ASP
1	1-A	811	LEU
1	1-A	949	VAL
1	1-A	999	VAL
2	1-E	111	SER
2	1-E	231	ARG
3	1-B	36	PRO
3	1-B	68	GLU
3	1-B	109	LEU
3	1-B	111	HIS
3	1-B	113	MET
3	1-B	254	PRO
3	1-B	255	SER
3	1-B	329	HIS
3	1-B	348	ASP
3	1-B	367	ASN
3	1-B	385	VAL
3	1-B	386	SER
3	1-B	466	SER
3	1-B	480	TYR
3	1-B	484	LYS
3	1-B	500	GLU
3	1-B	501	ILE
3	1-B	502	PRO
3	1-B	503	ILE
3	1-B	505	GLU
3	1-B	521	ILE
3	1-B	522	THR
3	1-B	547	PRO
3	1-B	767	THR
3	1-B	771	CYS
3	1-B	826	ALA
3	1-B	831	CYS
3	1-B	865	GLU
3	1-B	899	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1-B	929	PRO
3	1-B	930	VAL
3	1-B	934	PRO
3	1-B	935	ASP
3	1-B	938	VAL
4	1-C	27	GLU
4	1-C	89	LEU
4	1-C	200	PRO
4	1-C	228	HIS
4	1-C	270	GLY
4	1-C	273	ARG
4	1-C	325	ALA
4	1-C	326	ASN
4	1-C	328	LYS
4	1-C	329	ALA
4	1-C	332	ASP
4	1-C	350	SER
4	1-C	363	ASN
4	1-C	365	ARG
4	1-C	400	SER
4	1-C	410	SER
4	1-C	411	ILE
4	1-C	424	PHE
4	1-C	451	ASP
4	1-C	462	GLU
4	1-C	475	GLU
4	1-C	484	SER
4	1-C	502	HIS
4	1-C	614	PRO
4	1-C	615	LYS
4	1-C	638	SER
4	1-C	762	LEU
4	1-C	781	ASN
4	1-C	782	GLN
4	1-C	789	ALA
4	1-C	790	ASP
4	1-C	806	VAL
4	1-C	825	PRO
4	1-C	833	ARG
5	1-D	12	ALA
5	1-D	44	LYS
5	1-D	73	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1-D	96	ALA
6	1-F	97	ARG
6	1-F	117	ARG
6	1-F	131	PRO
7	1-G	77	PHE
7	1-G	100	GLU
7	1-G	106	THR
7	1-G	132	THR
7	1-G	151	LYS
7	1-G	171	PHE
7	1-G	243	GLU
7	1-G	261	ASN
7	1-G	275	VAL
7	1-G	277	LEU
7	1-G	283	LYS
7	1-G	299	PRO
7	1-G	373	ASP
7	1-G	394	HIS
7	1-G	446	CYS
7	1-G	484	HIS
7	1-G	608	THR
7	1-G	621	PRO
7	1-G	686	ALA
7	1-G	741	GLU
6	1-R	42	VAL
6	1-R	43	ILE
6	1-R	130	LEU
6	1-R	131	PRO
6	1-R	145	LEU
6	1-R	147	SER
6	1-R	151	ARG
6	1-R	175	ASN
8	1-Z	36	PRO
8	1-Z	37	SER
8	1-Z	84	TYR
7	1-K	134	SER
7	1-K	135	THR
7	1-K	170	SER
7	1-K	171	PHE
7	1-K	207	ASP
7	1-K	221	HIS
7	1-K	225	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	1-K	226	PRO
7	1-K	227	PHE
7	1-K	243	GLU
7	1-K	275	VAL
7	1-K	299	PRO
7	1-K	608	THR
7	1-K	621	PRO
7	1-K	686	ALA
7	1-K	741	GLU
7	1-K	813	CYS
8	1-L	37	SER
8	1-L	84	TYR
8	1-L	147	ALA
6	1-M	42	VAL
6	1-M	43	ILE
6	1-M	44	THR
6	1-M	51	PHE
6	1-M	71	GLN
6	1-M	80	HIS
6	1-M	118	ASN
6	1-M	149	ARG
3	1-N	36	PRO
3	1-N	68	GLU
3	1-N	109	LEU
3	1-N	111	HIS
3	1-N	113	MET
3	1-N	254	PRO
3	1-N	255	SER
3	1-N	329	HIS
3	1-N	348	ASP
3	1-N	367	ASN
3	1-N	385	VAL
3	1-N	386	SER
3	1-N	466	SER
3	1-N	480	TYR
3	1-N	484	LYS
3	1-N	500	GLU
3	1-N	501	ILE
3	1-N	502	PRO
3	1-N	503	ILE
3	1-N	505	GLU
3	1-N	521	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1-N	522	THR
3	1-N	547	PRO
4	1-H	27	GLU
4	1-H	89	LEU
4	1-H	200	PRO
4	1-H	228	HIS
4	1-H	270	GLY
4	1-H	273	ARG
4	1-H	325	ALA
4	1-H	326	ASN
4	1-H	328	LYS
4	1-H	329	ALA
4	1-H	332	ASP
4	1-H	350	SER
4	1-H	363	ASN
4	1-H	365	ARG
4	1-H	400	SER
4	1-H	410	SER
4	1-H	411	ILE
4	1-H	424	PHE
4	1-H	451	ASP
4	1-H	462	GLU
4	1-H	475	GLU
4	1-H	484	SER
4	1-H	502	HIS
4	1-H	614	PRO
4	1-H	615	LYS
4	1-H	638	SER
5	1-I	12	ALA
5	1-I	44	LYS
5	1-I	73	ASN
5	1-I	96	ALA
6	1-J	97	ARG
6	1-J	117	ARG
6	1-J	131	PRO
1	2-A	63	GLN
1	2-A	64	PRO
1	2-A	92	HIS
1	2-A	106	PRO
1	2-A	169	LYS
1	2-A	174	PRO
1	2-A	187	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-A	215	PRO
1	2-A	237	SER
1	2-A	250	ASN
1	2-A	252	VAL
1	2-A	271	LYS
1	2-A	278	MET
1	2-A	281	ARG
1	2-A	324	PRO
1	2-A	325	ALA
1	2-A	341	LEU
1	2-A	343	GLN
1	2-A	384	SER
1	2-A	454	ASP
1	2-A	457	PHE
1	2-A	466	LEU
1	2-A	479	GLN
1	2-A	492	LYS
1	2-A	566	LEU
1	2-A	583	ARG
1	2-A	584	GLU
1	2-A	592	ILE
1	2-A	593	ASP
1	2-A	619	LYS
1	2-A	642	VAL
1	2-A	671	LYS
1	2-A	728	ASP
1	2-A	779	ASP
1	2-A	788	ILE
1	2-A	796	GLN
1	2-A	797	PRO
1	2-A	798	PRO
1	2-A	803	PRO
1	2-A	805	ASP
1	2-A	811	LEU
1	2-A	949	VAL
1	2-A	999	VAL
2	2-E	111	SER
2	2-E	231	ARG
3	2-B	36	PRO
3	2-B	68	GLU
3	2-B	109	LEU
3	2-B	111	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2-B	113	MET
3	2-B	254	PRO
3	2-B	255	SER
3	2-B	329	HIS
3	2-B	348	ASP
3	2-B	367	ASN
3	2-B	385	VAL
3	2-B	386	SER
3	2-B	466	SER
3	2-B	480	TYR
3	2-B	484	LYS
3	2-B	500	GLU
3	2-B	501	ILE
3	2-B	502	PRO
3	2-B	503	ILE
3	2-B	505	GLU
3	2-B	521	ILE
3	2-B	522	THR
3	2-B	547	PRO
3	2-B	767	THR
3	2-B	771	CYS
3	2-B	826	ALA
3	2-B	831	CYS
3	2-B	865	GLU
3	2-B	899	LEU
3	2-B	929	PRO
3	2-B	930	VAL
3	2-B	934	PRO
3	2-B	935	ASP
3	2-B	938	VAL
4	2-C	27	GLU
4	2-C	89	LEU
4	2-C	200	PRO
4	2-C	228	HIS
4	2-C	270	GLY
4	2-C	273	ARG
4	2-C	325	ALA
4	2-C	326	ASN
4	2-C	328	LYS
4	2-C	329	ALA
4	2-C	332	ASP
4	2-C	350	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2-C	363	ASN
4	2-C	365	ARG
4	2-C	400	SER
4	2-C	410	SER
4	2-C	411	ILE
4	2-C	424	PHE
4	2-C	451	ASP
4	2-C	462	GLU
4	2-C	475	GLU
4	2-C	484	SER
4	2-C	502	HIS
4	2-C	614	PRO
4	2-C	615	LYS
4	2-C	638	SER
4	2-C	762	LEU
4	2-C	781	ASN
4	2-C	782	GLN
4	2-C	789	ALA
4	2-C	790	ASP
4	2-C	806	VAL
4	2-C	825	PRO
4	2-C	833	ARG
5	2-D	12	ALA
5	2-D	44	LYS
5	2-D	73	ASN
5	2-D	96	ALA
6	2-F	97	ARG
6	2-F	117	ARG
6	2-F	131	PRO
7	2-G	77	PHE
7	2-G	100	GLU
7	2-G	106	THR
7	2-G	132	THR
7	2-G	151	LYS
7	2-G	171	PHE
7	2-G	243	GLU
7	2-G	261	ASN
7	2-G	275	VAL
7	2-G	277	LEU
7	2-G	283	LYS
7	2-G	299	PRO
7	2-G	373	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	2-G	394	HIS
7	2-G	446	CYS
7	2-G	484	HIS
7	2-G	608	THR
7	2-G	621	PRO
7	2-G	686	ALA
7	2-G	741	GLU
6	2-R	42	VAL
6	2-R	43	ILE
6	2-R	130	LEU
6	2-R	131	PRO
6	2-R	145	LEU
6	2-R	147	SER
6	2-R	151	ARG
6	2-R	175	ASN
8	2-Z	36	PRO
8	2-Z	37	SER
8	2-Z	84	TYR
7	2-K	134	SER
7	2-K	135	THR
7	2-K	170	SER
7	2-K	171	PHE
7	2-K	207	ASP
7	2-K	221	HIS
7	2-K	225	SER
7	2-K	226	PRO
7	2-K	227	PHE
7	2-K	243	GLU
7	2-K	275	VAL
7	2-K	299	PRO
7	2-K	608	THR
7	2-K	621	PRO
7	2-K	741	GLU
7	2-K	813	CYS
8	2-L	37	SER
8	2-L	84	TYR
8	2-L	147	ALA
6	2-M	42	VAL
6	2-M	43	ILE
6	2-M	44	THR
6	2-M	51	PHE
6	2-M	71	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2-M	80	HIS
6	2-M	118	ASN
6	2-M	149	ARG
3	2-N	36	PRO
3	2-N	68	GLU
3	2-N	109	LEU
3	2-N	111	HIS
3	2-N	113	MET
3	2-N	254	PRO
3	2-N	255	SER
3	2-N	329	HIS
3	2-N	348	ASP
3	2-N	367	ASN
3	2-N	385	VAL
3	2-N	386	SER
3	2-N	466	SER
3	2-N	480	TYR
3	2-N	484	LYS
3	2-N	500	GLU
3	2-N	501	ILE
3	2-N	502	PRO
3	2-N	503	ILE
3	2-N	505	GLU
3	2-N	521	ILE
3	2-N	522	THR
3	2-N	547	PRO
4	2-H	27	GLU
4	2-H	89	LEU
4	2-H	200	PRO
4	2-H	228	HIS
4	2-H	270	GLY
4	2-H	273	ARG
4	2-H	325	ALA
4	2-H	326	ASN
4	2-H	328	LYS
4	2-H	329	ALA
4	2-H	332	ASP
4	2-H	350	SER
4	2-H	363	ASN
4	2-H	365	ARG
4	2-H	400	SER
4	2-H	410	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2-H	411	ILE
4	2-H	424	PHE
4	2-H	451	ASP
4	2-H	462	GLU
4	2-H	475	GLU
4	2-H	484	SER
4	2-H	502	HIS
4	2-H	614	PRO
4	2-H	615	LYS
4	2-H	638	SER
5	2-I	12	ALA
5	2-I	44	LYS
5	2-I	73	ASN
5	2-I	96	ALA
6	2-J	97	ARG
6	2-J	117	ARG
6	2-J	131	PRO
1	3-A	63	GLN
1	3-A	64	PRO
1	3-A	92	HIS
1	3-A	106	PRO
1	3-A	125	ARG
1	3-A	169	LYS
1	3-A	174	PRO
1	3-A	187	VAL
1	3-A	215	PRO
1	3-A	237	SER
1	3-A	250	ASN
1	3-A	252	VAL
1	3-A	271	LYS
1	3-A	278	MET
1	3-A	281	ARG
1	3-A	324	PRO
1	3-A	325	ALA
1	3-A	341	LEU
1	3-A	343	GLN
1	3-A	384	SER
1	3-A	454	ASP
1	3-A	457	PHE
1	3-A	466	LEU
1	3-A	479	GLN
1	3-A	492	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-A	566	LEU
1	3-A	583	ARG
1	3-A	584	GLU
1	3-A	592	ILE
1	3-A	593	ASP
1	3-A	619	LYS
1	3-A	642	VAL
1	3-A	671	LYS
1	3-A	728	ASP
1	3-A	779	ASP
1	3-A	788	ILE
1	3-A	796	GLN
1	3-A	797	PRO
1	3-A	798	PRO
1	3-A	803	PRO
1	3-A	805	ASP
1	3-A	811	LEU
1	3-A	949	VAL
1	3-A	999	VAL
2	3-E	111	SER
2	3-E	231	ARG
3	3-B	36	PRO
3	3-B	68	GLU
3	3-B	109	LEU
3	3-B	111	HIS
3	3-B	113	MET
3	3-B	254	PRO
3	3-B	255	SER
3	3-B	329	HIS
3	3-B	348	ASP
3	3-B	367	ASN
3	3-B	385	VAL
3	3-B	386	SER
3	3-B	466	SER
3	3-B	480	TYR
3	3-B	484	LYS
3	3-B	500	GLU
3	3-B	501	ILE
3	3-B	502	PRO
3	3-B	503	ILE
3	3-B	505	GLU
3	3-B	521	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3-B	522	THR
3	3-B	547	PRO
3	3-B	767	THR
3	3-B	771	CYS
3	3-B	826	ALA
3	3-B	831	CYS
3	3-B	865	GLU
3	3-B	899	LEU
3	3-B	929	PRO
3	3-B	930	VAL
3	3-B	934	PRO
3	3-B	935	ASP
3	3-B	938	VAL
4	3-C	27	GLU
4	3-C	89	LEU
4	3-C	200	PRO
4	3-C	228	HIS
4	3-C	270	GLY
4	3-C	273	ARG
4	3-C	325	ALA
4	3-C	326	ASN
4	3-C	328	LYS
4	3-C	329	ALA
4	3-C	332	ASP
4	3-C	350	SER
4	3-C	363	ASN
4	3-C	365	ARG
4	3-C	400	SER
4	3-C	410	SER
4	3-C	411	ILE
4	3-C	424	PHE
4	3-C	451	ASP
4	3-C	462	GLU
4	3-C	475	GLU
4	3-C	484	SER
4	3-C	502	HIS
4	3-C	614	PRO
4	3-C	615	LYS
4	3-C	638	SER
4	3-C	762	LEU
4	3-C	781	ASN
4	3-C	782	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	3-C	789	ALA
4	3-C	790	ASP
4	3-C	806	VAL
4	3-C	825	PRO
4	3-C	833	ARG
5	3-D	12	ALA
5	3-D	44	LYS
5	3-D	73	ASN
5	3-D	96	ALA
6	3-F	97	ARG
6	3-F	117	ARG
6	3-F	131	PRO
7	3-G	77	PHE
7	3-G	100	GLU
7	3-G	106	THR
7	3-G	132	THR
7	3-G	151	LYS
7	3-G	171	PHE
7	3-G	243	GLU
7	3-G	261	ASN
7	3-G	275	VAL
7	3-G	277	LEU
7	3-G	283	LYS
7	3-G	299	PRO
7	3-G	373	ASP
7	3-G	394	HIS
7	3-G	446	CYS
7	3-G	484	HIS
7	3-G	608	THR
7	3-G	621	PRO
7	3-G	686	ALA
7	3-G	741	GLU
6	3-R	42	VAL
6	3-R	43	ILE
6	3-R	130	LEU
6	3-R	131	PRO
6	3-R	145	LEU
6	3-R	147	SER
6	3-R	151	ARG
6	3-R	175	ASN
8	3-Z	36	PRO
8	3-Z	37	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	3-Z	84	TYR
7	3-K	134	SER
7	3-K	135	THR
7	3-K	170	SER
7	3-K	171	PHE
7	3-K	207	ASP
7	3-K	221	HIS
7	3-K	225	SER
7	3-K	226	PRO
7	3-K	227	PHE
7	3-K	243	GLU
7	3-K	275	VAL
7	3-K	299	PRO
7	3-K	608	THR
7	3-K	621	PRO
7	3-K	686	ALA
7	3-K	741	GLU
7	3-K	813	CYS
8	3-L	37	SER
8	3-L	84	TYR
8	3-L	147	ALA
6	3-M	42	VAL
6	3-M	43	ILE
6	3-M	44	THR
6	3-M	51	PHE
6	3-M	71	GLN
6	3-M	80	HIS
6	3-M	118	ASN
6	3-M	149	ARG
3	3-N	36	PRO
3	3-N	68	GLU
3	3-N	109	LEU
3	3-N	111	HIS
3	3-N	113	MET
3	3-N	254	PRO
3	3-N	255	SER
3	3-N	329	HIS
3	3-N	348	ASP
3	3-N	367	ASN
3	3-N	385	VAL
3	3-N	386	SER
3	3-N	466	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3-N	480	TYR
3	3-N	484	LYS
3	3-N	500	GLU
3	3-N	501	ILE
3	3-N	502	PRO
3	3-N	503	ILE
3	3-N	505	GLU
3	3-N	521	ILE
3	3-N	522	THR
3	3-N	547	PRO
4	3-H	27	GLU
4	3-H	89	LEU
4	3-H	200	PRO
4	3-H	228	HIS
4	3-H	270	GLY
4	3-H	273	ARG
4	3-H	325	ALA
4	3-H	326	ASN
4	3-H	328	LYS
4	3-H	329	ALA
4	3-H	332	ASP
4	3-H	350	SER
4	3-H	363	ASN
4	3-H	365	ARG
4	3-H	400	SER
4	3-H	410	SER
4	3-H	411	ILE
4	3-H	424	PHE
4	3-H	451	ASP
4	3-H	462	GLU
4	3-H	475	GLU
4	3-H	484	SER
4	3-H	502	HIS
4	3-H	614	PRO
4	3-H	615	LYS
4	3-H	638	SER
5	3-I	12	ALA
5	3-I	44	LYS
5	3-I	73	ASN
5	3-I	96	ALA
6	3-J	97	ARG
6	3-J	117	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	3-J	131	PRO
1	1-A	10	ALA
1	1-A	185	THR
1	1-A	282	THR
1	1-A	290	ASP
1	1-A	345	ASP
1	1-A	373	ALA
1	1-A	425	ARG
1	1-A	498	ALA
1	1-A	546	SER
1	1-A	564	LEU
1	1-A	572	ARG
1	1-A	622	GLY
1	1-A	624	SER
1	1-A	632	LYS
1	1-A	672	ASN
1	1-A	787	ASP
1	1-A	800	PRO
1	1-A	1178	ARG
3	1-B	49	ASP
3	1-B	69	LYS
3	1-B	162	ARG
3	1-B	186	PRO
3	1-B	383	ASN
3	1-B	445	ARG
3	1-B	498	LEU
3	1-B	499	GLY
3	1-B	551	GLU
3	1-B	740	PRO
3	1-B	741	VAL
3	1-B	751	GLN
3	1-B	764	THR
3	1-B	828	ASP
3	1-B	838	HIS
3	1-B	862	PHE
3	1-B	873	ASN
3	1-B	939	THR
4	1-C	88	THR
4	1-C	219	LYS
4	1-C	428	PHE
4	1-C	465	PRO
4	1-C	503	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	1-C	504	GLY
4	1-C	558	ASP
4	1-C	665	GLU
4	1-C	787	SER
4	1-C	793	GLU
4	1-C	797	LEU
5	1-D	24	MET
5	1-D	25	THR
5	1-D	42	THR
5	1-D	98	GLU
5	1-D	136	MET
7	1-G	96	SER
7	1-G	98	ILE
7	1-G	105	VAL
7	1-G	116	LYS
7	1-G	216	SER
7	1-G	278	PRO
7	1-G	310	THR
7	1-G	463	GLY
7	1-G	467	ASN
7	1-G	522	ASN
7	1-G	633	SER
7	1-G	718	THR
6	1-R	72	ASP
6	1-R	82	TYR
6	1-R	84	ASN
6	1-R	95	ASN
6	1-R	132	GLU
6	1-R	133	ALA
8	1-Z	73	ILE
7	1-K	38	PRO
7	1-K	116	LYS
7	1-K	245	GLY
7	1-K	297	SER
7	1-K	633	SER
7	1-K	718	THR
8	1-L	12	THR
8	1-L	69	TYR
8	1-L	132	GLY
6	1-M	70	GLY
6	1-M	129	ASP
6	1-M	164	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1-N	49	ASP
3	1-N	69	LYS
3	1-N	162	ARG
3	1-N	186	PRO
3	1-N	383	ASN
3	1-N	445	ARG
3	1-N	498	LEU
3	1-N	499	GLY
3	1-N	551	GLU
4	1-H	88	THR
4	1-H	219	LYS
4	1-H	428	PHE
4	1-H	465	PRO
4	1-H	503	GLU
4	1-H	504	GLY
4	1-H	558	ASP
4	1-H	665	GLU
5	1-I	24	MET
5	1-I	25	THR
5	1-I	42	THR
5	1-I	98	GLU
5	1-I	136	MET
1	2-A	10	ALA
1	2-A	125	ARG
1	2-A	185	THR
1	2-A	282	THR
1	2-A	290	ASP
1	2-A	345	ASP
1	2-A	373	ALA
1	2-A	425	ARG
1	2-A	498	ALA
1	2-A	546	SER
1	2-A	564	LEU
1	2-A	572	ARG
1	2-A	622	GLY
1	2-A	624	SER
1	2-A	632	LYS
1	2-A	672	ASN
1	2-A	787	ASP
1	2-A	800	PRO
1	2-A	1178	ARG
3	2-B	49	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2-B	69	LYS
3	2-B	162	ARG
3	2-B	186	PRO
3	2-B	383	ASN
3	2-B	445	ARG
3	2-B	498	LEU
3	2-B	499	GLY
3	2-B	551	GLU
3	2-B	740	PRO
3	2-B	741	VAL
3	2-B	764	THR
3	2-B	828	ASP
3	2-B	838	HIS
3	2-B	862	PHE
3	2-B	873	ASN
3	2-B	939	THR
4	2-C	88	THR
4	2-C	219	LYS
4	2-C	428	PHE
4	2-C	465	PRO
4	2-C	503	GLU
4	2-C	504	GLY
4	2-C	558	ASP
4	2-C	665	GLU
4	2-C	787	SER
4	2-C	793	GLU
4	2-C	797	LEU
5	2-D	24	MET
5	2-D	25	THR
5	2-D	42	THR
5	2-D	98	GLU
5	2-D	136	MET
7	2-G	96	SER
7	2-G	98	ILE
7	2-G	105	VAL
7	2-G	116	LYS
7	2-G	216	SER
7	2-G	278	PRO
7	2-G	310	THR
7	2-G	463	GLY
7	2-G	467	ASN
7	2-G	522	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	2-G	633	SER
7	2-G	718	THR
6	2-R	72	ASP
6	2-R	82	TYR
6	2-R	84	ASN
6	2-R	95	ASN
6	2-R	132	GLU
6	2-R	133	ALA
8	2-Z	73	ILE
7	2-K	38	PRO
7	2-K	116	LYS
7	2-K	245	GLY
7	2-K	297	SER
7	2-K	633	SER
7	2-K	686	ALA
7	2-K	718	THR
8	2-L	12	THR
8	2-L	69	TYR
8	2-L	132	GLY
6	2-M	70	GLY
6	2-M	129	ASP
6	2-M	164	GLU
3	2-N	49	ASP
3	2-N	69	LYS
3	2-N	162	ARG
3	2-N	186	PRO
3	2-N	383	ASN
3	2-N	445	ARG
3	2-N	498	LEU
3	2-N	499	GLY
3	2-N	551	GLU
4	2-H	88	THR
4	2-H	219	LYS
4	2-H	428	PHE
4	2-H	465	PRO
4	2-H	503	GLU
4	2-H	504	GLY
4	2-H	558	ASP
4	2-H	665	GLU
5	2-I	24	MET
5	2-I	25	THR
5	2-I	42	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	2-I	98	GLU
5	2-I	136	MET
1	3-A	10	ALA
1	3-A	185	THR
1	3-A	282	THR
1	3-A	290	ASP
1	3-A	345	ASP
1	3-A	373	ALA
1	3-A	425	ARG
1	3-A	498	ALA
1	3-A	546	SER
1	3-A	564	LEU
1	3-A	572	ARG
1	3-A	622	GLY
1	3-A	624	SER
1	3-A	632	LYS
1	3-A	672	ASN
1	3-A	787	ASP
1	3-A	800	PRO
1	3-A	1178	ARG
3	3-B	49	ASP
3	3-B	69	LYS
3	3-B	162	ARG
3	3-B	186	PRO
3	3-B	383	ASN
3	3-B	445	ARG
3	3-B	498	LEU
3	3-B	499	GLY
3	3-B	551	GLU
3	3-B	740	PRO
3	3-B	741	VAL
3	3-B	751	GLN
3	3-B	764	THR
3	3-B	828	ASP
3	3-B	838	HIS
3	3-B	862	PHE
3	3-B	873	ASN
3	3-B	939	THR
4	3-C	88	THR
4	3-C	219	LYS
4	3-C	428	PHE
4	3-C	465	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	3-C	503	GLU
4	3-C	504	GLY
4	3-C	558	ASP
4	3-C	665	GLU
4	3-C	787	SER
4	3-C	793	GLU
4	3-C	797	LEU
5	3-D	24	MET
5	3-D	25	THR
5	3-D	42	THR
5	3-D	98	GLU
5	3-D	136	MET
7	3-G	96	SER
7	3-G	98	ILE
7	3-G	105	VAL
7	3-G	116	LYS
7	3-G	216	SER
7	3-G	278	PRO
7	3-G	310	THR
7	3-G	463	GLY
7	3-G	467	ASN
7	3-G	522	ASN
7	3-G	633	SER
7	3-G	718	THR
6	3-R	72	ASP
6	3-R	82	TYR
6	3-R	84	ASN
6	3-R	95	ASN
6	3-R	132	GLU
6	3-R	133	ALA
8	3-Z	73	ILE
7	3-K	38	PRO
7	3-K	116	LYS
7	3-K	245	GLY
7	3-K	297	SER
7	3-K	633	SER
7	3-K	718	THR
8	3-L	12	THR
8	3-L	69	TYR
8	3-L	132	GLY
6	3-M	70	GLY
6	3-M	129	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	3-M	164	GLU
3	3-N	49	ASP
3	3-N	69	LYS
3	3-N	162	ARG
3	3-N	186	PRO
3	3-N	383	ASN
3	3-N	445	ARG
3	3-N	498	LEU
3	3-N	499	GLY
3	3-N	551	GLU
4	3-H	88	THR
4	3-H	219	LYS
4	3-H	428	PHE
4	3-H	465	PRO
4	3-H	503	GLU
4	3-H	504	GLY
4	3-H	558	ASP
4	3-H	665	GLU
5	3-I	24	MET
5	3-I	25	THR
5	3-I	42	THR
5	3-I	98	GLU
5	3-I	136	MET
1	1-A	61	LYS
1	1-A	62	GLN
1	1-A	168	ARG
1	1-A	176	ALA
1	1-A	183	GLY
1	1-A	218	PRO
1	1-A	251	ASN
1	1-A	323	ARG
1	1-A	340	PHE
1	1-A	349	SER
1	1-A	362	LYS
1	1-A	411	LYS
1	1-A	433	HIS
1	1-A	481	ARG
1	1-A	527	ASN
1	1-A	555	THR
1	1-A	585	CYS
1	1-A	686	ASN
1	1-A	731	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-A	755	LYS
3	1-B	216	ASP
3	1-B	779	GLY
3	1-B	871	ASN
4	1-C	140	GLY
4	1-C	156	ASN
4	1-C	250	ASP
4	1-C	259	SER
4	1-C	351	CYS
4	1-C	408	SER
4	1-C	454	ASN
4	1-C	708	ASN
4	1-C	763	PRO
5	1-D	46	HIS
5	1-D	138	SER
6	1-F	47	PRO
6	1-F	84	ASN
6	1-F	149	ARG
7	1-G	170	SER
7	1-G	282	ALA
7	1-G	297	SER
7	1-G	391	PRO
7	1-G	393	LYS
7	1-G	445	ASP
7	1-G	447	GLU
7	1-G	504	GLU
7	1-G	505	MET
7	1-G	628	PRO
7	1-G	641	GLU
7	1-G	687	TYR
7	1-G	720	VAL
7	1-G	761	ALA
6	1-R	114	ASP
8	1-Z	147	ALA
7	1-K	96	SER
7	1-K	248	ASP
7	1-K	628	PRO
7	1-K	641	GLU
7	1-K	687	TYR
7	1-K	720	VAL
7	1-K	761	ALA
8	1-L	36	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	1-M	127	LYS
6	1-M	135	SER
6	1-M	165	GLY
3	1-N	216	ASP
4	1-H	140	GLY
4	1-H	156	ASN
4	1-H	250	ASP
4	1-H	259	SER
4	1-H	351	CYS
4	1-H	408	SER
4	1-H	454	ASN
4	1-H	708	ASN
5	1-I	46	HIS
5	1-I	138	SER
6	1-J	47	PRO
6	1-J	84	ASN
6	1-J	149	ARG
1	2-A	61	LYS
1	2-A	62	GLN
1	2-A	168	ARG
1	2-A	176	ALA
1	2-A	183	GLY
1	2-A	218	PRO
1	2-A	251	ASN
1	2-A	323	ARG
1	2-A	340	PHE
1	2-A	349	SER
1	2-A	362	LYS
1	2-A	411	LYS
1	2-A	433	HIS
1	2-A	481	ARG
1	2-A	527	ASN
1	2-A	555	THR
1	2-A	585	CYS
1	2-A	686	ASN
1	2-A	731	GLY
1	2-A	755	LYS
3	2-B	216	ASP
3	2-B	751	GLN
3	2-B	779	GLY
3	2-B	871	ASN
4	2-C	140	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2-C	156	ASN
4	2-C	250	ASP
4	2-C	259	SER
4	2-C	351	CYS
4	2-C	408	SER
4	2-C	454	ASN
4	2-C	708	ASN
4	2-C	763	PRO
5	2-D	46	HIS
5	2-D	138	SER
6	2-F	47	PRO
6	2-F	84	ASN
6	2-F	149	ARG
7	2-G	170	SER
7	2-G	282	ALA
7	2-G	297	SER
7	2-G	391	PRO
7	2-G	393	LYS
7	2-G	445	ASP
7	2-G	447	GLU
7	2-G	504	GLU
7	2-G	505	MET
7	2-G	628	PRO
7	2-G	641	GLU
7	2-G	687	TYR
7	2-G	720	VAL
7	2-G	761	ALA
6	2-R	114	ASP
8	2-Z	147	ALA
7	2-K	96	SER
7	2-K	248	ASP
7	2-K	628	PRO
7	2-K	641	GLU
7	2-K	687	TYR
7	2-K	720	VAL
7	2-K	761	ALA
8	2-L	36	PRO
6	2-M	127	LYS
6	2-M	135	SER
6	2-M	165	GLY
3	2-N	216	ASP
4	2-H	140	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2-H	156	ASN
4	2-H	250	ASP
4	2-H	259	SER
4	2-H	351	CYS
4	2-H	408	SER
4	2-H	454	ASN
4	2-H	708	ASN
5	2-I	46	HIS
5	2-I	138	SER
6	2-J	47	PRO
6	2-J	84	ASN
6	2-J	149	ARG
1	3-A	61	LYS
1	3-A	62	GLN
1	3-A	168	ARG
1	3-A	176	ALA
1	3-A	183	GLY
1	3-A	218	PRO
1	3-A	251	ASN
1	3-A	323	ARG
1	3-A	340	PHE
1	3-A	349	SER
1	3-A	362	LYS
1	3-A	411	LYS
1	3-A	433	HIS
1	3-A	481	ARG
1	3-A	527	ASN
1	3-A	555	THR
1	3-A	585	CYS
1	3-A	686	ASN
1	3-A	731	GLY
1	3-A	755	LYS
3	3-B	216	ASP
3	3-B	779	GLY
3	3-B	871	ASN
4	3-C	140	GLY
4	3-C	156	ASN
4	3-C	250	ASP
4	3-C	259	SER
4	3-C	351	CYS
4	3-C	408	SER
4	3-C	454	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	3-C	708	ASN
4	3-C	763	PRO
5	3-D	46	HIS
5	3-D	138	SER
6	3-F	47	PRO
6	3-F	84	ASN
6	3-F	149	ARG
7	3-G	170	SER
7	3-G	282	ALA
7	3-G	297	SER
7	3-G	391	PRO
7	3-G	393	LYS
7	3-G	445	ASP
7	3-G	447	GLU
7	3-G	504	GLU
7	3-G	505	MET
7	3-G	628	PRO
7	3-G	641	GLU
7	3-G	687	TYR
7	3-G	720	VAL
7	3-G	761	ALA
6	3-R	114	ASP
8	3-Z	147	ALA
7	3-K	96	SER
7	3-K	248	ASP
7	3-K	628	PRO
7	3-K	641	GLU
7	3-K	687	TYR
7	3-K	720	VAL
7	3-K	761	ALA
8	3-L	36	PRO
6	3-M	127	LYS
6	3-M	135	SER
6	3-M	165	GLY
3	3-N	216	ASP
4	3-H	140	GLY
4	3-H	156	ASN
4	3-H	250	ASP
4	3-H	259	SER
4	3-H	351	CYS
4	3-H	408	SER
4	3-H	454	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	3-H	708	ASN
5	3-I	46	HIS
5	3-I	138	SER
6	3-J	47	PRO
6	3-J	84	ASN
6	3-J	149	ARG
1	1-A	73	TYR
1	1-A	103	HIS
1	1-A	170	LYS
1	1-A	205	ASP
1	1-A	236	GLU
1	1-A	330	GLY
1	1-A	398	LYS
1	1-A	424	ASN
1	1-A	488	ILE
1	1-A	556	GLY
1	1-A	783	GLU
1	1-A	786	PRO
1	1-A	801	ILE
2	1-E	113	ASP
3	1-B	128	ASN
3	1-B	384	ASN
3	1-B	425	SER
3	1-B	447	ASP
3	1-B	481	CYS
3	1-B	504	VAL
3	1-B	752	TYR
3	1-B	768	LEU
3	1-B	780	ASP
3	1-B	827	SER
3	1-B	837	ILE
3	1-B	901	GLY
3	1-B	928	LYS
4	1-C	165	ARG
4	1-C	321	GLU
4	1-C	346	LYS
4	1-C	401	SER
4	1-C	409	ASN
4	1-C	431	GLU
4	1-C	662	VAL
4	1-C	821	ALA
6	1-F	153	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	1-G	23	GLU
7	1-G	428	ASN
7	1-G	623	PHE
6	1-R	44	THR
6	1-R	129	ASP
6	1-R	158	THR
8	1-Z	34	THR
7	1-K	76	LEU
7	1-K	623	PHE
8	1-L	86	ASN
6	1-M	119	ALA
6	1-M	133	ALA
3	1-N	128	ASN
3	1-N	384	ASN
3	1-N	425	SER
3	1-N	447	ASP
3	1-N	481	CYS
3	1-N	504	VAL
4	1-H	165	ARG
4	1-H	321	GLU
4	1-H	346	LYS
4	1-H	401	SER
4	1-H	409	ASN
4	1-H	431	GLU
4	1-H	662	VAL
6	1-J	153	TRP
1	2-A	73	TYR
1	2-A	103	HIS
1	2-A	170	LYS
1	2-A	205	ASP
1	2-A	236	GLU
1	2-A	330	GLY
1	2-A	398	LYS
1	2-A	424	ASN
1	2-A	488	ILE
1	2-A	556	GLY
1	2-A	783	GLU
1	2-A	786	PRO
1	2-A	801	ILE
2	2-E	113	ASP
3	2-B	128	ASN
3	2-B	384	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2-B	425	SER
3	2-B	447	ASP
3	2-B	481	CYS
3	2-B	504	VAL
3	2-B	752	TYR
3	2-B	768	LEU
3	2-B	780	ASP
3	2-B	827	SER
3	2-B	837	ILE
3	2-B	901	GLY
3	2-B	928	LYS
4	2-C	165	ARG
4	2-C	321	GLU
4	2-C	346	LYS
4	2-C	401	SER
4	2-C	409	ASN
4	2-C	431	GLU
4	2-C	662	VAL
4	2-C	821	ALA
6	2-F	153	TRP
7	2-G	23	GLU
7	2-G	226	PRO
7	2-G	428	ASN
7	2-G	623	PHE
6	2-R	44	THR
6	2-R	129	ASP
8	2-Z	34	THR
7	2-K	76	LEU
7	2-K	623	PHE
8	2-L	86	ASN
6	2-M	119	ALA
6	2-M	133	ALA
3	2-N	128	ASN
3	2-N	384	ASN
3	2-N	425	SER
3	2-N	447	ASP
3	2-N	481	CYS
3	2-N	504	VAL
4	2-H	165	ARG
4	2-H	321	GLU
4	2-H	346	LYS
4	2-H	401	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2-H	409	ASN
4	2-H	431	GLU
4	2-H	662	VAL
6	2-J	153	TRP
1	3-A	73	TYR
1	3-A	103	HIS
1	3-A	170	LYS
1	3-A	205	ASP
1	3-A	236	GLU
1	3-A	330	GLY
1	3-A	398	LYS
1	3-A	424	ASN
1	3-A	488	ILE
1	3-A	556	GLY
1	3-A	783	GLU
1	3-A	786	PRO
1	3-A	801	ILE
2	3-E	113	ASP
3	3-B	128	ASN
3	3-B	384	ASN
3	3-B	425	SER
3	3-B	447	ASP
3	3-B	481	CYS
3	3-B	504	VAL
3	3-B	752	TYR
3	3-B	768	LEU
3	3-B	780	ASP
3	3-B	837	ILE
3	3-B	901	GLY
3	3-B	928	LYS
4	3-C	165	ARG
4	3-C	321	GLU
4	3-C	346	LYS
4	3-C	401	SER
4	3-C	409	ASN
4	3-C	431	GLU
4	3-C	662	VAL
4	3-C	821	ALA
6	3-F	153	TRP
7	3-G	23	GLU
7	3-G	226	PRO
7	3-G	428	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	3-G	623	PHE
6	3-R	44	THR
6	3-R	129	ASP
6	3-R	158	THR
8	3-Z	34	THR
7	3-K	76	LEU
7	3-K	623	PHE
8	3-L	86	ASN
6	3-M	119	ALA
6	3-M	133	ALA
3	3-N	128	ASN
3	3-N	384	ASN
3	3-N	425	SER
3	3-N	447	ASP
3	3-N	481	CYS
3	3-N	504	VAL
4	3-H	165	ARG
4	3-H	321	GLU
4	3-H	346	LYS
4	3-H	401	SER
4	3-H	409	ASN
4	3-H	431	GLU
4	3-H	662	VAL
6	3-J	153	TRP
1	1-A	182	ARG
1	1-A	195	ALA
1	1-A	364	PRO
1	1-A	452	ASN
1	1-A	517	LYS
1	1-A	531	LYS
1	1-A	621	VAL
1	1-A	644	ASP
1	1-A	810	LEU
3	1-B	270	SER
3	1-B	347	PRO
3	1-B	825	ALA
4	1-C	242	PRO
4	1-C	284	ASN
4	1-C	473	SER
4	1-C	737	LYS
5	1-D	40	MET
5	1-D	43	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	1-F	78	TRP
7	1-G	99	ALA
7	1-G	226	PRO
7	1-G	248	ASP
7	1-K	40	ASN
7	1-K	81	ASP
8	1-L	63	GLU
6	1-M	151	ARG
3	1-N	270	SER
3	1-N	347	PRO
4	1-H	242	PRO
4	1-H	284	ASN
4	1-H	473	SER
5	1-I	40	MET
5	1-I	43	GLY
6	1-J	78	TRP
1	2-A	182	ARG
1	2-A	195	ALA
1	2-A	364	PRO
1	2-A	452	ASN
1	2-A	517	LYS
1	2-A	531	LYS
1	2-A	621	VAL
1	2-A	644	ASP
1	2-A	810	LEU
3	2-B	270	SER
3	2-B	347	PRO
3	2-B	825	ALA
4	2-C	242	PRO
4	2-C	284	ASN
4	2-C	473	SER
4	2-C	737	LYS
5	2-D	40	MET
5	2-D	43	GLY
6	2-F	78	TRP
7	2-G	99	ALA
7	2-G	248	ASP
6	2-R	158	THR
7	2-K	40	ASN
7	2-K	81	ASP
8	2-L	63	GLU
6	2-M	151	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2-N	270	SER
3	2-N	347	PRO
4	2-H	242	PRO
4	2-H	284	ASN
4	2-H	473	SER
5	2-I	40	MET
5	2-I	43	GLY
6	2-J	78	TRP
1	3-A	182	ARG
1	3-A	195	ALA
1	3-A	364	PRO
1	3-A	452	ASN
1	3-A	517	LYS
1	3-A	531	LYS
1	3-A	621	VAL
1	3-A	644	ASP
1	3-A	810	LEU
3	3-B	270	SER
3	3-B	347	PRO
3	3-B	825	ALA
3	3-B	827	SER
4	3-C	242	PRO
4	3-C	284	ASN
4	3-C	473	SER
4	3-C	737	LYS
5	3-D	40	MET
5	3-D	43	GLY
6	3-F	78	TRP
7	3-G	99	ALA
7	3-G	248	ASP
7	3-K	40	ASN
7	3-K	81	ASP
8	3-L	63	GLU
6	3-M	151	ARG
3	3-N	270	SER
3	3-N	347	PRO
4	3-H	242	PRO
4	3-H	284	ASN
4	3-H	473	SER
5	3-I	40	MET
5	3-I	43	GLY
6	3-J	78	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-A	643	LYS
1	1-A	802	MET
3	1-B	86	ASP
3	1-B	104	THR
4	1-C	25	PRO
7	1-G	152	VAL
6	1-R	49	ILE
8	1-Z	54	ARG
7	1-K	37	THR
7	1-K	310	THR
7	1-K	694	PRO
3	1-N	86	ASP
3	1-N	104	THR
4	1-H	25	PRO
1	2-A	643	LYS
1	2-A	802	MET
3	2-B	86	ASP
3	2-B	104	THR
4	2-C	25	PRO
7	2-G	152	VAL
6	2-R	49	ILE
8	2-Z	54	ARG
7	2-K	37	THR
7	2-K	310	THR
7	2-K	694	PRO
3	2-N	86	ASP
3	2-N	104	THR
4	2-H	25	PRO
1	3-A	643	LYS
1	3-A	802	MET
3	3-B	86	ASP
3	3-B	104	THR
4	3-C	25	PRO
7	3-G	152	VAL
6	3-R	49	ILE
8	3-Z	54	ARG
7	3-K	37	THR
7	3-K	694	PRO
3	3-N	86	ASP
3	3-N	104	THR
4	3-H	25	PRO
4	1-C	312	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	1-K	274	ILE
4	1-H	312	GLY
4	2-C	312	GLY
7	2-K	274	ILE
4	2-H	312	GLY
4	3-C	312	GLY
7	3-K	274	ILE
4	3-H	312	GLY
1	1-A	22	PRO
1	1-A	503	VAL
1	1-A	615	VAL
2	1-E	213	SER
4	1-C	112	PRO
6	1-R	163	GLY
6	1-M	148	ILE
4	1-H	112	PRO
1	2-A	22	PRO
1	2-A	503	VAL
1	2-A	615	VAL
2	2-E	213	SER
4	2-C	112	PRO
6	2-R	163	GLY
6	2-M	148	ILE
4	2-H	112	PRO
1	3-A	22	PRO
1	3-A	503	VAL
1	3-A	615	VAL
2	3-E	213	SER
4	3-C	112	PRO
6	3-R	163	GLY
6	3-M	148	ILE
4	3-H	112	PRO
1	1-A	133	GLY
1	1-A	259	PRO
6	1-F	43	ILE
7	1-G	820	PRO
7	1-K	820	PRO
6	1-J	43	ILE
1	2-A	133	GLY
1	2-A	259	PRO
6	2-F	43	ILE
7	2-G	820	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2-J	43	ILE
1	3-A	133	GLY
1	3-A	259	PRO
6	3-F	43	ILE
7	3-G	820	PRO
7	3-K	820	PRO
6	3-J	43	ILE
7	1-G	694	PRO
7	2-G	694	PRO
7	3-G	694	PRO
1	1-A	575	GLY
2	1-E	45	SER
3	1-B	516	LYS
3	1-N	516	LYS
2	2-E	45	SER
3	2-N	516	LYS
1	3-A	575	GLY
3	3-B	516	LYS
3	3-N	516	LYS

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

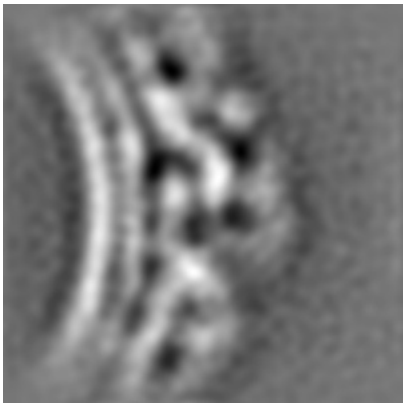
This section contains visualisations of the EMDB entry EMD-3722. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

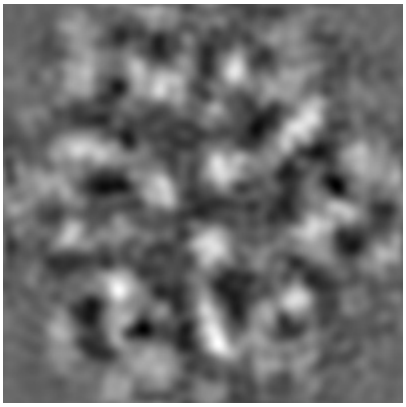
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



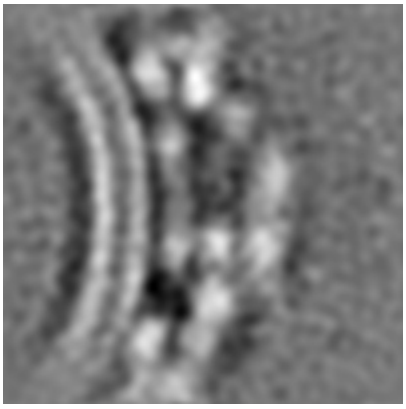
Z

The images above show the map projected in three orthogonal directions.

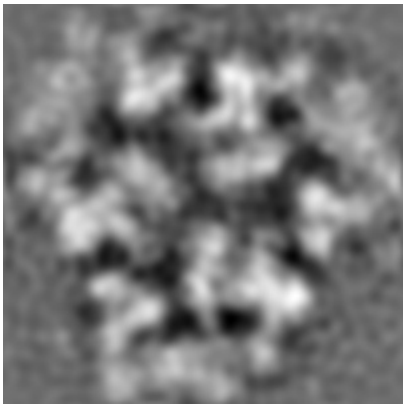
6.2 Central slices

6.2.1 Primary map

X Index: 106



Y Index: 106



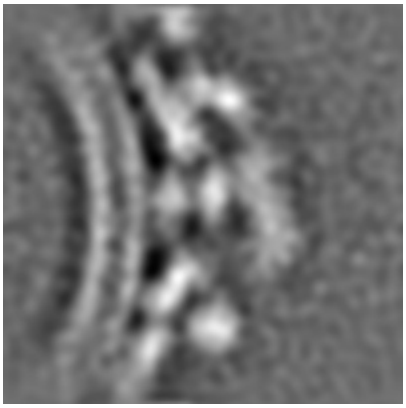
Z Index: 106

The images above show central slices of the map in three orthogonal directions.

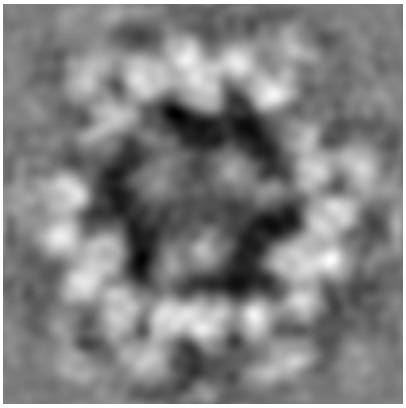
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 109



Y Index: 87

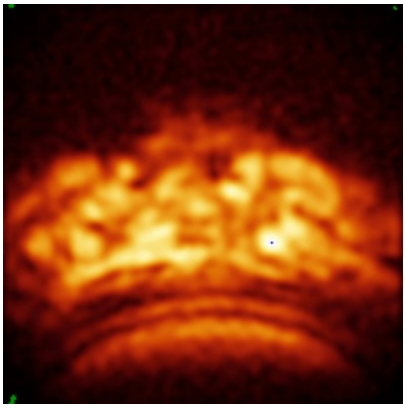


Z Index: 79

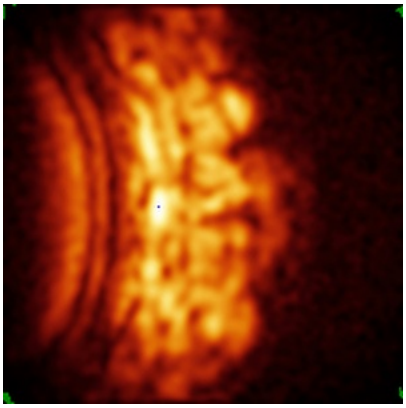
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

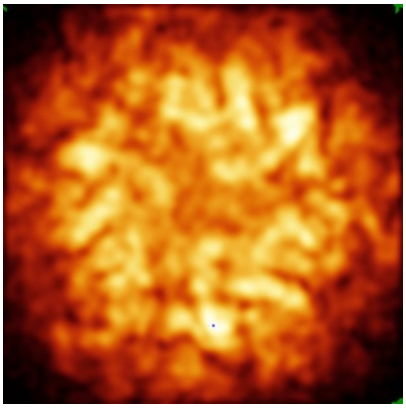
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

This section was not generated.

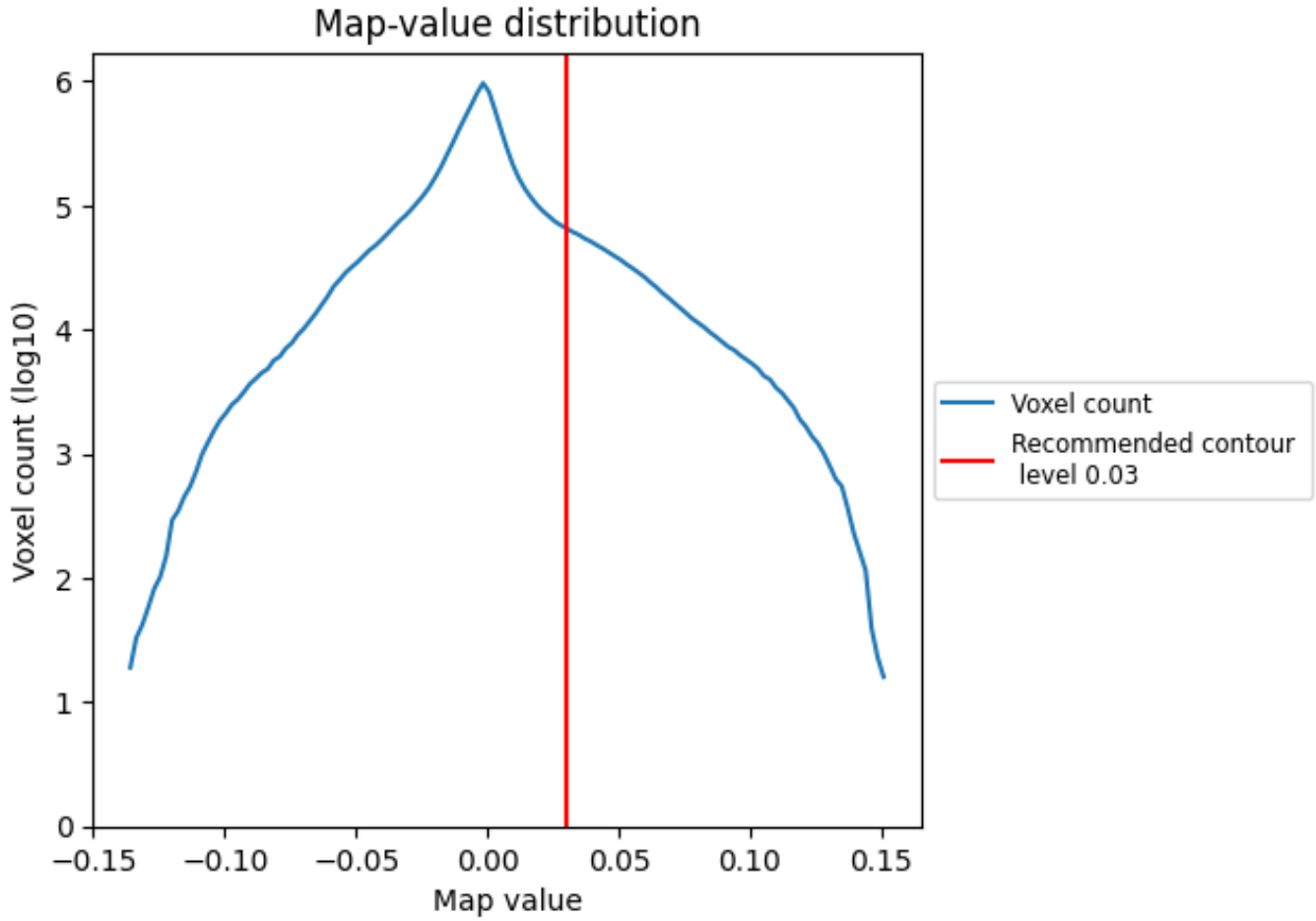
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

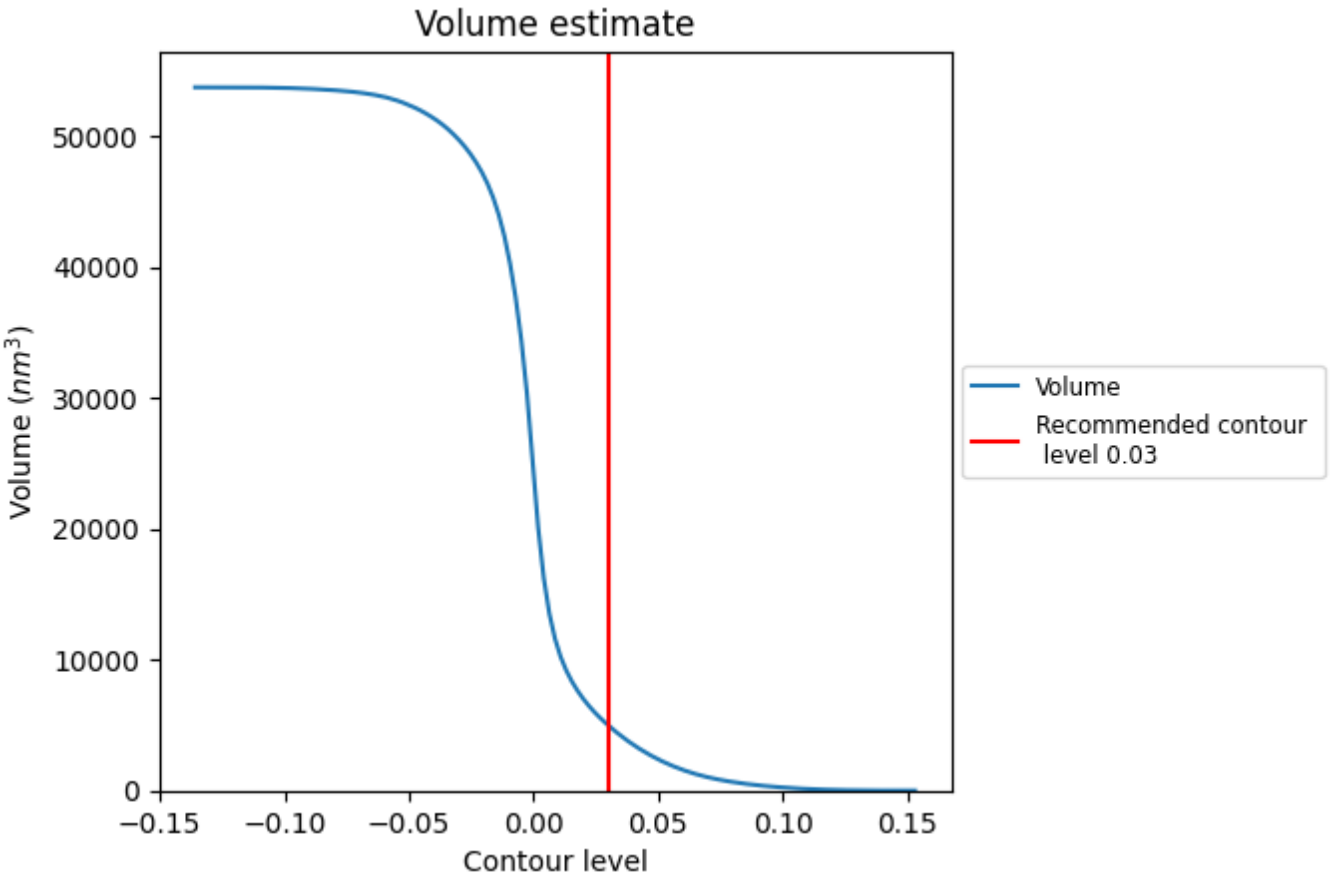
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

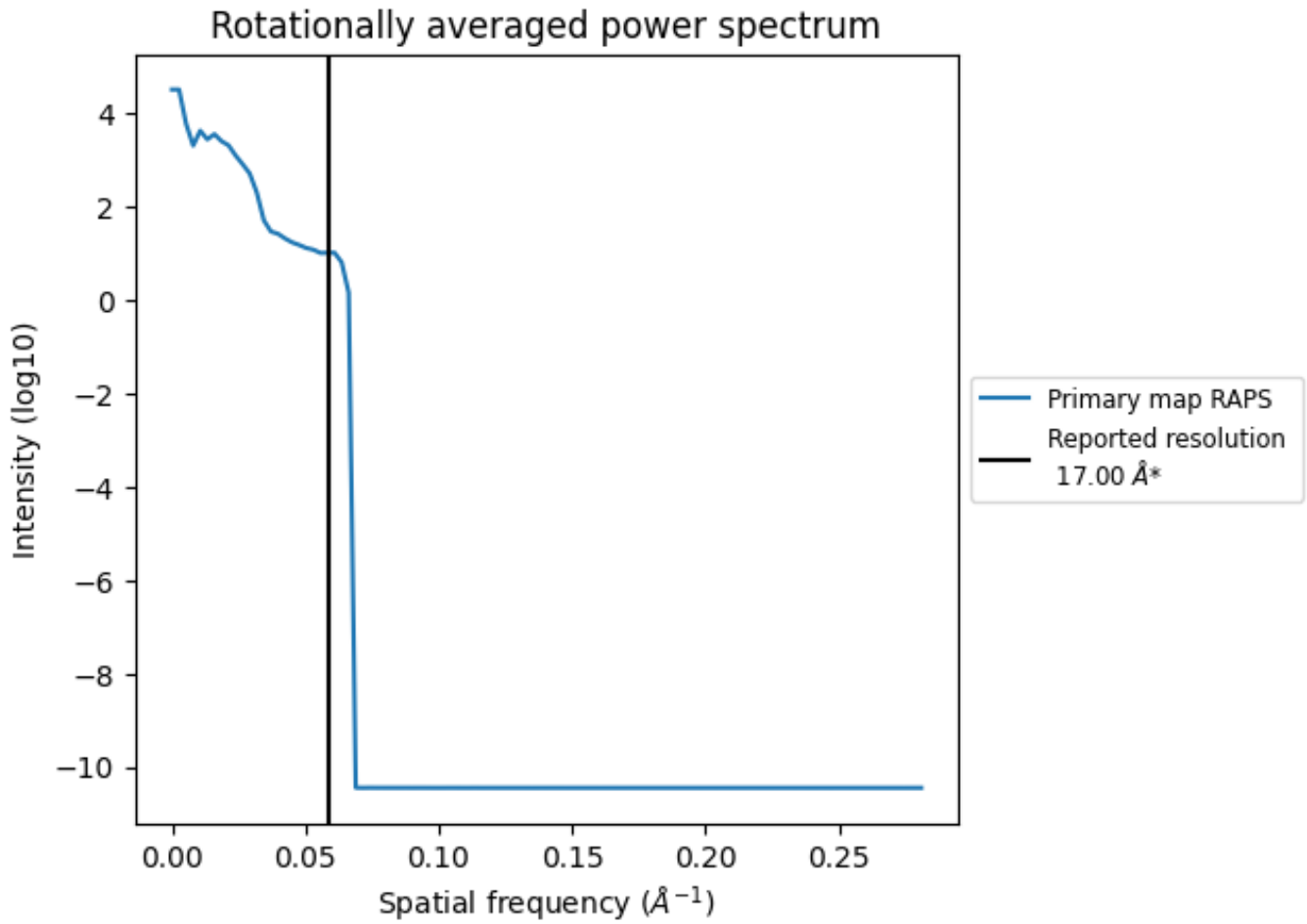
7.2 Volume estimate



The volume at the recommended contour level is 4989 nm^3; this corresponds to an approximate mass of 4507 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

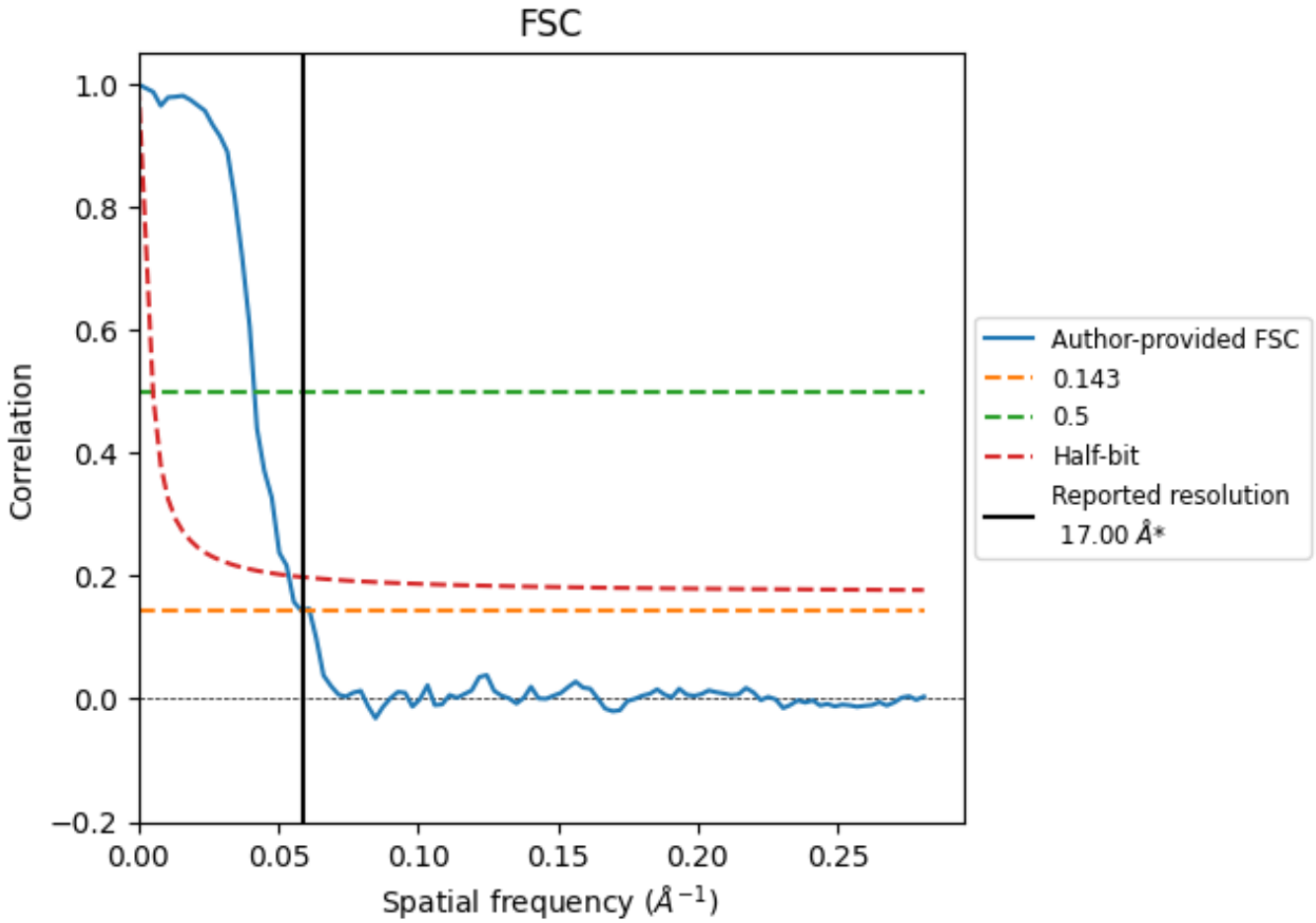


*Reported resolution corresponds to spatial frequency of 0.059 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.059 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	17.00	-	-
Author-provided FSC curve	16.34	24.15	18.62
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

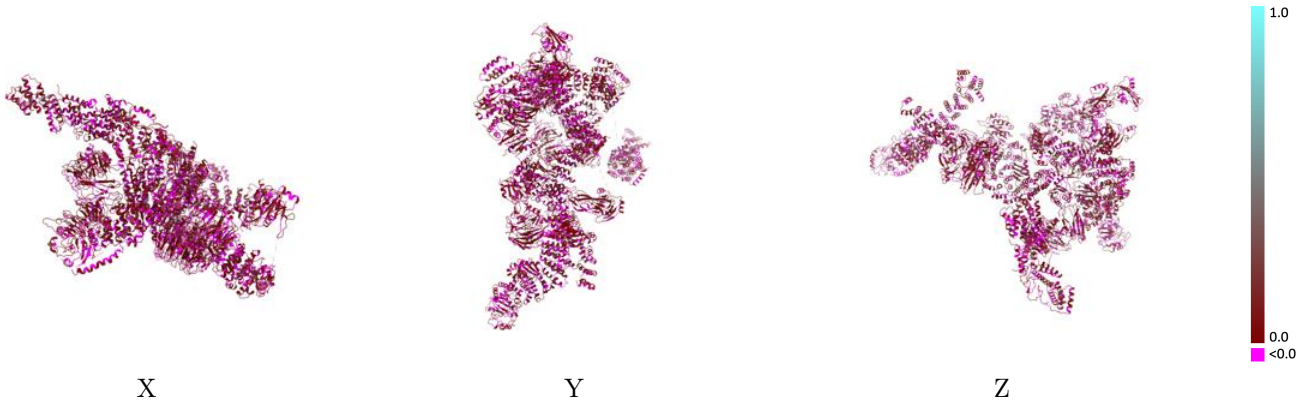
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3722 and PDB model 5NZT. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay

This section was not generated.

9.2 Q-score mapped to coordinate model

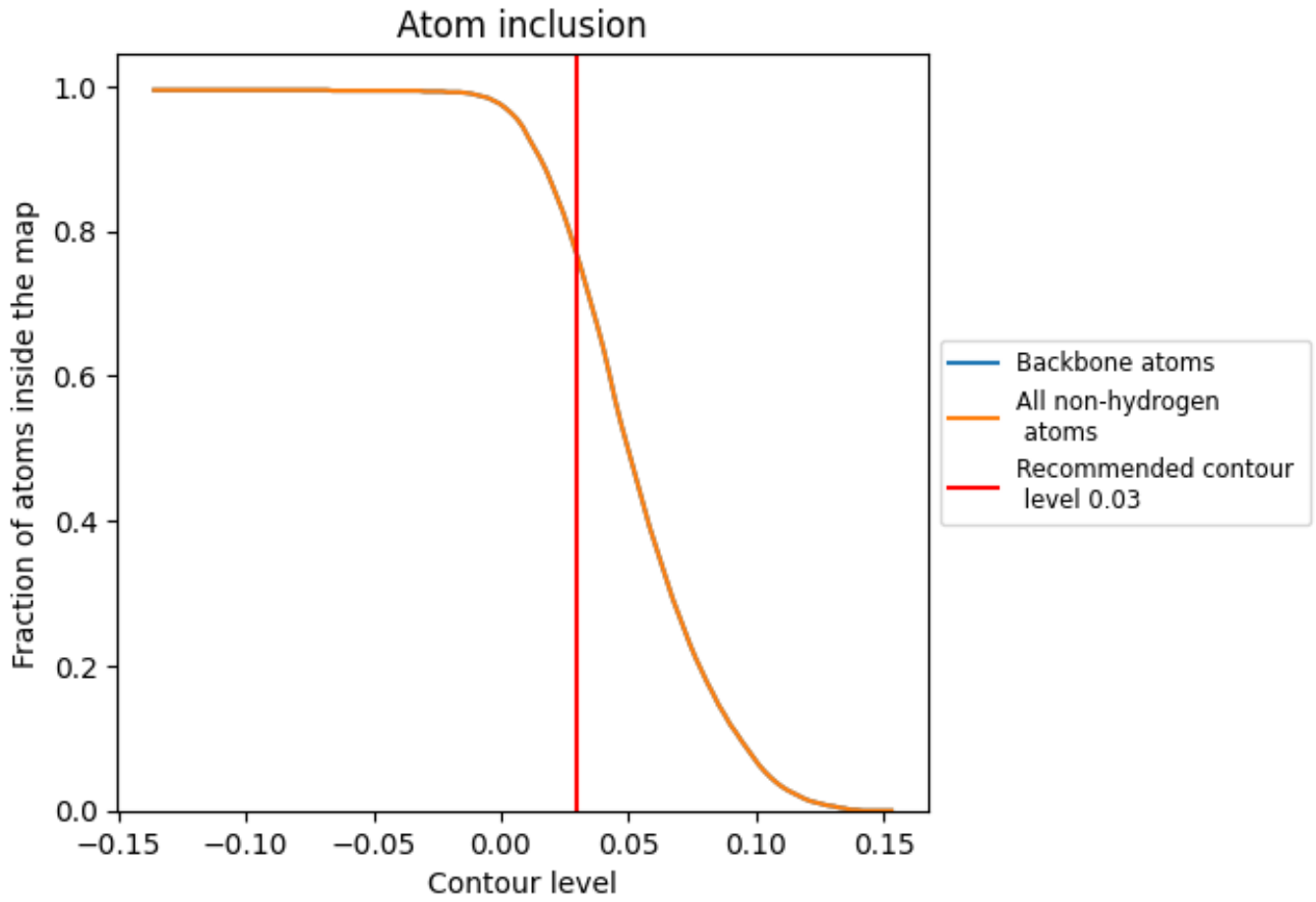


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7660	0.0610
A	0.8840	0.0690
B	0.7710	0.0610
C	0.8570	0.0670
D	0.7520	0.0670
E	0.7730	0.0450
F	0.8910	0.0640
G	0.9190	0.0650
H	0.7830	0.0660
I	0.3650	0.0270
J	0.3920	0.0360
K	0.5280	0.0530
L	0.5170	0.0500
M	0.8280	0.0690
N	0.5720	0.0570
R	0.8900	0.0720
Z	0.8470	0.0610