



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 04:56 AM GMT

PDB ID : 2Q3T
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At3g22680
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-30
Resolution : 1.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

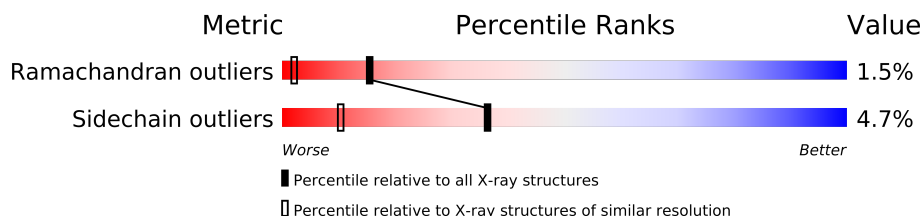
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	157	
1	10-A	157	
1	11-A	157	
1	12-A	157	
1	13-A	157	
1	14-A	157	
1	15-A	157	
1	16-A	157	
1	2-A	157	
1	3-A	157	
1	4-A	157	
1	5-A	157	
1	6-A	157	
1	7-A	157	
1	8-A	157	
1	9-A	157	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	1-A	300	X	-
2	SO4	11-A	300	X	-
2	SO4	14-A	301	X	-
2	SO4	15-A	301	X	-
2	SO4	2-A	301	X	-
2	SO4	7-A	301	X	-
2	SO4	9-A	301	X	-
3	CPS	1-A	200	X	-
3	CPS	10-A	200	X	-
3	CPS	11-A	200	X	-
3	CPS	12-A	200	X	-
3	CPS	13-A	200	X	-
3	CPS	14-A	200	X	-
3	CPS	15-A	200	X	-
3	CPS	16-A	200	X	-
3	CPS	2-A	200	X	-
3	CPS	3-A	200	X	-
3	CPS	5-A	200	X	-
3	CPS	6-A	200	X	-
3	CPS	7-A	200	X	-
3	CPS	8-A	200	X	-
3	CPS	9-A	200	X	-
4	EDO	1-A	402	X	-
4	EDO	10-A	404	X	-
4	EDO	11-A	403	X	-
4	EDO	12-A	404	X	-
4	EDO	13-A	403	X	-
4	EDO	13-A	404	X	-
4	EDO	14-A	401	X	-
4	EDO	14-A	402	X	-
4	EDO	14-A	403	X	-
4	EDO	15-A	403	X	-
4	EDO	15-A	404	X	-
4	EDO	16-A	403	X	-
4	EDO	3-A	403	X	-
4	EDO	3-A	404	X	-
4	EDO	4-A	402	X	-
4	EDO	4-A	404	X	-
4	EDO	5-A	402	X	-
4	EDO	5-A	404	X	-
4	EDO	8-A	402	X	-
4	EDO	8-A	403	X	-
4	EDO	8-A	404	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
4	EDO	9-A	402	X	-
4	EDO	9-A	404	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19808 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

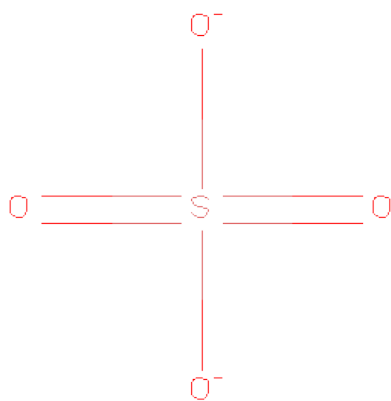
- Molecule 1 is a protein called Protein At3g22680.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	2-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	3-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	4-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	5-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	6-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	7-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	8-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	9-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	10-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	11-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	12-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	13-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	14-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	15-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			
1	16-A	121	Total	C	N	O	S	0	0	0
			1003	646	173	179	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q9LUJ3

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1-A	1	Total	O	S	0	0
			5	4	1		
2	1-A	1	Total	O	S	0	0
			5	4	1		
2	1-A	1	Total	O	S	0	0
			5	4	1		
2	2-A	1	Total	O	S	0	0
			5	4	1		
2	2-A	1	Total	O	S	0	0
			5	4	1		
2	2-A	1	Total	O	S	0	0
			5	4	1		
2	3-A	1	Total	O	S	0	0
			5	4	1		
2	3-A	1	Total	O	S	0	0
			5	4	1		
2	4-A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

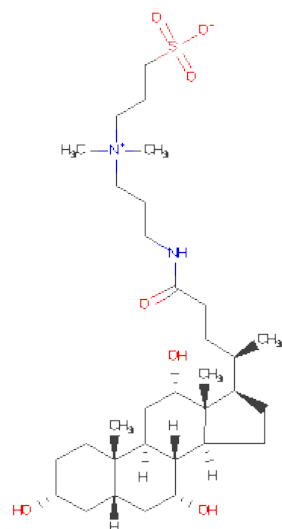
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	4-A	1	Total	O	S	0	0
			5	4	1		
2	4-A	1	Total	O	S	0	0
			5	4	1		
2	5-A	1	Total	O	S	0	0
			5	4	1		
2	5-A	1	Total	O	S	0	0
			5	4	1		
2	5-A	1	Total	O	S	0	0
			5	4	1		
2	6-A	1	Total	O	S	0	0
			5	4	1		
2	6-A	1	Total	O	S	0	0
			5	4	1		
2	6-A	1	Total	O	S	0	0
			5	4	1		
2	7-A	1	Total	O	S	0	0
			5	4	1		
2	7-A	1	Total	O	S	0	0
			5	4	1		
2	7-A	1	Total	O	S	0	0
			5	4	1		
2	8-A	1	Total	O	S	0	0
			5	4	1		
2	8-A	1	Total	O	S	0	0
			5	4	1		
2	8-A	1	Total	O	S	0	0
			5	4	1		
2	9-A	1	Total	O	S	0	0
			5	4	1		
2	9-A	1	Total	O	S	0	0
			5	4	1		
2	9-A	1	Total	O	S	0	0
			5	4	1		
2	10-A	1	Total	O	S	0	0
			5	4	1		
2	10-A	1	Total	O	S	0	0
			5	4	1		
2	10-A	1	Total	O	S	0	0
			5	4	1		
2	11-A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	11-A	1	Total	O	S	0	0
			5	4	1		
2	11-A	1	Total	O	S	0	0
			5	4	1		
2	12-A	1	Total	O	S	0	0
			5	4	1		
2	12-A	1	Total	O	S	0	0
			5	4	1		
2	12-A	1	Total	O	S	0	0
			5	4	1		
2	13-A	1	Total	O	S	0	0
			5	4	1		
2	13-A	1	Total	O	S	0	0
			5	4	1		
2	13-A	1	Total	O	S	0	0
			5	4	1		
2	14-A	1	Total	O	S	0	0
			5	4	1		
2	14-A	1	Total	O	S	0	0
			5	4	1		
2	14-A	1	Total	O	S	0	0
			5	4	1		
2	15-A	1	Total	O	S	0	0
			5	4	1		
2	15-A	1	Total	O	S	0	0
			5	4	1		
2	15-A	1	Total	O	S	0	0
			5	4	1		
2	16-A	1	Total	O	S	0	0
			5	4	1		
2	16-A	1	Total	O	S	0	0
			5	4	1		
2	16-A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (three-letter code: CPS) (formula: C₃₂H₅₈N₂O₇S).



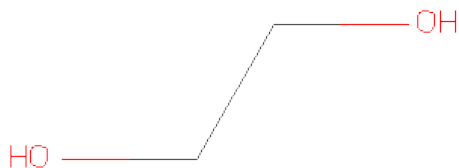
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	2-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	3-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	4-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	5-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	6-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	7-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	8-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	9-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	10-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	11-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	12-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	13-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	14-A	1	Total	C	N	O	0	0
			32	27	1	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	15-A	1	Total	C	N	O	0	0
			32	27	1	4		
3	16-A	1	Total	C	N	O	0	0
			32	27	1	4		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	1-A	1	Total	C	O	0	0
			4	2	2		
4	1-A	1	Total	C	O	0	0
			4	2	2		
4	1-A	1	Total	C	O	0	0
			4	2	2		
4	1-A	1	Total	C	O	0	0
			4	2	2		
4	2-A	1	Total	C	O	0	0
			4	2	2		
4	2-A	1	Total	C	O	0	0
			4	2	2		
4	2-A	1	Total	C	O	0	0
			4	2	2		
4	2-A	1	Total	C	O	0	0
			4	2	2		
4	3-A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	3-A	1	Total C O 4 2 2	0	0
4	3-A	1	Total C O 4 2 2	0	0
4	3-A	1	Total C O 4 2 2	0	0
4	4-A	1	Total C O 4 2 2	0	0
4	4-A	1	Total C O 4 2 2	0	0
4	4-A	1	Total C O 4 2 2	0	0
4	4-A	1	Total C O 4 2 2	0	0
4	5-A	1	Total C O 4 2 2	0	0
4	5-A	1	Total C O 4 2 2	0	0
4	5-A	1	Total C O 4 2 2	0	0
4	5-A	1	Total C O 4 2 2	0	0
4	6-A	1	Total C O 4 2 2	0	0
4	6-A	1	Total C O 4 2 2	0	0
4	6-A	1	Total C O 4 2 2	0	0
4	6-A	1	Total C O 4 2 2	0	0
4	7-A	1	Total C O 4 2 2	0	0
4	7-A	1	Total C O 4 2 2	0	0
4	7-A	1	Total C O 4 2 2	0	0
4	7-A	1	Total C O 4 2 2	0	0
4	8-A	1	Total C O 4 2 2	0	0
4	8-A	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	8-A	1	Total 4	C 2	O 2	0	0
4	8-A	1	Total 4	C 2	O 2	0	0
4	9-A	1	Total 4	C 2	O 2	0	0
4	9-A	1	Total 4	C 2	O 2	0	0
4	9-A	1	Total 4	C 2	O 2	0	0
4	9-A	1	Total 4	C 2	O 2	0	0
4	10-A	1	Total 4	C 2	O 2	0	0
4	10-A	1	Total 4	C 2	O 2	0	0
4	10-A	1	Total 4	C 2	O 2	0	0
4	10-A	1	Total 4	C 2	O 2	0	0
4	11-A	1	Total 4	C 2	O 2	0	0
4	11-A	1	Total 4	C 2	O 2	0	0
4	11-A	1	Total 4	C 2	O 2	0	0
4	11-A	1	Total 4	C 2	O 2	0	0
4	12-A	1	Total 4	C 2	O 2	0	0
4	12-A	1	Total 4	C 2	O 2	0	0
4	12-A	1	Total 4	C 2	O 2	0	0
4	12-A	1	Total 4	C 2	O 2	0	0
4	13-A	1	Total 4	C 2	O 2	0	0
4	13-A	1	Total 4	C 2	O 2	0	0
4	13-A	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	13-A	1	Total C O 4 2 2	0	0
4	14-A	1	Total C O 4 2 2	0	0
4	14-A	1	Total C O 4 2 2	0	0
4	14-A	1	Total C O 4 2 2	0	0
4	14-A	1	Total C O 4 2 2	0	0
4	15-A	1	Total C O 4 2 2	0	0
4	15-A	1	Total C O 4 2 2	0	0
4	15-A	1	Total C O 4 2 2	0	0
4	15-A	1	Total C O 4 2 2	0	0
4	16-A	1	Total C O 4 2 2	0	0
4	16-A	1	Total C O 4 2 2	0	0
4	16-A	1	Total C O 4 2 2	0	0
4	16-A	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-A	172	Total O 172 172	0	0
5	2-A	172	Total O 172 172	0	0
5	3-A	172	Total O 172 172	0	0
5	4-A	172	Total O 172 172	0	0
5	5-A	172	Total O 172 172	0	0
5	6-A	172	Total O 172 172	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	7-A	172	Total 172	O 172	0	0
5	8-A	172	Total 172	O 172	0	0
5	9-A	172	Total 172	O 172	0	0
5	10-A	172	Total 172	O 172	0	0
5	11-A	172	Total 172	O 172	0	0
5	12-A	172	Total 172	O 172	0	0
5	13-A	172	Total 172	O 172	0	0
5	14-A	172	Total 172	O 172	0	0
5	15-A	172	Total 172	O 172	0	0
5	16-A	172	Total 172	O 172	0	0

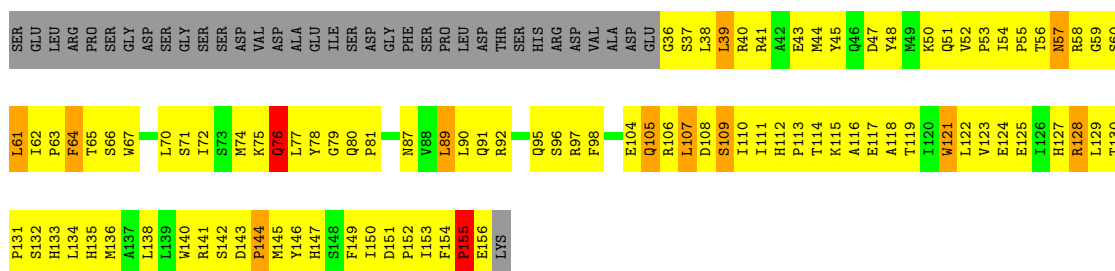
3 Residue-property plots

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

Note EDS failed to run properly.

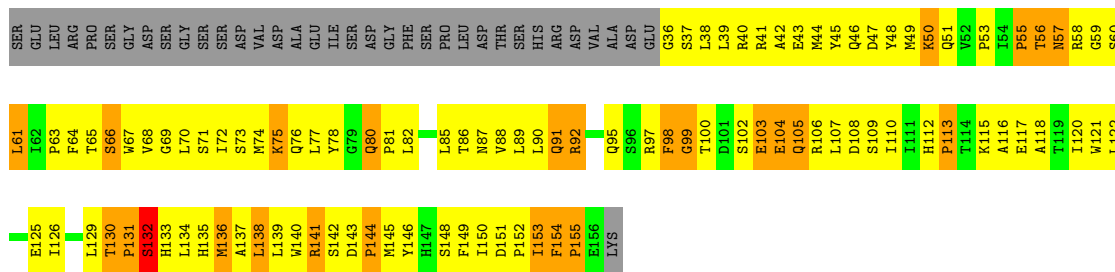
• Molecule 1: Protein At3g22680

Chain 1-A:



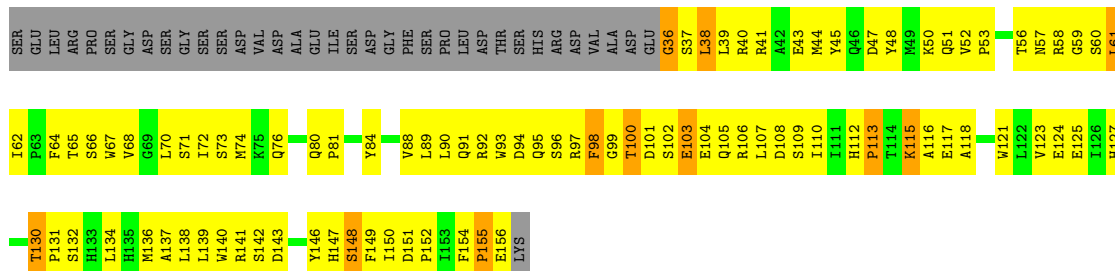
• Molecule 1: Protein At3g22680

Chain 2-A:



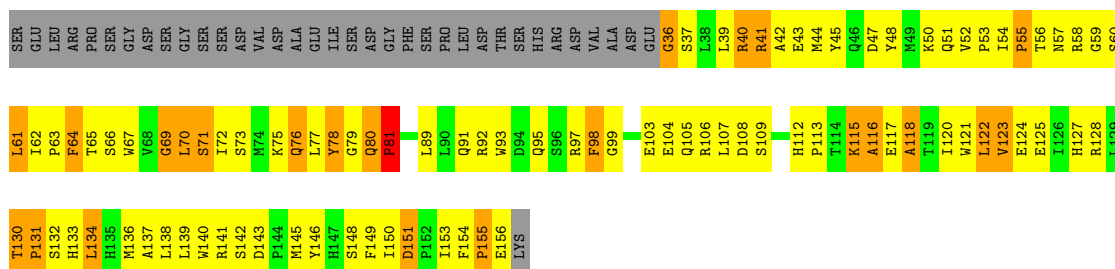
• Molecule 1: Protein At3g22680

Chain 3-A:



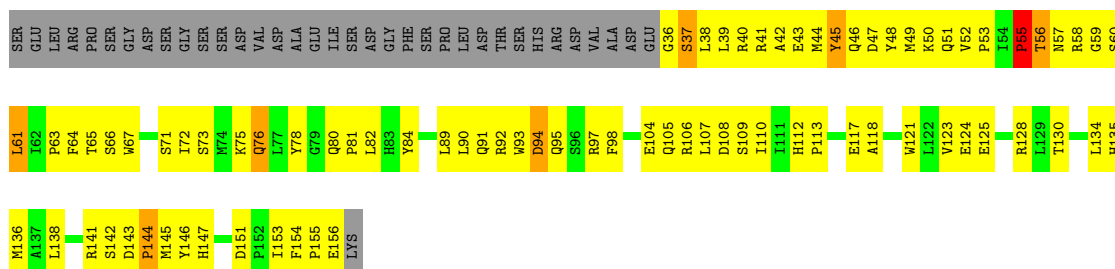
• Molecule 1: Protein At3g22680

Chain 4-A:



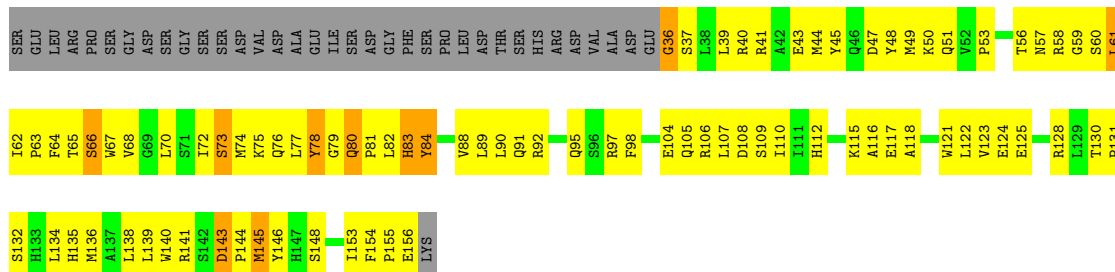
- Molecule 1: Protein At3g22680

Chain 5-A:



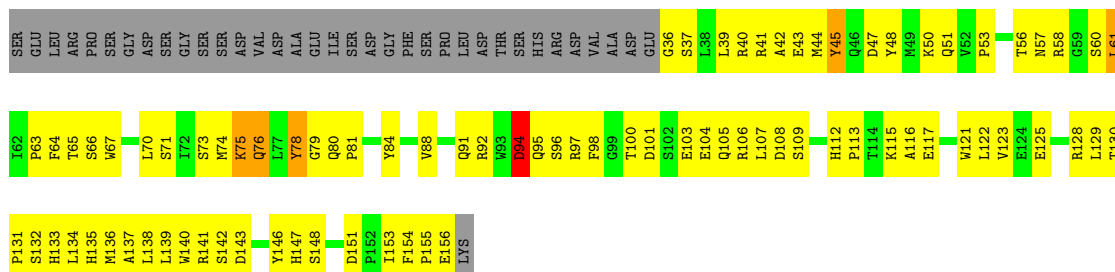
- Molecule 1: Protein At3g22680

Chain 6-A:



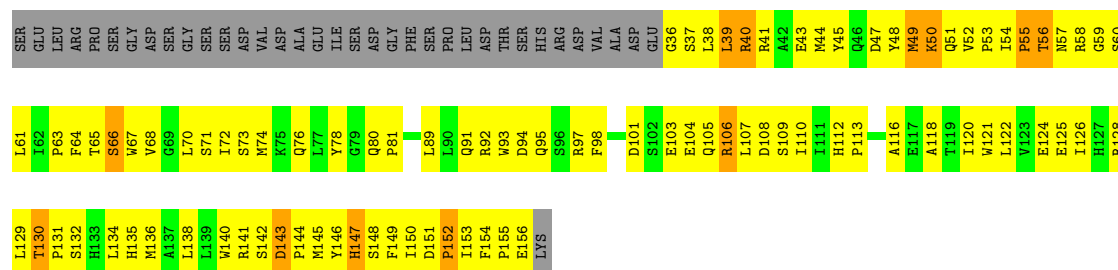
- Molecule 1: Protein At3g22680

Chain 7-A:



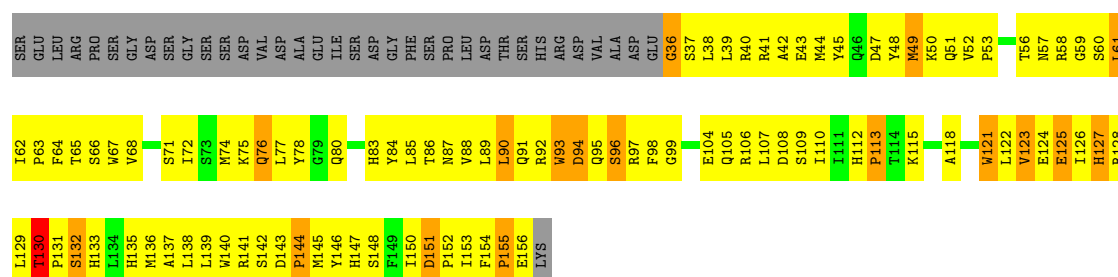
- Molecule 1: Protein At3g22680

Chain 8-A:



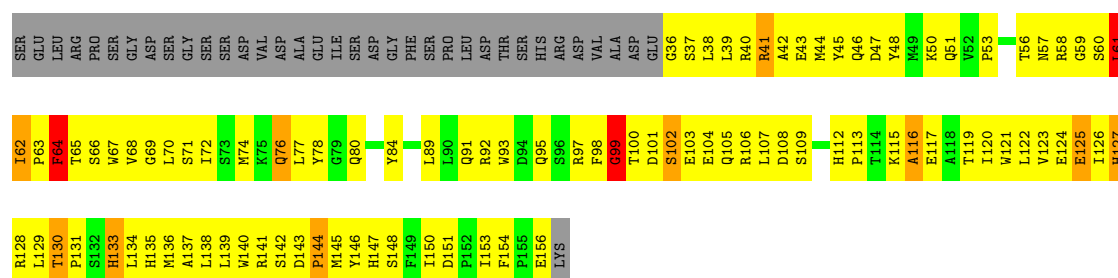
• Molecule 1: Protein At3g22680

Chain 9-A:



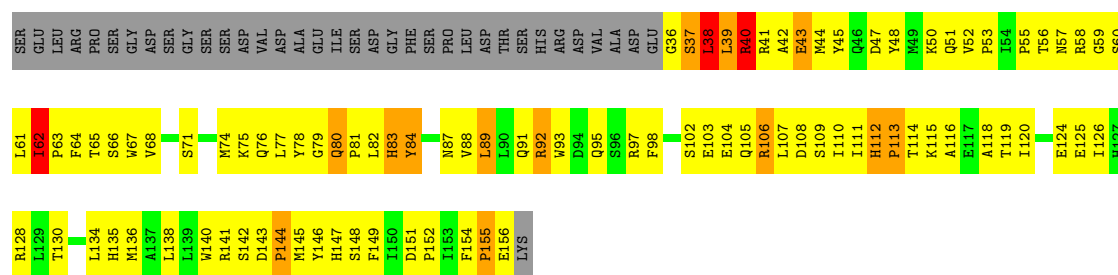
• Molecule 1: Protein At3g22680

Chain 10-A:



• Molecule 1: Protein At3g22680

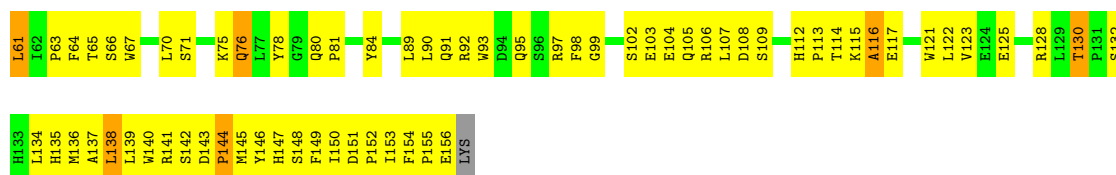
Chain 11-A:



• Molecule 1: Protein At3g22680

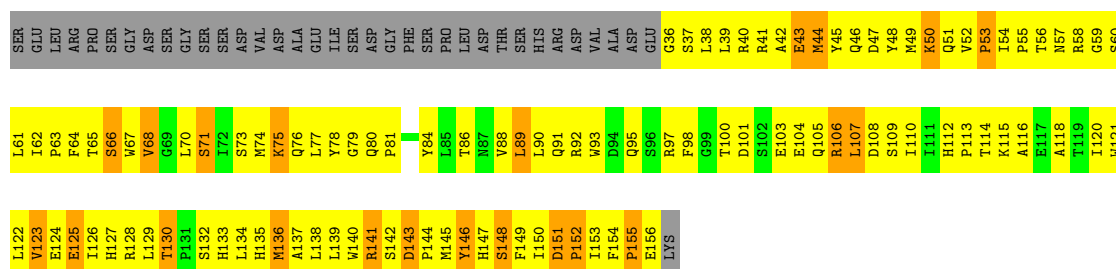
Chain 12-A:





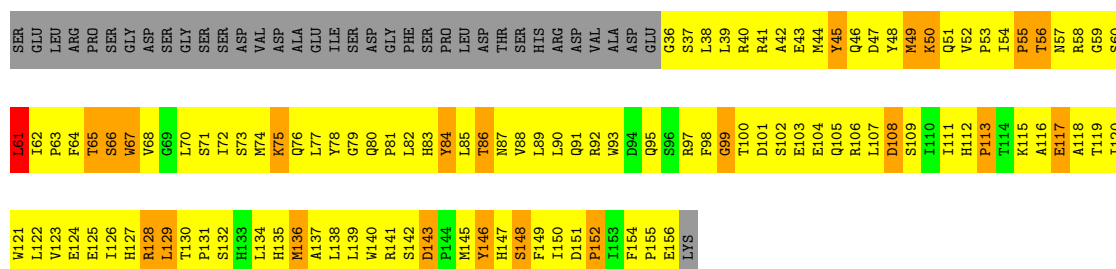
• Molecule 1: Protein At3g22680

Chain 13-A:



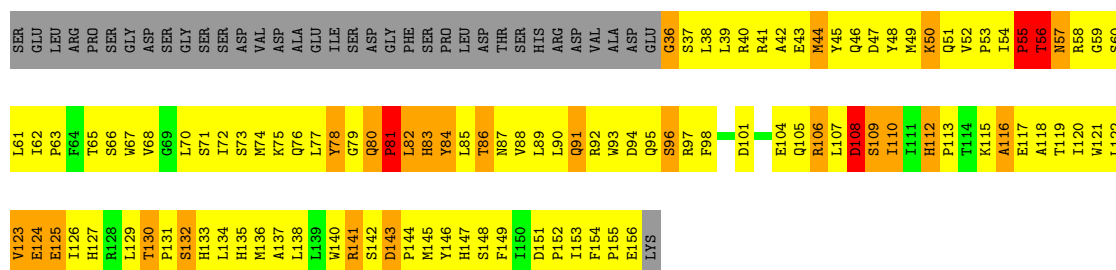
• Molecule 1: Protein At3g22680

Chain 14-A:



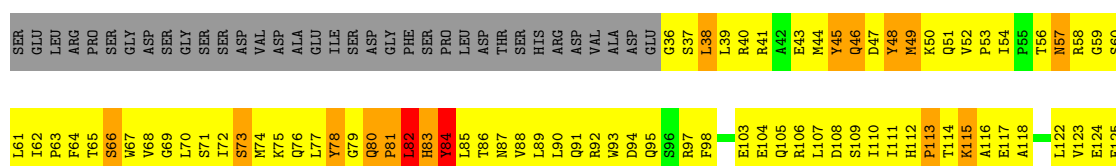
• Molecule 1: Protein At3g22680

Chain 15-A:



• Molecule 1: Protein At3g22680

Chain 16-A:



I126	H127	R128	L129	T130	P131	S132	H133	L134	M135	M136	A137	L138	L139	W140	R141	S142	D143	P144	M145	Y146	H147	S148	F149	I150	D151	P152	I153	F154	P155	E156	LYS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----

4 Data and refinement statistics i

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.45Å 83.45Å 60.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.03 – 1.60	Depositor
% Data completeness (in resolution range)	99.9 (31.03-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.43 (at 1.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.139 , 0.170	Depositor
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.019	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 32203 reflections	Xtriage
Total number of atoms	19808	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CPS, SO4, EDO

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	4.50	189/1034 (18.3%)	3.79	147/1407 (10.4%)
1	2-A	4.69	207/1034 (20.0%)	3.87	188/1407 (13.4%)
1	3-A	4.13	142/1034 (13.7%)	3.38	132/1407 (9.4%)
1	4-A	4.59	179/1034 (17.3%)	3.79	163/1407 (11.6%)
1	5-A	4.18	159/1034 (15.4%)	3.83	138/1407 (9.8%)
1	6-A	3.79	135/1034 (13.1%)	3.37	122/1407 (8.7%)
1	7-A	4.00	151/1034 (14.6%)	3.40	123/1407 (8.7%)
1	8-A	4.47	190/1034 (18.4%)	3.61	155/1407 (11.0%)
1	9-A	4.83	213/1034 (20.6%)	3.87	182/1407 (12.9%)
1	10-A	4.80	201/1034 (19.4%)	3.91	178/1407 (12.7%)
1	11-A	4.73	194/1034 (18.8%)	3.86	149/1407 (10.6%)
1	12-A	3.70	132/1034 (12.8%)	3.21	115/1407 (8.2%)
1	13-A	5.17	237/1034 (22.9%)	4.26	209/1407 (14.9%)
1	14-A	5.92	268/1034 (25.9%)	4.61	246/1407 (17.5%)
1	15-A	5.89	293/1034 (28.3%)	4.79	270/1407 (19.2%)
1	16-A	6.21	303/1034 (29.3%)	5.01	264/1407 (18.8%)
All	All	4.78	3193/16544 (19.3%)	3.94	2781/22512 (12.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	10
1	2-A	0	16
1	3-A	0	5
1	4-A	0	15
1	5-A	0	4
1	6-A	0	6
1	7-A	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	8-A	0	6
1	9-A	0	8
1	10-A	0	8
1	11-A	0	10
1	12-A	0	5
1	13-A	0	14
1	14-A	0	17
1	15-A	0	21
1	16-A	0	18
All	All	0	168

All (3193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	14-A	45	TYR	CD2-CE2	48.45	2.12	1.39
1	14-A	124	GLU	CD-OE1	42.84	1.72	1.25
1	16-A	93	TRP	CG-CD1	37.28	1.89	1.36
1	11-A	78	TYR	CD1-CE1	36.76	1.94	1.39
1	15-A	49	MET	CG-SD	36.34	2.75	1.81
1	16-A	93	TRP	CD1-NE1	35.92	1.99	1.38
1	16-A	83	HIS	C-O	35.24	1.90	1.23
1	1-A	109	SER	CB-OG	-33.51	0.98	1.42
1	10-A	43	GLU	CG-CD	32.36	2.00	1.51
1	9-A	84	TYR	CD1-CE1	31.82	1.87	1.39
1	13-A	136	MET	CG-SD	31.65	2.63	1.81
1	10-A	84	TYR	CD1-CE1	31.40	1.86	1.39
1	16-A	146	TYR	CD1-CE1	30.98	1.85	1.39
1	4-A	78	TYR	CE1-CZ	30.86	1.78	1.38
1	4-A	123	VAL	CB-CG1	30.39	2.16	1.52
1	15-A	109	SER	CB-OG	-30.04	1.03	1.42
1	13-A	50	LYS	CE-NZ	29.90	2.23	1.49
1	9-A	49	MET	CG-SD	27.99	2.54	1.81
1	2-A	98	PHE	CE2-CZ	27.88	1.90	1.37
1	11-A	118	ALA	CA-CB	27.56	2.10	1.52
1	16-A	144	PRO	C-O	27.55	1.78	1.23
1	4-A	138	LEU	CG-CD1	27.28	2.52	1.51
1	14-A	129	LEU	C-O	-26.59	0.72	1.23
1	14-A	64	PHE	CE2-CZ	26.52	1.87	1.37
1	2-A	45	TYR	CE1-CZ	25.86	1.72	1.38
1	14-A	141	ARG	CZ-NH1	-25.79	0.99	1.33
1	10-A	64	PHE	CE1-CZ	25.70	1.86	1.37
1	1-A	91	GLN	CB-CG	25.58	2.21	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	14-A	50	LYS	CA-CB	25.27	2.09	1.53
1	7-A	96	SER	CB-OG	25.22	1.75	1.42
1	8-A	64	PHE	CE2-CZ	25.20	1.85	1.37
1	15-A	115	LYS	CD-CE	25.20	2.14	1.51
1	2-A	50	LYS	CD-CE	24.87	2.13	1.51
1	6-A	73	SER	CB-OG	24.71	1.74	1.42
1	14-A	125	GLU	CD-OE2	24.47	1.52	1.25
1	10-A	140	TRP	CG-CD1	24.24	1.70	1.36
1	5-A	37	SER	CB-OG	-24.18	1.10	1.42
1	11-A	41	ARG	CG-CD	-24.01	0.92	1.51
1	5-A	80	GLN	CG-CD	23.85	2.05	1.51
1	14-A	64	PHE	CD2-CE2	23.83	1.86	1.39
1	14-A	137	ALA	CA-CB	23.80	2.02	1.52
1	15-A	109	SER	CA-CB	23.63	1.88	1.52
1	15-A	117	GLU	CB-CG	23.54	1.96	1.52
1	16-A	45	TYR	CD2-CE2	23.50	1.74	1.39
1	11-A	64	PHE	CD2-CE2	23.41	1.86	1.39
1	9-A	126	ILE	C-O	23.41	1.67	1.23
1	15-A	85	LEU	CG-CD1	23.38	2.38	1.51
1	12-A	50	LYS	CE-NZ	23.37	2.07	1.49
1	16-A	84	TYR	CE2-CZ	23.36	1.69	1.38
1	9-A	132	SER	C-O	23.33	1.67	1.23
1	14-A	85	LEU	CG-CD1	23.31	2.38	1.51
1	8-A	67	TRP	CE2-CZ2	23.20	1.79	1.39
1	4-A	123	VAL	CA-CB	23.13	2.03	1.54
1	13-A	53	PRO	CG-CD	23.11	2.27	1.50
1	5-A	84	TYR	CD1-CE1	22.98	1.73	1.39
1	7-A	115	LYS	CE-NZ	22.93	2.06	1.49
1	7-A	50	LYS	CE-NZ	22.89	2.06	1.49
1	16-A	50	LYS	CD-CE	22.88	2.08	1.51
1	16-A	71	SER	CB-OG	-22.73	1.12	1.42
1	15-A	88	VAL	CB-CG2	22.65	2.00	1.52
1	4-A	115	LYS	CE-NZ	22.55	2.05	1.49
1	5-A	80	GLN	CB-CG	-22.49	0.91	1.52
1	16-A	68	VAL	CB-CG2	22.48	2.00	1.52
1	16-A	47	ASP	CG-OD2	-22.47	0.73	1.25
1	13-A	123	VAL	C-O	22.45	1.66	1.23
1	8-A	140	TRP	CZ3-CH2	22.45	1.75	1.40
1	3-A	115	LYS	CE-NZ	22.36	2.04	1.49
1	13-A	148	SER	CA-CB	22.28	1.86	1.52
1	14-A	49	MET	CG-SD	-22.02	1.23	1.81
1	10-A	76	GLN	CD-OE1	21.94	1.72	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-A	52	VAL	CB-CG1	21.71	1.98	1.52
1	3-A	45	TYR	CE1-CZ	21.56	1.66	1.38
1	8-A	64	PHE	CD2-CE2	21.51	1.82	1.39
1	13-A	67	TRP	CE3-CZ3	-21.42	1.02	1.38
1	3-A	98	PHE	CE2-CZ	21.27	1.77	1.37
1	11-A	92	ARG	CD-NE	21.02	1.82	1.46
1	14-A	123	VAL	CB-CG2	21.00	1.97	1.52
1	3-A	149	PHE	CE1-CZ	21.00	1.77	1.37
1	15-A	93	TRP	CD1-NE1	20.98	1.73	1.38
1	16-A	123	VAL	CB-CG2	20.94	1.96	1.52
1	13-A	47	ASP	C-O	20.89	1.63	1.23
1	15-A	132	SER	CA-CB	20.82	1.84	1.52
1	13-A	45	TYR	C-O	20.65	1.62	1.23
1	1-A	37	SER	CB-OG	-20.58	1.15	1.42
1	14-A	48	TYR	CD1-CE1	-20.56	1.08	1.39
1	16-A	66	SER	CB-OG	-20.53	1.15	1.42
1	15-A	36	GLY	C-O	20.49	1.56	1.23
1	14-A	40	ARG	NE-CZ	20.32	1.59	1.33
1	9-A	140	TRP	CG-CD1	20.30	1.65	1.36
1	16-A	40	ARG	NE-CZ	20.23	1.59	1.33
1	3-A	98	PHE	CE1-CZ	-20.15	0.99	1.37
1	15-A	40	ARG	NE-CZ	20.14	1.59	1.33
1	13-A	40	ARG	NE-CZ	20.12	1.59	1.33
1	11-A	78	TYR	CE1-CZ	20.09	1.64	1.38
1	16-A	84	TYR	CD2-CE2	20.08	1.69	1.39
1	14-A	50	LYS	CB-CG	20.07	2.06	1.52
1	10-A	64	PHE	CD1-CE1	20.06	1.79	1.39
1	5-A	93	TRP	CG-CD1	20.04	1.64	1.36
1	11-A	78	TYR	CG-CD1	19.88	1.65	1.39
1	11-A	50	LYS	CB-CG	-19.70	0.99	1.52
1	16-A	82	LEU	CG-CD1	19.68	2.24	1.51
1	16-A	143	ASP	CG-OD2	19.65	1.70	1.25
1	8-A	68	VAL	CB-CG1	19.57	1.94	1.52
1	14-A	45	TYR	CG-CD2	19.43	1.64	1.39
1	12-A	116	ALA	CA-CB	19.39	1.93	1.52
1	13-A	68	VAL	CB-CG1	19.38	1.93	1.52
1	5-A	92	ARG	CZ-NH1	19.31	1.58	1.33
1	10-A	116	ALA	CA-CB	19.30	1.93	1.52
1	13-A	125	GLU	CD-OE2	19.20	1.46	1.25
1	2-A	67	TRP	CG-CD1	19.14	1.63	1.36
1	6-A	74	MET	SD-CE	19.09	2.84	1.77
1	11-A	60	SER	CB-OG	19.02	1.67	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-A	91	GLN	CB-CG	19.01	2.03	1.52
1	4-A	130	THR	CB-CG2	19.00	2.15	1.52
1	2-A	109	SER	CA-CB	18.98	1.81	1.52
1	14-A	36	GLY	N-CA	18.98	1.74	1.46
1	9-A	128	ARG	CZ-NH1	18.95	1.57	1.33
1	6-A	44	MET	CG-SD	18.93	2.30	1.81
1	2-A	92	ARG	CZ-NH2	18.88	1.57	1.33
1	15-A	113	PRO	CA-CB	18.83	1.91	1.53
1	13-A	89	LEU	CG-CD2	18.81	2.21	1.51
1	1-A	40	ARG	NE-CZ	18.72	1.57	1.33
1	9-A	36	GLY	N-CA	18.68	1.74	1.46
1	8-A	60	SER	CB-OG	18.68	1.66	1.42
1	9-A	40	ARG	CG-CD	18.68	1.98	1.51
1	9-A	138	LEU	C-O	18.68	1.58	1.23
1	15-A	115	LYS	CE-NZ	-18.67	1.02	1.49
1	16-A	141	ARG	CG-CD	18.53	1.98	1.51
1	1-A	45	TYR	CE1-CZ	18.49	1.62	1.38
1	9-A	109	SER	CA-CB	18.45	1.80	1.52
1	15-A	125	GLU	CD-OE2	18.43	1.46	1.25
1	15-A	78	TYR	CD2-CE2	18.43	1.67	1.39
1	10-A	121	TRP	C-O	18.37	1.58	1.23
1	16-A	82	LEU	C-O	18.36	1.58	1.23
1	14-A	45	TYR	CE1-CZ	18.30	1.62	1.38
1	16-A	86	THR	C-O	18.29	1.58	1.23
1	1-A	115	LYS	CA-CB	18.23	1.94	1.53
1	15-A	88	VAL	CB-CG1	18.21	1.91	1.52
1	2-A	141	ARG	CG-CD	18.20	1.97	1.51
1	1-A	78	TYR	CE1-CZ	18.20	1.62	1.38
1	5-A	43	GLU	CG-CD	18.17	1.79	1.51
1	4-A	67	TRP	CE3-CZ3	18.10	1.69	1.38
1	14-A	46	GLN	CB-CG	17.95	2.01	1.52
1	12-A	40	ARG	NE-CZ	17.86	1.56	1.33
1	4-A	80	GLN	CG-CD	17.86	1.92	1.51
1	2-A	98	PHE	CE1-CZ	-17.82	1.03	1.37
1	11-A	141	ARG	CG-CD	17.77	1.96	1.51
1	11-A	107	LEU	C-O	17.75	1.57	1.23
1	7-A	117	GLU	CG-CD	17.73	1.78	1.51
1	9-A	40	ARG	CZ-NH1	17.69	1.56	1.33
1	2-A	40	ARG	NE-CZ	17.63	1.55	1.33
1	14-A	148	SER	CA-CB	17.63	1.79	1.52
1	10-A	68	VAL	CB-CG2	17.63	1.89	1.52
1	1-A	123	VAL	CB-CG1	17.59	1.89	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-A	125	GLU	CD-OE2	17.54	1.45	1.25
1	15-A	53	PRO	CA-CB	17.53	1.88	1.53
1	8-A	40	ARG	NE-CZ	17.50	1.55	1.33
1	7-A	40	ARG	NE-CZ	17.49	1.55	1.33
1	8-A	67	TRP	CZ2-CH2	17.46	1.70	1.37
1	2-A	45	TYR	CD1-CE1	17.43	1.65	1.39
1	12-A	43	GLU	CG-CD	17.42	1.78	1.51
1	7-A	36	GLY	N-CA	17.38	1.72	1.46
1	6-A	40	ARG	NE-CZ	17.35	1.55	1.33
1	14-A	121	TRP	CG-CD1	17.35	1.61	1.36
1	3-A	40	ARG	NE-CZ	17.29	1.55	1.33
1	3-A	45	TYR	CD2-CE2	17.27	1.65	1.39
1	16-A	86	THR	CB-OG1	17.25	1.77	1.43
1	10-A	138	LEU	C-O	17.22	1.56	1.23
1	2-A	92	ARG	CZ-NH1	-17.16	1.10	1.33
1	15-A	106	ARG	CB-CG	17.10	1.98	1.52
1	2-A	89	LEU	CG-CD2	17.09	2.15	1.51
1	15-A	140	TRP	CZ3-CH2	17.05	1.67	1.40
1	10-A	76	GLN	CD-NE2	17.03	1.75	1.32
1	15-A	93	TRP	CG-CD1	17.00	1.60	1.36
1	10-A	44	MET	CG-SD	16.89	2.25	1.81
1	8-A	80	GLN	CG-CD	16.88	1.89	1.51
1	2-A	148	SER	CA-CB	16.87	1.78	1.52
1	7-A	91	GLN	CD-NE2	16.86	1.75	1.32
1	3-A	50	LYS	CE-NZ	16.85	1.91	1.49
1	15-A	98	PHE	CD1-CE1	-16.84	1.05	1.39
1	9-A	40	ARG	CZ-NH2	16.82	1.54	1.33
1	8-A	40	ARG	CA-CB	16.75	1.90	1.53
1	13-A	67	TRP	CG-CD1	16.69	1.60	1.36
1	16-A	141	ARG	NE-CZ	-16.67	1.11	1.33
1	8-A	45	TYR	CE1-CZ	16.65	1.60	1.38
1	6-A	109	SER	CA-CB	16.65	1.77	1.52
1	12-A	156	GLU	CD-OE1	16.59	1.43	1.25
1	10-A	40	ARG	NE-CZ	16.53	1.54	1.33
1	16-A	84	TYR	CE1-CZ	16.48	1.59	1.38
1	5-A	40	ARG	NE-CZ	16.42	1.54	1.33
1	14-A	97	ARG	NE-CZ	16.39	1.54	1.33
1	10-A	36	GLY	N-CA	16.38	1.70	1.46
1	4-A	40	ARG	NE-CZ	16.37	1.54	1.33
1	2-A	50	LYS	CE-NZ	16.33	1.89	1.49
1	15-A	126	ILE	CB-CG2	16.31	2.03	1.52
1	6-A	84	TYR	CD1-CE1	16.30	1.63	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	12-A	36	GLY	N-CA	16.27	1.70	1.46
1	16-A	36	GLY	N-CA	16.27	1.70	1.46
1	10-A	138	LEU	CG-CD2	16.26	2.12	1.51
1	8-A	49	MET	CG-SD	16.24	2.23	1.81
1	16-A	87	ASN	C-O	16.23	1.54	1.23
1	3-A	109	SER	CA-CB	16.18	1.77	1.52
1	11-A	41	ARG	CB-CG	16.15	1.96	1.52
1	16-A	67	TRP	C-O	16.14	1.54	1.23
1	15-A	81	PRO	CA-CB	16.10	1.85	1.53
1	14-A	65	THR	C-O	-16.07	0.92	1.23
1	13-A	45	TYR	CA-C	16.05	1.94	1.52
1	3-A	91	GLN	CD-OE1	16.04	1.59	1.24
1	13-A	141	ARG	NE-CZ	-16.04	1.12	1.33
1	8-A	44	MET	CG-SD	16.01	2.22	1.81
1	13-A	106	ARG	CZ-NH1	15.97	1.53	1.33
1	11-A	106	ARG	CZ-NH1	15.95	1.53	1.33
1	9-A	84	TYR	CE2-CZ	15.95	1.59	1.38
1	1-A	36	GLY	CA-C	15.88	1.77	1.51
1	5-A	40	ARG	CZ-NH2	15.88	1.53	1.33
1	5-A	109	SER	CA-CB	15.87	1.76	1.52
1	16-A	49	MET	CG-SD	-15.81	1.40	1.81
1	4-A	36	GLY	N-CA	15.81	1.69	1.46
1	16-A	106	ARG	CZ-NH1	15.80	1.53	1.33
1	2-A	92	ARG	CD-NE	15.78	1.73	1.46
1	14-A	117	GLU	CG-CD	15.73	1.75	1.51
1	16-A	45	TYR	CG-CD2	15.73	1.59	1.39
1	6-A	145	MET	CG-SD	15.72	2.22	1.81
1	11-A	41	ARG	CZ-NH1	15.72	1.53	1.33
1	8-A	106	ARG	CZ-NH1	15.71	1.53	1.33
1	4-A	122	LEU	CA-CB	15.71	1.89	1.53
1	13-A	141	ARG	CG-CD	15.64	1.91	1.51
1	16-A	146	TYR	CE1-CZ	15.62	1.58	1.38
1	10-A	128	ARG	CZ-NH1	15.58	1.53	1.33
1	15-A	84	TYR	CD2-CE2	15.57	1.62	1.39
1	14-A	115	LYS	CE-NZ	15.57	1.88	1.49
1	15-A	141	ARG	NE-CZ	-15.57	1.12	1.33
1	7-A	92	ARG	CZ-NH1	15.57	1.53	1.33
1	16-A	146	TYR	CE2-CZ	15.56	1.58	1.38
1	1-A	109	SER	CA-CB	15.48	1.76	1.52
1	16-A	43	GLU	CG-CD	15.46	1.75	1.51
1	16-A	109	SER	CB-OG	-15.45	1.22	1.42
1	1-A	40	ARG	CA-CB	15.43	1.87	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	116	ALA	C-O	15.42	1.52	1.23
1	2-A	40	ARG	CZ-NH2	15.41	1.53	1.33
1	16-A	84	TYR	CD1-CE1	-15.40	1.16	1.39
1	4-A	70	LEU	CB-CG	15.38	1.97	1.52
1	15-A	48	TYR	CD1-CE1	-15.38	1.16	1.39
1	15-A	58	ARG	CZ-NH2	15.38	1.53	1.33
1	1-A	45	TYR	CD1-CE1	15.35	1.62	1.39
1	14-A	106	ARG	CZ-NH2	15.34	1.52	1.33
1	15-A	117	GLU	CA-CB	15.31	1.87	1.53
1	14-A	140	TRP	CZ3-CH2	15.30	1.64	1.40
1	12-A	40	ARG	CZ-NH2	15.28	1.52	1.33
1	1-A	41	ARG	CB-CG	15.28	1.93	1.52
1	7-A	138	LEU	CG-CD1	15.27	2.08	1.51
1	15-A	50	LYS	CD-CE	15.24	1.89	1.51
1	9-A	137	ALA	C-O	15.22	1.52	1.23
1	9-A	125	GLU	CG-CD	-15.22	1.29	1.51
1	15-A	141	ARG	CG-CD	15.16	1.89	1.51
1	10-A	40	ARG	CZ-NH2	15.15	1.52	1.33
1	9-A	123	VAL	CA-CB	15.12	1.86	1.54
1	14-A	40	ARG	CZ-NH2	15.11	1.52	1.33
1	13-A	92	ARG	CG-CD	15.08	1.89	1.51
1	9-A	138	LEU	CG-CD2	15.06	2.07	1.51
1	2-A	88	VAL	CB-CG1	15.05	1.84	1.52
1	11-A	40	ARG	CG-CD	15.04	1.89	1.51
1	10-A	44	MET	CB-CG	14.96	1.99	1.51
1	4-A	81	PRO	CA-CB	14.95	1.83	1.53
1	15-A	104	GLU	CD-OE1	14.95	1.42	1.25
1	12-A	106	ARG	CZ-NH1	14.95	1.52	1.33
1	7-A	40	ARG	CZ-NH2	14.94	1.52	1.33
1	14-A	52	VAL	CB-CG1	14.90	1.84	1.52
1	4-A	77	LEU	CG-CD2	14.84	2.06	1.51
1	16-A	40	ARG	CZ-NH2	14.83	1.52	1.33
1	4-A	78	TYR	CE2-CZ	14.80	1.57	1.38
1	16-A	82	LEU	N-CA	14.77	1.75	1.46
1	7-A	106	ARG	CZ-NH1	14.71	1.52	1.33
1	9-A	97	ARG	NE-CZ	14.69	1.52	1.33
1	3-A	97	ARG	CG-CD	14.67	1.88	1.51
1	14-A	45	TYR	CD1-CE1	-14.63	1.17	1.39
1	8-A	148	SER	CB-OG	14.62	1.61	1.42
1	16-A	138	LEU	CG-CD1	14.62	2.06	1.51
1	7-A	117	GLU	CD-OE1	14.61	1.41	1.25
1	13-A	45	TYR	CE1-CZ	14.59	1.57	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-A	96	SER	CA-CB	14.59	1.74	1.52
1	15-A	44	MET	CG-SD	14.52	2.18	1.81
1	5-A	92	ARG	CZ-NH2	14.49	1.51	1.33
1	7-A	43	GLU	CG-CD	14.46	1.73	1.51
1	12-A	115	LYS	CE-NZ	14.44	1.85	1.49
1	3-A	45	TYR	CE2-CZ	-14.43	1.19	1.38
1	15-A	40	ARG	CG-CD	14.42	1.88	1.51
1	16-A	123	VAL	CB-CG1	14.42	1.83	1.52
1	13-A	65	THR	C-N	14.40	1.67	1.34
1	9-A	40	ARG	NE-CZ	14.40	1.51	1.33
1	4-A	73	SER	C-O	14.36	1.50	1.23
1	14-A	43	GLU	CG-CD	14.34	1.73	1.51
1	4-A	70	LEU	CG-CD2	14.32	2.04	1.51
1	4-A	125	GLU	CG-CD	-14.32	1.30	1.51
1	2-A	78	TYR	CD1-CE1	14.31	1.60	1.39
1	1-A	40	ARG	CB-CG	-14.27	1.14	1.52
1	9-A	129	LEU	C-O	14.25	1.50	1.23
1	3-A	98	PHE	CG-CD2	14.22	1.60	1.38
1	1-A	156	GLU	CD-OE1	14.21	1.41	1.25
1	4-A	109	SER	CA-CB	14.21	1.74	1.52
1	2-A	125	GLU	CD-OE2	14.20	1.41	1.25
1	15-A	53	PRO	N-CD	14.18	1.67	1.47
1	8-A	109	SER	CB-OG	-14.17	1.23	1.42
1	15-A	110	ILE	C-O	14.15	1.50	1.23
1	10-A	137	ALA	C-O	14.14	1.50	1.23
1	1-A	108	ASP	CB-CG	14.14	1.81	1.51
1	7-A	97	ARG	CG-CD	14.13	1.87	1.51
1	6-A	81	PRO	C-O	14.10	1.51	1.23
1	14-A	67	TRP	CE3-CZ3	-14.07	1.14	1.38
1	13-A	92	ARG	CD-NE	14.03	1.70	1.46
1	15-A	87	ASN	CB-CG	14.03	1.83	1.51
1	10-A	46	GLN	CB-CG	14.01	1.90	1.52
1	15-A	55	PRO	CG-CD	13.99	1.96	1.50
1	3-A	106	ARG	CZ-NH1	13.97	1.51	1.33
1	11-A	61	LEU	CA-CB	13.97	1.85	1.53
1	13-A	40	ARG	CG-CD	13.97	1.86	1.51
1	4-A	97	ARG	NE-CZ	13.96	1.51	1.33
1	1-A	38	LEU	CG-CD1	13.96	2.03	1.51
1	14-A	93	TRP	CZ3-CH2	13.95	1.62	1.40
1	2-A	154	PHE	CD1-CE1	13.93	1.67	1.39
1	8-A	76	GLN	C-O	13.93	1.49	1.23
1	11-A	50	LYS	CE-NZ	13.92	1.83	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-A	81	PRO	CB-CG	13.91	2.19	1.50
1	10-A	64	PHE	CG-CD2	13.90	1.59	1.38
1	16-A	67	TRP	CE3-CZ3	-13.86	1.14	1.38
1	15-A	37	SER	CB-OG	-13.84	1.24	1.42
1	15-A	118	ALA	CA-CB	13.82	1.81	1.52
1	13-A	109	SER	CA-CB	13.80	1.73	1.52
1	13-A	40	ARG	CZ-NH2	13.75	1.50	1.33
1	4-A	106	ARG	CZ-NH1	13.73	1.50	1.33
1	13-A	43	GLU	CG-CD	13.72	1.72	1.51
1	14-A	125	GLU	CB-CG	13.69	1.78	1.52
1	14-A	40	ARG	CG-CD	13.66	1.86	1.51
1	15-A	36	GLY	N-CA	13.63	1.66	1.46
1	15-A	40	ARG	CZ-NH2	13.61	1.50	1.33
1	15-A	56	THR	CA-CB	13.60	1.88	1.53
1	16-A	85	LEU	N-CA	13.60	1.73	1.46
1	10-A	68	VAL	CB-CG1	13.59	1.81	1.52
1	16-A	108	ASP	CB-CG	13.58	1.80	1.51
1	14-A	45	TYR	CG-CD1	13.53	1.56	1.39
1	1-A	50	LYS	CE-NZ	13.51	1.82	1.49
1	15-A	43	GLU	CG-CD	13.51	1.72	1.51
1	14-A	45	TYR	CE2-CZ	13.50	1.56	1.38
1	3-A	103	GLU	CB-CG	13.49	1.77	1.52
1	6-A	37	SER	CB-OG	-13.49	1.24	1.42
1	15-A	97	ARG	CZ-NH2	13.44	1.50	1.33
1	4-A	64	PHE	CE1-CZ	13.44	1.62	1.37
1	5-A	40	ARG	CG-CD	13.44	1.85	1.51
1	1-A	128	ARG	CB-CG	13.43	1.88	1.52
1	14-A	86	THR	CB-CG2	13.41	1.96	1.52
1	6-A	78	TYR	CG-CD1	13.40	1.56	1.39
1	13-A	123	VAL	CB-CG1	13.40	1.81	1.52
1	5-A	52	VAL	CB-CG1	13.39	1.80	1.52
1	9-A	123	VAL	CB-CG1	13.39	1.80	1.52
1	11-A	58	ARG	CZ-NH1	13.39	1.50	1.33
1	14-A	48	TYR	CE2-CZ	-13.37	1.21	1.38
1	14-A	102	SER	CB-OG	-13.35	1.24	1.42
1	5-A	58	ARG	CZ-NH2	13.34	1.50	1.33
1	10-A	109	SER	CA-CB	13.34	1.73	1.52
1	3-A	68	VAL	CB-CG1	13.34	1.80	1.52
1	8-A	58	ARG	CZ-NH2	13.33	1.50	1.33
1	6-A	106	ARG	CZ-NH1	13.31	1.50	1.33
1	15-A	86	THR	CB-CG2	13.29	1.96	1.52
1	15-A	83	HIS	CA-CB	13.28	1.83	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	10-A	123	VAL	CA-CB	13.28	1.82	1.54
1	16-A	122	LEU	CG-CD1	13.27	2.00	1.51
1	11-A	40	ARG	CD-NE	-13.27	1.23	1.46
1	15-A	131	PRO	CG-CD	13.24	1.94	1.50
1	9-A	43	GLU	CG-CD	13.23	1.71	1.51
1	15-A	58	ARG	CB-CG	13.23	1.88	1.52
1	16-A	85	LEU	CG-CD2	13.23	2.00	1.51
1	16-A	37	SER	CB-OG	-13.23	1.25	1.42
1	11-A	106	ARG	CB-CG	13.19	1.88	1.52
1	11-A	78	TYR	CE2-CZ	13.17	1.55	1.38
1	14-A	98	PHE	CE1-CZ	13.16	1.62	1.37
1	6-A	43	GLU	CG-CD	13.15	1.71	1.51
1	8-A	148	SER	CA-CB	13.15	1.72	1.52
1	16-A	40	ARG	CG-CD	13.14	1.84	1.51
1	6-A	40	ARG	CZ-NH2	13.14	1.50	1.33
1	14-A	125	GLU	N-CA	13.13	1.72	1.46
1	2-A	154	PHE	CE1-CZ	13.13	1.62	1.37
1	11-A	41	ARG	CD-NE	13.13	1.68	1.46
1	14-A	117	GLU	CB-CG	13.13	1.77	1.52
1	1-A	76	GLN	C-O	13.12	1.48	1.23
1	4-A	64	PHE	CA-CB	13.08	1.82	1.53
1	10-A	64	PHE	CG-CD1	13.07	1.58	1.38
1	2-A	44	MET	CG-SD	13.07	2.15	1.81
1	3-A	40	ARG	CA-CB	13.05	1.82	1.53
1	4-A	37	SER	CB-OG	-13.04	1.25	1.42
1	11-A	89	LEU	CA-CB	13.02	1.83	1.53
1	2-A	106	ARG	CZ-NH1	13.02	1.50	1.33
1	12-A	84	TYR	CD1-CE1	13.02	1.58	1.39
1	8-A	68	VAL	CB-CG2	13.01	1.80	1.52
1	1-A	98	PHE	CD1-CE1	-13.00	1.13	1.39
1	9-A	106	ARG	CZ-NH1	13.00	1.50	1.33
1	10-A	119	THR	CA-CB	13.00	1.87	1.53
1	13-A	67	TRP	CB-CG	12.98	1.73	1.50
1	8-A	38	LEU	CG-CD1	12.95	1.99	1.51
1	9-A	109	SER	CB-OG	12.94	1.59	1.42
1	13-A	90	LEU	C-O	12.93	1.48	1.23
1	1-A	125	GLU	CD-OE2	12.93	1.39	1.25
1	4-A	151	ASP	C-O	-12.90	0.98	1.23
1	3-A	115	LYS	CD-CE	12.90	1.83	1.51
1	8-A	67	TRP	CE3-CZ3	12.89	1.60	1.38
1	7-A	92	ARG	CZ-NH2	12.88	1.49	1.33
1	4-A	43	GLU	CG-CD	12.87	1.71	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	121	TRP	CD1-NE1	12.86	1.59	1.38
1	9-A	124	GLU	CA-CB	12.85	1.82	1.53
1	13-A	84	TYR	CD1-CE1	-12.83	1.20	1.39
1	2-A	76	GLN	CD-OE1	-12.82	0.95	1.24
1	10-A	141	ARG	CG-CD	12.82	1.84	1.51
1	1-A	78	TYR	CD1-CE1	12.81	1.58	1.39
1	4-A	77	LEU	CB-CG	12.80	1.89	1.52
1	10-A	74	MET	CB-CG	12.80	1.92	1.51
1	4-A	40	ARG	CA-CB	12.76	1.82	1.53
1	16-A	83	HIS	CB-CG	12.73	1.73	1.50
1	5-A	40	ARG	CZ-NH1	12.71	1.49	1.33
1	14-A	64	PHE	CA-C	-12.71	1.20	1.52
1	5-A	47	ASP	C-O	12.70	1.47	1.23
1	13-A	60	SER	CA-CB	12.70	1.72	1.52
1	15-A	67	TRP	CD2-CE3	12.69	1.59	1.40
1	15-A	48	TYR	CE2-CZ	-12.64	1.22	1.38
1	16-A	113	PRO	CA-CB	12.61	1.78	1.53
1	15-A	96	SER	C-O	12.61	1.47	1.23
1	1-A	40	ARG	CG-CD	12.59	1.83	1.51
1	1-A	64	PHE	CA-CB	12.58	1.81	1.53
1	3-A	105	GLN	CG-CD	12.58	1.79	1.51
1	15-A	78	TYR	CE1-CZ	12.56	1.54	1.38
1	15-A	127	HIS	CA-CB	12.56	1.81	1.53
1	8-A	66	SER	N-CA	12.55	1.71	1.46
1	1-A	140	TRP	CZ3-CH2	12.53	1.60	1.40
1	8-A	67	TRP	CZ3-CH2	12.51	1.60	1.40
1	14-A	50	LYS	N-CA	12.51	1.71	1.46
1	2-A	66	SER	CB-OG	12.51	1.58	1.42
1	11-A	50	LYS	CG-CD	12.50	1.95	1.52
1	13-A	133	HIS	C-O	12.49	1.47	1.23
1	16-A	115	LYS	CA-CB	12.48	1.81	1.53
1	12-A	97	ARG	NE-CZ	12.48	1.49	1.33
1	5-A	76	GLN	CD-OE1	-12.46	0.96	1.24
1	16-A	144	PRO	CA-C	12.46	1.77	1.52
1	1-A	53	PRO	CG-CD	12.43	1.91	1.50
1	10-A	40	ARG	CG-CD	12.42	1.82	1.51
1	3-A	88	VAL	CB-CG1	12.40	1.78	1.52
1	4-A	78	TYR	CD1-CE1	12.40	1.57	1.39
1	16-A	144	PRO	C-N	12.39	1.62	1.34
1	16-A	44	MET	CA-CB	12.35	1.81	1.53
1	14-A	117	GLU	CD-OE1	12.33	1.39	1.25
1	6-A	148	SER	CA-CB	12.32	1.71	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	10-A	64	PHE	CA-CB	12.32	1.81	1.53
1	10-A	100	THR	C-O	12.32	1.46	1.23
1	9-A	133	HIS	C-O	12.31	1.46	1.23
1	13-A	44	MET	CA-CB	12.31	1.81	1.53
1	15-A	50	LYS	CG-CD	12.31	1.94	1.52
1	16-A	145	MET	CG-SD	12.30	2.13	1.81
1	16-A	149	PHE	CD1-CE1	12.28	1.63	1.39
1	5-A	106	ARG	CZ-NH1	12.28	1.49	1.33
1	12-A	76	GLN	C-O	12.27	1.46	1.23
1	8-A	55	PRO	CG-CD	12.27	1.91	1.50
1	13-A	135	HIS	C-O	12.26	1.46	1.23
1	9-A	129	LEU	CG-CD2	12.24	1.97	1.51
1	4-A	128	ARG	CZ-NH1	12.21	1.49	1.33
1	14-A	64	PHE	CB-CG	12.18	1.72	1.51
1	3-A	109	SER	CB-OG	12.17	1.58	1.42
1	16-A	150	ILE	CB-CG2	12.16	1.90	1.52
1	8-A	37	SER	CB-OG	12.16	1.58	1.42
1	13-A	65	THR	C-O	12.15	1.46	1.23
1	14-A	145	MET	CG-SD	-12.15	1.49	1.81
1	9-A	37	SER	CA-CB	12.15	1.71	1.52
1	11-A	141	ARG	NE-CZ	-12.13	1.17	1.33
1	16-A	93	TRP	CD2-CE3	12.12	1.58	1.40
1	9-A	88	VAL	CB-CG1	12.11	1.78	1.52
1	10-A	106	ARG	CZ-NH1	12.11	1.48	1.33
1	14-A	127	HIS	CA-CB	12.09	1.80	1.53
1	3-A	88	VAL	CB-CG2	12.07	1.78	1.52
1	2-A	75	LYS	CB-CG	12.06	1.85	1.52
1	4-A	123	VAL	CB-CG2	12.06	1.78	1.52
1	12-A	109	SER	CB-OG	-12.06	1.26	1.42
1	3-A	127	HIS	C-O	12.04	1.46	1.23
1	2-A	125	GLU	CD-OE1	12.04	1.38	1.25
1	10-A	42	ALA	C-O	12.03	1.46	1.23
1	6-A	74	MET	CB-CG	12.02	1.89	1.51
1	6-A	145	MET	C-O	12.02	1.46	1.23
1	10-A	50	LYS	CE-NZ	12.01	1.79	1.49
1	16-A	146	TYR	CZ-OH	11.99	1.58	1.37
1	16-A	92	ARG	C-O	11.96	1.46	1.23
1	7-A	109	SER	CA-CB	11.95	1.70	1.52
1	9-A	92	ARG	CZ-NH1	-11.95	1.17	1.33
1	15-A	55	PRO	N-CD	11.94	1.64	1.47
1	16-A	60	SER	CA-CB	11.93	1.70	1.52
1	8-A	107	LEU	C-O	11.92	1.46	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	41	ARG	C-O	-11.92	1.00	1.23
1	14-A	136	MET	CB-CG	-11.91	1.13	1.51
1	12-A	109	SER	CA-CB	11.91	1.70	1.52
1	16-A	84	TYR	CG-CD1	11.91	1.54	1.39
1	13-A	122	LEU	CA-CB	11.90	1.81	1.53
1	10-A	125	GLU	CD-OE2	11.90	1.38	1.25
1	16-A	154	PHE	CG-CD2	11.90	1.56	1.38
1	3-A	97	ARG	CB-CG	11.90	1.84	1.52
1	15-A	97	ARG	CG-CD	11.89	1.81	1.51
1	15-A	60	SER	CA-CB	11.89	1.70	1.52
1	12-A	105	GLN	CG-CD	11.88	1.78	1.51
1	13-A	104	GLU	CD-OE1	11.88	1.38	1.25
1	9-A	40	ARG	CD-NE	11.86	1.66	1.46
1	15-A	97	ARG	CB-CG	11.86	1.84	1.52
1	7-A	98	PHE	CD1-CE1	-11.85	1.15	1.39
1	16-A	85	LEU	CA-CB	11.84	1.80	1.53
1	14-A	98	PHE	CD1-CE1	-11.83	1.15	1.39
1	4-A	40	ARG	CG-CD	11.83	1.81	1.51
1	6-A	36	GLY	N-CA	11.78	1.63	1.46
1	7-A	76	GLN	CD-OE1	-11.78	0.98	1.24
1	13-A	97	ARG	CZ-NH2	11.78	1.48	1.33
1	14-A	95	GLN	CD-OE1	11.78	1.49	1.24
1	3-A	149	PHE	CD2-CE2	11.76	1.62	1.39
1	14-A	130	THR	CB-OG1	11.74	1.66	1.43
1	2-A	107	LEU	N-CA	11.74	1.69	1.46
1	7-A	97	ARG	CB-CG	11.73	1.84	1.52
1	15-A	98	PHE	N-CA	11.71	1.69	1.46
1	2-A	67	TRP	CE3-CZ3	-11.71	1.18	1.38
1	16-A	67	TRP	CA-C	11.69	1.83	1.52
1	14-A	156	GLU	CD-OE1	-11.68	1.12	1.25
1	11-A	53	PRO	CG-CD	11.66	1.89	1.50
1	14-A	85	LEU	CB-CG	11.66	1.86	1.52
1	3-A	61	LEU	CG-CD1	11.65	1.95	1.51
1	10-A	43	GLU	C-O	11.65	1.45	1.23
1	14-A	60	SER	CA-CB	11.64	1.70	1.52
1	16-A	68	VAL	C-O	11.64	1.45	1.23
1	13-A	48	TYR	CD1-CE1	-11.62	1.22	1.39
1	15-A	85	LEU	C-O	11.62	1.45	1.23
1	4-A	40	ARG	CZ-NH2	11.61	1.48	1.33
1	13-A	141	ARG	CZ-NH1	11.61	1.48	1.33
1	15-A	72	ILE	CB-CG2	11.61	1.88	1.52
1	7-A	91	GLN	CB-CG	11.61	1.83	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-A	107	LEU	C-O	11.61	1.45	1.23
1	14-A	62	ILE	N-CA	-11.60	1.23	1.46
1	9-A	39	LEU	CG-CD1	11.59	1.94	1.51
1	13-A	76	GLN	C-O	11.59	1.45	1.23
1	16-A	141	ARG	C-O	11.58	1.45	1.23
1	1-A	43	GLU	CG-CD	11.55	1.69	1.51
1	7-A	143	ASP	CB-CG	11.55	1.76	1.51
1	1-A	91	GLN	CD-OE1	11.54	1.49	1.24
1	3-A	37	SER	CB-OG	-11.53	1.27	1.42
1	15-A	82	LEU	C-O	11.54	1.45	1.23
1	9-A	93	TRP	CZ3-CH2	11.53	1.58	1.40
1	1-A	113	PRO	C-O	11.53	1.46	1.23
1	4-A	155	PRO	CG-CD	11.52	1.88	1.50
1	15-A	120	ILE	CB-CG2	11.52	1.88	1.52
1	11-A	63	PRO	CA-CB	11.52	1.76	1.53
1	15-A	40	ARG	CA-CB	11.52	1.79	1.53
1	11-A	113	PRO	CA-CB	11.51	1.76	1.53
1	11-A	63	PRO	C-O	11.50	1.46	1.23
1	4-A	80	GLN	C-O	11.49	1.45	1.23
1	11-A	105	GLN	CG-CD	11.49	1.77	1.51
1	5-A	138	LEU	CG-CD1	11.48	1.94	1.51
1	1-A	118	ALA	CA-CB	11.46	1.76	1.52
1	14-A	70	LEU	CG-CD2	11.46	1.94	1.51
1	16-A	147	HIS	CA-CB	11.45	1.79	1.53
1	16-A	40	ARG	CA-CB	11.45	1.79	1.53
1	8-A	40	ARG	CG-CD	11.42	1.80	1.51
1	14-A	106	ARG	C-O	11.40	1.45	1.23
1	1-A	135	HIS	CA-CB	11.38	1.78	1.53
1	14-A	123	VAL	N-CA	11.38	1.69	1.46
1	8-A	107	LEU	CG-CD1	11.37	1.94	1.51
1	15-A	141	ARG	CZ-NH1	11.35	1.47	1.33
1	12-A	95	GLN	CD-OE1	11.35	1.49	1.24
1	2-A	98	PHE	CG-CD2	11.34	1.55	1.38
1	16-A	149	PHE	CG-CD1	11.34	1.55	1.38
1	13-A	40	ARG	CA-CB	11.33	1.78	1.53
1	13-A	46	GLN	CD-NE2	11.33	1.61	1.32
1	14-A	135	HIS	CA-C	11.32	1.82	1.52
1	15-A	76	GLN	C-O	11.32	1.44	1.23
1	16-A	122	LEU	CG-CD2	11.32	1.93	1.51
1	2-A	60	SER	CB-OG	11.30	1.56	1.42
1	7-A	117	GLU	CB-CG	11.30	1.73	1.52
1	13-A	66	SER	C-O	11.29	1.44	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-A	125	GLU	N-CA	11.29	1.69	1.46
1	15-A	105	GLN	CG-CD	11.27	1.76	1.51
1	5-A	128	ARG	CZ-NH1	11.27	1.47	1.33
1	8-A	58	ARG	CB-CG	11.27	1.82	1.52
1	16-A	45	TYR	CE1-CZ	11.26	1.53	1.38
1	13-A	45	TYR	N-CA	11.25	1.68	1.46
1	1-A	92	ARG	CZ-NH2	11.24	1.47	1.33
1	16-A	47	ASP	CB-CG	-11.24	1.28	1.51
1	15-A	121	TRP	CA-CB	11.24	1.78	1.53
1	8-A	36	GLY	C-O	11.23	1.41	1.23
1	2-A	71	SER	C-O	-11.22	1.02	1.23
1	7-A	109	SER	CB-OG	-11.21	1.27	1.42
1	4-A	95	GLN	CD-OE1	11.20	1.48	1.24
1	11-A	63	PRO	CG-CD	11.20	1.87	1.50
1	11-A	87	ASN	CG-OD1	-11.19	0.99	1.24
1	14-A	40	ARG	CA-CB	11.19	1.78	1.53
1	12-A	37	SER	CB-OG	-11.19	1.27	1.42
1	16-A	140	TRP	CZ3-CH2	11.18	1.57	1.40
1	10-A	66	SER	CB-OG	11.17	1.56	1.42
1	16-A	141	ARG	CZ-NH1	11.17	1.47	1.33
1	14-A	76	GLN	C-O	11.16	1.44	1.23
1	7-A	96	SER	CA-C	11.15	1.81	1.52
1	4-A	104	GLU	CD-OE1	11.13	1.37	1.25
1	1-A	154	PHE	CD1-CE1	11.12	1.61	1.39
1	2-A	107	LEU	C-O	11.12	1.44	1.23
1	3-A	40	ARG	CZ-NH2	11.12	1.47	1.33
1	9-A	121	TRP	CE3-CZ3	11.12	1.57	1.38
1	8-A	43	GLU	CG-CD	11.11	1.68	1.51
1	12-A	76	GLN	CD-OE1	-11.11	0.99	1.24
1	10-A	45	TYR	CG-CD1	11.11	1.53	1.39
1	6-A	82	LEU	CG-CD1	11.10	1.93	1.51
1	10-A	40	ARG	CA-CB	11.10	1.78	1.53
1	15-A	154	PHE	CG-CD2	11.10	1.55	1.38
1	16-A	146	TYR	C-O	11.10	1.44	1.23
1	4-A	124	GLU	CA-CB	11.10	1.78	1.53
1	2-A	106	ARG	C-O	-11.09	1.02	1.23
1	9-A	88	VAL	CB-CG2	11.08	1.76	1.52
1	5-A	40	ARG	CA-CB	11.08	1.78	1.53
1	15-A	140	TRP	CD2-CE2	11.08	1.54	1.41
1	14-A	152	PRO	CG-CD	11.06	1.87	1.50
1	3-A	102	SER	CA-CB	11.05	1.69	1.52
1	16-A	98	PHE	CE1-CZ	11.04	1.58	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	75	LYS	CE-NZ	11.04	1.76	1.49
1	4-A	69	GLY	CA-C	11.03	1.69	1.51
1	10-A	95	GLN	CD-OE1	11.03	1.48	1.24
1	11-A	78	TYR	CG-CD2	11.02	1.53	1.39
1	5-A	80	GLN	CD-NE2	11.02	1.60	1.32
1	16-A	67	TRP	CA-CB	11.02	1.78	1.53
1	16-A	67	TRP	CG-CD1	11.02	1.52	1.36
1	2-A	138	LEU	CB-CG	-11.01	1.20	1.52
1	16-A	129	LEU	CG-CD1	11.01	1.92	1.51
1	13-A	67	TRP	CD2-CE3	10.98	1.56	1.40
1	13-A	134	LEU	CA-CB	10.98	1.78	1.53
1	4-A	93	TRP	CZ3-CH2	10.97	1.57	1.40
1	2-A	51	GLN	CG-CD	10.97	1.76	1.51
1	13-A	36	GLY	N-CA	10.97	1.62	1.46
1	11-A	146	TYR	CD1-CE1	10.97	1.55	1.39
1	14-A	149	PHE	CD2-CE2	10.96	1.61	1.39
1	11-A	112	HIS	CA-CB	-10.95	1.29	1.53
1	11-A	107	LEU	CG-CD1	10.95	1.92	1.51
1	15-A	127	HIS	CB-CG	10.94	1.69	1.50
1	11-A	37	SER	CB-OG	-10.92	1.28	1.42
1	8-A	50	LYS	CG-CD	10.91	1.89	1.52
1	3-A	60	SER	CA-CB	10.91	1.69	1.52
1	9-A	93	TRP	CZ2-CH2	10.90	1.58	1.37
1	8-A	53	PRO	N-CD	10.90	1.63	1.47
1	1-A	141	ARG	CZ-NH1	10.89	1.47	1.33
1	16-A	49	MET	SD-CE	-10.89	1.16	1.77
1	7-A	98	PHE	N-CA	10.89	1.68	1.46
1	15-A	104	GLU	CG-CD	-10.88	1.35	1.51
1	1-A	39	LEU	CA-CB	10.87	1.78	1.53
1	15-A	84	TYR	CD1-CE1	-10.86	1.23	1.39
1	4-A	64	PHE	CD1-CE1	10.86	1.60	1.39
1	16-A	155	PRO	CG-CD	10.84	1.86	1.50
1	7-A	40	ARG	CA-CB	10.83	1.77	1.53
1	15-A	82	LEU	CA-C	10.83	1.81	1.52
1	13-A	140	TRP	CZ3-CH2	10.83	1.57	1.40
1	15-A	51	GLN	CB-CG	-10.82	1.23	1.52
1	12-A	43	GLU	CD-OE2	-10.81	1.13	1.25
1	9-A	40	ARG	CA-CB	10.80	1.77	1.53
1	2-A	58	ARG	CB-CG	10.80	1.81	1.52
1	13-A	92	ARG	CB-CG	10.80	1.81	1.52
1	14-A	85	LEU	CG-CD2	10.79	1.91	1.51
1	6-A	40	ARG	CA-CB	10.78	1.77	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	13-A	98	PHE	CE1-CZ	10.78	1.57	1.37
1	6-A	84	TYR	CG-CD2	10.77	1.53	1.39
1	16-A	93	TRP	CG-CD2	10.77	1.61	1.43
1	10-A	40	ARG	CZ-NH1	10.76	1.47	1.33
1	14-A	59	GLY	CA-C	-10.76	1.34	1.51
1	15-A	42	ALA	CA-CB	10.76	1.75	1.52
1	3-A	36	GLY	N-CA	10.76	1.62	1.46
1	11-A	61	LEU	CG-CD2	10.76	1.91	1.51
1	16-A	71	SER	CA-CB	10.75	1.69	1.52
1	1-A	154	PHE	CE1-CZ	10.75	1.57	1.37
1	2-A	65	THR	C-O	10.75	1.43	1.23
1	15-A	110	ILE	N-CA	10.74	1.67	1.46
1	2-A	141	ARG	NE-CZ	-10.74	1.19	1.33
1	13-A	145	MET	CG-SD	-10.74	1.53	1.81
1	1-A	44	MET	CA-CB	10.74	1.77	1.53
1	7-A	117	GLU	CD-OE2	10.74	1.37	1.25
1	3-A	140	TRP	CZ3-CH2	10.73	1.57	1.40
1	11-A	40	ARG	C-O	-10.73	1.02	1.23
1	11-A	37	SER	CA-CB	-10.72	1.36	1.52
1	11-A	61	LEU	C-O	10.72	1.43	1.23
1	12-A	150	ILE	CB-CG2	10.72	1.86	1.52
1	8-A	64	PHE	CE1-CZ	10.70	1.57	1.37
1	11-A	64	PHE	CG-CD2	10.70	1.54	1.38
1	16-A	108	ASP	CA-CB	10.69	1.77	1.53
1	14-A	123	VAL	CB-CG1	10.68	1.75	1.52
1	1-A	155	PRO	CG-CD	10.68	1.85	1.50
1	10-A	98	PHE	CE1-CZ	10.68	1.57	1.37
1	16-A	115	LYS	N-CA	10.68	1.67	1.46
1	13-A	48	TYR	CB-CG	-10.67	1.35	1.51
1	15-A	50	LYS	CA-CB	10.66	1.77	1.53
1	11-A	102	SER	CB-OG	-10.64	1.28	1.42
1	4-A	98	PHE	CE1-CZ	10.63	1.57	1.37
1	12-A	155	PRO	CG-CD	10.63	1.85	1.50
1	2-A	105	GLN	CA-C	10.63	1.80	1.52
1	13-A	45	TYR	CD1-CE1	10.62	1.55	1.39
1	4-A	79	GLY	CA-C	-10.61	1.34	1.51
1	15-A	97	ARG	CZ-NH1	10.61	1.46	1.33
1	5-A	95	GLN	CD-OE1	10.60	1.47	1.24
1	2-A	58	ARG	CZ-NH2	10.59	1.46	1.33
1	8-A	67	TRP	CD2-CE2	10.59	1.54	1.41
1	13-A	51	GLN	CD-OE1	10.58	1.47	1.24
1	9-A	121	TRP	CD2-CE3	10.57	1.56	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	12-A	40	ARG	CA-CB	10.57	1.77	1.53
1	11-A	87	ASN	CG-ND2	10.56	1.59	1.32
1	8-A	106	ARG	CB-CG	10.56	1.81	1.52
1	10-A	150	ILE	CB-CG2	10.55	1.85	1.52
1	7-A	96	SER	N-CA	10.54	1.67	1.46
1	5-A	42	ALA	C-O	10.53	1.43	1.23
1	15-A	123	VAL	CA-C	10.52	1.80	1.52
1	1-A	104	GLU	CD-OE1	10.50	1.37	1.25
1	15-A	67	TRP	CD2-CE2	10.50	1.53	1.41
1	11-A	89	LEU	CB-CG	10.50	1.82	1.52
1	4-A	70	LEU	CG-CD1	10.49	1.90	1.51
1	5-A	41	ARG	CZ-NH2	10.48	1.46	1.33
1	15-A	81	PRO	CB-CG	10.48	2.02	1.50
1	1-A	76	GLN	CD-OE1	-10.46	1.00	1.24
1	9-A	76	GLN	CG-CD	-10.46	1.26	1.51
1	1-A	106	ARG	CZ-NH1	10.46	1.46	1.33
1	9-A	137	ALA	CA-CB	10.46	1.74	1.52
1	16-A	46	GLN	CD-OE1	10.44	1.47	1.24
1	5-A	93	TRP	CZ2-CH2	10.44	1.57	1.37
1	8-A	67	TRP	CA-CB	10.44	1.76	1.53
1	5-A	60	SER	CB-OG	10.43	1.55	1.42
1	9-A	155	PRO	CG-CD	10.42	1.85	1.50
1	16-A	98	PHE	CD1-CE1	-10.42	1.18	1.39
1	7-A	128	ARG	CZ-NH1	10.41	1.46	1.33
1	11-A	87	ASN	CB-CG	10.41	1.75	1.51
1	9-A	61	LEU	N-CA	10.41	1.67	1.46
1	12-A	98	PHE	CE1-CZ	10.41	1.57	1.37
1	13-A	90	LEU	CA-CB	10.39	1.77	1.53
1	9-A	141	ARG	CG-CD	10.39	1.77	1.51
1	2-A	77	LEU	CG-CD1	-10.38	1.13	1.51
1	14-A	104	GLU	CB-CG	-10.38	1.32	1.52
1	16-A	122	LEU	CB-CG	10.38	1.82	1.52
1	11-A	91	GLN	CD-OE1	10.37	1.46	1.24
1	13-A	125	GLU	CB-CG	10.37	1.71	1.52
1	13-A	93	TRP	CZ3-CH2	10.36	1.56	1.40
1	15-A	80	GLN	CB-CG	-10.35	1.24	1.52
1	16-A	106	ARG	C-O	10.35	1.43	1.23
1	5-A	98	PHE	CE1-CZ	10.34	1.57	1.37
1	9-A	104	GLU	CD-OE1	10.34	1.37	1.25
1	14-A	51	GLN	CD-OE1	10.34	1.46	1.24
1	10-A	121	TRP	CD1-NE1	10.34	1.55	1.38
1	14-A	156	GLU	C-O	10.34	1.43	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9-A	50	LYS	C-O	10.34	1.43	1.23
1	2-A	104	GLU	CB-CG	10.33	1.71	1.52
1	13-A	93	TRP	CE3-CZ3	10.33	1.56	1.38
1	13-A	42	ALA	CA-CB	10.33	1.74	1.52
1	14-A	36	GLY	C-O	10.32	1.40	1.23
1	1-A	40	ARG	CZ-NH2	10.31	1.46	1.33
1	16-A	73	SER	C-O	10.31	1.43	1.23
1	14-A	150	ILE	CB-CG2	-10.30	1.21	1.52
1	13-A	59	GLY	CA-C	-10.29	1.35	1.51
1	1-A	141	ARG	CG-CD	10.29	1.77	1.51
1	13-A	89	LEU	CG-CD1	10.29	1.90	1.51
1	8-A	45	TYR	CD2-CE2	10.29	1.54	1.39
1	2-A	109	SER	CB-OG	10.29	1.55	1.42
1	9-A	106	ARG	CZ-NH2	10.28	1.46	1.33
1	6-A	117	GLU	CD-OE2	10.28	1.36	1.25
1	5-A	93	TRP	CA-CB	10.27	1.76	1.53
1	16-A	36	GLY	C-O	10.27	1.40	1.23
1	2-A	50	LYS	CG-CD	10.27	1.87	1.52
1	9-A	106	ARG	C-O	-10.27	1.03	1.23
1	11-A	114	THR	CB-OG1	10.25	1.63	1.43
1	1-A	121	TRP	C-O	10.24	1.42	1.23
1	15-A	82	LEU	CG-CD2	10.24	1.89	1.51
1	1-A	154	PHE	CG-CD1	10.23	1.54	1.38
1	12-A	117	GLU	CG-CD	10.23	1.67	1.51
1	2-A	98	PHE	CD2-CE2	10.23	1.59	1.39
1	10-A	50	LYS	CG-CD	10.22	1.87	1.52
1	16-A	86	THR	N-CA	-10.22	1.25	1.46
1	5-A	58	ARG	CB-CG	10.21	1.80	1.52
1	14-A	124	GLU	C-O	10.21	1.42	1.23
1	14-A	146	TYR	CB-CG	10.21	1.67	1.51
1	2-A	40	ARG	CA-CB	10.20	1.76	1.53
1	15-A	81	PRO	C-N	-10.20	1.10	1.34
1	7-A	141	ARG	CG-CD	10.19	1.77	1.51
1	2-A	117	GLU	CD-OE1	10.18	1.36	1.25
1	8-A	40	ARG	CZ-NH2	10.18	1.46	1.33
1	14-A	54	ILE	C-O	10.18	1.42	1.23
1	16-A	104	GLU	CB-CG	-10.17	1.32	1.52
1	11-A	107	LEU	CB-CG	10.15	1.81	1.52
1	16-A	78	TYR	CE1-CZ	-10.14	1.25	1.38
1	8-A	63	PRO	N-CA	10.14	1.64	1.47
1	13-A	67	TRP	CA-CB	10.14	1.76	1.53
1	6-A	104	GLU	CG-CD	10.14	1.67	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	50	LYS	CG-CD	10.13	1.86	1.52
1	11-A	62	ILE	CB-CG2	10.13	1.84	1.52
1	2-A	46	GLN	CD-OE1	10.12	1.46	1.24
1	14-A	85	LEU	C-O	10.11	1.42	1.23
1	3-A	59	GLY	CA-C	-10.11	1.35	1.51
1	14-A	56	THR	CA-CB	10.11	1.79	1.53
1	4-A	151	ASP	CG-OD1	10.10	1.48	1.25
1	14-A	126	ILE	N-CA	10.10	1.66	1.46
1	10-A	128	ARG	CA-C	10.09	1.79	1.52
1	5-A	53	PRO	N-CD	10.08	1.61	1.47
1	4-A	64	PHE	CG-CD2	10.07	1.53	1.38
1	11-A	146	TYR	CZ-OH	10.07	1.54	1.37
1	10-A	123	VAL	CB-CG1	10.07	1.74	1.52
1	9-A	76	GLN	CD-NE2	10.07	1.58	1.32
1	11-A	109	SER	CA-C	10.07	1.79	1.52
1	16-A	85	LEU	C-N	10.06	1.57	1.34
1	13-A	123	VAL	CA-CB	10.05	1.75	1.54
1	8-A	105	GLN	CG-CD	10.05	1.74	1.51
1	9-A	76	GLN	C-O	10.03	1.42	1.23
1	4-A	98	PHE	CD1-CE1	-10.01	1.19	1.39
1	12-A	141	ARG	CZ-NH1	10.00	1.46	1.33
1	15-A	59	GLY	N-CA	10.00	1.61	1.46
1	6-A	98	PHE	CE1-CZ	9.99	1.56	1.37
1	14-A	140	TRP	CD2-CE2	9.99	1.53	1.41
1	11-A	144	PRO	N-CA	9.98	1.64	1.47
1	16-A	149	PHE	CE2-CZ	9.98	1.56	1.37
1	8-A	125	GLU	CD-OE2	9.96	1.36	1.25
1	15-A	78	TYR	CD1-CE1	-9.96	1.24	1.39
1	15-A	59	GLY	C-O	9.96	1.39	1.23
1	7-A	43	GLU	CD-OE2	-9.95	1.14	1.25
1	2-A	106	ARG	CB-CG	9.95	1.79	1.52
1	14-A	84	TYR	CD2-CE2	9.95	1.54	1.39
1	15-A	84	TYR	C-N	9.95	1.56	1.34
1	9-A	98	PHE	CE1-CZ	9.94	1.56	1.37
1	11-A	104	GLU	CB-CG	-9.94	1.33	1.52
1	16-A	150	ILE	C-O	9.94	1.42	1.23
1	13-A	156	GLU	C-O	9.93	1.42	1.23
1	2-A	102	SER	CB-OG	-9.93	1.29	1.42
1	14-A	125	GLU	CG-CD	-9.93	1.37	1.51
1	9-A	84	TYR	CZ-OH	-9.93	1.21	1.37
1	8-A	36	GLY	N-CA	9.92	1.60	1.46
1	15-A	98	PHE	CD2-CE2	9.91	1.59	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	155	PRO	CG-CD	9.91	1.83	1.50
1	16-A	86	THR	CA-C	9.91	1.78	1.52
1	16-A	67	TRP	CD1-NE1	9.90	1.54	1.38
1	16-A	129	LEU	C-O	9.90	1.42	1.23
1	11-A	144	PRO	C-O	9.89	1.43	1.23
1	2-A	77	LEU	CA-CB	9.89	1.76	1.53
1	2-A	75	LYS	CD-CE	9.88	1.75	1.51
1	13-A	54	ILE	C-O	9.88	1.42	1.23
1	13-A	61	LEU	C-O	9.88	1.42	1.23
1	15-A	47	ASP	C-O	9.88	1.42	1.23
1	8-A	53	PRO	CA-CB	9.87	1.73	1.53
1	6-A	146	TYR	CG-CD2	-9.87	1.26	1.39
1	3-A	92	ARG	CZ-NH2	9.87	1.45	1.33
1	16-A	71	SER	C-O	-9.87	1.04	1.23
1	10-A	98	PHE	CD1-CE1	-9.86	1.19	1.39
1	15-A	54	ILE	CA-CB	9.86	1.77	1.54
1	14-A	59	GLY	C-O	9.85	1.39	1.23
1	14-A	118	ALA	N-CA	9.85	1.66	1.46
1	15-A	113	PRO	CG-CD	9.84	1.83	1.50
1	10-A	76	GLN	C-O	9.83	1.42	1.23
1	12-A	40	ARG	CG-CD	9.81	1.76	1.51
1	2-A	40	ARG	CG-CD	9.81	1.76	1.51
1	10-A	135	HIS	CA-CB	9.81	1.75	1.53
1	6-A	153	ILE	C-O	9.80	1.42	1.23
1	11-A	145	MET	CG-SD	9.80	2.06	1.81
1	2-A	106	ARG	C-N	9.79	1.56	1.34
1	3-A	115	LYS	CG-CD	9.79	1.85	1.52
1	1-A	98	PHE	CD2-CE2	9.79	1.58	1.39
1	14-A	115	LYS	CA-CB	9.79	1.75	1.53
1	14-A	45	TYR	CZ-OH	-9.78	1.21	1.37
1	9-A	128	ARG	CG-CD	9.77	1.76	1.51
1	14-A	64	PHE	C-O	-9.75	1.04	1.23
1	13-A	108	ASP	CB-CG	9.75	1.72	1.51
1	16-A	58	ARG	CD-NE	9.75	1.63	1.46
1	11-A	38	LEU	CG-CD1	9.74	1.88	1.51
1	10-A	119	THR	CB-OG1	9.74	1.62	1.43
1	8-A	107	LEU	CG-CD2	9.74	1.87	1.51
1	13-A	54	ILE	CB-CG2	9.74	1.83	1.52
1	13-A	58	ARG	CD-NE	9.73	1.62	1.46
1	1-A	142	SER	CB-OG	9.73	1.54	1.42
1	3-A	104	GLU	CB-CG	-9.72	1.33	1.52
1	3-A	141	ARG	CZ-NH1	9.72	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9-A	43	GLU	CD-OE2	-9.72	1.15	1.25
1	14-A	51	GLN	CB-CG	-9.72	1.26	1.52
1	9-A	124	GLU	CA-C	9.71	1.78	1.52
1	4-A	141	ARG	CZ-NH1	9.70	1.45	1.33
1	14-A	88	VAL	CB-CG2	9.69	1.73	1.52
1	5-A	104	GLU	CD-OE1	9.66	1.36	1.25
1	9-A	84	TYR	CD2-CE2	-9.66	1.24	1.39
1	1-A	61	LEU	N-CA	9.65	1.65	1.46
1	16-A	56	THR	CA-CB	9.64	1.78	1.53
1	8-A	39	LEU	CA-CB	9.64	1.75	1.53
1	10-A	104	GLU	CG-CD	9.63	1.66	1.51
1	12-A	80	GLN	CG-CD	9.63	1.73	1.51
1	13-A	146	TYR	CB-CG	9.63	1.66	1.51
1	16-A	114	THR	CB-OG1	9.63	1.62	1.43
1	11-A	67	TRP	CE3-CZ3	-9.62	1.22	1.38
1	7-A	135	HIS	CA-C	9.62	1.77	1.52
1	3-A	76	GLN	C-O	9.62	1.41	1.23
1	5-A	106	ARG	CZ-NH2	9.61	1.45	1.33
1	15-A	93	TRP	CD2-CE3	9.61	1.54	1.40
1	5-A	73	SER	CB-OG	9.61	1.54	1.42
1	13-A	37	SER	C-O	9.61	1.41	1.23
1	12-A	98	PHE	CD1-CE1	-9.59	1.20	1.39
1	16-A	116	ALA	C-O	9.59	1.41	1.23
1	11-A	62	ILE	CA-CB	-9.58	1.32	1.54
1	5-A	141	ARG	CZ-NH1	9.58	1.45	1.33
1	4-A	121	TRP	CZ3-CH2	9.58	1.55	1.40
1	2-A	154	PHE	CG-CD1	9.56	1.53	1.38
1	6-A	117	GLU	CG-CD	9.56	1.66	1.51
1	9-A	135	HIS	CA-CB	9.55	1.75	1.53
1	4-A	50	LYS	CE-NZ	9.55	1.73	1.49
1	2-A	74	MET	CB-CG	9.54	1.81	1.51
1	6-A	118	ALA	CA-CB	9.54	1.72	1.52
1	11-A	88	VAL	CA-C	9.54	1.77	1.52
1	15-A	82	LEU	N-CA	9.54	1.65	1.46
1	16-A	45	TYR	CG-CD1	9.53	1.51	1.39
1	8-A	140	TRP	CE3-CZ3	9.53	1.54	1.38
1	10-A	67	TRP	CE3-CZ3	9.53	1.54	1.38
1	8-A	81	PRO	N-CD	9.52	1.61	1.47
1	14-A	123	VAL	CA-CB	-9.52	1.34	1.54
1	6-A	125	GLU	CG-CD	-9.51	1.37	1.51
1	6-A	141	ARG	CZ-NH1	9.51	1.45	1.33
1	9-A	131	PRO	CA-CB	9.51	1.72	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-A	40	ARG	CG-CD	9.51	1.75	1.51
1	14-A	105	GLN	CG-CD	9.51	1.73	1.51
1	5-A	50	LYS	CB-CG	9.50	1.78	1.52
1	13-A	115	LYS	CE-NZ	9.50	1.72	1.49
1	12-A	102	SER	CB-OG	-9.49	1.29	1.42
1	14-A	138	LEU	CG-CD2	9.48	1.86	1.51
1	16-A	122	LEU	C-O	9.48	1.41	1.23
1	16-A	47	ASP	C-O	9.47	1.41	1.23
1	16-A	59	GLY	CA-C	-9.46	1.36	1.51
1	16-A	117	GLU	CD-OE2	9.46	1.36	1.25
1	3-A	91	GLN	CG-CD	9.46	1.72	1.51
1	16-A	64	PHE	CD2-CE2	9.46	1.58	1.39
1	13-A	67	TRP	CD1-NE1	9.45	1.54	1.38
1	13-A	104	GLU	CB-CG	-9.45	1.34	1.52
1	9-A	92	ARG	CG-CD	9.44	1.75	1.51
1	11-A	36	GLY	N-CA	9.44	1.60	1.46
1	14-A	58	ARG	CB-CG	9.43	1.78	1.52
1	16-A	47	ASP	CG-OD1	-9.43	1.03	1.25
1	3-A	40	ARG	CG-CD	9.42	1.75	1.51
1	5-A	42	ALA	N-CA	9.42	1.65	1.46
1	11-A	83	HIS	CA-CB	9.42	1.74	1.53
1	1-A	71	SER	C-O	-9.41	1.05	1.23
1	9-A	36	GLY	C-O	9.41	1.38	1.23
1	15-A	92	ARG	C-O	9.41	1.41	1.23
1	10-A	121	TRP	CB-CG	9.40	1.67	1.50
1	9-A	135	HIS	CA-C	9.39	1.77	1.52
1	6-A	79	GLY	N-CA	9.38	1.60	1.46
1	4-A	93	TRP	CZ2-CH2	9.37	1.55	1.37
1	12-A	141	ARG	CG-CD	9.37	1.75	1.51
1	10-A	129	LEU	CG-CD2	9.37	1.86	1.51
1	12-A	115	LYS	CG-CD	9.37	1.84	1.52
1	16-A	109	SER	CA-CB	9.37	1.67	1.52
1	16-A	93	TRP	N-CA	9.37	1.65	1.46
1	15-A	106	ARG	CZ-NH2	9.36	1.45	1.33
1	13-A	52	VAL	CB-CG2	9.36	1.72	1.52
1	7-A	134	LEU	CG-CD2	9.35	1.86	1.51
1	4-A	121	TRP	CE3-CZ3	9.34	1.54	1.38
1	6-A	146	TYR	CB-CG	9.34	1.65	1.51
1	14-A	141	ARG	CG-CD	9.34	1.75	1.51
1	15-A	149	PHE	CD2-CE2	9.34	1.57	1.39
1	16-A	124	GLU	CB-CG	9.33	1.69	1.52
1	11-A	154	PHE	CG-CD2	-9.33	1.24	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	55	PRO	CG-CD	9.32	1.81	1.50
1	10-A	37	SER	CA-CB	9.31	1.67	1.52
1	14-A	131	PRO	CG-CD	9.30	1.81	1.50
1	15-A	146	TYR	CD1-CE1	9.30	1.53	1.39
1	1-A	64	PHE	CG-CD2	9.29	1.52	1.38
1	9-A	113	PRO	CA-CB	9.28	1.72	1.53
1	16-A	50	LYS	CE-NZ	9.28	1.72	1.49
1	14-A	82	LEU	CG-CD1	9.27	1.86	1.51
1	11-A	62	ILE	CG1-CD1	9.27	2.14	1.50
1	13-A	126	ILE	CA-CB	9.27	1.76	1.54
1	6-A	40	ARG	CG-CD	9.27	1.75	1.51
1	16-A	98	PHE	CD2-CE2	9.26	1.57	1.39
1	6-A	74	MET	N-CA	9.25	1.64	1.46
1	11-A	62	ILE	CA-C	-9.25	1.28	1.52
1	13-A	95	GLN	CD-OE1	9.25	1.44	1.24
1	15-A	155	PRO	CG-CD	9.25	1.81	1.50
1	6-A	74	MET	CG-SD	9.24	2.05	1.81
1	10-A	135	HIS	CA-C	9.24	1.76	1.52
1	8-A	156	GLU	CD-OE1	9.24	1.35	1.25
1	10-A	39	LEU	CG-CD1	9.24	1.86	1.51
1	15-A	117	GLU	CA-C	9.23	1.76	1.52
1	10-A	134	LEU	CG-CD2	9.23	1.85	1.51
1	14-A	84	TYR	CD1-CE1	-9.23	1.25	1.39
1	14-A	145	MET	SD-CE	9.23	2.29	1.77
1	1-A	41	ARG	CD-NE	9.22	1.62	1.46
1	9-A	42	ALA	C-O	9.22	1.40	1.23
1	8-A	52	VAL	CB-CG1	9.21	1.72	1.52
1	10-A	137	ALA	CA-CB	9.21	1.71	1.52
1	4-A	141	ARG	CG-CD	9.20	1.75	1.51
1	15-A	115	LYS	CG-CD	9.20	1.83	1.52
1	16-A	78	TYR	CA-CB	9.20	1.74	1.53
1	2-A	141	ARG	CD-NE	9.20	1.62	1.46
1	10-A	67	TRP	CD2-CE3	9.20	1.54	1.40
1	11-A	98	PHE	CE1-CZ	9.20	1.54	1.37
1	13-A	149	PHE	N-CA	9.20	1.64	1.46
1	8-A	140	TRP	CD2-CE3	9.20	1.54	1.40
1	2-A	134	LEU	CG-CD2	9.20	1.85	1.51
1	9-A	138	LEU	CG-CD1	9.20	1.85	1.51
1	5-A	36	GLY	CA-C	9.19	1.66	1.51
1	2-A	132	SER	CA-C	9.18	1.76	1.52
1	9-A	98	PHE	CD1-CE1	-9.18	1.21	1.39
1	10-A	125	GLU	CB-CG	9.16	1.69	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	13-A	98	PHE	CD1-CE1	-9.16	1.21	1.39
1	4-A	67	TRP	CE2-CZ2	9.16	1.55	1.39
1	16-A	80	GLN	CD-NE2	9.16	1.55	1.32
1	3-A	70	LEU	CG-CD2	9.15	1.85	1.51
1	5-A	43	GLU	CD-OE1	-9.14	1.15	1.25
1	11-A	91	GLN	CD-NE2	9.14	1.55	1.32
1	15-A	56	THR	CB-CG2	-9.13	1.22	1.52
1	5-A	141	ARG	CG-CD	9.13	1.74	1.51
1	5-A	46	GLN	CA-C	9.12	1.76	1.52
1	16-A	109	SER	CA-C	9.11	1.76	1.52
1	1-A	37	SER	CA-CB	-9.11	1.39	1.52
1	5-A	84	TYR	CG-CD2	9.11	1.50	1.39
1	1-A	105	GLN	CA-C	9.11	1.76	1.52
1	7-A	141	ARG	CZ-NH1	9.11	1.44	1.33
1	12-A	106	ARG	CG-CD	9.11	1.74	1.51
1	1-A	51	GLN	CD-OE1	9.10	1.44	1.24
1	2-A	43	GLU	CD-OE2	-9.10	1.15	1.25
1	3-A	141	ARG	CG-CD	9.09	1.74	1.51
1	12-A	104	GLU	CB-CG	-9.09	1.34	1.52
1	3-A	88	VAL	CA-CB	9.09	1.73	1.54
1	6-A	84	TYR	CG-CD1	9.09	1.50	1.39
1	10-A	68	VAL	CA-CB	9.09	1.73	1.54
1	14-A	104	GLU	CD-OE2	-9.09	1.15	1.25
1	15-A	98	PHE	CG-CD2	9.09	1.52	1.38
1	15-A	141	ARG	C-O	9.09	1.40	1.23
1	9-A	97	ARG	CZ-NH1	9.08	1.44	1.33
1	5-A	98	PHE	CD1-CE1	-9.08	1.21	1.39
1	6-A	141	ARG	CG-CD	9.06	1.74	1.51
1	16-A	143	ASP	CB-CG	9.06	1.70	1.51
1	9-A	44	MET	SD-CE	9.06	2.28	1.77
1	13-A	109	SER	CB-OG	-9.06	1.30	1.42
1	8-A	104	GLU	CB-CG	-9.05	1.34	1.52
1	9-A	67	TRP	CE3-CZ3	9.05	1.53	1.38
1	9-A	141	ARG	CZ-NH1	9.04	1.44	1.33
1	14-A	121	TRP	CD2-CE2	9.02	1.52	1.41
1	15-A	106	ARG	CZ-NH1	9.02	1.44	1.33
1	15-A	56	THR	CB-OG1	9.02	1.61	1.43
1	16-A	78	TYR	CG-CD1	9.01	1.50	1.39
1	8-A	98	PHE	CE1-CZ	9.00	1.54	1.37
1	2-A	137	ALA	N-CA	9.00	1.64	1.46
1	1-A	41	ARG	CG-CD	8.99	1.74	1.51
1	16-A	117	GLU	CG-CD	8.99	1.65	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9-A	124	GLU	CD-OE1	8.98	1.35	1.25
1	4-A	121	TRP	CD2-CE3	8.98	1.53	1.40
1	16-A	143	ASP	CG-OD1	8.98	1.46	1.25
1	6-A	78	TYR	CD1-CE1	8.97	1.52	1.39
1	9-A	94	ASP	C-O	8.97	1.40	1.23
1	6-A	98	PHE	CD1-CE1	-8.96	1.21	1.39
1	16-A	69	GLY	C-O	8.95	1.38	1.23
1	11-A	125	GLU	CD-OE2	8.94	1.35	1.25
1	8-A	107	LEU	CB-CG	8.93	1.78	1.52
1	9-A	118	ALA	CA-CB	8.93	1.71	1.52
1	2-A	91	GLN	CA-CB	8.88	1.73	1.53
1	11-A	156	GLU	CD-OE1	-8.88	1.15	1.25
1	4-A	73	SER	CB-OG	8.88	1.53	1.42
1	16-A	126	ILE	CB-CG2	8.88	1.80	1.52
1	13-A	43	GLU	CA-CB	8.87	1.73	1.53
1	16-A	44	MET	C-O	8.87	1.40	1.23
1	16-A	70	LEU	C-O	-8.87	1.06	1.23
1	7-A	36	GLY	C-O	8.87	1.37	1.23
1	11-A	149	PHE	CD2-CE2	8.86	1.56	1.39
1	4-A	58	ARG	CD-NE	8.86	1.61	1.46
1	13-A	51	GLN	C-O	8.86	1.40	1.23
1	12-A	36	GLY	C-O	8.86	1.37	1.23
1	5-A	104	GLU	CB-CG	-8.86	1.35	1.52
1	15-A	51	GLN	CA-CB	8.86	1.73	1.53
1	1-A	58	ARG	CD-NE	8.84	1.61	1.46
1	6-A	79	GLY	CA-C	8.84	1.66	1.51
1	15-A	106	ARG	CG-CD	8.84	1.74	1.51
1	3-A	80	GLN	CA-CB	8.83	1.73	1.53
1	5-A	93	TRP	CD2-CE2	8.83	1.51	1.41
1	9-A	122	LEU	CA-CB	8.83	1.74	1.53
1	2-A	66	SER	C-O	-8.82	1.06	1.23
1	7-A	94	ASP	CG-OD2	8.82	1.45	1.25
1	13-A	151	ASP	CG-OD1	8.82	1.45	1.25
1	14-A	111	ILE	CB-CG2	8.82	1.80	1.52
1	15-A	119	THR	CB-CG2	8.81	1.81	1.52
1	5-A	93	TRP	CE2-CZ2	8.81	1.54	1.39
1	8-A	155	PRO	CG-CD	8.81	1.79	1.50
1	2-A	37	SER	N-CA	8.80	1.64	1.46
1	12-A	58	ARG	CD-NE	8.79	1.61	1.46
1	9-A	86	THR	C-O	8.79	1.40	1.23
1	4-A	104	GLU	CB-CG	-8.78	1.35	1.52
1	10-A	99	GLY	C-O	8.77	1.37	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	129	LEU	C-O	8.77	1.40	1.23
1	6-A	58	ARG	CD-NE	8.77	1.61	1.46
1	4-A	78	TYR	C-O	-8.76	1.06	1.23
1	9-A	156	GLU	CD-OE1	8.75	1.35	1.25
1	15-A	57	ASN	CB-CG	8.75	1.71	1.51
1	10-A	117	GLU	CD-OE2	8.75	1.35	1.25
1	10-A	45	TYR	CD2-CE2	8.74	1.52	1.39
1	3-A	58	ARG	CD-NE	8.74	1.61	1.46
1	4-A	75	LYS	CA-CB	8.74	1.73	1.53
1	5-A	94	ASP	CB-CG	8.73	1.70	1.51
1	8-A	109	SER	CA-CB	8.73	1.66	1.52
1	10-A	117	GLU	CD-OE1	8.73	1.35	1.25
1	8-A	148	SER	C-O	8.72	1.40	1.23
1	14-A	58	ARG	CD-NE	8.72	1.61	1.46
1	9-A	127	HIS	N-CA	8.72	1.63	1.46
1	16-A	145	MET	CB-CG	8.71	1.79	1.51
1	2-A	140	TRP	C-O	-8.70	1.06	1.23
1	11-A	62	ILE	N-CA	-8.70	1.28	1.46
1	8-A	140	TRP	CD2-CE2	8.70	1.51	1.41
1	13-A	80	GLN	CA-CB	8.70	1.73	1.53
1	14-A	124	GLU	CD-OE2	8.69	1.35	1.25
1	11-A	92	ARG	CG-CD	8.69	1.73	1.51
1	7-A	58	ARG	CD-NE	8.68	1.61	1.46
1	12-A	71	SER	CA-CB	8.68	1.66	1.52
1	11-A	92	ARG	CZ-NH1	-8.68	1.21	1.33
1	16-A	83	HIS	CA-CB	8.68	1.73	1.53
1	14-A	75	LYS	CD-CE	8.67	1.73	1.51
1	10-A	140	TRP	CD1-NE1	8.65	1.52	1.38
1	10-A	120	ILE	CG1-CD1	8.64	2.10	1.50
1	16-A	86	THR	CB-CG2	8.63	1.80	1.52
1	11-A	58	ARG	CD-NE	8.63	1.61	1.46
1	14-A	46	GLN	CA-CB	8.62	1.73	1.53
1	10-A	51	GLN	CD-OE1	8.62	1.43	1.24
1	1-A	97	ARG	CB-CG	8.61	1.75	1.52
1	11-A	142	SER	CA-CB	8.61	1.65	1.52
1	9-A	123	VAL	CB-CG2	8.59	1.70	1.52
1	14-A	122	LEU	N-CA	8.59	1.63	1.46
1	16-A	153	ILE	C-O	8.59	1.39	1.23
1	4-A	118	ALA	CA-CB	8.59	1.70	1.52
1	5-A	145	MET	CG-SD	8.58	2.03	1.81
1	4-A	67	TRP	CD2-CE2	8.58	1.51	1.41
1	6-A	105	GLN	CB-CG	-8.58	1.29	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	38	LEU	CG-CD2	8.57	1.83	1.51
1	1-A	40	ARG	CA-C	8.57	1.75	1.52
1	9-A	49	MET	SD-CE	-8.56	1.29	1.77
1	11-A	107	LEU	N-CA	8.56	1.63	1.46
1	4-A	98	PHE	C-O	-8.56	1.07	1.23
1	1-A	134	LEU	CG-CD1	8.55	1.83	1.51
1	4-A	81	PRO	N-CD	8.55	1.59	1.47
1	12-A	121	TRP	CZ3-CH2	8.55	1.53	1.40
1	1-A	146	TYR	CD1-CE1	8.55	1.52	1.39
1	15-A	80	GLN	CG-CD	8.55	1.70	1.51
1	8-A	141	ARG	CG-CD	8.54	1.73	1.51
1	1-A	121	TRP	CB-CG	8.54	1.65	1.50
1	8-A	150	ILE	CG1-CD1	8.54	2.09	1.50
1	2-A	151	ASP	C-O	-8.54	1.07	1.23
1	3-A	72	ILE	CB-CG2	8.54	1.79	1.52
1	8-A	40	ARG	CB-CG	-8.54	1.29	1.52
1	11-A	144	PRO	CA-C	8.53	1.70	1.52
1	7-A	133	HIS	C-O	8.52	1.39	1.23
1	11-A	140	TRP	CZ3-CH2	8.52	1.53	1.40
1	3-A	67	TRP	CA-CB	8.52	1.72	1.53
1	14-A	136	MET	C-O	8.52	1.39	1.23
1	3-A	43	GLU	CD-OE2	-8.51	1.16	1.25
1	13-A	113	PRO	N-CD	8.51	1.59	1.47
1	14-A	97	ARG	CG-CD	8.51	1.73	1.51
1	8-A	140	TRP	CZ2-CH2	8.51	1.53	1.37
1	9-A	93	TRP	C-O	8.51	1.39	1.23
1	2-A	138	LEU	CG-CD1	-8.50	1.20	1.51
1	15-A	122	LEU	C-O	8.50	1.39	1.23
1	9-A	139	LEU	C-O	8.50	1.39	1.23
1	4-A	36	GLY	C-O	8.49	1.37	1.23
1	4-A	39	LEU	CG-CD1	8.49	1.83	1.51
1	5-A	46	GLN	C-N	8.48	1.53	1.34
1	2-A	140	TRP	CZ3-CH2	8.48	1.53	1.40
1	15-A	119	THR	C-O	8.47	1.39	1.23
1	13-A	106	ARG	CZ-NH2	8.47	1.44	1.33
1	15-A	96	SER	C-N	8.46	1.53	1.34
1	16-A	108	ASP	C-O	8.46	1.39	1.23
1	9-A	127	HIS	CA-CB	8.46	1.72	1.53
1	15-A	121	TRP	CB-CG	8.45	1.65	1.50
1	4-A	76	GLN	CB-CG	-8.45	1.29	1.52
1	15-A	41	ARG	CA-CB	8.45	1.72	1.53
1	7-A	98	PHE	CD2-CE2	8.44	1.56	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-A	151	ASP	C-O	8.44	1.39	1.23
1	1-A	38	LEU	CG-CD2	8.44	1.83	1.51
1	2-A	141	ARG	CZ-NH1	8.44	1.44	1.33
1	15-A	41	ARG	CA-C	8.44	1.74	1.52
1	2-A	144	PRO	N-CA	8.43	1.61	1.47
1	5-A	48	TYR	CZ-OH	8.43	1.52	1.37
1	7-A	140	TRP	CG-CD1	8.43	1.48	1.36
1	15-A	153	ILE	C-O	8.43	1.39	1.23
1	8-A	40	ARG	CA-C	8.43	1.74	1.52
1	8-A	67	TRP	CA-C	8.43	1.74	1.52
1	1-A	60	SER	CA-CB	8.42	1.65	1.52
1	4-A	124	GLU	CA-C	8.42	1.74	1.52
1	5-A	156	GLU	CB-CG	8.42	1.68	1.52
1	1-A	50	LYS	CB-CG	-8.41	1.29	1.52
1	10-A	58	ARG	CD-NE	8.41	1.60	1.46
1	16-A	83	HIS	CD2-NE2	8.41	1.59	1.42
1	10-A	41	ARG	CZ-NH2	8.41	1.44	1.33
1	2-A	40	ARG	CZ-NH1	8.41	1.44	1.33
1	5-A	37	SER	C-O	8.41	1.39	1.23
1	6-A	90	LEU	C-O	8.41	1.39	1.23
1	8-A	68	VAL	C-N	8.40	1.48	1.33
1	3-A	95	GLN	C-O	8.39	1.39	1.23
1	6-A	156	GLU	CD-OE1	8.39	1.34	1.25
1	6-A	128	ARG	CZ-NH1	8.38	1.44	1.33
1	4-A	156	GLU	CG-CD	8.38	1.64	1.51
1	1-A	149	PHE	CD2-CE2	8.37	1.55	1.39
1	7-A	94	ASP	CA-CB	8.38	1.72	1.53
1	9-A	67	TRP	CD2-CE2	8.38	1.51	1.41
1	11-A	97	ARG	CZ-NH2	8.37	1.44	1.33
1	14-A	140	TRP	CE3-CZ3	8.37	1.52	1.38
1	8-A	56	THR	C-O	-8.37	1.07	1.23
1	16-A	68	VAL	CA-C	8.37	1.74	1.52
1	11-A	65	THR	CA-CB	8.37	1.75	1.53
1	15-A	141	ARG	CZ-NH2	8.37	1.44	1.33
1	9-A	153	ILE	C-O	8.36	1.39	1.23
1	15-A	92	ARG	CZ-NH2	8.36	1.44	1.33
1	4-A	149	PHE	CD2-CE2	8.36	1.55	1.39
1	9-A	80	GLN	CA-CB	8.36	1.72	1.53
1	12-A	153	ILE	C-O	8.36	1.39	1.23
1	15-A	78	TYR	CG-CD1	-8.35	1.28	1.39
1	8-A	140	TRP	CG-CD1	8.35	1.48	1.36
1	13-A	89	LEU	C-O	8.34	1.39	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	11-A	98	PHE	CD1-CE1	-8.34	1.22	1.39
1	9-A	41	ARG	CZ-NH2	8.33	1.43	1.33
1	1-A	127	HIS	CA-CB	8.33	1.72	1.53
1	9-A	124	GLU	CG-CD	8.33	1.64	1.51
1	10-A	120	ILE	CB-CG2	8.33	1.78	1.52
1	11-A	107	LEU	CG-CD2	8.33	1.82	1.51
1	14-A	87	ASN	N-CA	8.33	1.63	1.46
1	15-A	45	TYR	CE1-CZ	8.32	1.49	1.38
1	8-A	59	GLY	N-CA	8.32	1.58	1.46
1	1-A	64	PHE	CD1-CE1	8.31	1.55	1.39
1	15-A	121	TRP	N-CA	8.31	1.62	1.46
1	3-A	156	GLU	C-O	8.31	1.39	1.23
1	5-A	55	PRO	N-CD	8.31	1.59	1.47
1	5-A	93	TRP	N-CA	8.30	1.62	1.46
1	8-A	129	LEU	C-O	8.30	1.39	1.23
1	14-A	119	THR	CB-CG2	8.29	1.79	1.52
1	16-A	115	LYS	CE-NZ	8.28	1.69	1.49
1	1-A	97	ARG	CG-CD	8.28	1.72	1.51
1	5-A	82	LEU	CG-CD2	8.28	1.82	1.51
1	10-A	80	GLN	CA-CB	8.28	1.72	1.53
1	14-A	113	PRO	N-CD	8.28	1.59	1.47
1	15-A	118	ALA	CA-C	8.28	1.74	1.52
1	15-A	151	ASP	CG-OD1	8.28	1.44	1.25
1	10-A	36	GLY	C-O	8.27	1.36	1.23
1	6-A	45	TYR	CE1-CZ	8.27	1.49	1.38
1	10-A	108	ASP	CB-CG	8.26	1.69	1.51
1	9-A	105	GLN	CA-C	8.26	1.74	1.52
1	16-A	115	LYS	C-N	8.26	1.53	1.34
1	7-A	40	ARG	CZ-NH1	8.26	1.43	1.33
1	6-A	144	PRO	C-O	8.25	1.39	1.23
1	16-A	93	TRP	NE1-CE2	8.25	1.48	1.37
1	11-A	64	PHE	CD1-CE1	8.25	1.55	1.39
1	13-A	59	GLY	C-O	8.24	1.36	1.23
1	13-A	141	ARG	CZ-NH2	8.24	1.43	1.33
1	8-A	55	PRO	N-CD	8.24	1.59	1.47
1	1-A	116	ALA	C-O	8.24	1.39	1.23
1	9-A	151	ASP	CB-CG	8.23	1.69	1.51
1	15-A	54	ILE	CB-CG1	8.23	1.77	1.54
1	16-A	106	ARG	CG-CD	8.23	1.72	1.51
1	5-A	36	GLY	C-O	-8.22	1.10	1.23
1	2-A	64	PHE	CD1-CE1	8.22	1.55	1.39
1	11-A	154	PHE	CE1-CZ	8.22	1.52	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	14-A	126	ILE	CA-CB	8.22	1.73	1.54
1	2-A	134	LEU	CA-CB	8.22	1.72	1.53
1	9-A	44	MET	CB-CG	8.22	1.77	1.51
1	5-A	142	SER	CB-OG	8.21	1.52	1.42
1	9-A	50	LYS	CB-CG	8.21	1.74	1.52
1	14-A	137	ALA	C-O	8.21	1.39	1.23
1	14-A	139	LEU	N-CA	8.21	1.62	1.46
1	10-A	131	PRO	N-CD	8.21	1.59	1.47
1	15-A	88	VAL	C-O	8.21	1.39	1.23
1	16-A	72	ILE	CB-CG2	8.21	1.78	1.52
1	3-A	91	GLN	CD-NE2	8.20	1.53	1.32
1	13-A	91	GLN	CD-OE1	-8.20	1.05	1.24
1	9-A	37	SER	C-O	8.20	1.39	1.23
1	13-A	63	PRO	CG-CD	8.19	1.77	1.50
1	1-A	108	ASP	CG-OD1	8.19	1.44	1.25
1	15-A	153	ILE	CA-CB	8.19	1.73	1.54
1	2-A	141	ARG	C-O	8.19	1.39	1.23
1	16-A	117	GLU	CB-CG	8.19	1.67	1.52
1	9-A	104	GLU	CB-CG	-8.18	1.36	1.52
1	10-A	67	TRP	CD2-CE2	8.18	1.51	1.41
1	15-A	138	LEU	CG-CD1	8.18	1.82	1.51
1	16-A	51	GLN	C-O	8.18	1.38	1.23
1	15-A	87	ASN	CG-ND2	8.18	1.53	1.32
1	10-A	138	LEU	CG-CD1	8.17	1.82	1.51
1	13-A	118	ALA	CA-CB	8.17	1.69	1.52
1	13-A	38	LEU	CG-CD2	8.17	1.82	1.51
1	1-A	121	TRP	CG-CD1	8.16	1.48	1.36
1	3-A	148	SER	C-O	-8.16	1.07	1.23
1	14-A	122	LEU	C-O	8.16	1.38	1.23
1	2-A	37	SER	CA-CB	8.15	1.65	1.52
1	6-A	138	LEU	CG-CD1	8.15	1.82	1.51
1	2-A	63	PRO	N-CD	8.15	1.59	1.47
1	7-A	71	SER	CA-CB	8.15	1.65	1.52
1	14-A	136	MET	CA-C	8.15	1.74	1.52
1	14-A	46	GLN	CD-NE2	8.14	1.53	1.32
1	8-A	65	THR	CA-CB	8.13	1.74	1.53
1	3-A	138	LEU	CG-CD2	8.13	1.81	1.51
1	5-A	144	PRO	N-CA	8.13	1.61	1.47
1	11-A	60	SER	CA-CB	8.13	1.65	1.52
1	12-A	67	TRP	CD2-CE2	8.13	1.51	1.41
1	13-A	89	LEU	CB-CG	8.13	1.76	1.52
1	1-A	154	PHE	CE2-CZ	-8.12	1.22	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	10-A	60	SER	CA-CB	8.12	1.65	1.52
1	2-A	132	SER	CA-CB	8.12	1.65	1.52
1	8-A	53	PRO	CA-C	8.11	1.69	1.52
1	14-A	67	TRP	CD1-NE1	8.11	1.51	1.38
1	15-A	130	THR	C-O	8.10	1.38	1.23
1	16-A	74	MET	CG-SD	8.10	2.02	1.81
1	14-A	66	SER	N-CA	8.10	1.62	1.46
1	3-A	150	ILE	CB-CG1	8.10	1.76	1.54
1	8-A	107	LEU	N-CA	8.10	1.62	1.46
1	15-A	46	GLN	CD-NE2	8.10	1.53	1.32
1	10-A	41	ARG	CG-CD	8.09	1.72	1.51
1	4-A	134	LEU	CG-CD2	8.09	1.81	1.51
1	10-A	43	GLU	CA-C	8.09	1.74	1.52
1	5-A	36	GLY	N-CA	8.08	1.58	1.46
1	5-A	51	GLN	CG-CD	8.08	1.69	1.51
1	15-A	116	ALA	CA-CB	8.08	1.69	1.52
1	16-A	72	ILE	C-O	-8.08	1.07	1.23
1	2-A	80	GLN	CD-NE2	8.08	1.53	1.32
1	5-A	51	GLN	CB-CG	-8.08	1.30	1.52
1	16-A	81	PRO	C-O	-8.08	1.07	1.23
1	16-A	44	MET	CB-CG	8.07	1.77	1.51
1	2-A	91	GLN	C-O	8.07	1.38	1.23
1	11-A	63	PRO	N-CA	8.07	1.60	1.47
1	3-A	118	ALA	CA-CB	8.07	1.69	1.52
1	8-A	70	LEU	CG-CD2	8.07	1.81	1.51
1	3-A	59	GLY	C-O	8.07	1.36	1.23
1	8-A	153	ILE	C-O	8.06	1.38	1.23
1	2-A	125	GLU	CG-CD	8.06	1.64	1.51
1	16-A	112	HIS	CG-CD2	8.06	1.49	1.35
1	5-A	67	TRP	CE2-CZ2	8.06	1.53	1.39
1	13-A	141	ARG	CD-NE	8.06	1.60	1.46
1	9-A	107	LEU	C-O	8.05	1.38	1.23
1	2-A	72	ILE	C-O	8.05	1.38	1.23
1	2-A	91	GLN	CA-C	8.04	1.73	1.52
1	8-A	64	PHE	C-O	8.04	1.38	1.23
1	15-A	93	TRP	CG-CD2	8.04	1.57	1.43
1	2-A	110	ILE	N-CA	8.04	1.62	1.46
1	15-A	106	ARG	C-N	8.04	1.52	1.34
1	16-A	123	VAL	CA-CB	-8.03	1.37	1.54
1	6-A	60	SER	CA-CB	8.03	1.65	1.52
1	8-A	150	ILE	CB-CG2	8.02	1.77	1.52
1	16-A	153	ILE	CA-CB	8.02	1.73	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	13-A	41	ARG	CA-C	8.02	1.73	1.52
1	8-A	98	PHE	CD1-CE1	-8.01	1.23	1.39
1	5-A	93	TRP	CA-C	8.01	1.73	1.52
1	13-A	49	MET	CA-C	8.01	1.73	1.52
1	15-A	141	ARG	CD-NE	8.00	1.60	1.46
1	10-A	44	MET	SD-CE	8.00	2.22	1.77
1	2-A	139	LEU	CG-CD2	7.99	1.81	1.51
1	13-A	43	GLU	CB-CG	7.99	1.67	1.52
1	6-A	121	TRP	CZ3-CH2	7.97	1.52	1.40
1	4-A	67	TRP	CZ3-CH2	7.96	1.52	1.40
1	12-A	60	SER	CB-OG	7.96	1.52	1.42
1	14-A	37	SER	C-O	7.96	1.38	1.23
1	4-A	73	SER	C-N	7.96	1.52	1.34
1	7-A	106	ARG	CG-CD	7.96	1.71	1.51
1	11-A	154	PHE	CD1-CE1	7.96	1.55	1.39
1	13-A	135	HIS	CA-CB	7.95	1.71	1.53
1	16-A	92	ARG	C-N	7.95	1.52	1.34
1	16-A	48	TYR	CG-CD2	7.94	1.49	1.39
1	11-A	84	TYR	CD1-CE1	7.94	1.51	1.39
1	3-A	40	ARG	CB-CG	-7.94	1.31	1.52
1	13-A	86	THR	CA-CB	7.93	1.74	1.53
1	15-A	83	HIS	CA-C	7.93	1.73	1.52
1	3-A	106	ARG	CZ-NH2	7.93	1.43	1.33
1	11-A	80	GLN	CD-NE2	7.93	1.52	1.32
1	15-A	51	GLN	CG-CD	7.92	1.69	1.51
1	2-A	66	SER	N-CA	7.92	1.62	1.46
1	6-A	84	TYR	CE1-CZ	7.92	1.48	1.38
1	13-A	51	GLN	CB-CG	-7.92	1.31	1.52
1	4-A	76	GLN	CD-OE1	-7.91	1.06	1.24
1	5-A	91	GLN	CA-C	7.91	1.73	1.52
1	16-A	98	PHE	CB-CG	7.90	1.64	1.51
1	5-A	67	TRP	CD2-CE2	7.90	1.50	1.41
1	10-A	141	ARG	CZ-NH1	7.90	1.43	1.33
1	1-A	138	LEU	CG-CD2	7.89	1.81	1.51
1	1-A	146	TYR	CZ-OH	7.89	1.51	1.37
1	9-A	136	MET	CG-SD	7.89	2.01	1.81
1	14-A	104	GLU	CG-CD	7.88	1.63	1.51
1	16-A	66	SER	N-CA	7.88	1.62	1.46
1	11-A	89	LEU	CA-C	7.88	1.73	1.52
1	8-A	65	THR	CB-CG2	7.87	1.78	1.52
1	14-A	140	TRP	CA-CB	7.87	1.71	1.53
1	4-A	131	PRO	CA-CB	7.87	1.69	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	51	GLN	CB-CG	-7.87	1.31	1.52
1	10-A	145	MET	CB-CG	7.87	1.76	1.51
1	8-A	145	MET	CG-SD	-7.86	1.60	1.81
1	8-A	147	HIS	CA-CB	7.86	1.71	1.53
1	16-A	143	ASP	C-N	7.86	1.49	1.34
1	14-A	56	THR	CB-CG2	-7.86	1.26	1.52
1	9-A	113	PRO	CG-CD	7.86	1.76	1.50
1	2-A	105	GLN	CG-CD	7.86	1.69	1.51
1	15-A	88	VAL	CA-CB	7.85	1.71	1.54
1	16-A	58	ARG	C-O	7.85	1.38	1.23
1	14-A	109	SER	CA-CB	7.85	1.64	1.52
1	9-A	154	PHE	CE2-CZ	-7.84	1.22	1.37
1	9-A	139	LEU	N-CA	7.84	1.62	1.46
1	7-A	123	VAL	CB-CG1	-7.84	1.36	1.52
1	3-A	97	ARG	CZ-NH2	7.83	1.43	1.33
1	15-A	49	MET	SD-CE	-7.83	1.33	1.77
1	15-A	56	THR	C-O	-7.83	1.08	1.23
1	14-A	80	GLN	CA-CB	7.83	1.71	1.53
1	13-A	128	ARG	N-CA	7.82	1.61	1.46
1	14-A	146	TYR	CG-CD2	-7.82	1.28	1.39
1	1-A	104	GLU	CB-CG	-7.82	1.37	1.52
1	11-A	76	GLN	C-O	7.82	1.38	1.23
1	16-A	112	HIS	CA-CB	-7.81	1.36	1.53
1	16-A	150	ILE	CG1-CD1	7.81	2.04	1.50
1	16-A	89	LEU	C-O	-7.81	1.08	1.23
1	8-A	154	PHE	CG-CD2	7.81	1.50	1.38
1	4-A	106	ARG	CZ-NH2	7.81	1.43	1.33
1	6-A	154	PHE	CE1-CZ	7.81	1.52	1.37
1	9-A	110	ILE	N-CA	7.80	1.61	1.46
1	15-A	152	PRO	CG-CD	7.80	1.76	1.50
1	2-A	122	LEU	CB-CG	7.80	1.75	1.52
1	5-A	94	ASP	CG-OD1	7.79	1.43	1.25
1	12-A	117	GLU	N-CA	7.79	1.61	1.46
1	14-A	64	PHE	CE1-CZ	7.79	1.52	1.37
1	3-A	95	GLN	CA-CB	-7.79	1.36	1.53
1	11-A	43	GLU	CA-CB	7.79	1.71	1.53
1	15-A	56	THR	C-N	-7.79	1.16	1.34
1	11-A	40	ARG	N-CA	7.78	1.61	1.46
1	16-A	134	LEU	CG-CD2	7.77	1.80	1.51
1	6-A	97	ARG	NE-CZ	7.77	1.43	1.33
1	8-A	59	GLY	C-O	7.77	1.36	1.23
1	16-A	106	ARG	CZ-NH2	7.77	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	135	HIS	CB-CG	7.75	1.64	1.50
1	7-A	143	ASP	CA-CB	7.75	1.71	1.53
1	14-A	113	PRO	CG-CD	7.74	1.76	1.50
1	7-A	139	LEU	N-CA	7.74	1.61	1.46
1	15-A	156	GLU	CD-OE1	7.74	1.34	1.25
1	13-A	48	TYR	C-O	7.73	1.38	1.23
1	14-A	128	ARG	CD-NE	7.73	1.59	1.46
1	11-A	39	LEU	CG-CD1	7.73	1.80	1.51
1	16-A	108	ASP	CG-OD2	-7.72	1.07	1.25
1	13-A	112	HIS	CG-CD2	7.72	1.48	1.35
1	14-A	117	GLU	CA-C	7.71	1.73	1.52
1	7-A	134	LEU	CG-CD1	7.71	1.80	1.51
1	11-A	98	PHE	CD2-CE2	7.71	1.54	1.39
1	10-A	115	LYS	C-O	7.71	1.38	1.23
1	15-A	79	GLY	N-CA	7.71	1.57	1.46
1	14-A	107	LEU	CA-C	7.71	1.73	1.52
1	6-A	73	SER	CA-CB	7.70	1.64	1.52
1	1-A	123	VAL	CB-CG2	-7.70	1.36	1.52
1	4-A	64	PHE	C-O	7.70	1.38	1.23
1	1-A	141	ARG	C-O	7.69	1.38	1.23
1	2-A	64	PHE	CE1-CZ	7.69	1.51	1.37
1	6-A	36	GLY	C-O	7.69	1.35	1.23
1	1-A	72	ILE	C-O	7.69	1.38	1.23
1	14-A	128	ARG	N-CA	7.69	1.61	1.46
1	14-A	67	TRP	CG-CD1	7.68	1.47	1.36
1	3-A	43	GLU	CD-OE1	-7.68	1.17	1.25
1	15-A	43	GLU	CA-CB	7.67	1.70	1.53
1	9-A	59	GLY	CA-C	7.67	1.64	1.51
1	13-A	121	TRP	CZ3-CH2	7.67	1.52	1.40
1	10-A	37	SER	N-CA	7.66	1.61	1.46
1	11-A	138	LEU	CG-CD1	7.66	1.80	1.51
1	14-A	141	ARG	CZ-NH2	-7.66	1.23	1.33
1	12-A	146	TYR	CG-CD1	-7.66	1.29	1.39
1	3-A	147	HIS	CA-CB	7.66	1.70	1.53
1	7-A	115	LYS	CA-CB	7.66	1.70	1.53
1	8-A	146	TYR	CB-CG	7.66	1.63	1.51
1	8-A	57	ASN	CB-CG	7.65	1.68	1.51
1	12-A	42	ALA	CA-CB	7.65	1.68	1.52
1	10-A	116	ALA	N-CA	7.65	1.61	1.46
1	5-A	48	TYR	CG-CD2	7.65	1.49	1.39
1	10-A	60	SER	CB-OG	7.65	1.52	1.42
1	9-A	37	SER	N-CA	7.65	1.61	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	13-A	93	TRP	CA-CB	7.64	1.70	1.53
1	13-A	127	HIS	N-CA	-7.64	1.31	1.46
1	7-A	60	SER	CB-OG	7.64	1.52	1.42
1	13-A	152	PRO	CG-CD	7.64	1.75	1.50
1	14-A	93	TRP	CZ2-CH2	7.64	1.51	1.37
1	10-A	37	SER	C-O	7.64	1.37	1.23
1	5-A	52	VAL	CB-CG2	7.63	1.68	1.52
1	2-A	126	ILE	CB-CG2	7.63	1.76	1.52
1	16-A	54	ILE	CB-CG2	7.63	1.76	1.52
1	5-A	97	ARG	NE-CZ	7.62	1.43	1.33
1	11-A	146	TYR	CB-CG	7.62	1.63	1.51
1	12-A	56	THR	C-O	7.62	1.37	1.23
1	13-A	156	GLU	CD-OE1	-7.62	1.17	1.25
1	7-A	113	PRO	CA-CB	7.62	1.68	1.53
1	16-A	41	ARG	NE-CZ	7.62	1.43	1.33
1	3-A	84	TYR	CD1-CE1	-7.61	1.27	1.39
1	13-A	45	TYR	CG-CD2	7.61	1.49	1.39
1	13-A	98	PHE	CG-CD2	7.61	1.50	1.38
1	9-A	93	TRP	CE2-CZ2	7.60	1.52	1.39
1	3-A	134	LEU	CG-CD2	7.60	1.79	1.51
1	14-A	135	HIS	CA-CB	7.60	1.70	1.53
1	6-A	146	TYR	CA-CB	7.59	1.70	1.53
1	13-A	142	SER	CB-OG	7.59	1.52	1.42
1	2-A	71	SER	CA-CB	7.59	1.64	1.52
1	9-A	128	ARG	CZ-NH2	7.58	1.43	1.33
1	16-A	51	GLN	CA-CB	7.58	1.70	1.53
1	10-A	142	SER	CA-CB	7.58	1.64	1.52
1	2-A	43	GLU	CG-CD	7.57	1.63	1.51
1	15-A	98	PHE	CA-CB	-7.57	1.37	1.53
1	3-A	91	GLN	C-O	-7.56	1.08	1.23
1	5-A	46	GLN	N-CA	7.56	1.61	1.46
1	13-A	128	ARG	CZ-NH2	7.56	1.42	1.33
1	11-A	66	SER	CA-CB	-7.55	1.41	1.52
1	3-A	99	GLY	N-CA	7.55	1.57	1.46
1	15-A	57	ASN	CG-ND2	7.55	1.51	1.32
1	5-A	108	ASP	CB-CG	7.55	1.67	1.51
1	10-A	119	THR	CB-CG2	7.55	1.77	1.52
1	12-A	113	PRO	CA-CB	7.55	1.68	1.53
1	13-A	41	ARG	CA-CB	7.55	1.70	1.53
1	7-A	105	GLN	CB-CG	-7.54	1.32	1.52
1	5-A	57	ASN	CB-CG	7.54	1.68	1.51
1	3-A	98	PHE	N-CA	7.54	1.61	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	66	SER	CB-OG	-7.54	1.32	1.42
1	7-A	37	SER	C-O	7.54	1.37	1.23
1	11-A	40	ARG	CA-C	7.54	1.72	1.52
1	8-A	145	MET	C-O	7.53	1.37	1.23
1	6-A	66	SER	N-CA	7.53	1.61	1.46
1	4-A	67	TRP	CD2-CE3	7.53	1.51	1.40
1	15-A	60	SER	C-O	7.53	1.37	1.23
1	13-A	151	ASP	CB-CG	7.52	1.67	1.51
1	16-A	152	PRO	CG-CD	7.52	1.75	1.50
1	15-A	127	HIS	C-O	7.52	1.37	1.23
1	16-A	45	TYR	CZ-OH	-7.51	1.25	1.37
1	5-A	93	TRP	CD1-NE1	7.51	1.50	1.38
1	10-A	156	GLU	CD-OE2	-7.50	1.17	1.25
1	9-A	58	ARG	CD-NE	7.50	1.59	1.46
1	6-A	123	VAL	CA-CB	7.50	1.70	1.54
1	16-A	97	ARG	CZ-NH2	7.50	1.42	1.33
1	14-A	140	TRP	CG-CD1	7.50	1.47	1.36
1	5-A	50	LYS	CA-CB	7.50	1.70	1.53
1	2-A	103	GLU	CB-CG	-7.49	1.38	1.52
1	14-A	149	PHE	C-O	7.49	1.37	1.23
1	10-A	139	LEU	N-CA	7.49	1.61	1.46
1	15-A	151	ASP	C-O	7.49	1.37	1.23
1	8-A	56	THR	C-N	-7.48	1.16	1.34
1	11-A	41	ARG	CZ-NH2	7.48	1.42	1.33
1	12-A	117	GLU	CB-CG	7.48	1.66	1.52
1	1-A	138	LEU	CG-CD1	7.47	1.79	1.51
1	3-A	116	ALA	CA-CB	7.47	1.68	1.52
1	13-A	124	GLU	CD-OE1	-7.47	1.17	1.25
1	1-A	64	PHE	CE1-CZ	7.47	1.51	1.37
1	4-A	109	SER	CB-OG	-7.47	1.32	1.42
1	13-A	126	ILE	CA-C	7.47	1.72	1.52
1	6-A	50	LYS	CE-NZ	7.46	1.67	1.49
1	16-A	97	ARG	CZ-NH1	7.46	1.42	1.33
1	2-A	113	PRO	CG-CD	7.46	1.75	1.50
1	5-A	146	TYR	CG-CD1	-7.46	1.29	1.39
1	6-A	108	ASP	CB-CG	7.46	1.67	1.51
1	7-A	98	PHE	CE1-CZ	7.46	1.51	1.37
1	7-A	95	GLN	C-O	7.46	1.37	1.23
1	1-A	106	ARG	CD-NE	-7.46	1.33	1.46
1	8-A	91	GLN	CD-OE1	7.46	1.40	1.24
1	5-A	53	PRO	CA-C	7.45	1.67	1.52
1	13-A	66	SER	C-N	7.45	1.51	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	74	MET	CG-SD	7.45	2.00	1.81
1	6-A	78	TYR	CA-CB	7.45	1.70	1.53
1	9-A	89	LEU	CG-CD2	7.45	1.79	1.51
1	13-A	47	ASP	CG-OD2	7.45	1.42	1.25
1	13-A	98	PHE	CB-CG	7.45	1.64	1.51
1	3-A	117	GLU	CD-OE1	7.44	1.33	1.25
1	12-A	142	SER	CB-OG	7.44	1.51	1.42
1	14-A	59	GLY	N-CA	7.44	1.57	1.46
1	2-A	121	TRP	CG-CD1	7.44	1.47	1.36
1	13-A	105	GLN	CA-C	7.44	1.72	1.52
1	9-A	146	TYR	CA-CB	7.44	1.70	1.53
1	15-A	91	GLN	CD-NE2	-7.44	1.14	1.32
1	3-A	67	TRP	CA-C	7.43	1.72	1.52
1	15-A	37	SER	C-O	7.42	1.37	1.23
1	12-A	137	ALA	N-CA	7.42	1.61	1.46
1	15-A	125	GLU	CG-CD	7.41	1.63	1.51
1	7-A	148	SER	CA-CB	7.41	1.64	1.52
1	15-A	134	LEU	CG-CD1	7.41	1.79	1.51
1	1-A	140	TRP	CG-CD1	7.40	1.47	1.36
1	7-A	76	GLN	C-N	-7.40	1.17	1.34
1	14-A	150	ILE	CB-CG1	7.40	1.74	1.54
1	13-A	56	THR	CA-CB	7.40	1.72	1.53
1	15-A	86	THR	CA-CB	7.40	1.72	1.53
1	10-A	139	LEU	C-O	7.40	1.37	1.23
1	10-A	42	ALA	N-CA	7.39	1.61	1.46
1	14-A	75	LYS	CE-NZ	7.39	1.67	1.49
1	15-A	105	GLN	CA-C	7.39	1.72	1.52
1	14-A	130	THR	N-CA	7.39	1.61	1.46
1	5-A	38	LEU	CG-CD1	7.38	1.79	1.51
1	15-A	43	GLU	CB-CG	7.38	1.66	1.52
1	1-A	146	TYR	CG-CD1	-7.38	1.29	1.39
1	8-A	146	TYR	CG-CD2	-7.37	1.29	1.39
1	15-A	122	LEU	CB-CG	7.37	1.74	1.52
1	7-A	98	PHE	CA-CB	-7.36	1.37	1.53
1	7-A	155	PRO	CG-CD	7.36	1.75	1.50
1	16-A	48	TYR	CE2-CZ	7.36	1.48	1.38
1	16-A	89	LEU	CA-C	7.36	1.72	1.52
1	1-A	64	PHE	C-O	7.36	1.37	1.23
1	7-A	117	GLU	N-CA	7.36	1.61	1.46
1	11-A	146	TYR	CG-CD1	-7.36	1.29	1.39
1	13-A	116	ALA	C-O	7.36	1.37	1.23
1	13-A	50	LYS	CD-CE	7.36	1.69	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	41	ARG	CB-CG	7.36	1.72	1.52
1	16-A	147	HIS	CG-CD2	-7.36	1.23	1.35
1	16-A	84	TYR	CA-CB	7.35	1.70	1.53
1	4-A	61	LEU	N-CA	7.34	1.61	1.46
1	7-A	78	TYR	CG-CD1	7.34	1.48	1.39
1	1-A	54	ILE	CB-CG2	7.34	1.75	1.52
1	13-A	155	PRO	CG-CD	7.34	1.74	1.50
1	15-A	66	SER	CA-CB	-7.33	1.42	1.52
1	5-A	63	PRO	N-CD	7.32	1.58	1.47
1	10-A	45	TYR	CE1-CZ	-7.32	1.29	1.38
1	10-A	78	TYR	N-CA	7.32	1.60	1.46
1	11-A	78	TYR	CZ-OH	7.32	1.50	1.37
1	5-A	105	GLN	CA-C	7.32	1.72	1.52
1	9-A	88	VAL	CA-CB	7.32	1.70	1.54
1	7-A	39	LEU	CG-CD1	7.31	1.78	1.51
1	7-A	138	LEU	CG-CD2	7.31	1.78	1.51
1	7-A	156	GLU	CG-CD	7.31	1.62	1.51
1	11-A	37	SER	CA-C	7.30	1.72	1.52
1	16-A	64	PHE	CG-CD1	7.30	1.49	1.38
1	13-A	91	GLN	CA-CB	7.30	1.70	1.53
1	7-A	104	GLU	CB-CG	-7.30	1.38	1.52
1	1-A	78	TYR	CE2-CZ	7.29	1.48	1.38
1	7-A	60	SER	CA-CB	7.29	1.63	1.52
1	13-A	134	LEU	CB-CG	-7.29	1.31	1.52
1	8-A	51	GLN	CA-CB	7.29	1.70	1.53
1	8-A	45	TYR	CD1-CE1	-7.28	1.28	1.39
1	12-A	40	ARG	CZ-NH1	7.28	1.42	1.33
1	2-A	64	PHE	CG-CD2	7.28	1.49	1.38
1	11-A	39	LEU	CA-CB	7.28	1.70	1.53
1	15-A	146	TYR	CB-CG	7.28	1.62	1.51
1	13-A	37	SER	N-CA	7.28	1.60	1.46
1	15-A	53	PRO	CB-CG	7.27	1.86	1.50
1	4-A	131	PRO	CG-CD	7.27	1.74	1.50
1	12-A	154	PHE	CG-CD2	7.27	1.49	1.38
1	13-A	134	LEU	C-O	7.27	1.37	1.23
1	11-A	68	VAL	CB-CG2	7.26	1.68	1.52
1	1-A	92	ARG	CD-NE	7.26	1.58	1.46
1	4-A	63	PRO	N-CD	7.26	1.58	1.47
1	5-A	37	SER	N-CA	7.26	1.60	1.46
1	6-A	95	GLN	CD-OE1	7.26	1.40	1.24
1	7-A	41	ARG	CZ-NH2	7.25	1.42	1.33
1	1-A	75	LYS	CA-CB	7.25	1.70	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	14-A	90	LEU	N-CA	7.25	1.60	1.46
1	3-A	36	GLY	C-O	7.25	1.35	1.23
1	11-A	95	GLN	CD-OE1	7.25	1.39	1.24
1	7-A	98	PHE	CG-CD2	7.24	1.49	1.38
1	7-A	135	HIS	CA-CB	7.23	1.69	1.53
1	1-A	98	PHE	CE1-CZ	7.23	1.51	1.37
1	9-A	93	TRP	CA-C	7.23	1.71	1.52
1	12-A	41	ARG	CZ-NH2	7.23	1.42	1.33
1	13-A	146	TYR	CD2-CE2	7.22	1.50	1.39
1	1-A	110	ILE	N-CA	7.22	1.60	1.46
1	3-A	100	THR	CA-C	-7.21	1.34	1.52
1	5-A	90	LEU	C-O	7.21	1.37	1.23
1	9-A	129	LEU	CA-C	7.21	1.71	1.52
1	7-A	116	ALA	CA-CB	7.21	1.67	1.52
1	16-A	84	TYR	N-CA	7.21	1.60	1.46
1	6-A	67	TRP	CA-CB	7.21	1.69	1.53
1	16-A	142	SER	CA-CB	7.21	1.63	1.52
1	13-A	71	SER	CB-OG	-7.20	1.32	1.42
1	15-A	123	VAL	CB-CG2	-7.20	1.37	1.52
1	1-A	146	TYR	CB-CG	7.20	1.62	1.51
1	4-A	122	LEU	CG-CD2	7.19	1.78	1.51
1	9-A	130	THR	CB-OG1	7.19	1.57	1.43
1	9-A	41	ARG	CD-NE	7.19	1.58	1.46
1	5-A	51	GLN	CA-CB	7.19	1.69	1.53
1	16-A	75	LYS	CB-CG	7.19	1.72	1.52
1	12-A	117	GLU	CD-OE1	7.19	1.33	1.25
1	8-A	121	TRP	CG-CD1	7.18	1.46	1.36
1	10-A	98	PHE	CD2-CE2	7.18	1.53	1.39
1	14-A	41	ARG	NE-CZ	7.18	1.42	1.33
1	6-A	43	GLU	CD-OE2	-7.18	1.17	1.25
1	13-A	84	TYR	CD2-CE2	7.18	1.50	1.39
1	2-A	46	GLN	CG-CD	7.17	1.67	1.51
1	14-A	100	THR	N-CA	-7.17	1.32	1.46
1	15-A	45	TYR	CA-C	7.16	1.71	1.52
1	3-A	98	PHE	C-O	-7.16	1.09	1.23
1	9-A	106	ARG	CB-CG	7.16	1.71	1.52
1	9-A	145	MET	CB-CG	7.16	1.74	1.51
1	4-A	140	TRP	CZ3-CH2	7.16	1.51	1.40
1	7-A	106	ARG	CZ-NH2	7.16	1.42	1.33
1	2-A	76	GLN	C-N	-7.16	1.17	1.34
1	2-A	57	ASN	CB-CG	7.16	1.67	1.51
1	2-A	144	PRO	CA-C	7.15	1.67	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	56	THR	CA-CB	7.15	1.72	1.53
1	13-A	48	TYR	CE2-CZ	7.15	1.47	1.38
1	15-A	48	TYR	CB-CG	-7.15	1.41	1.51
1	13-A	140	TRP	CD2-CE2	7.15	1.50	1.41
1	2-A	69	GLY	CA-C	7.15	1.63	1.51
1	12-A	106	ARG	CZ-NH2	7.15	1.42	1.33
1	14-A	142	SER	CB-OG	7.14	1.51	1.42
1	9-A	106	ARG	C-N	7.14	1.50	1.34
1	11-A	81	PRO	CA-CB	7.14	1.67	1.53
1	7-A	123	VAL	C-O	7.14	1.36	1.23
1	15-A	83	HIS	CB-CG	-7.14	1.37	1.50
1	9-A	156	GLU	CB-CG	7.14	1.65	1.52
1	15-A	124	GLU	CD-OE2	7.13	1.33	1.25
1	11-A	48	TYR	CE2-CZ	7.13	1.47	1.38
1	12-A	116	ALA	N-CA	7.13	1.60	1.46
1	8-A	37	SER	CA-C	7.13	1.71	1.52
1	16-A	59	GLY	C-O	7.13	1.35	1.23
1	9-A	125	GLU	CB-CG	7.13	1.65	1.52
1	15-A	107	LEU	N-CA	7.13	1.60	1.46
1	16-A	141	ARG	CZ-NH2	7.12	1.42	1.33
1	13-A	98	PHE	CD2-CE2	7.12	1.53	1.39
1	8-A	63	PRO	CA-CB	7.12	1.67	1.53
1	10-A	120	ILE	CB-CG1	7.12	1.74	1.54
1	16-A	48	TYR	CD1-CE1	7.12	1.50	1.39
1	5-A	92	ARG	CD-NE	7.12	1.58	1.46
1	9-A	60	SER	CA-CB	7.12	1.63	1.52
1	16-A	146	TYR	CA-CB	7.12	1.69	1.53
1	11-A	116	ALA	C-O	7.12	1.36	1.23
1	15-A	41	ARG	CZ-NH2	7.12	1.42	1.33
1	5-A	41	ARG	CZ-NH1	7.11	1.42	1.33
1	9-A	131	PRO	CG-CD	7.11	1.74	1.50
1	16-A	47	ASP	N-CA	7.11	1.60	1.46
1	5-A	144	PRO	CA-C	7.11	1.67	1.52
1	8-A	141	ARG	CZ-NH2	-7.10	1.23	1.33
1	5-A	138	LEU	N-CA	7.10	1.60	1.46
1	5-A	125	GLU	CD-OE2	7.10	1.33	1.25
1	6-A	106	ARG	CZ-NH2	7.09	1.42	1.33
1	2-A	137	ALA	C-N	7.09	1.50	1.34
1	8-A	91	GLN	CD-NE2	7.09	1.50	1.32
1	12-A	112	HIS	C-O	7.08	1.36	1.23
1	11-A	91	GLN	CG-CD	7.08	1.67	1.51
1	8-A	150	ILE	CB-CG1	7.08	1.73	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-A	110	ILE	CA-CB	-7.08	1.38	1.54
1	8-A	66	SER	CA-C	7.08	1.71	1.52
1	12-A	37	SER	C-O	7.08	1.36	1.23
1	5-A	43	GLU	CD-OE2	7.07	1.33	1.25
1	11-A	41	ARG	C-O	-7.07	1.09	1.23
1	13-A	47	ASP	CA-C	7.07	1.71	1.52
1	15-A	40	ARG	CB-CG	-7.07	1.33	1.52
1	16-A	37	SER	C-O	7.06	1.36	1.23
1	1-A	66	SER	CB-OG	7.06	1.51	1.42
1	15-A	143	ASP	CG-OD2	7.06	1.41	1.25
1	13-A	121	TRP	CA-C	7.05	1.71	1.52
1	1-A	39	LEU	CA-C	-7.05	1.34	1.52
1	2-A	51	GLN	CA-CB	7.04	1.69	1.53
1	5-A	40	ARG	CD-NE	7.04	1.58	1.46
1	9-A	95	GLN	CD-OE1	7.03	1.39	1.24
1	16-A	81	PRO	C-N	7.02	1.50	1.34
1	9-A	131	PRO	N-CD	7.02	1.57	1.47
1	14-A	149	PHE	CD1-CE1	-7.01	1.25	1.39
1	9-A	143	ASP	CA-CB	7.01	1.69	1.53
1	6-A	37	SER	C-O	7.00	1.36	1.23
1	7-A	146	TYR	CA-CB	7.00	1.69	1.53
1	14-A	41	ARG	CZ-NH2	7.00	1.42	1.33
1	15-A	88	VAL	N-CA	7.00	1.60	1.46
1	7-A	154	PHE	CE1-CZ	7.00	1.50	1.37
1	14-A	78	TYR	CG-CD2	7.00	1.48	1.39
1	1-A	124	GLU	CD-OE1	-7.00	1.18	1.25
1	1-A	106	ARG	CB-CG	6.99	1.71	1.52
1	11-A	92	ARG	CZ-NH2	6.99	1.42	1.33
1	15-A	147	HIS	CA-CB	6.99	1.69	1.53
1	6-A	122	LEU	CA-CB	6.99	1.69	1.53
1	8-A	146	TYR	CA-CB	6.99	1.69	1.53
1	12-A	37	SER	CA-CB	6.98	1.63	1.52
1	12-A	56	THR	CA-CB	6.98	1.71	1.53
1	3-A	100	THR	N-CA	6.98	1.60	1.46
1	3-A	66	SER	N-CA	6.97	1.60	1.46
1	7-A	75	LYS	CB-CG	6.97	1.71	1.52
1	6-A	49	MET	SD-CE	6.97	2.16	1.77
1	1-A	71	SER	CA-CB	6.97	1.63	1.52
1	5-A	56	THR	CA-CB	6.97	1.71	1.53
1	16-A	62	ILE	CB-CG2	6.97	1.74	1.52
1	3-A	38	LEU	CG-CD2	6.96	1.77	1.51
1	9-A	64	PHE	CA-CB	6.96	1.69	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	53	PRO	N-CD	6.96	1.57	1.47
1	8-A	147	HIS	N-CA	-6.96	1.32	1.46
1	15-A	78	TYR	CG-CD2	6.96	1.48	1.39
1	12-A	149	PHE	CD1-CE1	6.96	1.53	1.39
1	14-A	132	SER	CB-OG	6.96	1.51	1.42
1	15-A	106	ARG	NE-CZ	6.95	1.42	1.33
1	16-A	118	ALA	CA-CB	6.95	1.67	1.52
1	5-A	71	SER	CA-CB	6.94	1.63	1.52
1	13-A	75	LYS	CA-C	6.94	1.71	1.52
1	2-A	37	SER	C-O	6.94	1.36	1.23
1	3-A	115	LYS	CB-CG	6.94	1.71	1.52
1	6-A	74	MET	CA-CB	6.94	1.69	1.53
1	13-A	133	HIS	CA-C	-6.94	1.34	1.52
1	4-A	60	SER	CB-OG	6.94	1.51	1.42
1	7-A	67	TRP	CE3-CZ3	-6.94	1.26	1.38
1	5-A	50	LYS	CD-CE	6.93	1.68	1.51
1	16-A	130	THR	C-O	6.93	1.36	1.23
1	7-A	37	SER	CA-CB	6.92	1.63	1.52
1	13-A	155	PRO	CB-CG	-6.92	1.15	1.50
1	14-A	91	GLN	C-O	6.92	1.36	1.23
1	7-A	131	PRO	N-CD	6.92	1.57	1.47
1	13-A	155	PRO	CA-C	-6.92	1.39	1.52
1	15-A	125	GLU	C-O	6.92	1.36	1.23
1	15-A	124	GLU	C-N	6.92	1.50	1.34
1	4-A	64	PHE	CG-CD1	6.91	1.49	1.38
1	3-A	139	LEU	CG-CD2	6.91	1.77	1.51
1	2-A	104	GLU	CD-OE2	6.91	1.33	1.25
1	10-A	128	ARG	CG-CD	6.91	1.69	1.51
1	10-A	115	LYS	CG-CD	6.90	1.75	1.52
1	3-A	110	ILE	N-CA	6.89	1.60	1.46
1	14-A	148	SER	CB-OG	-6.89	1.33	1.42
1	6-A	145	MET	CB-CG	6.89	1.73	1.51
1	5-A	67	TRP	CE3-CZ3	6.89	1.50	1.38
1	1-A	64	PHE	CB-CG	6.88	1.63	1.51
1	3-A	37	SER	C-O	6.88	1.36	1.23
1	8-A	67	TRP	CG-CD1	-6.88	1.27	1.36
1	16-A	41	ARG	CD-NE	6.88	1.58	1.46
1	2-A	64	PHE	CG-CD1	6.88	1.49	1.38
1	13-A	52	VAL	CB-CG1	-6.88	1.38	1.52
1	9-A	125	GLU	CA-CB	6.87	1.69	1.53
1	3-A	137	ALA	N-CA	6.87	1.60	1.46
1	1-A	51	GLN	CB-CG	-6.87	1.34	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	105	GLN	CB-CG	-6.87	1.34	1.52
1	4-A	108	ASP	CB-CG	6.86	1.66	1.51
1	2-A	56	THR	CA-CB	6.86	1.71	1.53
1	1-A	43	GLU	CD-OE1	6.86	1.33	1.25
1	8-A	78	TYR	CD2-CE2	6.86	1.49	1.39
1	8-A	109	SER	CA-C	6.86	1.70	1.52
1	9-A	92	ARG	CD-NE	6.86	1.58	1.46
1	7-A	153	ILE	C-O	6.86	1.36	1.23
1	12-A	80	GLN	CA-CB	6.86	1.69	1.53
1	4-A	113	PRO	CA-CB	6.85	1.67	1.53
1	15-A	90	LEU	C-O	6.85	1.36	1.23
1	5-A	59	GLY	N-CA	6.85	1.56	1.46
1	15-A	152	PRO	CA-CB	6.85	1.67	1.53
1	16-A	61	LEU	CA-CB	6.84	1.69	1.53
1	10-A	112	HIS	CG-CD2	6.84	1.47	1.35
1	14-A	62	ILE	C-N	6.84	1.47	1.34
1	8-A	72	ILE	CB-CG2	6.83	1.74	1.52
1	2-A	77	LEU	CB-CG	6.83	1.72	1.52
1	2-A	103	GLU	CA-C	6.83	1.70	1.52
1	2-A	41	ARG	CZ-NH2	6.82	1.42	1.33
1	12-A	146	TYR	CB-CG	6.82	1.61	1.51
1	7-A	103	GLU	CG-CD	6.82	1.62	1.51
1	2-A	78	TYR	CG-CD1	6.82	1.48	1.39
1	13-A	91	GLN	N-CA	6.82	1.59	1.46
1	2-A	103	GLU	C-O	6.81	1.36	1.23
1	4-A	130	THR	CB-OG1	6.81	1.56	1.43
1	4-A	54	ILE	C-O	6.81	1.36	1.23
1	2-A	141	ARG	N-CA	6.81	1.59	1.46
1	3-A	148	SER	CB-OG	-6.81	1.33	1.42
1	16-A	113	PRO	CA-C	-6.81	1.39	1.52
1	9-A	122	LEU	CG-CD2	6.80	1.77	1.51
1	9-A	83	HIS	CA-CB	6.80	1.69	1.53
1	13-A	48	TYR	CA-C	6.80	1.70	1.52
1	8-A	54	ILE	C-N	-6.79	1.21	1.34
1	11-A	155	PRO	CG-CD	6.79	1.73	1.50
1	15-A	85	LEU	CB-CG	6.79	1.72	1.52
1	16-A	58	ARG	CB-CG	6.79	1.70	1.52
1	16-A	83	HIS	C-N	6.79	1.49	1.34
1	14-A	98	PHE	CA-CB	-6.79	1.39	1.53
1	14-A	129	LEU	CA-C	-6.79	1.35	1.52
1	1-A	63	PRO	N-CD	6.79	1.57	1.47
1	15-A	67	TRP	CG-CD1	6.79	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	91	GLN	N-CA	6.79	1.59	1.46
1	6-A	105	GLN	CA-C	6.79	1.70	1.52
1	6-A	60	SER	CB-OG	6.78	1.51	1.42
1	10-A	84	TYR	CD2-CE2	-6.78	1.29	1.39
1	3-A	96	SER	C-O	6.78	1.36	1.23
1	7-A	98	PHE	CB-CG	6.77	1.62	1.51
1	11-A	149	PHE	CD1-CE1	-6.77	1.25	1.39
1	13-A	93	TRP	CD1-NE1	6.76	1.49	1.38
1	15-A	65	THR	CA-CB	6.76	1.71	1.53
1	16-A	127	HIS	CB-CG	6.76	1.62	1.50
1	15-A	151	ASP	N-CA	6.75	1.59	1.46
1	4-A	91	GLN	CD-OE1	6.75	1.38	1.24
1	13-A	75	LYS	CD-CE	6.75	1.68	1.51
1	14-A	124	GLU	CB-CG	6.75	1.65	1.52
1	14-A	41	ARG	CA-CB	6.75	1.68	1.53
1	12-A	156	GLU	CD-OE2	6.75	1.33	1.25
1	10-A	144	PRO	N-CA	6.75	1.58	1.47
1	12-A	57	ASN	CA-C	6.75	1.70	1.52
1	2-A	88	VAL	CB-CG2	6.74	1.67	1.52
1	15-A	148	SER	CA-CB	6.74	1.63	1.52
1	11-A	43	GLU	C-O	6.74	1.36	1.23
1	14-A	155	PRO	CB-CG	-6.74	1.16	1.50
1	16-A	57	ASN	CA-C	6.74	1.70	1.52
1	8-A	37	SER	N-CA	6.74	1.59	1.46
1	2-A	59	GLY	N-CA	6.74	1.56	1.46
1	5-A	144	PRO	C-O	6.74	1.36	1.23
1	8-A	145	MET	CB-CG	6.74	1.73	1.51
1	10-A	97	ARG	C-O	6.73	1.36	1.23
1	1-A	95	GLN	CD-OE1	6.73	1.38	1.24
1	9-A	98	PHE	CA-CB	-6.73	1.39	1.53
1	11-A	141	ARG	CZ-NH1	6.73	1.41	1.33
1	14-A	65	THR	CA-CB	6.73	1.70	1.53
1	2-A	131	PRO	CA-C	6.72	1.66	1.52
1	4-A	64	PHE	CB-CG	6.72	1.62	1.51
1	1-A	56	THR	CA-CB	6.72	1.70	1.53
1	7-A	156	GLU	CA-C	6.72	1.70	1.52
1	11-A	44	MET	N-CA	-6.72	1.32	1.46
1	15-A	58	ARG	CG-CD	6.72	1.68	1.51
1	11-A	47	ASP	CG-OD2	6.72	1.40	1.25
1	8-A	149	PHE	CD2-CE2	6.72	1.52	1.39
1	16-A	146	TYR	CG-CD2	6.71	1.47	1.39
1	3-A	96	SER	CB-OG	-6.71	1.33	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	10-A	128	ARG	CZ-NH2	6.71	1.41	1.33
1	12-A	146	TYR	CZ-OH	6.71	1.49	1.37
1	1-A	140	TRP	CA-CB	6.71	1.68	1.53
1	9-A	136	MET	CA-C	6.71	1.70	1.52
1	8-A	60	SER	CA-CB	6.71	1.63	1.52
1	10-A	113	PRO	N-CD	6.71	1.57	1.47
1	13-A	41	ARG	CZ-NH2	6.71	1.41	1.33
1	16-A	156	GLU	C-O	6.71	1.36	1.23
1	10-A	62	ILE	CA-CB	6.71	1.70	1.54
1	4-A	146	TYR	CG-CD1	-6.70	1.30	1.39
1	12-A	142	SER	CA-CB	6.70	1.63	1.52
1	16-A	51	GLN	CG-CD	6.70	1.66	1.51
1	2-A	146	TYR	CZ-OH	6.70	1.49	1.37
1	7-A	41	ARG	CD-NE	6.70	1.57	1.46
1	7-A	97	ARG	CZ-NH2	6.70	1.41	1.33
1	4-A	45	TYR	CE1-CZ	6.70	1.47	1.38
1	14-A	63	PRO	CB-CG	6.69	1.83	1.50
1	16-A	76	GLN	N-CA	6.69	1.59	1.46
1	1-A	145	MET	CG-SD	6.68	1.98	1.81
1	8-A	104	GLU	CD-OE2	6.68	1.33	1.25
1	2-A	81	PRO	CA-CB	6.68	1.67	1.53
1	6-A	92	ARG	CG-CD	6.68	1.68	1.51
1	9-A	88	VAL	CA-C	6.68	1.70	1.52
1	9-A	107	LEU	N-CA	6.67	1.59	1.46
1	14-A	120	ILE	C-O	6.67	1.36	1.23
1	16-A	148	SER	N-CA	-6.67	1.33	1.46
1	12-A	41	ARG	CD-NE	6.66	1.57	1.46
1	8-A	147	HIS	C-N	-6.66	1.18	1.34
1	14-A	146	TYR	CD2-CE2	6.66	1.49	1.39
1	2-A	102	SER	CA-CB	6.66	1.62	1.52
1	4-A	55	PRO	N-CD	6.66	1.57	1.47
1	5-A	41	ARG	CD-NE	6.66	1.57	1.46
1	9-A	61	LEU	CG-CD1	6.65	1.76	1.51
1	3-A	155	PRO	CG-CD	6.65	1.72	1.50
1	10-A	128	ARG	N-CA	6.65	1.59	1.46
1	14-A	48	TYR	CB-CG	-6.65	1.41	1.51
1	3-A	106	ARG	C-O	-6.65	1.10	1.23
1	3-A	146	TYR	CB-CG	6.65	1.61	1.51
1	11-A	60	SER	CA-C	-6.65	1.35	1.52
1	13-A	57	ASN	C-O	6.65	1.35	1.23
1	7-A	121	TRP	CZ3-CH2	6.64	1.50	1.40
1	8-A	81	PRO	CA-C	6.64	1.66	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-A	50	LYS	CG-CD	6.64	1.75	1.52
1	6-A	78	TYR	CG-CD2	6.64	1.47	1.39
1	15-A	110	ILE	C-N	6.64	1.49	1.34
1	1-A	125	GLU	CB-CG	6.63	1.64	1.52
1	12-A	48	TYR	CB-CG	-6.63	1.41	1.51
1	16-A	115	LYS	CA-C	6.63	1.70	1.52
1	2-A	149	PHE	N-CA	6.63	1.59	1.46
1	1-A	60	SER	CB-OG	6.63	1.50	1.42
1	10-A	122	LEU	CG-CD2	6.62	1.76	1.51
1	9-A	62	ILE	CB-CG2	6.62	1.73	1.52
1	10-A	124	GLU	CA-CB	6.62	1.68	1.53
1	6-A	72	ILE	CA-CB	-6.62	1.39	1.54
1	10-A	84	TYR	CZ-OH	-6.62	1.26	1.37
1	7-A	66	SER	CA-CB	-6.61	1.43	1.52
1	6-A	131	PRO	CG-CD	6.61	1.72	1.50
1	7-A	104	GLU	CD-OE2	6.61	1.32	1.25
1	14-A	128	ARG	C-O	6.61	1.35	1.23
1	2-A	70	LEU	C-O	-6.61	1.10	1.23
1	3-A	51	GLN	CD-OE1	6.61	1.38	1.24
1	4-A	37	SER	CA-CB	6.61	1.62	1.52
1	15-A	80	GLN	C-N	6.61	1.46	1.34
1	11-A	62	ILE	C-N	6.60	1.46	1.34
1	15-A	125	GLU	CB-CG	6.60	1.64	1.52
1	1-A	98	PHE	CG-CD2	6.60	1.48	1.38
1	14-A	63	PRO	N-CA	6.60	1.58	1.47
1	2-A	47	ASP	C-O	6.60	1.35	1.23
1	5-A	146	TYR	CB-CG	6.60	1.61	1.51
1	7-A	137	ALA	CA-CB	6.59	1.66	1.52
1	10-A	97	ARG	NE-CZ	6.59	1.41	1.33
1	11-A	102	SER	CA-CB	6.59	1.62	1.52
1	10-A	102	SER	C-O	-6.59	1.10	1.23
1	14-A	102	SER	CA-CB	6.59	1.62	1.52
1	15-A	95	GLN	CA-CB	-6.59	1.39	1.53
1	4-A	60	SER	CA-CB	6.58	1.62	1.52
1	6-A	146	TYR	CD2-CE2	6.58	1.49	1.39
1	4-A	48	TYR	CE1-CZ	6.58	1.47	1.38
1	10-A	131	PRO	CA-CB	6.58	1.66	1.53
1	11-A	64	PHE	CE1-CZ	6.58	1.49	1.37
1	1-A	79	GLY	CA-C	-6.58	1.41	1.51
1	4-A	151	ASP	N-CA	6.58	1.59	1.46
1	15-A	70	LEU	CG-CD2	6.58	1.76	1.51
1	3-A	48	TYR	CE2-CZ	6.58	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6-A	78	TYR	CE1-CZ	-6.57	1.30	1.38
1	16-A	98	PHE	CG-CD2	6.57	1.48	1.38
1	1-A	105	GLN	CG-CD	6.57	1.66	1.51
1	15-A	95	GLN	C-O	6.57	1.35	1.23
1	16-A	44	MET	C-N	6.57	1.49	1.34
1	6-A	67	TRP	CA-C	6.57	1.70	1.52
1	10-A	103	GLU	CB-CG	6.57	1.64	1.52
1	7-A	80	GLN	CA-CB	6.56	1.68	1.53
1	13-A	78	TYR	CG-CD2	6.56	1.47	1.39
1	16-A	116	ALA	CA-CB	6.56	1.66	1.52
1	8-A	81	PRO	CG-CD	6.56	1.72	1.50
1	16-A	41	ARG	CZ-NH2	6.56	1.41	1.33
1	10-A	124	GLU	CG-CD	6.54	1.61	1.51
1	12-A	102	SER	CA-CB	6.54	1.62	1.52
1	15-A	149	PHE	CD1-CE1	-6.54	1.26	1.39
1	16-A	65	THR	C-N	6.54	1.49	1.34
1	6-A	144	PRO	CA-CB	6.54	1.66	1.53
1	16-A	107	LEU	CA-CB	6.54	1.68	1.53
1	6-A	62	ILE	CB-CG2	6.54	1.73	1.52
1	10-A	62	ILE	CG1-CD1	6.54	1.95	1.50
1	2-A	120	ILE	CB-CG2	6.54	1.73	1.52
1	16-A	48	TYR	CD2-CE2	6.54	1.49	1.39
1	13-A	40	ARG	CB-CG	-6.53	1.34	1.52
1	4-A	155	PRO	CA-C	-6.53	1.39	1.52
1	6-A	104	GLU	CB-CG	-6.53	1.39	1.52
1	16-A	93	TRP	CD2-CE2	6.53	1.49	1.41
1	4-A	37	SER	C-O	6.53	1.35	1.23
1	14-A	52	VAL	CA-CB	6.52	1.68	1.54
1	8-A	104	GLU	CG-CD	6.52	1.61	1.51
1	10-A	76	GLN	CG-CD	6.52	1.66	1.51
1	5-A	67	TRP	CZ3-CH2	6.51	1.50	1.40
1	10-A	64	PHE	C-O	6.51	1.35	1.23
1	7-A	79	GLY	C-O	6.51	1.34	1.23
1	9-A	67	TRP	CD2-CE3	6.51	1.50	1.40
1	5-A	41	ARG	CG-CD	6.51	1.68	1.51
1	2-A	75	LYS	CA-C	6.51	1.69	1.52
1	6-A	76	GLN	CG-CD	6.50	1.66	1.51
1	6-A	41	ARG	CD-NE	6.50	1.57	1.46
1	1-A	140	TRP	CD2-CE2	6.50	1.49	1.41
1	10-A	41	ARG	CD-NE	6.50	1.57	1.46
1	10-A	156	GLU	CG-CD	6.50	1.61	1.51
1	14-A	152	PRO	C-O	6.50	1.36	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	64	PHE	CA-CB	6.49	1.68	1.53
1	14-A	147	HIS	CA-CB	6.49	1.68	1.53
1	10-A	139	LEU	CA-CB	6.49	1.68	1.53
1	1-A	43	GLU	CA-CB	6.48	1.68	1.53
1	2-A	138	LEU	N-CA	-6.48	1.33	1.46
1	16-A	115	LYS	CD-CE	6.48	1.67	1.51
1	7-A	48	TYR	CB-CG	-6.48	1.42	1.51
1	11-A	51	GLN	CD-NE2	6.48	1.49	1.32
1	13-A	141	ARG	C-O	6.47	1.35	1.23
1	10-A	67	TRP	CG-CD1	6.47	1.45	1.36
1	10-A	76	GLN	N-CA	6.47	1.59	1.46
1	6-A	146	TYR	CZ-OH	6.47	1.48	1.37
1	9-A	95	GLN	CA-CB	6.46	1.68	1.53
1	1-A	128	ARG	CD-NE	6.46	1.57	1.46
1	16-A	141	ARG	CD-NE	6.46	1.57	1.46
1	5-A	47	ASP	N-CA	6.46	1.59	1.46
1	12-A	71	SER	C-O	6.46	1.35	1.23
1	1-A	67	TRP	CD2-CE2	6.46	1.49	1.41
1	12-A	145	MET	CG-SD	6.46	1.98	1.81
1	9-A	139	LEU	CA-C	6.46	1.69	1.52
1	16-A	129	LEU	CG-CD2	6.46	1.75	1.51
1	11-A	93	TRP	C-O	6.45	1.35	1.23
1	16-A	67	TRP	C-N	6.45	1.48	1.34
1	4-A	151	ASP	CB-CG	6.44	1.65	1.51
1	9-A	48	TYR	CD1-CE1	6.44	1.49	1.39
1	7-A	108	ASP	CB-CG	6.44	1.65	1.51
1	13-A	138	LEU	CG-CD2	6.44	1.75	1.51
1	6-A	155	PRO	CG-CD	6.44	1.71	1.50
1	14-A	72	ILE	N-CA	6.44	1.59	1.46
1	14-A	156	GLU	CB-CG	6.43	1.64	1.52
1	15-A	80	GLN	N-CA	6.43	1.59	1.46
1	16-A	105	GLN	CB-CG	-6.43	1.35	1.52
1	4-A	138	LEU	CG-CD2	6.43	1.75	1.51
1	9-A	64	PHE	CD1-CE1	6.43	1.52	1.39
1	11-A	43	GLU	CD-OE1	-6.43	1.18	1.25
1	6-A	37	SER	CA-CB	6.43	1.62	1.52
1	14-A	87	ASN	CG-ND2	6.43	1.49	1.32
1	15-A	124	GLU	CA-CB	6.42	1.68	1.53
1	6-A	39	LEU	CG-CD1	6.42	1.75	1.51
1	6-A	95	GLN	CG-CD	6.42	1.65	1.51
1	7-A	95	GLN	CA-CB	-6.42	1.39	1.53
1	14-A	129	LEU	CA-CB	6.42	1.68	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	13-A	146	TYR	C-N	6.42	1.48	1.34
1	9-A	84	TYR	CE1-CZ	6.41	1.46	1.38
1	14-A	62	ILE	CG1-CD1	6.41	1.94	1.50
1	15-A	145	MET	SD-CE	6.41	2.13	1.77
1	14-A	84	TYR	CA-CB	6.41	1.68	1.53
1	13-A	124	GLU	CB-CG	6.41	1.64	1.52
1	11-A	98	PHE	CB-CG	6.40	1.62	1.51
1	1-A	108	ASP	CA-C	6.40	1.69	1.52
1	4-A	41	ARG	CD-NE	6.40	1.57	1.46
1	14-A	75	LYS	CA-C	6.40	1.69	1.52
1	1-A	133	HIS	C-O	6.40	1.35	1.23
1	9-A	76	GLN	N-CA	6.40	1.59	1.46
1	14-A	126	ILE	CB-CG2	6.40	1.72	1.52
1	15-A	80	GLN	CD-OE1	6.39	1.38	1.24
1	16-A	87	ASN	CG-ND2	6.39	1.48	1.32
1	4-A	92	ARG	CZ-NH1	-6.39	1.24	1.33
1	2-A	43	GLU	CD-OE1	-6.39	1.18	1.25
1	5-A	84	TYR	CB-CG	-6.39	1.42	1.51
1	14-A	126	ILE	CG1-CD1	6.39	1.94	1.50
1	4-A	75	LYS	C-O	6.39	1.35	1.23
1	12-A	125	GLU	CD-OE2	6.39	1.32	1.25
1	2-A	117	GLU	CD-OE2	6.38	1.32	1.25
1	1-A	71	SER	CA-C	6.38	1.69	1.52
1	2-A	71	SER	CA-C	6.38	1.69	1.52
1	10-A	56	THR	CA-CB	6.38	1.70	1.53
1	8-A	103	GLU	CG-CD	6.38	1.61	1.51
1	7-A	96	SER	C-N	6.37	1.48	1.34
1	9-A	141	ARG	CA-CB	6.37	1.68	1.53
1	7-A	141	ARG	CA-CB	6.37	1.68	1.53
1	2-A	154	PHE	C-N	6.37	1.46	1.34
1	6-A	64	PHE	CD2-CE2	6.37	1.51	1.39
1	9-A	49	MET	CB-CG	6.37	1.71	1.51
1	16-A	95	GLN	CD-OE1	6.37	1.38	1.24
1	3-A	94	ASP	C-O	6.36	1.35	1.23
1	6-A	98	PHE	CD2-CE2	6.36	1.51	1.39
1	13-A	91	GLN	C-O	-6.36	1.11	1.23
1	13-A	92	ARG	CZ-NH2	6.36	1.41	1.33
1	3-A	125	GLU	CD-OE2	6.36	1.32	1.25
1	10-A	135	HIS	C-O	6.36	1.35	1.23
1	4-A	92	ARG	CD-NE	6.35	1.57	1.46
1	11-A	152	PRO	CG-CD	6.35	1.71	1.50
1	7-A	63	PRO	N-CD	6.35	1.56	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	13-A	115	LYS	CB-CG	6.35	1.69	1.52
1	16-A	113	PRO	C-O	6.35	1.35	1.23
1	3-A	149	PHE	CD1-CE1	-6.35	1.26	1.39
1	8-A	126	ILE	CB-CG2	6.35	1.72	1.52
1	11-A	112	HIS	CG-CD2	6.35	1.46	1.35
1	8-A	149	PHE	CD1-CE1	-6.34	1.26	1.39
1	7-A	139	LEU	C-O	6.34	1.35	1.23
1	15-A	84	TYR	CG-CD1	6.34	1.47	1.39
1	16-A	38	LEU	CG-CD2	6.34	1.75	1.51
1	10-A	84	TYR	CG-CD2	6.33	1.47	1.39
1	6-A	143	ASP	CA-CB	6.33	1.67	1.53
1	13-A	59	GLY	N-CA	6.33	1.55	1.46
1	10-A	61	LEU	C-O	6.33	1.35	1.23
1	14-A	42	ALA	CA-CB	6.32	1.65	1.52
1	14-A	116	ALA	CA-CB	6.32	1.65	1.52
1	3-A	95	GLN	N-CA	6.32	1.58	1.46
1	12-A	107	LEU	C-O	6.32	1.35	1.23
1	13-A	43	GLU	CD-OE2	6.32	1.32	1.25
1	1-A	62	ILE	CB-CG2	6.32	1.72	1.52
1	16-A	53	PRO	N-CD	6.31	1.56	1.47
1	2-A	136	MET	CB-CG	6.31	1.71	1.51
1	4-A	134	LEU	CA-CB	6.31	1.68	1.53
1	13-A	147	HIS	N-CA	-6.31	1.33	1.46
1	14-A	51	GLN	CA-CB	6.31	1.67	1.53
1	15-A	72	ILE	N-CA	6.31	1.58	1.46
1	8-A	152	PRO	CG-CD	6.31	1.71	1.50
1	9-A	142	SER	CA-CB	6.30	1.62	1.52
1	15-A	50	LYS	CB-CG	-6.30	1.35	1.52
1	8-A	113	PRO	CA-CB	6.30	1.66	1.53
1	4-A	146	TYR	CB-CG	6.30	1.61	1.51
1	11-A	154	PHE	CD2-CE2	6.30	1.51	1.39
1	12-A	140	TRP	CZ3-CH2	6.30	1.50	1.40
1	15-A	143	ASP	CG-OD1	6.30	1.39	1.25
1	16-A	78	TYR	CD2-CE2	6.30	1.48	1.39
1	1-A	130	THR	C-O	6.29	1.35	1.23
1	2-A	92	ARG	N-CA	6.29	1.58	1.46
1	9-A	139	LEU	CA-CB	6.28	1.68	1.53
1	6-A	76	GLN	CD-OE1	-6.28	1.10	1.24
1	8-A	103	GLU	CD-OE2	6.28	1.32	1.25
1	14-A	50	LYS	CG-CD	6.28	1.73	1.52
1	12-A	107	LEU	CB-CG	6.27	1.70	1.52
1	4-A	122	LEU	CB-CG	6.27	1.70	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	11-A	93	TRP	CE2-CZ2	-6.27	1.29	1.39
1	14-A	104	GLU	N-CA	6.27	1.58	1.46
1	4-A	156	GLU	C-O	6.27	1.35	1.23
1	9-A	60	SER	CB-OG	6.27	1.50	1.42
1	16-A	146	TYR	CA-C	6.27	1.69	1.52
1	16-A	88	VAL	CA-C	6.26	1.69	1.52
1	11-A	43	GLU	CB-CG	6.26	1.64	1.52
1	6-A	154	PHE	CE2-CZ	-6.26	1.25	1.37
1	11-A	106	ARG	C-O	6.26	1.35	1.23
1	11-A	110	ILE	CB-CG2	6.26	1.72	1.52
1	5-A	134	LEU	CG-CD1	6.26	1.75	1.51
1	7-A	125	GLU	CG-CD	-6.26	1.42	1.51
1	13-A	110	ILE	CB-CG2	6.26	1.72	1.52
1	15-A	109	SER	C-O	6.26	1.35	1.23
1	4-A	48	TYR	CD1-CE1	6.25	1.48	1.39
1	1-A	51	GLN	C-O	6.25	1.35	1.23
1	8-A	95	GLN	CD-OE1	6.25	1.37	1.24
1	1-A	96	SER	CA-CB	6.25	1.62	1.52
1	2-A	55	PRO	CG-CD	6.25	1.71	1.50
1	12-A	66	SER	CA-CB	-6.24	1.43	1.52
1	5-A	48	TYR	CE2-CZ	-6.24	1.30	1.38
1	3-A	47	ASP	CG-OD2	6.24	1.39	1.25
1	11-A	103	GLU	CG-CD	6.24	1.61	1.51
1	15-A	59	GLY	CA-C	-6.23	1.41	1.51
1	15-A	105	GLN	N-CA	-6.23	1.33	1.46
1	13-A	149	PHE	CD2-CE2	6.23	1.51	1.39
1	16-A	92	ARG	CZ-NH2	6.23	1.41	1.33
1	12-A	146	TYR	CD1-CE1	6.23	1.48	1.39
1	9-A	75	LYS	CD-CE	6.22	1.66	1.51
1	7-A	129	LEU	C-O	6.22	1.35	1.23
1	11-A	41	ARG	CA-C	6.22	1.69	1.52
1	16-A	67	TRP	N-CA	6.22	1.58	1.46
1	7-A	125	GLU	CD-OE2	6.22	1.32	1.25
1	9-A	136	MET	SD-CE	-6.22	1.43	1.77
1	13-A	134	LEU	CA-C	-6.22	1.36	1.52
1	10-A	104	GLU	CD-OE1	6.21	1.32	1.25
1	13-A	123	VAL	C-N	6.21	1.48	1.34
1	4-A	48	TYR	CG-CD2	6.21	1.47	1.39
1	9-A	78	TYR	N-CA	6.21	1.58	1.46
1	11-A	88	VAL	C-O	6.21	1.35	1.23
1	11-A	140	TRP	CE3-CZ3	-6.21	1.27	1.38
1	16-A	59	GLY	N-CA	6.21	1.55	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	10-A	107	LEU	CA-CB	6.21	1.68	1.53
1	10-A	143	ASP	CA-CB	6.21	1.67	1.53
1	2-A	146	TYR	CB-CG	6.21	1.60	1.51
1	16-A	48	TYR	CE1-CZ	6.20	1.46	1.38
1	3-A	67	TRP	CE2-CZ2	6.20	1.50	1.39
1	15-A	124	GLU	CB-CG	-6.20	1.40	1.52
1	13-A	75	LYS	CE-NZ	6.20	1.64	1.49
1	15-A	120	ILE	CA-CB	6.19	1.69	1.54
1	12-A	67	TRP	CE3-CZ3	6.18	1.49	1.38
1	12-A	45	TYR	CD1-CE1	-6.18	1.30	1.39
1	15-A	119	THR	C-N	6.18	1.48	1.34
1	10-A	45	TYR	CE2-CZ	6.18	1.46	1.38
1	16-A	140	TRP	CD2-CE2	6.18	1.48	1.41
1	4-A	48	TYR	CA-CB	6.18	1.67	1.53
1	10-A	105	GLN	CA-C	6.18	1.69	1.52
1	4-A	106	ARG	CG-CD	6.18	1.67	1.51
1	6-A	116	ALA	CA-CB	6.18	1.65	1.52
1	12-A	123	VAL	CB-CG1	-6.17	1.39	1.52
1	3-A	45	TYR	CZ-OH	-6.17	1.27	1.37
1	4-A	115	LYS	CA-CB	6.17	1.67	1.53
1	9-A	64	PHE	CG-CD2	6.17	1.48	1.38
1	1-A	48	TYR	CA-CB	6.16	1.67	1.53
1	14-A	155	PRO	CG-CD	6.16	1.71	1.50
1	2-A	135	HIS	C-O	6.16	1.35	1.23
1	6-A	91	GLN	CD-OE1	-6.16	1.10	1.24
1	10-A	70	LEU	CG-CD2	6.16	1.74	1.51
1	1-A	64	PHE	CG-CD1	6.15	1.48	1.38
1	10-A	150	ILE	CG1-CD1	6.15	1.93	1.50
1	16-A	124	GLU	CD-OE2	6.15	1.32	1.25
1	3-A	155	PRO	CA-C	-6.15	1.40	1.52
1	2-A	144	PRO	C-O	6.15	1.35	1.23
1	3-A	57	ASN	C-O	6.15	1.35	1.23
1	9-A	90	LEU	C-O	6.14	1.35	1.23
1	11-A	114	THR	CA-CB	6.14	1.69	1.53
1	15-A	97	ARG	CA-C	6.14	1.69	1.52
1	1-A	113	PRO	N-CD	6.14	1.56	1.47
1	13-A	120	ILE	CA-C	6.14	1.69	1.52
1	11-A	40	ARG	CA-CB	6.13	1.67	1.53
1	13-A	64	PHE	CA-CB	6.13	1.67	1.53
1	6-A	146	TYR	CE2-CZ	-6.13	1.30	1.38
1	8-A	131	PRO	CA-C	6.13	1.65	1.52
1	7-A	97	ARG	C-O	6.13	1.34	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	14-A	38	LEU	CG-CD2	6.13	1.74	1.51
1	3-A	108	ASP	CB-CG	6.13	1.64	1.51
1	16-A	104	GLU	CD-OE2	6.13	1.32	1.25
1	1-A	37	SER	C-O	6.12	1.34	1.23
1	6-A	73	SER	C-O	6.12	1.34	1.23
1	15-A	38	LEU	CG-CD1	6.12	1.74	1.51
1	16-A	36	GLY	CA-C	6.12	1.61	1.51
1	9-A	42	ALA	N-CA	6.12	1.58	1.46
1	15-A	63	PRO	CG-CD	6.12	1.70	1.50
1	2-A	41	ARG	NE-CZ	6.12	1.41	1.33
1	10-A	144	PRO	CA-C	6.12	1.65	1.52
1	12-A	144	PRO	N-CA	6.12	1.57	1.47
1	3-A	156	GLU	CD-OE1	-6.11	1.19	1.25
1	12-A	134	LEU	CA-CB	6.11	1.67	1.53
1	7-A	154	PHE	CG-CD2	6.11	1.48	1.38
1	5-A	71	SER	CA-C	6.11	1.68	1.52
1	14-A	130	THR	CA-CB	6.11	1.69	1.53
1	15-A	88	VAL	CA-C	-6.11	1.37	1.52
1	4-A	57	ASN	C-O	6.10	1.34	1.23
1	11-A	143	ASP	C-O	-6.10	1.11	1.23
1	5-A	56	THR	C-N	-6.10	1.20	1.34
1	15-A	112	HIS	CA-C	6.10	1.68	1.52
1	7-A	103	GLU	CD-OE2	6.09	1.32	1.25
1	10-A	100	THR	CA-CB	6.09	1.69	1.53
1	14-A	86	THR	CA-CB	6.09	1.69	1.53
1	14-A	51	GLN	CG-CD	6.09	1.65	1.51
1	12-A	103	GLU	CG-CD	6.08	1.61	1.51
1	10-A	41	ARG	CZ-NH1	6.08	1.41	1.33
1	13-A	90	LEU	N-CA	6.08	1.58	1.46
1	15-A	113	PRO	C-O	-6.08	1.11	1.23
1	6-A	67	TRP	CD2-CE2	6.08	1.48	1.41
1	7-A	106	ARG	C-O	6.08	1.34	1.23
1	14-A	95	GLN	C-O	6.08	1.34	1.23
1	2-A	72	ILE	CA-C	6.08	1.68	1.52
1	10-A	141	ARG	CA-CB	6.08	1.67	1.53
1	12-A	108	ASP	CB-CG	6.08	1.64	1.51
1	15-A	126	ILE	C-O	6.08	1.34	1.23
1	16-A	86	THR	C-N	6.08	1.48	1.34
1	5-A	66	SER	CB-OG	6.07	1.50	1.42
1	10-A	48	TYR	CE2-CZ	6.07	1.46	1.38
1	9-A	59	GLY	C-O	6.07	1.33	1.23
1	2-A	41	ARG	CD-NE	6.07	1.56	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6-A	80	GLN	CA-CB	6.07	1.67	1.53
1	15-A	85	LEU	N-CA	6.07	1.58	1.46
1	5-A	98	PHE	CD2-CE2	6.07	1.51	1.39
1	10-A	77	LEU	C-O	6.07	1.34	1.23
1	10-A	140	TRP	CZ2-CH2	6.07	1.48	1.37
1	9-A	83	HIS	ND1-CE1	6.07	1.50	1.34
1	12-A	152	PRO	CG-CD	6.07	1.70	1.50
1	4-A	93	TRP	CE2-CZ2	6.06	1.50	1.39
1	5-A	38	LEU	C-O	6.05	1.34	1.23
1	11-A	52	VAL	CB-CG1	6.05	1.65	1.52
1	14-A	67	TRP	C-N	6.04	1.48	1.34
1	2-A	99	GLY	N-CA	6.04	1.55	1.46
1	7-A	97	ARG	CA-C	6.04	1.68	1.52
1	1-A	97	ARG	CZ-NH2	6.04	1.40	1.33
1	1-A	121	TRP	N-CA	6.04	1.58	1.46
1	12-A	105	GLN	CB-CG	-6.04	1.36	1.52
1	15-A	45	TYR	C-O	6.04	1.34	1.23
1	6-A	59	GLY	CA-C	-6.03	1.42	1.51
1	9-A	129	LEU	N-CA	6.03	1.58	1.46
1	13-A	148	SER	C-N	6.03	1.48	1.34
1	15-A	45	TYR	CD1-CE1	6.03	1.48	1.39
1	1-A	78	TYR	CG-CD2	6.03	1.47	1.39
1	8-A	149	PHE	CA-CB	6.03	1.67	1.53
1	11-A	112	HIS	C-O	6.03	1.34	1.23
1	14-A	146	TYR	C-N	6.03	1.48	1.34
1	2-A	135	HIS	CA-CB	6.02	1.67	1.53
1	5-A	110	ILE	N-CA	6.02	1.58	1.46
1	14-A	129	LEU	N-CA	-6.02	1.34	1.46
1	5-A	94	ASP	CA-CB	6.02	1.67	1.53
1	2-A	125	GLU	CB-CG	6.02	1.63	1.52
1	16-A	128	ARG	N-CA	6.02	1.58	1.46
1	3-A	130	THR	C-O	6.01	1.34	1.23
1	7-A	91	GLN	CD-OE1	6.01	1.37	1.24
1	14-A	92	ARG	CD-NE	6.01	1.56	1.46
1	14-A	101	ASP	C-O	-6.01	1.11	1.23
1	7-A	42	ALA	C-O	6.01	1.34	1.23
1	8-A	112	HIS	CG-CD2	6.01	1.46	1.35
1	14-A	99	GLY	N-CA	6.01	1.55	1.46
1	3-A	124	GLU	CD-OE1	-6.01	1.19	1.25
1	10-A	144	PRO	C-O	6.01	1.35	1.23
1	16-A	122	LEU	C-N	6.01	1.47	1.34
1	1-A	109	SER	C-O	6.00	1.34	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	40	ARG	CB-CG	-6.00	1.36	1.52
1	5-A	46	GLN	C-O	6.00	1.34	1.23
1	13-A	138	LEU	N-CA	6.00	1.58	1.46
1	2-A	37	SER	CA-C	6.00	1.68	1.52
1	16-A	90	LEU	CG-CD1	6.00	1.74	1.51
1	4-A	47	ASP	N-CA	6.00	1.58	1.46
1	6-A	145	MET	CA-C	6.00	1.68	1.52
1	11-A	57	ASN	C-O	6.00	1.34	1.23
1	14-A	118	ALA	CA-C	6.00	1.68	1.52
1	4-A	131	PRO	N-CD	6.00	1.56	1.47
1	13-A	55	PRO	CA-C	5.99	1.64	1.52
1	16-A	44	MET	CA-C	5.99	1.68	1.52
1	4-A	128	ARG	CG-CD	5.99	1.67	1.51
1	11-A	56	THR	CA-CB	5.99	1.69	1.53
1	8-A	48	TYR	CE2-CZ	5.99	1.46	1.38
1	9-A	97	ARG	CG-CD	5.99	1.67	1.51
1	15-A	89	LEU	CG-CD2	5.99	1.74	1.51
1	6-A	124	GLU	CA-CB	5.99	1.67	1.53
1	8-A	63	PRO	CB-CG	5.99	1.79	1.50
1	11-A	84	TYR	CD2-CE2	-5.99	1.30	1.39
1	1-A	121	TRP	CD2-CE2	5.98	1.48	1.41
1	8-A	51	GLN	CG-CD	5.98	1.64	1.51
1	7-A	146	TYR	CB-CG	5.98	1.60	1.51
1	8-A	120	ILE	CB-CG2	5.98	1.71	1.52
1	16-A	57	ASN	CG-OD1	-5.98	1.10	1.24
1	3-A	149	PHE	C-O	5.97	1.34	1.23
1	5-A	46	GLN	CD-OE1	5.97	1.37	1.24
1	15-A	115	LYS	C-O	5.96	1.34	1.23
1	16-A	151	ASP	CG-OD1	5.96	1.39	1.25
1	13-A	152	PRO	CB-CG	-5.96	1.20	1.50
1	15-A	112	HIS	C-O	5.96	1.34	1.23
1	2-A	74	MET	C-N	5.95	1.47	1.34
1	4-A	105	GLN	CB-CG	-5.95	1.36	1.52
1	9-A	64	PHE	CG-CD1	5.95	1.47	1.38
1	14-A	98	PHE	CD2-CE2	5.95	1.51	1.39
1	16-A	60	SER	CB-OG	5.95	1.50	1.42
1	10-A	51	GLN	CB-CG	-5.95	1.36	1.52
1	2-A	88	VAL	CA-CB	5.94	1.67	1.54
1	1-A	111	ILE	CB-CG2	5.94	1.71	1.52
1	3-A	72	ILE	CA-CB	5.94	1.68	1.54
1	12-A	123	VAL	C-O	5.94	1.34	1.23
1	6-A	73	SER	C-N	5.94	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	97	ARG	CZ-NH2	5.94	1.40	1.33
1	4-A	121	TRP	C-O	-5.94	1.12	1.23
1	14-A	37	SER	N-CA	5.94	1.58	1.46
1	3-A	67	TRP	CD2-CE2	5.94	1.48	1.41
1	9-A	47	ASP	C-O	5.94	1.34	1.23
1	13-A	156	GLU	CD-OE2	-5.94	1.19	1.25
1	5-A	135	HIS	CA-CB	5.93	1.67	1.53
1	6-A	80	GLN	CD-NE2	5.93	1.47	1.32
1	8-A	146	TYR	CE2-CZ	-5.93	1.30	1.38
1	9-A	126	ILE	C-N	5.93	1.47	1.34
1	1-A	153	ILE	CB-CG1	-5.92	1.37	1.54
1	10-A	140	TRP	CZ3-CH2	-5.92	1.30	1.40
1	2-A	95	GLN	CG-CD	5.92	1.64	1.51
1	1-A	108	ASP	C-O	5.92	1.34	1.23
1	13-A	45	TYR	CD2-CE2	-5.92	1.30	1.39
1	15-A	66	SER	CB-OG	5.92	1.50	1.42
1	16-A	84	TYR	CG-CD2	5.92	1.46	1.39
1	7-A	134	LEU	C-O	5.92	1.34	1.23
1	1-A	61	LEU	CG-CD1	5.91	1.73	1.51
1	2-A	70	LEU	CA-CB	5.91	1.67	1.53
1	2-A	74	MET	CA-CB	-5.91	1.41	1.53
1	11-A	120	ILE	CB-CG2	5.91	1.71	1.52
1	2-A	116	ALA	C-O	5.91	1.34	1.23
1	13-A	93	TRP	CG-CD1	5.91	1.45	1.36
1	13-A	57	ASN	CG-OD1	-5.91	1.10	1.24
1	4-A	149	PHE	CD1-CE1	-5.90	1.27	1.39
1	13-A	36	GLY	CA-C	5.90	1.61	1.51
1	8-A	98	PHE	CD2-CE2	5.90	1.51	1.39
1	13-A	81	PRO	CB-CG	5.90	1.79	1.50
1	5-A	53	PRO	CA-CB	5.90	1.65	1.53
1	3-A	67	TRP	CE3-CZ3	-5.90	1.28	1.38
1	8-A	134	LEU	CA-CB	5.90	1.67	1.53
1	10-A	150	ILE	CB-CG1	5.90	1.70	1.54
1	6-A	92	ARG	CD-NE	5.90	1.56	1.46
1	11-A	111	ILE	N-CA	5.90	1.58	1.46
1	4-A	41	ARG	CZ-NH2	5.89	1.40	1.33
1	5-A	128	ARG	CZ-NH2	5.89	1.40	1.33
1	7-A	107	LEU	CB-CG	5.89	1.69	1.52
1	16-A	148	SER	CA-CB	5.89	1.61	1.52
1	1-A	74	MET	CB-CG	5.88	1.70	1.51
1	15-A	36	GLY	CA-C	5.88	1.61	1.51
1	16-A	37	SER	CA-CB	5.88	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	88	VAL	CA-C	-5.88	1.37	1.52
1	5-A	128	ARG	CG-CD	5.88	1.66	1.51
1	11-A	77	LEU	CG-CD1	5.87	1.73	1.51
1	7-A	45	TYR	CD1-CE1	-5.87	1.30	1.39
1	9-A	127	HIS	C-O	5.87	1.34	1.23
1	1-A	91	GLN	CG-CD	5.87	1.64	1.51
1	14-A	41	ARG	CA-C	5.87	1.68	1.52
1	10-A	139	LEU	CA-C	5.87	1.68	1.52
1	11-A	45	TYR	CE1-CZ	5.87	1.46	1.38
1	13-A	114	THR	CB-OG1	5.87	1.54	1.43
1	15-A	52	VAL	CB-CG2	5.87	1.65	1.52
1	15-A	61	LEU	C-O	5.87	1.34	1.23
1	15-A	82	LEU	CA-CB	5.87	1.67	1.53
1	16-A	137	ALA	N-CA	5.87	1.58	1.46
1	2-A	67	TRP	CD1-NE1	5.86	1.48	1.38
1	14-A	41	ARG	CD-NE	5.86	1.56	1.46
1	2-A	151	ASP	CG-OD1	5.86	1.38	1.25
1	16-A	90	LEU	CG-CD2	5.86	1.73	1.51
1	9-A	66	SER	CA-CB	-5.85	1.44	1.52
1	14-A	127	HIS	CG-CD2	5.85	1.45	1.35
1	10-A	103	GLU	CG-CD	5.85	1.60	1.51
1	16-A	64	PHE	CA-CB	5.85	1.66	1.53
1	12-A	51	GLN	CD-OE1	5.85	1.36	1.24
1	4-A	156	GLU	CD-OE1	5.84	1.32	1.25
1	14-A	138	LEU	CA-CB	5.84	1.67	1.53
1	9-A	140	TRP	CD2-CE2	-5.84	1.34	1.41
1	2-A	138	LEU	C-N	5.84	1.47	1.34
1	3-A	117	GLU	CD-OE2	5.84	1.32	1.25
1	3-A	132	SER	CA-C	5.83	1.68	1.52
1	4-A	41	ARG	NE-CZ	5.83	1.40	1.33
1	15-A	95	GLN	N-CA	5.83	1.58	1.46
1	1-A	57	ASN	CA-C	5.83	1.68	1.52
1	10-A	130	THR	CB-OG1	5.83	1.54	1.43
1	3-A	96	SER	CA-C	5.83	1.68	1.52
1	8-A	116	ALA	C-O	5.83	1.34	1.23
1	11-A	78	TYR	CD2-CE2	-5.83	1.30	1.39
1	16-A	95	GLN	CA-CB	-5.83	1.41	1.53
1	13-A	98	PHE	CE2-CZ	5.82	1.48	1.37
1	2-A	140	TRP	CE3-CZ3	-5.82	1.28	1.38
1	7-A	37	SER	CB-OG	-5.82	1.34	1.42
1	1-A	48	TYR	CD1-CE1	5.82	1.48	1.39
1	5-A	46	GLN	CG-CD	5.82	1.64	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-A	156	GLU	C-O	5.82	1.34	1.23
1	4-A	124	GLU	C-O	-5.81	1.12	1.23
1	1-A	44	MET	CB-CG	5.81	1.70	1.51
1	8-A	50	LYS	CE-NZ	-5.81	1.34	1.49
1	15-A	118	ALA	C-N	5.81	1.47	1.34
1	7-A	95	GLN	N-CA	5.81	1.57	1.46
1	11-A	147	HIS	CA-CB	5.81	1.66	1.53
1	16-A	81	PRO	CA-C	-5.81	1.41	1.52
1	2-A	60	SER	CA-CB	5.81	1.61	1.52
1	2-A	120	ILE	C-O	-5.81	1.12	1.23
1	10-A	91	GLN	CD-NE2	5.81	1.47	1.32
1	12-A	149	PHE	CG-CD1	5.81	1.47	1.38
1	14-A	103	GLU	CD-OE1	5.81	1.32	1.25
1	4-A	97	ARG	CZ-NH1	5.81	1.40	1.33
1	7-A	107	LEU	C-O	5.80	1.34	1.23
1	16-A	138	LEU	CG-CD2	5.80	1.73	1.51
1	2-A	97	ARG	CZ-NH2	5.80	1.40	1.33
1	1-A	98	PHE	N-CA	5.80	1.57	1.46
1	10-A	154	PHE	CG-CD2	5.80	1.47	1.38
1	1-A	52	VAL	CB-CG2	5.80	1.65	1.52
1	3-A	142	SER	CA-CB	5.80	1.61	1.52
1	3-A	149	PHE	CG-CD2	5.80	1.47	1.38
1	8-A	80	GLN	CA-CB	5.80	1.66	1.53
1	16-A	151	ASP	C-N	5.79	1.45	1.34
1	2-A	86	THR	CA-CB	5.79	1.68	1.53
1	14-A	63	PRO	CA-CB	5.79	1.65	1.53
1	3-A	104	GLU	C-N	5.79	1.47	1.34
1	3-A	106	ARG	NE-CZ	5.79	1.40	1.33
1	8-A	63	PRO	CG-CD	5.79	1.69	1.50
1	8-A	78	TYR	C-O	5.79	1.34	1.23
1	13-A	112	HIS	CE1-NE2	5.79	1.46	1.32
1	4-A	97	ARG	CG-CD	5.78	1.66	1.51
1	9-A	128	ARG	CB-CG	5.78	1.68	1.52
1	2-A	66	SER	CA-C	5.78	1.68	1.52
1	8-A	146	TYR	CD2-CE2	5.78	1.48	1.39
1	15-A	67	TRP	CA-CB	5.78	1.66	1.53
1	11-A	59	GLY	N-CA	5.78	1.54	1.46
1	12-A	138	LEU	CG-CD1	-5.78	1.30	1.51
1	9-A	61	LEU	C-O	5.77	1.34	1.23
1	10-A	140	TRP	CD2-CE2	-5.77	1.34	1.41
1	16-A	115	LYS	C-O	-5.77	1.12	1.23
1	6-A	89	LEU	CG-CD2	5.77	1.73	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	12-A	139	LEU	CG-CD2	5.77	1.73	1.51
1	11-A	89	LEU	C-O	-5.77	1.12	1.23
1	1-A	37	SER	CA-C	5.77	1.68	1.52
1	5-A	143	ASP	C-N	-5.77	1.23	1.34
1	8-A	128	ARG	CZ-NH1	5.77	1.40	1.33
1	8-A	76	GLN	N-CA	5.76	1.57	1.46
1	15-A	129	LEU	C-O	5.76	1.34	1.23
1	16-A	117	GLU	CD-OE1	5.76	1.31	1.25
1	2-A	43	GLU	CA-CB	5.76	1.66	1.53
1	3-A	102	SER	CB-OG	-5.76	1.34	1.42
1	11-A	58	ARG	N-CA	5.76	1.57	1.46
1	13-A	138	LEU	C-N	5.76	1.47	1.34
1	4-A	76	GLN	N-CA	5.76	1.57	1.46
1	7-A	78	TYR	CA-CB	5.75	1.66	1.53
1	4-A	79	GLY	C-O	5.75	1.32	1.23
1	8-A	113	PRO	N-CA	-5.75	1.37	1.47
1	3-A	43	GLU	CA-CB	5.75	1.66	1.53
1	7-A	128	ARG	CG-CD	5.75	1.66	1.51
1	13-A	110	ILE	CB-CG1	5.75	1.70	1.54
1	15-A	74	MET	CB-CG	5.75	1.69	1.51
1	11-A	61	LEU	CB-CG	5.74	1.69	1.52
1	8-A	92	ARG	CD-NE	5.74	1.56	1.46
1	14-A	98	PHE	CA-C	5.74	1.67	1.52
1	3-A	155	PRO	CB-CG	-5.74	1.21	1.50
1	15-A	121	TRP	CE3-CZ3	5.74	1.48	1.38
1	16-A	95	GLN	C-O	5.74	1.34	1.23
1	8-A	98	PHE	CG-CD2	5.74	1.47	1.38
1	13-A	154	PHE	CD2-CE2	-5.73	1.27	1.39
1	1-A	149	PHE	CD1-CE1	-5.73	1.27	1.39
1	7-A	45	TYR	CE1-CZ	-5.73	1.31	1.38
1	13-A	92	ARG	C-O	5.73	1.34	1.23
1	13-A	76	GLN	N-CA	5.73	1.57	1.46
1	2-A	106	ARG	CD-NE	-5.73	1.36	1.46
1	9-A	43	GLU	C-O	5.73	1.34	1.23
1	13-A	98	PHE	CA-CB	-5.73	1.41	1.53
1	14-A	55	PRO	N-CD	5.73	1.55	1.47
1	10-A	113	PRO	N-CA	-5.72	1.37	1.47
1	11-A	155	PRO	CB-CG	-5.72	1.21	1.50
1	15-A	118	ALA	C-O	5.72	1.34	1.23
1	7-A	37	SER	N-CA	5.72	1.57	1.46
1	5-A	91	GLN	CA-CB	5.72	1.66	1.53
1	10-A	40	ARG	CD-NE	5.72	1.56	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	11-A	64	PHE	CA-CB	5.71	1.66	1.53
1	13-A	134	LEU	N-CA	-5.71	1.34	1.46
1	1-A	154	PHE	C-N	5.71	1.45	1.34
1	10-A	142	SER	CB-OG	-5.71	1.34	1.42
1	13-A	151	ASP	CA-CB	-5.71	1.41	1.53
1	11-A	119	THR	CB-CG2	5.71	1.71	1.52
1	12-A	92	ARG	CZ-NH2	5.71	1.40	1.33
1	11-A	156	GLU	CG-CD	-5.71	1.43	1.51
1	13-A	64	PHE	CD2-CE2	5.71	1.50	1.39
1	13-A	148	SER	C-O	5.71	1.34	1.23
1	1-A	63	PRO	CA-CB	5.71	1.65	1.53
1	6-A	64	PHE	CE2-CZ	5.71	1.48	1.37
1	16-A	110	ILE	CB-CG2	5.71	1.70	1.52
1	3-A	100	THR	CA-CB	-5.70	1.38	1.53
1	9-A	150	ILE	CB-CG2	5.70	1.70	1.52
1	15-A	113	PRO	CB-CG	5.70	1.78	1.50
1	14-A	93	TRP	CE2-CZ2	5.70	1.49	1.39
1	1-A	153	ILE	C-O	5.70	1.34	1.23
1	10-A	146	TYR	CB-CG	5.70	1.60	1.51
1	12-A	98	PHE	CA-CB	-5.69	1.41	1.53
1	5-A	78	TYR	CD1-CE1	5.69	1.47	1.39
1	10-A	119	THR	CA-C	5.69	1.67	1.52
1	2-A	50	LYS	CB-CG	-5.69	1.37	1.52
1	3-A	41	ARG	NE-CZ	5.69	1.40	1.33
1	8-A	147	HIS	CB-CG	5.69	1.60	1.50
1	9-A	92	ARG	CB-CG	5.69	1.68	1.52
1	9-A	132	SER	N-CA	5.69	1.57	1.46
1	16-A	78	TYR	CG-CD2	5.69	1.46	1.39
1	9-A	38	LEU	C-O	5.68	1.34	1.23
1	9-A	121	TRP	CZ3-CH2	5.68	1.49	1.40
1	3-A	58	ARG	C-O	5.68	1.34	1.23
1	6-A	51	GLN	CD-OE1	5.68	1.36	1.24
1	12-A	60	SER	CA-CB	5.68	1.61	1.52
1	13-A	91	GLN	CG-CD	5.68	1.64	1.51
1	1-A	80	GLN	CA-CB	5.68	1.66	1.53
1	3-A	59	GLY	N-CA	5.68	1.54	1.46
1	1-A	116	ALA	CA-CB	5.67	1.64	1.52
1	9-A	56	THR	CA-CB	5.67	1.68	1.53
1	9-A	68	VAL	CB-CG2	5.67	1.64	1.52
1	13-A	100	THR	CB-CG2	5.67	1.71	1.52
1	11-A	120	ILE	C-O	5.67	1.34	1.23
1	4-A	48	TYR	CG-CD1	5.67	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	45	TYR	CG-CD2	5.67	1.46	1.39
1	14-A	106	ARG	CD-NE	-5.67	1.36	1.46
1	3-A	76	GLN	N-CA	5.67	1.57	1.46
1	16-A	154	PHE	CD1-CE1	5.67	1.50	1.39
1	16-A	131	PRO	CA-C	5.67	1.64	1.52
1	1-A	128	ARG	CZ-NH1	-5.66	1.25	1.33
1	6-A	83	HIS	CA-C	-5.66	1.38	1.52
1	8-A	64	PHE	CG-CD1	-5.66	1.30	1.38
1	8-A	92	ARG	CZ-NH2	5.66	1.40	1.33
1	11-A	144	PRO	C-N	5.66	1.47	1.34
1	1-A	156	GLU	CD-OE2	5.66	1.31	1.25
1	10-A	64	PHE	CE2-CZ	5.66	1.48	1.37
1	7-A	41	ARG	NE-CZ	5.65	1.40	1.33
1	13-A	107	LEU	C-O	5.65	1.34	1.23
1	14-A	67	TRP	CA-CB	5.65	1.66	1.53
1	15-A	85	LEU	CG-CD2	5.65	1.72	1.51
1	16-A	68	VAL	C-N	5.65	1.43	1.33
1	9-A	96	SER	CA-CB	5.65	1.61	1.52
1	14-A	143	ASP	CA-CB	5.65	1.66	1.53
1	9-A	146	TYR	CG-CD1	-5.65	1.31	1.39
1	11-A	57	ASN	CG-OD1	-5.65	1.11	1.24
1	13-A	46	GLN	C-O	-5.65	1.12	1.23
1	13-A	137	ALA	N-CA	5.65	1.57	1.46
1	16-A	67	TRP	NE1-CE2	5.65	1.44	1.37
1	1-A	70	LEU	C-O	-5.64	1.12	1.23
1	2-A	56	THR	C-N	-5.64	1.21	1.34
1	4-A	80	GLN	N-CA	5.64	1.57	1.46
1	16-A	73	SER	C-N	5.64	1.47	1.34
1	10-A	43	GLU	C-N	5.64	1.47	1.34
1	4-A	67	TRP	CZ2-CH2	5.64	1.48	1.37
1	15-A	127	HIS	N-CA	5.63	1.57	1.46
1	14-A	121	TRP	CD1-NE1	5.63	1.47	1.38
1	2-A	133	HIS	CA-C	-5.63	1.38	1.52
1	1-A	115	LYS	N-CA	5.63	1.57	1.46
1	10-A	84	TYR	CE2-CZ	5.63	1.45	1.38
1	14-A	50	LYS	CE-NZ	-5.63	1.34	1.49
1	16-A	75	LYS	CA-C	5.63	1.67	1.52
1	2-A	42	ALA	CA-CB	5.62	1.64	1.52
1	3-A	56	THR	CA-CB	5.62	1.68	1.53
1	3-A	113	PRO	CG-CD	5.62	1.69	1.50
1	4-A	70	LEU	C-O	5.62	1.34	1.23
1	15-A	76	GLN	N-CA	5.62	1.57	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	146	TYR	CZ-OH	5.62	1.47	1.37
1	6-A	77	LEU	CA-C	5.62	1.67	1.52
1	14-A	101	ASP	N-CA	5.62	1.57	1.46
1	5-A	61	LEU	CG-CD2	5.62	1.72	1.51
1	5-A	84	TYR	CG-CD1	5.61	1.46	1.39
1	13-A	146	TYR	CD1-CE1	5.61	1.47	1.39
1	1-A	127	HIS	N-CA	-5.61	1.35	1.46
1	6-A	56	THR	CA-CB	5.61	1.68	1.53
1	6-A	145	MET	SD-CE	5.61	2.09	1.77
1	10-A	141	ARG	CD-NE	-5.61	1.36	1.46
1	7-A	88	VAL	CB-CG2	-5.61	1.41	1.52
1	9-A	84	TYR	C-O	5.61	1.34	1.23
1	9-A	152	PRO	CA-C	-5.61	1.41	1.52
1	10-A	125	GLU	CA-CB	5.61	1.66	1.53
1	15-A	54	ILE	C-O	5.61	1.34	1.23
1	15-A	149	PHE	C-O	5.61	1.34	1.23
1	9-A	57	ASN	C-O	5.60	1.33	1.23
1	10-A	63	PRO	C-O	-5.60	1.12	1.23
1	14-A	68	VAL	C-N	5.60	1.43	1.33
1	15-A	73	SER	C-N	5.60	1.47	1.34
1	10-A	78	TYR	CA-CB	5.60	1.66	1.53
1	1-A	57	ASN	CG-OD1	-5.60	1.11	1.24
1	2-A	78	TYR	CG-CD2	5.60	1.46	1.39
1	9-A	45	TYR	CE2-CZ	5.60	1.45	1.38
1	7-A	100	THR	CB-CG2	5.60	1.70	1.52
1	4-A	125	GLU	CB-CG	5.59	1.62	1.52
1	15-A	117	GLU	CD-OE1	5.59	1.31	1.25
1	8-A	54	ILE	CA-CB	5.59	1.67	1.54
1	10-A	64	PHE	CD2-CE2	5.59	1.50	1.39
1	12-A	42	ALA	C-O	5.59	1.33	1.23
1	7-A	135	HIS	C-O	5.59	1.33	1.23
1	8-A	97	ARG	NE-CZ	5.59	1.40	1.33
1	16-A	40	ARG	CB-CG	-5.59	1.37	1.52
1	5-A	143	ASP	C-O	-5.59	1.12	1.23
1	15-A	55	PRO	CB-CG	5.59	1.77	1.50
1	2-A	95	GLN	CD-OE1	5.58	1.36	1.24
1	5-A	60	SER	CA-CB	5.58	1.61	1.52
1	9-A	151	ASP	CA-C	5.58	1.67	1.52
1	10-A	146	TYR	CA-CB	5.58	1.66	1.53
1	12-A	84	TYR	CG-CD2	5.58	1.46	1.39
1	7-A	51	GLN	CD-NE2	5.58	1.46	1.32
1	15-A	55	PRO	CA-C	5.58	1.64	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	117	GLU	CD-OE1	-5.58	1.19	1.25
1	5-A	113	PRO	CA-CB	5.58	1.64	1.53
1	5-A	147	HIS	CA-CB	5.58	1.66	1.53
1	13-A	78	TYR	CD1-CE1	5.58	1.47	1.39
1	5-A	64	PHE	CG-CD1	5.57	1.47	1.38
1	7-A	56	THR	CA-CB	5.57	1.67	1.53
1	10-A	153	ILE	C-O	5.57	1.33	1.23
1	13-A	51	GLN	CA-CB	5.57	1.66	1.53
1	1-A	98	PHE	CB-CG	5.57	1.60	1.51
1	6-A	67	TRP	CE2-CZ2	5.57	1.49	1.39
1	11-A	134	LEU	CG-CD1	5.57	1.72	1.51
1	13-A	49	MET	CA-CB	5.57	1.66	1.53
1	3-A	107	LEU	C-O	5.57	1.33	1.23
1	9-A	78	TYR	CA-CB	5.57	1.66	1.53
1	5-A	38	LEU	CB-CG	5.57	1.68	1.52
1	6-A	76	GLN	C-N	-5.57	1.21	1.34
1	2-A	48	TYR	CD1-CE1	5.56	1.47	1.39
1	8-A	67	TRP	C-N	5.56	1.46	1.34
1	8-A	156	GLU	CA-C	5.56	1.67	1.52
1	12-A	39	LEU	CG-CD1	5.56	1.72	1.51
1	3-A	150	ILE	CG1-CD1	5.56	1.88	1.50
1	12-A	143	ASP	C-N	-5.56	1.23	1.34
1	14-A	97	ARG	CA-C	5.56	1.67	1.52
1	2-A	75	LYS	CG-CD	5.56	1.71	1.52
1	6-A	47	ASP	N-CA	5.56	1.57	1.46
1	2-A	63	PRO	C-O	-5.55	1.12	1.23
1	15-A	84	TYR	CA-CB	5.55	1.66	1.53
1	6-A	107	LEU	CB-CG	5.55	1.68	1.52
1	14-A	73	SER	C-N	5.55	1.46	1.34
1	2-A	143	ASP	CG-OD1	5.55	1.38	1.25
1	4-A	41	ARG	CA-CB	-5.55	1.41	1.53
1	5-A	143	ASP	CA-CB	5.55	1.66	1.53
1	1-A	142	SER	CA-CB	5.55	1.61	1.52
1	3-A	138	LEU	C-N	5.55	1.46	1.34
1	6-A	140	TRP	CZ3-CH2	5.55	1.49	1.40
1	11-A	44	MET	CG-SD	5.55	1.95	1.81
1	16-A	56	THR	CB-CG2	-5.54	1.34	1.52
1	6-A	41	ARG	CZ-NH2	5.54	1.40	1.33
1	11-A	140	TRP	CB-CG	5.54	1.60	1.50
1	4-A	95	GLN	CA-CB	5.54	1.66	1.53
1	8-A	140	TRP	CG-CD2	5.54	1.53	1.43
1	11-A	109	SER	CB-OG	-5.54	1.35	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-A	57	ASN	CG-OD1	5.54	1.36	1.24
1	2-A	87	ASN	CB-CG	5.54	1.63	1.51
1	5-A	135	HIS	CA-C	5.54	1.67	1.52
1	13-A	153	ILE	CA-CB	5.54	1.67	1.54
1	5-A	121	TRP	CZ3-CH2	5.53	1.49	1.40
1	6-A	128	ARG	CG-CD	5.53	1.65	1.51
1	8-A	135	HIS	CA-CB	5.53	1.66	1.53
1	14-A	156	GLU	CD-OE2	-5.53	1.19	1.25
1	11-A	82	LEU	N-CA	5.53	1.57	1.46
1	14-A	76	GLN	N-CA	5.53	1.57	1.46
1	15-A	58	ARG	CZ-NH1	5.53	1.40	1.33
1	6-A	57	ASN	CG-OD1	-5.53	1.11	1.24
1	8-A	138	LEU	CG-CD1	5.53	1.72	1.51
1	15-A	84	TYR	CA-C	5.53	1.67	1.52
1	15-A	87	ASN	C-O	5.53	1.33	1.23
1	13-A	134	LEU	CG-CD1	5.52	1.72	1.51
1	4-A	98	PHE	CA-CB	-5.52	1.41	1.53
1	12-A	151	ASP	CA-CB	-5.52	1.41	1.53
1	16-A	57	ASN	C-N	-5.52	1.21	1.34
1	10-A	61	LEU	CG-CD2	5.52	1.72	1.51
1	14-A	151	ASP	CG-OD1	5.52	1.38	1.25
1	4-A	40	ARG	N-CA	5.52	1.57	1.46
1	15-A	98	PHE	CE1-CZ	-5.52	1.26	1.37
1	16-A	48	TYR	N-CA	5.52	1.57	1.46
1	10-A	121	TRP	CA-CB	5.52	1.66	1.53
1	15-A	133	HIS	CG-CD2	5.52	1.45	1.35
1	16-A	73	SER	N-CA	5.52	1.57	1.46
1	5-A	118	ALA	CA-C	5.52	1.67	1.52
1	3-A	62	ILE	C-N	5.51	1.44	1.34
1	14-A	92	ARG	CZ-NH2	5.51	1.40	1.33
1	15-A	125	GLU	CA-CB	-5.51	1.41	1.53
1	2-A	148	SER	CB-OG	5.51	1.49	1.42
1	4-A	99	GLY	N-CA	5.51	1.54	1.46
1	11-A	63	PRO	CB-CG	5.51	1.77	1.50
1	7-A	133	HIS	CB-CG	-5.51	1.40	1.50
1	8-A	66	SER	CA-CB	5.50	1.61	1.52
1	5-A	146	TYR	CD1-CE1	5.50	1.47	1.39
1	14-A	120	ILE	CB-CG2	5.50	1.70	1.52
1	14-A	146	TYR	CD1-CE1	5.50	1.47	1.39
1	1-A	147	HIS	CA-CB	5.50	1.66	1.53
1	13-A	90	LEU	CA-C	5.50	1.67	1.52
1	15-A	45	TYR	CG-CD2	5.50	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	14-A	107	LEU	CA-CB	5.50	1.66	1.53
1	14-A	135	HIS	CB-CG	5.50	1.59	1.50
1	13-A	106	ARG	N-CA	5.49	1.57	1.46
1	16-A	143	ASP	C-O	-5.49	1.12	1.23
1	9-A	108	ASP	CB-CG	5.49	1.63	1.51
1	12-A	51	GLN	CD-NE2	5.49	1.46	1.32
1	2-A	130	THR	N-CA	-5.49	1.35	1.46
1	10-A	139	LEU	CG-CD1	5.49	1.72	1.51
1	13-A	91	GLN	CD-NE2	-5.49	1.19	1.32
1	1-A	143	ASP	C-N	-5.48	1.23	1.34
1	2-A	145	MET	CB-CG	5.48	1.68	1.51
1	2-A	133	HIS	CB-CG	5.48	1.59	1.50
1	13-A	105	GLN	CG-CD	5.48	1.63	1.51
1	8-A	67	TRP	NE1-CE2	5.47	1.44	1.37
1	13-A	65	THR	CB-CG2	5.47	1.70	1.52
1	5-A	124	GLU	CB-CG	5.47	1.62	1.52
1	16-A	112	HIS	CE1-NE2	5.47	1.45	1.32
1	1-A	89	LEU	CA-CB	5.47	1.66	1.53
1	2-A	105	GLN	CD-OE1	5.47	1.35	1.24
1	13-A	147	HIS	CA-CB	5.47	1.66	1.53
1	15-A	127	HIS	ND1-CE1	5.47	1.48	1.34
1	10-A	68	VAL	N-CA	5.47	1.57	1.46
1	16-A	68	VAL	CB-CG1	5.47	1.64	1.52
1	7-A	113	PRO	CA-C	5.46	1.63	1.52
1	10-A	102	SER	CB-OG	-5.46	1.35	1.42
1	5-A	45	TYR	CA-C	5.46	1.67	1.52
1	10-A	146	TYR	CG-CD1	-5.46	1.32	1.39
1	12-A	47	ASP	CG-OD2	5.46	1.38	1.25
1	14-A	154	PHE	CD2-CE2	-5.46	1.28	1.39
1	8-A	101	ASP	CB-CG	5.46	1.63	1.51
1	11-A	143	ASP	CA-CB	5.46	1.66	1.53
1	12-A	81	PRO	N-CD	5.46	1.55	1.47
1	12-A	137	ALA	C-O	5.46	1.33	1.23
1	13-A	103	GLU	C-O	-5.46	1.12	1.23
1	14-A	43	GLU	CD-OE2	-5.46	1.19	1.25
1	8-A	52	VAL	CB-CG2	5.46	1.64	1.52
1	4-A	124	GLU	CG-CD	5.45	1.60	1.51
1	7-A	57	ASN	CG-OD1	-5.45	1.11	1.24
1	6-A	84	TYR	CD2-CE2	5.45	1.47	1.39
1	10-A	120	ILE	C-O	5.45	1.33	1.23
1	14-A	134	LEU	CG-CD1	5.45	1.72	1.51
1	3-A	66	SER	C-O	-5.44	1.13	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	11-A	74	MET	CB-CG	5.44	1.68	1.51
1	3-A	136	MET	CB-CG	5.44	1.68	1.51
1	9-A	139	LEU	CG-CD1	5.44	1.72	1.51
1	14-A	148	SER	CA-C	5.44	1.67	1.52
1	14-A	150	ILE	C-O	5.44	1.33	1.23
1	15-A	140	TRP	CA-CB	5.44	1.66	1.53
1	8-A	142	SER	CB-OG	5.43	1.49	1.42
1	11-A	98	PHE	CG-CD2	5.43	1.46	1.38
1	16-A	114	THR	CA-CB	5.43	1.67	1.53
1	7-A	96	SER	C-O	5.43	1.33	1.23
1	11-A	124	GLU	CB-CG	5.43	1.62	1.52
1	13-A	140	TRP	CB-CG	5.43	1.60	1.50
1	6-A	51	GLN	CD-NE2	5.43	1.46	1.32
1	8-A	128	ARG	CG-CD	5.43	1.65	1.51
1	8-A	55	PRO	CB-CG	5.43	1.77	1.50
1	14-A	135	HIS	CD2-NE2	5.43	1.53	1.42
1	16-A	78	TYR	N-CA	-5.43	1.35	1.46
1	10-A	147	HIS	CA-CB	5.42	1.65	1.53
1	10-A	72	ILE	CB-CG2	5.42	1.69	1.52
1	3-A	52	VAL	CB-CG2	5.42	1.64	1.52
1	4-A	61	LEU	CG-CD2	5.42	1.71	1.51
1	8-A	113	PRO	C-O	5.42	1.34	1.23
1	14-A	107	LEU	N-CA	5.42	1.57	1.46
1	14-A	118	ALA	C-N	5.41	1.46	1.34
1	14-A	126	ILE	CB-CG1	5.41	1.69	1.54
1	14-A	136	MET	CG-SD	5.41	1.95	1.81
1	16-A	142	SER	C-N	5.41	1.46	1.34
1	4-A	125	GLU	CA-CB	5.41	1.65	1.53
1	4-A	52	VAL	C-O	5.41	1.33	1.23
1	5-A	67	TRP	CA-CB	5.41	1.65	1.53
1	8-A	50	LYS	CB-CG	-5.41	1.38	1.52
1	8-A	130	THR	C-O	5.41	1.33	1.23
1	12-A	128	ARG	CZ-NH1	5.41	1.40	1.33
1	12-A	143	ASP	C-O	-5.41	1.13	1.23
1	13-A	110	ILE	CG1-CD1	5.41	1.87	1.50
1	13-A	68	VAL	C-O	5.40	1.33	1.23
1	13-A	73	SER	C-N	5.40	1.46	1.34
1	5-A	46	GLN	CA-CB	-5.40	1.42	1.53
1	6-A	41	ARG	NE-CZ	5.40	1.40	1.33
1	6-A	48	TYR	CE2-CZ	5.40	1.45	1.38
1	1-A	54	ILE	C-O	5.40	1.33	1.23
1	16-A	152	PRO	CA-CB	5.40	1.64	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-A	41	ARG	N-CA	5.40	1.57	1.46
1	16-A	85	LEU	C-O	5.40	1.33	1.23
1	1-A	77	LEU	CG-CD1	5.39	1.71	1.51
1	8-A	41	ARG	CB-CG	5.39	1.67	1.52
1	12-A	106	ARG	CB-CG	5.39	1.67	1.52
1	3-A	51	GLN	CD-NE2	5.39	1.46	1.32
1	15-A	108	ASP	CB-CG	5.39	1.63	1.51
1	2-A	98	PHE	C-O	-5.39	1.13	1.23
1	8-A	153	ILE	CA-CB	5.39	1.67	1.54
1	10-A	99	GLY	N-CA	5.39	1.54	1.46
1	14-A	151	ASP	N-CA	5.39	1.57	1.46
1	9-A	97	ARG	CB-CG	5.39	1.67	1.52
1	16-A	41	ARG	CA-C	5.39	1.67	1.52
1	3-A	100	THR	CB-OG1	5.39	1.54	1.43
1	5-A	93	TRP	CZ3-CH2	5.39	1.48	1.40
1	1-A	131	PRO	CG-CD	5.39	1.68	1.50
1	5-A	57	ASN	CG-ND2	5.39	1.46	1.32
1	9-A	148	SER	N-CA	-5.39	1.35	1.46
1	9-A	98	PHE	CE2-CZ	5.38	1.47	1.37
1	12-A	104	GLU	CG-CD	5.38	1.60	1.51
1	8-A	129	LEU	CG-CD2	5.38	1.71	1.51
1	8-A	143	ASP	CA-CB	5.38	1.65	1.53
1	14-A	93	TRP	CE3-CZ3	5.38	1.47	1.38
1	13-A	106	ARG	NE-CZ	5.38	1.40	1.33
1	9-A	133	HIS	N-CA	5.38	1.57	1.46
1	12-A	54	ILE	CB-CG2	5.38	1.69	1.52
1	16-A	149	PHE	CA-CB	5.38	1.65	1.53
1	9-A	147	HIS	CA-CB	5.38	1.65	1.53
1	15-A	140	TRP	CZ2-CH2	5.38	1.47	1.37
1	1-A	114	THR	C-O	5.37	1.33	1.23
1	3-A	39	LEU	CG-CD1	5.37	1.71	1.51
1	4-A	66	SER	CA-CB	-5.37	1.44	1.52
1	13-A	75	LYS	CA-CB	5.37	1.65	1.53
1	1-A	61	LEU	C-O	5.37	1.33	1.23
1	1-A	124	GLU	CB-CG	5.37	1.62	1.52
1	6-A	74	MET	C-O	5.37	1.33	1.23
1	8-A	140	TRP	NE1-CE2	5.37	1.44	1.37
1	14-A	107	LEU	CB-CG	5.37	1.68	1.52
1	15-A	89	LEU	N-CA	5.37	1.57	1.46
1	7-A	112	HIS	CG-CD2	5.36	1.44	1.35
1	9-A	52	VAL	C-O	5.36	1.33	1.23
1	16-A	48	TYR	CG-CD1	5.36	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	11-A	64	PHE	N-CA	5.36	1.57	1.46
1	2-A	139	LEU	CB-CG	5.36	1.68	1.52
1	8-A	59	GLY	CA-C	-5.36	1.43	1.51
1	14-A	98	PHE	CE2-CZ	5.36	1.47	1.37
1	2-A	146	TYR	CG-CD1	-5.36	1.32	1.39
1	2-A	61	LEU	CG-CD2	5.36	1.71	1.51
1	4-A	113	PRO	CA-C	5.36	1.63	1.52
1	6-A	48	TYR	CD2-CE2	5.35	1.47	1.39
1	14-A	67	TRP	NE1-CE2	5.35	1.44	1.37
1	4-A	51	GLN	CD-NE2	5.35	1.46	1.32
1	14-A	139	LEU	CG-CD1	5.35	1.71	1.51
1	1-A	38	LEU	CA-CB	5.35	1.66	1.53
1	15-A	154	PHE	CG-CD1	-5.35	1.30	1.38
1	12-A	92	ARG	CD-NE	5.35	1.55	1.46
1	11-A	71	SER	CA-C	5.35	1.66	1.52
1	12-A	37	SER	N-CA	5.34	1.57	1.46
1	12-A	115	LYS	CD-CE	5.34	1.64	1.51
1	16-A	146	TYR	CB-CG	5.34	1.59	1.51
1	12-A	41	ARG	NE-CZ	5.34	1.40	1.33
1	7-A	51	GLN	CD-OE1	5.34	1.35	1.24
1	7-A	61	LEU	CG-CD2	5.34	1.71	1.51
1	7-A	132	SER	N-CA	5.34	1.57	1.46
1	3-A	64	PHE	CD2-CE2	5.34	1.50	1.39
1	8-A	67	TRP	N-CA	5.33	1.57	1.46
1	5-A	47	ASP	CA-C	-5.33	1.39	1.52
1	1-A	144	PRO	N-CA	5.33	1.56	1.47
1	2-A	55	PRO	N-CD	5.33	1.55	1.47
1	4-A	145	MET	CG-SD	5.33	1.95	1.81
1	5-A	44	MET	SD-CE	5.33	2.07	1.77
1	8-A	64	PHE	CA-CB	5.33	1.65	1.53
1	8-A	58	ARG	CG-CD	5.32	1.65	1.51
1	9-A	61	LEU	CG-CD2	5.32	1.71	1.51
1	11-A	67	TRP	CA-CB	5.32	1.65	1.53
1	14-A	63	PRO	C-O	5.32	1.33	1.23
1	5-A	64	PHE	CA-CB	5.32	1.65	1.53
1	4-A	120	ILE	CA-C	5.32	1.66	1.52
1	9-A	124	GLU	C-O	-5.32	1.13	1.23
1	11-A	113	PRO	C-O	5.32	1.33	1.23
1	11-A	135	HIS	CA-CB	5.32	1.65	1.53
1	2-A	76	GLN	CA-CB	5.32	1.65	1.53
1	1-A	59	GLY	N-CA	5.31	1.54	1.46
1	11-A	39	LEU	N-CA	-5.31	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-A	128	ARG	CZ-NH2	5.31	1.40	1.33
1	6-A	134	LEU	CG-CD1	5.31	1.71	1.51
1	14-A	123	VAL	C-O	5.31	1.33	1.23
1	6-A	146	TYR	C-O	-5.30	1.13	1.23
1	14-A	91	GLN	CD-OE1	5.30	1.35	1.24
1	9-A	48	TYR	CG-CD2	5.30	1.46	1.39
1	13-A	129	LEU	C-O	5.30	1.33	1.23
1	15-A	106	ARG	CD-NE	-5.30	1.37	1.46
1	13-A	57	ASN	CG-ND2	-5.30	1.19	1.32
1	8-A	44	MET	SD-CE	5.30	2.07	1.77
1	13-A	122	LEU	N-CA	-5.30	1.35	1.46
1	12-A	61	LEU	CG-CD2	5.30	1.71	1.51
1	2-A	133	HIS	CA-CB	5.30	1.65	1.53
1	4-A	98	PHE	CA-C	5.29	1.66	1.52
1	8-A	124	GLU	CB-CG	5.29	1.62	1.52
1	13-A	46	GLN	CB-CG	5.29	1.66	1.52
1	5-A	78	TYR	CG-CD2	5.29	1.46	1.39
1	11-A	142	SER	C-N	5.29	1.46	1.34
1	14-A	81	PRO	CB-CG	5.29	1.76	1.50
1	15-A	106	ARG	C-O	-5.29	1.13	1.23
1	2-A	82	LEU	N-CA	5.29	1.56	1.46
1	14-A	61	LEU	C-N	5.29	1.46	1.34
1	10-A	92	ARG	CD-NE	5.29	1.55	1.46
1	16-A	103	GLU	C-O	-5.29	1.13	1.23
1	2-A	143	ASP	C-O	-5.28	1.13	1.23
1	3-A	43	GLU	CB-CG	5.28	1.62	1.52
1	10-A	117	GLU	CG-CD	5.28	1.59	1.51
1	1-A	58	ARG	N-CA	5.28	1.56	1.46
1	2-A	70	LEU	CG-CD2	5.28	1.71	1.51
1	9-A	50	LYS	CE-NZ	-5.28	1.35	1.49
1	4-A	61	LEU	CA-CB	-5.28	1.41	1.53
1	11-A	63	PRO	C-N	5.28	1.46	1.34
1	12-A	128	ARG	CG-CD	5.28	1.65	1.51
1	1-A	121	TRP	CG-CD2	5.28	1.52	1.43
1	12-A	144	PRO	CA-C	5.28	1.63	1.52
1	14-A	105	GLN	CD-NE2	5.28	1.46	1.32
1	5-A	72	ILE	C-O	5.28	1.33	1.23
1	16-A	85	LEU	CB-CG	5.28	1.67	1.52
1	2-A	64	PHE	C-O	5.27	1.33	1.23
1	7-A	67	TRP	CD2-CE2	5.27	1.47	1.41
1	13-A	51	GLN	N-CA	-5.27	1.35	1.46
1	1-A	61	LEU	CG-CD2	5.27	1.71	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	63	PRO	CA-CB	5.27	1.64	1.53
1	9-A	77	LEU	C-O	5.27	1.33	1.23
1	14-A	61	LEU	CA-CB	5.27	1.65	1.53
1	7-A	97	ARG	CZ-NH1	5.27	1.39	1.33
1	9-A	85	LEU	C-N	5.27	1.46	1.34
1	3-A	90	LEU	CA-CB	5.26	1.65	1.53
1	12-A	98	PHE	CD2-CE2	5.26	1.49	1.39
1	12-A	78	TYR	CA-CB	5.26	1.65	1.53
1	14-A	124	GLU	CG-CD	5.26	1.59	1.51
1	9-A	146	TYR	CB-CG	5.26	1.59	1.51
1	7-A	155	PRO	CA-C	-5.26	1.42	1.52
1	10-A	145	MET	CG-SD	5.26	1.94	1.81
1	11-A	128	ARG	CG-CD	5.26	1.65	1.51
1	13-A	120	ILE	CB-CG2	5.26	1.69	1.52
1	16-A	56	THR	N-CA	-5.26	1.35	1.46
1	14-A	128	ARG	CA-C	5.25	1.66	1.52
1	15-A	138	LEU	CG-CD2	5.25	1.71	1.51
1	4-A	42	ALA	CA-CB	-5.25	1.41	1.52
1	4-A	117	GLU	CB-CG	5.25	1.62	1.52
1	9-A	98	PHE	C-O	-5.25	1.13	1.23
1	11-A	71	SER	CA-CB	5.25	1.60	1.52
1	16-A	72	ILE	CG1-CD1	5.25	1.86	1.50
1	10-A	59	GLY	CA-C	-5.25	1.43	1.51
1	14-A	98	PHE	N-CA	5.25	1.56	1.46
1	16-A	108	ASP	CG-OD1	-5.25	1.13	1.25
1	6-A	81	PRO	CA-CB	-5.25	1.43	1.53
1	3-A	57	ASN	CG-OD1	-5.24	1.12	1.24
1	8-A	48	TYR	CD2-CE2	5.24	1.47	1.39
1	12-A	106	ARG	C-O	5.24	1.33	1.23
1	7-A	142	SER	CA-CB	5.24	1.60	1.52
1	14-A	122	LEU	CA-CB	-5.24	1.41	1.53
1	10-A	62	ILE	N-CA	5.24	1.56	1.46
1	11-A	156	GLU	CA-C	5.24	1.66	1.52
1	4-A	107	LEU	CB-CG	5.24	1.67	1.52
1	13-A	46	GLN	CD-OE1	5.24	1.35	1.24
1	16-A	37	SER	N-CA	5.24	1.56	1.46
1	1-A	72	ILE	CA-C	5.24	1.66	1.52
1	8-A	39	LEU	N-CA	-5.23	1.35	1.46
1	9-A	124	GLU	CD-OE2	5.23	1.31	1.25
1	13-A	143	ASP	CA-CB	5.23	1.65	1.53
1	15-A	81	PRO	N-CA	5.23	1.56	1.47
1	16-A	104	GLU	CG-CD	5.23	1.59	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	139	LEU	CG-CD2	5.23	1.71	1.51
1	14-A	107	LEU	CG-CD2	5.23	1.71	1.51
1	4-A	103	GLU	C-O	-5.23	1.13	1.23
1	9-A	71	SER	CA-C	5.23	1.66	1.52
1	16-A	43	GLU	CD-OE2	-5.23	1.20	1.25
1	1-A	92	ARG	CZ-NH1	5.23	1.39	1.33
1	5-A	138	LEU	CG-CD2	5.22	1.71	1.51
1	10-A	135	HIS	CB-CG	5.22	1.59	1.50
1	1-A	45	TYR	CA-C	5.22	1.66	1.52
1	12-A	48	TYR	CE2-CZ	5.21	1.45	1.38
1	7-A	84	TYR	CD2-CE2	-5.21	1.31	1.39
1	6-A	121	TRP	CE3-CZ3	5.21	1.47	1.38
1	10-A	92	ARG	CZ-NH2	5.21	1.39	1.33
1	8-A	73	SER	CA-CB	5.21	1.60	1.52
1	9-A	135	HIS	CB-CG	5.21	1.59	1.50
1	7-A	147	HIS	CA-CB	5.21	1.65	1.53
1	11-A	64	PHE	CE2-CZ	5.21	1.47	1.37
1	12-A	150	ILE	CG1-CD1	5.21	1.86	1.50
1	13-A	38	LEU	C-O	5.21	1.33	1.23
1	16-A	110	ILE	CB-CG1	5.21	1.68	1.54
1	2-A	122	LEU	C-O	5.20	1.33	1.23
1	8-A	121	TRP	CD1-NE1	5.20	1.46	1.38
1	10-A	41	ARG	CB-CG	5.20	1.66	1.52
1	5-A	45	TYR	CG-CD1	5.20	1.46	1.39
1	5-A	55	PRO	CA-C	5.20	1.63	1.52
1	3-A	71	SER	CA-CB	5.20	1.60	1.52
1	7-A	64	PHE	CA-CB	5.20	1.65	1.53
1	13-A	45	TYR	CE2-CZ	5.20	1.45	1.38
1	16-A	105	GLN	CG-CD	5.19	1.62	1.51
1	1-A	143	ASP	C-O	-5.19	1.13	1.23
1	4-A	77	LEU	CA-CB	5.19	1.65	1.53
1	11-A	113	PRO	CA-C	-5.19	1.42	1.52
1	16-A	105	GLN	CA-C	5.19	1.66	1.52
1	1-A	61	LEU	CA-CB	-5.19	1.41	1.53
1	12-A	114	THR	CB-OG1	5.19	1.53	1.43
1	10-A	38	LEU	C-O	5.19	1.33	1.23
1	16-A	97	ARG	CG-CD	5.19	1.65	1.51
1	10-A	107	LEU	CB-CG	5.18	1.67	1.52
1	15-A	58	ARG	CA-CB	-5.18	1.42	1.53
1	13-A	145	MET	CB-CG	5.18	1.68	1.51
1	15-A	45	TYR	CE2-CZ	5.18	1.45	1.38
1	15-A	46	GLN	CA-CB	5.18	1.65	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-A	97	ARG	CB-CG	5.18	1.66	1.52
1	2-A	125	GLU	N-CA	5.18	1.56	1.46
1	14-A	49	MET	CA-CB	5.18	1.65	1.53
1	14-A	54	ILE	C-N	5.18	1.44	1.34
1	6-A	122	LEU	CG-CD2	5.18	1.71	1.51
1	11-A	126	ILE	CB-CG2	5.18	1.69	1.52
1	11-A	140	TRP	C-O	-5.18	1.13	1.23
1	14-A	108	ASP	CB-CG	5.18	1.62	1.51
1	15-A	127	HIS	CD2-NE2	5.18	1.52	1.42
1	7-A	94	ASP	CG-OD1	5.17	1.37	1.25
1	15-A	52	VAL	CA-CB	5.17	1.65	1.54
1	5-A	98	PHE	CA-CB	-5.17	1.42	1.53
1	9-A	105	GLN	CB-CG	-5.17	1.38	1.52
1	16-A	38	LEU	N-CA	5.17	1.56	1.46
1	1-A	55	PRO	CA-C	5.17	1.63	1.52
1	13-A	146	TYR	CA-CB	-5.17	1.42	1.53
1	13-A	155	PRO	C-O	5.17	1.33	1.23
1	14-A	124	GLU	CA-C	5.17	1.66	1.52
1	16-A	154	PHE	CG-CD1	-5.17	1.30	1.38
1	13-A	63	PRO	CA-CB	5.17	1.63	1.53
1	15-A	143	ASP	CA-CB	5.17	1.65	1.53
1	2-A	137	ALA	C-O	5.17	1.33	1.23
1	2-A	134	LEU	CA-C	-5.16	1.39	1.52
1	16-A	136	MET	CB-CG	5.16	1.67	1.51
1	15-A	46	GLN	C-O	-5.16	1.13	1.23
1	10-A	143	ASP	N-CA	5.16	1.56	1.46
1	11-A	118	ALA	N-CA	5.16	1.56	1.46
1	2-A	76	GLN	CA-C	5.16	1.66	1.52
1	7-A	78	TYR	CE1-CZ	-5.16	1.31	1.38
1	8-A	67	TRP	C-O	5.16	1.33	1.23
1	4-A	153	ILE	C-O	5.15	1.33	1.23
1	10-A	142	SER	C-N	5.15	1.46	1.34
1	5-A	117	GLU	CB-CG	5.15	1.61	1.52
1	15-A	120	ILE	CB-CG1	5.15	1.68	1.54
1	7-A	101	ASP	CB-CG	5.15	1.62	1.51
1	9-A	87	ASN	CA-CB	5.15	1.66	1.53
1	8-A	57	ASN	CG-OD1	5.15	1.35	1.24
1	15-A	77	LEU	CG-CD2	5.14	1.70	1.51
1	4-A	93	TRP	CA-C	5.14	1.66	1.52
1	4-A	98	PHE	CD2-CE2	5.14	1.49	1.39
1	15-A	84	TYR	CE1-CZ	5.14	1.45	1.38
1	14-A	40	ARG	CB-CG	-5.14	1.38	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9-A	51	GLN	CD-OE1	5.14	1.35	1.24
1	15-A	68	VAL	N-CA	5.14	1.56	1.46
1	11-A	144	PRO	CA-CB	5.14	1.63	1.53
1	1-A	130	THR	CB-CG2	5.14	1.69	1.52
1	2-A	58	ARG	CG-CD	5.14	1.64	1.51
1	3-A	101	ASP	CA-C	5.14	1.66	1.52
1	9-A	92	ARG	C-N	-5.14	1.22	1.34
1	6-A	98	PHE	CG-CD2	5.13	1.46	1.38
1	4-A	69	GLY	N-CA	5.13	1.53	1.46
1	6-A	110	ILE	N-CA	5.13	1.56	1.46
1	12-A	78	TYR	CG-CD1	5.13	1.45	1.39
1	13-A	151	ASP	N-CA	5.13	1.56	1.46
1	15-A	122	LEU	CA-C	5.12	1.66	1.52
1	8-A	122	LEU	CB-CG	5.12	1.67	1.52
1	5-A	97	ARG	CZ-NH2	5.12	1.39	1.33
1	14-A	61	LEU	CA-C	5.12	1.66	1.52
1	15-A	120	ILE	C-O	5.12	1.33	1.23
1	7-A	47	ASP	CG-OD2	5.12	1.37	1.25
1	14-A	151	ASP	C-O	5.12	1.33	1.23
1	1-A	111	ILE	CG1-CD1	5.12	1.85	1.50
1	4-A	92	ARG	CZ-NH2	5.12	1.39	1.33
1	7-A	154	PHE	CD1-CE1	5.12	1.49	1.39
1	7-A	92	ARG	CD-NE	5.12	1.55	1.46
1	12-A	99	GLY	CA-C	-5.12	1.43	1.51
1	3-A	102	SER	CA-C	5.11	1.66	1.52
1	13-A	113	PRO	C-O	5.11	1.33	1.23
1	16-A	74	MET	CA-CB	5.11	1.65	1.53
1	2-A	57	ASN	CG-ND2	5.11	1.45	1.32
1	2-A	113	PRO	N-CD	5.11	1.55	1.47
1	9-A	99	GLY	CA-C	-5.11	1.43	1.51
1	9-A	148	SER	CA-CB	5.11	1.60	1.52
1	14-A	137	ALA	N-CA	5.11	1.56	1.46
1	10-A	145	MET	N-CA	5.11	1.56	1.46
1	14-A	129	LEU	CG-CD2	5.11	1.70	1.51
1	8-A	91	GLN	CG-CD	5.10	1.62	1.51
1	10-A	121	TRP	N-CA	5.10	1.56	1.46
1	4-A	112	HIS	CG-CD2	5.10	1.44	1.35
1	5-A	67	TRP	CZ2-CH2	5.10	1.47	1.37
1	15-A	84	TYR	CZ-OH	5.10	1.46	1.37
1	15-A	155	PRO	CB-CG	5.10	1.75	1.50
1	8-A	98	PHE	CA-CB	-5.10	1.42	1.53
1	12-A	56	THR	CB-CG2	-5.10	1.35	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-A	53	PRO	CA-C	5.10	1.63	1.52
1	15-A	77	LEU	N-CA	5.10	1.56	1.46
1	15-A	140	TRP	CD1-NE1	5.10	1.46	1.38
1	11-A	145	MET	CB-CG	5.09	1.67	1.51
1	10-A	123	VAL	CB-CG2	5.09	1.63	1.52
1	12-A	113	PRO	CA-C	5.09	1.63	1.52
1	15-A	95	GLN	CD-OE1	5.09	1.35	1.24
1	13-A	149	PHE	CD1-CE1	-5.09	1.29	1.39
1	16-A	113	PRO	N-CA	-5.09	1.38	1.47
1	1-A	150	ILE	CB-CG1	5.09	1.68	1.54
1	10-A	113	PRO	CA-CB	5.09	1.63	1.53
1	2-A	69	GLY	N-CA	5.08	1.53	1.46
1	9-A	51	GLN	CA-CB	5.08	1.65	1.53
1	9-A	141	ARG	CD-NE	-5.08	1.37	1.46
1	7-A	146	TYR	CG-CD1	-5.08	1.32	1.39
1	2-A	38	LEU	C-O	5.08	1.33	1.23
1	6-A	70	LEU	CG-CD2	5.08	1.70	1.51
1	11-A	106	ARG	CZ-NH2	5.08	1.39	1.33
1	5-A	98	PHE	CG-CD2	5.08	1.46	1.38
1	5-A	105	GLN	CB-CG	-5.08	1.38	1.52
1	9-A	98	PHE	CA-C	5.08	1.66	1.52
1	14-A	39	LEU	CG-CD1	5.08	1.70	1.51
1	15-A	122	LEU	CA-CB	5.08	1.65	1.53
1	9-A	61	LEU	CA-CB	-5.08	1.42	1.53
1	16-A	135	HIS	CA-CB	5.08	1.65	1.53
1	7-A	156	GLU	CD-OE1	5.08	1.31	1.25
1	10-A	47	ASP	CG-OD2	5.08	1.37	1.25
1	1-A	109	SER	N-CA	5.07	1.56	1.46
1	2-A	153	ILE	CB-CG1	-5.07	1.39	1.54
1	9-A	115	LYS	CA-CB	5.07	1.65	1.53
1	4-A	143	ASP	CA-CB	5.07	1.65	1.53
1	8-A	129	LEU	CG-CD1	5.07	1.70	1.51
1	14-A	105	GLN	CD-OE1	5.07	1.35	1.24
1	16-A	80	GLN	C-N	5.07	1.43	1.34
1	9-A	97	ARG	N-CA	5.07	1.56	1.46
1	1-A	65	THR	CA-CB	5.07	1.66	1.53
1	16-A	82	LEU	CG-CD2	5.07	1.70	1.51
1	1-A	107	LEU	C-N	5.06	1.45	1.34
1	11-A	48	TYR	CB-CG	-5.06	1.44	1.51
1	12-A	113	PRO	C-O	5.06	1.33	1.23
1	9-A	71	SER	N-CA	5.06	1.56	1.46
1	4-A	134	LEU	CG-CD1	5.06	1.70	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	113	PRO	CA-CB	5.06	1.63	1.53
1	10-A	97	ARG	CA-C	5.06	1.66	1.52
1	4-A	92	ARG	C-N	-5.05	1.22	1.34
1	9-A	50	LYS	CD-CE	5.05	1.63	1.51
1	9-A	105	GLN	CD-NE2	5.05	1.45	1.32
1	10-A	100	THR	N-CA	5.05	1.56	1.46
1	12-A	147	HIS	CA-CB	5.05	1.65	1.53
1	13-A	125	GLU	C-O	5.05	1.32	1.23
1	13-A	130	THR	N-CA	5.05	1.56	1.46
1	14-A	140	TRP	CD1-NE1	5.05	1.46	1.38
1	15-A	135	HIS	CA-CB	5.05	1.65	1.53
1	16-A	91	GLN	CD-OE1	-5.05	1.12	1.24
1	16-A	48	TYR	CA-C	5.05	1.66	1.52
1	4-A	76	GLN	CG-CD	-5.05	1.39	1.51
1	15-A	62	ILE	CA-CB	5.05	1.66	1.54
1	4-A	81	PRO	CB-CG	5.04	1.75	1.50
1	9-A	48	TYR	CE1-CZ	5.04	1.45	1.38
1	3-A	137	ALA	C-N	5.04	1.45	1.34
1	15-A	104	GLU	C-O	5.04	1.32	1.23
1	10-A	148	SER	N-CA	-5.04	1.36	1.46
1	12-A	59	GLY	N-CA	5.04	1.53	1.46
1	16-A	146	TYR	C-N	5.04	1.45	1.34
1	9-A	138	LEU	CA-C	5.03	1.66	1.52
1	12-A	135	HIS	CA-CB	5.03	1.65	1.53
1	16-A	111	ILE	N-CA	5.03	1.56	1.46
1	1-A	145	MET	CB-CG	5.03	1.67	1.51
1	4-A	142	SER	CA-CB	5.03	1.60	1.52
1	6-A	84	TYR	CE2-CZ	-5.03	1.32	1.38
1	12-A	136	MET	CB-CG	5.03	1.67	1.51
1	14-A	78	TYR	CD2-CE2	5.03	1.46	1.39
1	10-A	112	HIS	CE1-NE2	5.03	1.44	1.32
1	12-A	58	ARG	CA-C	-5.03	1.39	1.52
1	4-A	77	LEU	CG-CD1	5.03	1.70	1.51
1	15-A	41	ARG	CB-CG	5.03	1.66	1.52
1	11-A	38	LEU	CA-CB	5.03	1.65	1.53
1	14-A	65	THR	CA-C	-5.03	1.39	1.52
1	5-A	82	LEU	CG-CD1	5.02	1.70	1.51
1	15-A	122	LEU	CG-CD1	5.02	1.70	1.51
1	5-A	91	GLN	C-O	5.02	1.32	1.23
1	7-A	148	SER	N-CA	-5.02	1.36	1.46
1	2-A	104	GLU	CG-CD	5.01	1.59	1.51
1	15-A	74	MET	SD-CE	5.01	2.06	1.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	15-A	136	MET	SD-CE	-5.01	1.49	1.77
1	13-A	143	ASP	CG-OD2	5.01	1.36	1.25
1	5-A	45	TYR	CD1-CE1	-5.01	1.31	1.39
1	9-A	50	LYS	N-CA	5.01	1.56	1.46
1	12-A	112	HIS	CG-CD2	5.01	1.44	1.35
1	13-A	74	MET	CB-CG	5.01	1.67	1.51
1	4-A	116	ALA	C-N	5.01	1.45	1.34
1	4-A	117	GLU	N-CA	5.01	1.56	1.46
1	11-A	83	HIS	C-O	5.01	1.32	1.23
1	1-A	74	MET	CA-CB	5.00	1.65	1.53
1	10-A	98	PHE	CG-CD2	5.00	1.46	1.38
1	16-A	117	GLU	CA-CB	5.00	1.65	1.53
1	12-A	116	ALA	C-O	-5.00	1.13	1.23
1	13-A	80	GLN	CB-CG	5.00	1.66	1.52
1	14-A	64	PHE	CA-CB	5.00	1.65	1.53

All (2781) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16-A	143	ASP	CB-CG-OD1	-59.30	64.92	118.30
1	11-A	40	ARG	NE-CZ-NH1	40.59	140.59	120.30
1	13-A	92	ARG	NE-CZ-NH1	38.80	139.70	120.30
1	5-A	92	ARG	NE-CZ-NH2	-38.57	101.01	120.30
1	7-A	92	ARG	NE-CZ-NH2	-37.16	101.72	120.30
1	5-A	94	ASP	CB-CG-OD1	35.87	150.59	118.30
1	15-A	41	ARG	NE-CZ-NH2	-35.72	102.44	120.30
1	1-A	92	ARG	NE-CZ-NH2	-35.66	102.47	120.30
1	13-A	41	ARG	NE-CZ-NH2	-33.82	103.39	120.30
1	13-A	92	ARG	NE-CZ-NH2	-33.77	103.42	120.30
1	5-A	41	ARG	NE-CZ-NH2	-33.67	103.47	120.30
1	10-A	41	ARG	NE-CZ-NH2	-33.02	103.79	120.30
1	16-A	82	LEU	CB-CG-CD2	-32.45	55.83	111.00
1	2-A	40	ARG	NE-CZ-NH1	-32.33	104.14	120.30
1	8-A	41	ARG	NE-CZ-NH2	-31.91	104.35	120.30
1	16-A	92	ARG	NE-CZ-NH2	-31.76	104.42	120.30
1	12-A	40	ARG	NE-CZ-NH1	-31.56	104.52	120.30
1	16-A	84	TYR	CZ-CE2-CD2	-31.44	91.51	119.80
1	5-A	40	ARG	NE-CZ-NH1	-31.09	104.75	120.30
1	7-A	40	ARG	NE-CZ-NH1	-31.04	104.78	120.30
1	10-A	40	ARG	NE-CZ-NH1	-30.48	105.06	120.30
1	14-A	92	ARG	NE-CZ-NH2	-30.46	105.07	120.30
1	4-A	151	ASP	CB-CG-OD1	29.66	145.00	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	15-A	92	ARG	NE-CZ-NH2	-29.57	105.52	120.30
1	14-A	40	ARG	NE-CZ-NH1	-29.25	105.67	120.30
1	2-A	92	ARG	NE-CZ-NH1	-29.11	105.75	120.30
1	9-A	40	ARG	NE-CZ-NH1	-29.08	105.76	120.30
1	16-A	40	ARG	NE-CZ-NH1	-29.04	105.78	120.30
1	10-A	41	ARG	NE-CZ-NH1	28.75	134.68	120.30
1	15-A	106	ARG	NE-CZ-NH2	28.57	134.59	120.30
1	15-A	106	ARG	NE-CZ-NH1	28.33	134.47	120.30
1	6-A	40	ARG	NE-CZ-NH1	-27.83	106.39	120.30
1	5-A	41	ARG	NE-CZ-NH1	27.76	134.18	120.30
1	16-A	93	TRP	CG-CD1-NE1	-27.72	82.38	110.10
1	11-A	40	ARG	NH1-CZ-NH2	-27.52	89.13	119.40
1	15-A	106	ARG	NH1-CZ-NH2	-27.51	89.14	119.40
1	4-A	78	TYR	CD1-CE1-CZ	-27.50	95.05	119.80
1	16-A	143	ASP	CB-CG-OD2	26.88	142.49	118.30
1	2-A	92	ARG	NE-CZ-NH2	26.81	133.70	120.30
1	9-A	41	ARG	NE-CZ-NH2	-26.77	106.91	120.30
1	9-A	41	ARG	NE-CZ-NH1	26.08	133.34	120.30
1	10-A	68	VAL	CG1-CB-CG2	-25.91	69.44	110.90
1	1-A	41	ARG	NE-CZ-NH2	-25.67	107.47	120.30
1	4-A	40	ARG	NE-CZ-NH1	-25.57	107.51	120.30
1	14-A	124	GLU	OE1-CD-OE2	25.34	153.71	123.30
1	11-A	92	ARG	NE-CZ-NH2	25.27	132.94	120.30
1	10-A	64	PHE	CB-CG-CD1	-25.21	103.15	120.80
1	12-A	41	ARG	NE-CZ-NH1	25.16	132.88	120.30
1	10-A	92	ARG	NE-CZ-NH2	-25.08	107.76	120.30
1	13-A	40	ARG	NE-CZ-NH1	-24.99	107.80	120.30
1	13-A	43	GLU	OE1-CD-OE2	24.98	153.27	123.30
1	12-A	92	ARG	NE-CZ-NH2	-24.78	107.91	120.30
1	15-A	43	GLU	OE1-CD-OE2	24.78	153.03	123.30
1	9-A	84	TYR	CD1-CE1-CZ	-24.53	97.72	119.80
1	14-A	106	ARG	NE-CZ-NH2	24.53	132.57	120.30
1	3-A	92	ARG	NE-CZ-NH2	-24.43	108.08	120.30
1	12-A	41	ARG	NE-CZ-NH2	-24.33	108.13	120.30
1	15-A	40	ARG	NE-CZ-NH1	-24.12	108.24	120.30
1	14-A	45	TYR	CB-CG-CD2	-23.95	106.63	121.00
1	14-A	45	TYR	CG-CD2-CE2	-23.91	102.18	121.30
1	11-A	38	LEU	CB-CG-CD1	-23.78	70.57	111.00
1	1-A	108	ASP	CB-CG-OD2	23.73	139.66	118.30
1	14-A	85	LEU	CB-CG-CD1	-23.50	71.05	111.00
1	16-A	146	TYR	CD1-CE1-CZ	-23.46	98.68	119.80
1	7-A	41	ARG	NE-CZ-NH1	23.22	131.91	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	92	ARG	NE-CZ-NH2	-23.08	108.76	120.30
1	11-A	41	ARG	NE-CZ-NH1	22.99	131.80	120.30
1	4-A	64	PHE	CB-CG-CD1	-22.91	104.77	120.80
1	8-A	41	ARG	NE-CZ-NH1	22.79	131.70	120.30
1	7-A	41	ARG	NE-CZ-NH2	-22.68	108.96	120.30
1	16-A	43	GLU	OE1-CD-OE2	22.61	150.43	123.30
1	14-A	43	GLU	OE1-CD-OE2	22.15	149.88	123.30
1	1-A	41	ARG	NE-CZ-NH1	22.14	131.37	120.30
1	6-A	41	ARG	NE-CZ-NH2	-21.85	109.38	120.30
1	3-A	40	ARG	NE-CZ-NH1	-21.74	109.43	120.30
1	2-A	41	ARG	NE-CZ-NH1	21.62	131.11	120.30
1	8-A	43	GLU	OE1-CD-OE2	21.56	149.17	123.30
1	3-A	41	ARG	NE-CZ-NH2	-21.34	109.63	120.30
1	16-A	41	ARG	NE-CZ-NH2	-21.25	109.67	120.30
1	3-A	61	LEU	CB-CG-CD1	-21.24	74.90	111.00
1	4-A	43	GLU	OE1-CD-OE2	21.22	148.77	123.30
1	2-A	41	ARG	NE-CZ-NH2	-21.12	109.74	120.30
1	14-A	41	ARG	NE-CZ-NH2	-21.08	109.76	120.30
1	4-A	92	ARG	NE-CZ-NH2	-21.00	109.80	120.30
1	6-A	41	ARG	NE-CZ-NH1	20.83	130.71	120.30
1	1-A	78	TYR	CD1-CE1-CZ	-20.79	101.09	119.80
1	6-A	92	ARG	NE-CZ-NH1	20.73	130.67	120.30
1	16-A	84	TYR	CG-CD2-CE2	20.73	137.88	121.30
1	15-A	85	LEU	CB-CG-CD1	-20.59	75.99	111.00
1	14-A	92	ARG	NE-CZ-NH1	20.56	130.58	120.30
1	6-A	84	TYR	CG-CD1-CE1	-20.43	104.96	121.30
1	15-A	115	LYS	CD-CE-NZ	-20.28	65.06	111.70
1	15-A	97	ARG	NE-CZ-NH2	-20.19	110.21	120.30
1	11-A	58	ARG	NE-CZ-NH1	20.06	130.33	120.30
1	2-A	50	LYS	CD-CE-NZ	20.04	157.78	111.70
1	1-A	64	PHE	CB-CG-CD1	-19.95	106.83	120.80
1	6-A	43	GLU	OE1-CD-OE2	19.95	147.23	123.30
1	9-A	128	ARG	NE-CZ-NH1	-19.79	110.40	120.30
1	4-A	41	ARG	NE-CZ-NH2	-19.64	110.48	120.30
1	14-A	47	ASP	CB-CG-OD2	-19.59	100.67	118.30
1	8-A	68	VAL	CG1-CB-CG2	19.48	142.06	110.90
1	16-A	41	ARG	NE-CZ-NH1	19.34	129.97	120.30
1	8-A	92	ARG	NE-CZ-NH2	-19.27	110.66	120.30
1	16-A	146	TYR	CB-CG-CD1	-19.16	109.51	121.00
1	14-A	47	ASP	CB-CG-OD1	19.05	135.45	118.30
1	15-A	41	ARG	NE-CZ-NH1	19.03	129.81	120.30
1	5-A	47	ASP	CB-CG-OD2	-18.89	101.30	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	11-A	89	LEU	CA-CB-CG	-18.76	72.15	115.30
1	13-A	41	ARG	NE-CZ-NH1	18.75	129.68	120.30
1	10-A	45	TYR	CG-CD2-CE2	-18.59	106.43	121.30
1	11-A	58	ARG	NE-CZ-NH2	-18.47	111.06	120.30
1	4-A	151	ASP	CB-CG-OD2	-18.23	101.89	118.30
1	9-A	47	ASP	CB-CG-OD1	18.21	134.69	118.30
1	9-A	47	ASP	CB-CG-OD2	-18.14	101.97	118.30
1	2-A	47	ASP	CB-CG-OD2	-18.12	102.00	118.30
1	10-A	140	TRP	CG-CD1-NE1	-17.93	92.17	110.10
1	14-A	41	ARG	NE-CZ-NH1	17.92	129.26	120.30
1	14-A	128	ARG	NE-CZ-NH1	17.79	129.19	120.30
1	13-A	97	ARG	NE-CZ-NH2	-17.76	111.42	120.30
1	13-A	123	VAL	CG1-CB-CG2	17.69	139.20	110.90
1	3-A	41	ARG	NE-CZ-NH1	17.59	129.09	120.30
1	16-A	93	TRP	CD1-CG-CD2	17.56	120.35	106.30
1	13-A	151	ASP	CB-CG-OD1	17.56	134.10	118.30
1	7-A	43	GLU	OE1-CD-OE2	17.50	144.31	123.30
1	16-A	115	LYS	CD-CE-NZ	17.46	151.87	111.70
1	5-A	92	ARG	NH1-CZ-NH2	17.42	138.56	119.40
1	1-A	43	GLU	OE1-CD-OE2	17.25	143.99	123.30
1	1-A	45	TYR	CD1-CE1-CZ	-17.23	104.29	119.80
1	7-A	143	ASP	CB-CG-OD2	17.19	133.77	118.30
1	12-A	138	LEU	CB-CG-CD1	17.17	140.19	111.00
1	13-A	108	ASP	CB-CG-OD2	-17.17	102.85	118.30
1	2-A	154	PHE	CZ-CE2-CD2	17.15	140.69	120.10
1	7-A	92	ARG	NH1-CZ-NH2	17.13	138.24	119.40
1	15-A	88	VAL	CG1-CB-CG2	-17.04	83.64	110.90
1	4-A	41	ARG	NE-CZ-NH1	17.00	128.80	120.30
1	1-A	121	TRP	CG-CD1-NE1	-16.96	93.14	110.10
1	15-A	93	TRP	CG-CD1-NE1	-16.94	93.16	110.10
1	1-A	92	ARG	NE-CZ-NH1	16.92	128.76	120.30
1	15-A	47	ASP	CB-CG-OD2	-16.90	103.09	118.30
1	8-A	49	MET	CG-SD-CE	-16.89	73.18	100.20
1	14-A	64	PHE	CZ-CE2-CD2	-16.84	99.89	120.10
1	9-A	140	TRP	CG-CD1-NE1	-16.78	93.32	110.10
1	4-A	134	LEU	CB-CG-CD2	-16.75	82.53	111.00
1	1-A	128	ARG	NE-CZ-NH1	16.71	128.66	120.30
1	14-A	146	TYR	CB-CG-CD2	-16.70	110.98	121.00
1	1-A	121	TRP	CB-CG-CD1	-16.70	105.29	127.00
1	13-A	146	TYR	CB-CG-CD2	-16.64	111.02	121.00
1	8-A	64	PHE	CZ-CE2-CD2	-16.63	100.14	120.10
1	5-A	84	TYR	CG-CD1-CE1	-16.61	108.01	121.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	115	LYS	CD-CE-NZ	16.58	149.84	111.70
1	13-A	58	ARG	NE-CZ-NH2	-16.56	112.02	120.30
1	4-A	64	PHE	CB-CG-CD2	16.55	132.38	120.80
1	2-A	45	TYR	CD1-CE1-CZ	-16.48	104.96	119.80
1	6-A	74	MET	CG-SD-CE	-16.41	73.95	100.20
1	10-A	92	ARG	NE-CZ-NH1	16.39	128.49	120.30
1	11-A	78	TYR	CD1-CE1-CZ	-16.38	105.06	119.80
1	5-A	94	ASP	OD1-CG-OD2	-16.36	92.21	123.30
1	5-A	43	GLU	OE1-CD-OE2	16.34	142.91	123.30
1	16-A	129	LEU	CB-CG-CD2	-16.33	83.24	111.00
1	16-A	92	ARG	NE-CZ-NH1	16.32	128.46	120.30
1	5-A	128	ARG	NE-CZ-NH2	-16.29	112.16	120.30
1	14-A	97	ARG	NH1-CZ-NH2	-16.15	101.63	119.40
1	15-A	141	ARG	NE-CZ-NH1	-16.10	112.25	120.30
1	16-A	141	ARG	NE-CZ-NH1	-16.08	112.26	120.30
1	14-A	97	ARG	NE-CZ-NH2	16.07	128.33	120.30
1	15-A	47	ASP	CB-CG-OD1	16.07	132.76	118.30
1	15-A	117	GLU	CA-CB-CG	-15.96	78.29	113.40
1	11-A	97	ARG	NE-CZ-NH2	-15.90	112.35	120.30
1	1-A	109	SER	CA-CB-OG	-15.86	68.39	111.20
1	1-A	64	PHE	CB-CG-CD2	15.82	131.87	120.80
1	9-A	68	VAL	CG1-CB-CG2	-15.82	85.59	110.90
1	6-A	82	LEU	CB-CG-CD1	15.80	137.86	111.00
1	9-A	43	GLU	OE1-CD-OE2	15.80	142.25	123.30
1	11-A	92	ARG	NH1-CZ-NH2	-15.68	102.15	119.40
1	13-A	141	ARG	NE-CZ-NH1	-15.63	112.48	120.30
1	10-A	128	ARG	NE-CZ-NH2	-15.49	112.55	120.30
1	11-A	154	PHE	CZ-CE2-CD2	15.45	138.64	120.10
1	2-A	64	PHE	CB-CG-CD1	-15.43	110.00	120.80
1	14-A	97	ARG	NE-CZ-NH1	15.40	128.00	120.30
1	2-A	47	ASP	CB-CG-OD1	15.37	132.14	118.30
1	13-A	146	TYR	CG-CD2-CE2	-15.38	109.00	121.30
1	1-A	154	PHE	CZ-CE2-CD2	15.37	138.54	120.10
1	8-A	92	ARG	NE-CZ-NH1	15.36	127.98	120.30
1	16-A	143	ASP	OD1-CG-OD2	15.35	152.46	123.30
1	9-A	49	MET	CG-SD-CE	15.32	124.71	100.20
1	14-A	108	ASP	OD1-CG-OD2	-15.31	94.20	123.30
1	7-A	94	ASP	CB-CG-OD2	-15.18	104.64	118.30
1	4-A	123	VAL	CG1-CB-CG2	-15.16	86.64	110.90
1	15-A	123	VAL	CG1-CB-CG2	15.08	135.03	110.90
1	16-A	73	SER	N-CA-CB	15.07	133.10	110.50
1	11-A	64	PHE	CG-CD2-CE2	-15.02	104.28	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	15-A	151	ASP	CB-CG-OD2	-14.98	104.82	118.30
1	1-A	121	TRP	CD1-CG-CD2	14.96	118.27	106.30
1	11-A	141	ARG	NE-CZ-NH1	-14.94	112.83	120.30
1	9-A	97	ARG	NE-CZ-NH1	14.85	127.72	120.30
1	15-A	78	TYR	CZ-CE2-CD2	-14.77	106.51	119.80
1	16-A	108	ASP	CB-CG-OD2	-14.70	105.07	118.30
1	11-A	107	LEU	CB-CG-CD2	-14.69	86.03	111.00
1	9-A	88	VAL	CG1-CB-CG2	-14.64	87.48	110.90
1	4-A	97	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	15-A	154	PHE	CB-CG-CD2	14.58	131.00	120.80
1	1-A	108	ASP	CB-CG-OD1	-14.58	105.18	118.30
1	15-A	146	TYR	CG-CD2-CE2	-14.53	109.68	121.30
1	8-A	40	ARG	NE-CZ-NH1	-14.50	113.05	120.30
1	14-A	124	GLU	CG-CD-OE1	-14.49	89.32	118.30
1	14-A	121	TRP	CG-CD1-NE1	-14.37	95.73	110.10
1	9-A	128	ARG	NH1-CZ-NH2	14.36	135.19	119.40
1	13-A	115	LYS	CD-CE-NZ	14.33	144.65	111.70
1	4-A	78	TYR	CG-CD1-CE1	14.31	132.75	121.30
1	3-A	151	ASP	CB-CG-OD1	14.30	131.17	118.30
1	3-A	138	LEU	CB-CG-CD2	-14.29	86.71	111.00
1	2-A	138	LEU	CB-CG-CD1	14.27	135.26	111.00
1	6-A	146	TYR	CB-CG-CD2	-14.24	112.46	121.00
1	14-A	48	TYR	CZ-CE2-CD2	-14.23	106.99	119.80
1	16-A	86	THR	CA-C-N	-14.22	85.91	117.20
1	12-A	92	ARG	NE-CZ-NH1	14.19	127.39	120.30
1	8-A	97	ARG	NE-CZ-NH2	-14.18	113.21	120.30
1	14-A	97	ARG	CD-NE-CZ	-14.12	103.83	123.60
1	15-A	50	LYS	CD-CE-NZ	14.11	144.16	111.70
1	11-A	154	PHE	CB-CG-CD2	14.11	130.67	120.80
1	5-A	47	ASP	CB-CG-OD1	14.09	130.98	118.30
1	8-A	80	GLN	CA-CB-CG	-14.09	82.41	113.40
1	15-A	92	ARG	NE-CZ-NH1	14.05	127.33	120.30
1	10-A	64	PHE	CB-CG-CD2	14.04	130.63	120.80
1	15-A	36	GLY	CA-C-O	-14.03	95.34	120.60
1	10-A	64	PHE	CD1-CE1-CZ	-13.96	103.35	120.10
1	9-A	136	MET	CA-CB-CG	-13.95	89.59	113.30
1	7-A	47	ASP	CB-CG-OD2	-13.77	105.90	118.30
1	8-A	106	ARG	NE-CZ-NH2	-13.74	113.43	120.30
1	15-A	48	TYR	CZ-CE2-CD2	-13.74	107.43	119.80
1	3-A	68	VAL	CG1-CB-CG2	13.74	132.88	110.90
1	14-A	46	GLN	CA-CB-CG	-13.72	83.22	113.40
1	15-A	124	GLU	C-N-CA	-13.66	87.54	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	12-A	47	ASP	CB-CG-OD2	-13.66	106.01	118.30
1	10-A	108	ASP	CB-CG-OD2	-13.65	106.01	118.30
1	13-A	90	LEU	CB-CG-CD2	13.57	134.07	111.00
1	16-A	146	TYR	CD1-CG-CD2	13.56	132.82	117.90
1	11-A	106	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	3-A	106	ARG	NE-CZ-NH1	13.48	127.04	120.30
1	8-A	107	LEU	CB-CG-CD2	-13.39	88.24	111.00
1	16-A	49	MET	CB-CG-SD	13.34	152.43	112.40
1	16-A	45	TYR	CG-CD2-CE2	-13.33	110.64	121.30
1	14-A	146	TYR	CG-CD2-CE2	-13.32	110.64	121.30
1	6-A	84	TYR	CD1-CE1-CZ	13.29	131.76	119.80
1	16-A	44	MET	CA-CB-CG	-13.22	90.83	113.30
1	4-A	70	LEU	CB-CG-CD2	-13.20	88.57	111.00
1	5-A	93	TRP	CB-CG-CD1	-13.15	109.90	127.00
1	16-A	154	PHE	CB-CG-CD2	13.15	130.00	120.80
1	15-A	96	SER	O-C-N	13.14	143.72	122.70
1	16-A	141	ARG	NE-CZ-NH2	-13.13	113.73	120.30
1	5-A	97	ARG	NE-CZ-NH2	-13.11	113.75	120.30
1	10-A	47	ASP	CB-CG-OD2	-13.07	106.54	118.30
1	14-A	141	ARG	NE-CZ-NH1	13.05	126.83	120.30
1	13-A	106	ARG	NE-CZ-NH1	13.04	126.82	120.30
1	8-A	146	TYR	CB-CG-CD2	-13.00	113.20	121.00
1	1-A	41	ARG	CD-NE-CZ	-12.94	105.49	123.60
1	11-A	78	TYR	CB-CG-CD2	-12.94	113.24	121.00
1	12-A	97	ARG	NE-CZ-NH1	12.94	126.77	120.30
1	16-A	58	ARG	NE-CZ-NH2	-12.94	113.83	120.30
1	16-A	41	ARG	CD-NE-CZ	-12.92	105.51	123.60
1	4-A	58	ARG	NE-CZ-NH2	-12.92	113.84	120.30
1	14-A	41	ARG	CD-NE-CZ	-12.91	105.52	123.60
1	6-A	108	ASP	CB-CG-OD1	-12.90	106.69	118.30
1	10-A	46	GLN	CA-CB-CG	-12.84	85.15	113.40
1	13-A	65	THR	C-N-CA	-12.83	89.62	121.70
1	16-A	115	LYS	CB-CA-C	-12.83	84.75	110.40
1	16-A	64	PHE	CB-CG-CD2	-12.81	111.83	120.80
1	15-A	49	MET	CB-CG-SD	-12.80	73.99	112.40
1	12-A	58	ARG	NE-CZ-NH2	-12.80	113.90	120.30
1	10-A	128	ARG	NH1-CZ-NH2	12.76	133.44	119.40
1	15-A	36	GLY	O-C-N	12.74	143.09	122.70
1	4-A	122	LEU	CB-CG-CD2	12.72	132.63	111.00
1	9-A	123	VAL	CG1-CB-CG2	-12.66	90.64	110.90
1	11-A	154	PHE	CE1-CZ-CE2	-12.66	97.21	120.00
1	1-A	115	LYS	CA-CB-CG	-12.66	85.55	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16-A	134	LEU	CB-CG-CD1	12.59	132.41	111.00
1	7-A	96	SER	N-CA-CB	-12.59	91.62	110.50
1	10-A	128	ARG	NE-CZ-NH1	-12.58	114.01	120.30
1	11-A	118	ALA	N-CA-CB	12.57	127.70	110.10
1	11-A	118	ALA	CB-CA-C	-12.55	91.27	110.10
1	14-A	49	MET	CB-CG-SD	-12.55	74.75	112.40
1	11-A	78	TYR	CG-CD1-CE1	-12.50	111.30	121.30
1	16-A	125	GLU	OE1-CD-OE2	-12.50	108.30	123.30
1	16-A	122	LEU	CD1-CG-CD2	-12.46	73.13	110.50
1	8-A	101	ASP	CB-CG-OD2	12.45	129.51	118.30
1	13-A	123	VAL	O-C-N	12.43	142.58	122.70
1	3-A	100	THR	CA-CB-CG2	-12.43	95.00	112.40
1	15-A	56	THR	OG1-CB-CG2	-12.42	81.43	110.00
1	2-A	108	ASP	CB-CG-OD2	-12.42	107.12	118.30
1	13-A	41	ARG	CD-NE-CZ	-12.40	106.24	123.60
1	1-A	128	ARG	NH1-CZ-NH2	-12.38	105.78	119.40
1	16-A	92	ARG	C-N-CA	-12.36	90.80	121.70
1	16-A	45	TYR	CB-CG-CD2	-12.36	113.59	121.00
1	4-A	138	LEU	CB-CG-CD2	-12.34	90.02	111.00
1	9-A	64	PHE	CB-CG-CD1	-12.34	112.17	120.80
1	16-A	81	PRO	C-N-CA	-12.33	90.86	121.70
1	13-A	44	MET	CA-CB-CG	-12.31	92.36	113.30
1	13-A	50	LYS	CB-CG-CD	-12.30	79.61	111.60
1	9-A	128	ARG	NE-CZ-NH2	-12.30	114.15	120.30
1	15-A	41	ARG	CD-NE-CZ	-12.30	106.38	123.60
1	5-A	108	ASP	CB-CG-OD1	-12.29	107.23	118.30
1	14-A	136	MET	CG-SD-CE	12.29	119.86	100.20
1	13-A	148	SER	CA-CB-OG	-12.29	78.03	111.20
1	1-A	106	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	1-A	58	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	3-A	146	TYR	CG-CD2-CE2	-12.25	111.50	121.30
1	6-A	58	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	5-A	146	TYR	CB-CG-CD1	-12.22	113.67	121.00
1	13-A	141	ARG	NE-CZ-NH2	-12.21	114.19	120.30
1	6-A	78	TYR	CB-CG-CD2	-12.19	113.69	121.00
1	2-A	145	MET	CG-SD-CE	12.18	119.69	100.20
1	5-A	93	TRP	CB-CA-C	-12.18	86.05	110.40
1	10-A	84	TYR	CD1-CE1-CZ	-12.16	108.86	119.80
1	9-A	89	LEU	CB-CG-CD2	-12.13	90.38	111.00
1	11-A	61	LEU	CB-CG-CD2	-12.11	90.41	111.00
1	4-A	70	LEU	CA-CB-CG	-12.11	87.45	115.30
1	14-A	115	LYS	CD-CE-NZ	-12.08	83.91	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	14-A	126	ILE	CG1-CB-CG2	12.08	137.98	111.40
1	9-A	92	ARG	NE-CZ-NH2	-12.08	114.26	120.30
1	14-A	143	ASP	CB-CG-OD1	12.03	129.12	118.30
1	8-A	50	LYS	CD-CE-NZ	12.02	139.35	111.70
1	9-A	151	ASP	CB-CG-OD2	12.01	129.11	118.30
1	5-A	40	ARG	NH1-CZ-NH2	12.01	132.61	119.40
1	14-A	88	VAL	CG1-CB-CG2	11.97	130.05	110.90
1	10-A	126	ILE	CG1-CB-CG2	11.97	137.73	111.40
1	16-A	92	ARG	O-C-N	11.94	141.81	122.70
1	13-A	89	LEU	CB-CG-CD2	-11.94	90.71	111.00
1	15-A	84	TYR	CG-CD2-CE2	-11.92	111.76	121.30
1	4-A	128	ARG	NE-CZ-NH2	-11.91	114.35	120.30
1	8-A	128	ARG	NE-CZ-NH2	-11.90	114.35	120.30
1	14-A	82	LEU	CB-CG-CD1	11.90	131.23	111.00
1	8-A	45	TYR	CB-CG-CD1	11.89	128.13	121.00
1	2-A	97	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	5-A	48	TYR	CZ-CE2-CD2	-11.87	109.12	119.80
1	16-A	48	TYR	CG-CD2-CE2	11.85	130.78	121.30
1	8-A	41	ARG	CD-NE-CZ	-11.84	107.02	123.60
1	11-A	38	LEU	CA-CB-CG	-11.82	88.12	115.30
1	16-A	129	LEU	CD1-CG-CD2	-11.81	75.06	110.50
1	12-A	146	TYR	CB-CG-CD1	-11.81	113.91	121.00
1	14-A	58	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	10-A	40	ARG	NH1-CZ-NH2	11.77	132.35	119.40
1	15-A	86	THR	OG1-CB-CG2	11.76	137.04	110.00
1	13-A	92	ARG	CB-CG-CD	-11.72	81.13	111.60
1	16-A	144	PRO	CA-C-N	-11.72	91.41	117.20
1	3-A	108	ASP	CB-CG-OD1	-11.71	107.76	118.30
1	12-A	50	LYS	CD-CE-NZ	11.66	138.52	111.70
1	3-A	84	TYR	CB-CG-CD1	11.65	127.99	121.00
1	9-A	40	ARG	NH1-CZ-NH2	11.63	132.20	119.40
1	16-A	146	TYR	CG-CD2-CE2	-11.63	112.00	121.30
1	3-A	115	LYS	CD-CE-NZ	-11.61	84.99	111.70
1	8-A	129	LEU	CB-CG-CD2	-11.61	91.26	111.00
1	11-A	65	THR	CA-CB-CG2	-11.61	96.15	112.40
1	5-A	37	SER	N-CA-CB	-11.60	93.10	110.50
1	1-A	146	TYR	CB-CG-CD1	-11.60	114.04	121.00
1	14-A	50	LYS	N-CA-CB	11.57	131.43	110.60
1	14-A	49	MET	CA-CB-CG	11.56	132.96	113.30
1	4-A	108	ASP	CB-CG-OD1	-11.55	107.91	118.30
1	11-A	64	PHE	CD1-CG-CD2	11.54	133.30	118.30
1	13-A	146	TYR	CD1-CG-CD2	11.52	130.57	117.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	58	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	6-A	78	TYR	CG-CD1-CE1	-11.49	112.11	121.30
1	5-A	93	TRP	CH2-CZ2-CE2	-11.48	105.92	117.40
1	16-A	136	MET	CG-SD-CE	11.46	118.53	100.20
1	15-A	141	ARG	NE-CZ-NH2	-11.45	114.57	120.30
1	16-A	125	GLU	CG-CD-OE1	11.45	141.20	118.30
1	14-A	130	THR	CA-CB-CG2	-11.45	96.38	112.40
1	13-A	47	ASP	CB-CG-OD2	-11.42	108.03	118.30
1	10-A	146	TYR	CG-CD2-CE2	-11.41	112.17	121.30
1	15-A	97	ARG	NH1-CZ-NH2	11.40	131.94	119.40
1	7-A	108	ASP	CB-CG-OD1	-11.39	108.05	118.30
1	3-A	41	ARG	CD-NE-CZ	-11.39	107.66	123.60
1	2-A	88	VAL	CG1-CB-CG2	-11.37	92.70	110.90
1	12-A	108	ASP	CB-CG-OD1	-11.38	108.06	118.30
1	11-A	89	LEU	CB-CA-C	11.37	131.81	110.20
1	15-A	125	GLU	CG-CD-OE1	11.37	141.04	118.30
1	15-A	96	SER	CA-C-O	-11.35	96.27	120.10
1	5-A	91	GLN	N-CA-C	-11.34	80.39	111.00
1	13-A	67	TRP	CG-CD1-NE1	-11.33	98.77	110.10
1	13-A	125	GLU	OE1-CD-OE2	-11.29	109.75	123.30
1	4-A	78	TYR	CB-CG-CD1	-11.28	114.23	121.00
1	16-A	47	ASP	CB-CA-C	-11.26	87.88	110.40
1	11-A	146	TYR	CB-CG-CD1	-11.26	114.25	121.00
1	2-A	130	THR	CA-C-O	-11.26	96.46	120.10
1	10-A	121	TRP	CB-CG-CD1	-11.24	112.39	127.00
1	14-A	50	LYS	CA-CB-CG	-11.22	88.72	113.40
1	2-A	40	ARG	NH1-CZ-NH2	11.20	131.72	119.40
1	2-A	117	GLU	OE1-CD-OE2	11.20	136.74	123.30
1	16-A	87	ASN	CA-C-N	-11.20	92.57	117.20
1	11-A	64	PHE	CB-CG-CD1	-11.18	112.97	120.80
1	4-A	146	TYR	CB-CG-CD1	-11.18	114.29	121.00
1	8-A	143	ASP	CB-CG-OD1	11.18	128.36	118.30
1	5-A	52	VAL	CG1-CB-CG2	11.18	128.78	110.90
1	2-A	138	LEU	CB-CG-CD2	-11.16	92.02	111.00
1	15-A	125	GLU	OE1-CD-OE2	-11.16	109.91	123.30
1	7-A	58	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	15-A	84	TYR	C-N-CA	-11.14	93.86	121.70
1	15-A	79	GLY	N-CA-C	11.13	140.91	113.10
1	7-A	40	ARG	NH1-CZ-NH2	11.12	131.63	119.40
1	8-A	65	THR	CA-CB-CG2	-11.11	96.85	112.40
1	8-A	45	TYR	CG-CD1-CE1	11.11	130.19	121.30
1	9-A	84	TYR	CZ-CE2-CD2	11.09	129.78	119.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	50	LYS	CD-CE-NZ	11.07	137.17	111.70
1	16-A	81	PRO	CA-CB-CG	-11.07	82.96	104.00
1	16-A	92	ARG	CA-C-O	-11.07	96.86	120.10
1	15-A	113	PRO	CA-CB-CG	-11.07	82.97	104.00
1	15-A	80	GLN	CG-CD-OE1	-11.04	99.51	121.60
1	8-A	148	SER	N-CA-CB	11.01	127.02	110.50
1	3-A	50	LYS	CD-CE-NZ	10.99	136.97	111.70
1	13-A	143	ASP	CB-CG-OD1	10.98	128.18	118.30
1	12-A	43	GLU	OE1-CD-OE2	10.97	136.46	123.30
1	10-A	45	TYR	CZ-CE2-CD2	10.96	129.67	119.80
1	6-A	44	MET	CG-SD-CE	-10.96	82.67	100.20
1	7-A	50	LYS	CD-CE-NZ	10.95	136.88	111.70
1	7-A	146	TYR	CG-CD2-CE2	-10.94	112.55	121.30
1	9-A	40	ARG	CG-CD-NE	-10.94	88.84	111.80
1	14-A	146	TYR	CD1-CG-CD2	10.93	129.92	117.90
1	15-A	146	TYR	CB-CG-CD2	-10.91	114.45	121.00
1	3-A	65	THR	CA-CB-CG2	-10.91	97.13	112.40
1	14-A	67	TRP	CD1-CG-CD2	10.90	115.02	106.30
1	6-A	66	SER	CA-CB-OG	10.88	140.57	111.20
1	1-A	114	THR	OG1-CB-CG2	-10.87	84.99	110.00
1	15-A	65	THR	CA-CB-CG2	-10.88	97.17	112.40
1	16-A	146	TYR	CE1-CZ-OH	-10.87	90.74	120.10
1	9-A	84	TYR	CG-CD1-CE1	10.86	129.98	121.30
1	13-A	123	VAL	CA-C-N	-10.85	93.34	117.20
1	2-A	91	GLN	C-N-CA	-10.84	94.61	121.70
1	14-A	45	TYR	CB-CG-CD1	10.84	127.50	121.00
1	2-A	143	ASP	CB-CG-OD1	10.83	128.05	118.30
1	11-A	141	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	12-A	40	ARG	NH1-CZ-NH2	10.82	131.30	119.40
1	15-A	136	MET	CG-SD-CE	10.80	117.49	100.20
1	4-A	77	LEU	CB-CG-CD1	-10.77	92.69	111.00
1	10-A	141	ARG	NE-CZ-NH2	-10.77	114.92	120.30
1	14-A	128	ARG	NH1-CZ-NH2	-10.76	107.56	119.40
1	9-A	108	ASP	CB-CG-OD1	-10.76	108.62	118.30
1	5-A	39	LEU	CB-CG-CD1	-10.75	92.72	111.00
1	14-A	64	PHE	CD1-CE1-CZ	10.75	133.00	120.10
1	6-A	154	PHE	CZ-CE2-CD2	10.75	133.00	120.10
1	10-A	58	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	7-A	141	ARG	NE-CZ-NH1	-10.74	114.93	120.30
1	16-A	69	GLY	C-N-CA	-10.74	94.84	121.70
1	5-A	106	ARG	NE-CZ-NH2	10.74	125.67	120.30
1	8-A	64	PHE	CB-CG-CD1	-10.73	113.29	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	141	ARG	NE-CZ-NH1	-10.72	114.94	120.30
1	9-A	146	TYR	CG-CD2-CE2	-10.72	112.72	121.30
1	1-A	74	MET	CA-CB-CG	-10.69	95.14	113.30
1	13-A	67	TRP	NE1-CE2-CD2	10.61	117.91	107.30
1	1-A	121	TRP	CD1-NE1-CE2	10.59	118.53	109.00
1	7-A	101	ASP	CB-CG-OD2	10.59	127.83	118.30
1	8-A	41	ARG	CA-CB-CG	10.59	136.70	113.40
1	5-A	48	TYR	CG-CD1-CE1	-10.57	112.84	121.30
1	12-A	80	GLN	CA-CB-CG	-10.56	90.16	113.40
1	2-A	136	MET	CG-SD-CE	10.55	117.09	100.20
1	15-A	49	MET	CA-CB-CG	-10.55	95.36	113.30
1	16-A	123	VAL	CG1-CB-CG2	10.55	127.78	110.90
1	7-A	74	MET	CA-CB-CG	-10.55	95.37	113.30
1	11-A	64	PHE	CD1-CE1-CZ	-10.53	107.46	120.10
1	13-A	97	ARG	NH1-CZ-NH2	10.51	130.97	119.40
1	4-A	92	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	10-A	107	LEU	CB-CG-CD2	-10.49	93.17	111.00
1	1-A	91	GLN	CB-CG-CD	-10.48	84.35	111.60
1	13-A	133	HIS	O-C-N	10.48	139.47	122.70
1	15-A	143	ASP	CB-CG-OD1	10.48	127.73	118.30
1	14-A	64	PHE	O-C-N	10.47	139.45	122.70
1	15-A	106	ARG	CD-NE-CZ	10.47	138.25	123.60
1	5-A	93	TRP	CB-CG-CD2	10.45	140.18	126.60
1	15-A	81	PRO	CA-C-N	-10.43	94.27	117.20
1	16-A	70	LEU	CB-CG-CD1	-10.42	93.29	111.00
1	9-A	91	GLN	N-CA-C	-10.40	82.92	111.00
1	14-A	97	ARG	O-C-N	10.39	139.33	122.70
1	4-A	122	LEU	CA-CB-CG	-10.39	91.40	115.30
1	8-A	44	MET	CG-SD-CE	-10.39	83.57	100.20
1	16-A	64	PHE	CG-CD2-CE2	-10.34	109.42	120.80
1	13-A	49	MET	CA-CB-CG	-10.34	95.73	113.30
1	15-A	93	TRP	CD1-CG-CD2	10.34	114.57	106.30
1	15-A	124	GLU	OE1-CD-OE2	-10.33	110.91	123.30
1	4-A	123	VAL	CA-CB-CG2	-10.32	95.42	110.90
1	16-A	40	ARG	CA-CB-CG	-10.32	90.70	113.40
1	2-A	129	LEU	CB-CG-CD2	-10.31	93.48	111.00
1	7-A	47	ASP	CB-CG-OD1	10.31	127.58	118.30
1	10-A	136	MET	CA-CB-CG	-10.31	95.78	113.30
1	9-A	127	HIS	O-C-N	10.29	139.17	122.70
1	2-A	98	PHE	CG-CD1-CE1	10.28	132.11	120.80
1	15-A	146	TYR	CD1-CE1-CZ	-10.27	110.56	119.80
1	15-A	146	TYR	CD1-CG-CD2	10.27	129.19	117.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	67	TRP	CZ3-CH2-CZ2	-10.25	109.30	121.60
1	14-A	53	PRO	N-CD-CG	-10.25	87.82	103.20
1	5-A	93	TRP	CG-CD1-NE1	-10.24	99.86	110.10
1	8-A	150	ILE	CB-CG1-CD1	-10.24	85.24	113.90
1	9-A	140	TRP	CD1-NE1-CE2	10.23	118.20	109.00
1	10-A	68	VAL	CA-CB-CG2	-10.21	95.58	110.90
1	3-A	106	ARG	NH1-CZ-NH2	-10.21	108.17	119.40
1	14-A	121	TRP	CD1-NE1-CE2	10.20	118.18	109.00
1	7-A	128	ARG	NE-CZ-NH1	-10.18	115.21	120.30
1	2-A	148	SER	CA-CB-OG	-10.17	83.74	111.20
1	15-A	39	LEU	CB-CG-CD2	10.17	128.29	111.00
1	2-A	81	PRO	O-C-N	10.16	138.96	122.70
1	6-A	73	SER	C-N-CA	-10.16	96.29	121.70
1	2-A	106	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	15-A	117	GLU	N-CA-CB	-10.15	92.33	110.60
1	13-A	48	TYR	CZ-CE2-CD2	-10.14	110.68	119.80
1	5-A	138	LEU	CB-CG-CD1	10.13	128.22	111.00
1	15-A	120	ILE	CA-CB-CG1	-10.12	91.76	111.00
1	11-A	64	PHE	CB-CG-CD2	-10.12	113.71	120.80
1	4-A	40	ARG	NH1-CZ-NH2	10.10	130.51	119.40
1	8-A	80	GLN	CB-CA-C	-10.10	90.19	110.40
1	2-A	39	LEU	CB-CG-CD1	-10.10	93.83	111.00
1	13-A	40	ARG	CA-CB-CG	-10.08	91.22	113.40
1	6-A	65	THR	CA-CB-CG2	-10.08	98.29	112.40
1	14-A	40	ARG	CA-CB-CG	-10.08	91.23	113.40
1	4-A	81	PRO	CA-CB-CG	-10.07	84.88	104.00
1	8-A	108	ASP	CB-CG-OD1	-10.06	109.24	118.30
1	14-A	156	GLU	OE1-CD-OE2	-10.06	111.22	123.30
1	1-A	40	ARG	CB-CA-C	-10.06	90.28	110.40
1	11-A	41	ARG	NE-CZ-NH2	-10.05	115.28	120.30
1	3-A	146	TYR	CB-CG-CD2	-10.04	114.97	121.00
1	5-A	48	TYR	CG-CD2-CE2	10.03	129.33	121.30
1	13-A	39	LEU	CB-CG-CD1	-10.03	93.95	111.00
1	15-A	39	LEU	CB-CG-CD1	-10.03	93.94	111.00
1	10-A	45	TYR	CB-CG-CD2	-9.99	115.00	121.00
1	10-A	123	VAL	CG1-CB-CG2	-9.99	94.91	110.90
1	5-A	128	ARG	NH1-CZ-NH2	9.99	130.39	119.40
1	7-A	117	GLU	OE1-CD-OE2	9.99	135.28	123.30
1	1-A	41	ARG	CG-CD-NE	-9.98	90.83	111.80
1	16-A	48	TYR	CG-CD1-CE1	-9.97	113.32	121.30
1	15-A	67	TRP	CD2-CE3-CZ3	-9.96	105.86	118.80
1	13-A	64	PHE	CB-CG-CD2	-9.95	113.83	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	40	ARG	NH1-CZ-NH2	9.95	130.34	119.40
1	11-A	115	LYS	CD-CE-NZ	-9.94	88.83	111.70
1	15-A	98	PHE	CG-CD2-CE2	-9.94	109.87	120.80
1	16-A	48	TYR	CD1-CE1-CZ	9.94	128.74	119.80
1	4-A	48	TYR	CZ-CE2-CD2	-9.94	110.86	119.80
1	15-A	94	ASP	CB-CG-OD2	-9.94	109.36	118.30
1	1-A	38	LEU	CB-CG-CD1	-9.93	94.13	111.00
1	4-A	57	ASN	O-C-N	9.93	138.58	122.70
1	1-A	44	MET	CA-CB-CG	-9.92	96.43	113.30
1	13-A	67	TRP	CB-CG-CD1	-9.91	114.11	127.00
1	16-A	48	TYR	CZ-CE2-CD2	-9.91	110.88	119.80
1	7-A	64	PHE	CB-CG-CD1	-9.89	113.87	120.80
1	16-A	82	LEU	CB-CA-C	9.89	129.00	110.20
1	15-A	110	ILE	O-C-N	9.88	138.51	122.70
1	2-A	146	TYR	CG-CD2-CE2	-9.87	113.41	121.30
1	2-A	91	GLN	CA-C-O	9.87	140.82	120.10
1	16-A	74	MET	CA-CB-CG	-9.85	96.55	113.30
1	11-A	92	ARG	CD-NE-CZ	-9.85	109.81	123.60
1	3-A	131	PRO	N-CD-CG	-9.85	88.43	103.20
1	3-A	146	TYR	CD1-CG-CD2	9.84	128.73	117.90
1	15-A	48	TYR	CG-CD1-CE1	-9.84	113.43	121.30
1	5-A	39	LEU	CB-CG-CD2	9.83	127.71	111.00
1	3-A	97	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	15-A	40	ARG	CA-CB-CG	-9.82	91.80	113.40
1	14-A	40	ARG	NH1-CZ-NH2	9.81	130.19	119.40
1	4-A	40	ARG	CB-CA-C	-9.80	90.79	110.40
1	16-A	40	ARG	NH1-CZ-NH2	9.80	130.18	119.40
1	2-A	108	ASP	OD1-CG-OD2	9.79	141.91	123.30
1	15-A	126	ILE	CA-CB-CG1	-9.78	92.41	111.00
1	2-A	63	PRO	N-CD-CG	-9.78	88.53	103.20
1	4-A	67	TRP	CG-CD2-CE3	-9.77	125.11	133.90
1	15-A	97	ARG	CG-CD-NE	9.76	132.30	111.80
1	4-A	97	ARG	CD-NE-CZ	-9.76	109.94	123.60
1	5-A	63	PRO	N-CD-CG	-9.76	88.56	103.20
1	16-A	81	PRO	N-CA-CB	9.75	115.00	103.30
1	1-A	40	ARG	CD-NE-CZ	9.72	137.21	123.60
1	15-A	82	LEU	CA-CB-CG	9.72	137.65	115.30
1	15-A	85	LEU	CA-CB-CG	-9.71	92.97	115.30
1	14-A	117	GLU	OE1-CD-OE2	9.70	134.94	123.30
1	16-A	37	SER	CA-CB-OG	-9.69	85.04	111.20
1	13-A	45	TYR	CD1-CE1-CZ	-9.69	111.08	119.80
1	2-A	74	MET	CA-CB-CG	-9.68	96.84	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	146	TYR	CG-CD2-CE2	-9.67	113.56	121.30
1	11-A	43	GLU	OE1-CD-OE2	9.67	134.91	123.30
1	9-A	106	ARG	NE-CZ-NH2	9.67	125.14	120.30
1	15-A	125	GLU	C-N-CA	-9.66	97.54	121.70
1	3-A	100	THR	O-C-N	9.65	138.15	122.70
1	6-A	41	ARG	CD-NE-CZ	-9.63	110.11	123.60
1	16-A	67	TRP	CD1-CG-CD2	9.63	114.01	106.30
1	3-A	88	VAL	CG1-CB-CG2	-9.63	95.50	110.90
1	15-A	124	GLU	O-C-N	9.61	138.08	122.70
1	4-A	41	ARG	CD-NE-CZ	-9.60	110.16	123.60
1	13-A	53	PRO	N-CD-CG	-9.58	88.83	103.20
1	11-A	108	ASP	CB-CG-OD1	-9.57	109.69	118.30
1	4-A	63	PRO	N-CD-CG	-9.56	88.86	103.20
1	14-A	146	TYR	CD1-CE1-CZ	-9.55	111.21	119.80
1	15-A	120	ILE	CG1-CB-CG2	-9.54	90.42	111.40
1	13-A	43	GLU	CG-CD-OE1	-9.53	99.24	118.30
1	4-A	48	TYR	CG-CD2-CE2	9.52	128.92	121.30
1	14-A	141	ARG	CD-NE-CZ	9.52	136.93	123.60
1	9-A	61	LEU	CD1-CG-CD2	-9.52	81.95	110.50
1	15-A	131	PRO	N-CD-CG	-9.52	88.92	103.20
1	14-A	140	TRP	CE3-CZ3-CH2	-9.51	110.74	121.20
1	13-A	68	VAL	CG1-CB-CG2	-9.51	95.69	110.90
1	7-A	143	ASP	OD1-CG-OD2	-9.49	105.26	123.30
1	14-A	39	LEU	CB-CG-CD2	9.49	127.14	111.00
1	16-A	82	LEU	CD1-CG-CD2	-9.49	82.03	110.50
1	11-A	141	ARG	NH1-CZ-NH2	9.49	129.84	119.40
1	2-A	78	TYR	CD1-CE1-CZ	-9.48	111.27	119.80
1	15-A	118	ALA	N-CA-CB	-9.48	96.82	110.10
1	13-A	80	GLN	CA-CB-CG	-9.47	92.56	113.40
1	9-A	121	TRP	CE3-CZ3-CH2	-9.46	110.79	121.20
1	2-A	146	TYR	CB-CG-CD1	-9.45	115.33	121.00
1	9-A	97	ARG	CD-NE-CZ	-9.44	110.38	123.60
1	15-A	136	MET	O-C-N	9.44	137.80	122.70
1	6-A	146	TYR	CD1-CG-CD2	9.44	128.28	117.90
1	6-A	78	TYR	CB-CG-CD1	9.43	126.66	121.00
1	2-A	153	ILE	CG1-CB-CG2	-9.43	90.66	111.40
1	1-A	114	THR	CA-CB-OG1	9.41	128.77	109.00
1	2-A	48	TYR	CG-CD2-CE2	9.41	128.83	121.30
1	4-A	138	LEU	CB-CG-CD1	9.41	127.00	111.00
1	10-A	146	TYR	CB-CG-CD1	-9.40	115.36	121.00
1	1-A	151	ASP	CB-CG-OD1	9.40	126.76	118.30
1	3-A	40	ARG	CB-CA-C	-9.39	91.62	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-A	125	GLU	OE1-CD-OE2	-9.38	112.04	123.30
1	4-A	123	VAL	N-CA-CB	9.38	132.13	111.50
1	10-A	146	TYR	CD1-CG-CD2	9.37	128.21	117.90
1	14-A	90	LEU	CB-CG-CD2	9.37	126.93	111.00
1	2-A	66	SER	CA-CB-OG	-9.36	85.93	111.20
1	3-A	74	MET	CA-CB-CG	-9.35	97.41	113.30
1	7-A	48	TYR	CZ-CE2-CD2	-9.35	111.39	119.80
1	7-A	128	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	15-A	84	TYR	CA-C-O	-9.34	100.49	120.10
1	4-A	98	PHE	C-N-CA	-9.34	102.69	122.30
1	13-A	146	TYR	CD1-CE1-CZ	-9.34	111.40	119.80
1	2-A	92	ARG	CD-NE-CZ	-9.33	110.54	123.60
1	9-A	48	TYR	CZ-CE2-CD2	-9.32	111.41	119.80
1	9-A	146	TYR	CD1-CG-CD2	9.32	128.16	117.90
1	10-A	47	ASP	CB-CG-OD1	9.32	126.69	118.30
1	14-A	121	TRP	CD1-CG-CD2	9.32	113.75	106.30
1	11-A	89	LEU	N-CA-CB	-9.30	91.80	110.40
1	10-A	151	ASP	CB-CG-OD2	9.28	126.65	118.30
1	3-A	117	GLU	OE1-CD-OE2	9.27	134.43	123.30
1	11-A	64	PHE	CE1-CZ-CE2	9.27	136.68	120.00
1	13-A	92	ARG	CG-CD-NE	-9.26	92.36	111.80
1	14-A	122	LEU	CB-CG-CD1	-9.26	95.26	111.00
1	3-A	134	LEU	CB-CG-CD1	9.26	126.74	111.00
1	16-A	78	TYR	CA-CB-CG	-9.25	95.82	113.40
1	7-A	146	TYR	CD1-CG-CD2	9.25	128.07	117.90
1	15-A	115	LYS	CG-CD-CE	9.25	139.65	111.90
1	16-A	144	PRO	O-C-N	9.25	137.50	122.70
1	1-A	123	VAL	CA-CB-CG1	9.24	124.75	110.90
1	14-A	61	LEU	CB-CG-CD1	-9.23	95.30	111.00
1	10-A	150	ILE	CB-CG1-CD1	-9.23	88.05	113.90
1	13-A	151	ASP	N-CA-CB	-9.23	93.98	110.60
1	2-A	39	LEU	CB-CG-CD2	9.22	126.68	111.00
1	15-A	121	TRP	CA-CB-CG	-9.21	96.20	113.70
1	2-A	98	PHE	CG-CD2-CE2	-9.20	110.68	120.80
1	14-A	152	PRO	O-C-N	-9.20	107.98	122.70
1	9-A	108	ASP	OD1-CG-OD2	9.19	140.76	123.30
1	10-A	77	LEU	C-N-CA	-9.19	98.73	121.70
1	13-A	65	THR	O-C-N	9.19	137.40	122.70
1	15-A	80	GLN	CA-CB-CG	-9.19	93.19	113.40
1	1-A	48	TYR	CZ-CE2-CD2	-9.19	111.53	119.80
1	15-A	84	TYR	CG-CD1-CE1	9.18	128.64	121.30
1	2-A	153	ILE	CB-CA-C	-9.17	93.25	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	36	GLY	O-C-N	-9.17	108.02	122.70
1	14-A	123	VAL	CA-CB-CG1	-9.17	97.14	110.90
1	4-A	130	THR	CA-CB-CG2	9.16	125.23	112.40
1	12-A	48	TYR	CZ-CE2-CD2	-9.16	111.55	119.80
1	15-A	67	TRP	C-N-CA	-9.16	98.80	121.70
1	15-A	97	ARG	CB-CG-CD	-9.16	87.78	111.60
1	15-A	154	PHE	CB-CG-CD1	-9.16	114.39	120.80
1	13-A	90	LEU	CA-CB-CG	-9.16	94.24	115.30
1	16-A	84	TYR	CA-CB-CG	-9.15	96.01	113.40
1	10-A	121	TRP	CD1-CG-CD2	9.15	113.62	106.30
1	9-A	93	TRP	CB-CA-C	-9.15	92.10	110.40
1	13-A	136	MET	CG-SD-CE	-9.15	85.56	100.20
1	14-A	123	VAL	CG1-CB-CG2	9.15	125.53	110.90
1	11-A	61	LEU	O-C-N	9.13	137.32	122.70
1	14-A	152	PRO	N-CD-CG	-9.13	89.50	103.20
1	5-A	151	ASP	CB-CG-OD2	9.13	126.52	118.30
1	7-A	40	ARG	CA-CB-CG	-9.13	93.31	113.40
1	10-A	44	MET	CA-CB-CG	-9.12	97.80	113.30
1	8-A	64	PHE	CD1-CE1-CZ	9.12	131.04	120.10
1	10-A	100	THR	O-C-N	9.11	137.28	122.70
1	7-A	81	PRO	O-C-N	9.10	137.27	122.70
1	8-A	146	TYR	CD1-CG-CD2	9.10	127.91	117.90
1	16-A	130	THR	CA-C-O	-9.10	101.00	120.10
1	3-A	93	TRP	C-N-CA	-9.09	98.97	121.70
1	13-A	148	SER	CA-C-N	-9.08	97.23	117.20
1	16-A	68	VAL	CG1-CB-CG2	9.07	125.41	110.90
1	11-A	61	LEU	N-CA-CB	-9.06	92.28	110.40
1	4-A	128	ARG	NH1-CZ-NH2	9.06	129.36	119.40
1	13-A	67	TRP	CA-CB-CG	-9.06	96.49	113.70
1	8-A	40	ARG	N-CA-CB	9.06	126.90	110.60
1	11-A	57	ASN	O-C-N	9.04	137.16	122.70
1	8-A	52	VAL	CG1-CB-CG2	9.03	125.35	110.90
1	13-A	108	ASP	OD1-CG-OD2	9.03	140.46	123.30
1	2-A	41	ARG	CD-NE-CZ	-9.02	110.97	123.60
1	8-A	40	ARG	CB-CA-C	-9.02	92.35	110.40
1	1-A	63	PRO	N-CD-CG	-9.02	89.67	103.20
1	13-A	58	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	2-A	91	GLN	CA-CB-CG	-9.02	93.56	113.40
1	14-A	45	TYR	CD1-CE1-CZ	9.02	127.91	119.80
1	2-A	106	ARG	C-N-CA	-9.01	99.18	121.70
1	6-A	115	LYS	CD-CE-NZ	9.00	132.40	111.70
1	14-A	148	SER	CA-CB-OG	-9.00	86.90	111.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	15-A	43	GLU	CG-CD-OE1	-8.99	100.31	118.30
1	4-A	97	ARG	O-C-N	8.99	137.08	122.70
1	15-A	50	LYS	N-CA-CB	-8.99	94.42	110.60
1	1-A	65	THR	CA-CB-CG2	-8.98	99.82	112.40
1	9-A	58	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	6-A	40	ARG	CA-CB-CG	-8.97	93.67	113.40
1	11-A	83	HIS	CB-CA-C	-8.97	92.47	110.40
1	9-A	123	VAL	CA-CB-CG1	-8.96	97.46	110.90
1	10-A	80	GLN	CA-CB-CG	-8.96	93.69	113.40
1	3-A	106	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	5-A	138	LEU	CB-CG-CD2	-8.95	95.78	111.00
1	7-A	146	TYR	CB-CG-CD2	-8.95	115.63	121.00
1	4-A	36	GLY	N-CA-C	8.95	135.47	113.10
1	8-A	140	TRP	CE3-CZ3-CH2	-8.95	111.36	121.20
1	11-A	42	ALA	N-CA-CB	-8.94	97.58	110.10
1	9-A	48	TYR	CG-CD2-CE2	8.94	128.45	121.30
1	10-A	97	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	8-A	154	PHE	CB-CG-CD2	8.93	127.05	120.80
1	14-A	128	ARG	O-C-N	-8.93	108.41	122.70
1	12-A	40	ARG	CA-CB-CG	-8.92	93.77	113.40
1	5-A	40	ARG	CA-CB-CG	-8.92	93.78	113.40
1	11-A	93	TRP	O-C-N	8.91	136.96	122.70
1	9-A	61	LEU	CA-CB-CG	-8.91	94.80	115.30
1	6-A	146	TYR	CG-CD2-CE2	-8.91	114.17	121.30
1	12-A	36	GLY	N-CA-C	8.90	135.35	113.10
1	14-A	120	ILE	C-N-CA	-8.89	99.47	121.70
1	16-A	68	VAL	CA-CB-CG2	-8.88	97.57	110.90
1	5-A	93	TRP	CD1-NE1-CE2	8.87	116.98	109.00
1	15-A	81	PRO	CA-CB-CG	-8.86	87.16	104.00
1	10-A	115	LYS	CA-CB-CG	-8.86	93.90	113.40
1	10-A	40	ARG	CA-CB-CG	-8.85	93.92	113.40
1	7-A	128	ARG	NH1-CZ-NH2	8.85	129.14	119.40
1	2-A	40	ARG	CA-CB-CG	-8.85	93.94	113.40
1	13-A	106	ARG	NH1-CZ-NH2	-8.85	109.67	119.40
1	14-A	125	GLU	N-CA-CB	-8.85	94.68	110.60
1	11-A	39	LEU	CA-CB-CG	-8.84	94.97	115.30
1	14-A	56	THR	OG1-CB-CG2	-8.84	89.67	110.00
1	6-A	48	TYR	CG-CD2-CE2	8.83	128.37	121.30
1	16-A	83	HIS	CG-ND1-CE1	8.83	120.56	108.20
1	16-A	93	TRP	CB-CG-CD2	-8.83	115.12	126.60
1	2-A	131	PRO	N-CD-CG	-8.82	89.96	103.20
1	10-A	42	ALA	N-CA-CB	-8.82	97.75	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-A	117	GLU	OE1-CD-OE2	8.82	133.89	123.30
1	14-A	45	TYR	CG-CD1-CE1	8.82	128.36	121.30
1	10-A	97	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	15-A	106	ARG	CB-CG-CD	-8.82	88.68	111.60
1	16-A	109	SER	N-CA-CB	-8.82	97.28	110.50
1	10-A	100	THR	N-CA-C	-8.81	87.22	111.00
1	14-A	128	ARG	CG-CD-NE	-8.81	93.30	111.80
1	13-A	138	LEU	CB-CG-CD1	-8.80	96.04	111.00
1	15-A	126	ILE	C-N-CA	-8.80	99.69	121.70
1	4-A	121	TRP	CE3-CZ3-CH2	-8.79	111.53	121.20
1	14-A	141	ARG	NH1-CZ-NH2	-8.77	109.75	119.40
1	8-A	140	TRP	CH2-CZ2-CE2	8.76	126.16	117.40
1	16-A	136	MET	O-C-N	8.76	136.72	122.70
1	11-A	61	LEU	CA-CB-CG	-8.76	95.15	115.30
1	6-A	97	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	7-A	140	TRP	CG-CD1-NE1	-8.76	101.34	110.10
1	1-A	48	TYR	CG-CD2-CE2	8.75	128.30	121.30
1	12-A	47	ASP	CB-CG-OD1	8.75	126.17	118.30
1	16-A	41	ARG	O-C-N	8.75	136.69	122.70
1	14-A	89	LEU	C-N-CA	-8.74	99.84	121.70
1	13-A	39	LEU	CB-CG-CD2	8.74	125.86	111.00
1	1-A	61	LEU	CA-CB-CG	-8.74	95.20	115.30
1	4-A	146	TYR	CG-CD2-CE2	-8.74	114.31	121.30
1	14-A	89	LEU	O-C-N	8.73	136.68	122.70
1	10-A	143	ASP	CB-CG-OD1	8.73	126.16	118.30
1	16-A	86	THR	O-C-N	8.73	136.67	122.70
1	5-A	97	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	16-A	131	PRO	N-CD-CG	-8.73	90.10	103.20
1	3-A	70	LEU	CB-CG-CD2	-8.73	96.16	111.00
1	12-A	97	ARG	O-C-N	8.73	136.66	122.70
1	9-A	124	GLU	CA-C-O	-8.71	101.81	120.10
1	3-A	45	TYR	CZ-CE2-CD2	-8.70	111.97	119.80
1	15-A	109	SER	CA-CB-OG	-8.69	87.73	111.20
1	15-A	92	ARG	C-N-CA	-8.68	100.01	121.70
1	9-A	93	TRP	CH2-CZ2-CE2	-8.67	108.73	117.40
1	15-A	53	PRO	CA-CB-CG	-8.67	87.53	104.00
1	1-A	64	PHE	CB-CA-C	-8.66	93.07	110.40
1	13-A	44	MET	N-CA-CB	8.66	126.19	110.60
1	16-A	82	LEU	N-CA-CB	8.66	127.72	110.40
1	2-A	77	LEU	CB-CG-CD2	-8.66	96.29	111.00
1	2-A	146	TYR	CD1-CG-CD2	8.65	127.42	117.90
1	13-A	97	ARG	O-C-N	8.65	136.55	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16-A	89	LEU	CB-CA-C	-8.65	93.76	110.20
1	9-A	146	TYR	CB-CG-CD1	-8.63	115.82	121.00
1	15-A	37	SER	CA-CB-OG	-8.63	87.91	111.20
1	16-A	97	ARG	O-C-N	8.63	136.50	122.70
1	11-A	118	ALA	CA-C-O	-8.62	101.99	120.10
1	3-A	53	PRO	N-CD-CG	-8.62	90.27	103.20
1	3-A	97	ARG	CB-CG-CD	-8.62	89.18	111.60
1	9-A	127	HIS	CA-C-O	-8.61	102.01	120.10
1	13-A	40	ARG	NH1-CZ-NH2	8.61	128.87	119.40
1	9-A	128	ARG	CG-CD-NE	-8.60	93.74	111.80
1	9-A	146	TYR	CB-CG-CD2	-8.59	115.85	121.00
1	15-A	98	PHE	CG-CD1-CE1	8.59	130.25	120.80
1	14-A	126	ILE	C-N-CA	-8.58	100.25	121.70
1	10-A	48	TYR	CZ-CE2-CD2	-8.58	112.08	119.80
1	11-A	81	PRO	CA-C-N	-8.57	98.34	117.20
1	9-A	128	ARG	CD-NE-CZ	-8.57	111.61	123.60
1	13-A	152	PRO	N-CD-CG	-8.56	90.36	103.20
1	14-A	52	VAL	CG1-CB-CG2	-8.55	97.22	110.90
1	15-A	106	ARG	C-N-CA	-8.55	100.33	121.70
1	11-A	48	TYR	CZ-CE2-CD2	-8.54	112.11	119.80
1	13-A	67	TRP	CD1-CG-CD2	8.54	113.14	106.30
1	15-A	83	HIS	CB-CA-C	8.54	127.48	110.40
1	9-A	108	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	7-A	97	ARG	CB-CG-CD	-8.53	89.42	111.60
1	8-A	72	ILE	CA-CB-CG2	-8.53	93.84	110.90
1	8-A	141	ARG	NE-CZ-NH1	-8.52	116.04	120.30
1	16-A	149	PHE	CG-CD1-CE1	-8.51	111.43	120.80
1	3-A	48	TYR	CZ-CE2-CD2	-8.51	112.14	119.80
1	5-A	84	TYR	CB-CG-CD1	-8.51	115.90	121.00
1	14-A	88	VAL	CA-CB-CG2	-8.50	98.15	110.90
1	16-A	142	SER	CB-CA-C	-8.50	93.94	110.10
1	3-A	99	GLY	O-C-N	-8.50	109.10	122.70
1	6-A	97	ARG	O-C-N	8.50	136.30	122.70
1	10-A	121	TRP	O-C-N	8.49	136.29	122.70
1	16-A	93	TRP	CD1-NE1-CE2	8.49	116.64	109.00
1	6-A	153	ILE	CA-CB-CG1	-8.49	94.87	111.00
1	15-A	92	ARG	CA-C-O	-8.48	102.28	120.10
1	1-A	61	LEU	CD1-CG-CD2	-8.48	85.06	110.50
1	1-A	78	TYR	CB-CG-CD1	-8.47	115.92	121.00
1	11-A	143	ASP	CB-CG-OD1	8.47	125.92	118.30
1	14-A	48	TYR	CB-CG-CD1	8.46	126.08	121.00
1	16-A	106	ARG	NE-CZ-NH1	-8.47	116.07	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	97	ARG	O-C-N	8.46	136.24	122.70
1	8-A	50	LYS	CB-CG-CD	-8.46	89.61	111.60
1	9-A	154	PHE	CZ-CE2-CD2	8.46	130.25	120.10
1	15-A	147	HIS	N-CA-CB	-8.46	95.38	110.60
1	2-A	89	LEU	CB-CG-CD2	-8.45	96.63	111.00
1	6-A	73	SER	CA-C-N	-8.44	98.64	117.20
1	2-A	129	LEU	CD1-CG-CD2	-8.43	85.21	110.50
1	1-A	92	ARG	NH1-CZ-NH2	8.43	128.67	119.40
1	15-A	84	TYR	N-CA-C	-8.43	88.25	111.00
1	2-A	43	GLU	OE1-CD-OE2	8.41	133.40	123.30
1	5-A	97	ARG	O-C-N	8.41	136.15	122.70
1	12-A	97	ARG	CD-NE-CZ	-8.41	111.83	123.60
1	6-A	143	ASP	CB-CG-OD1	8.40	125.86	118.30
1	15-A	67	TRP	CB-CG-CD1	-8.40	116.07	127.00
1	2-A	48	TYR	CZ-CE2-CD2	-8.40	112.24	119.80
1	4-A	65	THR	CA-CB-CG2	-8.40	100.64	112.40
1	10-A	67	TRP	CG-CD2-CE3	-8.40	126.34	133.90
1	11-A	62	ILE	N-CA-C	8.39	133.67	111.00
1	10-A	139	LEU	CB-CG-CD1	-8.39	96.73	111.00
1	15-A	127	HIS	N-CA-CB	-8.38	95.52	110.60
1	1-A	109	SER	CB-CA-C	-8.38	94.19	110.10
1	14-A	136	MET	C-N-CA	-8.37	100.77	121.70
1	10-A	121	TRP	CA-C-N	-8.37	98.78	117.20
1	16-A	89	LEU	N-CA-C	-8.37	88.39	111.00
1	7-A	36	GLY	N-CA-C	8.37	134.02	113.10
1	9-A	76	GLN	CG-CD-OE1	-8.36	104.88	121.60
1	15-A	81	PRO	CA-C-O	8.36	140.26	120.20
1	1-A	38	LEU	O-C-N	-8.35	109.34	122.70
1	3-A	98	PHE	O-C-N	-8.35	109.00	123.20
1	16-A	47	ASP	CA-C-O	-8.35	102.56	120.10
1	4-A	64	PHE	CB-CA-C	-8.35	93.71	110.40
1	5-A	52	VAL	CA-CB-CG2	-8.35	98.38	110.90
1	15-A	40	ARG	NH1-CZ-NH2	8.34	128.58	119.40
1	3-A	91	GLN	CA-CB-CG	-8.34	95.05	113.40
1	15-A	104	GLU	OE1-CD-OE2	8.34	133.31	123.30
1	16-A	145	MET	CA-CB-CG	-8.34	99.12	113.30
1	8-A	73	SER	N-CA-CB	8.33	122.99	110.50
1	3-A	108	ASP	OD1-CG-OD2	8.33	139.12	123.30
1	8-A	48	TYR	CG-CD2-CE2	8.33	127.96	121.30
1	16-A	67	TRP	N-CA-CB	-8.32	95.61	110.60
1	6-A	48	TYR	CZ-CE2-CD2	-8.32	112.31	119.80
1	5-A	89	LEU	CB-CG-CD2	-8.32	96.85	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16-A	115	LYS	CA-CB-CG	-8.32	95.10	113.40
1	7-A	76	GLN	O-C-N	-8.31	109.40	122.70
1	14-A	80	GLN	CA-CB-CG	-8.31	95.12	113.40
1	14-A	81	PRO	O-C-N	8.31	135.99	122.70
1	11-A	78	TYR	CD1-CG-CD2	8.30	127.03	117.90
1	16-A	123	VAL	CA-CB-CG2	-8.31	98.44	110.90
1	12-A	45	TYR	CG-CD2-CE2	-8.30	114.66	121.30
1	9-A	61	LEU	CB-CG-CD1	8.30	125.11	111.00
1	16-A	71	SER	O-C-N	8.30	135.98	122.70
1	13-A	65	THR	CA-CB-CG2	-8.28	100.80	112.40
1	14-A	85	LEU	C-N-CA	-8.27	101.02	121.70
1	3-A	80	GLN	CA-CB-CG	-8.27	95.21	113.40
1	12-A	53	PRO	N-CD-CG	-8.26	90.81	103.20
1	6-A	109	SER	CA-CB-OG	-8.26	88.90	111.20
1	9-A	139	LEU	CB-CG-CD1	-8.26	96.96	111.00
1	10-A	67	TRP	CD2-CE3-CZ3	-8.26	108.07	118.80
1	11-A	114	THR	CA-CB-CG2	-8.26	100.84	112.40
1	7-A	63	PRO	N-CD-CG	-8.25	90.83	103.20
1	8-A	48	TYR	CZ-CE2-CD2	-8.25	112.38	119.80
1	13-A	92	ARG	CD-NE-CZ	-8.25	112.05	123.60
1	13-A	148	SER	C-N-CA	-8.25	101.08	121.70
1	4-A	73	SER	N-CA-CB	-8.24	98.14	110.50
1	2-A	76	GLN	CA-CB-CG	8.23	131.50	113.40
1	4-A	55	PRO	CB-CA-C	-8.23	91.44	112.00
1	4-A	70	LEU	C-N-CA	-8.23	101.13	121.70
1	14-A	125	GLU	C-N-CA	-8.23	101.14	121.70
1	11-A	113	PRO	CA-CB-CG	-8.22	88.37	104.00
1	12-A	154	PHE	CB-CG-CD2	8.22	126.55	120.80
1	14-A	115	LYS	CA-CB-CG	-8.22	95.32	113.40
1	15-A	126	ILE	N-CA-C	8.22	133.19	111.00
1	16-A	87	ASN	O-C-N	8.19	135.81	122.70
1	11-A	87	ASN	CB-CG-OD1	-8.18	105.24	121.60
1	16-A	73	SER	CB-CA-C	-8.18	94.56	110.10
1	13-A	84	TYR	CG-CD1-CE1	8.17	127.84	121.30
1	13-A	136	MET	C-N-CA	-8.17	101.28	121.70
1	9-A	80	GLN	CA-CB-CG	-8.16	95.44	113.40
1	16-A	67	TRP	CG-CD1-NE1	-8.16	101.94	110.10
1	12-A	150	ILE	CB-CG1-CD1	-8.16	91.06	113.90
1	1-A	45	TYR	CB-CG-CD1	-8.15	116.11	121.00
1	2-A	108	ASP	CB-CG-OD1	-8.15	110.97	118.30
1	13-A	124	GLU	CG-CD-OE1	8.15	134.60	118.30
1	11-A	63	PRO	C-N-CA	-8.14	101.34	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	62	ILE	CB-CG1-CD1	-8.14	91.11	113.90
1	2-A	91	GLN	CA-C-N	-8.14	99.29	117.20
1	9-A	62	ILE	CB-CG1-CD1	-8.14	91.12	113.90
1	15-A	107	LEU	N-CA-CB	-8.14	94.12	110.40
1	6-A	61	LEU	CB-CA-C	8.13	125.66	110.20
1	14-A	106	ARG	CD-NE-CZ	8.13	134.98	123.60
1	11-A	41	ARG	CA-CB-CG	8.12	131.27	113.40
1	9-A	131	PRO	O-C-N	8.12	135.69	122.70
1	2-A	122	LEU	CB-CG-CD2	8.12	124.80	111.00
1	3-A	97	ARG	O-C-N	8.12	135.69	122.70
1	9-A	132	SER	C-N-CA	-8.12	101.41	121.70
1	7-A	146	TYR	CB-CG-CD1	-8.11	116.13	121.00
1	13-A	54	ILE	CG1-CB-CG2	8.11	129.24	111.40
1	10-A	120	ILE	CA-CB-CG1	-8.11	95.59	111.00
1	14-A	124	GLU	C-N-CA	-8.11	101.43	121.70
1	3-A	98	PHE	CG-CD1-CE1	8.11	129.72	120.80
1	10-A	150	ILE	CG1-CB-CG2	8.10	129.21	111.40
1	6-A	57	ASN	O-C-N	8.09	135.65	122.70
1	4-A	106	ARG	NE-CZ-NH1	-8.09	116.26	120.30
1	10-A	50	LYS	CD-CE-NZ	-8.08	93.11	111.70
1	9-A	77	LEU	C-N-CA	-8.08	101.50	121.70
1	12-A	64	PHE	CB-CG-CD1	-8.08	115.15	120.80
1	15-A	70	LEU	CB-CG-CD2	-8.08	97.27	111.00
1	4-A	40	ARG	CA-C-O	-8.07	103.15	120.10
1	5-A	47	ASP	O-C-N	8.07	135.62	122.70
1	14-A	97	ARG	CA-C-O	-8.07	103.15	120.10
1	15-A	98	PHE	CB-CG-CD1	8.07	126.45	120.80
1	15-A	151	ASP	O-C-N	8.07	136.43	121.10
1	4-A	146	TYR	CD1-CG-CD2	8.07	126.77	117.90
1	7-A	57	ASN	O-C-N	8.07	135.61	122.70
1	13-A	136	MET	CB-CA-C	-8.07	94.27	110.40
1	16-A	93	TRP	NE1-CE2-CD2	8.07	115.37	107.30
1	15-A	97	ARG	O-C-N	8.06	135.60	122.70
1	15-A	86	THR	CA-CB-CG2	-8.05	101.13	112.40
1	3-A	40	ARG	CA-CB-CG	-8.05	95.70	113.40
1	4-A	128	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	16-A	47	ASP	CB-CG-OD1	8.04	125.54	118.30
1	15-A	67	TRP	CA-CB-CG	-8.04	98.43	113.70
1	3-A	45	TYR	CG-CD2-CE2	8.03	127.72	121.30
1	14-A	97	ARG	CG-CD-NE	-8.03	94.94	111.80
1	14-A	137	ALA	N-CA-CB	8.02	121.33	110.10
1	16-A	90	LEU	CB-CG-CD1	-8.02	97.37	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	14-A	117	GLU	C-N-CA	-8.02	101.66	121.70
1	15-A	58	ARG	NE-CZ-NH1	-8.02	116.29	120.30
1	1-A	61	LEU	CB-CG-CD1	8.01	124.62	111.00
1	9-A	106	ARG	NH1-CZ-NH2	-8.00	110.60	119.40
1	3-A	92	ARG	CA-C-O	-8.00	103.30	120.10
1	1-A	38	LEU	CB-CG-CD2	-8.00	97.40	111.00
1	3-A	41	ARG	CA-CB-CG	7.99	130.98	113.40
1	5-A	45	TYR	CB-CG-CD1	7.99	125.79	121.00
1	14-A	39	LEU	CB-CG-CD1	-7.99	97.42	111.00
1	8-A	97	ARG	O-C-N	7.98	135.47	122.70
1	3-A	96	SER	CA-CB-OG	-7.98	89.65	111.20
1	14-A	113	PRO	N-CD-CG	-7.98	91.23	103.20
1	16-A	114	THR	CA-CB-CG2	-7.97	101.24	112.40
1	8-A	38	LEU	O-C-N	-7.96	109.96	122.70
1	16-A	154	PHE	CB-CG-CD1	-7.96	115.23	120.80
1	10-A	140	TRP	CD1-NE1-CE2	7.95	116.16	109.00
1	3-A	146	TYR	CB-CG-CD1	-7.95	116.23	121.00
1	9-A	61	LEU	CB-CG-CD2	-7.95	97.49	111.00
1	5-A	37	SER	CA-CB-OG	7.94	132.65	111.20
1	3-A	91	GLN	CB-CG-CD	-7.94	90.96	111.60
1	13-A	125	GLU	CG-CD-OE1	7.93	134.17	118.30
1	10-A	43	GLU	CB-CG-CD	-7.92	92.81	114.20
1	3-A	47	ASP	CB-CG-OD2	-7.92	111.18	118.30
1	9-A	49	MET	CA-CB-CG	7.91	126.75	113.30
1	16-A	53	PRO	N-CD-CG	-7.91	91.33	103.20
1	14-A	107	LEU	CB-CA-C	-7.91	95.17	110.20
1	14-A	122	LEU	CA-CB-CG	-7.91	97.11	115.30
1	10-A	46	GLN	CB-CG-CD	7.91	132.16	111.60
1	14-A	137	ALA	CB-CA-C	-7.90	98.25	110.10
1	3-A	147	HIS	C-N-CA	-7.90	101.96	121.70
1	16-A	36	GLY	N-CA-C	7.89	132.83	113.10
1	14-A	84	TYR	CG-CD2-CE2	-7.89	114.99	121.30
1	3-A	97	ARG	CA-CB-CG	-7.89	96.05	113.40
1	3-A	98	PHE	CZ-CE2-CD2	-7.89	110.64	120.10
1	8-A	38	LEU	CB-CG-CD1	-7.89	97.59	111.00
1	1-A	128	ARG	CG-CD-NE	-7.88	95.26	111.80
1	2-A	47	ASP	CA-C-O	-7.88	103.56	120.10
1	3-A	40	ARG	NH1-CZ-NH2	7.87	128.06	119.40
1	1-A	91	GLN	CA-CB-CG	-7.87	96.09	113.40
1	9-A	98	PHE	C-N-CA	-7.87	105.78	122.30
1	16-A	85	LEU	CB-CA-C	-7.86	95.26	110.20
1	5-A	45	TYR	CG-CD2-CE2	-7.86	115.01	121.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	11-A	112	HIS	CB-CA-C	-7.86	94.68	110.40
1	14-A	41	ARG	O-C-N	7.86	135.27	122.70
1	8-A	38	LEU	CB-CG-CD2	-7.86	97.64	111.00
1	5-A	40	ARG	CG-CD-NE	-7.85	95.31	111.80
1	7-A	78	TYR	CA-CB-CG	-7.85	98.48	113.40
1	8-A	147	HIS	C-N-CA	-7.85	102.07	121.70
1	15-A	117	GLU	CB-CA-C	7.85	126.10	110.40
1	10-A	146	TYR	CB-CG-CD2	-7.84	116.29	121.00
1	2-A	41	ARG	O-C-N	7.84	135.24	122.70
1	6-A	70	LEU	CB-CG-CD2	-7.84	97.67	111.00
1	13-A	133	HIS	CA-C-O	-7.84	103.64	120.10
1	14-A	85	LEU	CA-CB-CG	-7.83	97.30	115.30
1	10-A	108	ASP	OD1-CG-OD2	7.82	138.16	123.30
1	15-A	140	TRP	C-N-CA	-7.82	102.14	121.70
1	2-A	64	PHE	CG-CD1-CE1	-7.82	112.20	120.80
1	7-A	97	ARG	C-N-CA	-7.82	102.16	121.70
1	5-A	146	TYR	CD1-CG-CD2	7.81	126.49	117.90
1	15-A	97	ARG	C-N-CA	-7.81	102.17	121.70
1	7-A	41	ARG	O-C-N	7.81	135.19	122.70
1	15-A	146	TYR	CB-CG-CD1	-7.81	116.31	121.00
1	16-A	81	PRO	CB-CA-C	-7.81	92.48	112.00
1	5-A	89	LEU	CA-CB-CG	-7.81	97.34	115.30
1	1-A	128	ARG	N-CA-CB	-7.80	96.56	110.60
1	7-A	41	ARG	CD-NE-CZ	-7.80	112.68	123.60
1	10-A	128	ARG	CA-CB-CG	-7.80	96.25	113.40
1	2-A	140	TRP	C-N-CA	-7.79	102.21	121.70
1	10-A	68	VAL	CA-CB-CG1	-7.79	99.22	110.90
1	2-A	88	VAL	CA-CB-CG2	-7.79	99.22	110.90
1	16-A	39	LEU	CB-CG-CD2	7.78	124.23	111.00
1	14-A	67	TRP	CG-CD1-NE1	-7.78	102.32	110.10
1	12-A	41	ARG	O-C-N	7.78	135.15	122.70
1	9-A	67	TRP	CG-CD2-CE3	-7.77	126.91	133.90
1	14-A	106	ARG	NH1-CZ-NH2	-7.76	110.86	119.40
1	8-A	45	TYR	CZ-CE2-CD2	-7.76	112.82	119.80
1	12-A	89	LEU	CB-CG-CD2	-7.76	97.81	111.00
1	10-A	45	TYR	CG-CD1-CE1	7.75	127.50	121.30
1	9-A	44	MET	CA-CB-CG	-7.75	100.12	113.30
1	16-A	146	TYR	CA-C-O	7.75	136.37	120.10
1	7-A	97	ARG	CG-CD-NE	7.74	128.06	111.80
1	11-A	128	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	16-A	50	LYS	CG-CD-CE	-7.74	88.68	111.90
1	11-A	97	ARG	O-C-N	7.73	135.07	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	11-A	47	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	7-A	45	TYR	CG-CD2-CE2	-7.73	115.12	121.30
1	13-A	121	TRP	O-C-N	7.73	135.06	122.70
1	4-A	67	TRP	CE2-CD2-CE3	7.72	127.97	118.70
1	15-A	85	LEU	N-CA-CB	-7.72	94.95	110.40
1	12-A	138	LEU	CB-CG-CD2	-7.72	97.88	111.00
1	4-A	116	ALA	O-C-N	7.71	135.04	122.70
1	13-A	107	LEU	CA-C-O	-7.71	103.91	120.10
1	16-A	115	LYS	CG-CD-CE	-7.71	88.77	111.90
1	16-A	78	TYR	CG-CD2-CE2	-7.71	115.13	121.30
1	13-A	101	ASP	CB-CG-OD1	-7.71	111.36	118.30
1	13-A	50	LYS	CG-CD-CE	-7.71	88.78	111.90
1	3-A	43	GLU	OE1-CD-OE2	7.70	132.54	123.30
1	15-A	58	ARG	CB-CG-CD	-7.70	91.58	111.60
1	16-A	146	TYR	O-C-N	-7.69	110.39	122.70
1	15-A	53	PRO	CA-N-CD	7.69	122.46	111.70
1	3-A	150	ILE	CB-CG1-CD1	-7.68	92.38	113.90
1	16-A	122	LEU	CA-CB-CG	-7.68	97.63	115.30
1	13-A	148	SER	CB-CA-C	7.68	124.69	110.10
1	14-A	70	LEU	CB-CG-CD1	-7.68	97.94	111.00
1	15-A	98	PHE	N-CA-CB	-7.68	96.78	110.60
1	8-A	52	VAL	CA-CB-CG2	-7.67	99.39	110.90
1	16-A	78	TYR	CZ-CE2-CD2	7.67	126.71	119.80
1	14-A	85	LEU	CB-CG-CD2	-7.67	97.97	111.00
1	14-A	135	HIS	CB-CA-C	-7.67	95.07	110.40
1	14-A	124	GLU	CA-CB-CG	-7.66	96.54	113.40
1	5-A	50	LYS	N-CA-CB	-7.66	96.82	110.60
1	15-A	87	ASN	CB-CG-OD1	-7.65	106.30	121.60
1	7-A	96	SER	N-CA-C	-7.64	90.36	111.00
1	16-A	110	ILE	CG1-CB-CG2	7.64	128.20	111.40
1	13-A	49	MET	CB-CA-C	-7.64	95.13	110.40
1	10-A	100	THR	OG1-CB-CG2	7.63	127.56	110.00
1	2-A	81	PRO	CA-C-N	-7.63	100.42	117.20
1	11-A	36	GLY	N-CA-C	-7.63	94.03	113.10
1	2-A	131	PRO	CA-CB-CG	-7.62	89.53	104.00
1	9-A	45	TYR	CB-CG-CD1	7.62	125.57	121.00
1	1-A	40	ARG	N-CA-CB	7.61	124.30	110.60
1	3-A	72	ILE	CG1-CB-CG2	-7.61	94.66	111.40
1	6-A	72	ILE	CA-C-O	-7.60	104.13	120.10
1	2-A	36	GLY	CA-C-O	-7.60	106.92	120.60
1	3-A	91	GLN	N-CA-CB	-7.59	96.93	110.60
1	16-A	107	LEU	CA-C-O	-7.59	104.15	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	106	ARG	O-C-N	7.59	134.85	122.70
1	9-A	123	VAL	N-CA-CB	7.59	128.20	111.50
1	2-A	98	PHE	CZ-CE2-CD2	-7.59	111.00	120.10
1	7-A	78	TYR	CZ-CE2-CD2	7.59	126.63	119.80
1	3-A	94	ASP	CB-CG-OD2	-7.57	111.48	118.30
1	14-A	98	PHE	CA-C-N	-7.57	101.06	116.20
1	9-A	124	GLU	CA-C-N	7.57	133.85	117.20
1	12-A	80	GLN	CB-CA-C	-7.57	95.26	110.40
1	16-A	113	PRO	CA-CB-CG	-7.56	89.63	104.00
1	6-A	78	TYR	CD1-CE1-CZ	7.56	126.60	119.80
1	9-A	153	ILE	CA-CB-CG1	-7.55	96.65	111.00
1	15-A	118	ALA	CB-CA-C	7.55	121.43	110.10
1	12-A	146	TYR	CD1-CG-CD2	7.54	126.20	117.90
1	14-A	106	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	14-A	65	THR	CA-CB-CG2	-7.53	101.85	112.40
1	11-A	109	SER	N-CA-CB	-7.53	99.20	110.50
1	9-A	64	PHE	CB-CG-CD2	7.53	126.07	120.80
1	15-A	92	ARG	O-C-N	7.52	134.74	122.70
1	1-A	40	ARG	CA-CB-CG	-7.52	96.85	113.40
1	15-A	50	LYS	CG-CD-CE	-7.52	89.33	111.90
1	13-A	78	TYR	CD1-CE1-CZ	-7.52	113.03	119.80
1	9-A	41	ARG	O-C-N	7.52	134.73	122.70
1	16-A	147	HIS	CB-CA-C	-7.52	95.36	110.40
1	3-A	99	GLY	C-N-CA	-7.51	102.91	121.70
1	14-A	65	THR	CA-C-O	-7.51	104.32	120.10
1	5-A	45	TYR	CB-CG-CD2	-7.51	116.49	121.00
1	8-A	55	PRO	CA-N-CD	7.51	122.22	111.70
1	1-A	44	MET	N-CA-CB	7.51	124.12	110.60
1	2-A	74	MET	CA-C-O	-7.51	104.33	120.10
1	4-A	67	TRP	NE1-CE2-CZ2	7.51	138.66	130.40
1	14-A	48	TYR	CB-CG-CD2	-7.51	116.50	121.00
1	1-A	80	GLN	CB-CA-C	-7.50	95.39	110.40
1	3-A	151	ASP	OD1-CG-OD2	-7.50	109.05	123.30
1	5-A	47	ASP	CA-C-O	-7.50	104.35	120.10
1	15-A	109	SER	N-CA-CB	-7.50	99.25	110.50
1	15-A	71	SER	O-C-N	7.49	134.69	122.70
1	1-A	134	LEU	CB-CG-CD2	-7.48	98.28	111.00
1	8-A	40	ARG	CD-NE-CZ	7.48	134.08	123.60
1	15-A	58	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	9-A	132	SER	CA-C-N	-7.48	100.74	117.20
1	11-A	38	LEU	C-N-CA	-7.48	103.00	121.70
1	16-A	84	TYR	O-C-N	-7.48	110.73	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	11-A	50	LYS	CD-CE-NZ	7.48	128.90	111.70
1	13-A	136	MET	CA-CB-CG	7.48	126.02	113.30
1	16-A	43	GLU	CG-CD-OE2	-7.48	103.35	118.30
1	7-A	48	TYR	CG-CD2-CE2	7.47	127.28	121.30
1	4-A	67	TRP	CD2-CE3-CZ3	-7.47	109.09	118.80
1	15-A	48	TYR	CD1-CE1-CZ	7.46	126.52	119.80
1	14-A	54	ILE	CB-CA-C	-7.46	96.67	111.60
1	8-A	49	MET	CA-CB-CG	-7.45	100.64	113.30
1	7-A	154	PHE	CZ-CE2-CD2	7.45	129.04	120.10
1	10-A	70	LEU	CB-CG-CD2	-7.45	98.34	111.00
1	15-A	41	ARG	NH1-CZ-NH2	7.45	127.59	119.40
1	12-A	128	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	10-A	97	ARG	O-C-N	7.44	134.61	122.70
1	1-A	121	TRP	CB-CG-CD2	7.44	136.27	126.60
1	14-A	98	PHE	C-N-CA	-7.44	106.67	122.30
1	8-A	130	THR	CA-C-O	-7.44	104.48	120.10
1	15-A	55	PRO	CA-C-N	-7.43	100.84	117.20
1	3-A	98	PHE	C-N-CA	-7.43	106.70	122.30
1	9-A	143	ASP	CB-CG-OD1	7.43	124.99	118.30
1	4-A	151	ASP	N-CA-CB	-7.43	97.23	110.60
1	3-A	84	TYR	CB-CG-CD2	-7.42	116.55	121.00
1	10-A	45	TYR	CB-CG-CD1	7.42	125.45	121.00
1	11-A	154	PHE	CG-CD1-CE1	7.42	128.97	120.80
1	4-A	79	GLY	N-CA-C	7.42	131.65	113.10
1	3-A	80	GLN	CB-CA-C	-7.41	95.58	110.40
1	16-A	141	ARG	NH1-CZ-NH2	7.41	127.55	119.40
1	2-A	75	LYS	N-CA-CB	-7.41	97.27	110.60
1	2-A	137	ALA	N-CA-CB	-7.41	99.73	110.10
1	4-A	76	GLN	CA-C-O	-7.41	104.55	120.10
1	13-A	80	GLN	CB-CA-C	-7.40	95.59	110.40
1	15-A	67	TRP	CB-CG-CD2	7.40	136.22	126.60
1	13-A	64	PHE	CG-CD2-CE2	-7.39	112.67	120.80
1	11-A	134	LEU	CB-CG-CD2	-7.39	98.44	111.00
1	14-A	89	LEU	CB-CG-CD2	-7.39	98.44	111.00
1	13-A	101	ASP	CB-CG-OD2	7.39	124.95	118.30
1	10-A	84	TYR	CZ-CE2-CD2	7.39	126.45	119.80
1	3-A	125	GLU	CG-CD-OE1	7.39	133.07	118.30
1	14-A	80	GLN	CB-CA-C	-7.38	95.63	110.40
1	10-A	128	ARG	N-CA-C	-7.37	91.11	111.00
1	10-A	139	LEU	CA-CB-CG	-7.36	98.38	115.30
1	16-A	86	THR	C-N-CA	-7.36	103.31	121.70
1	1-A	146	TYR	CD1-CG-CD2	7.35	125.99	117.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13-A	124	GLU	OE1-CD-OE2	-7.35	114.48	123.30
1	10-A	131	PRO	CA-C-N	-7.35	101.03	117.20
1	16-A	146	TYR	CE1-CZ-CE2	7.35	131.55	119.80
1	6-A	78	TYR	CA-CB-CG	-7.34	99.45	113.40
1	10-A	141	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	15-A	132	SER	N-CA-CB	-7.34	99.49	110.50
1	5-A	109	SER	CA-CB-OG	-7.33	91.41	111.20
1	9-A	115	LYS	CA-CB-CG	-7.32	97.29	113.40
1	5-A	89	LEU	C-N-CA	-7.31	103.42	121.70
1	11-A	152	PRO	N-CD-CG	-7.31	92.23	103.20
1	8-A	108	ASP	OD1-CG-OD2	7.30	137.18	123.30
1	10-A	116	ALA	O-C-N	-7.30	111.03	122.70
1	4-A	97	ARG	CA-C-O	-7.29	104.78	120.10
1	6-A	47	ASP	CA-C-O	-7.29	104.78	120.10
1	4-A	77	LEU	O-C-N	7.29	134.36	122.70
1	16-A	91	GLN	N-CA-CB	-7.29	97.49	110.60
1	16-A	48	TYR	CB-CG-CD2	7.28	125.37	121.00
1	14-A	126	ILE	CA-CB-CG1	-7.28	97.17	111.00
1	10-A	80	GLN	CB-CA-C	-7.28	95.85	110.40
1	1-A	112	HIS	CA-CB-CG	-7.28	101.23	113.60
1	3-A	96	SER	N-CA-CB	-7.28	99.59	110.50
1	9-A	97	ARG	CA-C-O	-7.28	104.82	120.10
1	4-A	93	TRP	CH2-CZ2-CE2	-7.27	110.13	117.40
1	4-A	47	ASP	CA-C-O	-7.25	104.87	120.10
1	2-A	37	SER	CA-CB-OG	-7.25	91.63	111.20
1	15-A	142	SER	CA-CB-OG	-7.24	91.64	111.20
1	2-A	98	PHE	C-N-CA	-7.24	107.09	122.30
1	11-A	108	ASP	OD1-CG-OD2	7.24	137.06	123.30
1	9-A	93	TRP	CB-CG-CD2	7.24	136.01	126.60
1	13-A	62	ILE	CG1-CB-CG2	7.24	127.32	111.40
1	3-A	152	PRO	N-CD-CG	-7.24	92.35	103.20
1	5-A	67	TRP	NE1-CE2-CZ2	7.23	138.35	130.40
1	4-A	118	ALA	CA-C-N	-7.23	101.29	117.20
1	5-A	45	TYR	C-N-CA	-7.23	103.63	121.70
1	2-A	141	ARG	NE-CZ-NH1	-7.22	116.69	120.30
1	12-A	41	ARG	CD-NE-CZ	-7.22	113.49	123.60
1	10-A	53	PRO	N-CD-CG	-7.22	92.37	103.20
1	14-A	71	SER	O-C-N	7.22	134.25	122.70
1	16-A	89	LEU	O-C-N	-7.22	111.15	122.70
1	2-A	67	TRP	CG-CD1-NE1	-7.21	102.89	110.10
1	12-A	65	THR	CA-CB-CG2	-7.21	102.30	112.40
1	11-A	151	ASP	CB-CG-OD2	7.21	124.79	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	145	MET	CG-SD-CE	7.21	111.73	100.20
1	15-A	58	ARG	CG-CD-NE	-7.21	96.66	111.80
1	4-A	79	GLY	C-N-CA	-7.21	103.68	121.70
1	10-A	121	TRP	CD1-NE1-CE2	-7.21	102.51	109.00
1	14-A	107	LEU	CB-CG-CD1	-7.20	98.76	111.00
1	4-A	124	GLU	N-CA-CB	-7.20	97.64	110.60
1	13-A	40	ARG	CD-NE-CZ	7.19	133.67	123.60
1	5-A	44	MET	C-N-CA	-7.19	103.73	121.70
1	2-A	115	LYS	CA-CB-CG	-7.19	97.59	113.40
1	15-A	113	PRO	CA-C-O	-7.18	102.96	120.20
1	9-A	86	THR	O-C-N	7.18	134.18	122.70
1	15-A	40	ARG	CD-NE-CZ	7.18	133.65	123.60
1	15-A	84	TYR	O-C-N	7.17	134.18	122.70
1	15-A	49	MET	CG-SD-CE	-7.16	88.74	100.20
1	2-A	64	PHE	CB-CG-CD2	7.16	125.81	120.80
1	8-A	43	GLU	CG-CD-OE1	-7.16	103.98	118.30
1	15-A	75	LYS	O-C-N	7.16	134.15	122.70
1	14-A	37	SER	CA-CB-OG	-7.15	91.89	111.20
1	14-A	43	GLU	CG-CD-OE2	-7.15	104.00	118.30
1	5-A	118	ALA	CA-C-O	-7.15	105.09	120.10
1	1-A	108	ASP	O-C-N	-7.14	111.27	122.70
1	15-A	50	LYS	CB-CG-CD	-7.14	93.04	111.60
1	14-A	48	TYR	CD1-CE1-CZ	7.14	126.22	119.80
1	14-A	140	TRP	O-C-N	7.14	134.12	122.70
1	16-A	52	VAL	CG1-CB-CG2	7.14	122.32	110.90
1	15-A	112	HIS	CG-ND1-CE1	7.13	118.18	108.20
1	8-A	97	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	12-A	98	PHE	C-N-CA	-7.13	107.33	122.30
1	13-A	93	TRP	CE3-CZ3-CH2	-7.12	113.37	121.20
1	10-A	40	ARG	CG-CD-NE	-7.11	96.88	111.80
1	14-A	45	TYR	CD1-CG-CD2	7.11	125.72	117.90
1	10-A	57	ASN	O-C-N	7.11	134.07	122.70
1	15-A	107	LEU	CA-C-O	-7.10	105.18	120.10
1	15-A	117	GLU	OE1-CD-OE2	7.10	131.82	123.30
1	12-A	112	HIS	O-C-N	-7.10	107.61	121.10
1	14-A	68	VAL	CG1-CB-CG2	7.10	122.26	110.90
1	2-A	136	MET	N-CA-CB	-7.10	97.83	110.60
1	3-A	137	ALA	N-CA-CB	-7.10	100.16	110.10
1	10-A	70	LEU	CB-CG-CD1	7.10	123.07	111.00
1	6-A	61	LEU	CA-CB-CG	-7.09	98.98	115.30
1	6-A	128	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	16-A	92	ARG	CA-CB-CG	-7.09	97.79	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-A	98	PHE	CB-CG-CD1	7.09	125.76	120.80
1	4-A	154	PHE	CZ-CE2-CD2	7.08	128.60	120.10
1	6-A	53	PRO	N-CD-CG	-7.08	92.58	103.20
1	13-A	137	ALA	N-CA-CB	-7.08	100.18	110.10
1	2-A	92	ARG	CG-CD-NE	-7.08	96.93	111.80
1	4-A	50	LYS	CD-CE-NZ	7.08	127.99	111.70
1	8-A	36	GLY	CA-C-O	-7.08	107.86	120.60
1	9-A	36	GLY	N-CA-C	7.08	130.79	113.10
1	12-A	97	ARG	CA-C-O	-7.08	105.24	120.10
1	15-A	82	LEU	N-CA-CB	-7.08	96.25	110.40
1	7-A	65	THR	CA-CB-CG2	-7.07	102.50	112.40
1	9-A	80	GLN	CB-CA-C	-7.07	96.25	110.40
1	14-A	139	LEU	CB-CG-CD1	-7.07	98.98	111.00
1	13-A	53	PRO	C-N-CA	-7.07	104.03	121.70
1	1-A	121	TRP	N-CA-CB	-7.07	97.88	110.60
1	12-A	57	ASN	CA-C-N	-7.07	101.66	117.20
1	2-A	107	LEU	N-CA-CB	-7.06	96.28	110.40
1	8-A	66	SER	N-CA-C	-7.06	91.93	111.00
1	12-A	89	LEU	CA-CB-CG	-7.06	99.07	115.30
1	14-A	64	PHE	CB-CG-CD1	-7.05	115.86	120.80
1	14-A	93	TRP	CE3-CZ3-CH2	-7.05	113.44	121.20
1	5-A	92	ARG	CD-NE-CZ	-7.05	113.73	123.60
1	10-A	140	TRP	CA-CB-CG	-7.05	100.31	113.70
1	3-A	37	SER	CA-CB-OG	-7.05	92.17	111.20
1	9-A	127	HIS	CA-CB-CG	-7.05	101.62	113.60
1	11-A	78	TYR	CE1-CZ-CE2	7.05	131.07	119.80
1	1-A	57	ASN	CA-C-N	-7.04	101.70	117.20
1	3-A	40	ARG	CA-C-O	-7.04	105.31	120.10
1	8-A	58	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	5-A	65	THR	CA-CB-CG2	-7.04	102.54	112.40
1	10-A	116	ALA	CB-CA-C	-7.04	99.54	110.10
1	2-A	120	ILE	C-N-CA	-7.04	104.10	121.70
1	15-A	140	TRP	CE3-CZ3-CH2	-7.04	113.46	121.20
1	16-A	69	GLY	O-C-N	7.04	133.96	122.70
1	2-A	77	LEU	N-CA-CB	7.04	124.47	110.40
1	6-A	125	GLU	CG-CD-OE1	7.04	132.37	118.30
1	13-A	68	VAL	CA-C-N	-7.04	102.13	116.20
1	2-A	142	SER	CB-CA-C	-7.03	96.74	110.10
1	3-A	61	LEU	CD1-CG-CD2	-7.03	89.41	110.50
1	13-A	90	LEU	CB-CA-C	-7.03	96.84	110.20
1	15-A	92	ARG	NH1-CZ-NH2	7.03	127.13	119.40
1	11-A	136	MET	O-C-N	7.03	133.94	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	15-A	58	ARG	NH1-CZ-NH2	7.03	127.13	119.40
1	6-A	74	MET	N-CA-C	7.02	129.96	111.00
1	5-A	42	ALA	N-CA-CB	-7.02	100.27	110.10
1	14-A	150	ILE	CG1-CB-CG2	7.02	126.84	111.40
1	1-A	113	PRO	C-N-CA	-7.02	104.16	121.70
1	5-A	47	ASP	CB-CA-C	-7.01	96.37	110.40
1	10-A	41	ARG	O-C-N	7.01	133.92	122.70
1	16-A	150	ILE	CA-CB-CG2	7.01	124.92	110.90
1	9-A	98	PHE	CA-C-N	-7.01	102.18	116.20
1	12-A	137	ALA	N-CA-CB	-7.01	100.29	110.10
1	4-A	71	SER	N-CA-CB	7.00	121.00	110.50
1	6-A	83	HIS	N-CA-CB	-7.00	98.01	110.60
1	7-A	45	TYR	CG-CD1-CE1	7.00	126.90	121.30
1	9-A	107	LEU	CB-CG-CD2	-6.99	99.11	111.00
1	12-A	48	TYR	CG-CD2-CE2	6.99	126.89	121.30
1	10-A	48	TYR	CG-CD2-CE2	6.99	126.89	121.30
1	16-A	117	GLU	OE1-CD-OE2	6.99	131.68	123.30
1	1-A	153	ILE	CB-CA-C	-6.99	97.63	111.60
1	5-A	58	ARG	NE-CZ-NH1	-6.99	116.81	120.30
1	15-A	55	PRO	CA-N-CD	6.98	121.48	111.70
1	9-A	40	ARG	CA-CB-CG	-6.98	98.04	113.40
1	11-A	146	TYR	CD1-CG-CD2	6.98	125.58	117.90
1	2-A	97	ARG	O-C-N	6.98	133.86	122.70
1	6-A	148	SER	CB-CA-C	-6.98	96.84	110.10
1	10-A	67	TRP	C-N-CA	-6.98	104.26	121.70
1	3-A	99	GLY	CA-C-O	6.97	133.15	120.60
1	16-A	143	ASP	CB-CA-C	6.97	124.34	110.40
1	14-A	63	PRO	N-CA-C	-6.97	93.98	112.10
1	4-A	43	GLU	CG-CD-OE1	-6.96	104.39	118.30
1	13-A	93	TRP	CE2-CD2-CG	6.96	112.86	107.30
1	8-A	131	PRO	N-CD-CG	-6.95	92.77	103.20
1	8-A	67	TRP	N-CA-CB	-6.95	98.09	110.60
1	13-A	49	MET	N-CA-CB	-6.95	98.09	110.60
1	10-A	123	VAL	CA-CB-CG1	-6.95	100.48	110.90
1	6-A	118	ALA	CA-C-N	-6.95	101.92	117.20
1	9-A	47	ASP	CA-C-O	-6.95	105.51	120.10
1	5-A	153	ILE	CA-CB-CG1	-6.94	97.81	111.00
1	11-A	154	PHE	CD1-CG-CD2	-6.94	109.28	118.30
1	11-A	144	PRO	CA-C-N	-6.94	101.94	117.20
1	16-A	64	PHE	CG-CD1-CE1	-6.93	113.17	120.80
1	2-A	133	HIS	N-CA-CB	-6.93	98.12	110.60
1	16-A	40	ARG	CD-NE-CZ	6.93	133.31	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	97	ARG	CG-CD-NE	6.93	126.34	111.80
1	9-A	45	TYR	CB-CG-CD2	-6.92	116.84	121.00
1	14-A	131	PRO	O-C-N	6.92	133.78	122.70
1	13-A	90	LEU	N-CA-C	-6.92	92.31	111.00
1	2-A	148	SER	CA-C-N	-6.92	101.98	117.20
1	11-A	105	GLN	CB-CA-C	-6.92	96.56	110.40
1	16-A	61	LEU	CB-CG-CD2	-6.91	99.25	111.00
1	9-A	45	TYR	CG-CD2-CE2	-6.91	115.77	121.30
1	5-A	146	TYR	CG-CD2-CE2	-6.91	115.78	121.30
1	16-A	84	TYR	CD1-CE1-CZ	6.90	126.01	119.80
1	2-A	148	SER	C-N-CA	-6.90	104.44	121.70
1	6-A	83	HIS	O-C-N	6.90	133.74	122.70
1	16-A	117	GLU	O-C-N	6.90	133.74	122.70
1	8-A	98	PHE	C-N-CA	-6.90	107.81	122.30
1	10-A	131	PRO	O-C-N	6.90	133.74	122.70
1	9-A	131	PRO	CA-C-N	-6.90	102.03	117.20
1	3-A	48	TYR	CG-CD2-CE2	6.89	126.81	121.30
1	16-A	92	ARG	NH1-CZ-NH2	6.89	126.98	119.40
1	1-A	61	LEU	CB-CG-CD2	-6.89	99.29	111.00
1	5-A	41	ARG	C-N-CA	-6.88	104.49	121.70
1	15-A	58	ARG	CD-NE-CZ	-6.88	113.97	123.60
1	11-A	88	VAL	CA-C-O	6.88	134.55	120.10
1	2-A	137	ALA	C-N-CA	-6.88	104.51	121.70
1	12-A	75	LYS	O-C-N	6.88	133.70	122.70
1	16-A	65	THR	CA-CB-CG2	-6.87	102.79	112.40
1	11-A	48	TYR	CG-CD2-CE2	6.87	126.79	121.30
1	12-A	156	GLU	OE1-CD-OE2	6.87	131.54	123.30
1	16-A	81	PRO	CA-C-N	-6.87	102.09	117.20
1	10-A	121	TRP	N-CA-CB	-6.86	98.25	110.60
1	14-A	122	LEU	C-N-CA	-6.86	104.55	121.70
1	14-A	64	PHE	CA-C-O	-6.86	105.69	120.10
1	4-A	98	PHE	CA-C-N	-6.86	102.48	116.20
1	9-A	139	LEU	CA-CB-CG	-6.86	99.53	115.30
1	16-A	62	ILE	CG1-CB-CG2	6.86	126.48	111.40
1	5-A	55	PRO	CA-C-N	-6.85	102.13	117.20
1	11-A	39	LEU	CB-CA-C	-6.85	97.18	110.20
1	13-A	45	TYR	CA-CB-CG	-6.85	100.38	113.40
1	8-A	67	TRP	CE3-CZ3-CH2	6.85	128.73	121.20
1	13-A	57	ASN	O-C-N	6.85	133.65	122.70
1	6-A	128	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	7-A	98	PHE	N-CA-CB	-6.84	98.28	110.60
1	8-A	142	SER	N-CA-CB	-6.84	100.24	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	12-A	105	GLN	CB-CA-C	-6.84	96.71	110.40
1	6-A	49	MET	CA-CB-CG	6.84	124.92	113.30
1	14-A	128	ARG	C-N-CA	-6.84	104.61	121.70
1	1-A	36	GLY	CA-C-O	6.83	132.90	120.60
1	8-A	148	SER	CB-CA-C	-6.83	97.12	110.10
1	15-A	93	TRP	C-N-CA	-6.83	104.62	121.70
1	4-A	108	ASP	OD1-CG-OD2	6.83	136.27	123.30
1	5-A	98	PHE	CA-C-N	-6.83	102.55	116.20
1	5-A	75	LYS	O-C-N	6.83	133.62	122.70
1	15-A	93	TRP	CB-CG-CD2	-6.82	117.73	126.60
1	16-A	82	LEU	N-CA-C	-6.82	92.59	111.00
1	12-A	108	ASP	OD1-CG-OD2	6.82	136.25	123.30
1	13-A	132	SER	C-N-CA	-6.82	104.66	121.70
1	9-A	63	PRO	N-CD-CG	-6.81	92.98	103.20
1	15-A	123	VAL	N-CA-C	-6.81	92.60	111.00
1	3-A	81	PRO	O-C-N	6.80	133.59	122.70
1	2-A	148	SER	CB-CA-C	6.80	123.02	110.10
1	13-A	140	TRP	C-N-CA	-6.80	104.71	121.70
1	8-A	152	PRO	CA-N-CD	6.79	121.21	111.70
1	2-A	109	SER	N-CA-CB	-6.79	100.31	110.50
1	5-A	141	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	7-A	53	PRO	N-CD-CG	-6.79	93.02	103.20
1	11-A	42	ALA	CA-C-O	6.78	134.35	120.10
1	6-A	98	PHE	CA-C-N	-6.78	102.64	116.20
1	8-A	58	ARG	CB-CG-CD	-6.78	93.97	111.60
1	10-A	121	TRP	NE1-CE2-CD2	6.78	114.08	107.30
1	9-A	124	GLU	N-CA-CB	-6.78	98.40	110.60
1	12-A	45	TYR	CG-CD1-CE1	6.77	126.72	121.30
1	3-A	149	PHE	CB-CG-CD2	-6.77	116.06	120.80
1	8-A	60	SER	CA-CB-OG	-6.77	92.92	111.20
1	9-A	45	TYR	O-C-N	6.77	133.53	122.70
1	6-A	90	LEU	CB-CG-CD2	6.76	122.50	111.00
1	12-A	125	GLU	CG-CD-OE1	6.76	131.83	118.30
1	3-A	98	PHE	N-CA-CB	-6.76	98.43	110.60
1	10-A	154	PHE	CB-CG-CD2	6.76	125.53	120.80
1	12-A	98	PHE	CA-C-N	-6.76	102.68	116.20
1	2-A	118	ALA	O-C-N	6.76	133.51	122.70
1	5-A	61	LEU	CB-CA-C	6.76	123.04	110.20
1	14-A	40	ARG	CD-NE-CZ	6.76	133.06	123.60
1	15-A	107	LEU	O-C-N	6.75	133.51	122.70
1	13-A	128	ARG	CB-CA-C	-6.75	96.89	110.40
1	9-A	127	HIS	N-CA-CB	6.75	122.75	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	12-A	151	ASP	N-CA-CB	-6.75	98.46	110.60
1	10-A	89	LEU	CA-CB-CG	-6.74	99.79	115.30
1	14-A	139	LEU	CB-CG-CD2	-6.74	99.55	111.00
1	11-A	55	PRO	CB-CA-C	-6.74	95.16	112.00
1	7-A	78	TYR	CB-CG-CD1	6.73	125.04	121.00
1	2-A	49	MET	CA-CB-CG	6.73	124.74	113.30
1	4-A	61	LEU	CB-CG-CD1	6.72	122.43	111.00
1	13-A	41	ARG	NH1-CZ-NH2	6.72	126.79	119.40
1	1-A	140	TRP	C-N-CA	-6.72	104.90	121.70
1	9-A	113	PRO	CA-CB-CG	-6.72	91.24	104.00
1	14-A	121	TRP	CA-CB-CG	6.72	126.46	113.70
1	13-A	67	TRP	CG-CD2-CE3	6.71	139.94	133.90
1	1-A	78	TYR	CG-CD1-CE1	6.71	126.67	121.30
1	3-A	109	SER	CA-CB-OG	-6.70	93.10	111.20
1	10-A	64	PHE	CE1-CZ-CE2	6.70	132.07	120.00
1	16-A	45	TYR	C-N-CA	-6.70	104.94	121.70
1	14-A	147	HIS	N-CA-CB	-6.70	98.54	110.60
1	16-A	98	PHE	CB-CG-CD1	6.70	125.49	120.80
1	2-A	40	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	4-A	48	TYR	CG-CD1-CE1	-6.70	115.94	121.30
1	9-A	57	ASN	O-C-N	6.69	133.41	122.70
1	10-A	45	TYR	O-C-N	6.69	133.41	122.70
1	13-A	98	PHE	C-N-CA	-6.69	108.25	122.30
1	13-A	156	GLU	OE1-CD-OE2	-6.69	115.27	123.30
1	11-A	97	ARG	NH1-CZ-NH2	6.69	126.76	119.40
1	15-A	124	GLU	CB-CA-C	-6.69	97.03	110.40
1	5-A	47	ASP	C-N-CA	-6.69	104.98	121.70
1	11-A	92	ARG	CA-CB-CG	-6.68	98.69	113.40
1	2-A	76	GLN	CA-C-O	6.68	134.13	120.10
1	16-A	58	ARG	NH1-CZ-NH2	6.68	126.74	119.40
1	2-A	36	GLY	O-C-N	6.67	133.38	122.70
1	6-A	41	ARG	O-C-N	6.67	133.38	122.70
1	1-A	78	TYR	CE1-CZ-CE2	6.67	130.48	119.80
1	14-A	112	HIS	CG-ND1-CE1	6.67	117.54	108.20
1	9-A	92	ARG	CG-CD-NE	-6.67	97.79	111.80
1	13-A	89	LEU	CB-CG-CD1	-6.67	99.66	111.00
1	14-A	152	PRO	CA-C-O	6.67	136.21	120.20
1	1-A	107	LEU	N-CA-CB	-6.67	97.07	110.40
1	16-A	71	SER	CA-C-O	-6.67	106.10	120.10
1	14-A	45	TYR	O-C-N	6.67	133.36	122.70
1	16-A	48	TYR	C-N-CA	-6.66	105.05	121.70
1	3-A	123	VAL	CG1-CB-CG2	6.66	121.56	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	136	MET	O-C-N	6.66	133.36	122.70
1	15-A	87	ASN	CB-CG-ND2	6.66	132.69	116.70
1	1-A	43	GLU	CG-CD-OE2	-6.66	104.98	118.30
1	7-A	97	ARG	CA-CB-CG	-6.66	98.75	113.40
1	4-A	89	LEU	CB-CG-CD2	-6.66	99.68	111.00
1	3-A	92	ARG	NH1-CZ-NH2	6.65	126.72	119.40
1	4-A	76	GLN	CG-CD-NE2	6.65	132.67	116.70
1	8-A	94	ASP	CB-CG-OD2	6.65	124.29	118.30
1	12-A	80	GLN	CB-CG-CD	-6.65	94.30	111.60
1	4-A	45	TYR	O-C-N	6.65	133.34	122.70
1	2-A	48	TYR	CG-CD1-CE1	-6.65	115.98	121.30
1	6-A	136	MET	O-C-N	6.65	133.34	122.70
1	9-A	93	TRP	O-C-N	6.65	133.34	122.70
1	3-A	93	TRP	O-C-N	6.65	133.33	122.70
1	9-A	60	SER	CB-CA-C	-6.64	97.48	110.10
1	2-A	133	HIS	C-N-CA	-6.63	105.11	121.70
1	14-A	65	THR	OG1-CB-CG2	6.63	125.26	110.00
1	6-A	75	LYS	O-C-N	6.63	133.31	122.70
1	8-A	105	GLN	CB-CA-C	-6.63	97.14	110.40
1	3-A	142	SER	N-CA-CB	-6.63	100.56	110.50
1	7-A	108	ASP	OD1-CG-OD2	6.63	135.89	123.30
1	10-A	107	LEU	N-CA-CB	-6.63	97.14	110.40
1	16-A	138	LEU	CB-CG-CD2	-6.63	99.73	111.00
1	1-A	140	TRP	CE3-CZ3-CH2	-6.62	113.91	121.20
1	8-A	40	ARG	CA-CB-CG	-6.62	98.83	113.40
1	14-A	148	SER	N-CA-CB	-6.62	100.57	110.50
1	4-A	55	PRO	CA-CB-CG	-6.62	91.43	104.00
1	16-A	112	HIS	CB-CA-C	-6.62	97.17	110.40
1	1-A	145	MET	CA-CB-CG	-6.61	102.06	113.30
1	6-A	77	LEU	CB-CG-CD2	-6.60	99.78	111.00
1	2-A	98	PHE	CB-CG-CD2	-6.60	116.18	120.80
1	16-A	70	LEU	N-CA-C	6.60	128.82	111.00
1	14-A	130	THR	N-CA-C	6.60	128.82	111.00
1	16-A	66	SER	N-CA-C	-6.60	93.18	111.00
1	2-A	45	TYR	CE1-CZ-OH	-6.60	102.29	120.10
1	5-A	125	GLU	CG-CD-OE1	6.59	131.49	118.30
1	16-A	115	LYS	N-CA-CB	-6.59	98.73	110.60
1	6-A	97	ARG	CA-C-O	-6.58	106.28	120.10
1	9-A	88	VAL	CA-CB-CG2	-6.58	101.03	110.90
1	12-A	134	LEU	CB-CG-CD2	-6.58	99.82	111.00
1	7-A	43	GLU	CG-CD-OE2	-6.57	105.15	118.30
1	15-A	50	LYS	CA-CB-CG	-6.57	98.94	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	45	TYR	OH-CZ-CE2	6.57	137.83	120.10
1	14-A	36	GLY	N-CA-C	6.57	129.52	113.10
1	3-A	40	ARG	CD-NE-CZ	6.57	132.79	123.60
1	3-A	140	TRP	CE3-CZ3-CH2	-6.56	113.98	121.20
1	9-A	67	TRP	CD2-CE3-CZ3	-6.56	110.27	118.80
1	2-A	107	LEU	CB-CG-CD2	-6.56	99.86	111.00
1	11-A	140	TRP	CH2-CZ2-CE2	-6.55	110.85	117.40
1	7-A	125	GLU	CG-CD-OE1	6.55	131.40	118.30
1	10-A	44	MET	CG-SD-CE	-6.55	89.72	100.20
1	7-A	97	ARG	O-C-N	6.55	133.18	122.70
1	15-A	104	GLU	CG-CD-OE2	-6.55	105.20	118.30
1	12-A	90	LEU	CB-CG-CD2	6.55	122.13	111.00
1	13-A	123	VAL	N-CA-CB	6.55	125.91	111.50
1	6-A	123	VAL	CG1-CB-CG2	6.55	121.38	110.90
1	10-A	140	TRP	CD1-CG-CD2	6.55	111.54	106.30
1	15-A	126	ILE	CA-C-N	-6.54	102.80	117.20
1	2-A	135	HIS	C-N-CA	-6.54	105.34	121.70
1	8-A	68	VAL	CA-C-O	-6.54	106.37	120.10
1	13-A	47	ASP	CB-CG-OD1	6.53	124.18	118.30
1	13-A	61	LEU	CA-C-O	6.53	133.82	120.10
1	4-A	150	ILE	O-C-N	6.53	133.15	122.70
1	10-A	123	VAL	N-CA-CB	6.53	125.87	111.50
1	13-A	50	LYS	CD-CE-NZ	6.53	126.71	111.70
1	5-A	154	PHE	CZ-CE2-CD2	6.53	127.93	120.10
1	7-A	98	PHE	C-N-CA	-6.53	108.60	122.30
1	12-A	154	PHE	CZ-CE2-CD2	6.52	127.92	120.10
1	12-A	40	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	10-A	89	LEU	CB-CG-CD2	-6.52	99.92	111.00
1	12-A	78	TYR	CA-CB-CG	-6.52	101.02	113.40
1	2-A	55	PRO	C-N-CA	-6.51	105.41	121.70
1	6-A	145	MET	CG-SD-CE	-6.51	89.78	100.20
1	10-A	142	SER	CA-CB-OG	-6.51	93.62	111.20
1	8-A	148	SER	CA-C-O	6.51	133.78	120.10
1	4-A	78	TYR	CZ-CE2-CD2	-6.51	113.94	119.80
1	14-A	49	MET	N-CA-CB	-6.51	98.88	110.60
1	5-A	58	ARG	CB-CG-CD	-6.51	94.68	111.60
1	9-A	50	LYS	O-C-N	-6.51	112.29	122.70
1	15-A	98	PHE	CD1-CE1-CZ	6.51	127.91	120.10
1	13-A	67	TRP	CD2-CE2-CZ2	-6.51	114.49	122.30
1	11-A	41	ARG	NH1-CZ-NH2	-6.50	112.25	119.40
1	7-A	75	LYS	O-C-N	6.50	133.10	122.70
1	13-A	89	LEU	O-C-N	6.50	133.10	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	15-A	125	GLU	CB-CG-CD	-6.50	96.65	114.20
1	13-A	41	ARG	O-C-N	6.50	133.10	122.70
1	11-A	125	GLU	CG-CD-OE1	6.49	131.28	118.30
1	14-A	118	ALA	C-N-CA	-6.49	105.48	121.70
1	16-A	117	GLU	CA-CB-CG	-6.49	99.12	113.40
1	6-A	48	TYR	CD1-CE1-CZ	6.49	125.64	119.80
1	9-A	64	PHE	CG-CD1-CE1	-6.48	113.67	120.80
1	10-A	128	ARG	CG-CD-NE	-6.48	98.19	111.80
1	16-A	50	LYS	CB-CG-CD	-6.48	94.76	111.60
1	16-A	94	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	10-A	101	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	10-A	154	PHE	CZ-CE2-CD2	6.47	127.87	120.10
1	3-A	94	ASP	C-N-CA	-6.47	105.52	121.70
1	8-A	48	TYR	C-N-CA	-6.47	105.53	121.70
1	16-A	86	THR	CA-C-O	6.47	133.68	120.10
1	9-A	53	PRO	N-CD-CG	-6.46	93.50	103.20
1	9-A	132	SER	CA-C-O	6.46	133.68	120.10
1	11-A	77	LEU	CB-CG-CD2	-6.46	100.01	111.00
1	7-A	80	GLN	CB-CA-C	-6.46	97.48	110.40
1	1-A	80	GLN	CA-CB-CG	-6.46	99.19	113.40
1	13-A	110	ILE	CG1-CB-CG2	6.46	125.60	111.40
1	16-A	48	TYR	CB-CG-CD1	-6.46	117.13	121.00
1	9-A	45	TYR	CG-CD1-CE1	6.45	126.46	121.30
1	5-A	49	MET	CA-CB-CG	6.45	124.27	113.30
1	4-A	40	ARG	CA-CB-CG	-6.45	99.21	113.40
1	9-A	65	THR	CA-CB-CG2	-6.45	103.37	112.40
1	16-A	39	LEU	CB-CG-CD1	-6.45	100.03	111.00
1	13-A	122	LEU	O-C-N	6.45	133.02	122.70
1	16-A	134	LEU	CB-CG-CD2	6.45	121.96	111.00
1	7-A	154	PHE	CB-CG-CD2	6.45	125.31	120.80
1	16-A	107	LEU	CA-C-N	6.44	131.38	117.20
1	5-A	46	GLN	CB-CA-C	-6.44	97.53	110.40
1	10-A	128	ARG	CD-NE-CZ	-6.43	114.59	123.60
1	4-A	136	MET	O-C-N	6.43	132.99	122.70
1	2-A	154	PHE	CB-CG-CD1	-6.43	116.30	120.80
1	16-A	46	GLN	CG-CD-OE1	-6.43	108.74	121.60
1	11-A	84	TYR	CB-CG-CD1	6.43	124.86	121.00
1	15-A	81	PRO	N-CA-CB	6.42	111.01	103.30
1	1-A	75	LYS	N-CA-CB	-6.42	99.04	110.60
1	15-A	55	PRO	CB-CA-C	-6.42	95.95	112.00
1	15-A	132	SER	CA-CB-OG	-6.42	93.86	111.20
1	7-A	45	TYR	CB-CG-CD2	-6.42	117.15	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16-A	128	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	14-A	90	LEU	CA-CB-CG	-6.42	100.54	115.30
1	16-A	80	GLN	CG-CD-OE1	-6.41	108.77	121.60
1	6-A	43	GLU	CG-CD-OE2	-6.41	105.48	118.30
1	16-A	93	TRP	N-CA-C	6.41	128.31	111.00
1	6-A	45	TYR	O-C-N	6.41	132.95	122.70
1	11-A	98	PHE	CB-CG-CD1	6.41	125.28	120.80
1	1-A	63	PRO	C-N-CA	-6.40	105.69	121.70
1	15-A	80	GLN	CA-C-O	-6.40	106.66	120.10
1	6-A	108	ASP	OD1-CG-OD2	6.40	135.45	123.30
1	16-A	113	PRO	N-CA-C	6.40	128.73	112.10
1	4-A	57	ASN	CA-C-N	-6.39	103.13	117.20
1	8-A	45	TYR	CG-CD2-CE2	6.39	126.42	121.30
1	5-A	108	ASP	OD1-CG-OD2	6.39	135.44	123.30
1	2-A	154	PHE	CD1-CE1-CZ	-6.39	112.43	120.10
1	5-A	138	LEU	N-CA-CB	-6.39	97.62	110.40
1	1-A	154	PHE	CD1-CE1-CZ	-6.39	112.44	120.10
1	5-A	43	GLU	CG-CD-OE1	-6.39	105.53	118.30
1	16-A	51	GLN	CA-CB-CG	-6.39	99.35	113.40
1	5-A	123	VAL	CA-CB-CG1	-6.38	101.32	110.90
1	9-A	144	PRO	N-CD-CG	-6.38	93.62	103.20
1	14-A	129	LEU	O-C-N	-6.38	112.49	122.70
1	3-A	154	PHE	CZ-CE2-CD2	6.38	127.76	120.10
1	5-A	93	TRP	CA-C-O	-6.38	106.70	120.10
1	13-A	91	GLN	CA-CB-CG	-6.38	99.37	113.40
1	16-A	70	LEU	CA-CB-CG	6.38	129.97	115.30
1	13-A	53	PRO	N-CA-CB	6.38	110.95	103.30
1	5-A	45	TYR	CG-CD1-CE1	6.37	126.40	121.30
1	7-A	131	PRO	O-C-N	6.37	132.90	122.70
1	13-A	120	ILE	CG1-CB-CG2	6.37	125.41	111.40
1	2-A	132	SER	N-CA-CB	-6.37	100.95	110.50
1	3-A	100	THR	CA-C-O	-6.37	106.73	120.10
1	4-A	53	PRO	N-CD-CG	-6.36	93.65	103.20
1	8-A	58	ARG	CG-CD-NE	-6.36	98.44	111.80
1	8-A	141	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	15-A	115	LYS	CA-CB-CG	-6.36	99.40	113.40
1	15-A	121	TRP	C-N-CA	-6.36	105.79	121.70
1	4-A	122	LEU	CB-CG-CD1	-6.36	100.19	111.00
1	15-A	106	ARG	CA-C-N	-6.36	103.20	117.20
1	4-A	47	ASP	CB-CG-OD1	6.36	124.02	118.30
1	10-A	67	TRP	CE2-CD2-CE3	6.36	126.33	118.70
1	14-A	76	GLN	CA-C-O	-6.36	106.75	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13-A	133	HIS	C-N-CA	-6.35	105.83	121.70
1	9-A	126	ILE	O-C-N	6.35	132.85	122.70
1	2-A	44	MET	CG-SD-CE	-6.34	90.05	100.20
1	16-A	115	LYS	CA-C-N	6.34	131.16	117.20
1	2-A	121	TRP	CG-CD1-NE1	-6.34	103.76	110.10
1	1-A	98	PHE	CG-CD1-CE1	6.34	127.77	120.80
1	5-A	90	LEU	CB-CG-CD2	6.34	121.77	111.00
1	13-A	71	SER	O-C-N	6.34	132.84	122.70
1	6-A	128	ARG	NH1-CZ-NH2	6.33	126.37	119.40
1	12-A	117	GLU	CG-CD-OE2	-6.33	105.63	118.30
1	9-A	67	TRP	C-N-CA	-6.33	105.87	121.70
1	11-A	38	LEU	CD1-CG-CD2	-6.33	91.50	110.50
1	15-A	48	TYR	CG-CD2-CE2	6.33	126.36	121.30
1	12-A	136	MET	C-N-CA	-6.33	105.88	121.70
1	16-A	98	PHE	CG-CD1-CE1	6.33	127.76	120.80
1	15-A	132	SER	CB-CA-C	6.32	122.11	110.10
1	10-A	100	THR	C-N-CA	6.32	137.51	121.70
1	2-A	78	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	13-A	84	TYR	CG-CD2-CE2	-6.32	116.24	121.30
1	15-A	124	GLU	CA-C-N	-6.32	103.29	117.20
1	12-A	89	LEU	C-N-CA	-6.32	105.90	121.70
1	10-A	100	THR	CA-C-N	-6.32	103.31	117.20
1	14-A	126	ILE	CB-CA-C	-6.32	98.97	111.60
1	5-A	93	TRP	N-CA-C	-6.31	93.95	111.00
1	6-A	125	GLU	CG-CD-OE2	-6.31	105.67	118.30
1	8-A	120	ILE	C-N-CA	-6.31	105.92	121.70
1	15-A	40	ARG	CB-CG-CD	-6.31	95.19	111.60
1	14-A	93	TRP	CD2-CE3-CZ3	6.31	127.00	118.80
1	13-A	38	LEU	CB-CG-CD2	-6.31	100.27	111.00
1	14-A	89	LEU	CA-CB-CG	-6.31	100.79	115.30
1	10-A	128	ARG	CB-CA-C	-6.31	97.79	110.40
1	2-A	132	SER	CB-CA-C	-6.30	98.12	110.10
1	9-A	156	GLU	OE1-CD-OE2	6.30	130.86	123.30
1	8-A	141	ARG	CD-NE-CZ	6.30	132.42	123.60
1	14-A	46	GLN	CA-C-O	6.30	133.33	120.10
1	7-A	74	MET	CB-CG-SD	-6.29	93.52	112.40
1	14-A	64	PHE	CG-CD2-CE2	6.29	127.72	120.80
1	7-A	81	PRO	CA-C-N	-6.29	103.35	117.20
1	3-A	99	GLY	N-CA-C	-6.29	97.37	113.10
1	3-A	136	MET	C-N-CA	-6.29	105.98	121.70
1	4-A	78	TYR	CD1-CG-CD2	6.29	124.82	117.90
1	8-A	125	GLU	CG-CD-OE1	6.29	130.88	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	139	LEU	CB-CG-CD2	-6.29	100.31	111.00
1	16-A	86	THR	CA-CB-CG2	-6.29	103.60	112.40
1	12-A	145	MET	CA-CB-CG	-6.29	102.61	113.30
1	9-A	50	LYS	N-CA-CB	-6.28	99.29	110.60
1	4-A	41	ARG	CG-CD-NE	-6.28	98.61	111.80
1	10-A	71	SER	O-C-N	6.28	132.75	122.70
1	12-A	39	LEU	CB-CG-CD2	6.28	121.68	111.00
1	15-A	152	PRO	O-C-N	-6.28	112.65	122.70
1	8-A	64	PHE	CG-CD2-CE2	6.28	127.71	120.80
1	12-A	45	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	13-A	135	HIS	C-N-CA	-6.28	106.01	121.70
1	1-A	91	GLN	N-CA-CB	-6.27	99.31	110.60
1	15-A	53	PRO	N-CD-CG	-6.27	93.79	103.20
1	8-A	48	TYR	CB-CG-CD2	6.26	124.76	121.00
1	11-A	91	GLN	N-CA-CB	-6.26	99.33	110.60
1	6-A	82	LEU	CD1-CG-CD2	-6.26	91.71	110.50
1	10-A	144	PRO	N-CD-CG	-6.26	93.81	103.20
1	11-A	51	GLN	CA-CB-CG	-6.26	99.63	113.40
1	13-A	76	GLN	CA-C-O	-6.26	106.96	120.10
1	14-A	86	THR	CA-CB-CG2	-6.26	103.64	112.40
1	2-A	146	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	4-A	154	PHE	CB-CG-CD2	6.25	125.17	120.80
1	10-A	65	THR	CA-CB-CG2	-6.25	103.65	112.40
1	15-A	119	THR	CA-CB-CG2	-6.25	103.65	112.40
1	4-A	76	GLN	CA-C-N	6.25	130.94	117.20
1	4-A	124	GLU	CA-C-N	6.24	130.92	117.20
1	9-A	45	TYR	CZ-CE2-CD2	6.24	125.41	119.80
1	9-A	48	TYR	CG-CD1-CE1	-6.24	116.31	121.30
1	5-A	48	TYR	CA-C-N	-6.23	103.49	117.20
1	2-A	53	PRO	N-CD-CG	-6.23	93.86	103.20
1	3-A	125	GLU	CG-CD-OE2	-6.23	105.85	118.30
1	2-A	132	SER	CA-C-O	6.22	133.17	120.10
1	1-A	114	THR	CA-CB-CG2	6.22	121.11	112.40
1	2-A	90	LEU	CB-CG-CD2	6.22	121.58	111.00
1	16-A	98	PHE	CA-C-N	-6.22	103.76	116.20
1	13-A	40	ARG	CB-CG-CD	-6.22	95.43	111.60
1	15-A	93	TRP	O-C-N	6.22	132.65	122.70
1	5-A	98	PHE	C-N-CA	-6.22	109.25	122.30
1	11-A	44	MET	CA-CB-CG	-6.22	102.73	113.30
1	16-A	137	ALA	N-CA-CB	-6.22	101.40	110.10
1	16-A	146	TYR	OH-CZ-CE2	6.22	136.88	120.10
1	2-A	120	ILE	CA-CB-CG1	-6.21	99.19	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	42	ALA	N-CA-CB	-6.21	101.40	110.10
1	15-A	82	LEU	O-C-N	6.21	132.64	122.70
1	13-A	151	ASP	OD1-CG-OD2	-6.21	111.50	123.30
1	15-A	81	PRO	O-C-N	-6.21	112.77	122.70
1	15-A	88	VAL	C-N-CA	-6.21	106.19	121.70
1	4-A	81	PRO	CB-CA-C	6.20	127.51	112.00
1	16-A	118	ALA	N-CA-CB	-6.20	101.41	110.10
1	14-A	71	SER	C-N-CA	-6.20	106.20	121.70
1	14-A	127	HIS	CA-CB-CG	-6.20	103.06	113.60
1	16-A	81	PRO	CA-N-CD	6.20	120.38	111.70
1	1-A	56	THR	OG1-CB-CG2	6.20	124.25	110.00
1	13-A	48	TYR	CG-CD2-CE2	6.20	126.26	121.30
1	6-A	134	LEU	CD1-CG-CD2	-6.19	91.93	110.50
1	13-A	152	PRO	O-C-N	-6.19	112.80	122.70
1	16-A	85	LEU	CB-CG-CD2	6.19	121.52	111.00
1	1-A	150	ILE	CG1-CB-CG2	6.18	125.01	111.40
1	4-A	79	GLY	CA-C-N	-6.18	103.59	117.20
1	7-A	80	GLN	CA-CB-CG	-6.18	99.81	113.40
1	9-A	131	PRO	C-N-CA	-6.17	106.27	121.70
1	14-A	128	ARG	N-CA-CB	-6.17	99.50	110.60
1	5-A	97	ARG	CA-C-O	-6.17	107.15	120.10
1	5-A	118	ALA	O-C-N	6.17	132.57	122.70
1	6-A	72	ILE	CA-C-N	6.17	130.77	117.20
1	9-A	140	TRP	CA-CB-CG	-6.17	101.98	113.70
1	13-A	92	ARG	CA-CB-CG	-6.17	99.83	113.40
1	1-A	47	ASP	CB-CG-OD1	6.17	123.85	118.30
1	15-A	41	ARG	O-C-N	6.17	132.57	122.70
1	10-A	68	VAL	CA-C-N	-6.17	103.87	116.20
1	14-A	67	TRP	CB-CG-CD1	-6.17	118.98	127.00
1	14-A	117	GLU	CG-CD-OE2	-6.17	105.97	118.30
1	13-A	74	MET	CA-CB-CG	-6.16	102.82	113.30
1	14-A	67	TRP	CA-C-O	-6.16	107.16	120.10
1	12-A	142	SER	N-CA-CB	-6.16	101.26	110.50
1	7-A	139	LEU	CB-CG-CD2	-6.15	100.54	111.00
1	14-A	129	LEU	C-N-CA	6.15	137.08	121.70
1	15-A	113	PRO	N-CD-CG	-6.15	93.97	103.20
1	15-A	119	THR	C-N-CA	-6.15	106.32	121.70
1	7-A	117	GLU	N-CA-CB	-6.15	99.53	110.60
1	8-A	147	HIS	CA-C-O	6.15	133.01	120.10
1	3-A	90	LEU	C-N-CA	-6.15	106.33	121.70
1	13-A	106	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	14-A	87	ASN	N-CA-CB	-6.15	99.53	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-A	121	TRP	O-C-N	6.15	132.53	122.70
1	12-A	116	ALA	CB-CA-C	-6.15	100.88	110.10
1	6-A	123	VAL	CA-CB-CG1	-6.14	101.68	110.90
1	4-A	124	GLU	CA-C-O	-6.14	107.20	120.10
1	4-A	116	ALA	CA-C-O	-6.14	107.21	120.10
1	10-A	139	LEU	CB-CG-CD2	-6.14	100.56	111.00
1	14-A	130	THR	N-CA-CB	6.14	121.97	110.30
1	2-A	136	MET	C-N-CA	-6.14	106.36	121.70
1	6-A	98	PHE	C-N-CA	-6.13	109.42	122.30
1	16-A	130	THR	OG1-CB-CG2	6.13	124.11	110.00
1	14-A	57	ASN	O-C-N	6.13	132.51	122.70
1	14-A	108	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	15-A	91	GLN	N-CA-CB	-6.13	99.56	110.60
1	14-A	40	ARG	CB-CG-CD	-6.13	95.66	111.60
1	2-A	140	TRP	CH2-CZ2-CE2	-6.13	111.27	117.40
1	4-A	77	LEU	CA-CB-CG	-6.13	101.20	115.30
1	16-A	70	LEU	CB-CG-CD2	6.13	121.42	111.00
1	2-A	151	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	3-A	44	MET	CG-SD-CE	-6.12	90.40	100.20
1	4-A	153	ILE	CA-CB-CG1	-6.12	99.36	111.00
1	10-A	106	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	13-A	98	PHE	CZ-CE2-CD2	-6.12	112.75	120.10
1	3-A	103	GLU	OE1-CD-OE2	-6.12	115.96	123.30
1	5-A	58	ARG	CG-CD-NE	-6.12	98.95	111.80
1	10-A	76	GLN	CA-C-O	-6.12	107.25	120.10
1	14-A	127	HIS	N-CA-CB	-6.12	99.59	110.60
1	16-A	92	ARG	CB-CA-C	-6.12	98.17	110.40
1	6-A	36	GLY	N-CA-C	6.12	128.39	113.10
1	6-A	145	MET	CB-CG-SD	-6.12	94.05	112.40
1	3-A	57	ASN	O-C-N	6.11	132.48	122.70
1	10-A	143	ASP	N-CA-C	-6.11	94.49	111.00
1	14-A	43	GLU	CG-CD-OE1	-6.11	106.07	118.30
1	1-A	121	TRP	O-C-N	6.11	132.48	122.70
1	1-A	98	PHE	CB-CG-CD1	6.11	125.08	120.80
1	3-A	143	ASP	CB-CG-OD1	6.11	123.80	118.30
1	5-A	80	GLN	CG-CD-OE1	-6.11	109.38	121.60
1	2-A	71	SER	CA-C-O	-6.11	107.27	120.10
1	7-A	115	LYS	CA-CB-CG	-6.11	99.96	113.40
1	16-A	49	MET	CA-CB-CG	-6.11	102.92	113.30
1	1-A	41	ARG	O-C-N	6.11	132.47	122.70
1	15-A	97	ARG	CA-CB-CG	-6.10	99.97	113.40
1	14-A	66	SER	N-CA-C	-6.10	94.52	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	92	ARG	NH1-CZ-NH2	6.10	126.11	119.40
1	13-A	148	SER	N-CA-CB	-6.10	101.35	110.50
1	10-A	84	TYR	CB-CG-CD1	-6.10	117.34	121.00
1	16-A	75	LYS	CD-CE-NZ	-6.10	97.68	111.70
1	10-A	100	THR	CA-CB-CG2	-6.09	103.87	112.40
1	4-A	69	GLY	C-N-CA	6.09	136.92	121.70
1	11-A	63	PRO	CA-N-CD	6.09	120.23	111.70
1	7-A	140	TRP	CD1-NE1-CE2	6.09	114.48	109.00
1	8-A	45	TYR	CE1-CZ-OH	-6.08	103.68	120.10
1	4-A	61	LEU	CA-CB-CG	-6.08	101.32	115.30
1	8-A	64	PHE	CD1-CG-CD2	6.08	126.20	118.30
1	9-A	131	PRO	CB-CA-C	-6.07	96.82	112.00
1	12-A	70	LEU	CB-CG-CD2	-6.07	100.68	111.00
1	14-A	117	GLU	CA-CB-CG	-6.07	100.04	113.40
1	12-A	121	TRP	O-C-N	6.07	132.41	122.70
1	13-A	45	TYR	C-N-CA	-6.07	106.53	121.70
1	13-A	125	GLU	CA-CB-CG	-6.07	100.05	113.40
1	15-A	110	ILE	CA-C-N	-6.07	103.85	117.20
1	4-A	77	LEU	CA-C-O	-6.07	107.36	120.10
1	8-A	58	ARG	CD-NE-CZ	-6.07	115.11	123.60
1	8-A	144	PRO	N-CD-CG	-6.07	94.10	103.20
1	15-A	116	ALA	N-CA-CB	-6.07	101.61	110.10
1	7-A	153	ILE	CA-CB-CG1	-6.06	99.48	111.00
1	7-A	117	GLU	CG-CD-OE2	-6.06	106.17	118.30
1	9-A	92	ARG	CB-CG-CD	-6.06	95.84	111.60
1	16-A	43	GLU	CG-CD-OE1	-6.06	106.18	118.30
1	8-A	49	MET	N-CA-CB	-6.06	99.70	110.60
1	2-A	50	LYS	CB-CG-CD	-6.05	95.86	111.60
1	7-A	45	TYR	CZ-CE2-CD2	6.05	125.25	119.80
1	8-A	48	TYR	CD1-CE1-CZ	6.05	125.25	119.80
1	10-A	76	GLN	OE1-CD-NE2	-6.05	107.98	121.90
1	16-A	122	LEU	CB-CG-CD2	-6.05	100.72	111.00
1	15-A	78	TYR	C-N-CA	-6.05	109.60	122.30
1	11-A	41	ARG	CB-CG-CD	-6.05	95.88	111.60
1	16-A	41	ARG	C-N-CA	-6.04	106.59	121.70
1	4-A	78	TYR	CE1-CZ-CE2	6.04	129.47	119.80
1	6-A	156	GLU	CG-CD-OE2	-6.04	106.22	118.30
1	14-A	98	PHE	CZ-CE2-CD2	-6.04	112.85	120.10
1	1-A	47	ASP	CA-C-O	-6.03	107.43	120.10
1	4-A	115	LYS	CA-CB-CG	-6.03	100.13	113.40
1	9-A	130	THR	N-CA-CB	6.03	121.76	110.30
1	16-A	56	THR	OG1-CB-CG2	-6.03	96.13	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	64	PHE	CB-CG-CD1	-6.03	116.58	120.80
1	10-A	125	GLU	CB-CG-CD	-6.03	97.92	114.20
1	13-A	154	PHE	CZ-CE2-CD2	6.03	127.33	120.10
1	13-A	45	TYR	CB-CA-C	-6.03	98.35	110.40
1	14-A	44	MET	CA-CB-CG	-6.03	103.06	113.30
1	12-A	63	PRO	N-CD-CG	-6.02	94.17	103.20
1	8-A	136	MET	O-C-N	6.02	132.33	122.70
1	10-A	64	PHE	CD1-CG-CD2	6.02	126.12	118.30
1	13-A	150	ILE	O-C-N	6.02	132.33	122.70
1	14-A	106	ARG	CA-CB-CG	-6.02	100.17	113.40
1	14-A	111	ILE	CA-CB-CG2	6.01	122.93	110.90
1	16-A	64	PHE	CD1-CG-CD2	6.01	126.12	118.30
1	8-A	121	TRP	CG-CD1-NE1	-6.01	104.09	110.10
1	13-A	46	GLN	O-C-N	-6.01	113.08	122.70
1	9-A	140	TRP	CD1-CG-CD2	6.01	111.11	106.30
1	3-A	104	GLU	N-CA-C	-6.01	94.78	111.00
1	5-A	128	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	5-A	67	TRP	CA-CB-CG	-6.00	102.29	113.70
1	10-A	64	PHE	CB-CA-C	-6.00	98.39	110.40
1	13-A	154	PHE	CB-CG-CD2	6.00	125.00	120.80
1	13-A	38	LEU	CB-CG-CD1	6.00	121.20	111.00
1	11-A	107	LEU	CA-CB-CG	-6.00	101.50	115.30
1	9-A	76	GLN	CA-C-O	-6.00	107.51	120.10
1	8-A	154	PHE	CZ-CE2-CD2	5.99	127.29	120.10
1	13-A	136	MET	O-C-N	5.99	132.29	122.70
1	14-A	66	SER	CA-CB-OG	-5.99	95.02	111.20
1	9-A	67	TRP	CE2-CD2-CE3	5.99	125.89	118.70
1	12-A	148	SER	CA-C-N	-5.99	104.03	117.20
1	2-A	45	TYR	CG-CD2-CE2	5.99	126.09	121.30
1	5-A	58	ARG	CD-NE-CZ	-5.99	115.22	123.60
1	11-A	113	PRO	CA-N-CD	-5.98	103.13	111.50
1	2-A	143	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	13-A	48	TYR	CA-CB-CG	-5.98	102.04	113.40
1	16-A	78	TYR	CB-CG-CD1	5.98	124.59	121.00
1	11-A	118	ALA	O-C-N	5.97	132.26	122.70
1	16-A	111	ILE	C-N-CA	-5.97	106.77	121.70
1	15-A	105	GLN	C-N-CA	-5.97	106.77	121.70
1	3-A	98	PHE	CA-C-O	5.97	132.64	120.10
1	5-A	45	TYR	CZ-CE2-CD2	5.97	125.17	119.80
1	16-A	118	ALA	C-N-CA	-5.97	106.77	121.70
1	16-A	140	TRP	C-N-CA	-5.97	106.78	121.70
1	11-A	98	PHE	CA-C-N	-5.97	104.27	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	89	LEU	CA-CB-CG	5.96	129.02	115.30
1	5-A	42	ALA	CB-CA-C	5.96	119.05	110.10
1	5-A	91	GLN	N-CA-CB	-5.96	99.86	110.60
1	9-A	107	LEU	CA-C-O	-5.96	107.57	120.10
1	16-A	108	ASP	OD1-CG-OD2	5.96	134.63	123.30
1	7-A	131	PRO	C-N-CA	-5.96	106.80	121.70
1	13-A	89	LEU	N-CA-C	5.96	127.09	111.00
1	9-A	40	ARG	N-CA-CB	5.96	121.32	110.60
1	16-A	81	PRO	O-C-N	5.96	132.23	122.70
1	4-A	128	ARG	CD-NE-CZ	-5.96	115.26	123.60
1	4-A	123	VAL	CA-CB-CG1	-5.95	101.97	110.90
1	10-A	121	TRP	N-CA-C	5.95	127.07	111.00
1	14-A	83	HIS	CB-CA-C	-5.95	98.50	110.40
1	2-A	145	MET	CA-CB-CG	-5.95	103.19	113.30
1	8-A	68	VAL	CA-C-N	5.95	128.10	116.20
1	8-A	118	ALA	CA-C-O	-5.95	107.61	120.10
1	7-A	44	MET	CA-CB-CG	-5.95	103.19	113.30
1	1-A	97	ARG	CB-CG-CD	-5.94	96.14	111.60
1	5-A	48	TYR	CA-C-O	5.94	132.58	120.10
1	9-A	106	ARG	C-N-CA	-5.94	106.84	121.70
1	3-A	97	ARG	NH1-CZ-NH2	5.94	125.93	119.40
1	5-A	61	LEU	CB-CG-CD1	5.93	121.09	111.00
1	1-A	118	ALA	C-N-CA	-5.93	106.87	121.70
1	6-A	135	HIS	O-C-N	5.93	132.19	122.70
1	12-A	67	TRP	CG-CD2-CE3	-5.93	128.56	133.90
1	12-A	125	GLU	CG-CD-OE2	-5.93	106.44	118.30
1	9-A	89	LEU	CA-CB-CG	-5.93	101.67	115.30
1	15-A	50	LYS	O-C-N	-5.93	113.22	122.70
1	9-A	128	ARG	CB-CG-CD	-5.93	96.19	111.60
1	12-A	78	TYR	CG-CD2-CE2	-5.93	116.56	121.30
1	13-A	93	TRP	CH2-CZ2-CE2	5.93	123.33	117.40
1	10-A	128	ARG	CA-C-O	-5.92	107.67	120.10
1	15-A	112	HIS	O-C-N	-5.92	109.85	121.10
1	15-A	78	TYR	CD1-CE1-CZ	5.92	125.13	119.80
1	12-A	112	HIS	CG-ND1-CE1	5.92	116.48	108.20
1	16-A	73	SER	CA-CB-OG	-5.92	95.23	111.20
1	6-A	92	ARG	CG-CD-NE	-5.92	99.38	111.80
1	13-A	98	PHE	CA-C-N	-5.92	104.37	116.20
1	13-A	126	ILE	CB-CA-C	-5.91	99.78	111.60
1	4-A	62	ILE	CB-CG1-CD1	-5.91	97.35	113.90
1	9-A	93	TRP	CA-C-O	-5.91	107.69	120.10
1	15-A	92	ARG	N-CA-CB	-5.91	99.96	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-A	106	ARG	NE-CZ-NH1	-5.91	117.34	120.30
1	5-A	144	PRO	CA-C-N	-5.91	104.20	117.20
1	14-A	67	TRP	CG-CD2-CE3	5.91	139.22	133.90
1	15-A	119	THR	O-C-N	5.91	132.15	122.70
1	15-A	92	ARG	CA-CB-CG	-5.91	100.41	113.40
1	15-A	131	PRO	CA-N-CD	5.90	119.97	111.70
1	10-A	131	PRO	C-N-CA	-5.90	106.95	121.70
1	4-A	97	ARG	NH1-CZ-NH2	-5.90	112.91	119.40
1	7-A	113	PRO	CA-CB-CG	-5.90	92.79	104.00
1	9-A	118	ALA	CA-C-N	-5.90	104.22	117.20
1	11-A	64	PHE	CZ-CE2-CD2	-5.90	113.02	120.10
1	14-A	131	PRO	C-N-CA	-5.90	106.95	121.70
1	14-A	135	HIS	N-CA-CB	-5.90	99.98	110.60
1	2-A	58	ARG	CG-CD-NE	-5.90	99.41	111.80
1	16-A	129	LEU	CB-CG-CD1	-5.90	100.97	111.00
1	7-A	101	ASP	N-CA-CB	-5.90	99.98	110.60
1	16-A	130	THR	CA-CB-CG2	-5.90	104.14	112.40
1	10-A	107	LEU	CA-C-O	-5.89	107.72	120.10
1	11-A	39	LEU	N-CA-C	5.89	126.91	111.00
1	10-A	45	TYR	N-CA-CB	-5.89	99.99	110.60
1	6-A	124	GLU	N-CA-CB	-5.89	100.00	110.60
1	6-A	61	LEU	CB-CG-CD2	-5.89	100.99	111.00
1	14-A	131	PRO	CA-C-N	-5.89	104.24	117.20
1	13-A	62	ILE	CA-CB-CG2	-5.89	99.13	110.90
1	7-A	45	TYR	CB-CG-CD1	5.88	124.53	121.00
1	8-A	109	SER	N-CA-CB	-5.88	101.67	110.50
1	7-A	131	PRO	CA-C-N	-5.88	104.26	117.20
1	1-A	39	LEU	CB-CA-C	-5.88	99.03	110.20
1	3-A	107	LEU	CA-C-O	-5.88	107.75	120.10
1	11-A	81	PRO	O-C-N	5.88	132.11	122.70
1	15-A	71	SER	C-N-CA	-5.88	107.00	121.70
1	16-A	45	TYR	CA-CB-CG	-5.88	102.23	113.40
1	1-A	81	PRO	O-C-N	5.88	132.10	122.70
1	8-A	39	LEU	CB-CA-C	-5.88	99.03	110.20
1	11-A	104	GLU	CG-CD-OE1	-5.88	106.54	118.30
1	14-A	48	TYR	C-N-CA	-5.88	107.01	121.70
1	14-A	62	ILE	CB-CA-C	-5.88	99.85	111.60
1	8-A	151	ASP	CB-CA-C	-5.87	98.65	110.40
1	15-A	117	GLU	C-N-CA	-5.87	107.01	121.70
1	14-A	152	PRO	CA-CB-CG	-5.87	92.84	104.00
1	5-A	38	LEU	CA-CB-CG	-5.87	101.80	115.30
1	6-A	61	LEU	CB-CG-CD1	5.87	120.98	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	101	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	10-A	41	ARG	CG-CD-NE	-5.87	99.48	111.80
1	12-A	115	LYS	CD-CE-NZ	-5.87	98.21	111.70
1	4-A	148	SER	CA-C-N	-5.86	104.30	117.20
1	10-A	128	ARG	CA-C-N	5.86	130.10	117.20
1	16-A	70	LEU	C-N-CA	5.86	136.36	121.70
1	1-A	152	PRO	O-C-N	-5.86	113.32	122.70
1	8-A	151	ASP	N-CA-C	5.86	126.82	111.00
1	16-A	78	TYR	CB-CG-CD2	-5.86	117.48	121.00
1	1-A	97	ARG	CG-CD-NE	5.86	124.10	111.80
1	2-A	106	ARG	CA-C-N	-5.86	104.31	117.20
1	13-A	136	MET	CB-CG-SD	-5.86	94.83	112.40
1	12-A	45	TYR	CB-CG-CD1	5.86	124.51	121.00
1	15-A	125	GLU	CG-CD-OE2	-5.86	106.59	118.30
1	13-A	129	LEU	C-N-CA	-5.85	107.07	121.70
1	1-A	134	LEU	CD1-CG-CD2	-5.85	92.95	110.50
1	8-A	131	PRO	CA-CB-CG	-5.85	92.88	104.00
1	14-A	90	LEU	CB-CA-C	-5.85	99.08	110.20
1	2-A	37	SER	N-CA-CB	-5.85	101.73	110.50
1	15-A	98	PHE	C-N-CA	-5.85	110.02	122.30
1	15-A	123	VAL	CA-CB-CG1	-5.85	102.13	110.90
1	15-A	143	ASP	N-CA-CB	-5.85	100.07	110.60
1	2-A	107	LEU	O-C-N	5.84	132.05	122.70
1	13-A	61	LEU	CB-CG-CD1	-5.84	101.07	111.00
1	13-A	63	PRO	CA-N-CD	5.84	119.88	111.70
1	15-A	48	TYR	O-C-N	5.84	132.05	122.70
1	13-A	77	LEU	C-N-CA	-5.84	107.11	121.70
1	14-A	98	PHE	O-C-N	5.84	133.12	123.20
1	16-A	90	LEU	CB-CG-CD2	-5.84	101.08	111.00
1	4-A	63	PRO	C-N-CA	-5.83	107.12	121.70
1	12-A	136	MET	CG-SD-CE	5.83	109.53	100.20
1	11-A	60	SER	O-C-N	5.83	132.03	122.70
1	1-A	110	ILE	O-C-N	5.83	132.02	122.70
1	15-A	43	GLU	CG-CD-OE2	-5.83	106.65	118.30
1	9-A	109	SER	N-CA-CB	-5.82	101.77	110.50
1	16-A	108	ASP	CA-CB-CG	-5.82	100.59	113.40
1	1-A	135	HIS	CB-CA-C	-5.82	98.76	110.40
1	15-A	48	TYR	CE1-CZ-CE2	5.82	129.11	119.80
1	8-A	97	ARG	CA-C-O	-5.82	107.88	120.10
1	12-A	45	TYR	CZ-CE2-CD2	5.82	125.04	119.80
1	13-A	107	LEU	N-CA-CB	-5.82	98.76	110.40
1	6-A	40	ARG	CB-CA-C	-5.81	98.78	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	12-A	146	TYR	CG-CD2-CE2	-5.81	116.65	121.30
1	1-A	74	MET	CB-CA-C	-5.81	98.78	110.40
1	5-A	61	LEU	CA-CB-CG	-5.81	101.94	115.30
1	3-A	73	SER	N-CA-CB	5.81	119.21	110.50
1	10-A	63	PRO	N-CD-CG	-5.81	94.49	103.20
1	2-A	118	ALA	CA-C-O	-5.80	107.91	120.10
1	11-A	60	SER	CA-CB-OG	-5.80	95.54	111.20
1	15-A	124	GLU	N-CA-C	-5.80	95.34	111.00
1	1-A	48	TYR	CG-CD1-CE1	-5.80	116.66	121.30
1	5-A	107	LEU	CA-C-O	-5.80	107.92	120.10
1	10-A	45	TYR	CE1-CZ-OH	5.80	135.76	120.10
1	4-A	47	ASP	CA-C-N	5.80	129.96	117.20
1	16-A	40	ARG	CB-CG-CD	-5.80	96.53	111.60
1	9-A	97	ARG	NH1-CZ-NH2	-5.80	113.02	119.40
1	11-A	87	ASN	CB-CG-ND2	5.80	130.61	116.70
1	11-A	36	GLY	O-C-N	5.79	131.97	122.70
1	6-A	74	MET	CB-CA-C	-5.79	98.82	110.40
1	15-A	76	GLN	CA-C-O	-5.79	107.94	120.10
1	15-A	113	PRO	N-CA-CB	5.79	110.25	103.30
1	8-A	98	PHE	CB-CG-CD1	5.79	124.85	120.80
1	12-A	153	ILE	CA-CB-CG1	-5.79	100.00	111.00
1	15-A	72	ILE	N-CA-CB	-5.79	97.49	110.80
1	6-A	141	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	3-A	73	SER	CA-C-N	-5.78	104.48	117.20
1	9-A	76	GLN	CG-CD-NE2	5.78	130.58	116.70
1	14-A	124	GLU	CA-C-N	-5.78	104.48	117.20
1	11-A	109	SER	CA-CB-OG	-5.78	95.59	111.20
1	8-A	45	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	16-A	142	SER	N-CA-CB	5.78	119.17	110.50
1	10-A	121	TRP	CE2-CD2-CG	-5.78	102.68	107.30
1	16-A	45	TYR	CD1-CE1-CZ	5.78	125.00	119.80
1	15-A	110	ILE	CA-C-O	-5.78	107.97	120.10
1	14-A	74	MET	CA-CB-CG	-5.77	103.48	113.30
1	7-A	45	TYR	N-CA-CB	-5.77	100.21	110.60
1	9-A	138	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	11-A	108	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	13-A	109	SER	CB-CA-C	-5.77	99.13	110.10
1	14-A	40	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	2-A	58	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	13-A	49	MET	CG-SD-CE	5.77	109.43	100.20
1	9-A	107	LEU	N-CA-CB	-5.77	98.86	110.40
1	16-A	78	TYR	CD1-CE1-CZ	5.77	124.99	119.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	39	LEU	CA-CB-CG	-5.77	102.04	115.30
1	8-A	70	LEU	CD1-CG-CD2	-5.77	93.20	110.50
1	2-A	65	THR	CB-CA-C	-5.76	96.03	111.60
1	6-A	92	ARG	CB-CG-CD	-5.76	96.61	111.60
1	8-A	58	ARG	NH1-CZ-NH2	5.76	125.74	119.40
1	10-A	98	PHE	CA-C-N	-5.76	104.67	116.20
1	12-A	45	TYR	N-CA-CB	-5.76	100.22	110.60
1	12-A	78	TYR	CB-CG-CD1	5.76	124.46	121.00
1	7-A	40	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	9-A	137	ALA	CA-C-N	-5.76	104.53	117.20
1	3-A	108	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	6-A	91	GLN	N-CA-CB	-5.76	100.24	110.60
1	11-A	43	GLU	CA-C-N	-5.76	104.53	117.20
1	13-A	121	TRP	CA-C-O	-5.76	108.01	120.10
1	15-A	91	GLN	N-CA-C	5.76	126.54	111.00
1	5-A	145	MET	CA-CB-CG	-5.75	103.52	113.30
1	13-A	125	GLU	CB-CG-CD	-5.75	98.67	114.20
1	2-A	58	ARG	CB-CG-CD	-5.75	96.64	111.60
1	9-A	90	LEU	CA-C-O	-5.75	108.02	120.10
1	13-A	65	THR	CA-C-O	-5.75	108.02	120.10
1	15-A	72	ILE	CG1-CB-CG2	-5.75	98.75	111.40
1	14-A	61	LEU	N-CA-C	-5.75	95.49	111.00
1	12-A	104	GLU	CG-CD-OE1	-5.74	106.81	118.30
1	13-A	135	HIS	O-C-N	5.74	131.89	122.70
1	13-A	43	GLU	CA-CB-CG	-5.74	100.77	113.40
1	14-A	41	ARG	C-N-CA	-5.74	107.34	121.70
1	13-A	135	HIS	N-CA-C	5.74	126.50	111.00
1	1-A	50	LYS	CD-CE-NZ	-5.73	98.51	111.70
1	4-A	70	LEU	N-CA-C	-5.73	95.52	111.00
1	4-A	76	GLN	CB-CG-CD	5.73	126.50	111.60
1	2-A	61	LEU	CB-CA-C	5.73	121.09	110.20
1	4-A	43	GLU	CG-CD-OE2	-5.73	106.84	118.30
1	8-A	107	LEU	CB-CG-CD1	-5.73	101.26	111.00
1	15-A	81	PRO	C-N-CA	-5.73	107.37	121.70
1	8-A	43	GLU	CG-CD-OE2	-5.73	106.84	118.30
1	16-A	77	LEU	CD1-CG-CD2	-5.73	93.31	110.50
1	5-A	56	THR	OG1-CB-CG2	-5.73	96.83	110.00
1	9-A	143	ASP	OD1-CG-OD2	-5.72	112.42	123.30
1	15-A	46	GLN	O-C-N	-5.72	113.55	122.70
1	16-A	106	ARG	CB-CG-CD	-5.72	96.73	111.60
1	8-A	58	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	10-A	130	THR	CA-CB-CG2	-5.71	104.40	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	15-A	63	PRO	CA-N-CD	5.71	119.70	111.70
1	14-A	85	LEU	CD1-CG-CD2	-5.71	93.37	110.50
1	3-A	149	PHE	CG-CD2-CE2	-5.71	114.52	120.80
1	13-A	106	ARG	CD-NE-CZ	5.71	131.59	123.60
1	10-A	69	GLY	O-C-N	5.71	131.83	122.70
1	4-A	89	LEU	CA-CB-CG	-5.71	102.18	115.30
1	7-A	125	GLU	CG-CD-OE2	-5.71	106.89	118.30
1	16-A	62	ILE	CA-CB-CG2	-5.71	99.49	110.90
1	8-A	135	HIS	O-C-N	5.70	131.82	122.70
1	12-A	107	LEU	CB-CG-CD2	-5.70	101.31	111.00
1	16-A	148	SER	CB-CA-C	-5.70	99.27	110.10
1	7-A	122	LEU	CB-CG-CD1	-5.70	101.32	111.00
1	12-A	138	LEU	N-CA-C	5.70	126.38	111.00
1	3-A	149	PHE	CD1-CG-CD2	5.69	125.70	118.30
1	12-A	44	MET	CA-CB-CG	-5.69	103.62	113.30
1	8-A	41	ARG	O-C-N	5.69	131.81	122.70
1	3-A	113	PRO	N-CD-CG	-5.69	94.66	103.20
1	16-A	89	LEU	N-CA-CB	-5.69	99.02	110.40
1	16-A	135	HIS	C-N-CA	-5.69	107.48	121.70
1	12-A	140	TRP	C-N-CA	-5.69	107.48	121.70
1	4-A	151	ASP	OD1-CG-OD2	-5.68	112.50	123.30
1	2-A	134	LEU	CD1-CG-CD2	-5.68	93.45	110.50
1	6-A	48	TYR	CB-CG-CD2	5.68	124.41	121.00
1	16-A	146	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	4-A	37	SER	CA-CB-OG	-5.68	95.86	111.20
1	15-A	90	LEU	C-N-CA	-5.68	107.50	121.70
1	2-A	139	LEU	C-N-CA	-5.68	107.50	121.70
1	16-A	47	ASP	N-CA-C	-5.68	95.67	111.00
1	10-A	107	LEU	CA-CB-CG	-5.68	102.24	115.30
1	4-A	149	PHE	CZ-CE2-CD2	-5.68	113.29	120.10
1	5-A	58	ARG	NH1-CZ-NH2	5.68	125.64	119.40
1	15-A	89	LEU	O-C-N	5.68	131.78	122.70
1	2-A	138	LEU	CA-CB-CG	5.67	128.35	115.30
1	15-A	45	TYR	CA-CB-CG	-5.67	102.62	113.40
1	1-A	57	ASN	O-C-N	5.67	131.78	122.70
1	1-A	38	LEU	CB-CA-C	5.67	120.98	110.20
1	6-A	134	LEU	CB-CG-CD2	-5.67	101.36	111.00
1	14-A	75	LYS	O-C-N	5.67	131.78	122.70
1	16-A	40	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	1-A	60	SER	CB-CA-C	-5.67	99.33	110.10
1	7-A	76	GLN	CA-C-O	5.67	132.01	120.10
1	8-A	71	SER	CA-C-N	-5.67	104.72	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13-A	143	ASP	N-CA-CB	-5.67	100.39	110.60
1	6-A	40	ARG	C-N-CA	-5.67	107.53	121.70
1	9-A	142	SER	CA-CB-OG	-5.67	95.89	111.20
1	10-A	45	TYR	OH-CZ-CE2	-5.66	104.81	120.10
1	11-A	103	GLU	O-C-N	5.66	131.76	122.70
1	15-A	55	PRO	N-CD-CG	-5.66	94.70	103.20
1	16-A	132	SER	C-N-CA	-5.66	107.54	121.70
1	10-A	135	HIS	CB-CA-C	-5.66	99.08	110.40
1	14-A	78	TYR	CG-CD2-CE2	-5.66	116.77	121.30
1	14-A	58	ARG	NH1-CZ-NH2	5.66	125.62	119.40
1	4-A	67	TRP	NE1-CE2-CD2	-5.66	101.64	107.30
1	11-A	83	HIS	CG-ND1-CE1	5.66	116.12	108.20
1	10-A	148	SER	CA-C-N	-5.66	104.76	117.20
1	4-A	106	ARG	NE-CZ-NH2	5.65	123.13	120.30
1	5-A	40	ARG	C-N-CA	-5.65	107.57	121.70
1	7-A	112	HIS	CG-ND1-CE1	5.65	116.11	108.20
1	10-A	108	ASP	N-CA-C	5.65	126.26	111.00
1	10-A	120	ILE	CG1-CB-CG2	-5.65	98.97	111.40
1	4-A	41	ARG	C-N-CA	-5.65	107.58	121.70
1	12-A	43	GLU	CG-CD-OE2	-5.65	107.01	118.30
1	5-A	55	PRO	C-N-CA	-5.64	107.59	121.70
1	12-A	151	ASP	CB-CG-OD1	5.64	123.38	118.30
1	1-A	133	HIS	O-C-N	5.64	131.73	122.70
1	9-A	145	MET	CG-SD-CE	5.64	109.23	100.20
1	14-A	143	ASP	N-CA-CB	-5.64	100.45	110.60
1	12-A	116	ALA	O-C-N	-5.64	113.68	122.70
1	15-A	144	PRO	N-CD-CG	-5.64	94.74	103.20
1	14-A	70	LEU	CB-CG-CD2	-5.63	101.42	111.00
1	5-A	121	TRP	O-C-N	5.63	131.71	122.70
1	4-A	72	ILE	CA-C-O	-5.63	108.28	120.10
1	2-A	55	PRO	CA-C-N	-5.63	104.82	117.20
1	15-A	118	ALA	CA-C-O	-5.63	108.28	120.10
1	1-A	43	GLU	CA-CB-CG	-5.62	101.03	113.40
1	13-A	97	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	15-A	57	ASN	C-N-CA	-5.62	107.66	121.70
1	7-A	139	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	9-A	85	LEU	CB-CG-CD2	-5.62	101.45	111.00
1	9-A	112	HIS	CG-ND1-CE1	5.62	116.06	108.20
1	8-A	37	SER	CB-CA-C	-5.61	99.43	110.10
1	15-A	54	ILE	CA-CB-CG1	-5.61	100.34	111.00
1	1-A	87	ASN	C-N-CA	-5.61	107.69	121.70
1	4-A	109	SER	CA-CB-OG	-5.61	96.07	111.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-A	109	SER	CB-CA-C	-5.61	99.45	110.10
1	10-A	40	ARG	C-N-CA	-5.60	107.69	121.70
1	7-A	78	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	7-A	98	PHE	CG-CD1-CE1	5.60	126.96	120.80
1	5-A	48	TYR	OH-CZ-CE2	-5.60	104.98	120.10
1	15-A	140	TRP	O-C-N	5.60	131.66	122.70
1	16-A	47	ASP	C-N-CA	-5.60	107.70	121.70
1	5-A	138	LEU	N-CA-C	-5.60	95.89	111.00
1	16-A	91	GLN	N-CA-C	5.60	126.11	111.00
1	6-A	88	VAL	CG1-CB-CG2	5.60	119.85	110.90
1	7-A	75	LYS	N-CA-CB	5.60	120.67	110.60
1	4-A	73	SER	CA-C-N	-5.59	104.89	117.20
1	4-A	98	PHE	CA-C-O	5.59	131.85	120.10
1	4-A	112	HIS	CG-ND1-CE1	5.59	116.03	108.20
1	5-A	58	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	7-A	141	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	4-A	113	PRO	CA-CB-CG	-5.59	93.38	104.00
1	14-A	109	SER	CA-CB-OG	-5.59	96.10	111.20
1	15-A	94	ASP	O-C-N	5.59	131.64	122.70
1	4-A	64	PHE	CD1-CE1-CZ	-5.58	113.40	120.10
1	8-A	143	ASP	OD1-CG-OD2	-5.58	112.69	123.30
1	9-A	49	MET	N-CA-CB	-5.58	100.56	110.60
1	1-A	45	TYR	CA-CB-CG	-5.58	102.80	113.40
1	16-A	115	LYS	CA-C-O	-5.58	108.39	120.10
1	16-A	83	HIS	N-CA-CB	-5.57	100.57	110.60
1	10-A	138	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	2-A	91	GLN	O-C-N	-5.57	113.79	122.70
1	3-A	72	ILE	N-CA-CB	-5.57	98.00	110.80
1	5-A	123	VAL	CG1-CB-CG2	5.56	119.80	110.90
1	6-A	76	GLN	O-C-N	-5.56	113.80	122.70
1	2-A	105	GLN	C-N-CA	-5.56	107.80	121.70
1	2-A	144	PRO	CA-C-N	-5.56	104.97	117.20
1	12-A	61	LEU	CB-CG-CD1	5.56	120.45	111.00
1	13-A	64	PHE	CG-CD1-CE1	-5.56	114.68	120.80
1	5-A	81	PRO	C-N-CA	-5.56	107.81	121.70
1	16-A	89	LEU	CA-C-N	5.56	129.43	117.20
1	1-A	41	ARG	CA-CB-CG	5.55	125.62	113.40
1	2-A	58	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	10-A	124	GLU	N-CA-CB	-5.55	100.61	110.60
1	13-A	123	VAL	CA-CB-CG1	-5.55	102.57	110.90
1	10-A	121	TRP	NE1-CE2-CZ2	-5.55	124.30	130.40
1	3-A	44	MET	CA-CB-CG	-5.54	103.87	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	112	HIS	CG-ND1-CE1	5.54	115.96	108.20
1	2-A	113	PRO	N-CD-CG	-5.54	94.89	103.20
1	7-A	138	LEU	N-CA-CB	-5.54	99.32	110.40
1	10-A	84	TYR	CG-CD1-CE1	-5.54	116.87	121.30
1	13-A	148	SER	O-C-N	5.54	131.56	122.70
1	15-A	137	ALA	N-CA-CB	-5.54	102.35	110.10
1	2-A	80	GLN	CG-CD-OE1	-5.54	110.53	121.60
1	8-A	49	MET	C-N-CA	-5.54	107.86	121.70
1	9-A	86	THR	N-CA-CB	-5.54	99.78	110.30
1	14-A	119	THR	OG1-CB-CG2	5.54	122.73	110.00
1	7-A	71	SER	N-CA-CB	5.53	118.80	110.50
1	10-A	153	ILE	CA-CB-CG1	-5.53	100.49	111.00
1	2-A	47	ASP	O-C-N	5.53	131.55	122.70
1	6-A	43	GLU	CG-CD-OE1	-5.53	107.24	118.30
1	10-A	107	LEU	CD1-CG-CD2	-5.53	93.91	110.50
1	14-A	129	LEU	CB-CA-C	5.53	120.70	110.20
1	11-A	78	TYR	CA-CB-CG	-5.53	102.90	113.40
1	11-A	89	LEU	CD1-CG-CD2	-5.53	93.92	110.50
1	14-A	140	TRP	CA-CB-CG	-5.53	103.20	113.70
1	15-A	94	ASP	C-N-CA	-5.52	107.89	121.70
1	16-A	40	ARG	CB-CA-C	-5.52	99.36	110.40
1	16-A	53	PRO	N-CA-CB	5.52	109.93	103.30
1	16-A	98	PHE	C-N-CA	-5.52	110.70	122.30
1	4-A	95	GLN	O-C-N	-5.52	113.87	122.70
1	11-A	145	MET	CA-CB-CG	-5.52	103.92	113.30
1	3-A	41	ARG	O-C-N	5.52	131.53	122.70
1	13-A	56	THR	C-N-CA	-5.52	107.90	121.70
1	13-A	128	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	14-A	140	TRP	CB-CG-CD1	5.52	134.17	127.00
1	2-A	107	LEU	CA-C-O	-5.51	108.52	120.10
1	2-A	131	PRO	CB-CG-CD	5.51	128.01	106.50
1	8-A	121	TRP	CD1-CG-CD2	5.51	110.71	106.30
1	13-A	112	HIS	N-CA-CB	-5.51	100.67	110.60
1	8-A	55	PRO	N-CA-CB	-5.51	96.54	102.60
1	16-A	112	HIS	N-CA-CB	-5.51	100.68	110.60
1	9-A	124	GLU	OE1-CD-OE2	5.51	129.91	123.30
1	16-A	53	PRO	CB-CG-CD	5.51	127.98	106.50
1	4-A	60	SER	CB-CA-C	-5.51	99.64	110.10
1	15-A	43	GLU	CA-CB-CG	-5.51	101.28	113.40
1	5-A	51	GLN	CA-C-O	-5.50	108.54	120.10
1	3-A	137	ALA	C-N-CA	-5.50	107.95	121.70
1	8-A	103	GLU	O-C-N	5.50	131.50	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	11-A	57	ASN	CA-C-N	-5.50	105.10	117.20
1	2-A	43	GLU	CG-CD-OE2	-5.50	107.31	118.30
1	9-A	143	ASP	N-CA-C	-5.50	96.16	111.00
1	10-A	121	TRP	CB-CG-CD2	5.50	133.75	126.60
1	16-A	47	ASP	N-CA-CB	-5.50	100.71	110.60
1	9-A	57	ASN	CA-C-N	-5.49	105.11	117.20
1	5-A	41	ARG	O-C-N	5.49	131.49	122.70
1	13-A	79	GLY	O-C-N	5.49	131.49	122.70
1	6-A	143	ASP	OD1-CG-OD2	-5.49	112.87	123.30
1	10-A	141	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	11-A	92	ARG	N-CA-CB	-5.49	100.73	110.60
1	14-A	91	GLN	CG-CD-OE1	5.48	132.57	121.60
1	13-A	140	TRP	O-C-N	5.48	131.47	122.70
1	15-A	101	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	16-A	91	GLN	CA-CB-CG	-5.48	101.34	113.40
1	6-A	112	HIS	CG-ND1-CE1	5.48	115.87	108.20
1	13-A	64	PHE	CD1-CG-CD2	5.48	125.42	118.30
1	14-A	121	TRP	CB-CG-CD1	-5.48	119.88	127.00
1	16-A	130	THR	CA-C-N	5.48	132.44	117.10
1	16-A	65	THR	C-N-CA	-5.48	108.01	121.70
1	6-A	153	ILE	CB-CA-C	-5.47	100.65	111.60
1	1-A	106	ARG	C-N-CA	-5.47	108.02	121.70
1	5-A	64	PHE	CG-CD1-CE1	-5.47	114.78	120.80
1	8-A	81	PRO	C-N-CA	-5.47	108.02	121.70
1	15-A	61	LEU	CA-C-O	5.47	131.59	120.10
1	12-A	112	HIS	CA-C-O	5.47	131.59	120.10
1	1-A	132	SER	C-N-CA	-5.47	108.02	121.70
1	2-A	152	PRO	CA-N-CD	5.47	119.36	111.70
1	16-A	52	VAL	CA-CB-CG2	-5.47	102.69	110.90
1	8-A	61	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	7-A	73	SER	CA-C-N	-5.47	105.17	117.20
1	14-A	86	THR	CA-CB-OG1	-5.47	97.52	109.00
1	1-A	98	PHE	CB-CG-CD2	-5.46	116.98	120.80
1	10-A	140	TRP	NE1-CE2-CD2	5.46	112.77	107.30
1	16-A	105	GLN	CB-CA-C	-5.46	99.47	110.40
1	6-A	41	ARG	C-N-CA	-5.46	108.05	121.70
1	2-A	112	HIS	CG-ND1-CE1	5.46	115.84	108.20
1	13-A	68	VAL	O-C-N	5.46	132.48	123.20
1	15-A	89	LEU	N-CA-C	5.46	125.74	111.00
1	16-A	87	ASN	CA-C-O	5.46	131.56	120.10
1	2-A	63	PRO	O-C-N	-5.46	113.97	122.70
1	14-A	84	TYR	CG-CD1-CE1	5.46	125.67	121.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	98	PHE	CB-CG-CD1	5.46	124.62	120.80
1	1-A	59	GLY	O-C-N	-5.45	113.97	122.70
1	9-A	40	ARG	O-C-N	5.45	131.43	122.70
1	13-A	71	SER	C-N-CA	-5.45	108.07	121.70
1	15-A	41	ARG	CG-CD-NE	-5.45	100.35	111.80
1	4-A	44	MET	CA-CB-CG	-5.45	104.03	113.30
1	8-A	108	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	2-A	137	ALA	CB-CA-C	5.45	118.28	110.10
1	4-A	75	LYS	N-CA-CB	-5.45	100.79	110.60
1	3-A	73	SER	CA-C-O	5.45	131.54	120.10
1	8-A	150	ILE	CG1-CB-CG2	-5.45	99.41	111.40
1	1-A	119	THR	N-CA-C	5.45	125.71	111.00
1	7-A	151	ASP	N-CA-CB	-5.45	100.80	110.60
1	12-A	152	PRO	CA-N-CD	5.45	119.33	111.70
1	8-A	152	PRO	N-CD-CG	-5.44	95.03	103.20
1	14-A	41	ARG	CG-CD-NE	-5.44	100.37	111.80
1	7-A	91	GLN	N-CA-CB	-5.44	100.81	110.60
1	8-A	40	ARG	NH1-CZ-NH2	5.44	125.38	119.40
1	11-A	45	TYR	O-C-N	5.44	131.40	122.70
1	7-A	75	LYS	CA-CB-CG	-5.44	101.44	113.40
1	16-A	68	VAL	N-CA-C	-5.44	96.32	111.00
1	1-A	41	ARG	C-N-CA	-5.44	108.11	121.70
1	1-A	92	ARG	CA-C-O	-5.44	108.68	120.10
1	16-A	67	TRP	NE1-CE2-CD2	5.44	112.74	107.30
1	6-A	146	TYR	CD1-CE1-CZ	-5.43	114.91	119.80
1	9-A	153	ILE	CG1-CB-CG2	5.43	123.36	111.40
1	10-A	125	GLU	C-N-CA	-5.43	108.11	121.70
1	13-A	98	PHE	CB-CG-CD1	5.43	124.60	120.80
1	3-A	115	LYS	CB-CG-CD	-5.43	97.48	111.60
1	8-A	71	SER	C-N-CA	-5.43	108.12	121.70
1	10-A	69	GLY	CA-C-N	-5.43	105.25	117.20
1	16-A	116	ALA	C-N-CA	-5.43	108.13	121.70
1	12-A	67	TRP	NE1-CE2-CZ2	5.43	136.37	130.40
1	14-A	132	SER	N-CA-CB	-5.43	102.36	110.50
1	15-A	72	ILE	CA-CB-CG1	-5.42	100.70	111.00
1	5-A	91	GLN	CB-CA-C	-5.42	99.56	110.40
1	10-A	42	ALA	CB-CA-C	5.42	118.23	110.10
1	1-A	154	PHE	CB-CA-C	-5.42	99.56	110.40
1	15-A	85	LEU	C-N-CA	-5.42	108.15	121.70
1	4-A	73	SER	O-C-N	5.42	131.37	122.70
1	5-A	90	LEU	N-CA-C	5.41	125.62	111.00
1	12-A	37	SER	CA-CB-OG	-5.41	96.58	111.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	15-A	55	PRO	N-CA-CB	-5.41	96.65	102.60
1	1-A	60	SER	CA-C-N	-5.41	105.30	117.20
1	8-A	50	LYS	N-CA-CB	-5.41	100.86	110.60
1	9-A	95	GLN	CA-C-O	5.41	131.46	120.10
1	16-A	82	LEU	CA-CB-CG	-5.41	102.86	115.30
1	2-A	120	ILE	CG1-CB-CG2	-5.41	99.50	111.40
1	3-A	112	HIS	CG-ND1-CE1	5.41	115.77	108.20
1	13-A	43	GLU	CG-CD-OE2	-5.41	107.48	118.30
1	15-A	41	ARG	C-N-CA	-5.41	108.18	121.70
1	4-A	71	SER	C-N-CA	-5.41	108.18	121.70
1	15-A	65	THR	OG1-CB-CG2	5.41	122.44	110.00
1	16-A	152	PRO	N-CD-CG	-5.40	95.10	103.20
1	1-A	110	ILE	CB-CG1-CD1	-5.40	98.78	113.90
1	6-A	98	PHE	CB-CG-CD1	5.40	124.58	120.80
1	13-A	48	TYR	O-C-N	5.40	131.34	122.70
1	1-A	54	ILE	CG1-CB-CG2	5.40	123.28	111.40
1	10-A	84	TYR	CE1-CZ-OH	-5.40	105.53	120.10
1	13-A	80	GLN	CB-CG-CD	-5.40	97.56	111.60
1	14-A	121	TRP	N-CA-CB	-5.40	100.89	110.60
1	12-A	103	GLU	O-C-N	5.40	131.33	122.70
1	14-A	109	SER	CB-CA-C	-5.40	99.85	110.10
1	6-A	91	GLN	CA-CB-CG	-5.39	101.53	113.40
1	8-A	74	MET	CA-CB-CG	-5.39	104.13	113.30
1	14-A	45	TYR	N-CA-CB	-5.39	100.89	110.60
1	1-A	64	PHE	CG-CD1-CE1	-5.39	114.87	120.80
1	1-A	79	GLY	O-C-N	5.39	131.32	122.70
1	7-A	106	ARG	CB-CG-CD	-5.39	97.59	111.60
1	9-A	129	LEU	CA-C-O	5.39	131.42	120.10
1	9-A	138	LEU	CA-C-N	-5.39	105.35	117.20
1	11-A	145	MET	CG-SD-CE	5.39	108.82	100.20
1	3-A	104	GLU	CA-C-O	-5.38	108.80	120.10
1	5-A	53	PRO	N-CD-CG	-5.38	95.13	103.20
1	10-A	36	GLY	N-CA-C	5.38	126.55	113.10
1	10-A	74	MET	CG-SD-CE	-5.38	91.59	100.20
1	11-A	105	GLN	O-C-N	5.38	131.31	122.70
1	14-A	154	PHE	CZ-CE2-CD2	5.38	126.55	120.10
1	11-A	143	ASP	N-CA-C	-5.38	96.49	111.00
1	6-A	74	MET	CA-CB-CG	-5.37	104.17	113.30
1	6-A	82	LEU	C-N-CA	-5.37	108.27	121.70
1	8-A	98	PHE	CA-C-N	-5.37	105.45	116.20
1	15-A	104	GLU	C-N-CA	-5.37	108.27	121.70
1	2-A	68	VAL	O-C-N	5.37	132.33	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	11-A	75	LYS	O-C-N	5.37	131.29	122.70
1	14-A	41	ARG	CA-C-O	-5.37	108.82	120.10
1	5-A	48	TYR	CE1-CZ-CE2	5.37	128.39	119.80
1	9-A	133	HIS	CA-C-N	-5.37	105.40	117.20
1	11-A	80	GLN	CG-CD-OE1	-5.37	110.87	121.60
1	15-A	88	VAL	N-CA-CB	-5.37	99.70	111.50
1	12-A	61	LEU	CB-CA-C	5.36	120.39	110.20
1	13-A	42	ALA	CA-C-N	-5.36	105.40	117.20
1	12-A	115	LYS	CB-CG-CD	-5.36	97.66	111.60
1	13-A	88	VAL	C-N-CA	-5.36	108.30	121.70
1	15-A	40	ARG	CB-CA-C	-5.36	99.68	110.40
1	1-A	133	HIS	CA-C-O	-5.36	108.85	120.10
1	7-A	143	ASP	N-CA-C	-5.36	96.53	111.00
1	4-A	80	GLN	CB-CG-CD	5.36	125.53	111.60
1	6-A	144	PRO	CA-CB-CG	-5.36	93.82	104.00
1	7-A	70	LEU	CB-CG-CD2	-5.36	101.89	111.00
1	13-A	57	ASN	CA-C-N	-5.36	105.41	117.20
1	4-A	73	SER	CA-CB-OG	-5.36	96.74	111.20
1	11-A	43	GLU	CB-CA-C	5.36	121.11	110.40
1	4-A	41	ARG	CA-CB-CG	5.35	125.18	113.40
1	8-A	68	VAL	CA-CB-CG1	-5.35	102.87	110.90
1	2-A	117	GLU	CG-CD-OE1	-5.35	107.60	118.30
1	15-A	44	MET	CB-CG-SD	-5.35	96.35	112.40
1	15-A	152	PRO	N-CD-CG	-5.35	95.17	103.20
1	2-A	107	LEU	C-N-CA	-5.35	108.33	121.70
1	8-A	67	TRP	CD2-CE3-CZ3	5.35	125.75	118.80
1	12-A	150	ILE	CG1-CB-CG2	5.35	123.17	111.40
1	16-A	145	MET	C-N-CA	-5.34	108.34	121.70
1	7-A	44	MET	C-N-CA	-5.34	108.35	121.70
1	7-A	57	ASN	CA-C-N	-5.34	105.45	117.20
1	9-A	129	LEU	C-N-CA	-5.34	108.35	121.70
1	4-A	132	SER	C-N-CA	-5.34	108.35	121.70
1	12-A	132	SER	C-N-CA	-5.34	108.35	121.70
1	14-A	84	TYR	CA-C-O	-5.34	108.89	120.10
1	15-A	127	HIS	C-N-CA	-5.34	108.35	121.70
1	13-A	70	LEU	C-N-CA	-5.34	108.36	121.70
1	15-A	83	HIS	CG-CD2-NE2	-5.34	99.06	109.20
1	16-A	136	MET	C-N-CA	-5.34	108.36	121.70
1	14-A	72	ILE	N-CA-CB	-5.33	98.53	110.80
1	14-A	95	GLN	O-C-N	-5.33	114.17	122.70
1	9-A	135	HIS	CB-CA-C	-5.33	99.74	110.40
1	14-A	75	LYS	CD-CE-NZ	-5.33	99.44	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	136	MET	O-C-N	5.33	131.23	122.70
1	9-A	130	THR	CA-CB-CG2	-5.33	104.94	112.40
1	5-A	44	MET	CA-CB-CG	-5.33	104.24	113.30
1	10-A	107	LEU	C-N-CA	-5.33	108.38	121.70
1	6-A	109	SER	CB-CA-C	-5.33	99.98	110.10
1	16-A	73	SER	O-C-N	5.33	131.22	122.70
1	4-A	61	LEU	CD1-CG-CD2	-5.33	94.52	110.50
1	16-A	75	LYS	CA-C-N	-5.33	105.48	117.20
1	2-A	121	TRP	CD1-CG-CD2	5.32	110.56	106.30
1	12-A	78	TYR	CZ-CE2-CD2	5.32	124.59	119.80
1	15-A	143	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	2-A	56	THR	OG1-CB-CG2	-5.32	97.77	110.00
1	2-A	125	GLU	CB-CG-CD	-5.32	99.84	114.20
1	4-A	156	GLU	CA-C-O	5.32	131.27	120.10
1	8-A	47	ASP	N-CA-C	-5.32	96.65	111.00
1	10-A	138	LEU	CA-C-N	-5.32	105.50	117.20
1	15-A	95	GLN	CA-CB-CG	-5.31	101.72	113.40
1	8-A	55	PRO	N-CD-CG	-5.31	95.24	103.20
1	10-A	66	SER	CA-CB-OG	5.31	125.53	111.20
1	14-A	126	ILE	CA-C-N	-5.31	105.53	117.20
1	7-A	116	ALA	N-CA-C	-5.30	96.68	111.00
1	15-A	98	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	4-A	137	ALA	N-CA-CB	-5.30	102.68	110.10
1	10-A	137	ALA	CA-C-N	-5.30	105.54	117.20
1	2-A	149	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	4-A	133	HIS	C-N-CA	-5.30	108.45	121.70
1	8-A	110	ILE	CA-CB-CG2	-5.30	100.30	110.90
1	12-A	75	LYS	CA-C-O	-5.30	108.97	120.10
1	2-A	148	SER	O-C-N	5.30	131.18	122.70
1	6-A	45	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	1-A	122	LEU	CA-CB-CG	-5.30	103.12	115.30
1	9-A	42	ALA	CB-CA-C	5.30	118.05	110.10
1	11-A	53	PRO	N-CD-CG	-5.30	95.26	103.20
1	7-A	78	TYR	CG-CD2-CE2	-5.29	117.06	121.30
1	11-A	88	VAL	O-C-N	-5.29	114.23	122.70
1	4-A	45	TYR	CB-CG-CD2	-5.29	117.82	121.00
1	8-A	105	GLN	O-C-N	5.29	131.17	122.70
1	13-A	144	PRO	N-CD-CG	-5.29	95.26	103.20
1	14-A	48	TYR	CG-CD1-CE1	-5.29	117.07	121.30
1	6-A	47	ASP	CA-C-N	5.29	128.84	117.20
1	15-A	37	SER	N-CA-CB	-5.29	102.56	110.50
1	9-A	121	TRP	CZ3-CH2-CZ2	5.29	127.95	121.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	134	LEU	CD1-CG-CD2	-5.29	94.64	110.50
1	15-A	52	VAL	CA-C-O	-5.29	109.00	120.10
1	4-A	127	HIS	O-C-N	5.28	131.15	122.70
1	9-A	48	TYR	C-N-CA	-5.28	108.49	121.70
1	12-A	91	GLN	N-CA-C	-5.28	96.73	111.00
1	13-A	142	SER	CA-CB-OG	-5.28	96.94	111.20
1	14-A	61	LEU	CD1-CG-CD2	-5.28	94.66	110.50
1	14-A	148	SER	CA-C-N	-5.28	105.58	117.20
1	3-A	130	THR	CA-C-O	-5.28	109.01	120.10
1	10-A	127	HIS	CA-C-O	-5.28	109.01	120.10
1	13-A	93	TRP	CD2-CE3-CZ3	5.28	125.66	118.80
1	14-A	148	SER	CB-CA-C	5.28	120.13	110.10
1	6-A	57	ASN	CA-C-N	-5.28	105.59	117.20
1	9-A	41	ARG	C-N-CA	-5.28	108.51	121.70
1	13-A	123	VAL	CB-CA-C	5.28	121.42	111.40
1	16-A	116	ALA	CB-CA-C	-5.28	102.19	110.10
1	2-A	130	THR	O-C-N	5.27	131.12	121.10
1	4-A	79	GLY	O-C-N	5.27	131.14	122.70
1	15-A	149	PHE	CZ-CE2-CD2	-5.27	113.77	120.10
1	3-A	36	GLY	N-CA-C	5.27	126.28	113.10
1	12-A	70	LEU	CB-CG-CD1	5.27	119.96	111.00
1	10-A	93	TRP	CH2-CZ2-CE2	-5.27	112.13	117.40
1	11-A	125	GLU	CG-CD-OE2	-5.27	107.77	118.30
1	7-A	61	LEU	CB-CA-C	5.27	120.20	110.20
1	1-A	96	SER	N-CA-CB	-5.26	102.61	110.50
1	8-A	142	SER	CA-CB-OG	-5.26	96.99	111.20
1	14-A	81	PRO	CA-C-N	-5.26	105.62	117.20
1	1-A	121	TRP	CE2-CD2-CG	-5.26	103.09	107.30
1	5-A	125	GLU	CG-CD-OE2	-5.26	107.78	118.30
1	9-A	83	HIS	CA-CB-CG	-5.26	104.66	113.60
1	12-A	45	TYR	O-C-N	5.26	131.12	122.70
1	15-A	151	ASP	CB-CA-C	-5.26	99.88	110.40
1	13-A	108	ASP	N-CA-C	5.26	125.20	111.00
1	14-A	55	PRO	CA-C-N	-5.26	105.63	117.20
1	1-A	156	GLU	OE1-CD-OE2	5.26	129.61	123.30
1	2-A	138	LEU	CD1-CG-CD2	5.26	126.27	110.50
1	11-A	61	LEU	CB-CA-C	5.26	120.19	110.20
1	15-A	92	ARG	CB-CA-C	-5.26	99.89	110.40
1	9-A	74	MET	CA-CB-CG	-5.25	104.37	113.30
1	5-A	75	LYS	CA-C-O	-5.25	109.07	120.10
1	5-A	143	ASP	CB-CG-OD1	5.25	123.03	118.30
1	14-A	77	LEU	C-N-CA	-5.25	108.56	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	14-A	107	LEU	N-CA-CB	-5.25	99.89	110.40
1	9-A	95	GLN	O-C-N	-5.25	114.30	122.70
1	8-A	109	SER	CA-CB-OG	-5.25	97.03	111.20
1	15-A	74	MET	CA-CB-CG	-5.25	104.38	113.30
1	8-A	53	PRO	N-CD-CG	-5.25	95.33	103.20
1	16-A	105	GLN	O-C-N	5.24	131.09	122.70
1	2-A	89	LEU	O-C-N	5.24	131.08	122.70
1	3-A	71	SER	C-N-CA	-5.24	108.60	121.70
1	10-A	112	HIS	N-CA-CB	-5.24	101.17	110.60
1	16-A	48	TYR	CA-C-N	-5.24	105.67	117.20
1	6-A	95	GLN	O-C-N	-5.24	114.32	122.70
1	7-A	70	LEU	CB-CG-CD1	5.24	119.91	111.00
1	14-A	79	GLY	O-C-N	5.24	131.08	122.70
1	2-A	45	TYR	O-C-N	5.24	131.08	122.70
1	7-A	139	LEU	CA-CB-CG	-5.24	103.25	115.30
1	11-A	39	LEU	CA-C-O	-5.24	109.11	120.10
1	15-A	58	ARG	N-CA-CB	-5.23	101.18	110.60
1	16-A	112	HIS	CG-ND1-CE1	5.23	115.53	108.20
1	10-A	98	PHE	O-C-N	5.23	132.09	123.20
1	15-A	67	TRP	CE2-CD2-CE3	5.23	124.98	118.70
1	13-A	41	ARG	CG-CD-NE	-5.23	100.82	111.80
1	14-A	54	ILE	N-CA-C	-5.23	96.88	111.00
1	10-A	131	PRO	CB-CA-C	-5.23	98.93	112.00
1	12-A	93	TRP	CH2-CZ2-CE2	-5.23	112.17	117.40
1	1-A	135	HIS	N-CA-C	5.22	125.11	111.00
1	9-A	40	ARG	CB-CG-CD	5.22	125.18	111.60
1	15-A	148	SER	O-C-N	5.22	131.06	122.70
1	2-A	100	THR	CA-CB-CG2	-5.22	105.09	112.40
1	3-A	71	SER	O-C-N	5.22	131.06	122.70
1	12-A	122	LEU	CB-CG-CD1	-5.22	102.12	111.00
1	14-A	67	TRP	NE1-CE2-CD2	5.22	112.52	107.30
1	1-A	37	SER	CB-CA-C	-5.22	100.18	110.10
1	1-A	56	THR	C-N-CA	-5.22	108.65	121.70
1	10-A	67	TRP	CD1-NE1-CE2	5.22	113.70	109.00
1	4-A	41	ARG	O-C-N	5.22	131.05	122.70
1	11-A	63	PRO	CA-CB-CG	-5.22	94.08	104.00
1	2-A	130	THR	CA-C-N	5.22	131.71	117.10
1	6-A	140	TRP	O-C-N	5.22	131.05	122.70
1	16-A	68	VAL	CB-CA-C	5.22	121.31	111.40
1	6-A	115	LYS	CA-C-O	5.21	131.05	120.10
1	9-A	44	MET	CB-CG-SD	-5.21	96.76	112.40
1	14-A	103	GLU	CG-CD-OE2	-5.21	107.87	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13-A	149	PHE	N-CA-C	5.21	125.08	111.00
1	3-A	68	VAL	CA-CB-CG1	-5.21	103.08	110.90
1	9-A	41	ARG	CD-NE-CZ	-5.21	116.30	123.60
1	11-A	111	ILE	C-N-CA	-5.21	108.67	121.70
1	13-A	75	LYS	O-C-N	5.21	131.04	122.70
1	15-A	82	LEU	CB-CG-CD2	5.21	119.86	111.00
1	16-A	111	ILE	CB-CG1-CD1	-5.21	99.31	113.90
1	4-A	143	ASP	CB-CG-OD1	5.21	122.99	118.30
1	8-A	89	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	6-A	47	ASP	N-CA-C	-5.21	96.94	111.00
1	9-A	107	LEU	C-N-CA	-5.21	108.68	121.70
1	2-A	85	LEU	CB-CG-CD1	-5.21	102.15	111.00
1	8-A	136	MET	C-N-CA	-5.21	108.68	121.70
1	15-A	76	GLN	C-N-CA	-5.21	108.68	121.70
1	15-A	97	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	7-A	94	ASP	C-N-CA	-5.20	108.69	121.70
1	8-A	128	ARG	O-C-N	5.20	131.03	122.70
1	16-A	106	ARG	CA-CB-CG	-5.20	101.95	113.40
1	3-A	64	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	16-A	141	ARG	N-CA-C	5.20	125.05	111.00
1	11-A	79	GLY	N-CA-C	5.20	126.10	113.10
1	13-A	40	ARG	CB-CA-C	-5.20	100.00	110.40
1	14-A	132	SER	O-C-N	5.20	131.02	122.70
1	7-A	45	TYR	O-C-N	5.20	131.02	122.70
1	14-A	98	PHE	N-CA-C	-5.20	96.97	111.00
1	15-A	151	ASP	OD1-CG-OD2	5.20	133.18	123.30
1	5-A	143	ASP	N-CA-CB	-5.20	101.25	110.60
1	16-A	142	SER	CA-CB-OG	-5.20	97.17	111.20
1	10-A	71	SER	C-N-CA	-5.20	108.71	121.70
1	13-A	41	ARG	C-N-CA	-5.19	108.72	121.70
1	14-A	48	TYR	CE1-CZ-CE2	5.19	128.11	119.80
1	4-A	97	ARG	CG-CD-NE	-5.19	100.90	111.80
1	4-A	117	GLU	CA-CB-CG	-5.19	101.98	113.40
1	12-A	95	GLN	O-C-N	-5.19	114.39	122.70
1	2-A	154	PHE	CB-CA-C	-5.19	100.02	110.40
1	10-A	63	PRO	CA-N-CD	5.19	118.97	111.70
1	11-A	98	PHE	CG-CD1-CE1	5.19	126.51	120.80
1	15-A	41	ARG	N-CA-C	-5.19	96.99	111.00
1	13-A	49	MET	CA-C-O	-5.19	109.21	120.10
1	5-A	55	PRO	CA-N-CD	5.18	118.96	111.70
1	5-A	78	TYR	CD1-CE1-CZ	-5.18	115.13	119.80
1	7-A	45	TYR	C-N-CA	-5.18	108.74	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16-A	85	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	6-A	139	LEU	O-C-N	5.18	130.99	122.70
1	7-A	64	PHE	CG-CD1-CE1	-5.18	115.10	120.80
1	12-A	71	SER	N-CA-CB	5.18	118.27	110.50
1	14-A	62	ILE	CA-CB-CG1	-5.18	101.15	111.00
1	15-A	42	ALA	CB-CA-C	-5.18	102.33	110.10
1	14-A	105	GLN	O-C-N	5.18	130.99	122.70
1	1-A	138	LEU	CB-CG-CD2	-5.18	102.20	111.00
1	4-A	61	LEU	CB-CG-CD2	-5.18	102.20	111.00
1	4-A	142	SER	N-CA-CB	-5.18	102.74	110.50
1	8-A	72	ILE	CB-CG1-CD1	-5.18	99.41	113.90
1	16-A	49	MET	C-N-CA	-5.18	108.76	121.70
1	1-A	44	MET	CB-CG-SD	-5.17	96.88	112.40
1	9-A	97	ARG	CG-CD-NE	-5.17	100.94	111.80
1	14-A	46	GLN	CB-CG-CD	5.17	125.05	111.60
1	1-A	149	PHE	CZ-CE2-CD2	-5.17	113.89	120.10
1	14-A	149	PHE	CG-CD1-CE1	5.17	126.49	120.80
1	4-A	131	PRO	CB-CA-C	5.17	124.92	112.00
1	13-A	36	GLY	CA-C-N	-5.17	105.83	117.20
1	16-A	84	TYR	CB-CG-CD2	5.17	124.10	121.00
1	1-A	152	PRO	CA-C-O	5.17	132.60	120.20
1	1-A	106	ARG	CD-NE-CZ	5.16	130.83	123.60
1	14-A	80	GLN	CB-CG-CD	-5.16	98.18	111.60
1	14-A	142	SER	CA-CB-OG	-5.16	97.27	111.20
1	14-A	151	ASP	CA-C-N	-5.16	102.66	117.10
1	16-A	149	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	1-A	152	PRO	C-N-CA	5.16	134.59	121.70
1	2-A	152	PRO	C-N-CA	5.16	134.59	121.70
1	4-A	67	TRP	CD1-NE1-CE2	5.16	113.64	109.00
1	8-A	112	HIS	CG-ND1-CE1	5.16	115.42	108.20
1	16-A	93	TRP	CA-C-N	-5.16	105.86	117.20
1	16-A	124	GLU	O-C-N	5.16	130.95	122.70
1	6-A	36	GLY	CA-C-N	-5.15	105.86	117.20
1	2-A	143	ASP	N-CA-CB	-5.15	101.33	110.60
1	16-A	92	ARG	N-CA-CB	-5.15	101.33	110.60
1	6-A	145	MET	CB-CA-C	-5.15	100.11	110.40
1	15-A	126	ILE	O-C-N	5.15	130.93	122.70
1	1-A	75	LYS	CA-C-O	-5.14	109.30	120.10
1	2-A	150	ILE	CG1-CB-CG2	5.14	122.72	111.40
1	10-A	58	ARG	NH1-CZ-NH2	5.14	125.06	119.40
1	13-A	149	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	2-A	75	LYS	CG-CD-CE	-5.14	96.47	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	15-A	112	HIS	CA-CB-CG	-5.14	104.86	113.60
1	16-A	110	ILE	CA-CB-CG2	-5.14	100.62	110.90
1	1-A	108	ASP	C-N-CA	-5.14	108.85	121.70
1	8-A	89	LEU	CA-CB-CG	-5.14	103.48	115.30
1	9-A	67	TRP	NE1-CE2-CZ2	5.14	136.05	130.40
1	8-A	65	THR	N-CA-CB	-5.13	100.54	110.30
1	9-A	44	MET	C-N-CA	-5.13	108.86	121.70
1	13-A	107	LEU	C-N-CA	-5.13	108.87	121.70
1	15-A	81	PRO	N-CA-C	-5.13	98.75	112.10
1	2-A	130	THR	CA-CB-CG2	-5.13	105.22	112.40
1	7-A	122	LEU	C-N-CA	-5.13	108.87	121.70
1	1-A	121	TRP	CA-C-N	-5.13	105.92	117.20
1	3-A	131	PRO	CA-N-CD	5.13	118.88	111.70
1	4-A	123	VAL	CB-CA-C	-5.13	101.66	111.40
1	8-A	47	ASP	CA-C-O	-5.13	109.33	120.10
1	3-A	92	ARG	CA-C-N	5.13	128.48	117.20
1	11-A	111	ILE	CB-CG1-CD1	-5.13	99.54	113.90
1	14-A	55	PRO	C-N-CA	-5.12	108.89	121.70
1	8-A	93	TRP	CH2-CZ2-CE2	-5.12	112.28	117.40
1	11-A	87	ASN	C-N-CA	-5.12	108.89	121.70
1	9-A	45	TYR	C-N-CA	-5.12	108.90	121.70
1	2-A	58	ARG	NH1-CZ-NH2	5.12	125.03	119.40
1	15-A	127	HIS	CG-ND1-CE1	5.12	115.37	108.20
1	13-A	93	TRP	CB-CG-CD2	-5.12	119.95	126.60
1	2-A	145	MET	O-C-N	5.11	130.88	122.70
1	7-A	105	GLN	CB-CA-C	-5.11	100.18	110.40
1	13-A	91	GLN	N-CA-CB	-5.11	101.40	110.60
1	9-A	148	SER	CA-C-N	-5.11	105.97	117.20
1	10-A	63	PRO	O-C-N	-5.11	114.53	122.70
1	12-A	138	LEU	C-N-CA	-5.11	108.93	121.70
1	2-A	78	TYR	CA-CB-CG	-5.11	103.70	113.40
1	11-A	148	SER	O-C-N	5.11	130.87	122.70
1	16-A	63	PRO	CA-N-CD	5.11	118.85	111.70
1	13-A	139	LEU	CA-C-N	-5.10	105.97	117.20
1	2-A	58	ARG	CD-NE-CZ	-5.10	116.46	123.60
1	3-A	71	SER	CA-C-N	-5.10	105.98	117.20
1	6-A	107	LEU	CA-C-O	-5.10	109.39	120.10
1	4-A	109	SER	CB-CA-C	-5.10	100.42	110.10
1	15-A	42	ALA	CA-C-N	-5.10	105.99	117.20
1	1-A	97	ARG	O-C-N	5.09	130.85	122.70
1	3-A	102	SER	CB-CA-C	-5.09	100.42	110.10
1	3-A	151	ASP	CB-CA-C	-5.09	100.21	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	138	LEU	N-CA-CB	-5.09	100.21	110.40
1	15-A	131	PRO	N-CA-CB	5.09	109.41	103.30
1	5-A	38	LEU	CD1-CG-CD2	-5.09	95.22	110.50
1	6-A	40	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	12-A	45	TYR	C-N-CA	-5.09	108.97	121.70
1	15-A	85	LEU	CB-CG-CD2	-5.09	102.34	111.00
1	16-A	155	PRO	CA-CB-CG	5.09	114.47	104.80
1	2-A	151	ASP	CB-CA-C	-5.09	100.22	110.40
1	13-A	134	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	14-A	53	PRO	CA-CB-CG	-5.09	94.33	104.00
1	2-A	75	LYS	CB-CG-CD	-5.09	98.37	111.60
1	9-A	129	LEU	CB-CG-CD1	-5.09	102.35	111.00
1	11-A	142	SER	CB-CA-C	-5.08	100.44	110.10
1	13-A	100	THR	OG1-CB-CG2	-5.08	98.31	110.00
1	6-A	63	PRO	CA-N-CD	5.08	118.81	111.70
1	12-A	70	LEU	CA-C-N	-5.08	106.02	117.20
1	2-A	63	PRO	CA-N-CD	5.08	118.81	111.70
1	4-A	67	TRP	CA-CB-CG	-5.08	104.05	113.70
1	7-A	97	ARG	CA-C-N	-5.08	106.03	117.20
1	10-A	97	ARG	CA-C-O	-5.08	109.44	120.10
1	11-A	155	PRO	N-CD-CG	-5.08	95.58	103.20
1	7-A	73	SER	CA-C-O	5.08	130.76	120.10
1	10-A	156	GLU	CA-C-O	-5.08	109.44	120.10
1	16-A	106	ARG	CD-NE-CZ	5.08	130.71	123.60
1	4-A	148	SER	O-C-N	5.08	130.82	122.70
1	13-A	126	ILE	CA-CB-CG2	5.08	121.05	110.90
1	2-A	106	ARG	CB-CA-C	-5.07	100.25	110.40
1	2-A	113	PRO	CA-CB-CG	-5.07	94.36	104.00
1	2-A	125	GLU	N-CA-CB	-5.07	101.47	110.60
1	7-A	61	LEU	CB-CG-CD1	5.07	119.63	111.00
1	4-A	76	GLN	CG-CD-OE1	-5.07	111.46	121.60
1	2-A	100	THR	CA-C-N	-5.07	106.04	117.20
1	3-A	121	TRP	C-N-CA	-5.07	109.02	121.70
1	9-A	84	TYR	CB-CG-CD2	5.07	124.04	121.00
1	12-A	150	ILE	CA-CB-CG1	-5.07	101.37	111.00
1	16-A	152	PRO	O-C-N	-5.07	114.59	122.70
1	1-A	53	PRO	N-CD-CG	-5.07	95.60	103.20
1	5-A	106	ARG	NH1-CZ-NH2	-5.07	113.83	119.40
1	15-A	90	LEU	CB-CG-CD2	5.07	119.61	111.00
1	1-A	136	MET	C-N-CA	-5.07	109.04	121.70
1	7-A	136	MET	CA-CB-CG	-5.06	104.69	113.30
1	11-A	120	ILE	CG1-CB-CG2	-5.06	100.26	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	59	GLY	O-C-N	-5.06	114.60	122.70
1	5-A	84	TYR	CG-CD2-CE2	5.06	125.35	121.30
1	11-A	144	PRO	N-CD-CG	-5.06	95.61	103.20
1	5-A	57	ASN	C-N-CA	-5.05	109.07	121.70
1	12-A	64	PHE	CG-CD1-CE1	-5.05	115.24	120.80
1	16-A	117	GLU	CG-CD-OE1	-5.05	108.19	118.30
1	12-A	137	ALA	C-N-CA	-5.05	109.07	121.70
1	4-A	138	LEU	C-N-CA	-5.05	109.07	121.70
1	10-A	44	MET	C-N-CA	-5.05	109.07	121.70
1	15-A	73	SER	CA-C-N	-5.05	106.08	117.20
1	16-A	134	LEU	CD1-CG-CD2	-5.05	95.34	110.50
1	5-A	91	GLN	CA-C-O	-5.05	109.50	120.10
1	6-A	68	VAL	CG1-CB-CG2	5.05	118.98	110.90
1	2-A	154	PHE	O-C-N	5.05	130.69	121.10
1	9-A	124	GLU	N-CA-C	-5.05	97.38	111.00
1	13-A	76	GLN	O-C-N	5.04	130.77	122.70
1	11-A	143	ASP	N-CA-CB	-5.04	101.52	110.60
1	3-A	148	SER	N-CA-C	5.04	124.61	111.00
1	6-A	80	GLN	CB-CA-C	-5.04	100.32	110.40
1	12-A	40	ARG	CG-CD-NE	-5.04	101.21	111.80
1	13-A	92	ARG	CA-C-O	-5.04	109.51	120.10
1	2-A	125	GLU	CG-CD-OE1	5.04	128.38	118.30
1	11-A	110	ILE	CA-CB-CG2	-5.04	100.82	110.90
1	7-A	148	SER	CB-CA-C	-5.04	100.53	110.10
1	9-A	72	ILE	CG1-CB-CG2	5.04	122.48	111.40
1	11-A	84	TYR	N-CA-C	5.04	124.60	111.00
1	16-A	84	TYR	C-N-CA	-5.04	109.10	121.70
1	2-A	126	ILE	C-N-CA	-5.04	109.11	121.70
1	8-A	150	ILE	CA-CB-CG1	-5.04	101.43	111.00
1	10-A	40	ARG	CB-CA-C	-5.04	100.33	110.40
1	11-A	146	TYR	CB-CA-C	-5.04	100.33	110.40
1	8-A	132	SER	C-N-CA	-5.03	109.11	121.70
1	10-A	139	LEU	N-CA-CB	5.03	120.47	110.40
1	5-A	134	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	1-A	140	TRP	CA-CB-CG	-5.03	104.14	113.70
1	3-A	36	GLY	CA-C-N	-5.03	106.14	117.20
1	8-A	143	ASP	N-CA-CB	-5.03	101.55	110.60
1	14-A	97	ARG	C-N-CA	-5.03	109.13	121.70
1	2-A	75	LYS	CA-C-O	-5.03	109.55	120.10
1	12-A	39	LEU	CB-CG-CD1	-5.03	102.46	111.00
1	3-A	56	THR	CA-CB-CG2	-5.02	105.37	112.40
1	7-A	101	ASP	C-N-CA	-5.02	109.14	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	63	PRO	CB-CA-C	-5.02	99.45	112.00
1	9-A	123	VAL	O-C-N	-5.02	114.67	122.70
1	3-A	94	ASP	CA-C-N	-5.02	106.17	117.20
1	1-A	90	LEU	C-N-CA	-5.01	109.16	121.70
1	7-A	123	VAL	CA-CB-CG1	-5.01	103.38	110.90
1	9-A	106	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	12-A	130	THR	CA-C-O	-5.01	109.57	120.10
1	14-A	66	SER	CA-C-N	-5.01	106.17	117.20
1	13-A	44	MET	CB-CG-SD	-5.01	97.36	112.40
1	13-A	125	GLU	CA-C-N	-5.01	106.17	117.20
1	3-A	97	ARG	C-N-CA	-5.01	109.17	121.70
1	11-A	89	LEU	N-CA-C	-5.01	97.47	111.00
1	16-A	66	SER	CA-CB-OG	-5.01	97.67	111.20
1	6-A	132	SER	C-N-CA	-5.01	109.17	121.70
1	11-A	41	ARG	CB-CA-C	-5.01	100.38	110.40
1	11-A	134	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	13-A	38	LEU	N-CA-CB	5.01	120.42	110.40
1	14-A	105	GLN	CB-CA-C	-5.01	100.38	110.40
1	4-A	47	ASP	CB-CA-C	-5.01	100.38	110.40
1	7-A	40	ARG	CG-CD-NE	-5.01	101.28	111.80
1	14-A	64	PHE	CD1-CG-CD2	5.01	124.81	118.30
1	15-A	131	PRO	O-C-N	5.01	130.71	122.70
1	16-A	84	TYR	CE1-CZ-CE2	5.01	127.81	119.80
1	2-A	125	GLU	CG-CD-OE2	-5.01	108.29	118.30
1	3-A	92	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	5-A	36	GLY	CA-C-O	-5.01	111.59	120.60
1	15-A	53	PRO	CB-CG-CD	5.01	126.03	106.50
1	6-A	117	GLU	N-CA-CB	-5.00	101.59	110.60

There are no chirality outliers.

All (168) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	105	GLN	Mainchain
1	1-A	107	LEU	Mainchain
1	1-A	109	SER	Mainchain
1	1-A	128	ARG	Sidechain
1	1-A	129	LEU	Mainchain
1	1-A	144	PRO	Mainchain
1	1-A	39	LEU	Mainchain
1	1-A	57	ASN	Mainchain
1	1-A	76	GLN	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	1-A	89	LEU	Mainchain
1	10-A	116	ALA	Mainchain
1	10-A	125	GLU	Mainchain
1	10-A	127	HIS	Mainchain
1	10-A	133	HIS	Sidechain
1	10-A	144	PRO	Mainchain
1	10-A	62	ILE	Mainchain
1	10-A	64	PHE	Sidechain
1	10-A	99	GLY	Mainchain
1	11-A	106	ARG	Sidechain
1	11-A	112	HIS	Mainchain
1	11-A	144	PRO	Mainchain
1	11-A	38	LEU	Mainchain
1	11-A	39	LEU	Mainchain
1	11-A	40	ARG	Sidechain
1	11-A	43	GLU	Mainchain
1	11-A	62	ILE	Mainchain
1	11-A	84	TYR	Sidechain
1	11-A	92	ARG	Sidechain
1	12-A	116	ALA	Mainchain
1	12-A	144	PRO	Mainchain
1	12-A	45	TYR	Sidechain
1	12-A	57	ASN	Mainchain
1	12-A	76	GLN	Mainchain
1	13-A	106	ARG	Mainchain
1	13-A	107	LEU	Mainchain
1	13-A	123	VAL	Mainchain
1	13-A	125	GLU	Sidechain,Mainchain
1	13-A	141	ARG	Sidechain
1	13-A	143	ASP	Mainchain
1	13-A	146	TYR	Sidechain
1	13-A	148	SER	Mainchain
1	13-A	43	GLU	Mainchain
1	13-A	44	MET	Mainchain
1	13-A	66	SER	Mainchain
1	13-A	68	VAL	Mainchain
1	13-A	75	LYS	Mainchain
1	14-A	108	ASP	Sidechain
1	14-A	117	GLU	Mainchain
1	14-A	128	ARG	Sidechain
1	14-A	129	LEU	Mainchain
1	14-A	143	ASP	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	14-A	146	TYR	Sidechain
1	14-A	45	TYR	Sidechain
1	14-A	55	PRO	Mainchain
1	14-A	56	THR	Mainchain
1	14-A	61	LEU	Mainchain
1	14-A	65	THR	Mainchain
1	14-A	66	SER	Mainchain
1	14-A	67	TRP	Mainchain
1	14-A	75	LYS	Mainchain
1	14-A	84	TYR	Mainchain
1	14-A	86	THR	Mainchain
1	14-A	99	GLY	Mainchain
1	15-A	106	ARG	Mainchain
1	15-A	108	ASP	Sidechain
1	15-A	110	ILE	Mainchain
1	15-A	112	HIS	Mainchain
1	15-A	116	ALA	Mainchain
1	15-A	124	GLU	Mainchain
1	15-A	125	GLU	Mainchain
1	15-A	141	ARG	Sidechain
1	15-A	143	ASP	Mainchain
1	15-A	36	GLY	Mainchain
1	15-A	44	MET	Mainchain
1	15-A	55	PRO	Mainchain
1	15-A	56	THR	Mainchain
1	15-A	57	ASN	Mainchain
1	15-A	78	TYR	Sidechain,Mainchain
1	15-A	81	PRO	Mainchain
1	15-A	82	LEU	Mainchain
1	15-A	84	TYR	Mainchain
1	15-A	86	THR	Mainchain
1	15-A	96	SER	Mainchain
1	16-A	128	ARG	Mainchain
1	16-A	141	ARG	Sidechain
1	16-A	142	SER	Mainchain
1	16-A	144	PRO	Mainchain
1	16-A	146	TYR	Sidechain,Mainchain
1	16-A	45	TYR	Sidechain
1	16-A	46	GLN	Sidechain
1	16-A	48	TYR	Sidechain
1	16-A	57	ASN	Mainchain
1	16-A	73	SER	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	16-A	78	TYR	Sidechain
1	16-A	79	GLY	Mainchain
1	16-A	81	PRO	Mainchain
1	16-A	82	LEU	Mainchain
1	16-A	83	HIS	Mainchain
1	16-A	84	TYR	Sidechain,Mainchain
1	2-A	105	GLN	Mainchain
1	2-A	131	PRO	Mainchain
1	2-A	136	MET	Mainchain
1	2-A	141	ARG	Sidechain
1	2-A	144	PRO	Mainchain
1	2-A	153	ILE	Mainchain
1	2-A	154	PHE	Mainchain
1	2-A	55	PRO	Mainchain
1	2-A	56	THR	Mainchain
1	2-A	57	ASN	Mainchain
1	2-A	73	SER	Mainchain
1	2-A	75	LYS	Mainchain
1	2-A	91	GLN	Mainchain
1	2-A	92	ARG	Sidechain
1	2-A	98	PHE	Sidechain
1	2-A	99	GLY	Mainchain
1	3-A	100	THR	Mainchain
1	3-A	148	SER	Mainchain
1	3-A	36	GLY	Mainchain
1	3-A	89	LEU	Mainchain
1	3-A	98	PHE	Mainchain
1	4-A	116	ALA	Mainchain
1	4-A	118	ALA	Mainchain
1	4-A	123	VAL	Mainchain
1	4-A	151	ASP	Mainchain
1	4-A	36	GLY	Mainchain
1	4-A	40	ARG	Mainchain
1	4-A	41	ARG	Mainchain
1	4-A	69	GLY	Mainchain
1	4-A	70	LEU	Mainchain
1	4-A	71	SER	Mainchain
1	4-A	76	GLN	Mainchain
1	4-A	78	TYR	Mainchain
1	4-A	80	GLN	Mainchain
1	4-A	81	PRO	Mainchain
1	4-A	98	PHE	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	5-A	144	PRO	Mainchain
1	5-A	45	TYR	Mainchain
1	5-A	55	PRO	Mainchain
1	5-A	56	THR	Mainchain
1	6-A	143	ASP	Mainchain
1	6-A	145	MET	Mainchain
1	6-A	36	GLY	Mainchain
1	6-A	78	TYR	Sidechain
1	6-A	83	HIS	Mainchain
1	6-A	84	TYR	Mainchain
1	7-A	45	TYR	Sidechain
1	7-A	75	LYS	Mainchain
1	7-A	76	GLN	Mainchain
1	7-A	78	TYR	Sidechain
1	7-A	94	ASP	Sidechain
1	8-A	106	ARG	Sidechain
1	8-A	143	ASP	Mainchain
1	8-A	147	HIS	Sidechain
1	8-A	39	LEU	Mainchain
1	8-A	56	THR	Mainchain
1	8-A	66	SER	Mainchain
1	9-A	123	VAL	Mainchain
1	9-A	125	GLU	Mainchain
1	9-A	127	HIS	Mainchain
1	9-A	130	THR	Mainchain
1	9-A	144	PRO	Mainchain
1	9-A	36	GLY	Mainchain
1	9-A	90	LEU	Mainchain
1	9-A	94	ASP	Mainchain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1003	0	985	0	2
1	2-A	1003	0	985	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3-A	1003	0	986	0	0
1	4-A	1003	0	986	0	1
1	5-A	1003	0	985	0	1
1	6-A	1003	0	986	0	1
1	7-A	1003	0	985	0	0
1	8-A	1003	0	985	0	0
1	9-A	1003	0	986	0	4
1	10-A	1003	0	986	0	2
1	11-A	1003	0	986	0	2
1	12-A	1003	0	986	0	0
1	13-A	1003	0	986	0	0
1	14-A	1003	0	986	0	0
1	15-A	1003	0	984	0	0
1	16-A	1003	0	986	0	0
2	1-A	15	0	0	0	0
2	2-A	15	0	0	0	0
2	3-A	15	0	0	0	0
2	4-A	15	0	0	0	0
2	5-A	15	0	0	0	0
2	6-A	15	0	0	0	0
2	7-A	15	0	0	0	0
2	8-A	15	0	0	0	0
2	9-A	15	0	0	0	0
2	10-A	15	0	0	0	0
2	11-A	15	0	0	0	0
2	12-A	15	0	0	0	0
2	13-A	15	0	0	0	0
2	14-A	15	0	0	0	0
2	15-A	15	0	0	0	0
2	16-A	15	0	0	0	0
3	1-A	32	0	33	0	2
3	2-A	32	0	33	0	0
3	3-A	32	0	19	0	0
3	4-A	32	0	38	0	0
3	5-A	32	0	28	0	2
3	6-A	32	0	31	0	1
3	7-A	32	0	30	0	0
3	8-A	32	0	38	0	0
3	9-A	32	0	39	0	0
3	10-A	32	0	28	0	0
3	11-A	32	0	34	0	1
3	12-A	32	0	29	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	13-A	32	0	37	0	0
3	14-A	32	0	23	0	0
3	15-A	32	0	38	0	0
3	16-A	32	0	27	0	0
4	1-A	16	0	23	0	0
4	2-A	16	0	22	0	0
4	3-A	16	0	22	0	0
4	4-A	16	0	22	0	0
4	5-A	16	0	22	0	1
4	6-A	16	0	23	0	0
4	7-A	16	0	22	0	0
4	8-A	16	0	22	0	0
4	9-A	16	0	22	0	0
4	10-A	16	0	22	0	0
4	11-A	16	0	23	0	0
4	12-A	16	0	22	0	0
4	13-A	16	0	22	0	1
4	14-A	16	0	23	0	1
4	15-A	16	0	22	0	1
4	16-A	16	0	23	0	0
5	1-A	172	0	0	0	0
5	2-A	172	0	0	0	0
5	3-A	172	0	0	0	0
5	4-A	172	0	0	0	0
5	5-A	172	0	0	0	0
5	6-A	172	0	0	0	0
5	7-A	172	0	0	0	0
5	8-A	172	0	0	0	0
5	9-A	172	0	0	0	3
5	10-A	172	0	0	0	1
5	11-A	172	0	0	0	1
5	12-A	172	0	0	0	0
5	13-A	172	0	0	0	1
5	14-A	172	0	0	0	1
5	15-A	172	0	0	0	1
5	16-A	172	0	0	0	0
All	All	19808	0	16631	0	17

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

All (17) symmetry-related close contacts are listed below. The label for Atom-2 includes the

symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:76:GLN:OE1	3:A:200:CPS:O3[2_655]	1.59	0.61
1:A:76:GLN:NE2	5:A:569:HOH:O[2_655]	1.90	0.30
1:A:73:SER:OG	3:A:200:CPS:O2[2_655]	1.93	0.27
4:A:403:EDO:O1	5:A:547:HOH:O[2_655]	1.99	0.21
1:A:76:GLN:OE1	5:A:525:HOH:O[2_655]	2.00	0.20
1:A:115:LYS:NZ	1:A:122:LEU:CD2[4_555]	2.01	0.19
1:A:76:GLN:NE2	5:A:569:HOH:O[2_655]	2.01	0.19
1:A:37:SER:OG	5:A:471:HOH:O[3_664]	2.02	0.18
4:A:403:EDO:O1	5:A:547:HOH:O[2_655]	2.02	0.18
3:A:200:CPS:O3	4:A:403:EDO:O1[3_664]	2.05	0.15
1:A:41:ARG:NH1	1:A:61:LEU:O[3_664]	2.09	0.11
1:A:62:ILE:CD1	3:A:200:CPS:O2[2_655]	2.09	0.11
4:A:403:EDO:O1	5:A:547:HOH:O[2_655]	2.11	0.09
1:A:93:TRP:O	5:A:445:HOH:O[4_555]	2.12	0.08
1:A:96:SER:O	1:A:132:SER:N[4_555]	2.13	0.07
1:A:76:GLN:CB	3:A:200:CPS:O3[2_655]	2.18	0.02
1:A:76:GLN:OE1	3:A:200:CPS:O3[2_655]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	119/157 (76%)	114 (96%)	4 (3%)	1 (1%)	27	7
1	2-A	119/157 (76%)	107 (90%)	8 (7%)	4 (3%)	6	0
1	3-A	119/157 (76%)	111 (93%)	5 (4%)	3 (2%)	9	1
1	4-A	119/157 (76%)	114 (96%)	4 (3%)	1 (1%)	27	7
1	5-A	119/157 (76%)	117 (98%)	1 (1%)	1 (1%)	27	7
1	6-A	119/157 (76%)	116 (98%)	2 (2%)	1 (1%)	27	7
1	7-A	119/157 (76%)	117 (98%)	1 (1%)	1 (1%)	27	7
1	8-A	119/157 (76%)	116 (98%)	1 (1%)	2 (2%)	14	2
1	9-A	119/157 (76%)	114 (96%)	4 (3%)	1 (1%)	27	7
1	10-A	119/157 (76%)	114 (96%)	2 (2%)	3 (2%)	9	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	11-A	119/157 (76%)	110 (92%)	6 (5%)	3 (2%)	9	1
1	12-A	119/157 (76%)	117 (98%)	1 (1%)	1 (1%)	27	7
1	13-A	119/157 (76%)	113 (95%)	5 (4%)	1 (1%)	27	7
1	14-A	119/157 (76%)	116 (98%)	3 (2%)	0	100	100
1	15-A	119/157 (76%)	106 (89%)	10 (8%)	3 (2%)	9	1
1	16-A	119/157 (76%)	113 (95%)	3 (2%)	3 (2%)	9	1
All	All	1904/2512 (76%)	1815 (95%)	60 (3%)	29 (2%)	15	2

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	132	SER
1	3-A	103	GLU
1	10-A	102	SER
1	11-A	83	HIS
1	15-A	83	HIS
1	16-A	84	TYR
1	2-A	104	GLU
1	9-A	130	THR
1	16-A	38	LEU
1	2-A	103	GLU
1	8-A	152	PRO
1	11-A	38	LEU
1	15-A	81	PRO
1	2-A	130	THR
1	7-A	130	THR
1	8-A	130	THR
1	16-A	130	THR
1	3-A	38	LEU
1	10-A	130	THR
1	3-A	130	THR
1	10-A	99	GLY
1	11-A	130	THR
1	12-A	130	THR
1	5-A	130	THR
1	15-A	130	THR
1	4-A	130	THR
1	6-A	130	THR
1	1-A	155	PRO
1	13-A	130	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	112/143 (78%)	108 (96%)	4 (4%)	47	17
1	2-A	112/143 (78%)	104 (93%)	8 (7%)	21	4
1	3-A	112/143 (78%)	108 (96%)	4 (4%)	47	17
1	4-A	112/143 (78%)	105 (94%)	7 (6%)	25	5
1	5-A	112/143 (78%)	107 (96%)	5 (4%)	38	11
1	6-A	112/143 (78%)	109 (97%)	3 (3%)	57	26
1	7-A	112/143 (78%)	110 (98%)	2 (2%)	71	44
1	8-A	112/143 (78%)	108 (96%)	4 (4%)	47	17
1	9-A	112/143 (78%)	106 (95%)	6 (5%)	31	7
1	10-A	112/143 (78%)	109 (97%)	3 (3%)	57	26
1	11-A	112/143 (78%)	107 (96%)	5 (4%)	38	11
1	12-A	112/143 (78%)	110 (98%)	2 (2%)	71	44
1	13-A	112/143 (78%)	104 (93%)	8 (7%)	21	4
1	14-A	112/143 (78%)	105 (94%)	7 (6%)	25	5
1	15-A	112/143 (78%)	103 (92%)	9 (8%)	17	2
1	16-A	112/143 (78%)	104 (93%)	8 (7%)	21	4
All	All	1792/2288 (78%)	1707 (95%)	85 (5%)	36	10

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	61	LEU
1	1-A	64	PHE
1	1-A	121	TRP
1	1-A	155	PRO
1	2-A	50	LYS
1	2-A	61	LEU
1	2-A	66	SER
1	2-A	80	GLN
1	2-A	113	PRO
1	2-A	132	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-A	138	LEU
1	2-A	155	PRO
1	3-A	61	LEU
1	3-A	113	PRO
1	3-A	115	LYS
1	3-A	155	PRO
1	4-A	55	PRO
1	4-A	61	LEU
1	4-A	64	PHE
1	4-A	81	PRO
1	4-A	131	PRO
1	4-A	134	LEU
1	4-A	155	PRO
1	5-A	37	SER
1	5-A	55	PRO
1	5-A	61	LEU
1	5-A	94	ASP
1	5-A	155	PRO
1	6-A	61	LEU
1	6-A	66	SER
1	6-A	80	GLN
1	7-A	61	LEU
1	7-A	94	ASP
1	8-A	40	ARG
1	8-A	49	MET
1	8-A	50	LYS
1	8-A	55	PRO
1	9-A	49	MET
1	9-A	61	LEU
1	9-A	113	PRO
1	9-A	121	TRP
1	9-A	151	ASP
1	9-A	155	PRO
1	10-A	61	LEU
1	10-A	64	PHE
1	10-A	133	HIS
1	11-A	40	ARG
1	11-A	80	GLN
1	11-A	89	LEU
1	11-A	113	PRO
1	11-A	155	PRO
1	12-A	61	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	12-A	138	LEU
1	13-A	50	LYS
1	13-A	53	PRO
1	13-A	71	SER
1	13-A	89	LEU
1	13-A	136	MET
1	13-A	151	ASP
1	13-A	152	PRO
1	13-A	155	PRO
1	14-A	49	MET
1	14-A	50	LYS
1	14-A	61	LEU
1	14-A	113	PRO
1	14-A	136	MET
1	14-A	148	SER
1	14-A	152	PRO
1	15-A	50	LYS
1	15-A	55	PRO
1	15-A	56	THR
1	15-A	80	GLN
1	15-A	91	GLN
1	15-A	108	ASP
1	15-A	109	SER
1	15-A	123	VAL
1	15-A	132	SER
1	16-A	49	MET
1	16-A	66	SER
1	16-A	80	GLN
1	16-A	82	LEU
1	16-A	113	PRO
1	16-A	115	LYS
1	16-A	134	LEU
1	16-A	143	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	3-A	91	GLN
1	5-A	105	GLN
1	6-A	105	GLN
1	9-A	105	GLN
1	11-A	87	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	11-A	95	GLN
1	13-A	135	HIS
1	15-A	80	GLN
1	15-A	91	GLN
1	15-A	95	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

128 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CPS	1-A	200	-	35,35,45	18.98	30 (85%)	54,54,70	10.89	48 (88%)
2	SO4	1-A	300	-	4,4,4	4.07	4 (100%)	6,6,6	1.76	2 (33%)
2	SO4	1-A	301	-	4,4,4	2.94	1 (25%)	6,6,6	0.78	0
2	SO4	1-A	302	-	4,4,4	0.65	0	6,6,6	0.40	0
4	EDO	1-A	401	-	3,3,3	2.14	1 (33%)	2,2,2	0.60	0
4	EDO	1-A	402	-	3,3,3	2.82	2 (66%)	2,2,2	2.11	1 (50%)
4	EDO	1-A	403	-	3,3,3	2.83	2 (66%)	2,2,2	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	1-A	404	-	3,3,3	4.86	2 (66%)	2,2,2	1.19	0
3	CPS	10-A	200	-	35,35,45	19.64	34 (97%)	54,54,70	11.84	44 (81%)
2	SO4	10-A	300	-	4,4,4	1.14	0	6,6,6	0.91	0
2	SO4	10-A	301	-	4,4,4	6.44	3 (75%)	6,6,6	2.38	1 (16%)
2	SO4	10-A	302	-	4,4,4	1.43	1 (25%)	6,6,6	0.53	0
4	EDO	10-A	401	-	3,3,3	1.55	1 (33%)	2,2,2	0.34	0
4	EDO	10-A	402	-	3,3,3	2.42	2 (66%)	2,2,2	1.15	0
4	EDO	10-A	403	-	3,3,3	2.87	2 (66%)	2,2,2	1.39	0
4	EDO	10-A	404	-	3,3,3	3.07	2 (66%)	2,2,2	2.08	1 (50%)
3	CPS	11-A	200	-	35,35,45	16.56	31 (88%)	54,54,70	10.03	45 (83%)
2	SO4	11-A	300	-	4,4,4	9.66	3 (75%)	6,6,6	5.31	6 (100%)
2	SO4	11-A	301	-	4,4,4	2.33	2 (50%)	6,6,6	1.75	2 (33%)
2	SO4	11-A	302	-	4,4,4	0.71	0	6,6,6	0.33	0
4	EDO	11-A	401	-	3,3,3	1.54	1 (33%)	2,2,2	1.31	0
4	EDO	11-A	402	-	3,3,3	2.40	2 (66%)	2,2,2	1.43	0
4	EDO	11-A	403	-	3,3,3	3.59	2 (66%)	2,2,2	2.07	1 (50%)
4	EDO	11-A	404	-	3,3,3	3.44	2 (66%)	2,2,2	1.72	0
3	CPS	12-A	200	-	35,35,45	14.10	28 (80%)	54,54,70	10.13	44 (81%)
2	SO4	12-A	300	-	4,4,4	0.66	0	6,6,6	0.73	0
2	SO4	12-A	301	-	4,4,4	4.81	3 (75%)	6,6,6	0.52	0
2	SO4	12-A	302	-	4,4,4	0.55	0	6,6,6	0.34	0
4	EDO	12-A	401	-	3,3,3	1.54	1 (33%)	2,2,2	0.94	0
4	EDO	12-A	402	-	3,3,3	2.55	2 (66%)	2,2,2	1.16	0
4	EDO	12-A	403	-	3,3,3	2.88	2 (66%)	2,2,2	0.84	0
4	EDO	12-A	404	-	3,3,3	4.66	3 (100%)	2,2,2	0.68	0
3	CPS	13-A	200	-	35,35,45	21.72	31 (88%)	54,54,70	18.58	40 (74%)
2	SO4	13-A	300	-	4,4,4	2.81	2 (50%)	6,6,6	0.78	0
2	SO4	13-A	301	-	4,4,4	4.91	2 (50%)	6,6,6	2.41	1 (16%)
2	SO4	13-A	302	-	4,4,4	0.72	0	6,6,6	0.44	0
4	EDO	13-A	401	-	3,3,3	2.84	1 (33%)	2,2,2	0.72	0
4	EDO	13-A	402	-	3,3,3	5.01	2 (66%)	2,2,2	0.90	0
4	EDO	13-A	403	-	3,3,3	5.06	3 (100%)	2,2,2	1.97	1 (50%)
4	EDO	13-A	404	-	3,3,3	8.27	3 (100%)	2,2,2	1.14	0
3	CPS	14-A	200	-	35,35,45	23.57	30 (85%)	54,54,70	13.75	42 (77%)
2	SO4	14-A	300	-	4,4,4	7.30	2 (50%)	6,6,6	1.77	2 (33%)
2	SO4	14-A	301	-	4,4,4	4.18	3 (75%)	6,6,6	3.29	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	14-A	302	-	4,4,4	0.50	0	6,6,6	0.23	0
4	EDO	14-A	401	-	3,3,3	4.05	3 (100%)	2,2,2	0.56	0
4	EDO	14-A	402	-	3,3,3	2.72	3 (100%)	2,2,2	1.23	0
4	EDO	14-A	403	-	3,3,3	4.50	3 (100%)	2,2,2	2.35	1 (50%)
4	EDO	14-A	404	-	3,3,3	7.56	2 (66%)	2,2,2	0.89	0
3	CPS	15-A	200	-	35,35,45	23.59	34 (97%)	54,54,70	17.80	40 (74%)
2	SO4	15-A	300	-	4,4,4	2.84	2 (50%)	6,6,6	0.75	0
2	SO4	15-A	301	-	4,4,4	5.10	4 (100%)	6,6,6	4.46	3 (50%)
2	SO4	15-A	302	-	4,4,4	2.35	1 (25%)	6,6,6	0.31	0
4	EDO	15-A	401	-	3,3,3	3.10	1 (33%)	2,2,2	0.91	0
4	EDO	15-A	402	-	3,3,3	4.34	2 (66%)	2,2,2	0.67	0
4	EDO	15-A	403	-	3,3,3	4.86	3 (100%)	2,2,2	1.98	1 (50%)
4	EDO	15-A	404	-	3,3,3	7.76	3 (100%)	2,2,2	0.73	0
3	CPS	16-A	200	-	35,35,45	20.27	29 (82%)	54,54,70	10.10	42 (77%)
2	SO4	16-A	300	-	4,4,4	6.96	2 (50%)	6,6,6	1.90	1 (16%)
2	SO4	16-A	301	-	4,4,4	4.42	2 (50%)	6,6,6	0.90	0
2	SO4	16-A	302	-	4,4,4	1.07	1 (25%)	6,6,6	0.34	0
4	EDO	16-A	401	-	3,3,3	1.92	1 (33%)	2,2,2	1.65	1 (50%)
4	EDO	16-A	402	-	3,3,3	1.35	0	2,2,2	0.99	0
4	EDO	16-A	403	-	3,3,3	3.08	3 (100%)	2,2,2	2.79	2 (100%)
4	EDO	16-A	404	-	3,3,3	8.09	2 (66%)	2,2,2	1.83	0
3	CPS	2-A	200	-	35,35,45	21.42	30 (85%)	54,54,70	10.55	41 (75%)
2	SO4	2-A	300	-	4,4,4	0.80	0	6,6,6	0.82	0
2	SO4	2-A	301	-	4,4,4	9.58	4 (100%)	6,6,6	1.36	1 (16%)
2	SO4	2-A	302	-	4,4,4	1.36	1 (25%)	6,6,6	0.96	0
4	EDO	2-A	401	-	3,3,3	2.81	2 (66%)	2,2,2	0.86	0
4	EDO	2-A	402	-	3,3,3	2.33	2 (66%)	2,2,2	0.55	0
4	EDO	2-A	403	-	3,3,3	4.48	2 (66%)	2,2,2	0.80	0
4	EDO	2-A	404	-	3,3,3	4.91	2 (66%)	2,2,2	0.95	0
3	CPS	3-A	200	-	35,35,45	37.76	30 (85%)	54,54,70	18.21	47 (87%)
2	SO4	3-A	300	-	4,4,4	2.53	2 (50%)	6,6,6	0.75	0
2	SO4	3-A	301	-	4,4,4	4.22	2 (50%)	6,6,6	0.78	0
2	SO4	3-A	302	-	4,4,4	0.51	0	6,6,6	0.26	0
4	EDO	3-A	401	-	3,3,3	1.48	1 (33%)	2,2,2	0.72	0
4	EDO	3-A	402	-	3,3,3	2.42	2 (66%)	2,2,2	1.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	3-A	403	-	3,3,3	2.82	1 (33%)	2,2,2	2.69	2 (100%)
4	EDO	3-A	404	-	3,3,3	3.99	3 (100%)	2,2,2	0.73	0
3	CPS	4-A	200	-	35,35,45	19.19	29 (82%)	54,54,70	9.15	40 (74%)
2	SO4	4-A	300	-	4,4,4	1.28	0	6,6,6	0.83	0
2	SO4	4-A	301	-	4,4,4	4.17	2 (50%)	6,6,6	0.66	0
2	SO4	4-A	302	-	4,4,4	0.75	0	6,6,6	0.36	0
4	EDO	4-A	401	-	3,3,3	1.85	1 (33%)	2,2,2	0.23	0
4	EDO	4-A	402	-	3,3,3	2.43	3 (100%)	2,2,2	0.81	0
4	EDO	4-A	403	-	3,3,3	4.52	2 (66%)	2,2,2	0.56	0
4	EDO	4-A	404	-	3,3,3	5.28	3 (100%)	2,2,2	1.07	0
3	CPS	5-A	200	-	35,35,45	20.17	32 (91%)	54,54,70	12.02	49 (90%)
2	SO4	5-A	300	-	4,4,4	1.69	1 (25%)	6,6,6	0.85	0
2	SO4	5-A	301	-	4,4,4	2.72	1 (25%)	6,6,6	0.97	0
2	SO4	5-A	302	-	4,4,4	1.98	1 (25%)	6,6,6	0.33	0
4	EDO	5-A	401	-	3,3,3	1.03	0	2,2,2	0.91	0
4	EDO	5-A	402	-	3,3,3	2.98	2 (66%)	2,2,2	2.35	2 (100%)
4	EDO	5-A	403	-	3,3,3	3.36	2 (66%)	2,2,2	0.72	0
4	EDO	5-A	404	-	3,3,3	3.83	2 (66%)	2,2,2	1.96	1 (50%)
3	CPS	6-A	200	-	35,35,45	13.79	29 (82%)	54,54,70	8.71	42 (77%)
2	SO4	6-A	300	-	4,4,4	1.38	0	6,6,6	0.78	0
2	SO4	6-A	301	-	4,4,4	2.27	2 (50%)	6,6,6	1.31	1 (16%)
2	SO4	6-A	302	-	4,4,4	0.56	0	6,6,6	0.33	0
4	EDO	6-A	401	-	3,3,3	1.42	1 (33%)	2,2,2	2.14	1 (50%)
4	EDO	6-A	402	-	3,3,3	2.33	2 (66%)	2,2,2	0.29	0
4	EDO	6-A	403	-	3,3,3	3.99	2 (66%)	2,2,2	1.06	0
4	EDO	6-A	404	-	3,3,3	2.81	1 (33%)	2,2,2	1.62	0
3	CPS	7-A	200	-	35,35,45	17.58	31 (88%)	54,54,70	10.21	43 (79%)
2	SO4	7-A	300	-	4,4,4	0.50	0	6,6,6	0.76	0
2	SO4	7-A	301	-	4,4,4	7.69	3 (75%)	6,6,6	3.48	2 (33%)
2	SO4	7-A	302	-	4,4,4	0.59	0	6,6,6	0.34	0
4	EDO	7-A	401	-	3,3,3	1.01	0	2,2,2	0.68	0
4	EDO	7-A	402	-	3,3,3	2.44	2 (66%)	2,2,2	1.40	0
4	EDO	7-A	403	-	3,3,3	2.88	2 (66%)	2,2,2	0.87	0
4	EDO	7-A	404	-	3,3,3	2.92	2 (66%)	2,2,2	1.17	0
3	CPS	8-A	200	-	35,35,45	26.79	32 (91%)	54,54,70	13.86	41 (75%)
2	SO4	8-A	300	-	4,4,4	2.91	2 (50%)	6,6,6	1.20	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	8-A	301	-	4,4,4	5.41	3 (75%)	6,6,6	2.61	1 (16%)
2	SO4	8-A	302	-	4,4,4	0.94	0	6,6,6	0.52	0
4	EDO	8-A	401	-	3,3,3	1.35	0	2,2,2	0.75	0
4	EDO	8-A	402	-	3,3,3	2.44	3 (100%)	2,2,2	0.90	0
4	EDO	8-A	403	-	3,3,3	2.98	3 (100%)	2,2,2	2.53	2 (100%)
4	EDO	8-A	404	-	3,3,3	3.72	3 (100%)	2,2,2	0.75	0
3	CPS	9-A	200	-	35,35,45	21.27	31 (88%)	54,54,70	16.31	46 (85%)
2	SO4	9-A	300	-	4,4,4	2.64	2 (50%)	6,6,6	1.27	1 (16%)
2	SO4	9-A	301	-	4,4,4	5.58	3 (75%)	6,6,6	3.33	3 (50%)
2	SO4	9-A	302	-	4,4,4	0.72	0	6,6,6	0.29	0
4	EDO	9-A	401	-	3,3,3	1.26	0	2,2,2	0.70	0
4	EDO	9-A	402	-	3,3,3	2.49	3 (100%)	2,2,2	1.11	0
4	EDO	9-A	403	-	3,3,3	2.59	2 (66%)	2,2,2	1.10	0
4	EDO	9-A	404	-	3,3,3	3.52	2 (66%)	2,2,2	2.09	1 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CPS	1-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	1-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	1-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	1-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	1-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	1-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	1-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	1-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	10-A	200	-	4/4/12/15	0/13/78/90	0/0/4/4
2	SO4	10-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	10-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	10-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	10-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	10-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	10-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	10-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	11-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	11-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	11-A	301	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	11-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	11-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	11-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	11-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	11-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	12-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	12-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	12-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	12-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	12-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	12-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	12-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	12-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	13-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	13-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	13-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	13-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	13-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	13-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	13-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	13-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	14-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	14-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	14-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	14-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	14-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	14-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	14-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	14-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	15-A	200	-	4/4/12/15	0/13/78/90	0/0/4/4
2	SO4	15-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	15-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	15-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	15-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	15-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	15-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	15-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	16-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	16-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	16-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	16-A	302	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	16-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	16-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	16-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	16-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	2-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	2-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	2-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	2-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	2-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	2-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	2-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	2-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	3-A	200	-	7/7/12/15	0/13/78/90	0/0/4/4
2	SO4	3-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	3-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	3-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	3-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	3-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	3-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	3-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	4-A	200	-	4/4/12/15	0/13/78/90	0/0/4/4
2	SO4	4-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	4-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	4-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	4-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	4-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	4-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	4-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	5-A	200	-	4/4/12/15	0/13/78/90	0/0/4/4
2	SO4	5-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	5-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	5-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	5-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	5-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	5-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	5-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	6-A	200	-	8/8/12/15	0/13/78/90	0/0/4/4
2	SO4	6-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	6-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	6-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	6-A	401	-	-	0/1/1/1	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	6-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	6-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	6-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	7-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	7-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	7-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	7-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	7-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	7-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	7-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	7-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	8-A	200	-	5/5/12/15	0/13/78/90	0/0/4/4
2	SO4	8-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	8-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	8-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	8-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	8-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	8-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	8-A	404	-	-	0/1/1/1	0/0/0/0
3	CPS	9-A	200	-	3/3/12/15	0/13/78/90	0/0/4/4
2	SO4	9-A	300	-	-	0/0/0/0	0/0/0/0
2	SO4	9-A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	9-A	302	-	-	0/0/0/0	0/0/0/0
4	EDO	9-A	401	-	-	0/1/1/1	0/0/0/0
4	EDO	9-A	402	-	-	0/1/1/1	0/0/0/0
4	EDO	9-A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	9-A	404	-	-	0/1/1/1	0/0/0/0

All (680) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-A	200	CPS	C18-C17	157.14	4.19	1.53
3	3-A	200	CPS	C12-C13	93.99	4.25	1.51
3	8-A	200	CPS	C5-C9	84.77	3.01	1.55
3	3-A	200	CPS	C27-C26	-78.71	1.23	1.55
3	2-A	200	CPS	C3-C4	71.59	2.82	1.53
3	8-A	200	CPS	C20-C9	-65.04	0.24	1.54
3	2-A	200	CPS	C3-C19	-64.34	0.46	1.53
3	16-A	200	CPS	C27-C26	-56.19	1.32	1.55
3	14-A	200	CPS	C5-C9	56.06	2.52	1.55
3	14-A	200	CPS	C20-C9	52.17	2.58	1.54
3	4-A	200	CPS	C11-C2	51.04	2.52	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	13-A	200	CPS	C20-C9	50.72	2.55	1.54
3	1-A	200	CPS	C3-C19	-50.38	0.69	1.53
3	8-A	200	CPS	C27-C26	49.80	1.75	1.55
3	5-A	200	CPS	C5-C9	-49.52	0.70	1.55
3	9-A	200	CPS	C27-C26	47.66	1.74	1.55
3	8-A	200	CPS	C8-C9	46.93	2.65	1.54
3	15-A	200	CPS	C5-C6	46.25	2.35	1.55
3	15-A	200	CPS	C20-C9	45.58	2.45	1.54
3	1-A	200	CPS	C20-C9	-45.38	0.63	1.54
3	15-A	200	CPS	C18-C17	44.79	2.29	1.53
3	10-A	200	CPS	C14-C13	44.65	2.38	1.51
3	4-A	200	CPS	C10-C5	42.50	2.25	1.54
3	16-A	200	CPS	C3-C4	42.25	2.29	1.53
3	4-A	200	CPS	C5-C6	-41.86	0.83	1.55
3	7-A	200	CPS	C16-C17	-41.46	0.84	1.52
3	9-A	200	CPS	O4-C4	-41.39	0.70	1.43
3	10-A	200	CPS	C11-C2	-40.79	0.75	1.54
3	13-A	200	CPS	C18-C17	40.53	2.22	1.53
3	9-A	200	CPS	C3-C4	40.43	2.26	1.53
3	6-A	200	CPS	C14-C15	-40.22	0.84	1.53
3	11-A	200	CPS	C5-C9	-40.22	0.86	1.55
3	2-A	200	CPS	C5-C4	-40.21	0.90	1.54
3	8-A	200	CPS	C22-C20	40.03	2.71	1.54
3	10-A	200	CPS	O4-C4	-39.46	0.74	1.43
3	7-A	200	CPS	C5-C4	-39.40	0.91	1.54
3	14-A	200	CPS	C5-C6	39.22	2.23	1.55
3	12-A	200	CPS	C10-C5	38.73	2.18	1.54
3	11-A	200	CPS	C18-C17	38.34	2.18	1.53
3	15-A	200	CPS	C3-C4	-38.06	0.84	1.53
3	1-A	200	CPS	C5-C6	37.90	2.20	1.55
3	15-A	200	CPS	C10-C5	37.62	2.17	1.54
3	5-A	200	CPS	C18-C17	37.34	2.16	1.53
3	13-A	200	CPS	C27-C26	37.34	1.70	1.55
3	3-A	200	CPS	C11-C2	-37.21	0.82	1.54
3	14-A	200	CPS	C16-C17	36.90	2.14	1.52
3	13-A	200	CPS	C5-C6	36.53	2.18	1.55
3	3-A	200	CPS	C3-C19	36.50	2.14	1.53
3	14-A	200	CPS	C2-C19	-36.22	0.99	1.56
3	5-A	200	CPS	C8-C9	-36.08	0.68	1.54
3	7-A	200	CPS	C10-C5	35.99	2.14	1.54
3	15-A	200	CPS	C14-C13	-35.60	0.82	1.51
3	9-A	200	CPS	O1-C24	-35.17	0.45	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	15-A	200	CPS	C1-C12	-34.45	0.74	1.53
3	8-A	200	CPS	C21-C20	34.44	2.44	1.53
3	4-A	200	CPS	C27-C26	34.42	1.68	1.55
3	16-A	200	CPS	C23-C24	34.08	2.21	1.51
3	13-A	200	CPS	C1-C12	-33.66	0.76	1.53
3	15-A	200	CPS	C8-C9	33.42	2.33	1.54
3	14-A	200	CPS	C18-C17	33.39	2.09	1.53
3	5-A	200	CPS	C1-C12	33.38	2.30	1.53
3	10-A	200	CPS	C5-C6	33.26	2.12	1.55
3	11-A	200	CPS	C16-C17	-32.55	0.98	1.52
3	9-A	200	CPS	C1-C12	32.54	2.28	1.53
3	3-A	200	CPS	C3-C4	-32.51	0.94	1.53
3	13-A	200	CPS	C5-C9	32.46	2.11	1.55
3	4-A	200	CPS	C5-C4	32.43	2.06	1.54
3	1-A	200	CPS	C18-C17	-32.41	0.98	1.53
3	8-A	200	CPS	C1-C12	-32.31	0.79	1.53
3	15-A	200	CPS	C3-C19	32.28	2.07	1.53
3	16-A	200	CPS	C1-C12	32.00	2.27	1.53
3	7-A	200	CPS	C27-C26	31.80	1.67	1.55
3	8-A	200	CPS	C10-C5	31.70	2.07	1.54
3	13-A	200	CPS	C8-C9	31.69	2.29	1.54
3	14-A	200	CPS	O1-C24	-31.42	0.54	1.23
3	16-A	200	CPS	C2-C19	-31.33	1.07	1.56
3	2-A	200	CPS	C1-C2	-31.33	0.94	1.54
3	15-A	200	CPS	O1-C24	-31.29	0.54	1.23
3	16-A	200	CPS	C5-C6	31.12	2.09	1.55
3	2-A	200	CPS	C14-C15	30.78	2.06	1.53
3	11-A	200	CPS	C21-C20	30.45	2.34	1.53
3	13-A	200	CPS	C14-C13	-30.40	0.92	1.51
3	16-A	200	CPS	C10-C5	-30.06	1.04	1.54
3	7-A	200	CPS	O1-C24	-29.75	0.57	1.23
3	14-A	200	CPS	O4-C4	29.46	1.95	1.43
3	13-A	200	CPS	C3-C19	29.46	2.02	1.53
3	9-A	200	CPS	C5-C9	-29.41	1.04	1.55
3	14-A	200	CPS	C3-C19	29.27	2.02	1.53
3	15-A	200	CPS	C16-C17	28.33	1.99	1.52
3	9-A	200	CPS	C5-C6	28.30	2.04	1.55
3	4-A	200	CPS	C16-C17	28.30	1.99	1.52
3	12-A	200	CPS	C24-N1	-28.29	0.66	1.33
3	14-A	200	CPS	C8-C9	28.27	2.21	1.54
3	7-A	200	CPS	C24-N1	-28.00	0.66	1.33
3	9-A	200	CPS	C18-C17	27.91	2.00	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	16-A	200	CPS	C5-C4	-27.88	1.10	1.54
3	10-A	200	CPS	C3-C19	27.56	1.99	1.53
3	14-A	200	CPS	C8-C7	-27.22	0.75	1.54
3	1-A	200	CPS	C3-C4	27.08	2.02	1.53
3	10-A	200	CPS	C7-C6	-26.91	0.90	1.54
3	10-A	200	CPS	C18-C6	26.91	2.07	1.53
3	13-A	200	CPS	C16-C17	26.65	1.97	1.52
3	11-A	200	CPS	C7-C6	26.65	2.17	1.54
3	8-A	200	CPS	O3-C17	-26.58	0.82	1.43
3	10-A	200	CPS	C2-C15	26.24	2.00	1.55
3	5-A	200	CPS	C3-C19	26.12	1.97	1.53
3	16-A	200	CPS	O3-C17	-26.08	0.83	1.43
3	9-A	200	CPS	C24-N1	-25.98	0.71	1.33
3	4-A	200	CPS	C3-C19	25.83	1.96	1.53
3	6-A	200	CPS	C24-N1	-25.52	0.72	1.33
3	13-A	200	CPS	C5-C4	25.44	1.95	1.54
3	13-A	200	CPS	C2-C15	25.41	1.98	1.55
3	9-A	200	CPS	C3-C19	25.32	1.96	1.53
3	15-A	200	CPS	C2-C15	25.31	1.98	1.55
3	12-A	200	CPS	C27-C26	25.23	1.65	1.55
3	3-A	200	CPS	C5-C6	25.09	1.98	1.55
3	6-A	200	CPS	C1-C2	25.07	2.01	1.54
3	3-A	200	CPS	C7-C6	-24.75	0.95	1.54
3	9-A	200	CPS	C16-C15	24.62	1.96	1.53
3	11-A	200	CPS	C27-C26	-24.48	1.45	1.55
3	3-A	200	CPS	O4-C4	24.44	1.86	1.43
3	1-A	200	CPS	O3-C17	24.34	1.99	1.43
3	10-A	200	CPS	C27-C26	24.28	1.64	1.55
3	1-A	200	CPS	C11-C2	24.25	2.01	1.54
3	4-A	200	CPS	C23-C24	-24.00	1.01	1.51
3	3-A	200	CPS	C14-C13	-23.94	1.05	1.51
3	5-A	200	CPS	C11-C2	23.84	2.00	1.54
3	1-A	200	CPS	C14-C13	-23.79	1.05	1.51
3	15-A	200	CPS	C11-C2	-23.61	1.08	1.54
3	9-A	200	CPS	C8-C7	-23.39	0.86	1.54
3	3-A	200	CPS	O3-C17	-23.38	0.89	1.43
3	9-A	200	CPS	C2-C15	23.34	1.95	1.55
3	15-A	200	CPS	C22-C23	-23.09	0.76	1.52
3	5-A	200	CPS	C7-C6	-23.06	0.99	1.54
3	6-A	200	CPS	C23-C24	22.99	1.98	1.51
3	7-A	200	CPS	C2-C19	-22.99	1.20	1.56
3	14-A	200	CPS	C22-C23	-22.79	0.77	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-A	200	CPS	O4-C4	-22.73	1.03	1.43
3	6-A	200	CPS	C20-C9	-22.66	1.09	1.54
3	12-A	200	CPS	C5-C4	-22.59	1.18	1.54
3	16-A	200	CPS	O4-C4	22.55	1.83	1.43
3	12-A	200	CPS	C21-C20	22.48	2.13	1.53
3	14-A	200	CPS	C10-C5	-22.43	1.17	1.54
3	8-A	200	CPS	C25-C26	-22.37	1.30	1.53
3	11-A	200	CPS	O3-C17	-22.21	0.92	1.43
3	3-A	200	CPS	C1-C12	-22.21	1.02	1.53
3	5-A	200	CPS	C16-C17	-22.20	1.15	1.52
3	8-A	200	CPS	C5-C6	22.15	1.93	1.55
3	14-A	200	CPS	C3-C4	22.12	1.93	1.53
3	11-A	200	CPS	C14-C15	22.10	1.91	1.53
3	1-A	200	CPS	C14-C15	22.06	1.91	1.53
3	10-A	200	CPS	C3-C4	22.00	1.93	1.53
3	16-A	200	CPS	C16-C17	-21.90	1.16	1.52
3	10-A	200	CPS	C5-C4	-21.87	1.19	1.54
3	2-A	200	CPS	C11-C2	21.81	1.96	1.54
3	7-A	200	CPS	C1-C12	21.79	2.03	1.53
3	3-A	200	CPS	C5-C9	-21.49	1.18	1.55
3	11-A	200	CPS	C5-C6	21.36	1.92	1.55
3	10-A	200	CPS	C16-C15	-21.27	1.17	1.53
3	5-A	200	CPS	O2-C13	-21.27	0.77	1.43
3	10-A	200	CPS	C24-N1	-21.21	0.83	1.33
3	3-A	200	CPS	C5-C4	21.20	1.88	1.54
3	5-A	200	CPS	C2-C15	20.97	1.91	1.55
3	6-A	200	CPS	C21-C20	20.59	2.08	1.53
3	2-A	200	CPS	C2-C15	20.44	1.90	1.55
3	8-A	200	CPS	C18-C17	20.39	1.88	1.53
3	3-A	200	CPS	C22-C23	20.35	2.20	1.52
3	1-A	200	CPS	C12-C13	20.35	2.10	1.51
3	2-A	200	CPS	C22-C23	-20.26	0.85	1.52
3	9-A	200	CPS	C22-C23	-20.21	0.85	1.52
3	5-A	200	CPS	C12-C13	20.17	2.10	1.51
3	13-A	200	CPS	C22-C23	-20.13	0.85	1.52
3	5-A	200	CPS	O1-C24	-20.12	0.78	1.23
3	13-A	200	CPS	O1-C24	-20.02	0.79	1.23
3	3-A	200	CPS	C21-C20	19.88	2.06	1.53
3	5-A	200	CPS	C24-N1	19.86	1.80	1.33
3	4-A	200	CPS	C24-N1	19.78	1.80	1.33
3	12-A	200	CPS	C20-C9	-19.77	1.14	1.54
3	12-A	200	CPS	O1-C24	-19.73	0.79	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	12-A	200	CPS	C23-C24	19.70	1.92	1.51
3	5-A	200	CPS	O3-C17	19.52	1.88	1.43
3	14-A	200	CPS	C21-C20	-19.45	1.01	1.53
3	1-A	200	CPS	C1-C2	-19.43	1.17	1.54
3	10-A	200	CPS	C22-C20	19.39	2.11	1.54
3	4-A	200	CPS	C3-C4	-19.28	1.18	1.53
3	5-A	200	CPS	C5-C4	19.28	1.85	1.54
3	4-A	200	CPS	C20-C9	19.08	1.92	1.54
3	11-A	200	CPS	C22-C23	18.96	2.15	1.52
3	15-A	200	CPS	C14-C15	18.84	1.86	1.53
3	7-A	200	CPS	C23-C24	18.67	1.90	1.51
3	8-A	200	CPS	C2-C19	18.63	1.85	1.56
3	2-A	200	CPS	C5-C9	18.62	1.87	1.55
3	16-A	200	CPS	C8-C9	18.60	1.98	1.54
3	5-A	200	CPS	C16-C15	18.49	1.85	1.53
3	8-A	200	CPS	C7-C6	-18.39	1.10	1.54
3	7-A	200	CPS	C22-C23	-18.26	0.92	1.52
3	15-A	200	CPS	O3-C17	-18.13	1.01	1.43
3	10-A	200	CPS	C1-C2	-18.05	1.19	1.54
3	12-A	200	CPS	C22-C23	-18.01	0.93	1.52
3	4-A	200	CPS	O1-C24	-17.82	0.84	1.23
3	9-A	200	CPS	C10-C5	17.81	1.84	1.54
3	6-A	200	CPS	O3-C17	-17.79	1.02	1.43
3	15-A	200	CPS	C22-C20	17.59	2.05	1.54
3	11-A	200	CPS	C2-C15	17.36	1.85	1.55
3	8-A	200	CPS	C3-C19	17.30	1.82	1.53
3	14-A	200	CPS	C18-C6	-17.21	1.19	1.53
3	6-A	200	CPS	C22-C20	17.20	2.04	1.54
3	1-A	200	CPS	C18-C6	-17.15	1.19	1.53
3	13-A	200	CPS	C10-C5	17.06	1.82	1.54
3	7-A	200	CPS	C3-C4	16.89	1.83	1.53
3	7-A	200	CPS	C5-C9	-16.81	1.26	1.55
3	15-A	200	CPS	C16-C15	-16.80	1.24	1.53
3	6-A	200	CPS	C27-C26	16.69	1.61	1.55
3	7-A	200	CPS	C18-C17	16.58	1.81	1.53
3	14-A	200	CPS	C14-C13	-16.50	1.19	1.51
3	5-A	200	CPS	C22-C20	16.49	2.02	1.54
3	6-A	200	CPS	O1-C24	16.45	1.59	1.23
3	12-A	200	CPS	O4-C4	16.17	1.72	1.43
3	14-A	200	CPS	C18-C19	16.06	1.86	1.53
3	2-A	200	CPS	C22-C20	15.94	2.01	1.54
3	5-A	200	CPS	C10-C5	15.80	1.80	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	10-A	200	CPS	C10-C5	15.73	1.80	1.54
3	11-A	200	CPS	C1-C12	-15.72	1.17	1.53
3	5-A	200	CPS	C27-C26	15.56	1.61	1.55
3	5-A	200	CPS	C21-C20	-15.48	1.11	1.53
3	8-A	200	CPS	C3-C4	-15.26	1.25	1.53
3	3-A	200	CPS	C10-C5	-15.24	1.29	1.54
3	1-A	200	CPS	C2-C15	15.19	1.81	1.55
3	9-A	200	CPS	C23-C24	15.17	1.82	1.51
3	12-A	200	CPS	C22-C20	15.16	1.98	1.54
3	14-A	200	CPS	C25-N1	15.13	1.82	1.46
3	15-A	200	CPS	C25-N1	15.13	1.82	1.46
3	9-A	200	CPS	C11-C2	15.11	1.83	1.54
3	13-A	200	CPS	C22-C20	14.95	1.98	1.54
3	1-A	200	CPS	C10-C5	-14.94	1.29	1.54
3	16-A	200	CPS	C25-C26	-14.94	1.37	1.53
3	2-A	200	CPS	C12-C13	14.92	1.95	1.51
2	11-A	300	SO4	O2-S	-14.68	0.99	1.47
3	14-A	200	CPS	C23-C24	-14.68	1.20	1.51
3	9-A	200	CPS	C14-C13	14.65	1.80	1.51
3	7-A	200	CPS	O3-C17	-14.59	1.09	1.43
3	3-A	200	CPS	O1-C24	14.58	1.55	1.23
3	9-A	200	CPS	C16-C17	-14.50	1.28	1.52
3	4-A	200	CPS	O4-C4	14.41	1.69	1.43
3	4-A	200	CPS	C21-C20	14.11	1.90	1.53
2	14-A	300	SO4	O4-S	14.07	1.95	1.47
3	16-A	200	CPS	O1-C24	14.06	1.54	1.23
3	6-A	200	CPS	O4-C4	14.05	1.68	1.43
3	3-A	200	CPS	C16-C17	-13.97	1.29	1.52
3	2-A	200	CPS	C16-C15	-13.82	1.29	1.53
3	13-A	200	CPS	C14-C15	13.72	1.77	1.53
3	12-A	200	CPS	C5-C9	-13.72	1.31	1.55
2	2-A	301	SO4	O4-S	13.66	1.93	1.47
3	11-A	200	CPS	C23-C24	13.64	1.79	1.51
3	13-A	200	CPS	C16-C15	-13.59	1.30	1.53
3	8-A	200	CPS	C25-N1	13.51	1.78	1.46
3	9-A	200	CPS	C12-C13	13.46	1.90	1.51
2	16-A	300	SO4	O4-S	13.45	1.93	1.47
2	7-A	301	SO4	O4-S	13.39	1.92	1.47
3	4-A	200	CPS	O3-C17	13.31	1.74	1.43
3	13-A	200	CPS	C23-C24	-13.18	1.24	1.51
3	6-A	200	CPS	C3-C19	-13.10	1.32	1.53
3	12-A	200	CPS	O3-C17	-13.06	1.13	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	16-A	200	CPS	C18-C6	12.85	1.79	1.53
3	7-A	200	CPS	C11-C2	12.83	1.79	1.54
3	2-A	200	CPS	O4-C4	-12.73	1.21	1.43
3	13-A	200	CPS	C24-N1	12.65	1.63	1.33
3	5-A	200	CPS	C20-C9	12.63	1.79	1.54
3	7-A	200	CPS	C18-C6	-12.60	1.28	1.53
3	14-A	200	CPS	C7-C6	-12.58	1.24	1.54
3	16-A	200	CPS	C24-N1	-12.51	1.03	1.33
3	6-A	200	CPS	C14-C13	12.35	1.75	1.51
3	16-A	200	CPS	C7-C6	12.35	1.83	1.54
3	5-A	200	CPS	C18-C6	12.35	1.78	1.53
3	10-A	200	CPS	C23-C24	12.34	1.76	1.51
3	14-A	200	CPS	O3-C17	-12.32	1.15	1.43
2	11-A	300	SO4	O1-S	12.31	1.87	1.47
4	16-A	404	EDO	O1-C1	12.27	2.07	1.42
3	5-A	200	CPS	C23-C24	12.05	1.76	1.51
3	3-A	200	CPS	C24-N1	11.99	1.61	1.33
3	3-A	200	CPS	C23-C24	11.96	1.76	1.51
3	11-A	200	CPS	C8-C9	11.85	1.82	1.54
3	6-A	200	CPS	C22-C23	-11.81	1.13	1.52
3	9-A	200	CPS	O2-C13	-11.81	1.06	1.43
3	5-A	200	CPS	C1-C2	-11.77	1.31	1.54
3	11-A	200	CPS	C3-C19	-11.77	1.34	1.53
3	9-A	200	CPS	C25-N1	11.77	1.74	1.46
3	6-A	200	CPS	C18-C6	-11.73	1.30	1.53
3	1-A	200	CPS	C2-C19	-11.73	1.37	1.56
3	13-A	200	CPS	C7-C6	-11.70	1.26	1.54
3	5-A	200	CPS	C3-C4	-11.65	1.32	1.53
3	5-A	200	CPS	C5-C6	11.44	1.75	1.55
3	12-A	200	CPS	C1-C12	11.39	1.79	1.53
4	15-A	404	EDO	O2-C2	11.23	2.02	1.42
3	10-A	200	CPS	C2-C19	11.23	1.73	1.56
4	14-A	404	EDO	O2-C2	11.17	2.01	1.42
3	15-A	200	CPS	C7-C6	-11.15	1.28	1.54
3	10-A	200	CPS	C22-C23	-11.14	1.15	1.52
3	4-A	200	CPS	C8-C7	11.10	1.86	1.54
3	16-A	200	CPS	C11-C2	11.01	1.75	1.54
2	2-A	301	SO4	O2-S	10.95	1.82	1.47
2	10-A	301	SO4	O1-S	10.94	1.82	1.47
3	16-A	200	CPS	C1-C2	-10.82	1.33	1.54
3	14-A	200	CPS	C11-C2	-10.81	1.33	1.54
3	9-A	200	CPS	C1-C2	-10.77	1.33	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-A	200	CPS	C22-C20	10.62	1.85	1.54
3	10-A	200	CPS	C5-C9	-10.49	1.37	1.55
3	15-A	200	CPS	C18-C6	-10.49	1.32	1.53
3	15-A	200	CPS	C23-C24	-10.41	1.29	1.51
3	14-A	200	CPS	C14-C15	10.34	1.71	1.53
3	13-A	200	CPS	O3-C17	-10.31	1.19	1.43
3	8-A	200	CPS	C18-C19	-10.30	1.33	1.53
3	16-A	200	CPS	C8-C7	-10.28	1.24	1.54
3	1-A	200	CPS	C16-C17	-10.12	1.36	1.52
3	2-A	200	CPS	C25-N1	10.11	1.70	1.46
3	16-A	200	CPS	C12-C13	10.01	1.80	1.51
3	15-A	200	CPS	O4-C4	9.92	1.61	1.43
3	3-A	200	CPS	O2-C13	-9.86	1.12	1.43
3	14-A	200	CPS	C25-C26	9.86	1.63	1.53
3	2-A	200	CPS	C25-C26	-9.86	1.43	1.53
4	13-A	404	EDO	O2-C2	9.61	1.93	1.42
3	12-A	200	CPS	C2-C19	-9.50	1.41	1.56
3	14-A	200	CPS	C16-C15	-9.47	1.37	1.53
3	6-A	200	CPS	O2-C13	9.35	1.72	1.43
3	1-A	200	CPS	C7-C6	-9.28	1.32	1.54
3	7-A	200	CPS	C25-N1	9.27	1.68	1.46
3	1-A	200	CPS	C8-C7	9.04	1.80	1.54
3	14-A	200	CPS	C24-N1	8.96	1.54	1.33
3	9-A	200	CPS	C25-C26	8.92	1.62	1.53
3	12-A	200	CPS	C25-N1	8.80	1.67	1.46
3	7-A	200	CPS	C2-C15	8.75	1.70	1.55
3	10-A	200	CPS	C8-C7	-8.75	1.28	1.54
3	1-A	200	CPS	C16-C15	-8.73	1.38	1.53
3	16-A	200	CPS	C21-C20	8.69	1.76	1.53
3	16-A	200	CPS	C18-C17	-8.62	1.38	1.53
3	4-A	200	CPS	C1-C12	8.59	1.73	1.53
3	2-A	200	CPS	C1-C12	8.59	1.73	1.53
3	1-A	200	CPS	C22-C23	8.52	1.81	1.52
3	8-A	200	CPS	C18-C6	8.47	1.70	1.53
3	8-A	200	CPS	O2-C13	-8.41	1.17	1.43
3	13-A	200	CPS	C21-C20	-8.33	1.30	1.53
2	9-A	301	SO4	O1-S	-8.32	1.19	1.47
3	10-A	200	CPS	C12-C13	8.29	1.75	1.51
3	3-A	200	CPS	C1-C2	-8.23	1.38	1.54
3	15-A	200	CPS	C27-C26	8.19	1.58	1.55
3	8-A	200	CPS	C2-C15	8.03	1.69	1.55
2	12-A	301	SO4	O3-S	8.03	1.74	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	16-A	301	SO4	O3-S	8.02	1.74	1.47
3	1-A	200	CPS	C25-N1	7.99	1.65	1.46
3	13-A	200	CPS	C3-C4	7.97	1.67	1.53
3	12-A	200	CPS	C18-C19	-7.94	1.37	1.53
3	7-A	200	CPS	C16-C15	7.94	1.67	1.53
3	8-A	200	CPS	C1-C2	7.92	1.69	1.54
4	13-A	404	EDO	O1-C1	7.91	1.84	1.42
4	13-A	402	EDO	O1-C1	7.82	1.83	1.42
3	2-A	200	CPS	C8-C9	7.77	1.72	1.54
3	12-A	200	CPS	C14-C15	-7.73	1.40	1.53
2	13-A	301	SO4	O1-S	7.72	1.72	1.47
3	2-A	200	CPS	C8-C7	7.65	1.76	1.54
3	8-A	200	CPS	C22-C23	7.63	1.78	1.52
3	13-A	200	CPS	C8-C7	-7.62	1.31	1.54
3	15-A	200	CPS	C24-N1	7.60	1.51	1.33
3	2-A	200	CPS	O2-C13	7.50	1.67	1.43
3	5-A	200	CPS	C22-C23	-7.46	1.28	1.52
3	9-A	200	CPS	C18-C6	7.42	1.68	1.53
3	1-A	200	CPS	C25-C26	-7.37	1.45	1.53
2	3-A	301	SO4	O3-S	7.35	1.72	1.47
4	4-A	404	EDO	O2-C2	7.25	1.80	1.42
3	11-A	200	CPS	C25-N1	-7.23	1.29	1.46
3	1-A	200	CPS	O1-C24	7.20	1.39	1.23
3	7-A	200	CPS	C18-C19	-7.20	1.39	1.53
2	4-A	301	SO4	O3-S	7.17	1.71	1.47
4	13-A	404	EDO	C2-C1	7.08	1.95	1.47
3	10-A	200	CPS	O1-C24	7.00	1.38	1.23
3	11-A	200	CPS	C3-C4	6.99	1.66	1.53
3	12-A	200	CPS	C16-C17	-6.97	1.41	1.52
3	12-A	200	CPS	C14-C13	6.96	1.65	1.51
4	2-A	404	EDO	O2-C2	6.91	1.79	1.42
2	8-A	301	SO4	O1-S	6.90	1.69	1.47
2	2-A	301	SO4	O1-S	6.89	1.69	1.47
4	1-A	404	EDO	O1-C1	6.88	1.78	1.42
3	11-A	200	CPS	C24-N1	6.83	1.49	1.33
4	14-A	404	EDO	C2-C1	6.82	1.94	1.47
2	9-A	301	SO4	O4-S	6.81	1.70	1.47
3	6-A	200	CPS	C2-C19	-6.74	1.45	1.56
3	11-A	200	CPS	C1-C2	6.73	1.66	1.54
4	15-A	402	EDO	O1-C1	6.69	1.77	1.42
4	15-A	404	EDO	C2-C1	6.65	1.92	1.47
3	1-A	200	CPS	C5-C9	-6.62	1.44	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-A	200	CPS	C27-C26	6.61	1.57	1.55
4	16-A	404	EDO	C2-C1	6.58	1.92	1.47
3	1-A	200	CPS	C1-C12	6.56	1.68	1.53
3	8-A	200	CPS	C16-C17	-6.55	1.41	1.52
2	15-A	301	SO4	O4-S	6.50	1.69	1.47
4	4-A	403	EDO	O2-C2	-6.46	1.07	1.42
2	14-A	301	SO4	O4-S	6.46	1.69	1.47
3	15-A	200	CPS	C1-C2	-6.39	1.42	1.54
3	3-A	200	CPS	C18-C19	-6.36	1.41	1.53
4	2-A	403	EDO	O2-C2	-6.36	1.07	1.42
3	10-A	200	CPS	O2-C13	-6.36	1.23	1.43
3	8-A	200	CPS	C16-C15	6.32	1.64	1.53
2	10-A	301	SO4	O2-S	6.29	1.67	1.47
3	12-A	200	CPS	C18-C6	-6.25	1.41	1.53
3	8-A	200	CPS	O4-C4	6.25	1.54	1.43
3	13-A	200	CPS	C11-C2	6.20	1.66	1.54
3	2-A	200	CPS	C5-C6	-6.16	1.44	1.55
3	11-A	200	CPS	O1-C24	6.10	1.36	1.23
3	9-A	200	CPS	C7-C6	-6.00	1.40	1.54
3	9-A	200	CPS	C20-C9	6.00	1.66	1.54
3	3-A	200	CPS	C25-N1	-5.98	1.32	1.46
4	15-A	403	EDO	O1-C1	5.97	1.74	1.42
4	13-A	403	EDO	O1-C1	5.97	1.74	1.42
2	13-A	301	SO4	O2-S	5.97	1.66	1.47
3	6-A	200	CPS	C16-C15	-5.96	1.43	1.53
3	7-A	200	CPS	C22-C20	5.94	1.71	1.54
2	7-A	301	SO4	O1-S	-5.91	1.27	1.47
2	8-A	301	SO4	O3-S	5.90	1.67	1.47
3	16-A	200	CPS	C25-N1	5.89	1.60	1.46
3	7-A	200	CPS	C20-C9	-5.84	1.42	1.54
3	11-A	200	CPS	C10-C5	-5.82	1.44	1.54
4	13-A	403	EDO	O2-C2	-5.81	1.10	1.42
3	2-A	200	CPS	C23-C24	-5.79	1.39	1.51
3	10-A	200	CPS	C8-C9	5.76	1.68	1.54
3	7-A	200	CPS	C21-C20	5.75	1.68	1.53
3	2-A	200	CPS	C21-C20	-5.64	1.38	1.53
3	2-A	200	CPS	O3-C17	-5.59	1.30	1.43
3	15-A	200	CPS	C25-C26	5.57	1.59	1.53
2	8-A	301	SO4	O2-S	5.57	1.65	1.47
3	13-A	200	CPS	C25-C26	-5.56	1.47	1.53
3	3-A	200	CPS	C14-C15	5.55	1.63	1.53
3	6-A	200	CPS	C11-C2	5.45	1.64	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	14-A	403	EDO	O1-C1	5.42	1.71	1.42
3	4-A	200	CPS	C5-C9	5.40	1.64	1.55
3	2-A	200	CPS	C14-C13	-5.36	1.41	1.51
3	5-A	200	CPS	C2-C19	-5.36	1.47	1.56
2	15-A	301	SO4	O1-S	-5.35	1.29	1.47
3	6-A	200	CPS	C10-C5	-5.34	1.45	1.54
3	16-A	200	CPS	C22-C20	5.28	1.69	1.54
2	1-A	300	SO4	O3-S	-5.27	1.29	1.47
4	14-A	401	EDO	O1-C1	5.27	1.70	1.42
3	9-A	200	CPS	C22-C20	5.26	1.69	1.54
4	15-A	403	EDO	O2-C2	-5.24	1.13	1.42
3	4-A	200	CPS	C7-C6	5.24	1.66	1.54
3	2-A	200	CPS	C18-C17	-5.23	1.44	1.53
3	1-A	200	CPS	C18-C19	5.21	1.64	1.53
2	1-A	301	SO4	O3-S	5.20	1.65	1.47
3	2-A	200	CPS	C20-C9	5.19	1.64	1.54
3	8-A	200	CPS	C12-C13	5.19	1.66	1.51
3	1-A	200	CPS	C5-C4	-5.18	1.46	1.54
4	6-A	403	EDO	O2-C2	-5.16	1.14	1.42
3	2-A	200	CPS	C7-C6	-5.14	1.42	1.54
4	14-A	403	EDO	O2-C2	-5.10	1.14	1.42
3	7-A	200	CPS	C1-C2	-5.09	1.44	1.54
3	4-A	200	CPS	C22-C23	5.07	1.69	1.52
4	12-A	404	EDO	O2-C2	5.06	1.69	1.42
3	4-A	200	CPS	C25-C26	5.04	1.58	1.53
3	8-A	200	CPS	C5-C4	-4.98	1.46	1.54
3	15-A	200	CPS	C2-C19	-4.95	1.48	1.56
4	15-A	401	EDO	O2-C2	4.93	1.68	1.42
3	9-A	200	CPS	C2-C19	-4.92	1.48	1.56
3	12-A	200	CPS	O2-C13	4.90	1.58	1.43
3	15-A	200	CPS	C8-C7	-4.89	1.39	1.54
3	7-A	200	CPS	C25-C26	-4.86	1.48	1.53
2	15-A	301	SO4	O2-S	4.83	1.62	1.47
2	14-A	301	SO4	O3-S	4.83	1.63	1.47
3	4-A	200	CPS	C2-C15	4.81	1.63	1.55
3	13-A	200	CPS	C1-C2	-4.81	1.45	1.54
3	5-A	200	CPS	C18-C19	4.81	1.63	1.53
4	5-A	404	EDO	O1-C1	4.77	1.67	1.42
4	2-A	404	EDO	C2-C1	4.75	1.79	1.47
4	13-A	401	EDO	O1-C1	4.72	1.67	1.42
2	5-A	301	SO4	O3-S	4.69	1.63	1.47
3	1-A	200	CPS	C8-C9	-4.69	1.43	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	8-A	200	CPS	C14-C15	4.69	1.61	1.53
3	8-A	200	CPS	C24-N1	4.68	1.44	1.33
4	1-A	404	EDO	C2-C1	4.66	1.79	1.47
3	16-A	200	CPS	C5-C9	-4.63	1.47	1.55
3	6-A	200	CPS	C5-C4	-4.62	1.47	1.54
2	8-A	300	SO4	O3-S	-4.62	1.31	1.47
3	11-A	200	CPS	C2-C19	-4.62	1.48	1.56
4	5-A	403	EDO	O2-C2	-4.57	1.17	1.42
3	6-A	200	CPS	C16-C17	-4.55	1.45	1.52
4	4-A	404	EDO	C2-C1	4.50	1.78	1.47
4	12-A	404	EDO	O1-C1	-4.50	1.17	1.42
3	12-A	200	CPS	C25-C26	-4.48	1.48	1.53
2	7-A	301	SO4	O2-S	4.47	1.61	1.47
4	6-A	404	EDO	C2-C1	4.46	1.77	1.47
4	3-A	404	EDO	O2-C2	4.45	1.65	1.42
3	11-A	200	CPS	C22-C20	-4.42	1.41	1.54
4	5-A	404	EDO	C2-C1	4.42	1.77	1.47
3	10-A	200	CPS	C20-C9	4.40	1.63	1.54
4	9-A	404	EDO	C2-C1	4.40	1.77	1.47
4	11-A	404	EDO	C2-C1	4.39	1.77	1.47
4	12-A	404	EDO	C2-C1	4.38	1.77	1.47
3	7-A	200	CPS	C14-C13	4.38	1.60	1.51
4	8-A	404	EDO	C2-C1	4.37	1.77	1.47
4	11-A	403	EDO	O2-C2	-4.36	1.18	1.42
4	3-A	404	EDO	C2-C1	4.36	1.77	1.47
3	15-A	200	CPS	C5-C4	4.33	1.61	1.54
4	10-A	404	EDO	C2-C1	4.33	1.76	1.47
2	15-A	300	SO4	O3-S	-4.31	1.32	1.47
4	7-A	404	EDO	C2-C1	4.31	1.76	1.47
4	6-A	403	EDO	O1-C1	4.31	1.65	1.42
3	10-A	200	CPS	C1-C12	4.27	1.63	1.53
3	2-A	200	CPS	C18-C19	-4.25	1.45	1.53
4	4-A	403	EDO	O1-C1	4.25	1.64	1.42
3	5-A	200	CPS	C14-C15	4.25	1.61	1.53
3	11-A	200	CPS	C11-C2	4.23	1.62	1.54
4	2-A	401	EDO	C2-C1	4.22	1.76	1.47
2	15-A	302	SO4	O3-S	4.20	1.61	1.47
3	12-A	200	CPS	C12-C13	4.20	1.63	1.51
3	14-A	200	CPS	C2-C15	4.19	1.62	1.55
4	2-A	403	EDO	O1-C1	4.16	1.64	1.42
2	12-A	301	SO4	O1-S	4.16	1.60	1.47
3	4-A	200	CPS	C14-C15	-4.13	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	13-A	300	SO4	O3-S	-4.12	1.33	1.47
3	4-A	200	CPS	C16-C15	-4.12	1.46	1.53
2	1-A	300	SO4	O2-S	-4.10	1.33	1.47
3	15-A	200	CPS	O2-C13	4.10	1.56	1.43
4	1-A	403	EDO	O2-C2	-4.09	1.20	1.42
4	11-A	403	EDO	O1-C1	4.08	1.63	1.42
4	3-A	403	EDO	O1-C1	4.07	1.63	1.42
3	16-A	200	CPS	C14-C15	-4.07	1.46	1.53
4	12-A	403	EDO	O2-C2	-4.07	1.20	1.42
3	8-A	200	CPS	C14-C13	4.01	1.59	1.51
3	15-A	200	CPS	C12-C13	4.01	1.63	1.51
4	8-A	403	EDO	O1-C1	3.99	1.63	1.42
4	16-A	403	EDO	O1-C1	3.98	1.63	1.42
3	15-A	200	CPS	C21-C20	-3.98	1.42	1.53
2	6-A	301	SO4	O3-S	3.93	1.60	1.47
4	11-A	404	EDO	O1-C1	3.93	1.63	1.42
4	9-A	404	EDO	O1-C1	3.91	1.62	1.42
4	10-A	403	EDO	O1-C1	3.91	1.62	1.42
3	13-A	200	CPS	C2-C19	-3.90	1.50	1.56
4	7-A	403	EDO	O2-C2	-3.86	1.21	1.42
4	8-A	404	EDO	O2-C2	3.84	1.62	1.42
3	12-A	200	CPS	C11-C2	3.82	1.61	1.54
3	10-A	200	CPS	C16-C17	-3.80	1.46	1.52
3	6-A	200	CPS	C18-C17	-3.78	1.47	1.53
2	11-A	301	SO4	O3-S	3.75	1.60	1.47
2	9-A	300	SO4	O4-S	-3.73	1.34	1.47
2	9-A	300	SO4	O1-S	3.69	1.59	1.47
3	11-A	200	CPS	C16-C15	3.67	1.60	1.53
3	16-A	200	CPS	C14-C13	3.67	1.59	1.51
3	11-A	200	CPS	C25-C26	3.66	1.57	1.53
2	2-A	301	SO4	O3-S	3.63	1.59	1.47
3	11-A	200	CPS	C8-C7	-3.63	1.43	1.54
2	1-A	300	SO4	O1-S	3.62	1.58	1.47
3	11-A	200	CPS	C14-C13	-3.61	1.44	1.51
2	5-A	302	SO4	O3-S	3.61	1.59	1.47
4	13-A	402	EDO	C2-C1	3.58	1.71	1.47
2	13-A	300	SO4	O4-S	3.57	1.59	1.47
4	5-A	402	EDO	O1-C1	3.57	1.61	1.42
4	14-A	402	EDO	O1-C1	3.57	1.61	1.42
3	10-A	200	CPS	C14-C15	3.53	1.59	1.53
2	4-A	301	SO4	O1-S	3.52	1.58	1.47
2	3-A	301	SO4	O1-S	3.52	1.58	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	15-A	300	SO4	O4-S	3.47	1.59	1.47
2	8-A	300	SO4	O4-S	3.46	1.59	1.47
2	3-A	300	SO4	O3-S	-3.44	1.35	1.47
3	7-A	200	CPS	C3-C19	3.44	1.59	1.53
3	4-A	200	CPS	C8-C9	-3.43	1.46	1.54
3	9-A	200	CPS	C5-C4	-3.43	1.49	1.54
2	3-A	300	SO4	O4-S	3.42	1.58	1.47
4	5-A	403	EDO	O1-C1	3.39	1.60	1.42
2	14-A	300	SO4	O3-S	-3.38	1.35	1.47
4	14-A	401	EDO	C2-C1	3.38	1.70	1.47
4	1-A	402	EDO	O1-C1	3.34	1.59	1.42
3	12-A	200	CPS	C5-C6	3.34	1.61	1.55
4	4-A	404	EDO	O1-C1	-3.29	1.24	1.42
4	9-A	403	EDO	O1-C1	3.27	1.59	1.42
2	16-A	300	SO4	O3-S	-3.25	1.36	1.47
3	4-A	200	CPS	C18-C19	-3.25	1.47	1.53
3	11-A	200	CPS	O2-C13	3.24	1.53	1.43
3	7-A	200	CPS	C12-C13	3.23	1.61	1.51
4	15-A	404	EDO	O1-C1	-3.22	1.24	1.42
3	11-A	200	CPS	C12-C13	-3.20	1.42	1.51
4	5-A	402	EDO	C2-C1	3.20	1.69	1.47
3	7-A	200	CPS	C14-C15	-3.20	1.48	1.53
4	15-A	402	EDO	C2-C1	3.19	1.69	1.47
3	15-A	200	CPS	C5-C9	3.16	1.61	1.55
3	3-A	200	CPS	C16-C15	3.16	1.59	1.53
4	14-A	401	EDO	O2-C2	3.15	1.58	1.42
2	15-A	301	SO4	O3-S	3.13	1.57	1.47
2	16-A	301	SO4	O1-S	3.08	1.57	1.47
4	7-A	403	EDO	C2-C1	3.07	1.68	1.47
3	1-A	200	CPS	O4-C4	3.06	1.49	1.43
4	1-A	402	EDO	C2-C1	3.04	1.68	1.47
3	14-A	200	CPS	C12-C13	-3.04	1.42	1.51
4	3-A	404	EDO	O1-C1	-3.00	1.25	1.42
3	9-A	200	CPS	C8-C9	-2.91	1.47	1.54
2	1-A	300	SO4	O4-S	2.91	1.57	1.47
3	10-A	200	CPS	C25-N1	-2.90	1.39	1.46
4	9-A	402	EDO	C2-C1	2.88	1.67	1.47
4	12-A	402	EDO	C2-C1	2.88	1.67	1.47
2	5-A	300	SO4	O4-S	-2.86	1.37	1.47
3	4-A	200	CPS	C25-N1	-2.86	1.39	1.46
3	6-A	200	CPS	C18-C19	-2.86	1.48	1.53
4	4-A	402	EDO	C2-C1	2.82	1.66	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	9-A	301	SO4	O3-S	2.80	1.56	1.47
4	8-A	402	EDO	C2-C1	2.80	1.66	1.47
2	10-A	302	SO4	O3-S	2.80	1.56	1.47
4	11-A	402	EDO	O1-C1	2.79	1.56	1.42
3	12-A	200	CPS	C1-C2	2.78	1.59	1.54
4	8-A	404	EDO	O1-C1	-2.78	1.27	1.42
4	15-A	403	EDO	C2-C1	2.78	1.66	1.47
4	16-A	403	EDO	O2-C2	-2.78	1.27	1.42
2	12-A	301	SO4	O2-S	2.78	1.56	1.47
4	1-A	401	EDO	C2-C1	2.76	1.66	1.47
4	10-A	402	EDO	C2-C1	2.75	1.66	1.47
4	9-A	403	EDO	O2-C2	-2.75	1.27	1.42
4	13-A	403	EDO	C2-C1	2.73	1.66	1.47
3	4-A	200	CPS	C22-C20	-2.73	1.46	1.54
4	10-A	403	EDO	O2-C2	-2.72	1.27	1.42
4	7-A	402	EDO	O1-C1	2.71	1.56	1.42
4	3-A	402	EDO	O1-C1	2.71	1.56	1.42
4	12-A	402	EDO	O1-C1	2.71	1.56	1.42
4	7-A	402	EDO	C2-C1	2.69	1.65	1.47
4	6-A	402	EDO	C2-C1	2.67	1.65	1.47
4	12-A	403	EDO	C2-C1	2.66	1.65	1.47
4	10-A	404	EDO	O1-C1	2.66	1.56	1.42
4	3-A	402	EDO	C2-C1	2.66	1.65	1.47
4	4-A	401	EDO	C2-C1	2.65	1.65	1.47
3	6-A	200	CPS	C2-C15	-2.64	1.50	1.55
4	2-A	402	EDO	C2-C1	2.64	1.65	1.47
4	16-A	401	EDO	C2-C1	2.63	1.65	1.47
3	7-A	200	CPS	C8-C7	2.63	1.61	1.54
3	11-A	200	CPS	O4-C4	-2.60	1.39	1.43
3	3-A	200	CPS	C22-C20	-2.58	1.47	1.54
3	10-A	200	CPS	C18-C19	2.57	1.59	1.53
3	6-A	200	CPS	C25-C26	-2.56	1.50	1.53
4	11-A	402	EDO	C2-C1	2.55	1.64	1.47
3	2-A	200	CPS	C18-C6	-2.55	1.48	1.53
3	13-A	200	CPS	C18-C19	2.53	1.58	1.53
4	9-A	402	EDO	O1-C1	2.51	1.55	1.42
3	7-A	200	CPS	O4-C4	-2.50	1.39	1.43
4	10-A	402	EDO	O1-C1	2.50	1.55	1.42
3	6-A	200	CPS	C8-C9	2.49	1.60	1.54
4	11-A	401	EDO	C2-C1	2.48	1.64	1.47
4	8-A	403	EDO	O2-C2	-2.46	1.28	1.42
4	6-A	401	EDO	C2-C1	2.46	1.64	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1-A	403	EDO	C2-C1	2.46	1.64	1.47
4	8-A	402	EDO	O1-C1	2.45	1.55	1.42
2	11-A	301	SO4	O4-S	2.45	1.55	1.47
4	6-A	402	EDO	O1-C1	2.44	1.55	1.42
2	11-A	300	SO4	O3-S	-2.42	1.39	1.47
2	2-A	302	SO4	O4-S	2.42	1.55	1.47
3	6-A	200	CPS	C3-C4	2.40	1.57	1.53
4	4-A	402	EDO	O1-C1	2.37	1.54	1.42
4	10-A	401	EDO	C2-C1	2.36	1.63	1.47
3	10-A	200	CPS	C18-C17	-2.35	1.49	1.53
4	7-A	404	EDO	O1-C1	-2.35	1.29	1.42
4	14-A	403	EDO	C2-C1	2.34	1.63	1.47
4	2-A	402	EDO	O1-C1	2.33	1.54	1.42
3	4-A	200	CPS	C2-C19	-2.32	1.52	1.56
4	14-A	402	EDO	C2-C1	2.32	1.63	1.47
2	10-A	301	SO4	O4-S	2.31	1.55	1.47
4	3-A	401	EDO	C2-C1	2.27	1.62	1.47
3	6-A	200	CPS	C25-N1	2.24	1.51	1.46
3	12-A	200	CPS	C8-C7	2.24	1.60	1.54
4	12-A	401	EDO	O2-C2	2.23	1.54	1.42
4	16-A	403	EDO	C2-C1	2.23	1.62	1.47
2	6-A	301	SO4	O4-S	2.23	1.54	1.47
4	2-A	401	EDO	O1-C1	2.22	1.53	1.42
3	5-A	200	CPS	C8-C7	-2.22	1.47	1.54
3	10-A	200	CPS	O3-C17	2.20	1.48	1.43
3	16-A	200	CPS	C16-C15	-2.17	1.50	1.53
4	8-A	403	EDO	C2-C1	2.16	1.62	1.47
3	14-A	200	CPS	C22-C20	2.10	1.60	1.54
3	3-A	200	CPS	C8-C7	-2.09	1.47	1.54
3	10-A	200	CPS	C25-C26	2.05	1.55	1.53
4	4-A	402	EDO	O2-C2	2.04	1.52	1.42
3	8-A	200	CPS	C23-C24	-2.04	1.47	1.51
2	14-A	301	SO4	O1-S	2.03	1.53	1.47
4	14-A	402	EDO	O2-C2	2.03	1.52	1.42
3	13-A	200	CPS	O4-C4	-2.03	1.40	1.43
2	16-A	302	SO4	O3-S	2.01	1.54	1.47
4	8-A	402	EDO	O2-C2	2.01	1.52	1.42
4	9-A	402	EDO	O2-C2	2.01	1.52	1.42
3	3-A	200	CPS	C25-C26	-2.00	1.51	1.53

All (743) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-A	200	CPS	C14-C13-C12	-54.95	40.34	110.54
3	8-A	200	CPS	C8-C9-C5	-49.92	53.61	103.58
3	13-A	200	CPS	C7-C6-C5	-46.58	56.95	103.58
3	5-A	200	CPS	C7-C6-C5	-43.99	59.55	103.58
3	15-A	200	CPS	C6-C5-C4	-43.91	66.77	107.40
3	3-A	200	CPS	C1-C12-C13	-43.10	38.91	110.37
3	13-A	200	CPS	C10-C5-C4	-41.52	67.67	109.08
3	14-A	200	CPS	C11-C2-C19	-40.73	58.52	111.17
3	3-A	200	CPS	C19-C18-C17	-39.87	67.46	111.97
3	9-A	200	CPS	C7-C6-C5	-39.11	64.43	103.58
3	13-A	200	CPS	C8-C9-C5	-37.49	66.05	103.58
3	9-A	200	CPS	C14-C15-C2	-37.36	72.26	112.67
3	16-A	200	CPS	C21-C20-C22	-36.57	47.99	110.37
3	15-A	200	CPS	C3-C19-C18	-36.35	58.53	110.81
3	13-A	200	CPS	C5-C9-C20	-36.27	75.84	119.51
3	9-A	200	CPS	C15-C16-C17	-35.84	76.28	114.46
3	5-A	200	CPS	C14-C15-C2	-35.28	74.50	112.67
3	7-A	200	CPS	C10-C5-C9	-35.23	55.29	111.22
3	13-A	200	CPS	C6-C18-C17	-35.20	68.32	111.81
3	12-A	200	CPS	C10-C5-C9	-35.17	55.39	111.22
3	9-A	200	CPS	C19-C18-C17	-34.76	73.17	111.97
3	3-A	200	CPS	C3-C19-C18	-34.68	60.94	110.81
3	8-A	200	CPS	C16-C17-C18	-34.33	75.12	111.51
3	13-A	200	CPS	C6-C5-C4	-34.31	75.65	107.40
3	14-A	200	CPS	C8-C9-C5	-34.29	69.26	103.58
3	9-A	200	CPS	C9-C5-C4	34.06	149.11	117.67
3	3-A	200	CPS	C6-C18-C17	33.81	153.59	111.81
3	15-A	200	CPS	C6-C18-C17	-33.80	70.05	111.81
3	9-A	200	CPS	C2-C19-C18	33.24	147.25	111.90
3	15-A	200	CPS	C5-C6-C18	-33.08	77.30	114.81
3	13-A	200	CPS	C3-C19-C18	-33.08	63.24	110.81
3	10-A	200	CPS	O4-C4-C5	-32.10	58.39	111.13
3	9-A	200	CPS	C3-C19-C2	-31.89	79.64	113.73
3	14-A	200	CPS	C5-C9-C20	-31.87	81.14	119.51
3	13-A	200	CPS	C19-C2-C15	-31.75	64.50	108.67
3	15-A	200	CPS	C19-C2-C15	-31.63	64.67	108.67
3	3-A	200	CPS	C6-C5-C4	-31.45	78.29	107.40
3	13-A	200	CPS	C16-C15-C14	-31.44	73.76	111.14
3	2-A	200	CPS	C9-C5-C6	-31.41	67.97	100.07
3	15-A	200	CPS	C7-C6-C5	-31.33	72.22	103.58
3	14-A	200	CPS	C16-C15-C14	-31.13	74.13	111.14
3	1-A	200	CPS	C16-C15-C2	-30.99	79.15	112.67
3	15-A	200	CPS	C16-C15-C14	-30.87	74.44	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3-A	200	CPS	C16-C17-C18	-30.82	78.84	111.51
3	9-A	200	CPS	C5-C6-C18	-30.82	79.86	114.81
3	15-A	200	CPS	C14-C15-C2	-30.77	79.39	112.67
3	15-A	200	CPS	C16-C17-C18	-30.67	79.00	111.51
3	7-A	200	CPS	C9-C5-C4	29.98	145.34	117.67
3	15-A	200	CPS	C5-C9-C20	-29.92	83.48	119.51
3	3-A	200	CPS	C3-C4-C5	29.86	141.83	111.21
3	13-A	200	CPS	C3-C4-C5	-29.37	81.07	111.21
3	13-A	200	CPS	C10-C5-C9	29.25	157.66	111.22
3	3-A	200	CPS	O3-C17-C18	29.15	171.00	109.23
3	10-A	200	CPS	C19-C3-C4	-28.93	76.60	114.35
3	8-A	200	CPS	C2-C19-C18	-28.74	81.33	111.90
3	1-A	200	CPS	C6-C5-C4	-28.72	80.82	107.40
3	3-A	200	CPS	C10-C5-C4	28.66	137.67	109.08
3	13-A	200	CPS	C14-C15-C2	-28.60	81.73	112.67
3	10-A	200	CPS	C14-C15-C2	-28.60	81.74	112.67
3	1-A	200	CPS	C7-C6-C5	-28.13	75.42	103.58
3	9-A	200	CPS	C19-C3-C4	-28.04	77.75	114.35
3	8-A	200	CPS	C9-C5-C4	27.36	142.93	117.67
3	16-A	200	CPS	C16-C17-C18	27.09	140.22	111.51
3	13-A	200	CPS	C16-C17-C18	-26.12	83.82	111.51
3	14-A	200	CPS	C16-C17-C18	-25.96	83.99	111.51
3	4-A	200	CPS	C2-C19-C18	25.85	139.39	111.90
3	14-A	200	CPS	C7-C6-C5	-25.75	77.80	103.58
3	5-A	200	CPS	C5-C6-C18	-25.40	86.00	114.81
3	8-A	200	CPS	C3-C19-C2	-25.38	86.60	113.73
3	10-A	200	CPS	C3-C19-C2	-25.21	86.78	113.73
3	15-A	200	CPS	C10-C5-C4	-24.62	84.53	109.08
3	11-A	200	CPS	C8-C9-C5	24.28	127.88	103.58
3	8-A	200	CPS	C21-C20-C22	-24.28	68.96	110.37
3	3-A	200	CPS	C9-C5-C4	-24.17	95.35	117.67
3	10-A	200	CPS	C21-C20-C22	-24.07	69.31	110.37
3	3-A	200	CPS	C23-C22-C20	-23.51	77.23	114.46
3	11-A	200	CPS	C15-C16-C17	-23.49	89.43	114.46
3	4-A	200	CPS	C8-C9-C20	-22.94	69.67	112.06
3	13-A	200	CPS	C5-C6-C18	-22.75	89.01	114.81
3	8-A	200	CPS	C15-C16-C17	22.68	138.62	114.46
3	12-A	200	CPS	C16-C17-C18	22.50	135.35	111.51
3	4-A	200	CPS	C9-C5-C4	-22.47	96.92	117.67
3	10-A	200	CPS	C22-C20-C9	22.42	160.59	110.25
3	14-A	200	CPS	C9-C5-C6	-22.32	77.25	100.07
3	8-A	200	CPS	C5-C6-C18	-22.28	89.54	114.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-A	200	CPS	C16-C15-C14	21.88	137.15	111.14
3	11-A	200	CPS	C1-C2-C15	-21.59	84.00	107.79
3	15-A	200	CPS	C8-C9-C5	-21.42	82.14	103.58
3	8-A	200	CPS	C6-C18-C17	-21.37	85.42	111.81
3	14-A	200	CPS	C15-C16-C17	-21.25	91.82	114.46
3	10-A	200	CPS	C5-C6-C18	-21.23	90.73	114.81
3	14-A	200	CPS	C9-C5-C4	21.19	137.23	117.67
3	10-A	200	CPS	C19-C2-C15	-21.16	79.23	108.67
3	13-A	200	CPS	C21-C20-C22	-21.09	74.40	110.37
3	15-A	200	CPS	C10-C5-C6	-21.08	77.75	111.22
3	13-A	200	CPS	C15-C16-C17	-20.96	92.13	114.46
3	13-A	200	CPS	C19-C18-C17	-20.81	88.74	111.97
3	16-A	200	CPS	C1-C2-C19	-20.80	78.09	111.45
3	4-A	200	CPS	C9-C5-C6	20.54	121.06	100.07
3	2-A	200	CPS	C10-C5-C4	20.35	129.38	109.08
3	15-A	200	CPS	C3-C4-C5	-20.15	90.54	111.21
3	6-A	200	CPS	C10-C5-C9	-20.03	79.41	111.22
3	2-A	200	CPS	C16-C17-C18	19.81	132.50	111.51
3	11-A	200	CPS	C15-C14-C13	-19.73	83.99	112.95
3	12-A	200	CPS	O2-C13-C14	-19.54	70.93	109.87
3	1-A	200	CPS	C3-C4-C5	19.49	131.20	111.21
3	9-A	200	CPS	C11-C2-C1	19.45	141.25	108.17
3	2-A	200	CPS	C1-C2-C15	19.31	129.08	107.79
3	5-A	200	CPS	C19-C18-C17	-19.27	90.45	111.97
3	15-A	200	CPS	C9-C5-C4	19.25	135.44	117.67
3	2-A	200	CPS	C15-C14-C13	-19.25	84.70	112.95
3	1-A	200	CPS	C1-C12-C13	-19.13	78.65	110.37
3	14-A	200	CPS	C10-C5-C4	-19.12	90.01	109.08
3	9-A	200	CPS	O2-C13-C14	-19.03	71.93	109.87
3	6-A	200	CPS	C16-C17-C18	18.93	131.57	111.51
3	5-A	200	CPS	C3-C4-C5	18.80	130.50	111.21
3	9-A	200	CPS	C1-C2-C19	-18.55	81.70	111.45
3	2-A	200	CPS	C22-C20-C9	18.52	151.84	110.25
3	7-A	200	CPS	C10-C5-C6	18.45	140.52	111.22
3	12-A	200	CPS	C1-C2-C19	-18.40	81.95	111.45
3	3-A	200	CPS	C5-C9-C20	18.11	141.31	119.51
3	15-A	200	CPS	C23-C22-C20	-18.10	85.80	114.46
3	10-A	200	CPS	C9-C5-C6	-18.03	81.64	100.07
3	15-A	200	CPS	C3-C19-C2	-18.02	94.47	113.73
3	3-A	200	CPS	C3-C19-C2	-17.95	94.54	113.73
3	6-A	200	CPS	C1-C2-C15	-17.82	88.15	107.79
3	9-A	200	CPS	C19-C2-C15	-17.80	83.91	108.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	14-A	200	CPS	C6-C18-C17	-17.53	90.16	111.81
3	15-A	200	CPS	C15-C14-C13	17.47	138.60	112.95
3	15-A	200	CPS	O4-C4-C5	-17.39	82.55	111.13
3	11-A	200	CPS	C10-C5-C6	-17.36	83.65	111.22
3	6-A	200	CPS	O2-C13-C14	17.36	144.47	109.87
3	8-A	200	CPS	C16-C15-C2	-17.35	93.90	112.67
3	5-A	200	CPS	C9-C5-C6	17.34	117.79	100.07
3	15-A	200	CPS	C10-C5-C9	17.30	138.68	111.22
3	12-A	200	CPS	C3-C4-C5	17.13	128.78	111.21
3	3-A	200	CPS	C7-C6-C18	-17.07	94.04	118.30
3	15-A	200	CPS	C21-C20-C22	-16.90	81.54	110.37
3	12-A	200	CPS	C11-C2-C1	-16.84	79.54	108.17
3	4-A	200	CPS	C7-C6-C18	-16.69	94.58	118.30
3	8-A	200	CPS	C10-C5-C6	-16.66	84.77	111.22
3	15-A	200	CPS	C19-C18-C17	-16.64	93.39	111.97
3	14-A	200	CPS	C1-C2-C19	16.55	138.00	111.45
3	2-A	200	CPS	C3-C19-C2	16.55	131.42	113.73
3	2-A	200	CPS	C14-C15-C2	-16.43	94.90	112.67
3	11-A	200	CPS	C23-C22-C20	-16.40	88.49	114.46
3	5-A	200	CPS	C19-C2-C15	-16.38	85.88	108.67
3	14-A	200	CPS	C3-C4-C5	-16.31	94.48	111.21
3	4-A	200	CPS	C11-C2-C19	16.06	131.93	111.17
3	7-A	200	CPS	C3-C19-C2	16.06	130.90	113.73
3	1-A	200	CPS	C10-C5-C4	15.88	124.92	109.08
3	1-A	200	CPS	C10-C5-C6	15.88	136.43	111.22
3	1-A	200	CPS	C6-C18-C17	-15.87	92.21	111.81
3	16-A	200	CPS	C7-C6-C18	-15.86	95.76	118.30
3	6-A	200	CPS	C16-C15-C2	15.81	129.78	112.67
3	16-A	200	CPS	C8-C9-C20	-15.79	82.87	112.06
3	16-A	200	CPS	C7-C6-C5	-15.77	87.79	103.58
3	7-A	200	CPS	C1-C2-C15	15.70	125.10	107.79
3	11-A	200	CPS	C19-C2-C15	15.54	130.29	108.67
3	16-A	200	CPS	C12-C1-C2	-15.53	84.66	112.83
3	15-A	200	CPS	C19-C3-C4	-15.44	94.20	114.35
3	3-A	200	CPS	C19-C2-C15	-15.34	87.33	108.67
3	15-A	200	CPS	O2-C13-C14	15.27	140.31	109.87
3	2-A	200	CPS	C19-C18-C6	15.27	130.04	109.61
3	2-A	200	CPS	C11-C2-C1	-15.14	82.42	108.17
3	8-A	200	CPS	C10-C5-C4	-14.97	94.15	109.08
3	14-A	200	CPS	C23-C22-C20	-14.94	90.80	114.46
3	11-A	200	CPS	C6-C5-C4	14.94	121.22	107.40
3	5-A	200	CPS	C15-C16-C17	-14.91	98.58	114.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-A	200	CPS	C16-C15-C2	-14.89	96.57	112.67
3	2-A	200	CPS	C5-C9-C20	-14.83	101.66	119.51
3	3-A	200	CPS	C16-C15-C2	-14.81	96.66	112.67
3	4-A	200	CPS	C15-C16-C17	-14.80	98.69	114.46
3	4-A	200	CPS	C21-C20-C9	-14.79	87.05	112.96
3	12-A	200	CPS	C21-C20-C22	-14.79	85.14	110.37
3	6-A	200	CPS	C6-C5-C4	14.78	121.08	107.40
3	7-A	200	CPS	C16-C15-C2	-14.76	96.70	112.67
3	12-A	200	CPS	C10-C5-C6	14.66	134.50	111.22
3	1-A	200	CPS	C11-C2-C19	-14.57	92.34	111.17
3	1-A	200	CPS	C15-C16-C17	14.52	129.93	114.46
3	6-A	200	CPS	C10-C5-C4	14.47	123.51	109.08
3	15-A	200	CPS	C15-C16-C17	-14.42	99.10	114.46
3	7-A	200	CPS	C1-C2-C19	-14.39	88.37	111.45
3	3-A	200	CPS	C11-C2-C15	-14.30	85.52	110.26
3	7-A	200	CPS	C15-C16-C17	14.27	129.66	114.46
3	6-A	200	CPS	C1-C12-C13	-14.06	87.05	110.37
3	10-A	200	CPS	C14-C13-C12	-14.05	92.59	110.54
3	16-A	200	CPS	C1-C2-C15	14.01	123.23	107.79
3	1-A	200	CPS	C5-C9-C20	14.00	136.36	119.51
3	5-A	200	CPS	C1-C12-C13	-13.95	87.23	110.37
3	7-A	200	CPS	C12-C1-C2	-13.95	87.53	112.83
3	1-A	200	CPS	C11-C2-C15	-13.93	86.16	110.26
3	9-A	200	CPS	C6-C18-C17	-13.90	94.64	111.81
3	1-A	200	CPS	C19-C18-C6	13.77	128.04	109.61
3	3-A	200	CPS	C14-C15-C2	-13.77	97.78	112.67
3	13-A	200	CPS	C23-C22-C20	-13.76	92.67	114.46
3	2-A	200	CPS	C5-C6-C18	13.68	130.32	114.81
3	11-A	200	CPS	C5-C6-C18	-13.57	99.42	114.81
3	16-A	200	CPS	C11-C2-C19	13.49	128.60	111.17
3	4-A	200	CPS	C12-C1-C2	-13.43	88.47	112.83
3	11-A	200	CPS	C10-C5-C4	13.42	122.47	109.08
3	8-A	200	CPS	C3-C19-C18	-13.37	91.58	110.81
3	2-A	200	CPS	C15-C16-C17	-13.36	100.23	114.46
3	7-A	200	CPS	C11-C2-C19	13.34	128.41	111.17
3	6-A	200	CPS	C21-C20-C22	-13.32	87.65	110.37
3	12-A	200	CPS	C16-C15-C2	13.29	127.04	112.67
3	12-A	200	CPS	C11-C2-C19	13.23	128.27	111.17
3	7-A	200	CPS	O2-C13-C14	-13.14	83.68	109.87
3	6-A	200	CPS	C1-C2-C19	-13.09	90.46	111.45
3	5-A	200	CPS	C10-C5-C9	-13.01	90.57	111.22
3	12-A	200	CPS	C3-C19-C2	12.99	127.62	113.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-A	200	CPS	C7-C6-C18	12.95	136.70	118.30
3	12-A	200	CPS	C15-C16-C17	-12.93	100.69	114.46
3	13-A	200	CPS	C9-C5-C4	12.93	129.60	117.67
3	13-A	200	CPS	C3-C19-C2	-12.87	99.97	113.73
3	11-A	200	CPS	C3-C19-C18	12.86	129.31	110.81
3	14-A	200	CPS	C2-C19-C18	-12.85	98.23	111.90
3	12-A	200	CPS	C9-C5-C4	12.84	129.52	117.67
3	10-A	200	CPS	C10-C5-C9	12.81	131.56	111.22
3	4-A	200	CPS	C11-C2-C1	-12.79	86.42	108.17
3	4-A	200	CPS	C16-C15-C14	12.77	126.32	111.14
3	16-A	200	CPS	C5-C6-C18	-12.68	100.42	114.81
3	9-A	200	CPS	C6-C5-C4	-12.54	95.80	107.40
3	5-A	200	CPS	C6-C5-C4	-12.38	95.95	107.40
3	10-A	200	CPS	C11-C2-C1	12.30	129.10	108.17
3	8-A	200	CPS	C9-C5-C6	12.20	112.54	100.07
3	1-A	200	CPS	C11-C2-C1	12.18	128.89	108.17
3	11-A	200	CPS	O2-C13-C12	12.14	145.26	110.04
3	5-A	200	CPS	C21-C20-C9	12.14	134.21	112.96
3	9-A	200	CPS	C19-C18-C6	12.12	125.83	109.61
3	9-A	200	CPS	C1-C12-C13	-12.08	90.34	110.37
3	14-A	200	CPS	C3-C19-C2	12.07	126.63	113.73
3	3-A	200	CPS	C15-C16-C17	12.04	127.28	114.46
3	6-A	200	CPS	C3-C19-C18	11.95	128.00	110.81
3	9-A	200	CPS	C8-C9-C5	-11.93	91.64	103.58
3	3-A	200	CPS	O4-C4-C5	-11.81	91.73	111.13
3	11-A	200	CPS	C21-C20-C22	11.78	130.47	110.37
3	7-A	200	CPS	C5-C6-C18	11.78	128.17	114.81
3	14-A	200	CPS	C10-C5-C9	11.78	129.92	111.22
3	8-A	200	CPS	C11-C2-C19	-11.67	96.08	111.17
3	11-A	200	CPS	C7-C6-C18	-11.62	101.78	118.30
3	16-A	200	CPS	C9-C5-C4	-11.56	107.00	117.67
3	12-A	200	CPS	C1-C2-C15	11.52	120.50	107.79
3	10-A	200	CPS	C3-C4-C5	11.51	123.02	111.21
3	16-A	200	CPS	C10-C5-C4	11.51	120.56	109.08
3	1-A	200	CPS	C14-C15-C2	-11.46	100.28	112.67
3	9-A	200	CPS	C16-C15-C14	11.40	124.69	111.14
3	5-A	200	CPS	C23-C22-C20	-11.39	96.43	114.46
3	11-A	200	CPS	C1-C12-C13	11.32	129.14	110.37
3	12-A	200	CPS	C12-C1-C2	-11.30	92.34	112.83
3	3-A	200	CPS	C16-C15-C14	-11.27	97.74	111.14
3	3-A	200	CPS	C1-C2-C15	11.24	120.19	107.79
3	3-A	200	CPS	C12-C1-C2	11.21	133.16	112.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	8-A	200	CPS	C8-C7-C6	11.19	127.87	105.14
3	5-A	200	CPS	C8-C9-C5	-11.16	92.41	103.58
3	15-A	200	CPS	C1-C2-C19	11.11	129.27	111.45
3	9-A	200	CPS	C7-C6-C18	11.10	134.08	118.30
3	3-A	200	CPS	C8-C9-C5	-11.09	92.48	103.58
3	8-A	200	CPS	C15-C14-C13	-11.02	96.77	112.95
3	6-A	200	CPS	C7-C6-C5	10.98	114.57	103.58
3	13-A	200	CPS	C1-C2-C15	-10.96	95.71	107.79
3	5-A	200	CPS	C10-C5-C6	10.75	128.28	111.22
3	10-A	200	CPS	C3-C19-C18	-10.74	95.36	110.81
3	12-A	200	CPS	O1-C24-N1	-10.74	101.66	122.94
3	16-A	200	CPS	C15-C16-C17	-10.66	103.10	114.46
3	2-A	200	CPS	C7-C6-C5	10.64	114.23	103.58
3	13-A	200	CPS	C11-C2-C1	10.63	126.24	108.17
3	11-A	200	CPS	C9-C5-C4	-10.60	107.88	117.67
3	15-A	200	CPS	O4-C4-C3	10.59	130.30	108.99
3	15-A	200	CPS	C1-C2-C15	-10.56	96.16	107.79
3	16-A	200	CPS	C10-C5-C6	-10.46	94.61	111.22
3	16-A	200	CPS	C22-C20-C9	10.45	133.72	110.25
3	11-A	200	CPS	C8-C7-C6	-10.40	84.02	105.14
3	5-A	200	CPS	C2-C19-C18	10.32	122.87	111.90
3	9-A	200	CPS	C10-C5-C9	-10.31	94.85	111.22
3	9-A	200	CPS	O3-C17-C18	-10.28	87.45	109.23
3	7-A	200	CPS	C3-C4-C5	10.23	121.70	111.21
3	11-A	200	CPS	C7-C6-C5	-10.23	93.34	103.58
3	10-A	200	CPS	C12-C1-C2	10.15	131.25	112.83
3	8-A	200	CPS	C7-C8-C9	10.14	125.73	105.14
3	9-A	200	CPS	C12-C1-C2	-10.13	94.45	112.83
3	7-A	200	CPS	O3-C17-C16	-10.08	85.52	110.09
3	10-A	200	CPS	C6-C18-C17	-10.07	99.37	111.81
3	16-A	200	CPS	C19-C3-C4	-10.05	101.23	114.35
3	8-A	200	CPS	C1-C2-C19	10.05	127.57	111.45
3	9-A	200	CPS	C16-C17-C18	-9.99	100.91	111.51
3	6-A	200	CPS	C5-C9-C20	9.96	131.50	119.51
3	13-A	200	CPS	C10-C5-C6	-9.92	95.46	111.22
3	4-A	200	CPS	C1-C2-C15	9.91	118.72	107.79
3	10-A	200	CPS	C15-C14-C13	9.90	127.48	112.95
3	11-A	200	CPS	C19-C18-C6	-9.83	96.46	109.61
3	7-A	200	CPS	O1-C24-N1	-9.78	103.55	122.94
3	10-A	200	CPS	C10-C5-C6	-9.77	95.71	111.22
3	7-A	200	CPS	C21-C20-C9	9.77	130.06	112.96
3	14-A	200	CPS	C3-C19-C18	-9.74	96.81	110.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-A	200	CPS	C3-C19-C18	-9.72	96.82	110.81
3	7-A	200	CPS	C11-C2-C1	-9.70	91.69	108.17
3	6-A	200	CPS	C25-N1-C24	-9.67	103.14	122.84
3	3-A	200	CPS	C10-C5-C6	9.67	126.58	111.22
3	12-A	200	CPS	C19-C2-C15	9.65	122.09	108.67
3	7-A	200	CPS	C19-C2-C15	9.61	122.04	108.67
3	10-A	200	CPS	C8-C9-C20	-9.59	94.33	112.06
3	3-A	200	CPS	C26-C25-N1	-9.44	95.18	110.16
3	14-A	200	CPS	C21-C20-C22	-9.43	94.28	110.37
3	8-A	200	CPS	C3-C4-C5	-9.39	101.58	111.21
2	11-A	300	SO4	O2-S-O1	-9.39	78.48	109.53
3	10-A	200	CPS	C1-C2-C15	-9.32	97.52	107.79
3	7-A	200	CPS	C19-C18-C6	9.31	122.07	109.61
3	13-A	200	CPS	O2-C13-C14	9.31	128.42	109.87
3	13-A	200	CPS	C23-C24-N1	9.25	133.33	116.50
3	1-A	200	CPS	C12-C1-C2	-9.22	96.11	112.83
3	6-A	200	CPS	C23-C22-C20	-9.20	99.89	114.46
3	15-A	200	CPS	C14-C13-C12	-9.17	98.82	110.54
3	6-A	200	CPS	C8-C9-C5	9.14	112.73	103.58
3	4-A	200	CPS	C19-C18-C17	-9.11	101.79	111.97
3	11-A	200	CPS	C25-N1-C24	-9.11	104.29	122.84
3	4-A	200	CPS	O4-C4-C3	-9.10	90.68	108.99
3	10-A	200	CPS	C15-C16-C17	9.03	124.08	114.46
3	3-A	200	CPS	C11-C2-C19	8.99	122.78	111.17
3	13-A	200	CPS	C15-C14-C13	8.97	126.12	112.95
3	4-A	200	CPS	C5-C9-C20	8.96	130.30	119.51
3	1-A	200	CPS	C8-C9-C5	8.94	112.53	103.58
3	1-A	200	CPS	C21-C20-C9	8.93	128.60	112.96
3	2-A	200	CPS	C10-C5-C9	-8.91	97.07	111.22
3	6-A	200	CPS	O4-C4-C5	8.90	125.75	111.13
3	7-A	200	CPS	C7-C6-C18	8.88	130.92	118.30
3	2-A	200	CPS	C8-C9-C20	-8.83	95.74	112.06
3	2-A	200	CPS	C10-C5-C6	8.82	125.22	111.22
3	1-A	200	CPS	C16-C17-C18	8.79	120.82	111.51
2	15-A	301	SO4	O2-S-O1	8.71	138.34	109.53
3	2-A	200	CPS	C21-C20-C22	-8.70	95.53	110.37
3	4-A	200	CPS	O4-C4-C5	8.69	125.41	111.13
3	6-A	200	CPS	C15-C14-C13	-8.68	100.20	112.95
3	12-A	200	CPS	O4-C4-C3	8.67	126.43	108.99
3	16-A	200	CPS	C6-C18-C17	-8.67	101.11	111.81
3	9-A	200	CPS	C21-C20-C22	8.62	125.08	110.37
3	5-A	200	CPS	C9-C5-C4	8.61	125.62	117.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6-A	200	CPS	C15-C16-C17	-8.57	105.33	114.46
3	7-A	200	CPS	C15-C14-C13	8.56	125.51	112.95
3	5-A	200	CPS	O3-C17-C18	-8.56	91.10	109.23
3	2-A	200	CPS	C25-N1-C24	-8.54	105.45	122.84
3	1-A	200	CPS	O3-C17-C16	-8.51	89.33	110.09
3	16-A	200	CPS	C10-C5-C9	8.51	124.73	111.22
3	11-A	200	CPS	C1-C2-C19	-8.46	97.88	111.45
3	5-A	200	CPS	C11-C2-C1	8.39	122.44	108.17
3	9-A	200	CPS	C5-C9-C20	-8.37	109.43	119.51
3	5-A	200	CPS	C3-C19-C18	-8.35	98.80	110.81
3	5-A	200	CPS	C10-C5-C4	-8.34	100.76	109.08
3	3-A	200	CPS	C7-C8-C9	8.28	121.95	105.14
3	3-A	200	CPS	O2-C13-C12	8.25	133.97	110.04
3	15-A	200	CPS	C1-C12-C13	-8.22	96.74	110.37
3	13-A	200	CPS	O1-C24-C23	-8.21	105.60	121.92
3	10-A	200	CPS	C9-C5-C4	-8.20	110.10	117.67
3	11-A	200	CPS	C3-C4-C5	-8.20	102.79	111.21
3	11-A	200	CPS	C5-C9-C20	-8.20	109.64	119.51
3	11-A	200	CPS	C19-C18-C17	-8.19	102.82	111.97
3	8-A	200	CPS	C26-C25-N1	8.14	123.07	110.16
3	14-A	200	CPS	O1-C24-C23	-8.09	105.83	121.92
3	3-A	200	CPS	C21-C20-C22	8.07	124.15	110.37
3	5-A	200	CPS	C21-C20-C22	8.05	124.11	110.37
3	8-A	200	CPS	C19-C18-C17	-8.04	102.99	111.97
3	3-A	200	CPS	C9-C5-C6	8.00	108.25	100.07
3	9-A	200	CPS	O4-C4-C5	-7.96	98.06	111.13
3	9-A	200	CPS	O3-C17-C16	7.94	129.43	110.09
3	12-A	200	CPS	C5-C6-C18	7.93	123.80	114.81
3	1-A	200	CPS	C10-C5-C9	-7.91	98.65	111.22
3	2-A	200	CPS	C1-C12-C13	-7.91	97.25	110.37
3	8-A	200	CPS	C6-C5-C4	-7.90	100.09	107.40
3	3-A	200	CPS	C11-C2-C1	7.85	121.52	108.17
3	14-A	200	CPS	C14-C15-C2	-7.84	104.19	112.67
3	16-A	200	CPS	C25-N1-C24	-7.83	106.88	122.84
3	10-A	200	CPS	C16-C15-C14	-7.79	101.88	111.14
3	2-A	200	CPS	C6-C5-C4	-7.77	100.21	107.40
3	4-A	200	CPS	C14-C15-C2	-7.75	104.29	112.67
3	6-A	200	CPS	C11-C2-C19	7.75	121.18	111.17
3	5-A	200	CPS	C14-C13-C12	-7.65	100.76	110.54
3	6-A	200	CPS	C12-C1-C2	-7.63	98.99	112.83
3	12-A	200	CPS	C19-C18-C6	7.62	119.81	109.61
3	11-A	200	CPS	O4-C4-C5	7.61	123.63	111.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-A	200	CPS	C1-C2-C15	7.54	116.11	107.79
3	14-A	200	CPS	O2-C13-C14	7.50	124.83	109.87
3	13-A	200	CPS	C19-C3-C4	-7.48	104.59	114.35
3	5-A	200	CPS	C16-C15-C2	-7.47	104.59	112.67
3	11-A	200	CPS	C14-C15-C2	7.45	120.73	112.67
3	6-A	200	CPS	C6-C18-C17	7.44	121.01	111.81
3	16-A	200	CPS	O3-C17-C18	-7.44	93.48	109.23
3	11-A	200	CPS	C19-C3-C4	7.40	124.01	114.35
3	12-A	200	CPS	C5-C9-C20	7.37	128.38	119.51
3	16-A	200	CPS	O1-C24-N1	-7.36	108.34	122.94
3	11-A	200	CPS	C21-C20-C9	7.36	125.85	112.96
3	1-A	200	CPS	C23-C22-C20	-7.32	102.86	114.46
3	15-A	200	CPS	C7-C6-C18	7.32	128.70	118.30
3	14-A	200	CPS	C15-C14-C13	7.32	123.69	112.95
3	8-A	200	CPS	C11-C2-C1	7.31	120.61	108.17
3	11-A	200	CPS	C3-C19-C2	7.26	121.48	113.73
3	9-A	200	CPS	C26-C25-N1	7.24	121.65	110.16
3	12-A	200	CPS	C7-C6-C18	7.22	128.56	118.30
3	5-A	200	CPS	C25-N1-C24	-7.22	108.14	122.84
3	6-A	200	CPS	C19-C2-C15	7.22	118.71	108.67
3	3-A	200	CPS	C22-C23-C24	-7.19	92.60	112.90
3	9-A	200	CPS	C10-C5-C4	-7.18	101.92	109.08
3	14-A	200	CPS	C1-C12-C13	7.15	122.23	110.37
3	16-A	200	CPS	C19-C2-C15	7.14	118.60	108.67
3	6-A	200	CPS	C14-C15-C2	7.13	120.38	112.67
3	2-A	200	CPS	C19-C3-C4	-7.11	105.07	114.35
3	5-A	200	CPS	C1-C2-C19	-7.10	100.06	111.45
3	10-A	200	CPS	C10-C5-C4	7.07	116.13	109.08
3	1-A	200	CPS	C16-C15-C14	-7.07	102.74	111.14
3	15-A	200	CPS	C12-C1-C2	-7.02	100.09	112.83
3	5-A	200	CPS	O3-C17-C16	7.00	127.15	110.09
3	5-A	200	CPS	C19-C18-C6	7.00	118.97	109.61
3	10-A	200	CPS	C1-C12-C13	-6.99	98.78	110.37
3	8-A	200	CPS	C19-C2-C15	-6.95	99.00	108.67
3	11-A	200	CPS	C16-C15-C2	-6.89	105.22	112.67
3	12-A	200	CPS	C23-C24-N1	6.87	128.99	116.50
3	16-A	200	CPS	C16-C15-C2	6.81	120.04	112.67
3	2-A	200	CPS	C7-C8-C9	-6.81	91.32	105.14
3	3-A	200	CPS	C15-C14-C13	6.81	122.94	112.95
3	14-A	200	CPS	C6-C5-C4	-6.80	101.11	107.40
3	15-A	200	CPS	O1-C24-C23	-6.78	108.44	121.92
3	5-A	200	CPS	C11-C2-C19	6.76	119.90	111.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	13-A	200	CPS	C1-C2-C19	6.74	122.26	111.45
3	9-A	200	CPS	O1-C24-N1	-6.73	109.59	122.94
3	4-A	200	CPS	C19-C18-C6	6.72	118.61	109.61
3	14-A	200	CPS	C23-C24-N1	6.69	128.66	116.50
2	7-A	301	SO4	O2-S-O1	6.67	131.59	109.53
3	1-A	200	CPS	C9-C5-C4	-6.60	111.57	117.67
3	7-A	200	CPS	C8-C9-C20	6.51	124.08	112.06
3	7-A	200	CPS	C19-C3-C4	-6.49	105.88	114.35
3	1-A	200	CPS	O4-C4-C3	-6.43	96.05	108.99
3	2-A	200	CPS	C8-C7-C6	-6.43	92.08	105.14
3	2-A	200	CPS	O2-C13-C12	6.41	128.64	110.04
2	11-A	300	SO4	O4-S-O3	-6.40	82.01	109.08
3	15-A	200	CPS	C23-C24-N1	6.40	128.14	116.50
3	7-A	200	CPS	C23-C24-N1	6.40	128.14	116.50
3	4-A	200	CPS	C3-C19-C2	-6.38	106.91	113.73
2	9-A	301	SO4	O4-S-O3	-6.36	82.18	109.08
3	6-A	200	CPS	C7-C6-C18	6.33	127.30	118.30
3	7-A	200	CPS	C11-C2-C15	-6.31	99.34	110.26
3	8-A	200	CPS	O2-C13-C14	6.30	122.43	109.87
3	9-A	200	CPS	C25-N1-C24	6.24	135.55	122.84
2	8-A	301	SO4	O2-S-O1	-6.21	88.99	109.53
3	7-A	200	CPS	C16-C17-C18	-6.19	104.94	111.51
3	9-A	200	CPS	C11-C2-C15	-6.18	99.56	110.26
3	16-A	200	CPS	C19-C18-C6	6.17	117.87	109.61
3	10-A	200	CPS	O2-C13-C14	6.09	122.01	109.87
3	12-A	200	CPS	C15-C14-C13	6.09	121.89	112.95
3	5-A	200	CPS	C1-C2-C15	6.02	114.42	107.79
3	10-A	200	CPS	C5-C9-C20	-6.01	112.27	119.51
3	4-A	200	CPS	C10-C5-C4	-5.98	103.11	109.08
3	12-A	200	CPS	C19-C18-C17	5.98	118.64	111.97
3	11-A	200	CPS	C22-C20-C9	-5.98	96.83	110.25
3	1-A	200	CPS	O2-C13-C14	5.96	121.75	109.87
3	4-A	200	CPS	C19-C2-C15	-5.95	100.40	108.67
3	16-A	200	CPS	C16-C15-C14	-5.95	104.07	111.14
3	6-A	200	CPS	C19-C18-C6	5.88	117.49	109.61
2	15-A	301	SO4	O4-S-O3	-5.83	84.45	109.08
3	8-A	200	CPS	C1-C2-C15	-5.83	101.37	107.79
3	16-A	200	CPS	O4-C4-C3	-5.82	97.28	108.99
3	5-A	200	CPS	C7-C8-C9	5.82	116.95	105.14
3	4-A	200	CPS	C7-C8-C9	-5.79	93.38	105.14
3	1-A	200	CPS	C2-C19-C18	-5.77	105.77	111.90
3	12-A	200	CPS	C6-C18-C17	5.76	118.93	111.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-A	200	CPS	C26-C25-N1	5.73	119.25	110.16
3	12-A	200	CPS	C6-C5-C4	5.72	112.69	107.40
3	11-A	200	CPS	C2-C19-C18	-5.71	105.82	111.90
3	5-A	200	CPS	C22-C20-C9	-5.68	97.48	110.25
3	9-A	200	CPS	C11-C2-C19	5.66	118.48	111.17
3	15-A	200	CPS	C11-C2-C1	5.64	117.76	108.17
3	2-A	200	CPS	C26-C25-N1	5.63	119.09	110.16
3	1-A	200	CPS	C22-C20-C9	5.62	122.88	110.25
3	4-A	200	CPS	C6-C18-C17	5.62	118.76	111.81
3	16-A	200	CPS	C23-C22-C20	5.62	123.36	114.46
3	5-A	200	CPS	C3-C19-C2	-5.59	107.75	113.73
3	12-A	200	CPS	C8-C9-C20	5.58	122.38	112.06
3	1-A	200	CPS	C14-C13-C12	5.58	117.67	110.54
3	7-A	200	CPS	C10-C5-C4	-5.57	103.53	109.08
3	6-A	200	CPS	O1-C24-N1	-5.54	111.95	122.94
3	12-A	200	CPS	C8-C9-C5	5.54	109.12	103.58
3	2-A	200	CPS	C12-C1-C2	5.54	122.87	112.83
3	9-A	200	CPS	C15-C14-C13	5.53	121.07	112.95
3	6-A	200	CPS	C11-C2-C1	-5.53	98.78	108.17
3	1-A	200	CPS	C1-C2-C15	5.52	113.87	107.79
3	8-A	200	CPS	C14-C15-C2	5.46	118.58	112.67
3	15-A	200	CPS	C9-C5-C6	5.43	105.62	100.07
3	9-A	200	CPS	C7-C8-C9	5.41	116.14	105.14
3	6-A	200	CPS	C11-C2-C15	5.37	119.54	110.26
3	16-A	200	CPS	C2-C19-C18	5.35	117.58	111.90
3	5-A	200	CPS	O1-C24-N1	5.33	133.49	122.94
3	5-A	200	CPS	O2-C13-C14	-5.32	99.27	109.87
3	6-A	200	CPS	C19-C18-C17	5.31	117.90	111.97
2	10-A	301	SO4	O2-S-O1	5.31	127.08	109.53
3	10-A	200	CPS	C22-C23-C24	-5.26	98.05	112.90
3	13-A	200	CPS	C21-C20-C9	5.25	122.15	112.96
3	8-A	200	CPS	C19-C3-C4	-5.25	107.50	114.35
3	3-A	200	CPS	O2-C13-C14	5.22	120.27	109.87
3	5-A	200	CPS	C15-C14-C13	5.19	120.56	112.95
3	6-A	200	CPS	C26-C25-N1	5.15	118.33	110.16
2	13-A	301	SO4	O2-S-O1	-5.15	92.49	109.53
3	10-A	200	CPS	C8-C7-C6	-5.13	94.73	105.14
3	16-A	200	CPS	C26-C25-N1	-5.10	102.07	110.16
3	3-A	200	CPS	C8-C9-C20	-5.07	102.69	112.06
3	7-A	200	CPS	O2-C13-C12	-5.05	95.41	110.04
3	1-A	200	CPS	C8-C7-C6	4.98	115.24	105.14
3	13-A	200	CPS	O4-C4-C5	-4.97	102.97	111.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9-A	200	CPS	O2-C13-C12	4.96	124.44	110.04
3	4-A	200	CPS	C6-C5-C4	4.95	111.98	107.40
2	14-A	301	SO4	O2-S-O1	4.93	125.84	109.53
3	10-A	200	CPS	C7-C6-C5	-4.91	98.66	103.58
3	8-A	200	CPS	C8-C9-C20	-4.91	102.99	112.06
3	10-A	200	CPS	C16-C17-C18	-4.91	106.31	111.51
3	7-A	200	CPS	C1-C12-C13	-4.90	102.24	110.37
2	11-A	300	SO4	O4-S-O1	-4.89	65.71	110.12
3	8-A	200	CPS	C23-C24-N1	4.88	125.38	116.50
3	8-A	200	CPS	O3-C17-C18	4.86	119.53	109.23
3	2-A	200	CPS	C9-C5-C4	4.86	122.15	117.67
3	7-A	200	CPS	C9-C5-C6	4.85	105.02	100.07
3	11-A	200	CPS	C14-C13-C12	-4.84	104.35	110.54
3	13-A	200	CPS	C12-C1-C2	-4.82	104.09	112.83
3	13-A	200	CPS	C22-C23-C24	4.78	126.41	112.90
3	12-A	200	CPS	C26-C25-N1	4.78	117.75	110.16
3	3-A	200	CPS	C2-C19-C18	4.77	116.97	111.90
3	8-A	200	CPS	C7-C6-C18	-4.73	111.57	118.30
3	7-A	200	CPS	O3-C17-C18	-4.73	99.20	109.23
3	4-A	200	CPS	C16-C17-C18	-4.73	106.50	111.51
3	4-A	200	CPS	C14-C13-C12	4.72	116.57	110.54
3	5-A	200	CPS	O4-C4-C5	-4.71	103.39	111.13
2	14-A	301	SO4	O4-S-O1	-4.71	67.36	110.12
3	4-A	200	CPS	C22-C20-C9	-4.66	99.79	110.25
3	6-A	200	CPS	C22-C23-C24	-4.64	99.79	112.90
3	16-A	200	CPS	C11-C2-C15	-4.64	102.23	110.26
3	2-A	200	CPS	O4-C4-C3	-4.64	99.66	108.99
3	14-A	200	CPS	C22-C23-C24	4.63	125.98	112.90
3	2-A	200	CPS	C19-C18-C17	4.63	117.13	111.97
3	15-A	200	CPS	C11-C2-C15	-4.63	102.25	110.26
3	14-A	200	CPS	C12-C1-C2	4.62	121.20	112.83
3	5-A	200	CPS	C12-C1-C2	-4.58	104.52	112.83
2	7-A	301	SO4	O4-S-O3	-4.57	89.75	109.08
3	1-A	200	CPS	C25-N1-C24	-4.52	113.64	122.84
3	16-A	200	CPS	C3-C19-C2	4.51	118.55	113.73
3	1-A	200	CPS	C23-C24-N1	4.48	124.64	116.50
3	12-A	200	CPS	C3-C19-C18	4.48	117.24	110.81
3	9-A	200	CPS	C14-C13-C12	-4.47	104.83	110.54
3	6-A	200	CPS	C9-C5-C6	-4.45	95.52	100.07
3	1-A	200	CPS	C1-C2-C19	4.44	118.57	111.45
3	10-A	200	CPS	C11-C2-C15	4.42	117.90	110.26
3	16-A	200	CPS	C23-C24-N1	4.40	124.50	116.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-A	200	CPS	C19-C3-C4	-4.39	108.62	114.35
3	13-A	200	CPS	C1-C12-C13	-4.38	103.11	110.37
3	14-A	200	CPS	O2-C13-C12	4.34	122.63	110.04
3	14-A	200	CPS	O3-C17-C18	-4.33	100.05	109.23
3	11-A	200	CPS	O3-C17-C16	-4.31	99.57	110.09
3	11-A	200	CPS	O1-C24-N1	-4.31	114.40	122.94
3	7-A	200	CPS	O4-C4-C3	4.30	117.65	108.99
3	8-A	200	CPS	O1-C24-N1	-4.28	114.44	122.94
3	6-A	200	CPS	O1-C24-C23	4.27	130.42	121.92
3	9-A	200	CPS	C23-C22-C20	-4.24	107.74	114.46
3	1-A	200	CPS	O1-C24-C23	-4.20	113.58	121.92
3	3-A	200	CPS	C5-C6-C18	-4.17	110.08	114.81
3	14-A	200	CPS	C16-C15-C2	4.15	117.16	112.67
3	16-A	200	CPS	C9-C5-C6	-4.15	95.83	100.07
3	5-A	200	CPS	C23-C24-N1	-4.14	108.97	116.50
3	12-A	200	CPS	O4-C4-C5	-4.13	104.34	111.13
3	13-A	200	CPS	C26-C25-N1	4.12	116.70	110.16
2	9-A	301	SO4	O2-S-O1	4.10	123.11	109.53
3	5-A	200	CPS	C27-C26-C25	-4.09	105.26	114.46
3	2-A	200	CPS	O3-C17-C16	4.09	120.05	110.09
3	11-A	200	CPS	C10-C5-C9	4.07	117.68	111.22
3	14-A	200	CPS	C11-C2-C1	4.05	115.06	108.17
3	1-A	200	CPS	C7-C8-C9	-4.04	96.94	105.14
3	7-A	200	CPS	C3-C19-C18	-3.99	105.07	110.81
2	14-A	301	SO4	O4-S-O2	-3.99	73.90	110.12
3	1-A	200	CPS	C21-C20-C22	-3.98	103.58	110.37
3	7-A	200	CPS	C5-C9-C20	3.94	124.25	119.51
2	16-A	300	SO4	O4-S-O3	-3.94	92.43	109.08
3	4-A	200	CPS	C7-C6-C5	-3.88	99.70	103.58
3	14-A	200	CPS	C21-C20-C9	3.87	119.73	112.96
3	7-A	200	CPS	C8-C7-C6	-3.86	97.30	105.14
3	4-A	200	CPS	C19-C3-C4	-3.86	109.31	114.35
3	11-A	200	CPS	C7-C8-C9	3.84	112.93	105.14
3	2-A	200	CPS	C1-C2-C19	-3.83	105.31	111.45
3	2-A	200	CPS	C14-C13-C12	3.83	115.43	110.54
3	12-A	200	CPS	C14-C13-C12	-3.83	105.65	110.54
3	12-A	200	CPS	C22-C23-C24	-3.83	102.09	112.90
3	13-A	200	CPS	O3-C17-C16	-3.82	100.78	110.09
3	8-A	200	CPS	O4-C4-C3	-3.81	101.32	108.99
3	2-A	200	CPS	C2-C19-C18	3.80	115.94	111.90
3	3-A	200	CPS	O4-C4-C3	3.80	116.63	108.99
3	8-A	200	CPS	C22-C20-C9	3.79	118.77	110.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	15-A	200	CPS	C7-C8-C9	-3.78	97.46	105.14
3	1-A	200	CPS	C22-C23-C24	-3.76	102.27	112.90
3	9-A	200	CPS	C23-C24-N1	3.72	123.26	116.50
3	4-A	200	CPS	C8-C7-C6	-3.69	97.66	105.14
3	3-A	200	CPS	C10-C5-C9	-3.68	105.38	111.22
3	5-A	200	CPS	C16-C15-C14	3.64	115.47	111.14
2	1-A	300	SO4	O4-S-O3	-3.64	93.69	109.08
3	12-A	200	CPS	C22-C20-C9	3.63	118.39	110.25
3	3-A	200	CPS	C19-C18-C6	3.63	114.47	109.61
3	8-A	200	CPS	C10-C5-C9	-3.59	105.53	111.22
3	6-A	200	CPS	C3-C4-C5	-3.58	107.53	111.21
3	4-A	200	CPS	C16-C15-C2	-3.54	108.85	112.67
3	12-A	200	CPS	C1-C12-C13	-3.52	104.52	110.37
3	12-A	200	CPS	O1-C24-C23	3.51	128.90	121.92
3	5-A	200	CPS	O4-C4-C3	-3.50	101.96	108.99
3	3-A	200	CPS	C21-C20-C9	-3.47	106.89	112.96
3	7-A	200	CPS	C23-C22-C20	-3.46	108.97	114.46
3	12-A	200	CPS	O2-C13-C12	3.45	120.05	110.04
3	10-A	200	CPS	O1-C24-C23	-3.45	115.07	121.92
3	12-A	200	CPS	C10-C5-C4	3.44	112.52	109.08
3	16-A	200	CPS	C14-C13-C12	-3.44	106.15	110.54
3	16-A	200	CPS	C15-C14-C13	3.39	117.93	112.95
3	12-A	200	CPS	C8-C7-C6	-3.39	98.26	105.14
3	1-A	200	CPS	C5-C6-C18	-3.37	110.98	114.81
3	9-A	200	CPS	C10-C5-C6	3.36	116.55	111.22
3	10-A	200	CPS	C26-C25-N1	3.35	115.47	110.16
3	14-A	200	CPS	C7-C8-C9	3.30	111.85	105.14
3	10-A	200	CPS	C8-C9-C5	3.30	106.88	103.58
3	7-A	200	CPS	C16-C15-C14	-3.28	107.24	111.14
3	6-A	200	CPS	C14-C13-C12	-3.27	106.35	110.54
2	14-A	300	SO4	O4-S-O3	-3.27	95.26	109.08
3	2-A	200	CPS	C3-C4-C5	-3.27	107.85	111.21
3	10-A	200	CPS	C16-C15-C2	-3.19	109.22	112.67
3	3-A	200	CPS	C25-N1-C24	-3.17	116.38	122.84
3	13-A	200	CPS	C27-C26-C25	-3.17	107.33	114.46
3	4-A	200	CPS	C23-C24-N1	-3.17	110.74	116.50
3	16-A	200	CPS	C3-C19-C18	3.17	115.36	110.81
3	5-A	200	CPS	C22-C23-C24	-3.17	103.95	112.90
3	2-A	200	CPS	C11-C2-C15	3.16	115.73	110.26
3	15-A	200	CPS	C8-C7-C6	3.15	111.53	105.14
3	7-A	200	CPS	C7-C6-C5	-3.14	100.44	103.58
3	8-A	200	CPS	O2-C13-C12	3.13	119.13	110.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-A	200	CPS	C21-C20-C9	-3.12	107.50	112.96
3	5-A	200	CPS	C8-C7-C6	-3.09	98.86	105.14
3	6-A	200	CPS	C2-C19-C18	3.08	115.18	111.90
3	7-A	200	CPS	C22-C20-C9	3.08	117.17	110.25
3	1-A	200	CPS	C15-C14-C13	3.07	117.46	112.95
3	8-A	200	CPS	C25-N1-C24	-3.07	116.58	122.84
2	11-A	301	SO4	O2-S-O1	3.02	119.52	109.53
3	11-A	200	CPS	C16-C17-C18	-3.02	108.31	111.51
3	1-A	200	CPS	C19-C18-C17	-2.96	108.66	111.97
3	5-A	200	CPS	C16-C17-C18	2.94	114.62	111.51
3	16-A	200	CPS	C5-C9-C20	2.93	123.03	119.51
3	6-A	200	CPS	C5-C6-C18	2.92	118.12	114.81
4	14-A	403	EDO	O1-C1-C2	-2.92	91.73	112.13
3	7-A	200	CPS	C22-C23-C24	-2.90	104.72	112.90
3	11-A	200	CPS	C16-C15-C14	-2.89	107.71	111.14
4	16-A	403	EDO	O2-C2-C1	2.88	132.30	112.13
3	14-A	200	CPS	O3-C17-C16	2.88	117.10	110.09
3	5-A	200	CPS	C6-C18-C17	-2.87	108.27	111.81
2	2-A	301	SO4	O2-S-O1	-2.86	100.07	109.53
3	11-A	200	CPS	C11-C2-C15	2.85	115.19	110.26
3	6-A	200	CPS	C3-C19-C2	2.85	116.77	113.73
3	14-A	200	CPS	O4-C4-C3	-2.83	103.30	108.99
3	11-A	200	CPS	C23-C24-N1	2.83	121.65	116.50
3	12-A	200	CPS	C23-C22-C20	-2.81	110.01	114.46
3	4-A	200	CPS	C22-C23-C24	2.80	120.82	112.90
3	16-A	200	CPS	C22-C23-C24	2.80	120.81	112.90
4	3-A	403	EDO	O1-C1-C2	-2.80	92.57	112.13
4	15-A	403	EDO	O1-C1-C2	-2.79	92.58	112.13
3	6-A	200	CPS	C21-C20-C9	2.78	117.83	112.96
3	7-A	200	CPS	O1-C24-C23	2.78	127.44	121.92
3	11-A	200	CPS	C8-C9-C20	-2.77	106.93	112.06
4	13-A	403	EDO	O1-C1-C2	-2.77	92.74	112.13
3	10-A	200	CPS	C1-C2-C19	-2.74	107.06	111.45
4	8-A	403	EDO	O1-C1-C2	-2.74	92.97	112.13
3	14-A	200	CPS	C19-C18-C6	2.72	113.25	109.61
3	1-A	200	CPS	C9-C5-C6	2.72	102.84	100.07
3	9-A	200	CPS	C27-C26-C25	-2.70	108.38	114.46
3	1-A	200	CPS	C3-C19-C18	2.70	114.70	110.81
3	3-A	200	CPS	O1-C24-C23	-2.70	116.55	121.92
3	2-A	200	CPS	O1-C24-C23	2.69	127.27	121.92
4	16-A	403	EDO	O1-C1-C2	-2.69	93.34	112.13
3	4-A	200	CPS	O1-C24-N1	2.67	128.23	122.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4-A	200	CPS	C10-C5-C6	-2.65	107.01	111.22
4	11-A	403	EDO	O1-C1-C2	-2.64	93.67	112.13
3	16-A	200	CPS	O1-C24-C23	2.63	127.15	121.92
3	14-A	200	CPS	C10-C5-C6	2.62	115.38	111.22
3	11-A	200	CPS	C27-C26-C25	-2.59	108.64	114.46
3	1-A	200	CPS	O2-C13-C12	-2.58	102.55	110.04
3	7-A	200	CPS	C14-C15-C2	-2.58	109.88	112.67
3	10-A	200	CPS	O3-C17-C18	-2.58	103.76	109.23
4	3-A	403	EDO	O2-C2-C1	2.58	130.18	112.13
3	6-A	200	CPS	C16-C15-C14	-2.57	108.08	111.14
3	8-A	200	CPS	C22-C23-C24	2.56	120.14	112.90
4	5-A	402	EDO	O2-C2-C1	-2.54	94.34	112.13
3	4-A	200	CPS	O3-C17-C16	-2.54	103.89	110.09
2	15-A	301	SO4	O3-S-O1	-2.53	87.13	110.12
3	14-A	200	CPS	C25-N1-C24	-2.52	117.70	122.84
3	1-A	200	CPS	C8-C9-C20	-2.51	107.42	112.06
3	10-A	200	CPS	C25-N1-C24	-2.47	117.80	122.84
3	13-A	200	CPS	C2-C19-C18	2.47	114.52	111.90
3	6-A	200	CPS	O3-C17-C16	2.46	116.09	110.09
4	10-A	404	EDO	O2-C2-C1	-2.46	94.94	112.13
3	2-A	200	CPS	C23-C22-C20	-2.45	110.57	114.46
3	3-A	200	CPS	C7-C6-C5	2.44	106.03	103.58
4	9-A	404	EDO	O2-C2-C1	-2.44	95.07	112.13
3	4-A	200	CPS	C3-C4-C5	-2.44	108.71	111.21
2	11-A	301	SO4	O4-S-O3	-2.44	98.78	109.08
2	11-A	300	SO4	O3-S-O1	-2.42	88.10	110.12
3	12-A	200	CPS	C25-N1-C24	-2.42	117.90	122.84
4	6-A	401	EDO	O2-C2-C1	-2.42	95.24	112.13
3	16-A	200	CPS	C8-C9-C5	2.41	105.99	103.58
3	14-A	200	CPS	C11-C2-C15	2.40	114.41	110.26
3	4-A	200	CPS	C10-C5-C9	2.38	115.00	111.22
3	9-A	200	CPS	O1-C24-C23	2.38	126.66	121.92
3	10-A	200	CPS	C21-C20-C9	-2.38	108.79	112.96
3	13-A	200	CPS	C9-C5-C6	2.38	102.50	100.07
3	1-A	200	CPS	C3-C19-C2	2.37	116.26	113.73
3	16-A	200	CPS	C14-C15-C2	-2.37	110.11	112.67
3	10-A	200	CPS	C11-C2-C19	2.36	114.22	111.17
2	11-A	300	SO4	O4-S-O2	2.35	131.48	110.12
3	5-A	200	CPS	O1-C24-C23	-2.34	117.27	121.92
4	1-A	402	EDO	O2-C2-C1	-2.33	95.85	112.13
3	12-A	200	CPS	C21-C20-C9	2.31	117.02	112.96
2	8-A	300	SO4	O4-S-O3	-2.31	99.32	109.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-A	200	CPS	C19-C2-C15	2.31	111.88	108.67
4	8-A	403	EDO	O2-C2-C1	2.30	128.23	112.13
3	4-A	200	CPS	C25-N1-C24	-2.27	118.22	122.84
3	5-A	200	CPS	C8-C9-C20	-2.26	107.88	112.06
3	13-A	200	CPS	O4-C4-C3	2.25	113.51	108.99
3	10-A	200	CPS	C6-C5-C4	2.24	109.47	107.40
3	15-A	200	CPS	C8-C9-C20	-2.23	107.93	112.06
2	9-A	300	SO4	O4-S-O2	-2.22	89.98	110.12
3	3-A	200	CPS	C19-C3-C4	-2.22	111.46	114.35
2	6-A	301	SO4	O4-S-O3	-2.22	99.70	109.08
4	16-A	401	EDO	O1-C1-C2	-2.22	96.63	112.13
2	14-A	300	SO4	O2-S-O1	-2.21	102.21	109.53
3	12-A	200	CPS	C9-C5-C6	-2.21	97.80	100.07
3	16-A	200	CPS	C19-C18-C17	-2.21	109.50	111.97
4	5-A	404	EDO	O2-C2-C1	-2.20	96.74	112.13
3	11-A	200	CPS	O4-C4-C3	-2.19	104.59	108.99
2	11-A	300	SO4	O3-S-O2	2.18	129.90	110.12
3	14-A	200	CPS	C5-C6-C18	-2.17	112.34	114.81
3	11-A	200	CPS	C26-C25-N1	-2.15	106.75	110.16
2	1-A	300	SO4	O4-S-O2	2.14	129.58	110.12
4	5-A	402	EDO	O1-C1-C2	-2.13	97.23	112.13
3	4-A	200	CPS	C27-C26-C25	-2.12	109.69	114.46
3	10-A	200	CPS	O4-C4-C3	2.12	113.26	108.99
3	14-A	200	CPS	C1-C2-C15	2.12	110.12	107.79
3	10-A	200	CPS	C7-C8-C9	-2.10	100.89	105.14
3	8-A	200	CPS	O3-C17-C16	-2.07	105.05	110.09
2	9-A	301	SO4	O3-S-O1	-2.01	91.84	110.12
3	2-A	200	CPS	C7-C6-C18	-2.01	115.45	118.30

All (79) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	10-A	200	CPS	C18
3	10-A	200	CPS	C6
3	10-A	200	CPS	C19
3	10-A	200	CPS	C20
3	4-A	200	CPS	C18
3	4-A	200	CPS	C6
3	4-A	200	CPS	C19
3	4-A	200	CPS	C20
3	14-A	200	CPS	C13
3	14-A	200	CPS	C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
3	14-A	200	CPS	C6
3	14-A	200	CPS	C19
3	14-A	200	CPS	C20
3	11-A	200	CPS	C13
3	11-A	200	CPS	C18
3	11-A	200	CPS	C6
3	11-A	200	CPS	C19
3	11-A	200	CPS	C20
3	15-A	200	CPS	C18
3	15-A	200	CPS	C6
3	15-A	200	CPS	C19
3	15-A	200	CPS	C20
3	12-A	200	CPS	C4
3	12-A	200	CPS	C18
3	12-A	200	CPS	C19
3	12-A	200	CPS	C20
3	12-A	200	CPS	C9
3	1-A	200	CPS	C18
3	1-A	200	CPS	C20
3	1-A	200	CPS	C6
3	1-A	200	CPS	C19
3	1-A	200	CPS	C9
3	6-A	200	CPS	C18
3	6-A	200	CPS	C17
3	6-A	200	CPS	C9
3	6-A	200	CPS	C15
3	6-A	200	CPS	C6
3	6-A	200	CPS	C19
3	6-A	200	CPS	C20
3	6-A	200	CPS	C4
3	16-A	200	CPS	C20
3	16-A	200	CPS	C18
3	16-A	200	CPS	C6
3	16-A	200	CPS	C17
3	16-A	200	CPS	C19
3	3-A	200	CPS	C15
3	3-A	200	CPS	C18
3	3-A	200	CPS	C6
3	3-A	200	CPS	C17
3	3-A	200	CPS	C13
3	3-A	200	CPS	C20
3	3-A	200	CPS	C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
3	13-A	200	CPS	C13
3	13-A	200	CPS	C18
3	13-A	200	CPS	C6
3	13-A	200	CPS	C19
3	13-A	200	CPS	C20
3	7-A	200	CPS	C20
3	7-A	200	CPS	C6
3	7-A	200	CPS	C5
3	7-A	200	CPS	C18
3	7-A	200	CPS	C19
3	2-A	200	CPS	C20
3	2-A	200	CPS	C6
3	2-A	200	CPS	C18
3	2-A	200	CPS	C17
3	2-A	200	CPS	C19
3	8-A	200	CPS	C18
3	8-A	200	CPS	C13
3	8-A	200	CPS	C6
3	8-A	200	CPS	C19
3	8-A	200	CPS	C20
3	5-A	200	CPS	C18
3	5-A	200	CPS	C6
3	5-A	200	CPS	C19
3	5-A	200	CPS	C20
3	9-A	200	CPS	C18
3	9-A	200	CPS	C6
3	9-A	200	CPS	C19

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.