



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:26 PM UTC

PDB ID : 7TK5 / pdb_00007tk5
EMDB ID : EMD-25957
Title : Yeast ATP synthase State 1binding(d) with 10 mM ATP backbone model
Authors : Guo, H.; Rubinstein, J.L.
Deposited on : 2022-01-17
Resolution : 7.80 Å(reported)
Based on initial model : 2HLD

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

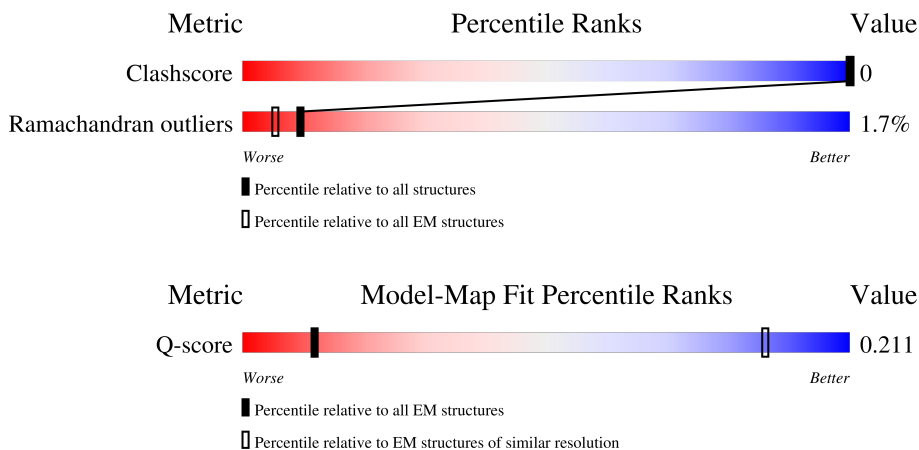
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 7.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	370 (7.30 - 8.30)

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

Mol	Chain	Length	Quality of chain
1	0	76	<div style="display: flex; justify-content: space-between;"> <div style="width: 42%;">■ 42%</div> <div style="width: 53%;">■ 53%</div> </div>
1	1	76	<div style="display: flex; justify-content: space-between;"> <div style="width: 42%;">■ 42%</div> <div style="width: 53%;">■ 53%</div> </div>
1	2	76	<div style="display: flex; justify-content: space-between;"> <div style="width: 47%;">■ 47%</div> <div style="width: 43%;">■ 43%</div> </div>
1	3	76	<div style="display: flex; justify-content: space-between;"> <div style="width: 29%;">■ 29%</div> <div style="width: 50%;">■ 50%</div> <div style="width: 46%;">■ 46%</div> </div>
1	4	76	<div style="display: flex; justify-content: space-between;"> <div style="width: 43%;">■ 43%</div> <div style="width: 47%;">■ 47%</div> <div style="width: 51%;">■ 51%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	5	76	43% 63% 34% ..
1	6	76	26% 50% 46% ..
1	7	76	25% 57% 39% .
1	8	76	37% 43% 54% ..
1	9	76	36% 51% 46% .
2	A	510	13% 57% 40% ..
2	B	510	10% 61% 38% .
2	C	510	11% 60% 38% .
3	D	478	17% 61% 37% .
3	E	478	24% 53% 44% ..
3	F	478	11% 57% 41% .
4	G	278	29% 51% 44% 5%
5	H	138	44% 54% 33% 13%
6	I	61	41% 44% 33% 21%
7	O	195	6% 56% 39% ..
8	T	249	37% 49% 41% 10%
9	U	209	5% 40% 34% 26%
10	V	173	13% 61% 37% ..
11	W	95	32% 44% 45% 11%
12	X	92	29% 36% 29% 33%
13	Y	59	24% 37% 25% 37%
14	Z	48	38% 75% 25%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 20227 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP synthase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	75	300	150	75	75	0	0
1	1	75	300	150	75	75	0	0
1	2	75	300	150	75	75	0	0
1	3	74	296	148	74	74	0	0
1	4	75	300	150	75	75	0	0
1	5	75	300	150	75	75	0	0
1	6	74	296	148	74	74	0	0
1	7	73	292	146	73	73	0	0
1	8	75	300	150	75	75	0	0
1	9	74	296	148	74	74	0	0

- Molecule 2 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	A	499	1996	998	499	499	0	0
2	B	505	2020	1010	505	505	0	0
2	C	498	1992	996	498	498	0	0

- Molecule 3 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	470	Total	C	N	O	0	0
			1880	940	470	470		
3	E	468	Total	C	N	O	0	0
			1872	936	468	468		
3	F	469	Total	C	N	O	0	0
			1876	938	469	469		

- Molecule 4 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	265	Total	C	N	O	0	0
			1060	530	265	265		

- Molecule 5 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	120	Total	C	N	O	0	0
			479	240	120	119		

- Molecule 6 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	48	Total	C	N	O	0	0
			193	96	48	49		

- Molecule 7 is a protein called ATP synthase subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	187	Total	C	N	O	0	0
			748	374	187	187		

- Molecule 8 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	T	224	Total	C	N	O	0	0
			897	448	224	225		

- Molecule 9 is a protein called ATP synthase subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	155	Total	C	N	O	0	0
			620	310	155	155		

- Molecule 10 is a protein called ATP synthase subunit d.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	V	171	685	342	171	172	0	0

- Molecule 11 is a protein called ATP synthase subunit f.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	W	85	340	170	85	85	0	0

- Molecule 12 is a protein called ATP synthase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	X	62	248	124	62	62	0	0

- Molecule 13 is a protein called ATP synthase subunit J.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	Y	37	148	74	37	37	0	0

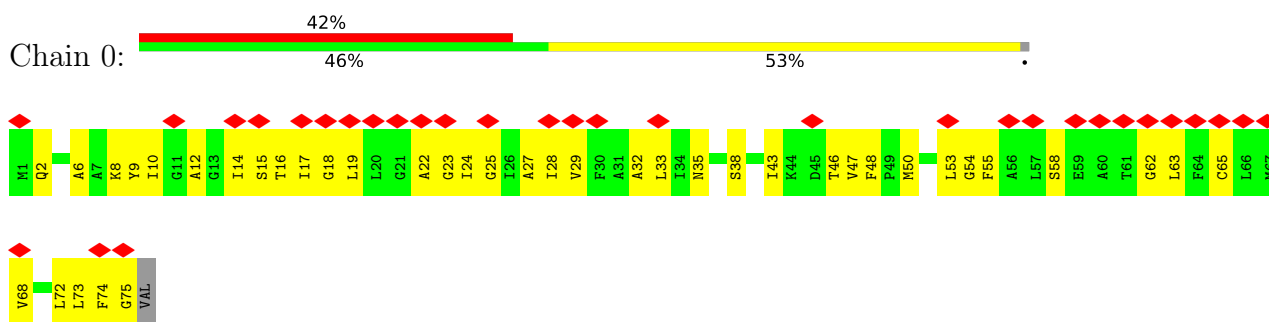
- Molecule 14 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	Z	48	193	96	48	49	0	0

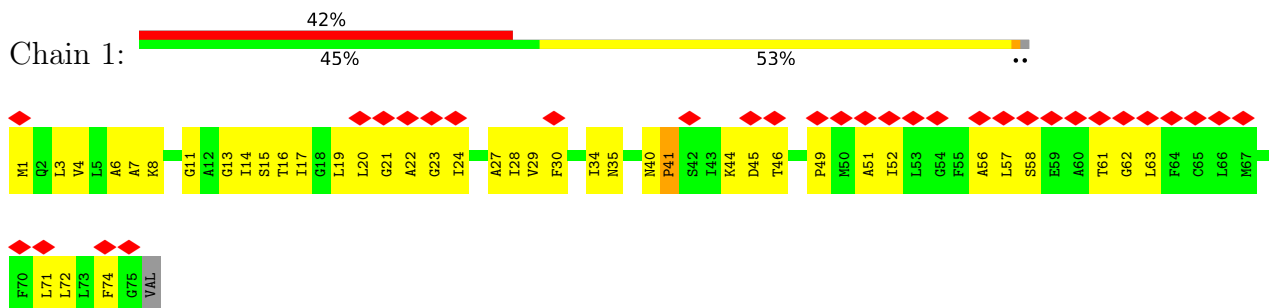
3 Residue-property plots [i](#)

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

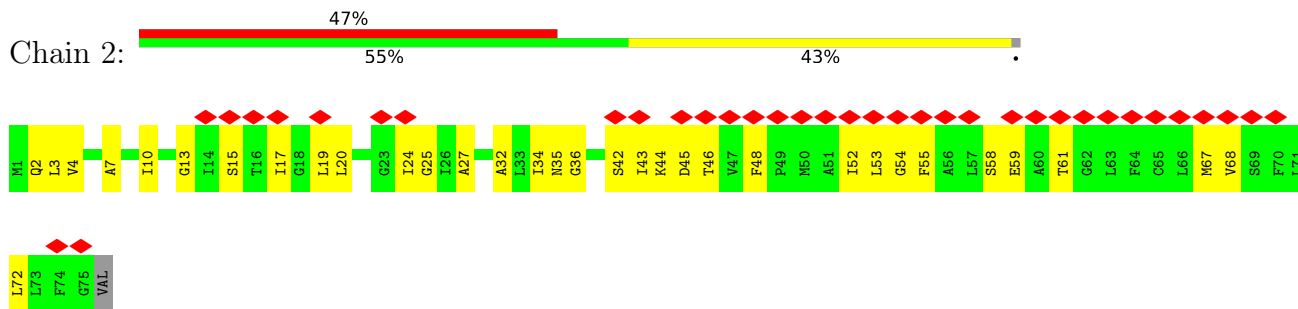
- Molecule 1: ATP synthase subunit 9, mitochondrial



- Molecule 1: ATP synthase subunit 9, mitochondrial

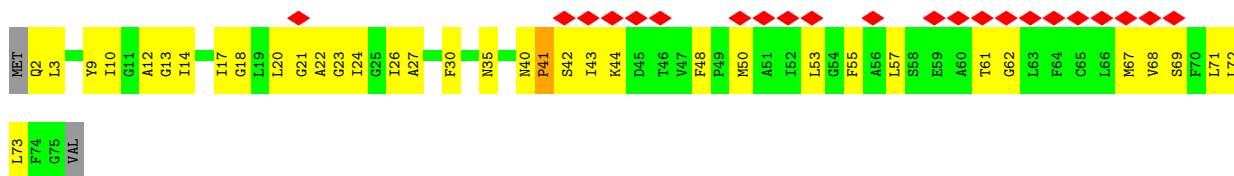


- Molecule 1: ATP synthase subunit 9, mitochondrial

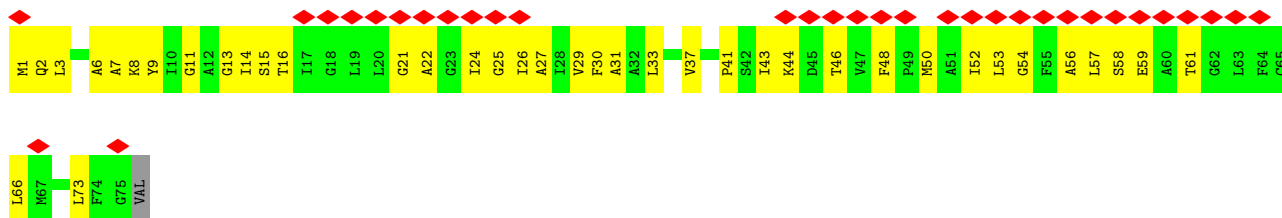
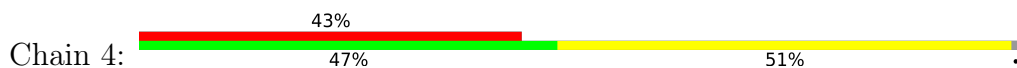


- Molecule 1: ATP synthase subunit 9, mitochondrial

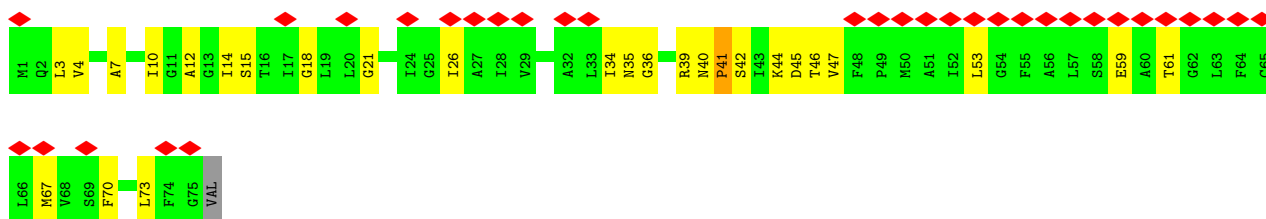
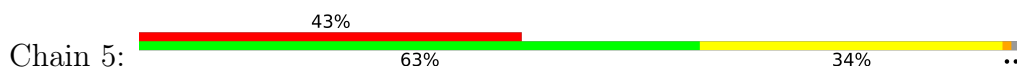




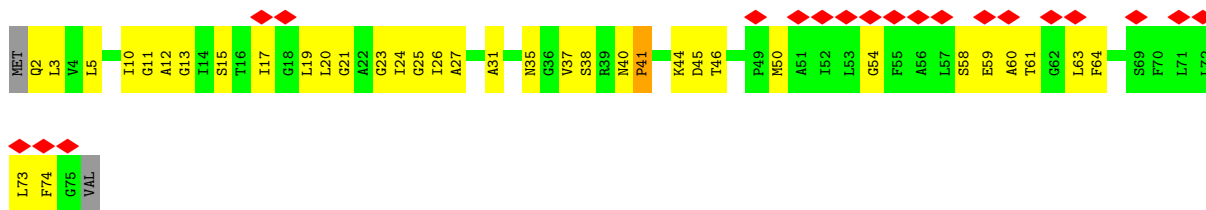
• Molecule 1: ATP synthase subunit 9, mitochondrial



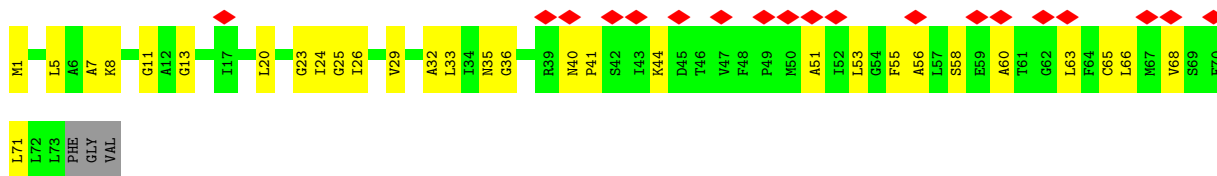
• Molecule 1: ATP synthase subunit 9, mitochondrial



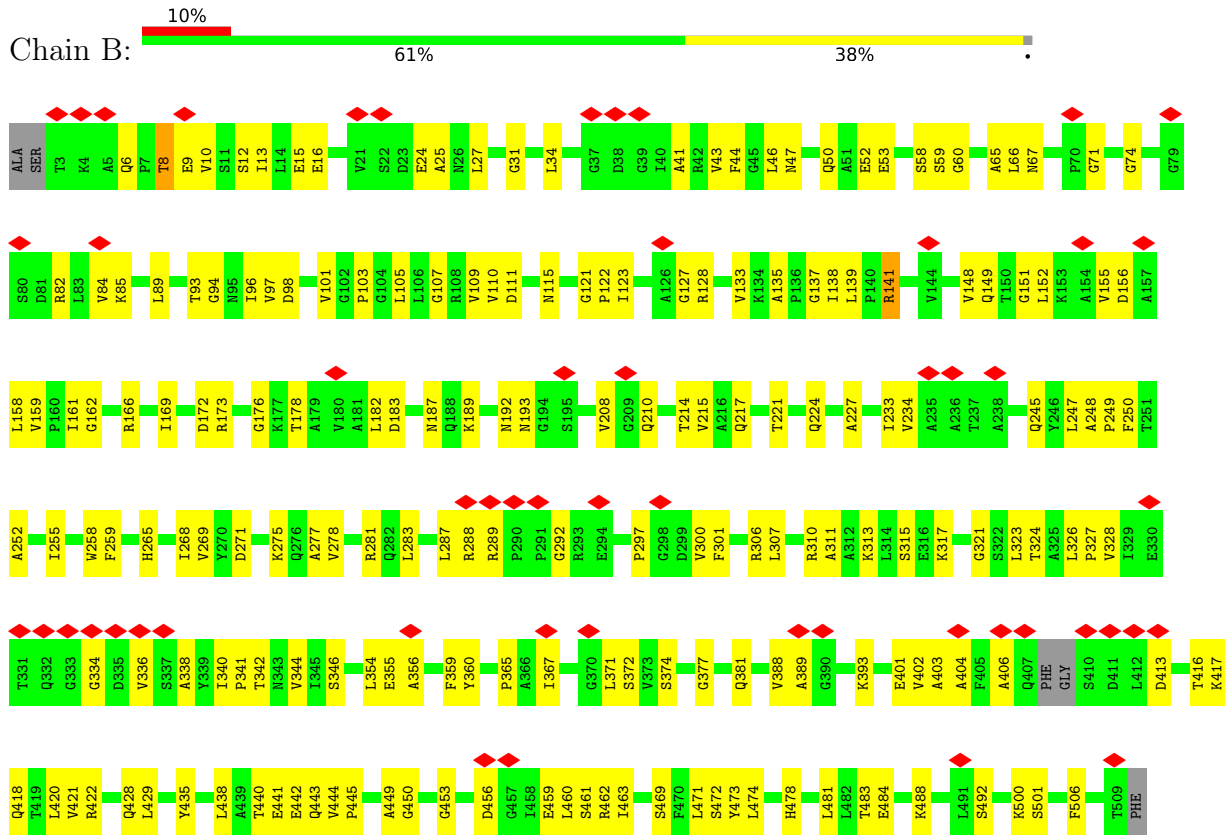
• Molecule 1: ATP synthase subunit 9, mitochondrial



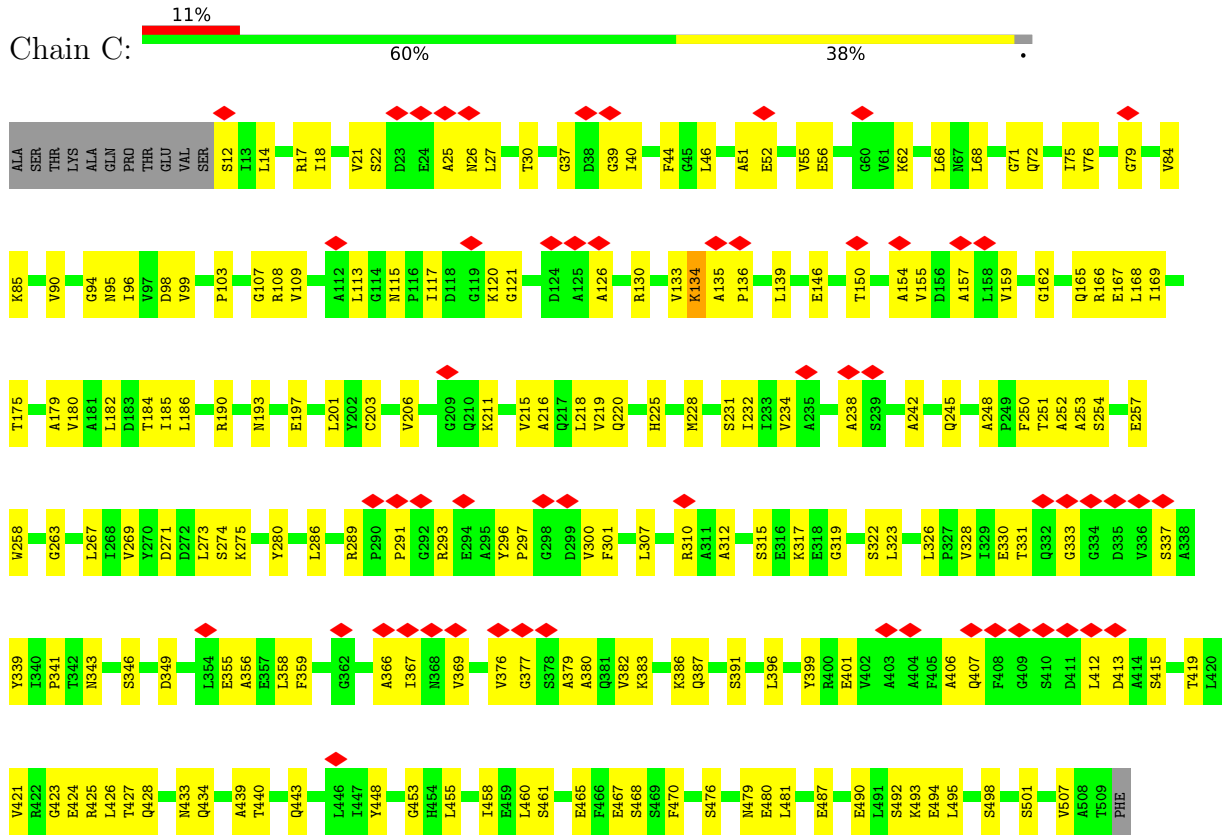
• Molecule 1: ATP synthase subunit 9, mitochondrial

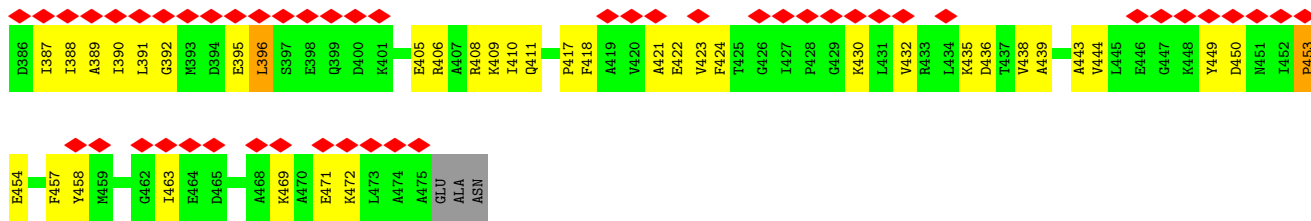


• Molecule 1: ATP synthase subunit 9, mitochondrial

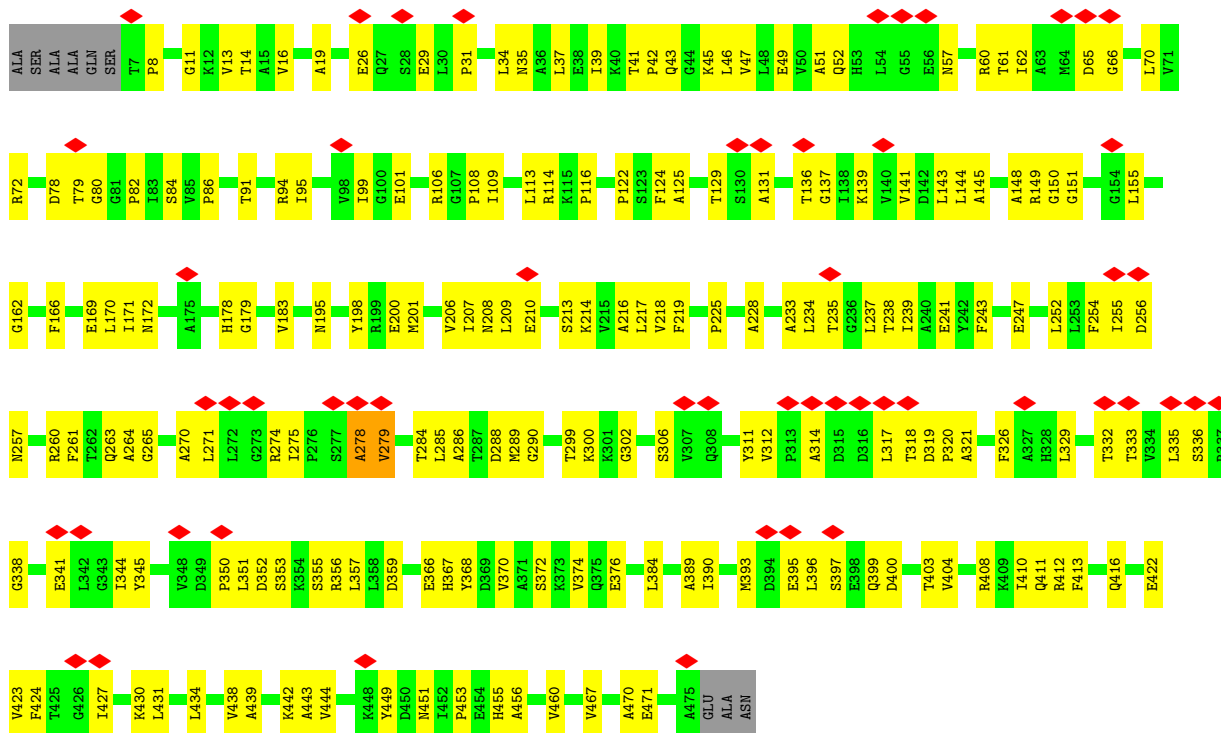


• Molecule 2: ATP synthase subunit alpha

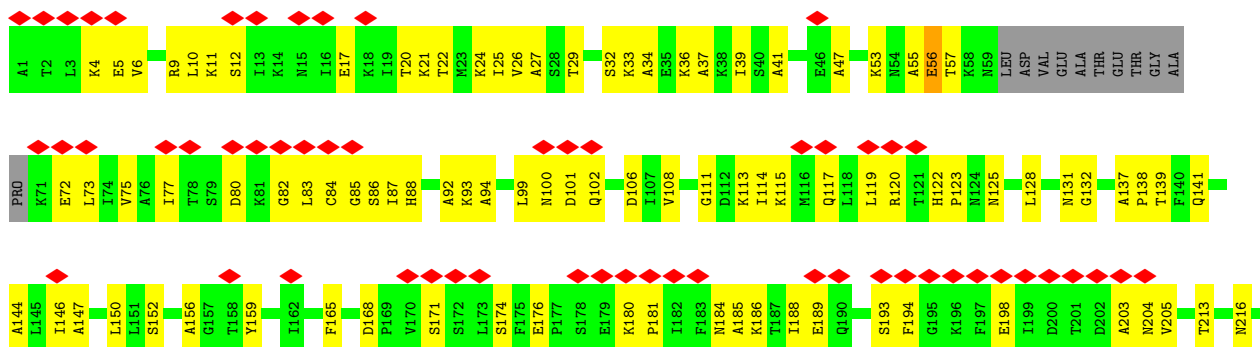


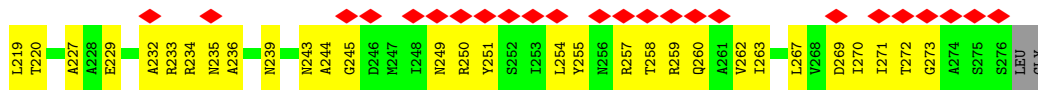


• Molecule 3: ATP synthase subunit beta

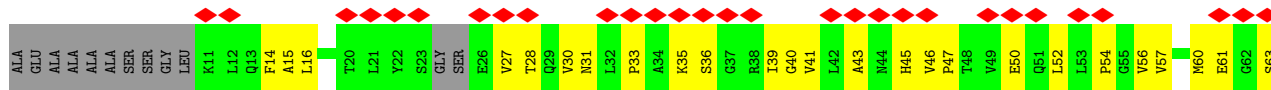
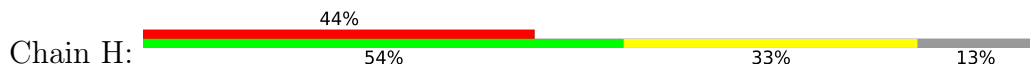


• Molecule 4: ATP synthase subunit gamma

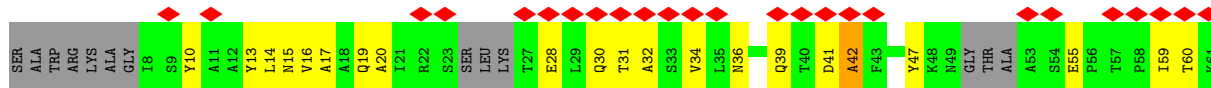
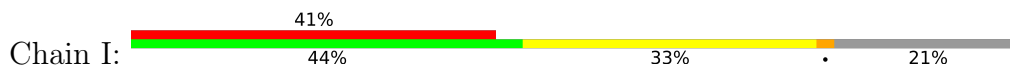




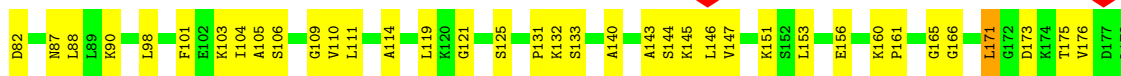
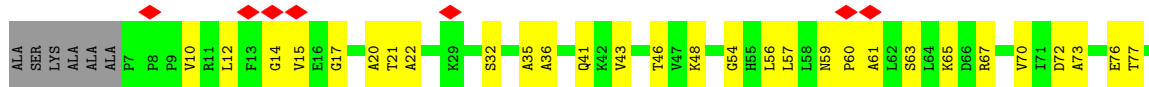
• Molecule 5: ATP synthase subunit delta



• Molecule 6: ATP synthase subunit epsilon

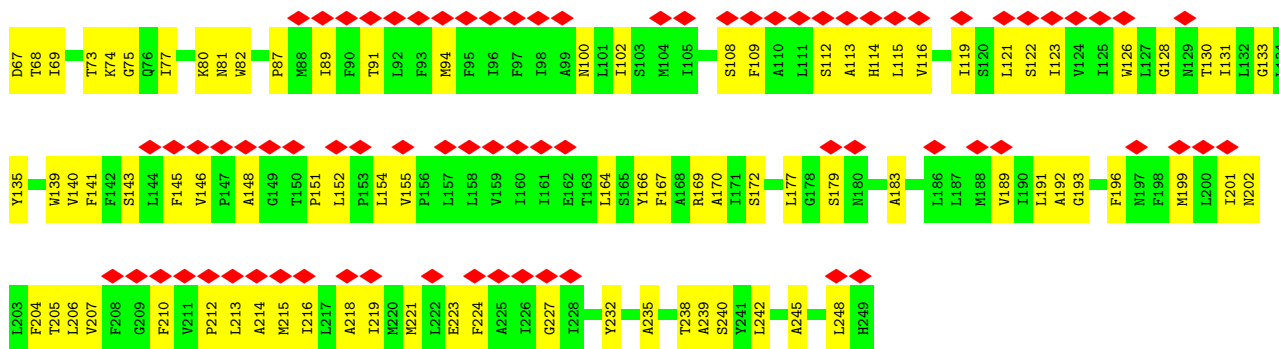


• Molecule 7: ATP synthase subunit 5

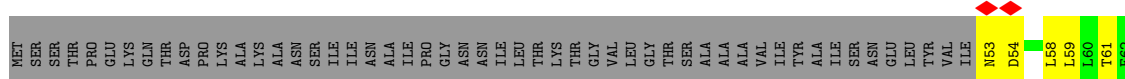


• Molecule 8: ATP synthase subunit a

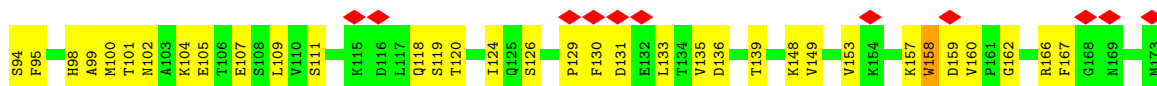
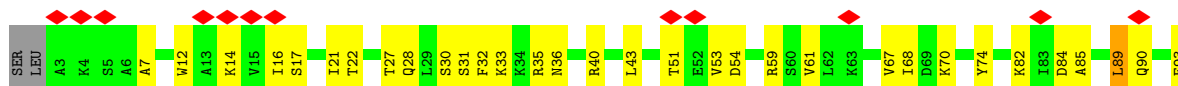




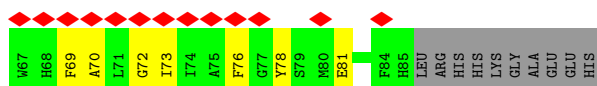
• Molecule 9: ATP synthase subunit 4



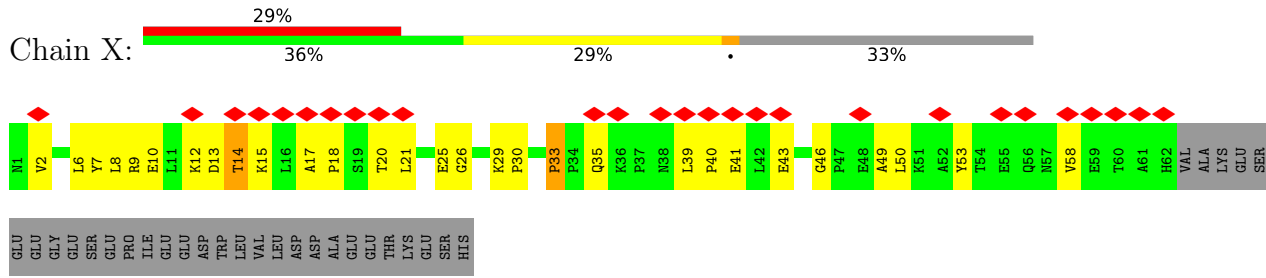
• Molecule 10: ATP synthase subunit d



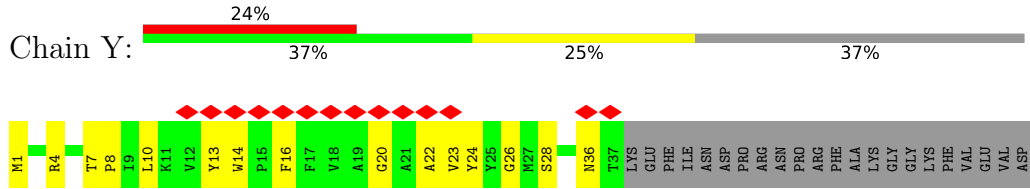
• Molecule 11: ATP synthase subunit f



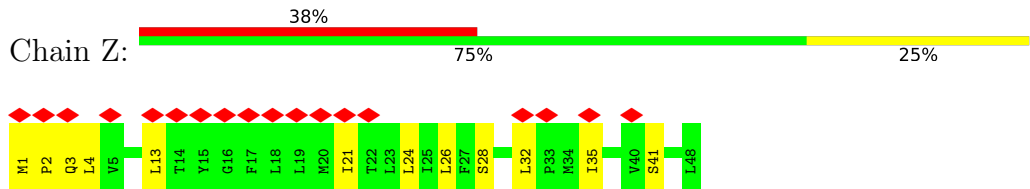
• Molecule 12: ATP synthase subunit H



• Molecule 13: ATP synthase subunit J



• Molecule 14: ATP synthase protein 8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3473	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	103896	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.600	Depositor
Minimum map value	-0.536	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.114	Depositor
Recommended contour level	0.65	Depositor
Map size (Å)	344.96, 344.96, 344.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3475, 1.3475, 1.3475	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	2.67	18/299 (6.0%)	3.40	57/372 (15.3%)
1	1	2.62	21/299 (7.0%)	3.33	51/372 (13.7%)
1	2	2.56	18/299 (6.0%)	3.39	42/372 (11.3%)
1	3	2.36	9/295 (3.1%)	3.28	56/367 (15.3%)
1	4	2.43	14/299 (4.7%)	3.23	52/372 (14.0%)
1	5	2.51	10/299 (3.3%)	3.05	27/372 (7.3%)
1	6	2.58	14/295 (4.7%)	3.21	41/367 (11.2%)
1	7	2.65	14/291 (4.8%)	3.14	35/362 (9.7%)
1	8	2.73	18/299 (6.0%)	3.28	50/372 (13.4%)
1	9	2.48	14/295 (4.7%)	3.09	42/367 (11.4%)
2	A	2.55	108/1994 (5.4%)	2.86	198/2489 (8.0%)
2	B	2.53	106/2018 (5.3%)	2.82	175/2519 (6.9%)
2	C	2.52	94/1991 (4.7%)	2.80	192/2487 (7.7%)
3	D	2.56	90/1879 (4.8%)	2.85	176/2347 (7.5%)
3	E	2.58	105/1871 (5.6%)	2.87	210/2337 (9.0%)
3	F	2.56	94/1875 (5.0%)	2.82	185/2342 (7.9%)
4	G	2.51	53/1058 (5.0%)	3.08	141/1319 (10.7%)
5	H	2.65	31/474 (6.5%)	2.57	26/584 (4.5%)
6	I	2.54	13/190 (6.8%)	2.84	22/231 (9.5%)
7	O	2.65	48/747 (6.4%)	2.81	79/932 (8.5%)
8	T	2.50	49/896 (5.5%)	2.94	105/1117 (9.4%)
9	U	2.43	26/619 (4.2%)	3.16	92/772 (11.9%)
10	V	2.52	33/684 (4.8%)	2.88	70/852 (8.2%)
11	W	2.57	22/339 (6.5%)	2.85	33/422 (7.8%)
12	X	2.45	12/247 (4.9%)	3.05	38/307 (12.4%)
13	Y	2.72	10/147 (6.8%)	2.88	12/182 (6.6%)
14	Z	2.38	6/192 (3.1%)	2.80	13/237 (5.5%)
All	All	2.55	1050/20191 (5.2%)	2.92	2220/25171 (8.8%)

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	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	8	0	1
1	9	0	1
2	A	0	1
2	B	0	1
3	D	0	1
3	E	0	1
3	F	0	1
5	H	0	1
All	All	0	12

All (1050) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	292	GLY	CA-C	-12.98	1.38	1.51
3	F	427	ILE	CA-C	-11.24	1.43	1.53
2	C	135	ALA	CA-C	10.29	1.64	1.53
3	E	388	ILE	CA-C	-9.89	1.40	1.52
7	O	119	LEU	N-CA	-9.88	1.34	1.45
3	D	296	ILE	CA-C	-9.71	1.42	1.53
3	D	373	LYS	CA-C	-9.67	1.40	1.52
2	B	98	ASP	C-N	9.67	1.44	1.33
1	5	12	ALA	C-N	9.49	1.45	1.33
3	F	149	ARG	CA-C	-9.42	1.40	1.52
2	B	152	LEU	CA-C	-9.37	1.41	1.52
3	F	312	VAL	N-CA	-9.31	1.39	1.46
3	D	128	SER	CA-C	-9.19	1.41	1.52
5	H	71	SER	C-N	8.90	1.44	1.33
11	W	73	ILE	N-CA	-8.79	1.34	1.46
10	V	136	ASP	N-CA	-8.71	1.35	1.46
2	C	356	ALA	CA-C	-8.69	1.41	1.52
3	E	216	ALA	CA-C	-8.65	1.42	1.52
2	C	90	VAL	CA-C	-8.60	1.42	1.52
3	E	128	SER	CA-C	-8.51	1.42	1.52
2	B	121	GLY	CA-C	-8.51	1.39	1.51
9	U	125	ASP	CA-C	-8.51	1.42	1.52
3	D	395	GLU	N-CA	-8.50	1.36	1.46
3	E	439	ALA	CA-C	-8.50	1.41	1.52
2	A	40	ILE	N-CA	-8.47	1.35	1.46
3	D	102	PRO	C-N	8.44	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	357	GLU	N-CA	-8.41	1.36	1.46
2	B	483	THR	CA-C	-8.38	1.41	1.52
3	F	306	SER	CA-C	-8.36	1.42	1.52
1	9	68	VAL	C-N	8.34	1.44	1.33
3	E	14	THR	CA-C	8.32	1.63	1.52
10	V	126	SER	CA-C	-8.25	1.41	1.52
3	F	218	VAL	N-CA	-8.22	1.36	1.46
1	5	42	SER	C-N	8.20	1.43	1.34
2	C	267	LEU	CA-C	-8.19	1.42	1.52
7	O	153	LEU	CA-C	-8.14	1.43	1.52
7	O	105	ALA	CA-C	-8.12	1.42	1.52
3	D	251	VAL	C-N	8.11	1.44	1.33
3	E	210	GLU	CA-C	-8.09	1.43	1.53
2	B	406	ALA	CA-C	-8.08	1.42	1.52
2	C	254	SER	CA-C	-8.07	1.42	1.52
8	T	62	GLN	C-N	8.07	1.45	1.33
3	E	82	PRO	N-CA	-8.06	1.37	1.47
2	A	238	ALA	N-CA	-8.06	1.36	1.46
6	I	30	GLN	C-N	8.04	1.44	1.33
3	D	115	LYS	N-CA	-8.01	1.38	1.45
1	1	56	ALA	CA-C	-8.00	1.42	1.52
3	D	12	LYS	CA-C	-7.98	1.43	1.52
1	4	53	LEU	N-CA	-7.96	1.36	1.46
3	D	134	LEU	C-N	7.95	1.44	1.33
3	D	138	ILE	C-N	7.95	1.44	1.33
2	C	461	SER	C-N	7.92	1.44	1.33
2	A	118	ASP	C-N	7.91	1.43	1.33
1	4	7	ALA	N-CA	-7.90	1.36	1.46
8	T	60	ILE	CA-C	-7.90	1.41	1.52
11	W	72	GLY	CA-C	-7.88	1.43	1.52
3	D	275	ILE	CA-C	-7.85	1.47	1.53
4	G	159	TYR	CA-C	-7.84	1.44	1.53
1	1	63	LEU	N-CA	-7.81	1.36	1.46
3	E	50	VAL	CA-C	-7.81	1.44	1.52
2	C	159	VAL	CA-C	7.80	1.59	1.52
2	C	231	SER	CA-C	-7.79	1.43	1.52
3	F	285	LEU	CA-C	-7.78	1.42	1.52
2	B	127	GLY	C-N	7.77	1.44	1.33
3	F	11	GLY	CA-C	-7.77	1.43	1.51
2	C	76	VAL	C-N	7.74	1.43	1.33
5	H	31	ASN	C-N	7.74	1.43	1.33
3	E	295	ARG	C-N	7.74	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	51	ALA	CA-C	-7.73	1.42	1.52
2	A	88	GLU	CA-C	-7.72	1.43	1.52
3	D	291	LEU	N-CA	-7.72	1.37	1.46
9	U	166	GLN	N-CA	-7.71	1.37	1.46
1	5	45	ASP	CA-C	-7.71	1.42	1.52
3	F	66	GLY	CA-C	-7.69	1.43	1.52
9	U	88	VAL	C-N	7.69	1.44	1.33
3	E	297	THR	CA-C	7.67	1.61	1.52
2	C	396	LEU	CA-C	7.67	1.62	1.52
2	A	236	ALA	CA-C	-7.66	1.43	1.52
3	D	152	LYS	CA-C	-7.65	1.41	1.53
2	B	44	PHE	CA-C	-7.64	1.43	1.52
2	C	428	GLN	N-CA	-7.64	1.36	1.46
3	E	279	VAL	CA-C	-7.64	1.43	1.52
5	H	104	LEU	N-CA	-7.63	1.37	1.46
1	8	51	ALA	N-CA	-7.63	1.37	1.46
2	A	360	TYR	CA-C	-7.62	1.42	1.52
1	7	24	ILE	N-CA	-7.61	1.37	1.46
3	E	55	GLY	CA-C	-7.61	1.44	1.52
3	D	157	GLY	CA-C	-7.59	1.43	1.51
2	B	346	SER	C-N	7.59	1.43	1.33
7	O	73	ALA	C-N	7.58	1.43	1.33
2	C	166	ARG	CA-C	-7.58	1.43	1.52
3	D	130	SER	N-CA	-7.56	1.36	1.46
7	O	121	GLY	N-CA	-7.56	1.38	1.45
1	5	59	GLU	C-N	7.56	1.43	1.33
3	D	358	LEU	CA-C	-7.54	1.42	1.52
1	9	59	GLU	C-N	7.54	1.43	1.33
2	A	389	ALA	C-N	7.53	1.42	1.33
10	V	43	LEU	C-N	7.52	1.43	1.33
7	O	14	GLY	C-N	7.51	1.40	1.33
9	U	130	THR	C-N	7.50	1.43	1.34
3	D	468	ALA	C-N	7.49	1.44	1.33
5	H	70	ILE	CA-C	-7.49	1.43	1.52
3	D	69	GLY	CA-C	7.49	1.59	1.51
3	F	237	LEU	CA-C	-7.48	1.42	1.52
8	T	232	TYR	C-N	7.48	1.43	1.33
1	8	14	ILE	CA-C	7.46	1.62	1.52
1	7	5	LEU	CA-C	-7.44	1.43	1.52
2	B	461	SER	CA-C	-7.42	1.43	1.52
4	G	73	LEU	N-CA	-7.42	1.37	1.45
2	C	136	PRO	CA-C	-7.41	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	125	SER	CA-C	-7.41	1.43	1.52
8	T	219	ILE	N-CA	-7.41	1.37	1.46
6	I	55	GLU	CA-C	-7.39	1.43	1.52
2	B	328	VAL	C-O	-7.38	1.16	1.24
4	G	243	ASN	CA-C	7.36	1.62	1.52
2	C	193	ASN	C-N	7.36	1.40	1.33
2	A	315	SER	C-N	7.35	1.44	1.34
13	Y	36	ASN	CA-C	-7.35	1.43	1.52
2	B	307	LEU	CA-C	-7.33	1.43	1.52
3	D	170	LEU	C-N	7.32	1.43	1.33
4	G	227	ALA	CA-C	-7.32	1.43	1.52
2	A	349	ASP	CA-C	-7.31	1.43	1.52
13	Y	10	LEU	CA-C	-7.30	1.43	1.52
1	8	15	SER	CA-C	-7.28	1.42	1.52
4	G	245	GLY	C-N	7.28	1.43	1.33
2	C	407	GLN	CA-C	-7.27	1.43	1.53
7	O	20	ALA	C-N	7.27	1.43	1.33
2	C	25	ALA	CA-C	-7.26	1.43	1.52
3	E	261	PHE	C-N	7.26	1.43	1.33
3	E	25	PHE	CA-C	-7.26	1.44	1.52
3	D	115	LYS	C-N	7.26	1.42	1.33
7	O	182	THR	CA-C	-7.25	1.43	1.52
1	2	54	GLY	CA-C	-7.24	1.44	1.52
13	Y	7	THR	CA-C	-7.24	1.44	1.52
2	B	183	ASP	C-N	7.24	1.43	1.33
2	C	201	LEU	CA-C	-7.24	1.44	1.52
6	I	28	GLU	CA-C	-7.24	1.43	1.52
2	B	354	LEU	C-N	7.21	1.43	1.33
3	E	110	LYS	C-N	7.21	1.42	1.33
2	C	269	VAL	CA-C	-7.20	1.44	1.52
2	A	234	VAL	CA-C	7.20	1.61	1.52
10	V	14	LYS	CA-C	7.20	1.62	1.52
2	A	152	LEU	N-CA	-7.19	1.37	1.46
4	G	82	GLY	N-CA	-7.19	1.37	1.45
3	E	371	ALA	CA-C	-7.19	1.43	1.52
3	F	372	SER	C-N	7.18	1.43	1.33
3	E	353	SER	CA-C	-7.18	1.43	1.53
2	C	220	GLN	N-CA	-7.17	1.37	1.46
1	6	12	ALA	N-CA	-7.17	1.37	1.46
12	X	40	PRO	CA-C	-7.16	1.44	1.52
3	D	269	SER	CA-C	7.15	1.61	1.52
2	A	428	GLN	C-N	7.15	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	328	VAL	C-N	7.13	1.42	1.33
2	C	480	GLU	CA-C	-7.13	1.43	1.52
3	D	224	GLU	C-N	7.12	1.41	1.33
1	3	22	ALA	CA-C	-7.10	1.43	1.52
2	B	155	VAL	CA-C	-7.09	1.43	1.52
3	E	244	ARG	N-CA	-7.08	1.38	1.46
2	A	435	TYR	C-N	7.05	1.39	1.33
2	C	254	SER	C-N	7.05	1.42	1.33
7	O	32	SER	CA-C	-7.05	1.44	1.53
2	C	203	CYS	C-N	7.04	1.42	1.33
3	D	404	VAL	CA-C	-7.04	1.43	1.52
3	E	74	GLU	C-N	7.03	1.42	1.33
1	2	67	MET	CA-C	-7.02	1.43	1.52
2	A	219	VAL	C-O	-7.02	1.16	1.24
3	F	166	PHE	N-CA	-7.01	1.37	1.46
4	G	273	GLY	CA-C	-6.99	1.44	1.52
2	B	84	VAL	N-CA	-6.96	1.37	1.46
3	E	417	PRO	N-CA	-6.95	1.39	1.46
2	C	250	PHE	CA-C	6.94	1.62	1.52
3	E	139	LYS	CA-C	-6.94	1.43	1.52
8	T	91	THR	CA-C	6.93	1.62	1.52
3	F	356	ARG	C-N	6.91	1.43	1.33
2	A	257	GLU	N-CA	-6.90	1.38	1.46
2	C	79	GLY	CA-C	-6.90	1.44	1.51
2	C	322	SER	CA-C	-6.90	1.44	1.52
8	T	130	THR	N-CA	6.89	1.54	1.46
2	B	371	LEU	C-N	6.89	1.42	1.33
2	B	137	GLY	CA-C	-6.87	1.42	1.51
10	V	31	SER	CA-C	-6.86	1.44	1.52
3	F	109	ILE	C-N	6.85	1.42	1.33
3	D	282	GLN	CA-C	-6.85	1.46	1.53
3	F	72	ARG	C-N	6.84	1.41	1.33
3	E	170	LEU	C-N	6.84	1.42	1.33
7	O	17	GLY	C-N	6.84	1.43	1.34
1	0	9	TYR	N-CA	-6.83	1.37	1.46
6	I	20	ALA	C-N	6.83	1.42	1.34
1	3	35	ASN	CA-C	-6.82	1.44	1.52
2	B	123	ILE	C-N	6.82	1.42	1.33
5	H	63	SER	C-N	6.82	1.42	1.33
1	1	35	ASN	C-N	6.81	1.42	1.33
3	F	41	THR	CA-C	-6.81	1.44	1.52
2	B	111	ASP	CA-C	-6.80	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	LYS	CA-C	-6.78	1.44	1.52
6	I	42	ALA	CA-C	-6.78	1.43	1.52
4	G	260	GLN	C-N	6.77	1.42	1.33
8	T	30	SER	C-N	6.77	1.43	1.33
2	A	60	GLY	CA-C	6.77	1.60	1.51
3	E	69	GLY	C-N	6.77	1.42	1.33
1	1	74	PHE	N-CA	6.76	1.54	1.46
3	D	65	ASP	N-CA	-6.76	1.37	1.45
2	B	393	LYS	C-N	6.76	1.43	1.33
1	2	35	ASN	C-N	6.75	1.42	1.33
1	6	63	LEU	C-N	6.75	1.42	1.33
3	E	190	ARG	C-N	6.75	1.43	1.34
2	C	419	THR	C-O	-6.75	1.16	1.24
4	G	150	LEU	C-N	6.75	1.42	1.33
5	H	50	GLU	CA-C	-6.75	1.44	1.52
4	G	119	LEU	CA-C	-6.74	1.44	1.52
9	U	85	MET	C-O	-6.73	1.16	1.24
2	B	359	PHE	CA-C	-6.73	1.44	1.52
1	5	15	SER	CA-C	6.72	1.61	1.52
2	A	325	ALA	N-CA	6.72	1.54	1.45
3	E	321	ALA	CA-C	6.72	1.60	1.52
2	B	492	SER	C-N	6.71	1.42	1.33
3	F	139	LYS	N-CA	-6.71	1.38	1.46
1	9	53	LEU	CA-C	-6.70	1.44	1.52
8	T	152	LEU	C-N	6.70	1.40	1.34
2	B	324	THR	CA-C	-6.69	1.44	1.52
3	E	194	GLY	CA-C	-6.68	1.44	1.52
3	D	183	VAL	N-CA	-6.68	1.38	1.46
7	O	103	LYS	CA-C	-6.67	1.44	1.52
1	6	25	GLY	C-N	6.67	1.42	1.33
8	T	49	ASN	N-CA	-6.67	1.37	1.46
2	B	98	ASP	CA-C	-6.67	1.44	1.52
7	O	35	ALA	CA-C	-6.67	1.44	1.52
2	B	327	PRO	N-CA	-6.64	1.38	1.47
3	F	413	PHE	CA-C	-6.64	1.44	1.52
8	T	143	SER	C-N	6.64	1.43	1.34
1	6	10	ILE	N-CA	6.63	1.54	1.46
3	D	89	ARG	CA-C	6.63	1.61	1.52
3	D	225	PRO	CA-C	6.63	1.58	1.52
5	H	30	VAL	CA-C	-6.63	1.44	1.52
3	D	112	LYS	CA-C	-6.62	1.43	1.52
1	6	46	THR	N-CA	-6.62	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	311	ALA	C-N	6.61	1.41	1.33
2	A	222	LEU	C-N	6.61	1.43	1.33
2	A	475	LYS	CA-C	-6.61	1.44	1.52
5	H	46	VAL	CA-C	-6.60	1.46	1.52
1	7	51	ALA	N-CA	-6.60	1.38	1.46
9	U	148	HIS	C-N	6.59	1.42	1.33
2	C	333	GLY	C-N	6.59	1.41	1.33
3	D	395	GLU	C-O	-6.59	1.17	1.24
11	W	9	VAL	N-CA	-6.57	1.38	1.46
3	D	173	ASN	CA-C	-6.56	1.47	1.53
8	T	66	TYR	CA-C	-6.56	1.44	1.52
3	F	384	LEU	C-N	6.55	1.42	1.33
3	E	19	ALA	N-CA	6.55	1.53	1.46
2	B	215	VAL	CA-C	-6.55	1.44	1.52
1	8	54	GLY	C-N	6.55	1.42	1.33
3	F	335	LEU	N-CA	6.55	1.54	1.46
8	T	87	PRO	N-CA	6.54	1.56	1.47
3	E	72	ARG	CA-C	-6.53	1.44	1.52
2	A	161	ILE	CA-C	-6.52	1.45	1.52
3	F	467	VAL	CA-C	-6.51	1.44	1.52
3	E	243	PHE	CA-C	-6.51	1.44	1.52
5	H	124	ALA	C-O	-6.51	1.16	1.24
1	0	63	LEU	C-O	-6.50	1.16	1.24
3	D	21	VAL	CA-C	-6.50	1.44	1.52
4	G	32	SER	CA-C	-6.50	1.44	1.52
5	H	77	VAL	CA-C	-6.50	1.45	1.52
11	W	54	LYS	CA-C	-6.50	1.43	1.52
2	A	250	PHE	N-CA	-6.50	1.38	1.46
1	9	60	ALA	C-N	6.49	1.42	1.34
3	E	228	ALA	C-N	6.49	1.42	1.33
3	F	84	SER	C-N	6.49	1.40	1.33
2	B	442	GLU	N-CA	-6.49	1.38	1.46
2	B	166	ARG	N-CA	-6.48	1.37	1.46
2	A	337	SER	CA-C	-6.48	1.44	1.52
2	B	122	PRO	CA-C	6.48	1.60	1.52
2	B	356	ALA	C-N	6.48	1.42	1.33
1	8	68	VAL	C-N	6.47	1.42	1.33
2	A	313	LYS	N-CA	-6.47	1.38	1.46
7	O	70	VAL	CA-C	6.47	1.61	1.52
3	E	391	LEU	C-N	6.47	1.42	1.33
10	V	107	GLU	C-O	-6.47	1.16	1.24
2	C	460	LEU	CA-C	6.46	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	471	LEU	CA-C	-6.44	1.44	1.52
8	T	207	VAL	C-N	6.44	1.41	1.33
10	V	94	SER	N-CA	6.44	1.54	1.46
1	0	62	GLY	C-N	6.43	1.42	1.33
2	C	269	VAL	N-CA	-6.43	1.38	1.46
3	F	422	GLU	CA-C	-6.43	1.44	1.52
3	E	111	SER	CA-C	-6.42	1.44	1.52
11	W	33	SER	CA-C	-6.42	1.44	1.52
3	E	176	LYS	C-O	-6.42	1.16	1.24
9	U	126	VAL	N-CA	-6.42	1.39	1.46
2	C	14	LEU	C-N	6.42	1.42	1.33
1	6	13	GLY	CA-C	-6.41	1.45	1.52
11	W	40	PRO	N-CA	-6.41	1.39	1.47
1	2	24	ILE	C-N	6.41	1.41	1.33
2	C	425	ARG	CA-C	-6.40	1.44	1.52
10	V	12	TRP	CA-C	-6.40	1.44	1.52
2	C	343	ASN	CA-C	-6.39	1.44	1.52
3	F	108	PRO	CA-C	6.39	1.60	1.52
1	1	51	ALA	C-N	6.39	1.42	1.33
3	E	121	PRO	CA-C	-6.39	1.46	1.52
2	C	37	GLY	N-CA	-6.39	1.37	1.45
2	A	142	ARG	N-CA	-6.39	1.38	1.46
3	D	427	ILE	N-CA	-6.39	1.40	1.46
2	B	417	LYS	C-N	6.38	1.42	1.33
1	2	27	ALA	CA-C	-6.38	1.44	1.52
2	A	253	ALA	N-CA	-6.38	1.38	1.46
4	G	120	ARG	CA-C	-6.38	1.44	1.52
2	C	46	LEU	CA-C	-6.38	1.45	1.53
3	E	15	ALA	CA-C	-6.38	1.44	1.52
3	F	148	ALA	N-CA	-6.38	1.37	1.45
3	E	384	LEU	CA-C	-6.37	1.44	1.52
2	A	305	SER	N-CA	-6.37	1.38	1.46
2	B	420	LEU	C-N	6.37	1.42	1.33
13	Y	14	TRP	N-CA	-6.37	1.39	1.46
1	6	27	ALA	C-N	6.37	1.42	1.33
1	5	14	ILE	C-N	6.36	1.42	1.34
2	B	344	VAL	CA-C	6.36	1.60	1.52
10	V	82	LYS	C-N	6.35	1.39	1.33
9	U	194	LEU	C-N	6.35	1.42	1.33
8	T	114	HIS	CA-C	-6.34	1.44	1.52
9	U	198	ILE	CA-C	-6.34	1.43	1.52
3	E	39	ILE	C-N	6.33	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	T	52	LYS	C-N	6.32	1.41	1.33
2	A	151	GLY	CA-C	-6.31	1.42	1.51
4	G	37	ALA	CA-C	6.31	1.60	1.52
4	G	57	THR	CA-C	6.31	1.56	1.52
7	O	61	ALA	CA-C	-6.30	1.44	1.52
1	8	20	LEU	N-CA	-6.30	1.38	1.46
2	A	339	TYR	C-N	6.30	1.40	1.33
3	E	255	ILE	N-CA	-6.30	1.39	1.46
4	G	236	ALA	N-CA	-6.30	1.38	1.46
2	B	342	THR	N-CA	-6.29	1.38	1.46
3	F	35	ASN	CA-C	6.29	1.61	1.53
2	C	225	HIS	C-N	6.29	1.42	1.33
1	1	20	LEU	C-N	6.28	1.41	1.33
10	V	90	GLN	C-N	6.28	1.42	1.33
3	D	176	LYS	N-CA	-6.28	1.38	1.46
3	E	457	PHE	C-N	6.28	1.42	1.33
3	E	313	PRO	N-CA	-6.27	1.39	1.47
3	E	41	THR	C-N	6.27	1.40	1.34
3	E	449	TYR	CA-C	-6.27	1.46	1.53
3	F	424	PHE	CA-C	-6.27	1.45	1.52
3	E	271	LEU	CA-C	-6.26	1.44	1.52
2	A	323	LEU	N-CA	-6.26	1.38	1.46
4	G	84	CYS	C-N	6.26	1.42	1.33
2	B	453	GLY	CA-C	6.26	1.59	1.51
3	E	214	LYS	N-CA	-6.26	1.39	1.46
8	T	69	ILE	CA-C	-6.25	1.44	1.53
2	A	149	GLN	CA-C	-6.25	1.45	1.52
7	O	60	PRO	C-N	6.25	1.42	1.33
3	E	49	GLU	C-N	6.25	1.40	1.33
8	T	68	THR	C-N	6.25	1.41	1.33
1	9	7	ALA	CA-C	-6.25	1.44	1.52
1	3	67	MET	C-N	6.25	1.41	1.33
12	X	33	PRO	CA-C	-6.24	1.46	1.52
1	7	60	ALA	C-N	6.24	1.42	1.33
3	F	219	PHE	N-CA	-6.24	1.38	1.46
10	V	149	VAL	N-CA	-6.24	1.39	1.46
1	7	32	ALA	C-N	6.24	1.41	1.33
2	B	85	LYS	CA-C	-6.23	1.44	1.52
1	8	32	ALA	CA-C	-6.23	1.44	1.52
3	F	122	PRO	C-N	6.23	1.42	1.33
2	A	232	ILE	C-O	-6.23	1.17	1.24
3	D	330	ASP	CA-C	6.23	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	188	ILE	CA-C	6.23	1.60	1.52
2	B	15	GLU	N-CA	6.22	1.54	1.46
5	H	16	LEU	N-CA	-6.22	1.40	1.46
2	A	466	PHE	CA-C	-6.22	1.44	1.52
2	B	315	SER	N-CA	-6.21	1.38	1.45
8	T	55	GLY	CA-C	-6.21	1.45	1.51
3	D	464	GLU	C-N	6.20	1.42	1.33
2	A	62	LYS	C-N	6.20	1.41	1.33
3	E	177	ALA	CA-C	-6.20	1.45	1.52
7	O	77	THR	CA-C	-6.20	1.44	1.52
10	V	32	PHE	CA-C	6.19	1.60	1.52
8	T	201	ILE	C-N	6.18	1.42	1.33
3	F	275	ILE	N-CA	-6.18	1.41	1.46
3	D	350	PRO	N-CA	-6.17	1.39	1.47
1	0	32	ALA	C-N	6.17	1.41	1.33
1	0	33	LEU	CA-C	-6.17	1.45	1.52
2	B	221	THR	C-N	6.17	1.42	1.33
9	U	111	SER	N-CA	6.16	1.53	1.46
3	F	376	GLU	C-N	6.16	1.41	1.33
2	A	487	GLU	CA-C	-6.15	1.44	1.52
10	V	102	ASN	C-N	6.15	1.42	1.33
1	8	60	ALA	C-N	6.15	1.42	1.33
12	X	8	LEU	N-CA	6.15	1.53	1.46
2	A	37	GLY	C-N	6.14	1.41	1.33
3	E	203	GLU	CA-C	-6.14	1.44	1.52
2	A	76	VAL	CA-C	-6.14	1.45	1.52
4	G	93	LYS	C-N	6.13	1.42	1.34
3	D	87	VAL	C-O	6.13	1.30	1.23
3	D	257	ASN	N-CA	-6.13	1.37	1.46
3	F	260	ARG	N-CA	-6.13	1.38	1.46
3	E	124	PHE	C-N	6.13	1.42	1.33
2	A	55	VAL	N-CA	-6.12	1.39	1.46
1	8	9	TYR	C-N	6.12	1.41	1.33
3	D	10	THR	CA-C	-6.12	1.45	1.52
2	C	307	LEU	N-CA	-6.12	1.39	1.46
9	U	172	LEU	CA-C	-6.12	1.44	1.52
3	F	353	SER	CA-C	6.11	1.59	1.52
1	0	18	GLY	CA-C	-6.11	1.45	1.52
3	E	408	ARG	N-CA	6.11	1.54	1.46
1	0	74	PHE	CA-C	-6.11	1.45	1.52
11	W	64	LYS	C-N	6.10	1.41	1.34
9	U	72	TYR	CA-C	6.10	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	24	ILE	CA-C	-6.09	1.44	1.52
2	C	12	SER	C-N	6.09	1.41	1.33
6	I	19	GLN	N-CA	-6.09	1.39	1.46
2	A	400	ARG	CA-C	-6.09	1.45	1.52
2	B	187	ASN	CA-C	-6.09	1.44	1.52
2	A	72	GLN	CA-C	-6.09	1.45	1.52
2	B	377	GLY	CA-C	-6.09	1.47	1.53
3	F	254	PHE	N-CA	-6.09	1.38	1.46
3	D	333	THR	CA-C	-6.08	1.45	1.52
11	W	60	ASN	N-CA	-6.08	1.38	1.46
4	G	229	GLU	C-N	6.08	1.41	1.33
12	X	30	PRO	C-N	6.08	1.41	1.33
1	8	17	ILE	CA-C	6.07	1.60	1.52
2	B	265	HIS	CA-C	-6.07	1.44	1.53
2	C	232	ILE	N-CA	-6.07	1.39	1.46
3	E	153	ILE	C-N	6.07	1.36	1.33
2	C	424	GLU	C-N	6.07	1.41	1.33
3	D	236	GLY	CA-C	-6.06	1.45	1.52
3	E	298	THR	C-N	-6.06	1.23	1.33
3	E	306	SER	C-N	6.05	1.41	1.33
2	C	349	ASP	N-CA	-6.05	1.38	1.46
4	G	165	PHE	CA-C	-6.05	1.45	1.52
9	U	89	SER	C-N	6.05	1.42	1.33
14	Z	24	LEU	CA-C	-6.05	1.45	1.52
2	A	282	GLN	C-N	6.04	1.42	1.33
2	C	481	LEU	CA-C	-6.04	1.45	1.52
3	E	111	SER	C-N	6.04	1.41	1.33
7	O	143	ALA	C-N	6.04	1.41	1.33
2	A	362	GLY	CA-C	-6.03	1.44	1.51
7	O	41	GLN	CA-C	-6.03	1.45	1.52
8	T	245	ALA	CA-C	6.03	1.60	1.52
2	B	440	THR	CA-C	-6.02	1.45	1.52
1	6	19	LEU	N-CA	-6.02	1.38	1.46
11	W	2	SER	CA-C	-6.01	1.44	1.52
2	B	105	LEU	C-N	6.01	1.41	1.33
9	U	182	SER	CA-C	-6.01	1.45	1.52
3	F	13	VAL	CA-C	-6.01	1.46	1.52
3	F	114	ARG	CA-C	-6.00	1.45	1.52
3	D	153	ILE	CA-C	-6.00	1.44	1.52
2	A	149	GLN	C-N	6.00	1.42	1.33
3	D	132	GLU	CA-C	-5.99	1.45	1.52
1	0	19	LEU	C-N	5.99	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	321	ALA	C-O	-5.99	1.18	1.24
1	2	7	ALA	C-N	5.99	1.41	1.33
2	A	121	GLY	C-N	5.99	1.41	1.33
3	E	34	LEU	C-N	5.99	1.41	1.33
7	O	147	VAL	C-O	-5.99	1.17	1.24
1	4	26	ILE	N-CA	5.98	1.53	1.46
7	O	181	SER	C-N	5.98	1.41	1.33
3	D	111	SER	CA-C	-5.98	1.44	1.52
2	A	330	GLU	CA-C	-5.97	1.45	1.52
2	C	168	LEU	CA-C	-5.97	1.45	1.52
10	V	36	ASN	CA-C	-5.97	1.45	1.52
12	X	17	ALA	CA-C	-5.97	1.48	1.52
7	O	191	LEU	N-CA	5.97	1.53	1.46
2	B	317	LYS	CA-C	5.97	1.60	1.52
2	A	474	LEU	N-CA	-5.96	1.39	1.46
3	F	471	GLU	C-N	5.96	1.41	1.33
2	B	381	GLN	C-N	5.96	1.41	1.33
3	F	14	THR	CA-C	-5.96	1.45	1.52
2	C	179	ALA	CA-C	-5.95	1.44	1.52
4	G	258	THR	N-CA	-5.95	1.39	1.46
1	9	27	ALA	C-N	5.95	1.41	1.33
3	D	91	THR	C-N	5.95	1.41	1.33
12	X	25	GLU	C-N	5.94	1.41	1.33
2	A	275	LYS	N-CA	-5.94	1.38	1.46
2	C	391	SER	C-O	5.93	1.32	1.24
3	F	79	THR	N-CA	-5.93	1.39	1.46
2	C	386	LYS	C-O	-5.93	1.17	1.24
2	A	346	SER	C-N	5.92	1.41	1.33
3	E	444	VAL	C-N	5.92	1.42	1.33
2	A	51	ALA	C-N	5.92	1.42	1.33
2	C	494	GLU	CA-C	5.92	1.60	1.52
4	G	189	GLU	C-N	5.92	1.42	1.33
2	A	139	LEU	CA-C	5.92	1.60	1.52
3	F	257	ASN	C-N	5.92	1.41	1.34
12	X	12	LYS	N-CA	-5.92	1.39	1.46
3	F	290	GLY	C-N	5.92	1.42	1.33
7	O	165	GLY	CA-C	-5.92	1.43	1.51
2	C	21	VAL	C-N	5.91	1.41	1.33
2	C	275	LYS	N-CA	-5.91	1.38	1.46
2	B	34	LEU	N-CA	-5.91	1.40	1.46
3	D	99	ILE	C-N	5.90	1.40	1.32
8	T	146	VAL	CA-C	5.90	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	26	GLU	N-CA	-5.90	1.38	1.46
2	A	99	VAL	CA-C	-5.90	1.46	1.52
1	2	19	LEU	C-N	5.89	1.41	1.33
3	E	294	GLU	CA-C	-5.89	1.44	1.52
3	F	237	LEU	N-CA	-5.89	1.39	1.46
2	B	462	ARG	C-N	5.89	1.41	1.33
7	O	60	PRO	N-CA	-5.88	1.39	1.47
9	U	157	TRP	N-CA	-5.88	1.39	1.46
3	F	455	HIS	C-N	5.88	1.42	1.34
5	H	15	ALA	N-CA	-5.88	1.38	1.45
2	C	312	ALA	CA-C	-5.88	1.45	1.52
7	O	57	LEU	N-CA	-5.88	1.38	1.46
1	2	68	VAL	N-CA	-5.88	1.39	1.46
1	9	2	GLN	C-N	5.87	1.41	1.33
2	B	101	VAL	C-N	5.87	1.42	1.33
2	C	495	LEU	C-N	5.86	1.41	1.33
2	A	162	GLY	N-CA	5.86	1.50	1.44
3	D	371	ALA	CA-C	-5.86	1.44	1.52
7	O	114	ALA	N-CA	-5.86	1.39	1.46
10	V	53	VAL	CA-C	5.85	1.60	1.52
2	B	89	LEU	C-N	5.84	1.40	1.33
2	A	135	ALA	CA-C	-5.84	1.45	1.52
3	F	306	SER	C-N	5.84	1.40	1.33
12	X	41	GLU	C-N	5.84	1.41	1.33
2	A	356	ALA	C-O	-5.84	1.17	1.24
5	H	101	ILE	CA-C	-5.83	1.45	1.52
10	V	157	LYS	C-N	5.83	1.41	1.33
1	6	31	ALA	C-N	5.82	1.41	1.33
2	A	232	ILE	C-N	5.82	1.41	1.33
3	F	47	VAL	N-CA	-5.82	1.39	1.46
3	F	169	GLU	N-CA	5.81	1.53	1.46
2	B	53	GLU	N-CA	-5.81	1.37	1.45
5	H	123	ALA	N-CA	-5.81	1.39	1.46
2	A	435	TYR	CA-C	-5.81	1.45	1.52
2	B	484	GLU	C-O	-5.81	1.17	1.24
2	C	39	GLY	C-N	5.81	1.39	1.33
2	C	242	ALA	C-O	-5.80	1.19	1.24
3	D	102	PRO	CA-C	5.80	1.60	1.52
3	E	321	ALA	C-O	-5.80	1.19	1.24
3	E	331	ALA	CA-C	-5.80	1.45	1.52
8	T	227	GLY	C-N	5.80	1.41	1.33
1	4	30	PHE	C-N	5.80	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	458	TYR	C-N	5.80	1.41	1.33
3	F	49	GLU	N-CA	-5.80	1.39	1.46
1	0	73	LEU	C-O	5.79	1.30	1.24
3	F	443	ALA	C-N	5.79	1.41	1.33
12	X	10	GLU	N-CA	-5.79	1.39	1.46
2	A	418	GLN	C-O	-5.78	1.17	1.24
3	D	109	ILE	N-CA	-5.78	1.39	1.46
8	T	191	LEU	CA-C	5.78	1.60	1.52
3	D	113	LEU	CA-C	5.78	1.59	1.52
2	A	201	LEU	N-CA	-5.78	1.39	1.46
2	A	202	TYR	N-CA	-5.77	1.38	1.46
8	T	116	VAL	CA-C	-5.77	1.44	1.52
3	F	198	TYR	CA-C	-5.77	1.45	1.52
3	F	129	THR	CA-C	-5.76	1.45	1.52
10	V	139	THR	N-CA	-5.76	1.39	1.46
3	D	275	ILE	C-N	5.76	1.40	1.33
5	H	80	ASP	N-CA	-5.76	1.39	1.46
2	A	180	VAL	N-CA	-5.75	1.39	1.46
3	D	209	LEU	C-N	5.75	1.41	1.33
5	H	77	VAL	C-O	-5.75	1.18	1.24
3	E	143	LEU	C-N	5.75	1.41	1.33
3	E	23	VAL	CA-C	-5.74	1.45	1.52
1	2	43	ILE	CA-C	-5.74	1.44	1.52
3	E	134	LEU	CA-C	-5.74	1.45	1.52
2	A	73	VAL	N-CA	-5.74	1.39	1.46
13	Y	26	GLY	CA-C	-5.73	1.44	1.51
4	G	156	ALA	CA-C	-5.73	1.45	1.52
5	H	43	ALA	CA-C	-5.73	1.45	1.52
1	4	15	SER	C-N	5.72	1.41	1.34
2	C	120	LYS	N-CA	-5.72	1.40	1.46
2	C	300	VAL	C-N	5.72	1.41	1.33
3	F	368	TYR	C-N	5.72	1.41	1.33
2	A	136	PRO	N-CA	-5.72	1.40	1.47
2	B	297	PRO	CA-C	-5.71	1.44	1.52
7	O	56	LEU	C-N	5.71	1.41	1.33
3	E	181	PHE	CA-C	-5.71	1.45	1.52
7	O	43	VAL	C-N	5.71	1.41	1.33
4	G	25	ILE	C-N	5.70	1.41	1.33
1	8	64	PHE	C-N	5.70	1.41	1.33
1	7	36	GLY	CA-C	-5.70	1.45	1.52
10	V	89	LEU	C-O	-5.70	1.16	1.24
1	9	28	ILE	C-N	5.70	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	193	SER	CA-C	-5.70	1.45	1.52
3	E	148	ALA	CA-C	-5.69	1.45	1.52
5	H	41	VAL	CA-C	-5.69	1.45	1.52
3	F	400	ASP	C-N	5.68	1.41	1.33
3	D	285	LEU	CA-C	-5.68	1.45	1.52
14	Z	2	PRO	N-CA	-5.68	1.41	1.47
2	C	238	ALA	N-CA	5.68	1.53	1.46
2	C	387	GLN	N-CA	-5.68	1.39	1.46
3	E	205	GLY	CA-C	-5.68	1.44	1.51
10	V	119	SER	N-CA	5.68	1.53	1.46
3	F	359	ASP	CA-C	5.67	1.59	1.52
8	T	154	LEU	CA-C	-5.67	1.45	1.52
2	A	69	GLU	N-CA	-5.67	1.40	1.46
1	4	27	ALA	C-N	5.66	1.41	1.33
3	D	194	GLY	CA-C	-5.66	1.45	1.52
3	E	432	VAL	C-N	5.66	1.41	1.33
3	F	320	PRO	C-N	5.66	1.41	1.33
1	0	27	ALA	CA-C	-5.66	1.45	1.52
2	B	65	ALA	CA-C	-5.66	1.45	1.52
5	H	124	ALA	C-N	5.66	1.41	1.33
2	A	274	SER	CA-C	-5.66	1.45	1.52
3	F	217	LEU	C-N	5.65	1.41	1.33
9	U	87	LYS	C-N	5.65	1.41	1.33
2	A	375	ARG	C-N	-5.65	1.28	1.33
2	B	107	GLY	CA-C	-5.65	1.43	1.51
4	G	233	ARG	C-N	5.65	1.41	1.33
1	9	50	MET	CA-C	-5.65	1.45	1.52
2	C	330	GLU	CA-C	-5.65	1.45	1.52
1	7	71	LEU	CA-C	-5.65	1.45	1.52
1	6	50	MET	C-N	5.64	1.41	1.33
4	G	174	SER	CA-C	-5.64	1.45	1.52
2	B	8	THR	CA-C	-5.63	1.45	1.52
3	E	372	SER	N-CA	-5.63	1.39	1.46
3	E	125	ALA	C-N	5.63	1.42	1.33
8	T	199	MET	C-N	5.63	1.41	1.33
4	G	72	GLU	CA-C	-5.62	1.45	1.52
1	8	5	LEU	N-CA	-5.62	1.39	1.46
3	F	390	ILE	CA-C	-5.62	1.45	1.52
3	F	470	ALA	C-N	5.62	1.41	1.33
4	G	122	HIS	C-N	-5.62	1.28	1.33
3	F	183	VAL	N-CA	5.61	1.52	1.46
1	1	3	LEU	N-CA	5.61	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	35	ASN	N-CA	-5.61	1.39	1.46
10	V	129	PRO	N-CA	5.61	1.52	1.46
1	6	17	ILE	C-N	5.61	1.41	1.33
2	B	268	ILE	C-N	5.61	1.40	1.33
3	E	241	GLU	C-N	5.61	1.41	1.33
3	F	29	GLU	C-N	5.61	1.39	1.33
9	U	136	GLU	C-O	-5.60	1.16	1.24
3	D	472	LYS	C-N	5.60	1.41	1.34
1	9	54	GLY	CA-C	-5.60	1.45	1.52
2	C	275	LYS	C-N	5.60	1.41	1.33
4	G	122	HIS	CA-C	-5.60	1.45	1.52
10	V	7	ALA	C-N	5.60	1.42	1.33
2	B	103	PRO	C-N	5.60	1.41	1.33
2	C	218	LEU	C-N	5.60	1.41	1.33
2	B	417	LYS	CA-C	-5.59	1.45	1.52
2	B	59	SER	N-CA	-5.59	1.38	1.46
4	G	147	ALA	N-CA	5.58	1.53	1.46
2	C	492	SER	CA-C	-5.58	1.46	1.52
2	C	280	TYR	C-N	5.58	1.41	1.33
2	B	472	SER	C-N	5.58	1.41	1.33
7	O	144	SER	CA-C	-5.58	1.45	1.53
2	B	450	GLY	C-N	5.57	1.40	1.33
2	A	277	ALA	C-N	5.57	1.41	1.33
9	U	193	VAL	N-CA	-5.57	1.39	1.46
1	2	25	GLY	C-O	5.57	1.30	1.23
3	D	392	GLY	N-CA	-5.57	1.39	1.45
2	B	214	THR	CA-C	-5.57	1.45	1.52
4	G	186	LYS	N-CA	-5.57	1.39	1.46
2	B	74	GLY	C-N	5.56	1.43	1.33
3	D	274	ARG	CA-C	-5.56	1.45	1.52
3	E	330	ASP	N-CA	5.56	1.53	1.46
2	A	282	GLN	C-O	5.55	1.30	1.24
6	I	59	ILE	N-CA	-5.55	1.39	1.46
2	B	248	ALA	N-CA	-5.55	1.38	1.46
7	O	65	LYS	CA-C	-5.55	1.45	1.52
7	O	101	PHE	CA-C	-5.55	1.46	1.52
2	C	326	LEU	CA-C	-5.55	1.46	1.52
3	D	245	ASP	C-O	-5.55	1.17	1.24
3	D	410	ILE	N-CA	5.55	1.53	1.46
3	E	436	ASP	C-N	5.54	1.41	1.33
7	O	109	GLY	C-O	-5.54	1.17	1.23
13	Y	22	ALA	C-N	5.54	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	84	VAL	N-CA	-5.54	1.39	1.46
8	T	205	THR	C-N	5.54	1.41	1.33
4	G	165	PHE	N-CA	-5.54	1.39	1.46
2	B	404	ALA	CA-C	-5.53	1.45	1.52
8	T	170	ALA	CA-C	5.53	1.60	1.52
8	T	219	ILE	C-O	-5.53	1.17	1.24
1	4	56	ALA	CA-C	-5.53	1.45	1.52
2	A	477	ASN	N-CA	-5.53	1.39	1.46
3	E	285	LEU	N-CA	-5.53	1.39	1.46
8	T	152	LEU	CA-C	5.53	1.59	1.52
1	0	75	GLY	CA-C	5.53	1.61	1.52
8	T	140	VAL	N-CA	5.52	1.53	1.46
2	A	12	SER	C-N	5.52	1.40	1.33
2	C	421	VAL	C-O	-5.52	1.17	1.24
2	B	365	PRO	C-N	5.51	1.40	1.33
3	D	387	ILE	N-CA	-5.51	1.40	1.46
2	B	109	VAL	C-N	5.51	1.41	1.33
3	F	370	VAL	N-CA	-5.51	1.40	1.46
2	B	402	VAL	CA-C	5.51	1.59	1.52
2	B	422	ARG	C-N	5.51	1.41	1.33
2	A	467	GLU	CA-C	-5.51	1.45	1.52
6	I	36	ASN	C-N	5.51	1.41	1.33
1	0	72	LEU	N-CA	5.50	1.53	1.46
2	A	29	GLU	N-CA	-5.50	1.39	1.46
2	A	443	GLN	N-CA	-5.50	1.39	1.46
2	B	41	ALA	N-CA	-5.50	1.39	1.45
2	A	367	ILE	CA-C	-5.50	1.45	1.52
3	E	410	ILE	CA-C	-5.49	1.45	1.52
2	B	215	VAL	C-N	5.49	1.41	1.33
3	D	265	GLY	C-O	5.49	1.30	1.23
9	U	59	LEU	CA-C	-5.49	1.45	1.52
1	5	67	MET	C-N	5.49	1.40	1.33
2	A	245	GLN	C-O	5.49	1.30	1.24
3	D	172	ASN	N-CA	-5.49	1.39	1.46
10	V	53	VAL	N-CA	-5.49	1.39	1.46
3	F	424	PHE	C-N	5.49	1.41	1.33
2	C	297	PRO	N-CA	-5.48	1.40	1.47
3	E	301	LYS	CA-C	-5.48	1.45	1.52
3	E	375	GLN	C-N	5.48	1.41	1.33
2	C	274	SER	C-N	5.48	1.41	1.33
2	C	190	ARG	C-O	-5.48	1.17	1.24
3	F	449	TYR	N-CA	-5.48	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	25	GLY	C-N	5.47	1.40	1.33
3	E	469	LYS	C-N	5.47	1.41	1.33
11	W	70	ALA	C-N	5.47	1.41	1.33
2	C	44	PHE	N-CA	5.47	1.52	1.46
1	1	16	THR	CA-C	5.47	1.60	1.52
1	1	21	GLY	C-O	-5.47	1.17	1.23
2	B	421	VAL	C-N	5.47	1.41	1.33
1	4	25	GLY	N-CA	-5.47	1.39	1.45
2	A	462	ARG	C-N	5.47	1.40	1.33
1	7	20	LEU	C-N	5.46	1.41	1.33
2	A	278	VAL	N-CA	-5.46	1.40	1.46
8	T	152	LEU	N-CA	-5.46	1.40	1.46
1	7	13	GLY	C-N	5.46	1.40	1.33
3	F	91	THR	C-N	5.46	1.41	1.33
2	A	422	ARG	C-N	5.45	1.40	1.33
4	G	156	ALA	C-N	5.45	1.40	1.33
2	C	419	THR	N-CA	-5.45	1.39	1.46
3	E	318	THR	C-N	5.44	1.41	1.33
3	E	195	ASN	C-N	5.44	1.41	1.33
7	O	156	GLU	N-CA	-5.44	1.38	1.45
2	C	319	GLY	CA-C	-5.44	1.44	1.51
7	O	147	VAL	C-N	5.44	1.41	1.33
7	O	161	PRO	C-N	5.44	1.41	1.33
1	4	50	MET	CA-C	-5.44	1.45	1.52
3	F	319	ASP	N-CA	5.44	1.53	1.46
2	B	224	GLN	C-O	-5.44	1.17	1.24
9	U	128	LYS	N-CA	-5.43	1.39	1.46
11	W	59	ASP	C-N	5.43	1.41	1.33
1	1	49	PRO	C-N	5.43	1.41	1.34
2	C	376	VAL	C-N	5.43	1.43	1.33
4	G	34	ALA	CA-C	5.43	1.59	1.52
3	D	177	ALA	C-N	5.42	1.41	1.33
3	E	290	GLY	C-N	5.42	1.40	1.33
2	A	416	THR	C-N	5.42	1.41	1.34
1	2	72	LEU	N-CA	-5.41	1.39	1.46
4	G	270	ILE	N-CA	-5.41	1.40	1.46
8	T	145	PHE	N-CA	5.41	1.52	1.46
1	0	68	VAL	CA-C	-5.41	1.45	1.52
4	G	100	ASN	C-N	5.41	1.41	1.33
1	7	26	ILE	N-CA	5.41	1.52	1.46
11	W	4	LEU	N-CA	-5.41	1.39	1.45
2	B	488	LYS	N-CA	-5.41	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	89	ARG	N-CA	-5.41	1.38	1.46
3	F	31	PRO	N-CA	-5.41	1.40	1.47
2	B	367	ILE	N-CA	5.41	1.52	1.46
7	O	166	GLY	C-N	5.41	1.40	1.33
2	B	401	GLU	CA-C	-5.40	1.46	1.52
8	T	131	ILE	CA-C	-5.40	1.45	1.52
1	1	1	MET	N-CA	5.40	1.56	1.46
3	F	329	LEU	N-CA	-5.40	1.39	1.45
8	T	89	ILE	CA-C	5.40	1.60	1.52
7	O	146	LEU	N-CA	-5.40	1.39	1.46
1	1	62	GLY	C-N	5.39	1.41	1.34
1	8	33	LEU	CA-C	-5.39	1.46	1.52
2	A	315	SER	CA-C	-5.39	1.46	1.53
6	I	31	THR	C-N	5.39	1.41	1.33
8	T	121	LEU	N-CA	-5.39	1.39	1.46
1	5	46	THR	C-N	5.38	1.40	1.33
8	T	135	TYR	C-N	5.38	1.41	1.34
2	A	133	VAL	N-CA	-5.38	1.40	1.46
2	B	416	THR	CA-C	-5.38	1.45	1.52
2	C	109	VAL	CA-C	5.38	1.59	1.52
1	1	29	VAL	CA-C	-5.38	1.46	1.52
6	I	13	TYR	C-N	5.38	1.41	1.34
1	7	58	SER	N-CA	5.38	1.52	1.46
3	F	351	LEU	N-CA	-5.38	1.38	1.46
2	B	139	LEU	C-O	-5.37	1.19	1.24
13	Y	1	MET	C-N	5.37	1.41	1.33
2	C	146	GLU	C-N	-5.37	1.26	1.33
1	0	68	VAL	C-N	5.37	1.40	1.33
3	E	273	GLY	N-CA	-5.36	1.37	1.45
2	C	424	GLU	N-CA	-5.36	1.39	1.46
1	8	23	GLY	C-N	5.36	1.40	1.33
3	F	352	ASP	CA-C	-5.36	1.45	1.53
2	C	134	LYS	N-CA	5.36	1.53	1.46
3	E	235	THR	C-N	5.36	1.41	1.33
8	T	235	ALA	C-N	5.36	1.40	1.33
3	F	136	THR	N-CA	-5.35	1.39	1.46
9	U	181	GLN	CA-C	-5.35	1.45	1.52
1	7	58	SER	C-N	5.35	1.41	1.33
3	E	136	THR	CA-C	-5.35	1.45	1.52
3	F	350	PRO	N-CA	-5.35	1.40	1.47
10	V	119	SER	CA-C	-5.35	1.45	1.52
11	W	76	PHE	CA-C	-5.35	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	43	VAL	C-N	5.34	1.40	1.33
2	B	271	ASP	C-N	5.34	1.40	1.33
2	C	310	ARG	C-N	5.34	1.41	1.33
2	C	453	GLY	C-N	5.34	1.41	1.33
2	A	341	PRO	C-N	5.34	1.41	1.33
1	8	13	GLY	CA-C	-5.33	1.46	1.52
2	B	252	ALA	C-N	5.33	1.41	1.34
1	2	61	THR	C-N	5.33	1.40	1.33
2	A	345	ILE	N-CA	-5.33	1.40	1.46
4	G	257	ARG	C-O	5.33	1.30	1.24
2	A	146	GLU	C-N	5.33	1.40	1.33
9	U	104	LYS	C-O	-5.33	1.17	1.24
11	W	23	ARG	C-N	5.33	1.40	1.33
1	5	44	LYS	C-N	5.33	1.41	1.33
3	D	317	LEU	N-CA	5.33	1.52	1.46
1	3	50	MET	CA-C	-5.32	1.45	1.52
3	D	59	VAL	C-O	-5.32	1.17	1.24
4	G	125	ASN	C-N	5.32	1.39	1.33
5	H	14	PHE	C-O	-5.32	1.17	1.24
11	W	58	GLY	CA-C	-5.32	1.47	1.52
5	H	57	VAL	CA-C	-5.32	1.46	1.52
8	T	224	PHE	CA-C	-5.32	1.46	1.52
12	X	8	LEU	CA-C	-5.32	1.46	1.52
2	A	159	VAL	CA-C	-5.31	1.47	1.52
7	O	67	ARG	N-CA	5.31	1.52	1.46
3	F	234	LEU	C-N	5.31	1.40	1.33
11	W	66	LEU	C-O	-5.31	1.18	1.24
4	G	250	ARG	C-O	-5.31	1.18	1.24
3	D	45	LYS	C-N	5.30	1.40	1.33
3	D	363	VAL	C-N	5.30	1.40	1.32
3	F	416	GLN	CA-C	-5.30	1.46	1.52
10	V	27	THR	C-N	5.30	1.41	1.34
1	3	20	LEU	N-CA	-5.30	1.39	1.46
1	6	60	ALA	C-N	5.30	1.41	1.33
10	V	109	LEU	C-O	5.30	1.30	1.24
2	B	247	LEU	CA-C	5.30	1.60	1.52
2	B	374	SER	C-N	5.30	1.41	1.33
3	E	263	GLN	N-CA	-5.30	1.39	1.46
2	B	471	LEU	C-N	5.30	1.41	1.33
4	G	17	GLU	C-N	5.30	1.40	1.33
5	H	52	LEU	C-O	-5.30	1.17	1.24
1	4	22	ALA	C-N	5.29	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	158	LEU	C-N	5.29	1.39	1.33
5	H	134	GLN	CA-C	-5.29	1.45	1.52
7	O	151	LYS	C-O	-5.29	1.17	1.24
8	T	123	ILE	C-N	5.29	1.40	1.33
2	A	208	VAL	N-CA	-5.29	1.40	1.46
2	B	149	GLN	CA-C	-5.29	1.46	1.52
3	E	270	ALA	N-CA	-5.29	1.39	1.46
1	0	55	PHE	CA-C	5.28	1.59	1.52
1	1	7	ALA	C-N	5.28	1.40	1.33
1	9	22	ALA	C-N	5.28	1.40	1.33
9	U	100	VAL	CA-C	-5.28	1.46	1.52
1	3	57	LEU	N-CA	5.28	1.52	1.46
1	9	33	LEU	N-CA	5.28	1.52	1.46
2	B	161	ILE	CA-C	-5.28	1.46	1.52
14	Z	41	SER	CA-C	-5.28	1.46	1.52
1	2	2	GLN	C-N	5.28	1.40	1.33
2	A	271	ASP	N-CA	-5.28	1.40	1.46
4	G	115	LYS	C-N	5.27	1.40	1.33
11	W	54	LYS	N-CA	-5.27	1.39	1.46
2	A	237	THR	CA-C	-5.27	1.46	1.52
2	B	16	GLU	C-O	-5.27	1.17	1.24
3	D	291	LEU	C-O	-5.27	1.18	1.24
5	H	85	VAL	C-N	5.27	1.40	1.33
3	D	79	THR	C-N	5.27	1.41	1.33
2	C	358	LEU	CA-C	5.27	1.60	1.52
3	F	412	ARG	CA-C	5.26	1.59	1.52
8	T	179	SER	C-N	5.26	1.40	1.33
8	T	242	LEU	C-N	5.26	1.40	1.33
10	V	89	LEU	CA-C	5.26	1.59	1.52
2	A	255	ILE	CA-C	5.26	1.59	1.52
3	E	207	ILE	C-O	5.26	1.29	1.24
3	F	317	LEU	C-N	5.26	1.41	1.33
3	F	439	ALA	CA-C	-5.26	1.46	1.52
9	U	152	ALA	N-CA	-5.26	1.40	1.46
2	A	388	VAL	N-CA	-5.25	1.39	1.46
7	O	104	ILE	CA-C	-5.25	1.46	1.52
12	X	58	VAL	CA-C	-5.25	1.46	1.52
2	B	288	ARG	CA-C	-5.25	1.46	1.53
3	E	221	GLN	CA-C	-5.25	1.45	1.53
3	F	238	THR	C-O	-5.25	1.17	1.24
7	O	48	LYS	C-N	5.25	1.41	1.33
3	E	56	GLU	CA-C	-5.24	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	75	VAL	CA-C	5.24	1.58	1.52
14	Z	1	MET	N-CA	5.24	1.56	1.46
2	B	217	GLN	N-CA	-5.24	1.40	1.46
3	D	78	ASP	N-CA	-5.24	1.40	1.46
3	F	62	ILE	CA-C	-5.24	1.46	1.52
5	H	27	VAL	C-N	5.24	1.41	1.33
2	C	434	GLN	C-N	5.23	1.41	1.33
13	Y	10	LEU	N-CA	-5.23	1.39	1.46
11	W	57	ASP	N-CA	-5.23	1.39	1.45
2	C	470	PHE	C-N	5.23	1.41	1.33
3	D	387	ILE	CA-C	-5.23	1.46	1.52
2	A	162	GLY	CA-C	-5.23	1.47	1.52
7	O	176	VAL	C-N	5.22	1.40	1.33
1	3	73	LEU	CA-C	-5.22	1.46	1.52
2	A	134	LYS	N-CA	-5.22	1.39	1.45
3	F	442	LYS	CA-C	-5.22	1.46	1.52
4	G	113	LYS	N-CA	-5.21	1.40	1.46
2	A	64	MET	C-N	5.21	1.43	1.34
2	A	367	ILE	C-N	5.21	1.40	1.33
2	B	269	VAL	CA-C	-5.21	1.46	1.52
4	G	22	THR	N-CA	5.21	1.52	1.46
3	D	348	VAL	N-CA	-5.21	1.40	1.46
3	F	336	SER	C-N	5.21	1.41	1.34
3	D	361	ALA	CA-C	5.21	1.59	1.52
1	1	45	ASP	CA-C	-5.21	1.46	1.52
1	8	29	VAL	N-CA	-5.21	1.40	1.46
13	Y	20	GLY	CA-C	-5.21	1.46	1.52
3	F	39	ILE	C-N	5.21	1.40	1.33
2	C	315	SER	C-N	5.20	1.41	1.33
2	A	358	LEU	C-N	5.20	1.40	1.33
2	A	93	THR	CA-C	5.20	1.59	1.52
6	I	32	ALA	N-CA	-5.19	1.40	1.46
3	E	225	PRO	C-N	5.19	1.40	1.33
4	G	245	GLY	N-CA	-5.19	1.39	1.45
3	E	387	ILE	C-N	5.19	1.40	1.33
3	F	355	SER	CA-C	-5.19	1.46	1.52
3	F	366	GLU	CA-C	-5.19	1.46	1.52
1	1	61	THR	C-N	5.18	1.40	1.33
3	F	367	HIS	CA-C	-5.18	1.46	1.52
5	H	61	GLU	C-N	5.18	1.40	1.33
1	9	20	LEU	C-N	5.18	1.40	1.33
3	D	46	LEU	CA-C	-5.18	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	U	191	GLU	CA-C	-5.18	1.45	1.52
7	O	160	LYS	N-CA	-5.18	1.36	1.45
1	8	55	PHE	N-CA	-5.17	1.40	1.46
3	E	100	GLY	C-N	5.17	1.39	1.32
3	D	239	ILE	CA-C	-5.17	1.46	1.52
8	T	80	LYS	N-CA	-5.17	1.39	1.46
1	2	46	THR	C-N	5.17	1.40	1.33
2	B	71	GLY	C-N	5.17	1.39	1.33
2	B	326	LEU	CA-C	5.17	1.58	1.52
11	W	29	HIS	C-N	5.17	1.41	1.33
10	V	111	SER	CA-C	-5.16	1.46	1.52
11	W	44	ALA	CA-C	5.16	1.58	1.52
14	Z	4	LEU	N-CA	-5.16	1.40	1.46
3	F	41	THR	N-CA	-5.16	1.38	1.46
10	V	153	VAL	CA-C	5.16	1.59	1.52
1	1	52	ILE	CA-C	-5.16	1.46	1.52
2	A	423	GLY	CA-C	5.16	1.57	1.52
7	O	119	LEU	C-N	5.16	1.40	1.33
3	E	395	GLU	CA-C	5.16	1.58	1.52
12	X	14	THR	N-CA	5.16	1.52	1.46
2	B	47	ASN	C-N	5.15	1.42	1.33
3	D	44	GLY	CA-C	-5.15	1.44	1.51
2	A	430	LEU	CA-C	-5.15	1.45	1.52
11	W	81	GLU	CA-C	-5.15	1.46	1.52
2	C	495	LEU	N-CA	-5.15	1.40	1.46
3	E	203	GLU	C-N	5.15	1.41	1.33
1	1	13	GLY	N-CA	-5.14	1.39	1.45
1	9	32	ALA	N-CA	-5.14	1.39	1.46
4	G	6	VAL	N-CA	-5.14	1.40	1.46
1	4	14	ILE	N-CA	-5.14	1.40	1.46
8	T	109	PHE	CA-C	5.14	1.58	1.52
8	T	155	VAL	C-O	-5.14	1.20	1.24
3	E	339	ILE	CA-C	-5.14	1.46	1.52
8	T	91	THR	C-N	5.14	1.41	1.33
11	W	7	PRO	N-CA	-5.13	1.41	1.47
1	2	44	LYS	CA-C	-5.13	1.45	1.52
3	E	266	SER	N-CA	-5.13	1.40	1.46
2	C	406	ALA	CA-C	-5.13	1.45	1.52
2	A	265	HIS	C-N	5.13	1.39	1.33
4	G	53	LYS	C-N	5.13	1.41	1.33
2	A	410	SER	N-CA	5.12	1.55	1.46
2	B	158	LEU	C-O	-5.12	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	182	LEU	N-CA	-5.12	1.40	1.46
1	3	44	LYS	C-N	5.12	1.40	1.33
3	E	286	ALA	CA-C	-5.12	1.46	1.52
3	F	16	VAL	CA-C	-5.12	1.46	1.52
3	F	45	LYS	N-CA	-5.11	1.39	1.45
7	O	88	LEU	C-O	-5.11	1.18	1.24
10	V	95	PHE	CA-C	-5.11	1.46	1.52
6	I	47	TYR	CA-C	5.11	1.59	1.52
2	C	55	VAL	N-CA	-5.11	1.40	1.46
2	C	492	SER	N-CA	5.11	1.52	1.45
3	F	13	VAL	N-CA	-5.11	1.40	1.46
2	C	291	PRO	CA-C	5.11	1.59	1.52
2	C	252	ALA	CA-C	-5.11	1.46	1.52
3	D	402	LEU	C-N	5.11	1.40	1.33
7	O	186	LYS	C-N	5.11	1.40	1.33
1	4	11	GLY	C-N	5.10	1.40	1.33
3	D	80	GLY	N-CA	-5.10	1.38	1.45
2	C	293	ARG	CA-C	-5.10	1.46	1.52
3	F	345	TYR	CA-C	-5.10	1.46	1.52
6	I	14	LEU	C-N	5.10	1.40	1.33
7	O	12	LEU	N-CA	-5.10	1.40	1.46
3	E	286	ALA	N-CA	-5.10	1.40	1.46
3	E	336	SER	CA-C	-5.10	1.46	1.52
3	D	215	VAL	C-N	5.10	1.40	1.33
3	E	409	LYS	CA-C	-5.10	1.46	1.52
1	0	46	THR	C-N	5.10	1.40	1.33
5	H	92	PRO	C-N	5.10	1.40	1.33
2	A	489	GLY	C-N	5.09	1.39	1.33
3	D	184	PHE	N-CA	-5.09	1.40	1.46
5	H	105	LEU	C-O	5.09	1.30	1.24
4	G	24	LYS	N-CA	-5.09	1.40	1.46
3	F	408	ARG	N-CA	-5.09	1.40	1.46
5	H	133	LEU	C-N	5.09	1.40	1.34
4	G	271	ILE	CA-C	-5.09	1.46	1.52
1	1	13	GLY	C-N	5.09	1.40	1.33
8	T	215	MET	N-CA	-5.09	1.40	1.46
2	A	320	SER	CA-C	-5.08	1.46	1.53
2	B	67	ASN	CA-C	-5.08	1.46	1.52
10	V	95	PHE	N-CA	-5.08	1.40	1.46
2	C	165	GLN	CA-C	-5.08	1.46	1.52
1	3	27	ALA	N-CA	-5.08	1.40	1.46
2	B	388	VAL	C-N	5.08	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	349	ASP	C-N	-5.08	1.27	1.34
3	D	267	GLU	N-CA	5.08	1.52	1.46
7	O	105	ALA	N-CA	-5.08	1.40	1.46
2	C	66	LEU	CA-C	-5.08	1.45	1.52
3	F	139	LYS	CA-C	-5.08	1.46	1.52
13	Y	4	ARG	CA-C	-5.08	1.46	1.52
3	D	375	GLN	C-O	-5.07	1.18	1.24
5	H	85	VAL	C-O	-5.07	1.18	1.24
1	1	14	ILE	C-N	5.07	1.40	1.33
2	B	151	GLY	N-CA	-5.07	1.38	1.45
3	D	294	GLU	N-CA	5.07	1.52	1.46
3	F	338	GLY	CA-C	5.07	1.57	1.52
2	A	257	GLU	CA-C	5.07	1.59	1.52
1	2	4	VAL	CA-C	-5.07	1.46	1.52
8	T	49	ASN	C-N	5.07	1.40	1.33
2	C	94	GLY	CA-C	-5.06	1.44	1.51
3	E	94	ARG	CA-C	-5.06	1.46	1.52
3	D	141	VAL	C-N	5.06	1.40	1.33
3	D	366	GLU	CA-C	-5.06	1.46	1.52
3	F	460	VAL	CA-C	-5.06	1.46	1.52
10	V	33	LYS	CA-C	-5.06	1.46	1.52
2	C	155	VAL	N-CA	-5.05	1.40	1.46
1	7	55	PHE	N-CA	-5.05	1.40	1.46
2	A	335	ASP	C-N	5.05	1.40	1.33
2	B	300	VAL	C-N	5.05	1.40	1.33
4	G	267	LEU	C-N	5.05	1.40	1.33
3	F	172	ASN	C-N	5.05	1.40	1.33
1	8	55	PHE	C-N	5.04	1.40	1.33
1	5	21	GLY	CA-C	-5.04	1.45	1.51
3	E	361	ALA	N-CA	-5.04	1.40	1.46
2	B	25	ALA	C-N	5.04	1.40	1.33
3	D	247	GLU	C-N	5.04	1.38	1.33
3	F	137	GLY	CA-C	-5.04	1.44	1.51
1	6	61	THR	N-CA	-5.03	1.40	1.46
2	A	261	ASP	C-N	5.03	1.40	1.33
1	7	68	VAL	N-CA	-5.03	1.40	1.46
3	E	83	ILE	CA-C	5.03	1.59	1.53
4	G	77	ILE	CA-C	-5.03	1.46	1.52
3	E	29	GLU	N-CA	-5.03	1.39	1.45
9	U	143	LYS	CA-C	-5.03	1.46	1.52
2	B	258	TRP	C-N	5.02	1.40	1.33
1	4	26	ILE	CA-C	-5.02	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	60	MET	C-N	5.02	1.40	1.33
10	V	30	SER	C-N	5.02	1.40	1.33
10	V	70	LYS	CA-C	5.01	1.59	1.52
14	Z	21	ILE	C-N	5.01	1.40	1.33
2	A	324	THR	N-CA	-5.01	1.39	1.46
3	E	432	VAL	CA-C	-5.01	1.46	1.52
1	2	44	LYS	C-N	5.01	1.40	1.33
8	T	218	ALA	CA-C	-5.01	1.46	1.52
1	4	1	MET	CA-C	-5.01	1.42	1.52
2	A	209	GLY	C-N	5.01	1.40	1.33
2	A	499	LEU	C-N	5.01	1.40	1.33
2	C	341	PRO	C-N	5.01	1.40	1.33
1	1	4	VAL	N-CA	-5.00	1.40	1.46
1	0	18	GLY	C-N	5.00	1.40	1.34
3	E	169	GLU	CA-C	-5.00	1.46	1.52
4	G	117	GLN	N-CA	-5.00	1.40	1.46

All (2220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8	60	ALA	CA-C-N	13.67	138.60	120.28
1	8	60	ALA	C-N-CA	13.67	138.60	120.28
2	B	336	VAL	N-CA-C	-12.95	100.77	113.20
1	2	53	LEU	CA-C-N	12.25	133.57	119.98
1	2	53	LEU	C-N-CA	12.25	133.57	119.98
8	T	155	VAL	CA-C-O	-12.02	110.64	118.69
1	7	53	LEU	CA-C-N	11.78	133.05	119.98
1	7	53	LEU	C-N-CA	11.78	133.05	119.98
10	V	59	ARG	N-CA-C	-11.63	99.07	113.38
3	D	215	VAL	CA-C-O	11.59	130.60	121.09
4	G	204	ASN	CA-C-N	11.38	127.41	120.24
4	G	204	ASN	C-N-CA	11.38	127.41	120.24
8	T	192	ALA	CA-C-N	10.93	132.11	119.98
8	T	192	ALA	C-N-CA	10.93	132.11	119.98
3	E	193	GLU	CA-C-N	10.73	131.89	119.98
3	E	193	GLU	C-N-CA	10.73	131.89	119.98
12	X	2	VAL	CA-C-N	10.62	133.94	120.56
12	X	2	VAL	C-N-CA	10.62	133.94	120.56
2	A	443	GLN	CA-C-N	10.35	126.76	120.24
2	A	443	GLN	C-N-CA	10.35	126.76	120.24
3	D	256	ASP	N-CA-C	-10.26	93.74	109.24
1	4	58	SER	CA-C-N	10.18	133.92	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	58	SER	C-N-CA	10.18	133.92	120.28
10	V	67	VAL	N-CA-C	-10.14	104.08	113.71
4	G	171	SER	N-CA-C	-10.12	93.96	109.24
11	W	36	GLN	N-CA-C	-10.11	98.58	112.12
2	B	500	LYS	CA-C-N	10.04	133.49	120.44
2	B	500	LYS	C-N-CA	10.04	133.49	120.44
2	C	121	GLY	CA-C-N	10.04	130.67	119.83
2	C	121	GLY	C-N-CA	10.04	130.67	119.83
3	F	302	GLY	CA-C-N	9.89	134.80	120.95
3	F	302	GLY	C-N-CA	9.89	134.80	120.95
2	A	241	ALA	CA-C-N	9.86	131.79	120.06
2	A	241	ALA	C-N-CA	9.86	131.79	120.06
3	D	337	ARG	CA-C-N	9.82	130.88	119.98
3	D	337	ARG	C-N-CA	9.82	130.88	119.98
3	F	99	ILE	N-CA-C	-9.76	102.90	112.17
9	U	115	ASN	CA-C-N	9.68	132.76	120.56
9	U	115	ASN	C-N-CA	9.68	132.76	120.56
2	C	75	ILE	CA-C-N	9.64	134.42	122.37
2	C	75	ILE	C-N-CA	9.64	134.42	122.37
1	2	45	ASP	CA-C-N	9.63	133.96	120.29
1	2	45	ASP	C-N-CA	9.63	133.96	120.29
3	F	143	LEU	N-CA-C	9.59	121.50	111.14
3	F	60	ARG	CA-C-O	-9.45	109.84	120.32
13	Y	7	THR	N-CA-C	-9.43	95.91	110.14
1	2	61	THR	CA-C-N	9.42	130.37	120.00
1	2	61	THR	C-N-CA	9.42	130.37	120.00
2	B	178	THR	CA-C-N	9.40	132.88	120.28
2	B	178	THR	C-N-CA	9.40	132.88	120.28
2	C	40	ILE	N-CA-C	-9.33	96.12	108.06
3	D	464	GLU	N-CA-C	9.32	121.44	111.28
1	8	17	ILE	CA-C-N	9.32	130.47	120.03
1	8	17	ILE	C-N-CA	9.32	130.47	120.03
3	F	91	THR	N-CA-C	-9.20	101.57	113.17
7	O	72	ASP	CA-C-N	9.12	134.18	120.31
7	O	72	ASP	C-N-CA	9.12	134.18	120.31
3	F	264	ALA	CA-C-N	9.11	130.10	119.98
3	F	264	ALA	C-N-CA	9.11	130.10	119.98
3	D	334	VAL	N-CA-C	-9.05	94.11	108.86
2	C	66	LEU	N-CA-C	-9.04	102.65	114.31
2	C	428	GLN	CA-C-N	9.04	133.12	120.29
2	C	428	GLN	C-N-CA	9.04	133.12	120.29
3	E	264	ALA	CA-C-N	9.02	130.00	119.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	264	ALA	C-N-CA	9.02	130.00	119.98
3	E	424	PHE	N-CA-C	8.95	122.00	111.71
3	F	65	ASP	CA-C-O	-8.90	111.54	121.51
3	D	210	GLU	N-CA-C	-8.86	102.01	113.17
2	C	157	ALA	N-CA-C	8.79	120.48	111.07
1	6	61	THR	CA-C-O	-8.78	111.11	120.42
1	3	44	LYS	N-CA-C	8.77	121.79	111.71
3	D	215	VAL	N-CA-C	-8.75	95.33	107.75
1	2	55	PHE	O-C-N	8.72	131.06	122.07
1	7	11	GLY	O-C-N	8.69	130.53	122.19
10	V	118	GLN	CA-C-N	8.69	131.92	120.28
10	V	118	GLN	C-N-CA	8.69	131.92	120.28
3	F	151	GLY	N-CA-C	-8.66	100.24	112.37
10	V	40	ARG	CA-C-O	-8.65	110.64	120.24
3	D	94	ARG	CA-C-O	-8.64	111.35	121.46
3	F	353	SER	N-CA-C	-8.64	95.84	109.23
1	0	27	ALA	N-CA-C	8.63	120.69	111.28
1	5	10	ILE	CA-C-N	8.62	129.55	119.98
1	5	10	ILE	C-N-CA	8.62	129.55	119.98
2	B	74	GLY	CA-C-N	8.62	133.28	120.95
2	B	74	GLY	C-N-CA	8.62	133.28	120.95
3	D	333	THR	N-CA-C	-8.62	96.23	109.24
2	C	117	ILE	N-CA-C	-8.62	104.50	112.43
2	C	146	GLU	CA-C-O	-8.60	113.70	119.29
2	A	30	THR	CA-C-N	8.59	129.04	121.82
2	A	30	THR	C-N-CA	8.59	129.04	121.82
3	E	215	VAL	O-C-N	-8.57	113.27	122.61
3	F	148	ALA	CA-C-O	-8.55	111.93	121.51
3	D	440	SER	CA-C-O	-8.54	111.36	120.42
13	Y	23	VAL	CA-C-N	8.54	131.54	120.44
13	Y	23	VAL	C-N-CA	8.54	131.54	120.44
3	D	318	THR	N-CA-C	-8.53	102.88	113.28
2	B	58	SER	N-CA-C	-8.52	102.89	113.28
2	C	96	ILE	N-CA-C	-8.52	100.58	110.21
3	D	451	ASN	N-CA-C	-8.52	102.67	113.23
1	0	65	CYS	CA-C-N	8.50	133.23	120.31
1	0	65	CYS	C-N-CA	8.50	133.23	120.31
4	G	235	ASN	CA-C-N	8.49	131.99	120.44
4	G	235	ASN	C-N-CA	8.49	131.99	120.44
3	D	176	LYS	CA-C-N	8.49	131.48	120.44
3	D	176	LYS	C-N-CA	8.49	131.48	120.44
2	B	355	GLU	CA-C-N	8.48	131.64	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	355	GLU	C-N-CA	8.48	131.64	120.28
3	E	258	ILE	N-CA-C	-8.47	102.80	113.22
11	W	9	VAL	CA-C-N	8.47	131.85	120.50
11	W	9	VAL	C-N-CA	8.47	131.85	120.50
1	8	35	ASN	CA-C-N	8.47	129.34	119.94
1	8	35	ASN	C-N-CA	8.47	129.34	119.94
3	E	165	VAL	CA-C-N	8.46	131.62	120.28
3	E	165	VAL	C-N-CA	8.46	131.62	120.28
3	F	60	ARG	O-C-N	8.46	133.21	123.31
2	B	233	ILE	CA-C-N	8.45	134.00	123.10
2	B	233	ILE	C-N-CA	8.45	134.00	123.10
3	E	409	LYS	CA-C-N	8.45	132.41	120.42
3	E	409	LYS	C-N-CA	8.45	132.41	120.42
2	A	347	ILE	O-C-N	-8.42	113.70	121.87
8	T	139	TRP	N-CA-C	-8.42	102.57	113.17
2	C	133	VAL	N-CA-C	-8.40	104.56	112.96
4	G	56	GLU	CA-C-N	8.40	131.72	121.64
4	G	56	GLU	C-N-CA	8.40	131.72	121.64
3	E	211	GLY	CA-C-N	8.40	134.08	122.07
3	E	211	GLY	C-N-CA	8.40	134.08	122.07
2	B	429	LEU	CA-C-N	8.38	131.51	120.28
2	B	429	LEU	C-N-CA	8.38	131.51	120.28
4	G	139	THR	CA-C-N	8.38	132.34	120.28
4	G	139	THR	C-N-CA	8.38	132.34	120.28
8	T	201	ILE	CA-C-N	8.37	137.53	121.54
8	T	201	ILE	C-N-CA	8.37	137.53	121.54
4	G	125	ASN	N-CA-C	-8.36	104.21	114.75
3	F	200	GLU	CA-C-N	8.36	132.16	120.29
3	F	200	GLU	C-N-CA	8.36	132.16	120.29
7	O	21	THR	CA-C-N	8.36	131.82	120.54
7	O	21	THR	C-N-CA	8.36	131.82	120.54
3	D	107	GLY	CA-C-N	8.30	130.22	119.84
3	D	107	GLY	C-N-CA	8.30	130.22	119.84
3	D	247	GLU	N-CA-C	-8.29	103.30	113.41
8	T	74	LYS	N-CA-C	-8.27	102.64	112.89
2	A	336	VAL	N-CA-C	-8.25	103.14	111.88
7	O	156	GLU	N-CA-C	-8.24	96.74	109.52
3	F	208	ASN	CA-C-N	8.24	131.32	120.28
3	F	208	ASN	C-N-CA	8.24	131.32	120.28
1	2	17	ILE	CA-C-N	8.22	129.24	120.03
1	2	17	ILE	C-N-CA	8.22	129.24	120.03
9	U	58	LEU	N-CA-C	-8.21	102.41	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	185	ALA	CA-C-N	8.21	131.28	120.28
4	G	185	ALA	C-N-CA	8.21	131.28	120.28
4	G	251	TYR	N-CA-C	8.19	121.32	111.82
8	T	60	ILE	CA-C-N	8.19	131.09	120.44
8	T	60	ILE	C-N-CA	8.19	131.09	120.44
8	T	239	ALA	N-CA-C	-8.19	102.88	113.12
1	1	19	LEU	N-CA-C	8.18	121.12	111.71
1	1	27	ALA	N-CA-C	8.17	121.11	111.71
1	0	53	LEU	CA-C-N	8.14	129.01	119.98
1	0	53	LEU	C-N-CA	8.14	129.01	119.98
3	F	206	VAL	N-CA-C	-8.14	104.56	113.43
4	G	5	GLU	CA-C-N	8.13	130.81	120.56
4	G	5	GLU	C-N-CA	8.13	130.81	120.56
1	3	13	GLY	CA-C-N	8.13	130.81	120.56
1	3	13	GLY	C-N-CA	8.13	130.81	120.56
3	E	270	ALA	CA-C-N	8.13	131.17	120.28
3	E	270	ALA	C-N-CA	8.13	131.17	120.28
10	V	35	ARG	O-C-N	8.13	130.44	122.07
3	F	389	ALA	N-CA-C	8.11	120.20	111.36
3	F	326	PHE	CA-C-N	8.10	131.14	120.28
3	F	326	PHE	C-N-CA	8.10	131.14	120.28
3	E	167	ILE	CA-C-N	8.10	131.13	120.28
3	E	167	ILE	C-N-CA	8.10	131.13	120.28
2	A	383	LYS	CA-C-N	8.10	130.97	120.44
2	A	383	LYS	C-N-CA	8.10	130.97	120.44
2	B	169	ILE	N-CA-C	-8.09	95.94	107.75
9	U	99	HIS	CA-C-N	8.09	131.90	120.42
9	U	99	HIS	C-N-CA	8.09	131.90	120.42
3	F	284	THR	N-CA-C	-8.09	101.59	112.26
1	3	20	LEU	CA-C-N	8.08	128.88	120.00
1	3	20	LEU	C-N-CA	8.08	128.88	120.00
2	B	360	TYR	CA-C-N	8.07	131.09	120.28
2	B	360	TYR	C-N-CA	8.07	131.09	120.28
2	C	22	SER	N-CA-C	-8.05	97.14	109.95
3	D	400	ASP	CA-C-N	8.05	131.72	120.29
3	D	400	ASP	C-N-CA	8.05	131.72	120.29
2	A	199	LYS	N-CA-C	-8.03	102.75	114.39
3	E	173	ASN	N-CA-C	8.03	120.03	111.28
2	C	269	VAL	N-CA-C	-8.03	96.93	108.17
7	O	82	ASP	N-CA-C	-8.03	98.34	110.14
1	9	50	MET	CA-C-N	8.02	131.03	120.28
1	9	50	MET	C-N-CA	8.02	131.03	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	132	LYS	O-C-N	8.00	130.60	122.12
1	5	36	GLY	CA-C-N	8.00	131.78	120.42
1	5	36	GLY	C-N-CA	8.00	131.78	120.42
1	1	19	LEU	CA-C-N	7.99	130.99	120.28
1	1	19	LEU	C-N-CA	7.99	130.99	120.28
11	W	13	LYS	N-CA-C	-7.98	104.01	114.31
3	E	471	GLU	N-CA-C	7.98	119.76	111.14
2	A	154	ALA	N-CA-C	7.97	119.96	111.28
3	F	311	TYR	N-CA-C	-7.96	96.25	109.46
1	0	38	SER	O-C-N	7.96	130.56	122.12
3	D	390	ILE	CA-C-N	7.95	130.93	120.28
3	D	390	ILE	C-N-CA	7.95	130.93	120.28
4	G	86	SER	N-CA-C	-7.94	103.59	112.57
1	1	61	THR	O-C-N	7.94	130.54	122.12
1	0	23	GLY	CA-C-N	7.93	131.33	120.46
1	0	23	GLY	C-N-CA	7.93	131.33	120.46
4	G	141	GLN	CA-C-O	7.92	128.94	120.55
2	C	310	ARG	N-CA-C	-7.91	103.63	113.28
10	V	133	LEU	N-CA-C	-7.91	97.05	109.07
3	D	224	GLU	CA-C-O	-7.90	112.85	120.19
2	B	259	PHE	CA-C-N	7.88	130.84	120.28
2	B	259	PHE	C-N-CA	7.88	130.84	120.28
3	D	177	ALA	N-CA-C	7.87	119.49	111.07
10	V	17	SER	CA-C-N	7.87	132.27	120.31
10	V	17	SER	C-N-CA	7.87	132.27	120.31
3	D	473	LEU	CA-C-N	7.87	130.82	120.28
3	D	473	LEU	C-N-CA	7.87	130.82	120.28
10	V	27	THR	CA-C-N	7.84	132.22	120.31
10	V	27	THR	C-N-CA	7.84	132.22	120.31
2	A	399	TYR	CA-C-N	7.83	130.63	120.44
2	A	399	TYR	C-N-CA	7.83	130.63	120.44
1	7	24	ILE	CA-C-N	7.83	128.64	119.94
1	7	24	ILE	C-N-CA	7.83	128.64	119.94
2	B	27	LEU	N-CA-C	-7.83	101.95	114.09
3	F	95	ILE	N-CA-C	-7.83	97.14	108.11
11	W	20	ASN	CA-C-N	7.83	130.78	120.28
11	W	20	ASN	C-N-CA	7.83	130.78	120.28
3	D	220	GLY	N-CA-C	-7.83	94.62	113.18
3	E	206	VAL	N-CA-C	-7.83	105.50	113.10
8	T	59	LEU	N-CA-C	-7.83	103.18	112.89
3	E	214	LYS	CA-C-N	7.83	131.79	120.91
3	E	214	LYS	C-N-CA	7.83	131.79	120.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	5	LEU	CA-C-N	7.81	130.60	120.44
1	6	5	LEU	C-N-CA	7.81	130.60	120.44
3	F	396	LEU	O-C-N	7.79	131.87	122.84
3	D	395	GLU	N-CA-C	-7.78	105.75	114.62
5	H	56	VAL	N-CA-C	-7.76	96.42	107.75
10	V	27	THR	N-CA-C	-7.76	102.90	111.36
1	3	24	ILE	N-CA-C	-7.76	102.88	110.72
4	G	272	THR	CA-C-N	7.76	128.53	120.00
4	G	272	THR	C-N-CA	7.76	128.53	120.00
3	E	349	ASP	N-CA-C	-7.75	98.38	109.62
3	D	317	LEU	N-CA-C	-7.75	101.77	112.30
1	0	12	ALA	CA-C-N	7.74	128.51	120.00
1	0	12	ALA	C-N-CA	7.74	128.51	120.00
2	A	237	THR	CA-C-N	7.74	130.50	120.44
2	A	237	THR	C-N-CA	7.74	130.50	120.44
3	F	395	GLU	CA-C-O	7.74	127.59	118.69
8	T	100	ASN	N-CA-C	-7.74	102.35	112.41
3	D	290	GLY	O-C-N	7.73	129.61	122.19
2	B	443	GLN	CA-C-N	7.72	126.51	120.33
2	B	443	GLN	C-N-CA	7.72	126.51	120.33
3	F	321	ALA	O-C-N	-7.72	113.45	120.71
2	A	47	ASN	N-CA-C	7.72	119.69	111.28
1	8	6	ALA	CA-C-N	7.70	130.60	120.28
1	8	6	ALA	C-N-CA	7.70	130.60	120.28
4	G	33	LYS	CA-C-N	7.70	130.60	120.28
4	G	33	LYS	C-N-CA	7.70	130.60	120.28
4	G	146	ILE	CA-C-N	7.70	131.22	120.29
4	G	146	ILE	C-N-CA	7.70	131.22	120.29
1	7	58	SER	CA-C-N	7.70	130.59	120.28
1	7	58	SER	C-N-CA	7.70	130.59	120.28
2	B	159	VAL	CA-C-N	7.68	127.67	119.76
2	B	159	VAL	C-N-CA	7.68	127.67	119.76
4	G	123	PRO	N-CA-C	-7.68	103.90	114.80
8	T	141	PHE	CA-C-O	7.67	128.77	120.10
3	E	107	GLY	CA-C-N	7.67	128.13	119.93
3	E	107	GLY	C-N-CA	7.67	128.13	119.93
2	B	105	LEU	CA-C-N	7.66	131.67	120.95
2	B	105	LEU	C-N-CA	7.66	131.67	120.95
1	3	48	PHE	CA-C-N	7.65	127.55	119.05
1	3	48	PHE	C-N-CA	7.65	127.55	119.05
3	D	203	GLU	CA-C-O	-7.64	112.46	120.55
2	A	449	ALA	CA-C-N	7.63	128.41	119.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	449	ALA	C-N-CA	7.63	128.41	119.94
1	9	70	PHE	O-C-N	-7.63	114.03	122.12
3	E	287	THR	CA-C-N	7.63	130.50	120.28
3	E	287	THR	C-N-CA	7.63	130.50	120.28
1	3	18	GLY	O-C-N	7.62	130.04	122.19
1	2	24	ILE	CA-C-N	7.61	128.39	119.94
1	2	24	ILE	C-N-CA	7.61	128.39	119.94
2	B	443	GLN	N-CA-C	7.61	120.64	111.82
3	D	337	ARG	CA-C-O	-7.60	112.49	120.55
2	B	13	ILE	N-CA-C	-7.58	103.41	110.53
3	D	388	ILE	N-CA-C	7.56	118.33	110.62
10	V	90	GLN	N-CA-C	-7.54	104.21	113.41
11	W	78	TYR	CA-C-N	7.53	130.37	120.28
11	W	78	TYR	C-N-CA	7.53	130.37	120.28
3	D	269	SER	CA-C-O	-7.53	112.94	120.70
3	E	210	GLU	CA-C-N	7.53	129.03	120.53
3	E	210	GLU	C-N-CA	7.53	129.03	120.53
7	O	70	VAL	O-C-N	-7.52	114.57	121.87
9	U	81	ALA	CA-C-N	7.52	130.69	120.54
9	U	81	ALA	C-N-CA	7.52	130.69	120.54
1	0	17	ILE	CA-C-N	7.51	128.32	119.98
1	0	17	ILE	C-N-CA	7.51	128.32	119.98
3	F	170	LEU	CA-C-N	7.51	131.08	120.42
3	F	170	LEU	C-N-CA	7.51	131.08	120.42
4	G	114	ILE	CA-C-N	7.51	130.20	120.44
4	G	114	ILE	C-N-CA	7.51	130.20	120.44
1	6	58	SER	CA-C-N	7.50	130.33	120.28
1	6	58	SER	C-N-CA	7.50	130.33	120.28
2	C	507	VAL	N-CA-C	-7.50	103.99	113.22
2	C	301	PHE	CA-C-N	7.50	130.33	120.28
2	C	301	PHE	C-N-CA	7.50	130.33	120.28
3	F	51	ALA	CA-C-O	7.50	127.10	118.55
3	F	399	GLN	CA-C-O	7.50	128.37	120.42
9	U	125	ASP	CA-C-N	7.49	130.26	120.60
9	U	125	ASP	C-N-CA	7.49	130.26	120.60
1	6	54	GLY	CA-C-O	7.47	128.44	120.75
2	C	206	VAL	CA-C-O	-7.47	112.55	120.39
2	A	242	ALA	CA-C-N	7.46	127.34	119.05
2	A	242	ALA	C-N-CA	7.46	127.34	119.05
4	G	184	ASN	CA-C-N	7.46	130.89	120.29
4	G	184	ASN	C-N-CA	7.46	130.89	120.29
3	E	245	ASP	N-CA-C	7.45	119.48	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	242	ALA	CA-C-O	-7.45	110.76	117.98
7	O	143	ALA	N-CA-C	7.45	119.40	111.28
2	A	276	GLN	N-CA-C	-7.44	103.19	111.82
3	D	91	THR	CA-C-N	-7.44	110.33	120.82
3	D	91	THR	C-N-CA	-7.44	110.33	120.82
2	A	115	ASN	N-CA-C	-7.44	100.05	110.31
3	D	312	VAL	CA-C-O	-7.43	113.59	119.98
4	G	120	ARG	CA-C-O	-7.43	113.02	120.82
5	H	80	ASP	CA-C-N	7.42	134.14	122.93
5	H	80	ASP	C-N-CA	7.42	134.14	122.93
2	B	271	ASP	CA-C-N	7.41	135.04	121.70
2	B	271	ASP	C-N-CA	7.41	135.04	121.70
2	A	228	MET	CA-C-N	7.41	135.69	121.54
2	A	228	MET	C-N-CA	7.41	135.69	121.54
2	B	340	ILE	CA-C-O	-7.40	110.03	119.95
2	A	412	LEU	CA-C-N	7.39	131.91	120.75
2	A	412	LEU	C-N-CA	7.39	131.91	120.75
6	I	16	VAL	CA-C-N	7.39	130.18	120.28
6	I	16	VAL	C-N-CA	7.39	130.18	120.28
3	E	217	LEU	N-CA-C	-7.39	97.36	109.40
8	T	43	LEU	N-CA-C	-7.39	104.00	113.16
2	C	234	VAL	N-CA-C	-7.39	97.83	108.17
3	E	97	ASN	N-CA-C	-7.39	100.16	110.35
2	B	193	ASN	N-CA-C	-7.38	102.81	112.41
1	6	59	GLU	CA-C-N	7.38	130.16	120.28
1	6	59	GLU	C-N-CA	7.38	130.16	120.28
3	F	332	THR	N-CA-C	-7.37	97.81	109.23
2	A	16	GLU	N-CA-C	7.37	119.31	111.28
2	C	68	LEU	N-CA-C	-7.37	96.89	108.90
2	C	406	ALA	N-CA-C	7.35	121.34	112.38
3	D	410	ILE	CA-C-N	7.35	130.12	120.28
3	D	410	ILE	C-N-CA	7.35	130.12	120.28
2	B	469	SER	CA-C-N	7.34	130.43	120.44
2	B	469	SER	C-N-CA	7.34	130.43	120.44
1	6	24	ILE	O-C-N	7.34	128.99	121.87
1	6	37	VAL	O-C-N	-7.34	114.75	121.87
9	U	133	LEU	CA-C-O	-7.33	112.65	120.42
3	D	428	PRO	CA-C-N	7.32	128.42	120.44
3	D	428	PRO	C-N-CA	7.32	128.42	120.44
2	C	215	VAL	O-C-N	7.32	128.97	121.87
3	D	330	ASP	N-CA-C	7.31	120.12	111.71
9	U	82	ASP	CA-C-N	7.31	129.95	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	82	ASP	C-N-CA	7.31	129.95	120.44
1	0	48	PHE	CA-C-N	7.29	127.64	119.32
1	0	48	PHE	C-N-CA	7.29	127.64	119.32
2	C	507	VAL	CA-C-O	7.29	126.92	119.20
1	1	44	LYS	CA-C-O	-7.28	111.88	120.10
2	B	388	VAL	CA-C-N	7.27	131.20	120.87
2	B	388	VAL	C-N-CA	7.27	131.20	120.87
2	A	366	ALA	N-CA-C	-7.26	104.44	112.72
2	A	12	SER	CA-C-O	7.26	128.11	120.42
1	6	20	LEU	CA-C-N	7.25	128.03	119.98
1	6	20	LEU	C-N-CA	7.25	128.03	119.98
3	D	216	ALA	N-CA-C	-7.23	98.31	109.52
9	U	78	LYS	CA-C-N	7.23	129.97	120.28
9	U	78	LYS	C-N-CA	7.23	129.97	120.28
2	C	415	SER	N-CA-C	7.23	119.16	111.28
3	D	192	ARG	CA-C-N	7.23	129.97	120.28
3	D	192	ARG	C-N-CA	7.23	129.97	120.28
14	Z	41	SER	N-CA-C	-7.23	103.48	111.36
3	E	335	LEU	N-CA-C	-7.22	99.79	110.48
2	B	172	ASP	CA-C-N	7.22	131.06	120.95
2	B	172	ASP	C-N-CA	7.22	131.06	120.95
1	2	58	SER	CA-C-N	7.21	129.95	120.28
1	2	58	SER	C-N-CA	7.21	129.95	120.28
5	H	35	LYS	N-CA-C	-7.21	105.32	112.97
2	A	193	ASN	CA-C-N	7.21	128.29	120.44
2	A	193	ASN	C-N-CA	7.21	128.29	120.44
3	D	275	ILE	CA-C-O	-7.20	115.09	119.12
10	V	159	ASP	CA-C-O	7.20	128.98	120.70
1	2	34	ILE	N-CA-C	7.19	117.96	110.62
4	G	152	SER	CA-C-N	7.18	129.48	120.72
4	G	152	SER	C-N-CA	7.18	129.48	120.72
1	0	35	ASN	CA-C-N	7.17	127.76	119.94
1	0	35	ASN	C-N-CA	7.17	127.76	119.94
1	2	48	PHE	CA-C-N	7.17	127.01	119.05
1	2	48	PHE	C-N-CA	7.17	127.01	119.05
9	U	202	GLU	CA-C-N	7.17	130.19	120.44
9	U	202	GLU	C-N-CA	7.17	130.19	120.44
1	7	35	ASN	CA-C-N	7.16	127.89	119.94
1	7	35	ASN	C-N-CA	7.16	127.89	119.94
3	E	104	ASP	N-CA-C	-7.16	104.15	113.17
4	G	254	LEU	CA-C-N	7.15	129.86	120.28
4	G	254	LEU	C-N-CA	7.15	129.86	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	277	ALA	CA-C-O	-7.15	112.97	120.55
9	U	165	ARG	CA-C-N	7.15	129.86	120.28
9	U	165	ARG	C-N-CA	7.15	129.86	120.28
2	B	208	VAL	N-CA-C	-7.14	98.19	108.48
3	D	21	VAL	N-CA-C	-7.14	97.74	108.17
1	5	10	ILE	N-CA-C	7.13	117.23	110.53
3	D	275	ILE	CA-C-N	7.12	127.54	119.92
3	D	275	ILE	C-N-CA	7.12	127.54	119.92
1	1	24	ILE	CA-C-N	7.12	127.88	119.98
1	1	24	ILE	C-N-CA	7.12	127.88	119.98
3	F	470	ALA	CA-C-N	7.12	129.82	120.28
3	F	470	ALA	C-N-CA	7.12	129.82	120.28
2	A	123	ILE	N-CA-C	-7.11	97.61	107.99
2	A	296	TYR	CA-C-O	-7.11	112.98	120.87
3	F	206	VAL	CA-C-O	-7.11	112.21	118.96
4	G	239	ASN	CA-C-N	7.10	129.67	120.44
4	G	239	ASN	C-N-CA	7.10	129.67	120.44
5	H	39	ILE	N-CA-C	-7.10	97.28	108.86
2	B	82	ARG	CA-C-O	-7.10	113.39	120.70
3	E	406	ARG	CA-C-N	7.10	129.67	120.44
3	E	406	ARG	C-N-CA	7.10	129.67	120.44
9	U	152	ALA	O-C-N	7.10	129.76	122.09
2	B	278	VAL	O-C-N	-7.09	114.99	121.87
3	F	321	ALA	CA-C-N	7.09	126.58	118.85
3	F	321	ALA	C-N-CA	7.09	126.58	118.85
2	A	352	ILE	N-CA-C	-7.09	98.18	108.11
2	B	192	ASN	N-CA-C	-7.09	104.37	113.16
2	C	383	LYS	CA-C-O	7.09	128.06	120.55
1	5	61	THR	CA-C-N	7.09	127.81	119.94
1	5	61	THR	C-N-CA	7.09	127.81	119.94
2	C	280	TYR	CA-C-O	7.08	128.12	119.97
3	F	155	LEU	N-CA-C	-7.08	98.31	109.50
7	O	110	VAL	N-CA-C	7.08	117.84	110.62
2	A	290	PRO	N-CA-C	7.08	119.33	110.70
4	G	131	ASN	N-CA-C	-7.08	97.77	108.52
7	O	192	GLU	N-CA-C	-7.08	99.94	110.06
1	9	24	ILE	O-C-N	7.07	128.73	121.87
8	T	51	ASN	CA-C-N	7.07	130.75	120.71
8	T	51	ASN	C-N-CA	7.07	130.75	120.71
2	A	463	ILE	CA-C-N	7.07	127.79	119.94
2	A	463	ILE	C-N-CA	7.07	127.79	119.94
3	E	370	VAL	CA-C-N	7.07	129.63	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	370	VAL	C-N-CA	7.07	129.63	120.44
10	V	21	ILE	CA-C-O	-7.07	112.97	120.39
4	G	244	ALA	CA-C-N	7.07	127.82	119.98
4	G	244	ALA	C-N-CA	7.07	127.82	119.98
14	Z	28	SER	N-CA-C	7.07	119.06	111.36
2	C	455	LEU	CA-C-N	7.06	130.32	120.29
2	C	455	LEU	C-N-CA	7.06	130.32	120.29
4	G	262	VAL	N-CA-C	7.06	117.82	110.62
4	G	203	ALA	N-CA-C	-7.06	99.78	109.95
4	G	194	PHE	N-CA-C	-7.05	104.32	114.12
3	E	276	PRO	CA-C-O	-7.04	113.41	121.36
11	W	49	ALA	N-CA-C	-7.03	104.17	112.89
3	E	246	GLU	N-CA-C	7.03	122.72	113.30
2	B	428	GLN	CA-C-O	-7.03	113.10	120.55
7	O	15	VAL	N-CA-C	-7.03	98.70	108.12
3	E	450	ASP	N-CA-C	-7.03	104.02	112.59
1	1	74	PHE	CA-C-O	7.02	128.06	120.55
1	4	3	LEU	O-C-N	7.02	129.56	122.12
2	C	126	ALA	CA-C-O	7.02	126.48	118.97
1	4	52	ILE	CA-C-N	7.02	129.56	120.44
1	4	52	ILE	C-N-CA	7.02	129.56	120.44
3	F	289	MET	CA-C-N	7.01	127.76	119.98
3	F	289	MET	C-N-CA	7.01	127.76	119.98
3	D	175	ALA	CA-C-N	7.01	129.67	120.28
3	D	175	ALA	C-N-CA	7.01	129.67	120.28
3	E	411	GLN	CA-C-O	-7.00	113.13	120.55
3	E	472	LYS	CA-C-N	7.00	129.66	120.28
3	E	472	LYS	C-N-CA	7.00	129.66	120.28
4	G	88	HIS	CA-C-O	-7.00	113.13	120.55
2	C	95	ASN	CA-C-N	6.98	131.37	120.34
2	C	95	ASN	C-N-CA	6.98	131.37	120.34
9	U	107	ILE	CA-C-N	6.98	129.63	120.28
9	U	107	ILE	C-N-CA	6.98	129.63	120.28
2	A	382	VAL	CA-C-N	6.98	129.63	120.28
2	A	382	VAL	C-N-CA	6.98	129.63	120.28
14	Z	32	LEU	O-C-N	-6.98	114.27	120.48
2	B	460	LEU	CA-C-N	6.96	129.61	120.28
2	B	460	LEU	C-N-CA	6.96	129.61	120.28
2	A	297	PRO	CA-C-O	-6.96	113.17	122.08
10	V	148	LYS	CA-C-N	6.96	129.99	120.46
10	V	148	LYS	C-N-CA	6.96	129.99	120.46
3	E	417	PRO	CA-C-N	6.96	134.34	122.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	417	PRO	C-N-CA	6.96	134.34	122.37
7	O	171	LEU	N-CA-C	-6.96	95.99	110.80
3	F	78	ASP	CA-C-O	-6.95	112.85	120.43
3	F	233	ALA	N-CA-C	6.95	118.51	111.07
3	D	81	GLY	CA-C-N	6.95	128.52	119.84
3	D	81	GLY	C-N-CA	6.95	128.52	119.84
1	8	16	THR	CA-C-N	6.95	129.97	120.46
1	8	16	THR	C-N-CA	6.95	129.97	120.46
2	A	355	GLU	O-C-N	-6.94	115.11	123.16
3	E	352	ASP	N-CA-C	-6.94	103.15	112.94
3	F	70	LEU	N-CA-C	-6.94	97.92	108.96
1	4	21	GLY	O-C-N	-6.94	115.53	122.19
2	A	479	ASN	N-CA-C	-6.94	104.82	113.28
2	B	501	SER	N-CA-C	-6.93	103.65	111.07
6	I	20	ALA	N-CA-C	6.93	118.84	111.28
3	E	228	ALA	CA-C-N	6.93	129.57	120.28
3	E	228	ALA	C-N-CA	6.93	129.57	120.28
4	G	120	ARG	O-C-N	6.93	129.21	122.07
1	1	71	LEU	N-CA-C	6.92	118.82	111.28
3	E	65	ASP	CA-C-N	6.92	127.59	120.60
3	E	65	ASP	C-N-CA	6.92	127.59	120.60
3	F	263	GLN	N-CA-C	6.92	118.82	111.28
8	T	240	SER	O-C-N	6.92	129.45	122.12
1	1	45	ASP	CA-C-N	6.92	129.84	120.44
1	1	45	ASP	C-N-CA	6.92	129.84	120.44
3	E	338	GLY	CA-C-N	6.91	129.93	120.46
3	E	338	GLY	C-N-CA	6.91	129.93	120.46
7	O	46	THR	CA-C-N	6.91	130.24	120.42
7	O	46	THR	C-N-CA	6.91	130.24	120.42
1	2	15	SER	CA-C-N	6.91	131.66	120.60
1	2	15	SER	C-N-CA	6.91	131.66	120.60
14	Z	26	LEU	CA-C-N	6.91	129.42	120.44
14	Z	26	LEU	C-N-CA	6.91	129.42	120.44
1	2	59	GLU	CA-C-N	6.91	129.54	120.28
1	2	59	GLU	C-N-CA	6.91	129.54	120.28
2	A	177	LYS	CA-C-N	6.91	129.53	120.28
2	A	177	LYS	C-N-CA	6.91	129.53	120.28
1	8	61	THR	CA-C-N	6.89	127.58	120.00
1	8	61	THR	C-N-CA	6.89	127.58	120.00
1	0	2	GLN	O-C-N	6.89	129.42	122.12
3	F	404	VAL	CA-C-N	6.88	129.50	120.28
3	F	404	VAL	C-N-CA	6.88	129.50	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7	32	ALA	O-C-N	6.87	129.41	122.12
4	G	29	THR	CA-C-N	6.86	130.03	120.29
4	G	29	THR	C-N-CA	6.86	130.03	120.29
5	H	40	GLY	N-CA-C	-6.86	99.45	111.46
4	G	94	ALA	CA-C-N	6.86	129.34	120.56
4	G	94	ALA	C-N-CA	6.86	129.34	120.56
11	W	18	ALA	O-C-N	-6.85	113.44	121.32
3	F	241	GLU	CA-C-N	6.85	129.46	120.28
3	F	241	GLU	C-N-CA	6.85	129.46	120.28
2	C	498	SER	CA-C-N	6.85	129.46	120.28
2	C	498	SER	C-N-CA	6.85	129.46	120.28
1	4	46	THR	CA-C-N	6.84	131.53	120.30
1	4	46	THR	C-N-CA	6.84	131.53	120.30
2	C	62	LYS	N-CA-C	-6.84	98.77	109.72
1	0	8	LYS	N-CA-C	6.83	118.73	111.28
9	U	136	GLU	CA-C-N	6.83	130.35	120.38
9	U	136	GLU	C-N-CA	6.83	130.35	120.38
1	5	10	ILE	CA-C-O	-6.82	113.48	121.05
3	E	454	GLU	CA-C-N	6.82	133.11	122.26
3	E	454	GLU	C-N-CA	6.82	133.11	122.26
2	C	427	THR	CA-C-O	6.82	127.78	120.55
4	G	176	GLU	CA-C-O	-6.81	112.75	119.69
1	9	57	LEU	CA-C-N	6.81	129.29	120.44
1	9	57	LEU	C-N-CA	6.81	129.29	120.44
2	C	490	GLU	CA-C-N	-6.81	113.39	122.99
2	C	490	GLU	C-N-CA	-6.81	113.39	122.99
1	1	46	THR	N-CA-C	6.81	118.49	111.14
12	X	6	LEU	CA-C-N	6.80	129.28	120.44
12	X	6	LEU	C-N-CA	6.80	129.28	120.44
7	O	121	GLY	N-CA-C	-6.79	101.00	111.12
11	W	6	PRO	N-CA-C	6.79	118.98	110.70
2	A	280	TYR	CA-C-N	6.78	129.26	120.44
2	A	280	TYR	C-N-CA	6.78	129.26	120.44
3	E	174	ILE	CA-C-N	6.77	129.36	120.28
3	E	174	ILE	C-N-CA	6.77	129.36	120.28
1	9	34	ILE	O-C-N	-6.77	115.30	121.87
4	G	99	LEU	N-CA-C	-6.77	104.76	113.16
10	V	148	LYS	N-CA-C	6.77	118.66	111.28
2	C	492	SER	N-CA-C	-6.77	100.19	110.14
9	U	187	PRO	CA-C-N	6.77	130.03	120.28
9	U	187	PRO	C-N-CA	6.77	130.03	120.28
4	G	9	ARG	O-C-N	-6.76	114.44	122.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	T	183	ALA	CA-C-N	6.76	127.44	119.94
8	T	183	ALA	C-N-CA	6.76	127.44	119.94
9	U	151	LYS	CA-C-N	6.76	129.64	120.44
9	U	151	LYS	C-N-CA	6.76	129.64	120.44
1	1	34	ILE	CA-C-N	6.76	129.23	120.44
1	1	34	ILE	C-N-CA	6.76	129.23	120.44
1	5	21	GLY	CA-C-O	6.76	127.74	120.30
3	E	167	ILE	O-C-N	-6.76	115.32	121.87
13	Y	16	PHE	CA-C-N	6.75	130.58	120.31
13	Y	16	PHE	C-N-CA	6.75	130.58	120.31
1	5	53	LEU	CA-C-N	6.75	127.47	119.98
1	5	53	LEU	C-N-CA	6.75	127.47	119.98
1	3	48	PHE	CA-C-O	-6.74	110.92	120.16
3	F	357	LEU	N-CA-C	-6.74	104.27	113.30
3	D	81	GLY	CA-C-O	-6.74	111.89	121.52
3	E	297	THR	O-C-N	-6.73	116.56	123.29
2	C	301	PHE	CA-C-O	-6.73	113.28	120.42
7	O	105	ALA	CA-C-N	6.73	129.30	120.28
7	O	105	ALA	C-N-CA	6.73	129.30	120.28
1	3	10	ILE	CA-C-N	6.73	127.45	119.98
1	3	10	ILE	C-N-CA	6.73	127.45	119.98
2	C	150	THR	N-CA-C	-6.73	105.36	113.97
3	F	106	ARG	N-CA-C	-6.73	105.84	112.97
4	G	229	GLU	N-CA-C	6.72	118.26	111.07
3	E	216	ALA	O-C-N	-6.72	114.69	123.16
1	1	74	PHE	N-CA-C	-6.72	103.20	111.40
2	B	371	LEU	O-C-N	-6.71	114.00	122.26
1	1	71	LEU	CA-C-O	6.71	127.66	120.55
3	D	365	GLN	N-CA-C	6.70	118.59	111.28
12	X	25	GLU	CA-C-N	6.70	127.42	119.98
12	X	25	GLU	C-N-CA	6.70	127.42	119.98
2	C	154	ALA	O-C-N	6.70	129.22	122.12
6	I	41	ASP	N-CA-C	6.70	119.20	110.43
1	9	62	GLY	CA-C-N	6.69	129.25	120.28
1	9	62	GLY	C-N-CA	6.69	129.25	120.28
4	G	84	CYS	N-CA-C	-6.69	94.53	107.44
2	C	72	GLN	CA-C-N	6.69	131.00	122.37
2	C	72	GLN	C-N-CA	6.69	131.00	122.37
9	U	90	ASP	CA-C-N	6.69	129.12	120.56
9	U	90	ASP	C-N-CA	6.69	129.12	120.56
7	O	72	ASP	CA-C-O	-6.69	113.46	120.55
7	O	70	VAL	CA-C-N	6.69	128.98	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	70	VAL	C-N-CA	6.69	128.98	120.56
8	T	91	THR	N-CA-C	-6.69	105.09	113.18
3	F	265	GLY	CA-C-N	6.68	129.24	120.28
3	F	265	GLY	C-N-CA	6.68	129.24	120.28
8	T	38	LEU	CA-C-N	6.68	128.98	120.56
8	T	38	LEU	C-N-CA	6.68	128.98	120.56
10	V	100	MET	CA-C-O	-6.68	113.82	120.70
12	X	43	GLU	CA-C-O	6.68	127.73	120.32
1	4	44	LYS	CA-C-N	6.67	129.76	120.29
1	4	44	LYS	C-N-CA	6.67	129.76	120.29
9	U	139	GLU	CA-C-N	6.67	129.54	120.54
9	U	139	GLU	C-N-CA	6.67	129.54	120.54
12	X	8	LEU	CA-C-N	6.66	129.10	120.44
12	X	8	LEU	C-N-CA	6.66	129.10	120.44
3	D	320	PRO	CA-C-N	6.66	128.04	119.78
3	D	320	PRO	C-N-CA	6.66	128.04	119.78
2	B	441	GLU	CA-C-N	6.66	130.43	120.31
2	B	441	GLU	C-N-CA	6.66	130.43	120.31
3	D	440	SER	O-C-N	6.66	129.74	122.15
8	T	224	PHE	O-C-N	6.66	129.28	122.09
12	X	50	LEU	CA-C-N	6.65	129.19	120.28
12	X	50	LEU	C-N-CA	6.65	129.19	120.28
4	G	80	ASP	CA-C-N	6.65	130.31	120.87
4	G	80	ASP	C-N-CA	6.65	130.31	120.87
1	1	17	ILE	CA-C-N	6.65	128.45	120.14
1	1	17	ILE	C-N-CA	6.65	128.45	120.14
8	T	133	GLY	O-C-N	6.64	128.63	122.19
1	1	17	ILE	N-CA-C	6.64	119.35	111.05
3	F	225	PRO	CA-C-N	6.64	125.87	118.97
3	F	225	PRO	C-N-CA	6.64	125.87	118.97
2	A	121	GLY	O-C-N	6.64	128.41	121.77
3	D	327	ALA	CA-C-O	6.64	127.54	120.70
4	G	36	LYS	CA-C-N	6.63	129.06	120.44
4	G	36	LYS	C-N-CA	6.63	129.06	120.44
2	A	362	GLY	O-C-N	6.63	129.30	122.54
3	F	125	ALA	N-CA-C	-6.63	105.23	113.38
1	9	53	LEU	CA-C-N	6.62	127.33	119.98
1	9	53	LEU	C-N-CA	6.62	127.33	119.98
9	U	66	THR	CA-C-N	6.62	127.33	119.98
9	U	66	THR	C-N-CA	6.62	127.33	119.98
1	1	6	ALA	O-C-N	-6.62	114.60	122.15
3	D	28	SER	CA-C-N	6.62	134.19	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	28	SER	C-N-CA	6.62	134.19	121.54
2	B	148	VAL	N-CA-C	-6.61	98.85	108.11
1	4	48	PHE	CA-C-O	-6.61	112.25	118.73
1	7	13	GLY	CA-C-N	6.61	129.52	120.46
1	7	13	GLY	C-N-CA	6.61	129.52	120.46
2	C	465	GLU	CA-C-N	6.61	129.14	120.28
2	C	465	GLU	C-N-CA	6.61	129.14	120.28
3	F	78	ASP	CA-C-N	6.61	129.13	120.28
3	F	78	ASP	C-N-CA	6.61	129.13	120.28
2	A	393	LYS	N-CA-C	-6.60	104.00	111.07
8	T	113	ALA	CA-C-N	6.60	131.82	121.99
8	T	113	ALA	C-N-CA	6.60	131.82	121.99
13	Y	36	ASN	N-CA-C	-6.60	104.36	112.88
3	D	451	ASN	CA-C-N	6.58	127.08	122.60
3	D	451	ASN	C-N-CA	6.58	127.08	122.60
3	D	166	PHE	CA-C-O	-6.58	113.92	120.70
3	D	289	MET	CA-C-N	6.57	127.28	119.98
3	D	289	MET	C-N-CA	6.57	127.28	119.98
5	H	87	ALA	O-C-N	-6.57	115.54	123.10
11	W	78	TYR	CA-C-O	-6.57	113.58	120.55
2	B	9	GLU	CA-C-O	6.56	127.52	119.97
10	V	99	ALA	O-C-N	6.56	129.07	122.12
2	B	110	VAL	N-CA-C	-6.56	98.02	108.90
3	D	118	HIS	O-C-N	6.55	130.85	123.19
2	C	267	LEU	O-C-N	-6.54	115.75	123.41
3	D	104	ASP	N-CA-C	-6.54	105.03	114.12
2	C	425	ARG	CA-C-N	6.54	129.33	120.44
2	C	425	ARG	C-N-CA	6.54	129.33	120.44
3	F	235	THR	N-CA-C	-6.54	104.15	111.28
9	U	91	VAL	CA-C-N	6.54	128.94	120.44
9	U	91	VAL	C-N-CA	6.54	128.94	120.44
4	G	47	ALA	CA-C-N	6.54	129.57	120.29
4	G	47	ALA	C-N-CA	6.54	129.57	120.29
4	G	219	LEU	CA-C-N	6.53	129.03	120.28
4	G	219	LEU	C-N-CA	6.53	129.03	120.28
1	3	12	ALA	CA-C-N	6.53	127.23	119.98
1	3	12	ALA	C-N-CA	6.53	127.23	119.98
4	G	101	ASP	N-CA-C	-6.53	105.47	113.50
1	3	18	GLY	CA-C-O	-6.53	113.79	120.45
3	E	207	ILE	N-CA-C	-6.53	98.06	107.78
3	F	46	LEU	N-CA-C	-6.53	97.73	108.76
1	9	20	LEU	CA-C-N	6.53	127.18	120.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9	20	LEU	C-N-CA	6.53	127.18	120.00
1	3	55	PHE	CA-C-N	6.52	129.02	120.28
1	3	55	PHE	C-N-CA	6.52	129.02	120.28
2	C	206	VAL	O-C-N	6.52	130.31	123.26
3	D	237	LEU	N-CA-C	6.52	118.39	111.28
6	I	55	GLU	CA-C-N	6.52	126.87	119.83
6	I	55	GLU	C-N-CA	6.52	126.87	119.83
3	E	177	ALA	N-CA-C	6.52	118.18	111.14
2	C	46	LEU	O-C-N	6.52	130.40	122.58
3	D	269	SER	CA-C-N	6.52	129.55	120.29
3	D	269	SER	C-N-CA	6.52	129.55	120.29
2	C	443	GLN	CA-C-N	6.51	124.34	120.24
2	C	443	GLN	C-N-CA	6.51	124.34	120.24
6	I	15	ASN	CA-C-N	6.51	129.38	120.46
6	I	15	ASN	C-N-CA	6.51	129.38	120.46
1	5	3	LEU	N-CA-C	6.51	118.46	111.36
2	B	346	SER	O-C-N	6.51	130.28	122.27
3	F	423	VAL	O-C-N	6.51	128.29	121.91
2	A	128	ARG	N-CA-C	-6.51	97.76	108.76
1	2	44	LYS	CA-C-N	6.50	129.52	120.29
1	2	44	LYS	C-N-CA	6.50	129.52	120.29
2	A	456	ASP	CA-C-N	6.50	128.26	120.14
2	A	456	ASP	C-N-CA	6.50	128.26	120.14
4	G	144	ALA	CA-C-N	6.50	129.52	120.29
4	G	144	ALA	C-N-CA	6.50	129.52	120.29
4	G	259	ARG	CA-C-N	6.50	128.99	120.28
4	G	259	ARG	C-N-CA	6.50	128.99	120.28
2	A	105	LEU	CA-C-O	6.49	126.94	119.35
2	B	463	ILE	CA-C-N	6.49	127.18	119.98
2	B	463	ILE	C-N-CA	6.49	127.18	119.98
1	6	54	GLY	CA-C-N	6.49	128.87	120.44
1	6	54	GLY	C-N-CA	6.49	128.87	120.44
1	3	17	ILE	CA-C-N	6.49	128.30	120.13
1	3	17	ILE	C-N-CA	6.49	128.30	120.13
7	O	179	SER	CA-C-N	6.48	130.34	122.63
7	O	179	SER	C-N-CA	6.48	130.34	122.63
2	A	447	ILE	O-C-N	6.48	129.12	121.80
2	A	277	ALA	O-C-N	6.47	129.53	122.15
2	C	258	TRP	O-C-N	6.47	129.53	122.15
4	G	82	GLY	N-CA-C	-6.47	102.70	112.41
2	B	128	ARG	N-CA-C	-6.47	99.49	109.52
2	B	481	LEU	CA-C-N	6.47	130.14	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	481	LEU	C-N-CA	6.47	130.14	120.31
4	G	128	LEU	N-CA-C	-6.47	99.20	109.23
9	U	90	ASP	N-CA-C	-6.47	104.31	111.36
2	C	169	ILE	N-CA-C	-6.47	98.55	107.99
3	E	86	PRO	O-C-N	-6.47	115.11	123.06
3	E	55	GLY	N-CA-C	-6.46	104.53	112.68
3	E	351	LEU	O-C-N	-6.46	114.58	122.34
1	0	32	ALA	N-CA-C	6.46	118.32	111.28
3	D	242	TYR	CA-C-N	6.46	129.23	120.44
3	D	242	TYR	C-N-CA	6.46	129.23	120.44
4	G	10	LEU	O-C-N	-6.46	115.27	122.12
2	B	310	ARG	N-CA-C	-6.46	105.22	113.23
5	H	93	LEU	CA-C-N	6.46	130.12	120.31
5	H	93	LEU	C-N-CA	6.46	130.12	120.31
2	B	162	GLY	N-CA-C	-6.45	101.35	110.96
2	A	36	VAL	CA-C-N	6.45	129.25	121.38
2	A	36	VAL	C-N-CA	6.45	129.25	121.38
3	E	155	LEU	CA-C-O	-6.45	113.70	121.05
2	C	307	LEU	CA-C-N	6.45	130.11	120.31
2	C	307	LEU	C-N-CA	6.45	130.11	120.31
1	1	72	LEU	CA-C-O	6.44	127.33	120.70
2	A	182	LEU	CA-C-N	6.43	128.90	120.28
2	A	182	LEU	C-N-CA	6.43	128.90	120.28
2	C	328	VAL	CA-C-N	6.43	131.65	123.10
2	C	328	VAL	C-N-CA	6.43	131.65	123.10
2	A	148	VAL	N-CA-C	-6.43	98.79	108.17
2	A	469	SER	CA-C-N	6.43	128.89	120.28
2	A	469	SER	C-N-CA	6.43	128.89	120.28
1	0	14	ILE	CA-C-N	6.42	128.89	120.28
1	0	14	ILE	C-N-CA	6.42	128.89	120.28
2	C	216	ALA	N-CA-C	6.42	118.36	111.36
3	D	369	ASP	N-CA-C	-6.42	104.36	111.36
1	4	54	GLY	CA-C-N	6.42	129.20	120.54
1	4	54	GLY	C-N-CA	6.42	129.20	120.54
2	A	274	SER	CA-C-N	6.42	130.06	120.31
2	A	274	SER	C-N-CA	6.42	130.06	120.31
1	6	26	ILE	CA-C-N	6.41	129.40	120.29
1	6	26	ILE	C-N-CA	6.41	129.40	120.29
8	T	35	ILE	CA-C-O	-6.41	114.05	120.85
8	T	64	ALA	CA-C-N	6.41	129.25	120.46
8	T	64	ALA	C-N-CA	6.41	129.25	120.46
2	C	180	VAL	O-C-N	6.41	128.09	121.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	58	SER	CA-C-N	6.41	128.87	120.28
1	1	58	SER	C-N-CA	6.41	128.87	120.28
8	T	57	ARG	N-CA-C	-6.41	104.94	112.89
1	1	41	PRO	N-CA-C	6.41	125.66	112.47
2	A	381	GLN	CA-C-O	-6.41	113.97	121.46
3	F	145	ALA	CA-C-O	-6.41	114.76	121.29
3	D	468	ALA	N-CA-C	6.40	118.26	111.28
4	G	22	THR	N-CA-C	-6.40	104.22	111.07
3	E	169	GLU	CA-C-N	6.40	128.86	120.28
3	E	169	GLU	C-N-CA	6.40	128.86	120.28
10	V	89	LEU	CA-C-N	6.40	133.55	122.09
10	V	89	LEU	C-N-CA	6.40	133.55	122.09
12	X	20	THR	O-C-N	6.40	130.08	122.79
1	0	24	ILE	CA-C-O	6.39	127.60	120.95
2	C	263	GLY	O-C-N	-6.39	114.39	122.70
1	0	58	SER	CA-C-N	6.39	128.84	120.28
1	0	58	SER	C-N-CA	6.39	128.84	120.28
1	7	1	MET	CA-C-N	6.39	129.16	120.54
1	7	1	MET	C-N-CA	6.39	129.16	120.54
1	7	25	GLY	CA-C-N	6.39	128.84	120.60
1	7	25	GLY	C-N-CA	6.39	128.84	120.60
2	C	185	ILE	CA-C-N	6.39	129.36	120.29
2	C	185	ILE	C-N-CA	6.39	129.36	120.29
4	G	106	ASP	CA-C-O	6.39	127.19	120.36
3	F	411	GLN	CA-C-O	6.38	127.18	120.42
1	3	20	LEU	N-CA-C	6.38	119.05	111.33
4	G	12	SER	CA-C-N	6.38	129.19	120.46
4	G	12	SER	C-N-CA	6.38	129.19	120.46
1	2	20	LEU	CA-C-N	6.37	127.05	119.98
1	2	20	LEU	C-N-CA	6.37	127.05	119.98
6	I	10	TYR	CA-C-N	6.37	132.29	121.14
6	I	10	TYR	C-N-CA	6.37	132.29	121.14
1	7	29	VAL	N-CA-C	6.37	116.54	110.42
3	E	388	ILE	O-C-N	6.37	128.39	121.83
2	C	315	SER	N-CA-C	-6.36	99.92	110.17
2	B	96	ILE	N-CA-C	-6.36	103.11	110.05
4	G	21	LYS	CA-C-N	6.36	128.71	120.44
4	G	21	LYS	C-N-CA	6.36	128.71	120.44
2	B	97	VAL	CA-C-N	6.36	132.57	122.59
2	B	97	VAL	C-N-CA	6.36	132.57	122.59
1	3	26	ILE	CA-C-N	6.35	128.79	120.28
1	3	26	ILE	C-N-CA	6.35	128.79	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	2	GLN	CA-C-N	6.35	129.31	120.29
1	6	2	GLN	C-N-CA	6.35	129.31	120.29
1	0	74	PHE	N-CA-C	-6.35	103.66	112.30
1	9	10	ILE	CA-C-N	6.35	127.03	119.98
1	9	10	ILE	C-N-CA	6.35	127.03	119.98
3	E	42	PRO	N-CA-C	-6.35	105.70	114.27
2	B	367	ILE	CA-C-N	6.35	129.77	120.82
2	B	367	ILE	C-N-CA	6.35	129.77	120.82
1	9	63	LEU	N-CA-C	-6.34	104.37	111.28
2	A	58	SER	N-CA-C	-6.34	103.89	112.26
6	I	47	TYR	N-CA-C	-6.34	99.99	108.74
3	E	235	THR	CA-C-N	6.33	127.01	119.98
3	E	235	THR	C-N-CA	6.33	127.01	119.98
9	U	152	ALA	CA-C-O	-6.33	114.18	120.70
7	O	186	LYS	CA-C-N	6.32	128.66	120.44
7	O	186	LYS	C-N-CA	6.32	128.66	120.44
2	C	197	GLU	N-CA-C	-6.32	104.26	112.23
2	B	115	ASN	CA-C-O	-6.32	112.78	120.05
2	B	245	GLN	CA-C-N	6.32	128.75	120.28
2	B	245	GLN	C-N-CA	6.32	128.75	120.28
2	B	306	ARG	CA-C-N	6.32	128.65	120.44
2	B	306	ARG	C-N-CA	6.32	128.65	120.44
1	2	48	PHE	O-C-N	-6.31	114.78	120.71
3	D	146	PRO	CA-C-O	-6.31	113.74	121.31
5	H	78	GLN	CA-C-N	6.31	125.88	119.19
5	H	78	GLN	C-N-CA	6.31	125.88	119.19
8	T	205	THR	N-CA-C	-6.31	105.41	113.23
8	T	66	TYR	O-C-N	6.31	129.34	122.15
8	T	242	LEU	CA-C-O	6.31	127.23	119.79
2	B	289	ARG	N-CA-C	-6.30	101.61	110.31
1	5	47	VAL	CA-C-N	6.29	128.69	120.26
1	5	47	VAL	C-N-CA	6.29	128.69	120.26
3	F	82	PRO	N-CA-C	6.29	121.09	111.34
3	F	341	GLU	N-CA-C	6.29	118.22	111.36
3	F	410	ILE	N-CA-C	-6.29	104.37	110.72
8	T	33	THR	CA-C-O	-6.29	113.75	120.42
3	F	35	ASN	N-CA-C	-6.29	101.67	110.35
2	C	428	GLN	N-CA-C	6.29	119.11	111.82
7	O	12	LEU	O-C-N	6.29	130.62	123.27
3	F	444	VAL	CA-C-N	6.28	129.33	120.28
3	F	444	VAL	C-N-CA	6.28	129.33	120.28
11	W	41	ALA	N-CA-C	-6.28	97.42	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	108	VAL	N-CA-C	-6.28	98.69	107.80
4	G	269	ASP	CA-C-N	6.28	128.47	120.56
4	G	269	ASP	C-N-CA	6.28	128.47	120.56
2	B	121	GLY	O-C-N	-6.28	115.49	121.77
3	E	172	ASN	N-CA-C	-6.28	104.35	111.07
2	B	189	LYS	CA-C-N	6.27	129.20	120.29
2	B	189	LYS	C-N-CA	6.27	129.20	120.29
1	2	67	MET	CA-C-O	-6.27	113.77	120.42
2	A	137	GLY	CA-C-N	6.27	128.59	120.56
2	A	137	GLY	C-N-CA	6.27	128.59	120.56
2	C	333	GLY	CA-C-N	6.27	132.09	120.87
2	C	333	GLY	C-N-CA	6.27	132.09	120.87
10	V	31	SER	CA-C-N	6.27	129.00	120.54
10	V	31	SER	C-N-CA	6.27	129.00	120.54
1	3	2	GLN	CA-C-N	6.27	129.31	120.28
1	3	2	GLN	C-N-CA	6.27	129.31	120.28
8	T	82	TRP	CA-C-O	6.27	127.19	120.55
2	C	355	GLU	CA-C-N	6.26	128.68	120.28
2	C	355	GLU	C-N-CA	6.26	128.68	120.28
2	A	180	VAL	CA-C-N	6.26	129.18	120.29
2	A	180	VAL	C-N-CA	6.26	129.18	120.29
3	E	321	ALA	CA-C-O	-6.26	112.59	118.73
1	1	3	LEU	N-CA-C	6.26	117.90	111.14
7	O	145	LYS	N-CA-C	-6.26	104.95	112.59
1	1	8	LYS	O-C-N	6.25	128.59	122.09
3	F	279	VAL	CA-C-N	6.25	130.64	122.26
3	F	279	VAL	C-N-CA	6.25	130.64	122.26
10	V	120	THR	O-C-N	6.25	128.75	122.12
2	C	419	THR	CA-C-O	6.25	127.14	120.70
3	F	451	ASN	N-CA-C	-6.25	104.96	112.59
2	A	31	GLY	O-C-N	-6.25	118.16	123.60
3	D	68	GLU	O-C-N	-6.24	115.03	123.15
2	C	18	ILE	O-C-N	6.24	128.26	121.83
2	C	126	ALA	O-C-N	-6.23	114.94	122.48
3	F	352	ASP	N-CA-C	-6.23	98.21	108.49
2	A	126	ALA	N-CA-C	-6.23	104.94	114.16
8	T	65	ILE	O-C-N	-6.22	115.83	121.87
8	T	122	SER	CA-C-N	6.22	129.26	120.42
8	T	122	SER	C-N-CA	6.22	129.26	120.42
11	W	60	ASN	O-C-N	6.22	130.59	123.31
3	E	418	PHE	CA-C-N	6.22	128.62	120.28
3	E	418	PHE	C-N-CA	6.22	128.62	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9	61	THR	N-CA-C	-6.21	104.56	111.71
3	D	414	LEU	N-CA-C	-6.21	105.18	112.89
3	F	124	PHE	N-CA-C	-6.21	105.73	113.38
2	B	141	ARG	O-C-N	6.21	130.85	122.59
1	4	33	LEU	CA-C-N	6.21	128.97	120.46
1	4	33	LEU	C-N-CA	6.21	128.97	120.46
2	B	283	LEU	CA-C-N	6.21	129.10	120.29
2	B	283	LEU	C-N-CA	6.21	129.10	120.29
2	A	78	PHE	N-CA-C	-6.20	105.35	113.17
7	O	98	LEU	CA-C-N	6.20	128.16	120.34
7	O	98	LEU	C-N-CA	6.20	128.16	120.34
2	A	324	THR	N-CA-C	-6.20	99.54	109.96
1	5	4	VAL	CA-C-N	6.20	129.09	120.29
1	5	4	VAL	C-N-CA	6.20	129.09	120.29
1	2	52	ILE	CA-C-N	6.19	128.49	120.44
1	2	52	ILE	C-N-CA	6.19	128.49	120.44
1	8	71	LEU	CA-C-N	6.19	129.72	120.31
1	8	71	LEU	C-N-CA	6.19	129.72	120.31
1	9	73	LEU	CA-C-O	-6.19	114.33	120.70
2	B	255	ILE	CA-C-N	6.19	126.85	119.98
2	B	255	ILE	C-N-CA	6.19	126.85	119.98
2	B	138	ILE	CA-C-N	6.18	127.82	120.09
2	B	138	ILE	C-N-CA	6.18	127.82	120.09
3	E	347	ALA	CA-C-N	6.18	129.78	120.75
3	E	347	ALA	C-N-CA	6.18	129.78	120.75
3	F	274	ARG	N-CA-C	-6.18	99.64	109.23
8	T	102	ILE	N-CA-C	-6.18	106.97	112.90
9	U	109	SER	CA-C-N	6.18	128.93	120.46
9	U	109	SER	C-N-CA	6.18	128.93	120.46
1	6	3	LEU	O-C-N	-6.18	115.11	122.15
2	B	413	ASP	N-CA-C	-6.17	101.64	110.59
2	A	219	VAL	O-C-N	6.17	127.96	121.91
9	U	105	ASP	CA-C-N	6.17	128.54	120.28
9	U	105	ASP	C-N-CA	6.17	128.54	120.28
14	Z	41	SER	CA-C-N	6.17	128.55	120.28
14	Z	41	SER	C-N-CA	6.17	128.55	120.28
14	Z	3	GLN	N-CA-C	-6.17	104.36	113.61
1	8	65	CYS	CA-C-N	6.16	128.53	120.28
1	8	65	CYS	C-N-CA	6.16	128.53	120.28
2	C	238	ALA	N-CA-C	-6.16	105.72	113.18
3	E	91	THR	N-CA-C	-6.16	105.05	113.30
2	B	135	ALA	CA-C-O	-6.16	113.99	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	261	PHE	CA-C-O	-6.15	114.36	120.82
2	B	321	GLY	CA-C-O	-6.15	114.24	122.24
1	7	56	ALA	CA-C-N	6.15	128.52	120.28
1	7	56	ALA	C-N-CA	6.15	128.52	120.28
2	C	289	ARG	CA-C-N	6.15	126.71	120.38
2	C	289	ARG	C-N-CA	6.15	126.71	120.38
8	T	216	ILE	CA-C-N	6.15	128.43	120.44
8	T	216	ILE	C-N-CA	6.15	128.43	120.44
3	F	179	GLY	O-C-N	6.15	130.69	122.70
2	B	43	VAL	CA-C-O	-6.14	114.50	121.75
11	W	54	LYS	N-CA-C	6.14	120.85	113.23
5	H	87	ALA	N-CA-C	-6.14	99.81	108.96
12	X	20	THR	CA-C-N	6.14	128.50	120.28
12	X	20	THR	C-N-CA	6.14	128.50	120.28
1	0	18	GLY	CA-C-O	-6.14	114.43	120.75
1	3	53	LEU	N-CA-C	-6.14	104.59	111.28
3	E	290	GLY	CA-C-N	6.14	128.42	120.44
3	E	290	GLY	C-N-CA	6.14	128.42	120.44
2	A	356	ALA	CA-C-N	6.13	128.41	120.44
2	A	356	ALA	C-N-CA	6.13	128.41	120.44
1	7	53	LEU	O-C-N	-6.13	115.63	122.12
2	C	26	ASN	N-CA-C	-6.12	105.85	113.38
2	C	467	GLU	O-C-N	6.12	128.61	122.12
3	D	460	VAL	CA-C-N	6.12	130.59	122.75
3	D	460	VAL	C-N-CA	6.12	130.59	122.75
3	E	129	THR	N-CA-C	-6.12	104.43	113.61
4	G	4	LYS	CA-C-O	6.12	127.01	119.97
2	A	403	ALA	O-C-N	6.12	128.61	122.12
4	G	263	ILE	O-C-N	6.12	127.80	121.87
1	7	7	ALA	N-CA-C	6.11	117.94	111.28
2	A	241	ALA	N-CA-C	6.11	118.66	110.35
3	D	98	VAL	O-C-N	-6.11	114.04	122.05
3	F	317	LEU	N-CA-C	-6.11	105.47	113.17
10	V	28	GLN	O-C-N	6.11	129.79	122.27
3	F	252	LEU	N-CA-C	-6.11	99.68	108.60
12	X	50	LEU	CA-C-O	6.11	127.23	120.82
1	8	1	MET	CA-C-N	6.11	128.38	120.44
1	8	1	MET	C-N-CA	6.11	128.38	120.44
8	T	189	VAL	CA-C-N	6.10	129.09	120.42
8	T	189	VAL	C-N-CA	6.10	129.09	120.42
1	8	62	GLY	CA-C-N	6.10	128.46	120.28
1	8	62	GLY	C-N-CA	6.10	128.46	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	387	ILE	CA-C-N	6.10	129.08	120.42
3	E	387	ILE	C-N-CA	6.10	129.08	120.42
1	3	61	THR	CA-C-N	6.10	126.71	120.00
1	3	61	THR	C-N-CA	6.10	126.71	120.00
2	A	59	SER	N-CA-C	-6.10	104.46	113.61
3	E	21	VAL	O-C-N	-6.10	116.67	123.26
3	E	140	VAL	N-CA-C	6.10	116.28	110.42
14	Z	13	LEU	CA-C-O	6.10	126.99	119.79
2	A	26	ASN	N-CA-C	-6.10	97.81	110.80
2	A	295	ALA	CA-C-O	-6.10	114.03	121.28
2	B	234	VAL	O-C-N	6.09	129.36	123.14
1	9	9	TYR	CA-C-O	-6.09	114.09	120.55
2	A	392	LEU	CA-C-N	6.08	128.35	120.44
2	A	392	LEU	C-N-CA	6.08	128.35	120.44
3	E	173	ASN	CA-C-O	-6.08	114.10	120.55
3	F	207	ILE	N-CA-C	-6.08	98.36	107.37
4	G	188	ILE	O-C-N	6.08	127.77	121.87
1	0	10	ILE	CA-C-N	6.08	126.73	119.98
1	0	10	ILE	C-N-CA	6.08	126.73	119.98
2	A	232	ILE	N-CA-C	-6.08	99.45	108.45
1	0	16	THR	N-CA-C	6.08	118.70	111.71
1	0	22	ALA	CA-C-N	6.07	126.68	119.94
1	0	22	ALA	C-N-CA	6.07	126.68	119.94
3	D	243	PHE	CA-C-N	6.07	128.33	120.44
3	D	243	PHE	C-N-CA	6.07	128.33	120.44
3	E	237	LEU	N-CA-C	-6.07	104.66	111.28
2	A	444	VAL	O-C-N	-6.07	115.76	120.07
4	G	87	ILE	CA-C-N	6.07	128.41	120.28
4	G	87	ILE	C-N-CA	6.07	128.41	120.28
1	6	20	LEU	CA-C-O	-6.06	114.12	120.55
2	B	393	LYS	O-C-N	-6.06	115.69	122.12
1	5	26	ILE	N-CA-C	6.06	116.24	110.42
3	F	300	LYS	N-CA-C	-6.06	104.59	112.23
1	8	73	LEU	N-CA-C	-6.06	104.60	111.14
3	D	56	GLU	CA-C-N	6.06	133.11	121.54
3	D	56	GLU	C-N-CA	6.06	133.11	121.54
3	F	438	VAL	CA-C-N	6.06	128.32	120.44
3	F	438	VAL	C-N-CA	6.06	128.32	120.44
1	4	8	LYS	CA-C-N	6.06	128.68	120.44
1	4	8	LYS	C-N-CA	6.06	128.68	120.44
2	A	376	VAL	CA-C-O	6.06	124.19	119.46
1	8	22	ALA	CA-C-O	-6.06	114.00	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	13	GLY	CA-C-N	6.05	128.75	120.46
1	2	13	GLY	C-N-CA	6.05	128.75	120.46
2	C	476	SER	N-CA-C	6.05	117.67	111.14
3	D	111	SER	N-CA-C	-6.05	105.56	113.12
3	E	171	ILE	CA-C-N	6.05	128.30	120.44
3	E	171	ILE	C-N-CA	6.05	128.30	120.44
3	F	384	LEU	N-CA-C	6.05	120.28	113.02
3	F	19	ALA	N-CA-C	-6.05	103.10	111.81
1	2	10	ILE	CA-C-N	6.04	126.69	119.98
1	2	10	ILE	C-N-CA	6.04	126.69	119.98
1	0	47	VAL	O-C-N	-6.04	115.61	121.83
9	U	110	VAL	CA-C-N	6.04	128.38	120.28
9	U	110	VAL	C-N-CA	6.04	128.38	120.28
5	H	82	GLN	N-CA-C	-6.04	98.43	108.34
1	6	23	GLY	CA-C-N	6.04	128.73	120.46
1	6	23	GLY	C-N-CA	6.04	128.73	120.46
5	H	47	PRO	N-CA-C	-6.04	100.03	112.47
8	T	115	LEU	CA-C-O	6.04	126.91	119.79
1	3	40	ASN	CA-C-N	-6.03	112.30	119.84
1	3	40	ASN	C-N-CA	-6.03	112.30	119.84
2	A	189	LYS	N-CA-C	-6.03	104.70	111.28
2	A	296	TYR	CA-C-N	6.03	126.00	120.03
2	A	296	TYR	C-N-CA	6.03	126.00	120.03
3	D	136	THR	N-CA-C	-6.03	105.88	113.72
7	O	104	ILE	CA-C-N	6.03	128.64	120.44
7	O	104	ILE	C-N-CA	6.03	128.64	120.44
3	D	427	ILE	O-C-N	-6.03	115.98	121.41
3	F	144	LEU	N-CA-C	-6.03	106.06	113.41
2	C	493	LYS	N-CA-C	6.03	117.52	111.07
4	G	39	ILE	CA-C-N	6.02	128.84	120.29
4	G	39	ILE	C-N-CA	6.02	128.84	120.29
4	G	243	ASN	N-CA-C	6.02	117.85	111.28
10	V	95	PHE	CA-C-N	6.02	128.35	120.28
10	V	95	PHE	C-N-CA	6.02	128.35	120.28
1	1	28	ILE	CA-C-N	6.02	128.15	120.56
1	1	28	ILE	C-N-CA	6.02	128.15	120.56
1	4	57	LEU	N-CA-C	6.02	117.92	111.36
2	C	219	VAL	CA-C-O	-6.02	114.47	120.85
3	F	113	LEU	N-CA-C	-6.02	99.59	109.40
1	4	2	GLN	CA-C-N	6.01	128.34	120.28
1	4	2	GLN	C-N-CA	6.01	128.34	120.28
3	F	288	ASP	CA-C-O	-6.01	114.51	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	249	ASN	N-CA-C	6.01	117.91	111.36
1	0	54	GLY	O-C-N	6.01	127.96	122.19
1	3	9	TYR	CA-C-N	6.01	128.25	120.56
1	3	9	TYR	C-N-CA	6.01	128.25	120.56
3	F	314	ALA	CA-C-N	6.01	130.89	122.36
3	F	314	ALA	C-N-CA	6.01	130.89	122.36
2	A	148	VAL	CA-C-O	6.00	126.97	120.43
3	E	132	GLU	CA-C-N	6.00	128.54	120.50
3	E	132	GLU	C-N-CA	6.00	128.54	120.50
3	E	345	TYR	CA-C-O	-6.00	114.91	119.59
2	C	440	THR	CA-C-N	6.00	128.92	120.28
2	C	440	THR	C-N-CA	6.00	128.92	120.28
3	E	347	ALA	N-CA-C	-6.00	104.61	113.61
1	4	53	LEU	O-C-N	-6.00	115.89	122.07
3	D	214	LYS	N-CA-C	-6.00	103.42	111.87
12	X	35	GLN	N-CA-C	-6.00	105.83	113.02
10	V	135	VAL	CA-C-N	5.99	128.31	120.28
10	V	135	VAL	C-N-CA	5.99	128.31	120.28
3	E	43	GLN	N-CA-C	-5.99	105.94	113.18
2	B	66	LEU	N-CA-C	-5.99	105.06	112.72
3	E	311	TYR	N-CA-C	-5.99	100.43	109.95
5	H	31	ASN	O-C-N	5.98	130.31	123.31
8	T	81	ASN	N-CA-C	-5.98	103.74	113.19
3	E	38	GLU	CA-C-N	5.98	130.90	123.12
3	E	38	GLU	C-N-CA	5.98	130.90	123.12
2	C	423	GLY	CA-C-N	5.97	128.28	120.28
2	C	423	GLY	C-N-CA	5.97	128.28	120.28
2	C	301	PHE	O-C-N	5.97	128.95	122.15
3	E	430	LYS	O-C-N	-5.97	116.99	123.26
1	4	29	VAL	CA-C-N	5.97	128.87	120.28
1	4	29	VAL	C-N-CA	5.97	128.87	120.28
2	A	219	VAL	CA-C-O	-5.96	114.85	121.17
9	U	150	ALA	CA-C-N	5.96	128.76	120.29
9	U	150	ALA	C-N-CA	5.96	128.76	120.29
2	B	156	ASP	O-C-N	5.96	130.47	122.96
1	9	32	ALA	CA-C-N	5.96	128.19	120.44
1	9	32	ALA	C-N-CA	5.96	128.19	120.44
2	B	506	PHE	CA-C-N	5.96	128.62	120.46
2	B	506	PHE	C-N-CA	5.96	128.62	120.46
3	D	262	THR	CA-C-O	5.96	126.86	120.55
3	D	11	GLY	O-C-N	5.95	128.61	123.37
8	T	204	PHE	CA-C-O	-5.95	111.31	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	284	SER	O-C-N	5.95	128.93	122.15
3	F	427	ILE	CA-C-N	5.95	127.27	119.84
3	F	427	ILE	C-N-CA	5.95	127.27	119.84
1	8	63	LEU	N-CA-C	-5.94	104.80	111.28
2	A	220	GLN	N-CA-C	-5.94	104.92	111.82
3	D	165	VAL	O-C-N	5.94	127.73	121.91
3	F	214	LYS	N-CA-C	-5.94	106.07	113.38
1	0	29	VAL	CA-C-N	5.94	128.73	120.29
1	0	29	VAL	C-N-CA	5.94	128.73	120.29
2	A	180	VAL	CA-C-O	-5.94	114.77	120.95
3	F	319	ASP	CA-C-N	5.94	125.81	119.28
3	F	319	ASP	C-N-CA	5.94	125.81	119.28
1	7	23	GLY	CA-C-O	5.94	127.41	121.00
8	T	232	TYR	N-CA-C	-5.94	104.75	112.23
1	9	55	PHE	CA-C-N	5.94	128.16	120.44
1	9	55	PHE	C-N-CA	5.94	128.16	120.44
7	O	147	VAL	CA-C-O	-5.93	114.16	120.39
10	V	100	MET	CA-C-N	5.93	128.15	120.44
10	V	100	MET	C-N-CA	5.93	128.15	120.44
1	0	38	SER	CA-C-O	-5.93	114.27	120.55
1	7	36	GLY	CA-C-N	5.93	128.58	120.46
1	7	36	GLY	C-N-CA	5.93	128.58	120.46
2	C	228	MET	N-CA-C	-5.93	104.66	112.72
4	G	205	VAL	CA-C-O	-5.93	113.81	118.85
12	X	53	TYR	CA-C-N	5.93	128.15	120.44
12	X	53	TYR	C-N-CA	5.93	128.15	120.44
2	B	50	GLN	N-CA-C	-5.93	101.99	110.59
3	D	235	THR	O-C-N	5.93	128.40	122.12
10	V	61	VAL	N-CA-C	-5.93	106.54	112.17
2	C	433	ASN	N-CA-C	-5.93	99.69	108.99
7	O	32	SER	CA-C-N	5.93	129.34	122.35
7	O	32	SER	C-N-CA	5.93	129.34	122.35
3	D	201	MET	N-CA-C	5.92	120.51	113.28
3	E	236	GLY	CA-C-N	5.92	128.22	120.28
3	E	236	GLY	C-N-CA	5.92	128.22	120.28
3	F	239	ILE	N-CA-C	-5.92	104.74	110.72
3	E	367	HIS	N-CA-C	-5.92	104.83	111.28
3	E	377	THR	CA-C-N	5.92	128.69	120.29
3	E	377	THR	C-N-CA	5.92	128.69	120.29
2	C	17	ARG	CA-C-O	-5.91	113.17	119.97
2	C	399	TYR	CA-C-N	5.91	128.21	120.28
2	C	399	TYR	C-N-CA	5.91	128.21	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	51	THR	O-C-N	-5.91	115.24	122.34
3	D	340	SER	CA-C-N	5.91	128.68	120.29
3	D	340	SER	C-N-CA	5.91	128.68	120.29
2	C	126	ALA	N-CA-C	-5.91	106.41	113.97
7	O	20	ALA	O-C-N	5.91	128.88	122.15
2	C	46	LEU	CA-C-N	5.91	130.59	120.72
2	C	46	LEU	C-N-CA	5.91	130.59	120.72
1	3	27	ALA	N-CA-C	5.91	117.72	111.28
2	C	359	PHE	CA-C-N	5.90	128.67	120.29
2	C	359	PHE	C-N-CA	5.90	128.67	120.29
3	F	255	ILE	CA-C-O	5.90	126.86	120.43
2	A	498	SER	CA-C-N	5.90	128.67	120.29
2	A	498	SER	C-N-CA	5.90	128.67	120.29
2	B	60	GLY	CA-C-O	5.90	124.31	118.77
1	4	66	LEU	CA-C-O	-5.90	114.30	120.55
3	E	162	GLY	CA-C-N	5.90	128.46	120.38
3	E	162	GLY	C-N-CA	5.90	128.46	120.38
3	D	464	GLU	CA-C-N	5.89	128.66	120.29
3	D	464	GLU	C-N-CA	5.89	128.66	120.29
4	G	9	ARG	CA-C-O	5.89	126.67	120.42
8	T	223	GLU	CA-C-N	5.89	128.46	120.44
8	T	223	GLU	C-N-CA	5.89	128.46	120.44
9	U	100	VAL	CA-C-N	5.89	128.18	120.28
9	U	100	VAL	C-N-CA	5.89	128.18	120.28
4	G	22	THR	CA-C-N	5.89	128.10	120.44
4	G	22	THR	C-N-CA	5.89	128.10	120.44
3	F	94	ARG	N-CA-C	-5.89	100.55	109.85
7	O	161	PRO	CA-C-N	5.89	128.65	120.29
7	O	161	PRO	C-N-CA	5.89	128.65	120.29
3	D	152	LYS	CA-C-N	5.89	128.39	120.50
3	D	152	LYS	C-N-CA	5.89	128.39	120.50
7	O	180	ILE	CA-C-N	5.89	128.17	120.28
7	O	180	ILE	C-N-CA	5.89	128.17	120.28
1	9	60	ALA	CA-C-N	5.88	128.75	120.28
1	9	60	ALA	C-N-CA	5.88	128.75	120.28
1	3	43	ILE	CA-C-N	5.88	128.75	120.28
1	3	43	ILE	C-N-CA	5.88	128.75	120.28
1	5	46	THR	CA-C-O	5.88	126.77	120.24
2	A	31	GLY	N-CA-C	-5.88	102.55	111.14
3	E	48	LEU	CA-C-O	-5.88	114.35	120.70
2	B	93	THR	N-CA-C	-5.88	104.95	111.36
1	3	41	PRO	N-CA-C	5.88	124.57	112.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	30	PHE	CA-C-N	5.87	128.15	120.28
1	1	30	PHE	C-N-CA	5.87	128.15	120.28
3	F	376	GLU	CA-C-N	5.87	128.07	120.44
3	F	376	GLU	C-N-CA	5.87	128.07	120.44
10	V	130	PHE	N-CA-C	-5.87	105.20	112.72
1	8	40	ASN	O-C-N	5.87	128.07	121.32
8	T	73	THR	CA-C-N	5.86	131.39	121.14
8	T	73	THR	C-N-CA	5.86	131.39	121.14
2	C	206	VAL	N-CA-C	-5.86	99.91	108.11
3	D	415	SER	CA-C-O	5.86	127.63	121.19
1	0	35	ASN	N-CA-C	5.86	117.66	111.28
1	9	44	LYS	CA-C-O	-5.86	114.34	120.55
2	B	60	GLY	O-C-N	-5.86	116.42	122.51
3	D	334	VAL	O-C-N	-5.86	116.73	123.00
8	T	67	ASP	N-CA-C	-5.86	104.85	112.23
7	O	12	LEU	N-CA-C	-5.85	98.74	108.34
2	A	385	LEU	CA-C-N	5.85	128.40	120.44
2	A	385	LEU	C-N-CA	5.85	128.40	120.44
3	D	398	GLU	CA-C-O	-5.85	114.35	120.55
2	C	448	TYR	N-CA-C	-5.85	104.90	111.28
3	D	340	SER	N-CA-C	5.85	117.66	111.28
3	E	224	GLU	CA-C-O	-5.85	114.58	120.96
3	E	392	GLY	N-CA-C	-5.85	104.21	111.70
8	T	167	PHE	N-CA-C	-5.85	105.73	112.92
1	6	35	ASN	O-C-N	5.85	128.09	122.07
3	E	64	MET	N-CA-C	-5.85	106.77	114.31
4	G	102	GLN	O-C-N	-5.84	114.60	121.32
3	F	162	GLY	CA-C-N	5.84	128.10	120.28
3	F	162	GLY	C-N-CA	5.84	128.10	120.28
12	X	39	LEU	O-C-N	5.84	126.17	121.38
1	2	55	PHE	CA-C-N	5.84	128.03	120.44
1	2	55	PHE	C-N-CA	5.84	128.03	120.44
2	C	271	ASP	N-CA-C	-5.84	99.39	108.90
10	V	82	LYS	N-CA-C	-5.84	100.08	108.60
2	C	182	LEU	CA-C-N	5.83	128.10	120.28
2	C	182	LEU	C-N-CA	5.83	128.10	120.28
12	X	33	PRO	CA-C-O	-5.83	112.10	120.56
2	A	209	GLY	O-C-N	5.83	127.88	122.57
3	E	463	ILE	CA-C-N	5.83	128.09	120.28
3	E	463	ILE	C-N-CA	5.83	128.09	120.28
5	H	88	ILE	N-CA-C	-5.83	105.40	111.58
10	V	51	THR	CA-C-N	5.83	132.82	121.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	51	THR	C-N-CA	5.83	132.82	121.63
1	4	24	ILE	CA-C-N	5.83	126.41	119.94
1	4	24	ILE	C-N-CA	5.83	126.41	119.94
3	D	323	ALA	N-CA-C	5.83	117.63	111.28
4	G	244	ALA	N-CA-C	-5.83	105.01	111.36
7	O	184	ILE	O-C-N	-5.83	116.22	121.87
2	A	473	TYR	CA-C-N	5.82	128.56	120.29
2	A	473	TYR	C-N-CA	5.82	128.56	120.29
9	U	108	ASP	CA-C-N	5.82	128.40	120.54
9	U	108	ASP	C-N-CA	5.82	128.40	120.54
10	V	16	ILE	O-C-N	-5.82	114.09	122.12
3	E	341	GLU	CA-C-N	5.82	132.57	122.56
3	E	341	GLU	C-N-CA	5.82	132.57	122.56
2	B	445	PRO	CA-C-N	5.82	128.07	120.28
2	B	445	PRO	C-N-CA	5.82	128.07	120.28
3	F	216	ALA	CA-C-O	-5.82	114.83	121.58
3	F	374	VAL	N-CA-C	5.82	116.00	110.42
3	F	412	ARG	CA-C-N	5.82	128.07	120.28
3	F	412	ARG	C-N-CA	5.82	128.07	120.28
7	O	151	LYS	CA-C-N	5.81	129.53	120.75
7	O	151	LYS	C-N-CA	5.81	129.53	120.75
14	Z	35	ILE	CA-C-N	5.81	129.15	120.31
14	Z	35	ILE	C-N-CA	5.81	129.15	120.31
4	G	86	SER	CA-C-N	5.81	128.42	120.46
4	G	86	SER	C-N-CA	5.81	128.42	120.46
3	D	465	ASP	CA-C-N	5.81	128.67	120.42
3	D	465	ASP	C-N-CA	5.81	128.67	120.42
2	A	291	PRO	N-CA-C	-5.81	102.47	111.13
4	G	115	LYS	CA-C-O	-5.81	114.72	120.82
1	1	11	GLY	CA-C-N	5.81	128.06	120.28
1	1	11	GLY	C-N-CA	5.81	128.06	120.28
1	1	62	GLY	CA-C-N	5.81	128.64	120.28
1	1	62	GLY	C-N-CA	5.81	128.64	120.28
2	A	169	ILE	N-CA-C	-5.80	97.27	109.34
2	B	449	ALA	CA-C-O	-5.80	114.73	120.82
1	3	14	ILE	CA-C-O	-5.80	115.02	121.17
7	O	22	ALA	CA-C-N	5.80	127.98	120.44
7	O	22	ALA	C-N-CA	5.80	127.98	120.44
3	F	91	THR	O-C-N	-5.79	115.10	122.34
1	9	18	GLY	O-C-N	5.79	128.38	122.24
3	D	349	ASP	CA-C-O	-5.79	112.23	120.16
3	E	164	THR	N-CA-C	-5.79	105.05	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	U	173	ALA	N-CA-C	5.79	117.67	111.36
1	6	15	SER	O-C-N	5.79	128.99	122.22
2	B	444	VAL	CA-C-O	5.79	122.57	118.69
3	D	14	THR	O-C-N	5.78	129.85	122.10
1	3	3	LEU	CA-C-O	-5.78	113.57	120.10
1	8	46	THR	CA-C-N	5.78	129.77	120.30
1	8	46	THR	C-N-CA	5.78	129.77	120.30
7	O	36	ALA	CA-C-N	5.78	128.02	120.28
7	O	36	ALA	C-N-CA	5.78	128.02	120.28
2	B	250	PHE	CA-C-O	5.78	126.67	120.55
1	0	15	SER	CA-C-N	5.77	128.59	120.28
1	0	15	SER	C-N-CA	5.77	128.59	120.28
1	6	3	LEU	CA-C-O	5.77	126.54	120.42
1	1	23	GLY	CA-C-N	5.77	128.61	120.42
1	1	23	GLY	C-N-CA	5.77	128.61	120.42
2	A	17	ARG	CA-C-N	5.77	128.61	120.42
2	A	17	ARG	C-N-CA	5.77	128.61	120.42
2	B	338	ALA	N-CA-C	5.77	117.77	110.33
3	E	89	ARG	O-C-N	5.77	129.98	122.42
1	6	64	PHE	N-CA-C	5.77	117.24	111.07
9	U	124	PHE	O-C-N	5.77	128.01	122.07
3	E	202	LYS	CA-C-O	5.77	126.53	120.42
2	A	428	GLN	CA-C-N	5.76	128.47	120.29
2	A	428	GLN	C-N-CA	5.76	128.47	120.29
2	A	13	ILE	O-C-N	5.76	128.31	121.80
2	C	273	LEU	CA-C-O	5.76	126.47	119.38
3	F	456	ALA	CA-C-O	5.76	126.59	119.97
3	D	83	ILE	CA-C-O	-5.76	115.03	121.36
10	V	54	ASP	O-C-N	5.76	130.08	123.29
1	9	54	GLY	O-C-N	5.75	127.72	122.19
2	B	456	ASP	N-CA-C	-5.75	105.75	112.89
1	2	42	SER	N-CA-C	-5.75	104.98	112.23
1	4	16	THR	CA-C-N	5.75	128.64	120.53
1	4	16	THR	C-N-CA	5.75	128.64	120.53
8	T	130	THR	CA-C-N	5.75	128.58	120.42
8	T	130	THR	C-N-CA	5.75	128.58	120.42
1	2	27	ALA	CA-C-N	5.75	128.33	120.46
1	2	27	ALA	C-N-CA	5.75	128.33	120.46
2	A	253	ALA	CA-C-N	5.74	127.98	120.28
2	A	253	ALA	C-N-CA	5.74	127.98	120.28
3	E	356	ARG	CA-C-N	5.74	131.55	122.60
3	E	356	ARG	C-N-CA	5.74	131.55	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	69	PHE	CA-C-O	-5.74	113.37	119.97
2	C	376	VAL	CA-C-O	5.74	126.13	119.36
2	A	28	ASN	N-CA-C	-5.74	106.32	113.38
5	H	43	ALA	CA-C-N	5.74	129.01	120.87
5	H	43	ALA	C-N-CA	5.74	129.01	120.87
3	D	151	GLY	N-CA-C	-5.73	101.62	112.51
3	E	261	PHE	CA-C-O	5.73	126.50	120.42
8	T	82	TRP	N-CA-C	5.73	117.53	111.28
2	C	339	TYR	CA-C-N	-5.73	111.53	122.13
2	C	339	TYR	C-N-CA	-5.73	111.53	122.13
3	E	89	ARG	N-CA-C	-5.73	106.33	113.38
3	E	265	GLY	O-C-N	5.73	127.69	122.19
3	E	396	LEU	O-C-N	-5.73	114.97	122.59
6	I	34	VAL	CA-C-N	5.73	128.53	120.28
6	I	34	VAL	C-N-CA	5.73	128.53	120.28
7	O	173	ASP	N-CA-C	-5.73	104.70	112.26
9	U	54	ASP	N-CA-C	-5.73	104.67	111.03
2	B	422	ARG	CA-C-N	5.72	126.33	119.98
2	B	422	ARG	C-N-CA	5.72	126.33	119.98
4	G	83	LEU	N-CA-C	5.72	119.53	111.52
2	B	324	THR	CA-C-O	-5.72	114.34	120.46
3	E	129	THR	CA-C-N	5.72	132.46	121.54
3	E	129	THR	C-N-CA	5.72	132.46	121.54
1	8	30	PHE	O-C-N	-5.72	115.24	122.27
3	E	187	VAL	CA-C-N	5.72	130.72	120.77
3	E	187	VAL	C-N-CA	5.72	130.72	120.77
3	F	430	LYS	N-CA-C	-5.72	98.77	108.26
2	A	451	VAL	N-CA-C	5.71	116.45	110.62
1	3	50	MET	N-CA-C	5.71	117.50	111.28
3	E	422	GLU	O-C-N	5.71	128.17	122.12
5	H	71	SER	N-CA-C	-5.71	106.08	113.16
1	0	28	ILE	CA-C-N	5.71	127.86	120.56
1	0	28	ILE	C-N-CA	5.71	127.86	120.56
2	B	46	LEU	CA-C-O	-5.71	114.90	122.03
8	T	177	LEU	CA-C-N	5.71	126.28	119.94
8	T	177	LEU	C-N-CA	5.71	126.28	119.94
2	C	79	GLY	O-C-N	-5.70	117.20	122.79
7	O	175	THR	CA-C-O	-5.70	114.44	121.06
1	8	24	ILE	O-C-N	5.70	127.70	121.83
3	F	101	GLU	CA-C-N	5.70	125.61	119.85
3	F	101	GLU	C-N-CA	5.70	125.61	119.85
1	5	73	LEU	O-C-N	5.70	127.94	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	247	LEU	N-CA-C	-5.70	106.10	113.16
2	C	413	ASP	N-CA-C	-5.70	102.09	110.52
1	2	55	PHE	CA-C-O	-5.69	114.84	120.82
2	B	139	LEU	CA-C-O	-5.69	112.82	118.34
4	G	219	LEU	CA-C-O	-5.69	114.52	120.55
3	E	389	ALA	CA-C-N	5.69	127.84	120.56
3	E	389	ALA	C-N-CA	5.69	127.84	120.56
2	C	107	GLY	O-C-N	-5.69	116.27	122.41
1	4	6	ALA	CA-C-N	5.69	128.47	120.28
1	4	6	ALA	C-N-CA	5.69	128.47	120.28
2	C	115	ASN	CA-C-O	-5.69	115.48	120.60
3	E	121	PRO	CA-C-O	-5.68	112.32	120.56
7	O	131	PRO	O-C-N	5.68	130.03	122.30
8	T	169	ARG	N-CA-C	-5.68	105.85	112.89
8	T	245	ALA	CA-C-N	5.68	129.64	120.55
8	T	245	ALA	C-N-CA	5.68	129.64	120.55
10	V	94	SER	N-CA-C	-5.68	105.17	111.36
1	9	3	LEU	N-CA-C	5.67	117.47	111.28
2	C	439	ALA	N-CA-C	-5.67	102.36	110.59
1	7	35	ASN	N-CA-C	5.67	117.14	111.07
8	T	221	MET	O-C-N	5.67	128.21	122.09
3	F	422	GLU	CA-C-N	5.67	127.70	120.56
3	F	422	GLU	C-N-CA	5.67	127.70	120.56
10	V	160	VAL	O-C-N	-5.66	114.64	121.10
11	W	52	LYS	N-CA-C	5.66	117.45	111.28
3	D	169	GLU	CA-C-N	5.66	127.87	120.28
3	D	169	GLU	C-N-CA	5.66	127.87	120.28
2	B	372	SER	CA-C-O	5.66	126.55	120.38
2	C	211	LYS	CA-C-N	5.66	127.86	120.28
2	C	211	LYS	C-N-CA	5.66	127.86	120.28
3	E	200	GLU	O-C-N	5.66	128.12	122.12
9	U	161	GLU	CA-C-O	-5.66	114.88	120.82
2	B	59	SER	N-CA-C	5.66	120.18	113.28
1	5	34	ILE	O-C-N	5.66	127.36	121.87
3	D	365	GLN	CA-C-N	5.66	127.79	120.44
3	D	365	GLN	C-N-CA	5.66	127.79	120.44
6	I	30	GLN	N-CA-C	-5.66	100.81	109.41
2	A	185	ILE	N-CA-C	5.65	116.39	110.62
2	B	389	ALA	CA-C-N	5.65	132.49	121.41
2	B	389	ALA	C-N-CA	5.65	132.49	121.41
9	U	150	ALA	O-C-N	-5.65	116.13	122.12
2	C	366	ALA	O-C-N	5.65	129.78	122.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	175	ALA	N-CA-C	5.65	117.44	111.28
3	E	284	THR	CA-C-N	5.65	128.12	120.44
3	E	284	THR	C-N-CA	5.65	128.12	120.44
7	O	185	GLN	O-C-N	5.65	128.11	122.12
1	0	38	SER	CA-C-N	5.65	128.89	120.31
1	0	38	SER	C-N-CA	5.65	128.89	120.31
3	E	304	VAL	CA-C-N	5.65	131.60	122.29
3	E	304	VAL	C-N-CA	5.65	131.60	122.29
3	E	348	VAL	N-CA-C	-5.65	102.29	109.80
10	V	124	ILE	N-CA-C	5.64	118.14	111.09
13	Y	28	SER	N-CA-C	-5.64	105.03	111.07
1	6	61	THR	N-CA-C	-5.64	105.21	111.36
1	8	38	SER	O-C-N	-5.64	115.33	122.27
2	A	150	THR	N-CA-C	-5.64	106.94	113.88
4	G	234	ARG	CA-C-O	5.64	126.51	120.70
10	V	104	LYS	CA-C-N	5.64	127.84	120.28
10	V	104	LYS	C-N-CA	5.64	127.84	120.28
2	A	254	SER	CA-C-O	5.64	126.53	120.55
3	E	81	GLY	CA-C-N	5.64	125.59	119.78
3	E	81	GLY	C-N-CA	5.64	125.59	119.78
5	H	61	GLU	N-CA-C	-5.64	99.09	108.34
3	E	86	PRO	CA-C-O	5.64	128.55	121.67
7	O	146	LEU	N-CA-C	-5.64	106.57	113.50
7	O	140	ALA	CA-C-O	5.63	126.52	120.55
2	C	257	GLU	N-CA-C	5.63	118.19	111.71
3	D	193	GLU	CA-C-N	5.63	126.19	119.94
3	D	193	GLU	C-N-CA	5.63	126.19	119.94
10	V	105	GLU	O-C-N	5.63	128.09	122.12
6	I	39	GLN	N-CA-C	5.62	119.15	111.39
7	O	188	ASN	O-C-N	5.62	127.86	122.07
3	F	108	PRO	CA-C-N	5.62	129.67	121.80
3	F	108	PRO	C-N-CA	5.62	129.67	121.80
1	9	69	SER	O-C-N	5.62	127.85	122.07
1	1	44	LYS	N-CA-C	5.61	118.17	111.71
3	F	255	ILE	O-C-N	-5.61	117.01	123.07
2	B	281	ARG	CA-C-N	5.61	127.80	120.28
2	B	281	ARG	C-N-CA	5.61	127.80	120.28
3	E	435	LYS	N-CA-C	-5.61	105.25	111.36
4	G	100	ASN	N-CA-C	-5.61	106.10	113.17
1	0	10	ILE	N-CA-C	5.60	115.80	110.53
2	B	249	PRO	CA-C-N	5.60	127.78	120.28
2	B	249	PRO	C-N-CA	5.60	127.78	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	19	LYS	CA-C-N	5.60	132.38	121.41
2	A	19	LYS	C-N-CA	5.60	132.38	121.41
1	1	22	ALA	CA-C-N	5.59	126.19	119.98
1	1	22	ALA	C-N-CA	5.59	126.19	119.98
3	F	399	GLN	O-C-N	-5.59	115.77	122.15
2	B	313	LYS	O-C-N	-5.59	116.64	122.96
1	1	34	ILE	N-CA-C	5.59	116.32	110.62
1	8	57	LEU	N-CA-C	5.59	117.45	111.36
2	C	323	LEU	N-CA-C	-5.59	100.57	109.96
3	F	359	ASP	N-CA-C	-5.59	101.03	108.74
3	E	121	PRO	CA-C-N	5.59	126.37	120.11
3	E	121	PRO	C-N-CA	5.59	126.37	120.11
3	F	278	ALA	CA-C-N	5.59	132.03	121.97
3	F	278	ALA	C-N-CA	5.59	132.03	121.97
8	T	206	LEU	CA-C-N	5.59	128.58	120.98
8	T	206	LEU	C-N-CA	5.59	128.58	120.98
11	W	34	LEU	O-C-N	-5.59	117.91	121.88
3	D	440	SER	N-CA-C	5.58	117.45	111.36
4	G	55	ALA	CA-C-N	5.58	132.21	121.54
4	G	55	ALA	C-N-CA	5.58	132.21	121.54
9	U	71	LYS	N-CA-C	5.58	117.45	111.36
7	O	76	GLU	CA-C-N	5.58	128.79	120.31
7	O	76	GLU	C-N-CA	5.58	128.79	120.31
3	F	52	GLN	CA-C-N	5.58	130.85	122.99
3	F	52	GLN	C-N-CA	5.58	130.85	122.99
1	8	54	GLY	CA-C-N	5.58	127.69	120.44
1	8	54	GLY	C-N-CA	5.58	127.69	120.44
8	T	140	VAL	CA-C-N	5.58	128.31	120.28
8	T	140	VAL	C-N-CA	5.58	128.31	120.28
13	Y	23	VAL	N-CA-C	5.58	116.35	110.72
1	9	17	ILE	CA-C-N	5.57	127.11	120.14
1	9	17	ILE	C-N-CA	5.57	127.11	120.14
2	A	80	SER	CA-C-N	5.57	130.99	122.29
2	A	80	SER	C-N-CA	5.57	130.99	122.29
2	A	130	ARG	CA-C-N	5.57	130.16	120.68
2	A	130	ARG	C-N-CA	5.57	130.16	120.68
2	A	191	TRP	CA-C-N	5.57	128.20	120.29
2	A	191	TRP	C-N-CA	5.57	128.20	120.29
12	X	18	PRO	CA-C-N	5.57	128.76	120.90
12	X	18	PRO	C-N-CA	5.57	128.76	120.90
3	D	129	THR	CA-C-N	5.57	128.67	120.82
3	D	129	THR	C-N-CA	5.57	128.67	120.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	195	ASN	N-CA-C	5.57	117.35	111.28
2	A	504	GLU	CA-C-N	5.57	127.68	120.44
2	A	504	GLU	C-N-CA	5.57	127.68	120.44
12	X	9	ARG	N-CA-C	-5.57	105.11	111.07
2	C	458	ILE	N-CA-C	-5.56	100.57	108.58
3	D	337	ARG	O-C-N	5.56	128.02	122.12
3	E	127	GLN	CA-C-N	5.56	129.15	120.75
3	E	127	GLN	C-N-CA	5.56	129.15	120.75
11	W	5	ILE	CA-C-N	5.56	126.11	120.38
11	W	5	ILE	C-N-CA	5.56	126.11	120.38
1	4	61	THR	CA-C-N	5.56	126.15	119.98
1	4	61	THR	C-N-CA	5.56	126.15	119.98
2	C	162	GLY	CA-C-O	-5.56	115.62	121.57
4	G	213	THR	CA-C-N	5.56	128.18	120.29
4	G	213	THR	C-N-CA	5.56	128.18	120.29
5	H	129	VAL	CA-C-O	-5.56	114.62	120.57
7	O	186	LYS	N-CA-C	5.55	117.01	111.07
11	W	72	GLY	O-C-N	-5.55	116.86	122.19
1	4	15	SER	CA-C-N	5.55	128.27	120.28
1	4	15	SER	C-N-CA	5.55	128.27	120.28
2	A	150	THR	CA-C-O	5.55	125.51	119.24
2	B	121	GLY	CA-C-N	5.54	125.55	119.90
2	B	121	GLY	C-N-CA	5.54	125.55	119.90
3	D	404	VAL	CA-C-O	-5.54	115.19	120.95
2	B	31	GLY	N-CA-C	-5.54	103.06	111.14
10	V	162	GLY	N-CA-C	-5.54	107.79	114.66
1	8	55	PHE	O-C-N	5.54	127.77	122.07
7	O	106	SER	N-CA-C	5.54	117.31	111.28
2	A	179	ALA	O-C-N	5.53	128.46	122.15
3	D	301	LYS	CA-C-O	-5.53	114.78	120.54
8	T	193	GLY	O-C-N	5.53	127.50	122.19
1	8	28	ILE	N-CA-C	5.53	116.26	110.62
4	G	102	GLN	CA-C-N	5.53	125.15	119.56
4	G	102	GLN	C-N-CA	5.53	125.15	119.56
12	X	33	PRO	CA-C-N	5.53	126.75	119.84
12	X	33	PRO	C-N-CA	5.53	126.75	119.84
3	E	60	ARG	O-C-N	-5.53	116.61	123.36
2	C	56	GLU	CA-C-O	-5.53	114.66	120.58
3	D	319	ASP	CA-C-O	-5.53	114.28	120.25
2	A	256	GLY	CA-C-N	5.53	127.68	120.28
2	A	256	GLY	C-N-CA	5.53	127.68	120.28
2	B	473	TYR	CA-C-N	5.53	127.62	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	473	TYR	C-N-CA	5.53	127.62	120.44
1	3	14	ILE	O-C-N	5.52	127.32	121.91
3	F	210	GLU	N-CA-C	-5.52	107.55	114.56
1	7	63	LEU	CA-C-N	5.52	127.67	120.28
1	7	63	LEU	C-N-CA	5.52	127.67	120.28
10	V	167	PHE	CA-C-N	5.52	132.22	121.41
10	V	167	PHE	C-N-CA	5.52	132.22	121.41
3	F	43	GLN	N-CA-C	-5.51	106.60	113.38
3	F	141	VAL	CA-C-N	5.51	127.94	120.44
3	F	141	VAL	C-N-CA	5.51	127.94	120.44
10	V	120	THR	CA-C-N	5.51	127.61	120.44
10	V	120	THR	C-N-CA	5.51	127.61	120.44
2	C	154	ALA	CA-C-O	-5.51	114.71	120.55
4	G	26	VAL	CA-C-N	5.51	127.67	120.28
4	G	26	VAL	C-N-CA	5.51	127.67	120.28
3	D	464	GLU	O-C-N	5.51	127.96	122.12
2	B	440	THR	O-C-N	5.50	127.95	122.12
2	C	232	ILE	N-CA-C	-5.50	100.41	108.11
1	1	8	LYS	CA-C-O	-5.50	115.02	120.90
9	U	173	ALA	CA-C-N	5.50	128.67	120.31
9	U	173	ALA	C-N-CA	5.50	128.67	120.31
12	X	13	ASP	CA-C-N	5.50	132.04	121.54
12	X	13	ASP	C-N-CA	5.50	132.04	121.54
2	A	505	SER	CA-C-N	5.50	127.64	120.28
2	A	505	SER	C-N-CA	5.50	127.64	120.28
6	I	34	VAL	CA-C-O	5.49	126.99	121.17
2	A	474	LEU	CA-C-N	5.49	127.64	120.28
2	A	474	LEU	C-N-CA	5.49	127.64	120.28
7	O	133	SER	CA-C-O	-5.49	115.06	120.82
1	1	14	ILE	CA-C-N	5.49	127.63	120.28
1	1	14	ILE	C-N-CA	5.49	127.63	120.28
2	C	30	THR	N-CA-C	-5.49	100.40	108.79
7	O	183	LYS	CA-C-O	-5.49	114.74	120.55
1	4	31	ALA	CA-C-N	5.48	128.07	120.29
1	4	31	ALA	C-N-CA	5.48	128.07	120.29
3	D	466	VAL	CA-C-N	5.48	128.21	120.42
3	D	466	VAL	C-N-CA	5.48	128.21	120.42
3	E	453	PRO	CA-C-N	5.48	128.64	120.31
3	E	453	PRO	C-N-CA	5.48	128.64	120.31
8	T	69	ILE	N-CA-C	-5.48	105.33	113.39
9	U	61	THR	N-CA-C	5.48	117.25	111.28
1	4	59	GLU	O-C-N	5.47	127.92	122.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	227	ALA	N-CA-C	-5.47	107.61	114.56
7	O	101	PHE	CA-C-N	5.47	129.86	120.72
7	O	101	PHE	C-N-CA	5.47	129.86	120.72
8	T	240	SER	CA-C-N	5.47	128.06	120.29
8	T	240	SER	C-N-CA	5.47	128.06	120.29
2	B	418	GLN	O-C-N	5.47	127.92	122.12
3	D	404	VAL	O-C-N	5.47	127.18	121.87
3	E	339	ILE	CA-C-N	5.47	128.16	120.28
3	E	339	ILE	C-N-CA	5.47	128.16	120.28
8	T	213	LEU	CA-C-N	5.47	128.62	120.31
8	T	213	LEU	C-N-CA	5.47	128.62	120.31
2	B	275	LYS	CA-C-O	-5.47	112.66	119.38
2	C	113	LEU	CA-C-O	5.47	124.91	118.90
1	5	70	PHE	O-C-N	5.46	127.70	122.07
2	C	175	THR	N-CA-C	-5.46	107.18	112.97
7	O	181	SER	CA-C-N	5.46	127.60	120.28
7	O	181	SER	C-N-CA	5.46	127.60	120.28
13	Y	24	TYR	O-C-N	5.46	127.69	122.07
10	V	22	THR	CA-C-N	5.46	131.61	120.80
10	V	22	THR	C-N-CA	5.46	131.61	120.80
2	A	123	ILE	CA-C-N	5.46	129.22	121.42
2	A	123	ILE	C-N-CA	5.46	129.22	121.42
2	A	244	LEU	CA-C-N	5.46	128.04	120.29
2	A	244	LEU	C-N-CA	5.46	128.04	120.29
3	E	123	SER	CA-C-N	5.46	128.60	120.31
3	E	123	SER	C-N-CA	5.46	128.60	120.31
9	U	124	PHE	CA-C-N	5.46	127.53	120.44
9	U	124	PHE	C-N-CA	5.46	127.53	120.44
1	3	24	ILE	CA-C-N	5.45	126.15	119.99
1	3	24	ILE	C-N-CA	5.45	126.15	119.99
1	6	73	LEU	O-C-N	5.45	127.76	122.09
2	A	299	ASP	N-CA-C	-5.45	106.51	112.72
3	D	443	ALA	CA-C-N	5.45	127.93	120.46
3	D	443	ALA	C-N-CA	5.45	127.93	120.46
3	F	431	LEU	CA-C-O	-5.45	114.47	120.30
3	E	84	SER	CA-C-N	5.45	132.21	122.13
3	E	84	SER	C-N-CA	5.45	132.21	122.13
2	C	343	ASN	CA-C-N	5.45	128.15	120.42
2	C	343	ASN	C-N-CA	5.45	128.15	120.42
2	C	407	GLN	CA-C-O	5.44	127.81	121.11
7	O	151	LYS	N-CA-C	-5.44	99.86	108.73
2	C	401	GLU	CA-C-N	5.44	128.15	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	GLU	C-N-CA	5.44	128.15	120.42
3	D	395	GLU	CA-C-N	5.44	128.44	120.71
3	D	395	GLU	C-N-CA	5.44	128.44	120.71
3	F	94	ARG	CA-C-O	5.44	127.83	121.46
3	E	443	ALA	CA-C-N	5.44	127.91	120.46
3	E	443	ALA	C-N-CA	5.44	127.91	120.46
3	E	265	GLY	N-CA-C	5.44	119.26	112.73
3	F	393	MET	N-CA-C	5.44	119.54	113.02
10	V	74	TYR	CA-C-N	5.44	127.52	120.56
10	V	74	TYR	C-N-CA	5.44	127.52	120.56
2	C	85	LYS	N-CA-C	-5.43	100.17	108.76
4	G	232	ALA	CA-C-N	5.43	127.56	120.28
4	G	232	ALA	C-N-CA	5.43	127.56	120.28
2	C	109	VAL	N-CA-C	-5.43	100.62	108.71
4	G	180	LYS	O-C-N	5.43	126.65	121.71
1	1	6	ALA	CA-C-O	5.43	126.18	120.42
1	4	2	GLN	N-CA-C	5.43	117.20	111.28
1	6	11	GLY	CA-C-N	5.43	127.50	120.44
1	6	11	GLY	C-N-CA	5.43	127.50	120.44
2	C	184	THR	CA-C-N	5.43	127.90	120.46
2	C	184	THR	C-N-CA	5.43	127.90	120.46
4	G	111	GLY	CA-C-N	5.43	128.00	120.29
4	G	111	GLY	C-N-CA	5.43	128.00	120.29
5	H	56	VAL	O-C-N	5.43	128.96	123.20
8	T	143	SER	CA-C-N	5.43	128.56	120.31
8	T	143	SER	C-N-CA	5.43	128.56	120.31
10	V	85	ALA	CA-C-N	5.43	130.96	122.17
10	V	85	ALA	C-N-CA	5.43	130.96	122.17
1	3	21	GLY	CA-C-O	-5.43	114.91	120.66
1	5	18	GLY	O-C-N	5.43	127.78	122.19
9	U	94	ALA	CA-C-N	5.43	127.55	120.28
9	U	94	ALA	C-N-CA	5.43	127.55	120.28
10	V	111	SER	CA-C-N	5.42	127.49	120.44
10	V	111	SER	C-N-CA	5.42	127.49	120.44
2	C	167	GLU	O-C-N	-5.42	116.97	123.31
1	6	74	PHE	CA-C-O	5.42	126.05	119.38
2	A	70	PRO	N-CA-C	5.42	120.67	113.57
3	F	116	PRO	CA-C-O	-5.42	114.81	121.31
2	C	253	ALA	CA-C-N	5.42	127.54	120.28
2	C	253	ALA	C-N-CA	5.42	127.54	120.28
2	A	132	GLN	N-CA-C	-5.42	99.58	108.41
6	I	17	ALA	N-CA-C	-5.42	105.38	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	3	LEU	O-C-N	5.41	127.86	122.12
2	B	141	ARG	N-CA-C	-5.41	99.27	110.80
2	C	245	GLN	CA-C-N	5.41	127.98	120.29
2	C	245	GLN	C-N-CA	5.41	127.98	120.29
3	E	223	ASN	N-CA-C	-5.41	107.04	113.97
1	8	51	ALA	CA-C-N	5.41	127.87	120.46
1	8	51	ALA	C-N-CA	5.41	127.87	120.46
6	I	30	GLN	O-C-N	5.41	130.35	122.94
4	G	139	THR	CA-C-O	-5.41	115.29	121.40
9	U	99	HIS	CA-C-O	-5.41	112.60	119.31
2	C	286	LEU	N-CA-C	-5.40	105.91	112.88
3	F	213	SER	CA-C-N	5.40	131.60	122.26
3	F	213	SER	C-N-CA	5.40	131.60	122.26
1	7	44	LYS	CA-C-O	5.40	126.25	120.20
4	G	92	ALA	CA-C-N	5.40	127.51	120.28
4	G	92	ALA	C-N-CA	5.40	127.51	120.28
2	A	464	GLY	N-CA-C	-5.39	106.24	112.50
5	H	28	THR	N-CA-C	-5.39	99.31	110.80
9	U	197	SER	N-CA-C	-5.39	105.30	111.07
10	V	109	LEU	N-CA-C	5.39	116.96	111.14
2	B	287	LEU	CA-C-N	5.39	129.79	122.19
2	B	287	LEU	C-N-CA	5.39	129.79	122.19
3	D	398	GLU	O-C-N	5.39	127.83	122.12
2	B	404	ALA	N-CA-C	5.38	117.15	111.28
3	D	424	PHE	CA-C-O	5.38	125.57	119.27
2	C	487	GLU	N-CA-C	5.38	117.22	111.36
6	I	32	ALA	N-CA-C	5.38	117.22	111.36
2	C	383	LYS	O-C-N	-5.38	116.42	122.12
8	T	112	SER	N-CA-C	-5.37	106.65	114.12
3	F	400	ASP	O-C-N	-5.37	116.03	122.15
4	G	220	THR	CA-C-N	5.37	127.92	120.29
4	G	220	THR	C-N-CA	5.37	127.92	120.29
8	T	94	MET	N-CA-C	5.37	117.21	111.36
8	T	212	PRO	CA-C-N	5.37	127.47	120.28
8	T	212	PRO	C-N-CA	5.37	127.47	120.28
2	C	479	ASN	CA-C-N	5.36	127.90	120.29
2	C	479	ASN	C-N-CA	5.36	127.90	120.29
3	D	163	LYS	O-C-N	5.36	127.88	122.09
7	O	171	LEU	CA-C-O	5.36	128.18	120.51
3	D	262	THR	CA-C-N	5.36	127.90	120.29
3	D	262	THR	C-N-CA	5.36	127.90	120.29
1	3	62	GLY	O-C-N	5.36	127.38	122.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	130	ARG	CA-C-N	5.36	127.99	120.28
2	C	130	ARG	C-N-CA	5.36	127.99	120.28
3	D	212	GLU	CA-C-N	5.36	132.14	122.02
3	D	212	GLU	C-N-CA	5.36	132.14	122.02
3	E	343	GLY	CA-C-N	5.36	130.39	123.11
3	E	343	GLY	C-N-CA	5.36	130.39	123.11
4	G	123	PRO	CA-C-N	5.36	131.77	122.56
4	G	123	PRO	C-N-CA	5.36	131.77	122.56
2	B	428	GLN	CA-C-N	5.35	127.45	120.28
2	B	428	GLN	C-N-CA	5.35	127.45	120.28
2	C	296	TYR	CA-C-O	-5.35	114.77	120.23
3	F	243	PHE	N-CA-C	5.35	117.19	111.36
11	W	49	ALA	CA-C-N	5.35	128.45	120.31
11	W	49	ALA	C-N-CA	5.35	128.45	120.31
5	H	132	ASN	CA-C-O	5.35	126.22	120.55
2	C	337	SER	N-CA-C	-5.35	106.34	112.92
1	4	73	LEU	CA-C-N	5.35	129.72	120.58
1	4	73	LEU	C-N-CA	5.35	129.72	120.58
2	A	427	THR	CA-C-N	5.35	127.98	120.28
2	A	427	THR	C-N-CA	5.35	127.98	120.28
2	B	377	GLY	N-CA-C	-5.35	106.75	111.67
1	0	72	LEU	CA-C-N	5.34	127.44	120.28
1	0	72	LEU	C-N-CA	5.34	127.44	120.28
2	A	142	ARG	CA-C-N	5.34	128.30	120.71
2	A	142	ARG	C-N-CA	5.34	128.30	120.71
2	B	459	GLU	CA-C-O	-5.34	115.50	121.81
2	C	501	SER	CA-C-N	5.34	127.39	120.44
2	C	501	SER	C-N-CA	5.34	127.39	120.44
3	E	390	ILE	CA-C-N	5.34	127.88	120.29
3	E	390	ILE	C-N-CA	5.34	127.88	120.29
2	A	179	ALA	CA-C-O	-5.34	114.76	120.42
2	C	387	GLN	N-CA-C	-5.34	105.37	111.14
3	E	294	GLU	O-C-N	-5.34	115.90	122.20
4	G	159	TYR	O-C-N	-5.34	115.45	121.43
4	G	11	LYS	CA-C-N	5.33	127.38	120.44
4	G	11	LYS	C-N-CA	5.33	127.38	120.44
2	C	346	SER	CA-C-N	5.33	127.77	120.46
2	C	346	SER	C-N-CA	5.33	127.77	120.46
2	B	12	SER	CA-C-N	5.33	127.39	120.56
2	B	12	SER	C-N-CA	5.33	127.39	120.56
3	E	25	PHE	N-CA-C	-5.33	101.43	109.85
11	W	43	LYS	CA-C-O	-5.33	115.02	120.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	136	ASP	O-C-N	5.33	127.77	122.12
11	W	53	ALA	N-CA-C	5.33	117.09	111.28
8	T	55	GLY	CA-C-O	5.33	126.88	122.24
7	O	111	LEU	N-CA-C	5.33	117.09	111.28
12	X	21	LEU	N-CA-C	5.33	117.08	111.28
4	G	24	LYS	O-C-N	-5.32	116.48	122.12
9	U	160	TYR	CA-C-N	5.32	127.36	120.44
9	U	160	TYR	C-N-CA	5.32	127.36	120.44
10	V	68	ILE	CA-C-N	5.32	128.40	120.31
10	V	68	ILE	C-N-CA	5.32	128.40	120.31
1	8	9	TYR	CA-C-N	5.32	127.26	120.56
1	8	9	TYR	C-N-CA	5.32	127.26	120.56
2	C	186	LEU	CA-C-O	-5.32	114.78	120.42
2	C	331	THR	CA-C-N	5.32	130.23	122.41
2	C	331	THR	C-N-CA	5.32	130.23	122.41
2	C	382	VAL	CA-C-N	5.32	127.41	120.28
2	C	382	VAL	C-N-CA	5.32	127.41	120.28
2	C	470	PHE	CA-C-N	5.32	127.84	120.29
2	C	470	PHE	C-N-CA	5.32	127.84	120.29
8	T	154	LEU	CA-C-N	5.32	124.58	120.33
8	T	154	LEU	C-N-CA	5.32	124.58	120.33
3	E	268	VAL	CA-C-N	5.31	127.67	120.44
3	E	268	VAL	C-N-CA	5.31	127.67	120.44
1	8	21	GLY	CA-C-O	5.31	126.22	120.75
2	A	462	ARG	CA-C-N	5.31	127.74	120.46
2	A	462	ARG	C-N-CA	5.31	127.74	120.46
3	D	121	PRO	O-C-N	-5.31	115.19	121.46
1	3	71	LEU	CA-C-N	5.31	127.66	120.44
1	3	71	LEU	C-N-CA	5.31	127.66	120.44
3	F	423	VAL	CA-C-N	5.31	127.66	120.44
3	F	423	VAL	C-N-CA	5.31	127.66	120.44
4	G	270	ILE	CA-C-N	5.31	127.96	120.42
4	G	270	ILE	C-N-CA	5.31	127.96	120.42
2	A	120	LYS	N-CA-C	-5.31	106.76	113.18
3	F	285	LEU	N-CA-C	5.31	117.06	111.28
3	E	167	ILE	CA-C-O	5.31	126.47	120.95
2	B	133	VAL	N-CA-C	5.30	117.27	109.63
3	E	405	GLU	CA-C-N	5.30	127.39	120.28
3	E	405	GLU	C-N-CA	5.30	127.39	120.28
8	T	192	ALA	N-CA-C	5.30	117.06	111.28
1	0	15	SER	CA-C-O	-5.30	114.93	120.55
1	1	57	LEU	N-CA-C	5.30	117.14	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	113	LEU	N-CA-C	-5.30	106.49	113.17
3	D	21	VAL	O-C-N	-5.30	117.34	123.07
11	W	1	VAL	CA-C-O	-5.30	111.79	120.80
2	C	453	GLY	N-CA-C	-5.30	107.96	115.43
1	9	12	ALA	CA-C-N	5.30	125.97	119.99
1	9	12	ALA	C-N-CA	5.30	125.97	119.99
2	A	411	ASP	CA-C-O	-5.30	114.92	120.80
2	C	96	ILE	CA-C-O	-5.30	116.25	122.13
8	T	94	MET	CA-C-O	-5.29	114.81	120.42
11	W	23	ARG	CA-C-O	-5.29	115.26	120.82
1	8	24	ILE	N-CA-C	-5.29	105.38	110.72
2	A	111	ASP	N-CA-C	-5.29	101.66	109.86
3	D	408	ARG	CA-C-N	5.29	127.37	120.28
3	D	408	ARG	C-N-CA	5.29	127.37	120.28
3	E	210	GLU	N-CA-C	-5.29	103.47	111.56
3	E	423	VAL	CA-C-N	5.29	127.90	120.28
3	E	423	VAL	C-N-CA	5.29	127.90	120.28
3	F	57	ASN	CA-C-N	-5.29	115.35	122.86
3	F	57	ASN	C-N-CA	-5.29	115.35	122.86
1	3	68	VAL	CA-C-N	5.29	127.36	120.28
1	3	68	VAL	C-N-CA	5.29	127.36	120.28
1	1	15	SER	O-C-N	5.29	127.72	122.12
2	A	383	LYS	CA-C-O	-5.28	114.95	120.55
1	4	9	TYR	N-CA-C	5.28	116.84	111.14
2	C	412	LEU	O-C-N	-5.28	115.71	122.94
2	B	94	GLY	N-CA-C	-5.28	107.83	115.27
3	F	344	ILE	N-CA-C	-5.28	100.28	107.99
1	6	38	SER	N-CA-C	5.28	117.94	111.82
2	A	214	THR	CA-C-O	-5.28	114.95	120.55
3	D	278	ALA	CA-C-N	5.28	131.47	121.97
3	D	278	ALA	C-N-CA	5.28	131.47	121.97
3	F	150	GLY	CA-C-N	5.28	125.93	120.60
3	F	150	GLY	C-N-CA	5.28	125.93	120.60
3	F	270	ALA	CA-C-O	5.28	126.01	120.42
1	6	45	ASP	CA-C-N	5.27	129.52	120.71
1	6	45	ASP	C-N-CA	5.27	129.52	120.71
9	U	177	ILE	CA-C-N	5.27	127.35	120.28
9	U	177	ILE	C-N-CA	5.27	127.35	120.28
8	T	126	TRP	CA-C-O	-5.27	114.83	120.42
9	U	169	GLN	CA-C-N	5.27	128.32	120.31
9	U	169	GLN	C-N-CA	5.27	128.32	120.31
3	D	450	ASP	N-CA-C	-5.26	106.90	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	76	VAL	CA-C-N	5.26	128.94	121.42
2	A	76	VAL	C-N-CA	5.26	128.94	121.42
9	U	83	ALA	O-C-N	-5.26	116.65	122.07
1	0	43	ILE	CA-C-N	5.26	127.33	120.28
1	0	43	ILE	C-N-CA	5.26	127.33	120.28
3	E	357	LEU	N-CA-C	-5.26	106.10	112.88
3	F	408	ARG	CA-C-N	5.25	127.75	120.29
3	F	408	ARG	C-N-CA	5.25	127.75	120.29
8	T	164	LEU	N-CA-C	-5.25	105.45	111.07
9	U	103	VAL	N-CA-C	-5.25	105.26	110.62
1	5	41	PRO	N-CA-C	5.25	123.29	112.47
2	B	372	SER	O-C-N	-5.25	117.09	123.29
9	U	144	VAL	CA-C-N	5.25	127.27	120.44
9	U	144	VAL	C-N-CA	5.25	127.27	120.44
12	X	15	LYS	CA-C-N	5.25	130.40	123.05
12	X	15	LYS	C-N-CA	5.25	130.40	123.05
1	4	57	LEU	CA-C-N	5.25	127.27	120.44
1	4	57	LEU	C-N-CA	5.25	127.27	120.44
1	6	24	ILE	CA-C-O	-5.25	115.49	120.95
3	F	228	ALA	N-CA-C	5.25	117.08	111.36
3	F	286	ALA	CA-C-O	5.25	126.11	120.70
1	0	50	MET	N-CA-C	5.25	117.00	111.28
2	B	10	VAL	CA-C-N	5.25	127.31	120.28
2	B	10	VAL	C-N-CA	5.25	127.31	120.28
3	D	470	ALA	CA-C-N	5.25	127.31	120.28
3	D	470	ALA	C-N-CA	5.25	127.31	120.28
3	E	296	ILE	CA-C-O	-5.25	114.92	120.53
1	6	64	PHE	CA-C-N	5.24	127.31	120.28
1	6	64	PHE	C-N-CA	5.24	127.31	120.28
9	U	145	GLU	CA-C-O	-5.24	115.31	120.82
1	3	72	LEU	CA-C-N	5.24	127.57	120.44
1	3	72	LEU	C-N-CA	5.24	127.57	120.44
2	B	24	GLU	N-CA-C	5.24	117.91	110.10
3	E	374	VAL	O-C-N	5.24	127.23	121.83
9	U	200	GLU	CA-C-N	5.24	127.64	120.46
9	U	200	GLU	C-N-CA	5.24	127.64	120.46
3	D	307	VAL	O-C-N	-5.24	117.39	122.99
1	0	35	ASN	CA-C-O	5.24	126.10	120.55
9	U	150	ALA	N-CA-C	5.24	116.99	111.28
2	C	455	LEU	O-C-N	-5.24	116.02	122.25
2	C	467	GLU	CA-C-O	-5.24	115.00	120.55
3	D	41	THR	O-C-N	-5.23	118.36	121.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	175	THR	O-C-N	5.23	129.34	123.27
8	T	152	LEU	O-C-N	-5.23	115.79	120.92
1	8	50	MET	CA-C-O	5.23	126.10	120.55
3	E	366	GLU	CA-C-N	5.23	127.29	120.28
3	E	366	GLU	C-N-CA	5.23	127.29	120.28
4	G	132	GLY	N-CA-C	-5.23	107.82	115.72
7	O	160	LYS	N-CA-C	-5.23	101.03	109.40
2	A	20	GLY	CA-C-N	5.23	129.67	123.19
2	A	20	GLY	C-N-CA	5.23	129.67	123.19
2	A	227	ALA	CA-C-O	-5.23	113.03	120.51
9	U	119	THR	N-CA-C	5.23	117.06	111.36
9	U	162	ALA	O-C-N	5.23	127.66	122.12
11	W	6	PRO	O-C-N	-5.23	115.29	121.46
2	A	278	VAL	CA-C-O	-5.22	115.52	120.95
2	B	176	GLY	N-CA-C	-5.22	105.00	114.46
10	V	98	HIS	CA-C-N	5.22	127.28	120.28
10	V	98	HIS	C-N-CA	5.22	127.28	120.28
2	C	251	THR	N-CA-C	-5.22	106.75	113.23
3	F	65	ASP	O-C-N	5.22	129.54	122.96
9	U	131	VAL	CA-C-O	-5.22	114.98	120.57
1	8	59	GLU	CA-C-N	5.22	127.80	120.28
1	8	59	GLU	C-N-CA	5.22	127.80	120.28
2	B	334	GLY	CA-C-N	5.22	129.35	122.30
2	B	334	GLY	C-N-CA	5.22	129.35	122.30
2	B	492	SER	CA-C-O	-5.22	115.50	121.82
4	G	41	ALA	O-C-N	5.22	127.65	122.12
2	A	10	VAL	CA-C-N	5.22	127.27	120.28
2	A	10	VAL	C-N-CA	5.22	127.27	120.28
2	A	341	PRO	N-CA-C	5.22	120.39	113.40
2	A	280	TYR	O-C-N	-5.21	116.12	122.22
2	B	354	LEU	N-CA-C	-5.21	100.53	109.24
3	D	238	THR	O-C-N	5.21	128.68	122.27
3	E	307	VAL	CA-C-O	-5.21	114.95	120.48
5	H	45	HIS	O-C-N	-5.21	117.31	123.25
12	X	46	GLY	N-CA-C	5.21	122.98	112.34
3	D	336	SER	N-CA-C	-5.21	100.74	109.24
9	U	74	ALA	N-CA-C	5.21	120.56	113.16
3	E	107	GLY	O-C-N	5.21	126.98	121.77
7	O	90	LYS	CA-C-N	5.21	127.59	120.46
7	O	90	LYS	C-N-CA	5.21	127.59	120.46
2	A	505	SER	CA-C-O	5.21	126.29	120.82
11	W	64	LYS	CA-C-O	-5.21	113.29	118.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	X	29	LYS	CA-C-O	-5.21	114.63	120.25
2	B	60	GLY	CA-C-N	5.20	130.08	122.69
2	B	60	GLY	C-N-CA	5.20	130.08	122.69
3	D	283	PRO	N-CA-C	-5.20	105.90	114.75
3	F	108	PRO	CA-C-O	-5.20	115.32	121.67
3	F	247	GLU	CA-C-O	5.20	125.36	119.27
2	B	338	ALA	CA-C-O	-5.20	116.15	122.03
3	D	197	LEU	CA-C-N	5.20	127.25	120.28
3	D	197	LEU	C-N-CA	5.20	127.25	120.28
1	9	15	SER	CA-C-N	5.20	127.77	120.28
1	9	15	SER	C-N-CA	5.20	127.77	120.28
1	9	24	ILE	CA-C-O	-5.20	115.54	120.95
2	B	417	LYS	CA-C-O	-5.20	115.04	120.55
2	C	98	ASP	N-CA-C	-5.20	101.17	109.07
3	E	317	LEU	N-CA-C	-5.20	106.85	114.39
4	G	25	ILE	O-C-N	5.20	127.19	121.83
2	A	493	LYS	CA-C-N	5.20	127.24	120.28
2	A	493	LYS	C-N-CA	5.20	127.24	120.28
2	B	47	ASN	N-CA-C	-5.20	106.53	112.92
2	B	169	ILE	O-C-N	-5.20	117.69	123.20
3	D	427	ILE	N-CA-C	-5.20	102.23	107.89
1	1	62	GLY	CA-C-O	5.19	126.10	120.75
2	B	93	THR	O-C-N	5.19	128.07	122.15
2	B	214	THR	CA-C-N	5.19	127.57	120.46
2	B	214	THR	C-N-CA	5.19	127.57	120.46
12	X	49	ALA	CA-C-N	5.19	127.19	120.44
12	X	49	ALA	C-N-CA	5.19	127.19	120.44
1	6	21	GLY	CA-C-N	5.19	127.66	120.29
1	6	21	GLY	C-N-CA	5.19	127.66	120.29
2	A	28	ASN	O-C-N	-5.19	115.62	122.42
3	F	397	SER	CA-C-N	5.19	127.66	120.29
3	F	397	SER	C-N-CA	5.19	127.66	120.29
1	7	5	LEU	CA-C-N	5.19	127.23	120.28
1	7	5	LEU	C-N-CA	5.19	127.23	120.28
3	F	80	GLY	N-CA-C	-5.19	108.07	115.64
3	E	56	GLU	CA-C-N	5.18	129.55	122.34
3	E	56	GLU	C-N-CA	5.18	129.55	122.34
8	T	210	PHE	N-CA-C	-5.18	106.11	112.90
3	D	36	ALA	N-CA-C	-5.18	100.46	108.90
7	O	176	VAL	CA-C-O	-5.18	114.87	120.36
3	D	68	GLU	CA-C-N	5.18	127.93	120.11
3	D	68	GLU	C-N-CA	5.18	127.93	120.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	87	ASN	N-CA-C	-5.18	105.71	112.23
3	F	442	LYS	N-CA-C	-5.17	105.53	111.07
8	T	248	LEU	CA-C-N	5.17	131.01	121.70
8	T	248	LEU	C-N-CA	5.17	131.01	121.70
2	B	301	PHE	O-C-N	5.17	128.05	122.15
3	F	51	ALA	O-C-N	-5.17	116.62	122.10
3	F	234	LEU	CA-C-N	5.17	127.21	120.28
3	F	234	LEU	C-N-CA	5.17	127.21	120.28
1	8	61	THR	N-CA-C	-5.17	105.65	111.28
1	9	36	GLY	CA-C-O	-5.17	115.18	120.66
2	A	124	ASP	N-CA-C	-5.17	102.03	110.20
3	E	145	ALA	CA-C-N	5.17	125.08	119.76
3	E	145	ALA	C-N-CA	5.17	125.08	119.76
5	H	36	SER	N-CA-C	-5.17	105.26	112.03
7	O	57	LEU	CA-C-O	5.17	126.28	120.70
3	E	291	LEU	O-C-N	5.17	127.39	122.07
3	E	438	VAL	CA-C-N	5.17	127.20	120.28
3	E	438	VAL	C-N-CA	5.17	127.20	120.28
1	7	8	LYS	N-CA-C	5.16	116.60	111.07
3	E	277	SER	CA-C-N	5.16	129.47	122.19
3	E	277	SER	C-N-CA	5.16	129.47	122.19
2	A	309	GLU	CA-C-N	5.16	129.77	122.24
2	A	309	GLU	C-N-CA	5.16	129.77	122.24
2	B	277	ALA	O-C-N	5.16	127.59	122.12
2	B	341	PRO	CA-C-N	5.16	127.19	120.28
2	B	341	PRO	C-N-CA	5.16	127.19	120.28
3	E	47	VAL	O-C-N	-5.16	117.07	123.10
3	E	26	GLU	CA-C-N	5.16	128.17	120.95
3	E	26	GLU	C-N-CA	5.16	128.17	120.95
1	5	39	ARG	O-C-N	-5.15	115.93	122.17
3	E	421	ALA	N-CA-C	-5.15	106.30	112.59
1	0	54	GLY	CA-C-O	-5.15	115.44	120.75
1	8	24	ILE	CA-C-O	-5.15	115.39	120.85
1	9	22	ALA	CA-C-N	5.15	125.66	119.94
1	9	22	ALA	C-N-CA	5.15	125.66	119.94
2	A	242	ALA	O-C-N	-5.15	115.87	120.92
2	A	311	ALA	N-CA-C	-5.15	99.83	110.80
13	Y	8	PRO	CA-C-O	-5.15	115.13	121.31
1	4	13	GLY	CA-C-N	5.15	127.51	120.46
1	4	13	GLY	C-N-CA	5.15	127.51	120.46
7	O	76	GLU	CA-C-O	5.15	125.88	120.42
3	D	25	PHE	CA-C-O	5.14	127.83	121.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	X	20	THR	CA-C-O	-5.14	115.91	121.87
2	A	292	GLY	CA-C-O	-5.14	114.24	120.92
3	E	148	ALA	CA-C-N	5.14	129.01	120.94
3	E	148	ALA	C-N-CA	5.14	129.01	120.94
2	A	192	ASN	CA-C-N	5.13	127.67	120.28
2	A	192	ASN	C-N-CA	5.13	127.67	120.28
2	B	34	LEU	CA-C-O	5.13	126.19	119.98
3	D	218	VAL	N-CA-C	-5.13	98.66	109.34
2	B	122	PRO	CA-C-O	-5.13	115.56	121.36
1	4	13	GLY	CA-C-O	-5.13	115.46	121.00
1	7	65	CYS	CA-C-N	5.13	127.16	120.28
1	7	65	CYS	C-N-CA	5.13	127.16	120.28
2	C	52	GLU	CA-C-O	5.13	128.91	119.32
8	T	151	PRO	CA-C-N	5.13	126.16	120.06
8	T	151	PRO	C-N-CA	5.13	126.16	120.06
2	C	425	ARG	N-CA-C	5.12	116.87	111.28
2	C	21	VAL	N-CA-C	5.12	120.00	109.34
2	A	282	GLN	N-CA-C	-5.12	105.70	111.28
3	F	333	THR	CA-C-N	5.12	128.03	120.91
3	F	333	THR	C-N-CA	5.12	128.03	120.91
3	E	309	ALA	CA-C-O	5.12	125.89	120.36
9	U	185	GLY	CA-C-N	5.12	128.46	120.68
9	U	185	GLY	C-N-CA	5.12	128.46	120.68
13	Y	13	TYR	CA-C-N	5.12	126.49	120.09
13	Y	13	TYR	C-N-CA	5.12	126.49	120.09
2	A	418	GLN	CA-C-N	5.12	127.14	120.28
2	A	418	GLN	C-N-CA	5.12	127.14	120.28
3	F	61	THR	N-CA-C	5.12	117.79	109.24
8	T	166	TYR	N-CA-C	5.12	117.99	111.69
3	D	162	GLY	N-CA-C	-5.11	106.69	115.08
8	T	196	PHE	N-CA-C	-5.11	105.60	111.07
11	W	39	ALA	CA-C-N	5.11	124.42	118.85
11	W	39	ALA	C-N-CA	5.11	124.42	118.85
1	4	43	ILE	CA-C-N	5.11	127.84	120.38
1	4	43	ILE	C-N-CA	5.11	127.84	120.38
2	A	389	ALA	CA-C-N	5.11	125.51	119.94
2	A	389	ALA	C-N-CA	5.11	125.51	119.94
11	W	56	PHE	CA-C-N	5.11	129.51	120.87
11	W	56	PHE	C-N-CA	5.11	129.51	120.87
3	E	115	LYS	CA-C-N	5.11	125.05	119.78
3	E	115	LYS	C-N-CA	5.11	125.05	119.78
3	F	318	THR	N-CA-C	5.11	116.93	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	137	ALA	CA-C-N	5.11	126.23	119.84
4	G	137	ALA	C-N-CA	5.11	126.23	119.84
12	X	7	TYR	O-C-N	-5.11	116.81	122.07
3	F	439	ALA	CA-C-N	5.11	127.54	120.29
3	F	439	ALA	C-N-CA	5.11	127.54	120.29
1	2	36	GLY	CA-C-N	5.11	127.10	120.56
1	2	36	GLY	C-N-CA	5.11	127.10	120.56
3	E	471	GLU	CA-C-O	5.11	125.96	120.70
3	D	216	ALA	CA-C-O	-5.11	115.47	121.44
3	D	287	THR	N-CA-C	5.11	116.92	111.36
2	B	474	LEU	O-C-N	-5.10	116.81	122.07
2	C	139	LEU	CA-C-N	-5.10	115.62	120.83
2	C	139	LEU	C-N-CA	-5.10	115.62	120.83
3	D	228	ALA	CA-C-N	5.10	127.63	120.28
3	D	228	ALA	C-N-CA	5.10	127.63	120.28
2	B	346	SER	N-CA-C	5.10	117.74	111.82
3	D	11	GLY	N-CA-C	-5.10	103.07	111.38
3	F	37	LEU	N-CA-C	-5.10	100.72	109.24
7	O	35	ALA	CA-C-N	5.10	127.07	120.44
7	O	35	ALA	C-N-CA	5.10	127.07	120.44
8	T	128	GLY	N-CA-C	-5.10	108.33	114.66
9	U	179	ARG	O-C-N	-5.10	116.00	122.27
1	5	35	ASN	CA-C-N	5.10	125.60	119.94
1	5	35	ASN	C-N-CA	5.10	125.60	119.94
1	6	44	LYS	N-CA-C	5.10	117.50	111.33
2	A	394	LEU	N-CA-C	5.10	116.92	111.36
2	B	10	VAL	CA-C-O	-5.10	115.23	121.04
3	F	403	THR	O-C-N	5.10	127.52	122.12
2	C	108	ARG	CA-C-O	-5.10	115.15	121.06
3	F	299	THR	N-CA-C	-5.09	101.67	109.41
9	U	119	THR	CA-C-N	5.09	127.11	120.28
9	U	119	THR	C-N-CA	5.09	127.11	120.28
3	F	171	ILE	CA-C-N	5.09	127.11	120.28
3	F	171	ILE	C-N-CA	5.09	127.11	120.28
8	T	214	ALA	CA-C-N	5.09	127.52	120.29
8	T	214	ALA	C-N-CA	5.09	127.52	120.29
9	U	53	ASN	CA-C-N	5.09	127.56	120.63
9	U	53	ASN	C-N-CA	5.09	127.56	120.63
1	3	23	GLY	N-CA-C	5.09	118.84	112.73
1	3	30	PHE	CA-C-N	5.09	127.52	120.29
1	3	30	PHE	C-N-CA	5.09	127.52	120.29
3	D	177	ALA	CA-C-N	5.09	132.31	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	177	ALA	C-N-CA	5.09	132.31	122.07
2	C	468	SER	CA-C-N	5.09	127.51	120.29
2	C	468	SER	C-N-CA	5.09	127.51	120.29
3	E	275	ILE	CA-C-N	5.09	125.09	119.90
3	E	275	ILE	C-N-CA	5.09	125.09	119.90
3	F	201	MET	CA-C-O	-5.09	115.03	120.42
4	G	168	ASP	CA-C-N	5.09	126.20	119.84
4	G	168	ASP	C-N-CA	5.09	126.20	119.84
2	A	146	GLU	CA-C-N	5.08	125.09	120.21
2	A	146	GLU	C-N-CA	5.08	125.09	120.21
2	A	61	VAL	N-CA-C	-5.08	100.56	108.95
2	B	210	GLN	CA-C-N	5.08	128.92	120.94
2	B	210	GLN	C-N-CA	5.08	128.92	120.94
12	X	50	LEU	O-C-N	-5.08	116.83	122.07
1	3	53	LEU	CA-C-N	5.08	125.62	119.98
1	3	53	LEU	C-N-CA	5.08	125.62	119.98
3	E	321	ALA	O-C-N	5.08	125.00	120.48
3	F	42	PRO	N-CA-C	-5.08	106.11	114.75
3	F	434	LEU	CA-C-O	-5.08	115.03	120.42
1	4	37	VAL	N-CA-C	5.08	115.80	110.62
2	B	403	ALA	CA-C-N	5.08	127.09	120.28
2	B	403	ALA	C-N-CA	5.08	127.09	120.28
3	F	79	THR	CA-C-N	5.08	129.87	122.10
3	F	79	THR	C-N-CA	5.08	129.87	122.10
1	5	7	ALA	CA-C-O	-5.08	114.36	120.10
1	9	69	SER	CA-C-O	-5.08	115.49	120.82
3	E	300	LYS	O-C-N	5.08	128.29	122.25
3	F	101	GLU	O-C-N	-5.08	116.65	121.57
3	F	317	LEU	CA-C-N	5.08	127.50	120.29
3	F	317	LEU	C-N-CA	5.08	127.50	120.29
1	4	21	GLY	CA-C-N	5.07	127.08	120.28
1	4	21	GLY	C-N-CA	5.07	127.08	120.28
1	9	53	LEU	CA-C-O	-5.07	115.49	120.82
3	D	327	ALA	O-C-N	-5.07	116.61	122.09
2	C	99	VAL	CA-C-N	5.07	125.86	120.13
2	C	99	VAL	C-N-CA	5.07	125.86	120.13
1	8	43	ILE	CA-C-N	5.07	127.58	120.28
1	8	43	ILE	C-N-CA	5.07	127.58	120.28
4	G	32	SER	O-C-N	5.07	127.29	122.07
1	1	4	VAL	N-CA-C	5.07	115.84	110.72
3	D	33	ILE	N-CA-C	-5.07	101.11	109.12
6	I	36	ASN	O-C-N	5.07	128.82	122.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	69	SER	CA-C-O	-5.07	115.18	120.55
2	B	6	GLN	N-CA-C	-5.07	102.38	108.25
7	O	54	GLY	N-CA-C	-5.06	107.70	116.01
8	T	172	SER	CA-C-N	5.06	127.07	120.28
8	T	172	SER	C-N-CA	5.06	127.07	120.28
2	C	426	LEU	N-CA-C	-5.06	105.67	111.14
3	E	115	LYS	CA-C-O	-5.06	114.75	119.91
1	6	41	PRO	N-CA-C	5.06	122.89	112.47
2	B	417	LYS	O-C-N	5.06	127.48	122.12
3	F	13	VAL	CA-C-N	5.06	129.23	120.58
3	F	13	VAL	C-N-CA	5.06	129.23	120.58
4	G	152	SER	N-CA-C	5.06	116.60	111.14
2	A	82	ARG	N-CA-C	-5.06	106.62	112.89
3	E	58	THR	N-CA-C	-5.06	101.51	109.50
3	F	312	VAL	CA-C-O	5.05	122.13	119.15
2	A	429	LEU	CA-C-N	5.05	132.04	121.94
2	A	429	LEU	C-N-CA	5.05	132.04	121.94
3	F	79	THR	N-CA-C	5.05	116.79	111.28
1	4	29	VAL	O-C-N	-5.05	116.65	121.90
2	B	173	ARG	O-C-N	5.05	129.14	122.93
3	E	285	LEU	CA-C-N	5.05	127.05	120.28
3	E	285	LEU	C-N-CA	5.05	127.05	120.28
10	V	101	THR	CA-C-O	-5.05	115.52	120.82
2	C	367	ILE	O-C-N	5.05	128.33	123.03
3	D	233	ALA	N-CA-C	-5.05	105.86	111.36
3	F	300	LYS	CA-C-N	5.05	127.98	120.31
3	F	300	LYS	C-N-CA	5.05	127.98	120.31
1	1	71	LEU	CA-C-N	5.05	127.31	120.44
1	1	71	LEU	C-N-CA	5.05	127.31	120.44
2	C	494	GLU	CA-C-N	5.05	127.04	120.28
2	C	494	GLU	C-N-CA	5.05	127.04	120.28
2	C	377	GLY	CA-C-N	5.05	127.94	120.82
2	C	377	GLY	C-N-CA	5.05	127.94	120.82
8	T	75	GLY	CA-C-O	-5.04	115.25	120.90
10	V	93	GLU	O-C-N	5.04	128.47	122.27
3	E	339	ILE	N-CA-C	-5.04	105.48	110.62
3	F	209	LEU	CA-C-O	-5.04	115.21	120.55
9	U	161	GLU	CA-C-N	5.04	127.03	120.28
9	U	161	GLU	C-N-CA	5.04	127.03	120.28
6	I	19	GLN	CA-C-N	5.04	127.03	120.28
6	I	19	GLN	C-N-CA	5.04	127.03	120.28
3	D	25	PHE	O-C-N	-5.04	117.05	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	T	238	THR	N-CA-C	-5.04	106.97	113.02
7	O	59	ASN	N-CA-C	-5.04	100.74	109.15
1	0	6	ALA	O-C-N	5.04	127.26	122.07
1	7	66	LEU	CA-C-O	-5.04	115.21	120.55
2	A	146	GLU	CA-C-O	-5.04	114.59	120.03
1	8	2	GLN	O-C-N	5.03	127.25	122.07
1	8	37	VAL	CA-C-N	5.03	127.96	120.31
1	8	37	VAL	C-N-CA	5.03	127.96	120.31
4	G	27	ALA	CA-C-O	-5.03	115.21	120.55
2	C	317	LYS	CA-C-N	5.03	131.15	121.54
2	C	317	LYS	C-N-CA	5.03	131.15	121.54
3	D	437	THR	N-CA-C	5.03	117.66	111.82
4	G	216	ASN	CA-C-N	5.03	127.96	120.31
4	G	216	ASN	C-N-CA	5.03	127.96	120.31
8	T	119	ILE	CA-C-N	5.03	126.98	120.44
8	T	119	ILE	C-N-CA	5.03	126.98	120.44
3	E	288	ASP	N-CA-C	5.03	116.76	111.28
14	Z	24	LEU	CA-C-N	5.03	126.89	120.56
14	Z	24	LEU	C-N-CA	5.03	126.89	120.56
1	0	47	VAL	CA-C-N	5.02	126.37	120.09
1	0	47	VAL	C-N-CA	5.02	126.37	120.09
2	C	56	GLU	N-CA-C	5.02	116.50	108.41
4	G	20	THR	CA-C-O	5.02	125.75	119.97
8	T	63	GLU	CA-C-N	5.02	127.01	120.28
8	T	63	GLU	C-N-CA	5.02	127.01	120.28
10	V	158	TRP	CA-C-N	5.02	128.46	121.02
10	V	158	TRP	C-N-CA	5.02	128.46	121.02
2	A	157	ALA	O-C-N	5.02	128.86	122.03
3	D	457	PHE	N-CA-C	-5.02	106.84	113.17
2	A	119	GLY	CA-C-O	-5.02	113.41	119.68
2	B	217	GLN	N-CA-C	5.02	116.83	111.36
9	U	156	SER	CA-C-O	5.02	125.74	120.42
1	3	3	LEU	N-CA-C	5.02	117.48	111.71
2	B	438	LEU	N-CA-C	5.02	117.50	110.23
2	C	248	ALA	CA-C-N	5.02	124.62	119.05
2	C	248	ALA	C-N-CA	5.02	124.62	119.05
2	C	75	ILE	N-CA-C	-5.01	100.67	107.99
4	G	232	ALA	N-CA-C	5.01	116.75	111.28
4	G	29	THR	N-CA-C	5.01	117.12	111.11
2	C	167	GLU	CA-C-O	5.01	125.88	120.32
8	T	218	ALA	O-C-N	-5.01	116.81	122.12
1	0	50	MET	CA-C-N	5.01	127.40	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	50	MET	C-N-CA	5.01	127.40	120.29
2	A	176	GLY	CA-C-N	5.01	127.25	120.44
2	A	176	GLY	C-N-CA	5.01	127.25	120.44
2	C	300	VAL	CA-C-N	5.01	127.40	120.29
2	C	300	VAL	C-N-CA	5.01	127.40	120.29
4	G	255	TYR	O-C-N	-5.01	116.81	122.12
1	2	32	ALA	CA-C-O	-5.01	115.24	120.55
12	X	26	GLY	N-CA-C	-5.01	106.72	112.73
1	7	33	LEU	N-CA-C	-5.01	105.71	111.07
2	B	74	GLY	N-CA-C	-5.01	101.31	113.18
3	D	293	GLN	N-CA-C	5.01	116.82	111.36
10	V	51	THR	CA-C-O	5.00	125.42	119.56
3	F	271	LEU	CA-C-N	5.00	126.98	120.28
3	F	271	LEU	C-N-CA	5.00	126.98	120.28

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	40	ASN	Peptide
1	5	40	ASN	Peptide
1	6	40	ASN	Peptide
1	7	40	ASN	Peptide
1	8	40	ASN	Peptide
1	9	40	ASN	Peptide
2	A	381	GLN	Peptide
2	B	323	LEU	Mainchain
3	D	256	ASP	Peptide
3	E	128	SER	Mainchain
3	F	256	ASP	Peptide
5	H	54	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	300	0	95	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	300	0	95	0	0
1	2	300	0	95	0	0
1	3	296	0	91	0	0
1	4	300	0	95	0	0
1	5	300	0	95	0	0
1	6	296	0	91	0	0
1	7	292	0	91	0	0
1	8	300	0	95	0	0
1	9	296	0	91	0	0
2	A	1996	0	570	0	0
2	B	2020	0	575	0	0
2	C	1992	0	572	0	0
3	D	1880	0	538	0	0
3	E	1872	0	537	0	0
3	F	1876	0	537	0	0
4	G	1060	0	277	0	0
5	H	479	0	122	0	0
6	I	193	0	43	0	0
7	O	748	0	205	0	0
8	T	897	0	248	0	0
9	U	620	0	158	0	0
10	V	685	0	173	0	0
11	W	340	0	92	0	0
12	X	248	0	61	0	0
13	Y	148	0	40	0	0
14	Z	193	0	49	0	0
All	All	20227	0	5731	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	73/76 (96%)	73 (100%)	0	0	100	100
1	1	73/76 (96%)	71 (97%)	1 (1%)	1 (1%)	9	40
1	2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
1	3	72/76 (95%)	69 (96%)	1 (1%)	2 (3%)	4	24
1	4	73/76 (96%)	70 (96%)	2 (3%)	1 (1%)	9	40
1	5	73/76 (96%)	71 (97%)	1 (1%)	1 (1%)	9	40
1	6	72/76 (95%)	69 (96%)	2 (3%)	1 (1%)	9	40
1	7	71/76 (93%)	69 (97%)	1 (1%)	1 (1%)	9	40
1	8	73/76 (96%)	70 (96%)	2 (3%)	1 (1%)	9	40
1	9	72/76 (95%)	70 (97%)	1 (1%)	1 (1%)	9	40
2	A	495/510 (97%)	462 (93%)	22 (4%)	11 (2%)	5	29
2	B	501/510 (98%)	464 (93%)	32 (6%)	5 (1%)	12	49
2	C	496/510 (97%)	459 (92%)	30 (6%)	7 (1%)	9	40
3	D	468/478 (98%)	432 (92%)	30 (6%)	6 (1%)	9	42
3	E	466/478 (98%)	426 (91%)	29 (6%)	11 (2%)	4	27
3	F	467/478 (98%)	431 (92%)	28 (6%)	8 (2%)	7	36
4	G	261/278 (94%)	242 (93%)	14 (5%)	5 (2%)	6	32
5	H	110/138 (80%)	98 (89%)	11 (10%)	1 (1%)	14	51
6	I	42/61 (69%)	40 (95%)	0	2 (5%)	2	16
7	O	185/195 (95%)	168 (91%)	14 (8%)	3 (2%)	7	38
8	T	222/249 (89%)	211 (95%)	6 (3%)	5 (2%)	5	28
9	U	153/209 (73%)	153 (100%)	0	0	100	100
10	V	169/173 (98%)	156 (92%)	8 (5%)	5 (3%)	3	23
11	W	83/95 (87%)	69 (83%)	9 (11%)	5 (6%)	1	13
12	X	60/92 (65%)	52 (87%)	6 (10%)	2 (3%)	3	21
13	Y	35/59 (59%)	32 (91%)	3 (9%)	0	100	100
14	Z	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
All	All	4984/5321 (94%)	4642 (93%)	257 (5%)	85 (2%)	9	36

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	41	PRO
1	3	41	PRO
1	4	41	PRO
1	5	41	PRO
1	6	41	PRO
1	7	41	PRO
1	8	41	PRO
1	9	41	PRO
2	A	226	ASP
2	A	229	LYS
2	A	379	ALA
2	C	379	ALA
3	D	110	LYS
3	E	28	SER
3	E	130	SER
3	E	314	ALA
3	E	396	LEU
3	F	278	ALA
3	F	279	VAL
4	G	56	GLU
7	O	63	SER
8	T	202	ASN
11	W	11	SER
11	W	42	ILE
12	X	14	THR
2	A	227	ALA
2	B	141	ARG
2	B	435	TYR
2	C	369	VAL
3	D	29	GLU
3	D	131	ALA
3	D	302	GLY
3	E	303	SER
3	F	178	HIS
4	G	85	GLY
8	T	50	ASN
8	T	148	ALA
10	V	84	ASP
10	V	158	TRP
11	W	3	THR
11	W	31	TYR
1	3	42	SER
2	A	333	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	478	HIS
2	C	71	GLY
2	C	103	PRO
2	C	134	LYS
3	E	209	LEU
3	E	277	SER
3	E	315	ASP
3	E	453	PRO
5	H	33	PRO
7	O	171	LEU
8	T	108	SER
10	V	89	LEU
10	V	166	ARG
2	A	103	PRO
2	A	435	TYR
3	F	86	PRO
3	F	131	ALA
6	I	42	ALA
10	V	131	ASP
11	W	48	LEU
2	A	26	ASN
2	A	311	ALA
2	B	8	THR
2	B	52	GLU
2	C	27	LEU
2	C	380	ALA
3	D	57	ASN
3	D	86	PRO
3	E	16	VAL
4	G	181	PRO
4	G	198	GLU
3	F	8	PRO
3	F	34	LEU
4	G	138	PRO
6	I	60	THR
2	A	140	PRO
3	E	279	VAL
8	T	77	ILE
12	X	33	PRO
2	A	367	ILE
3	F	453	PRO
7	O	10	VAL

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

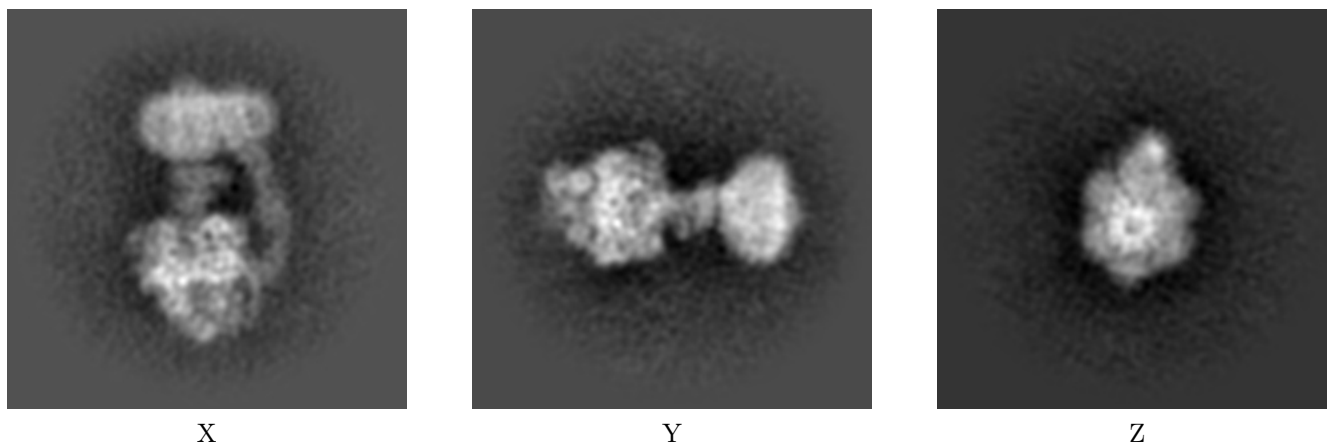
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25957. These allow visual inspection of the internal detail of the map and identification of artifacts.

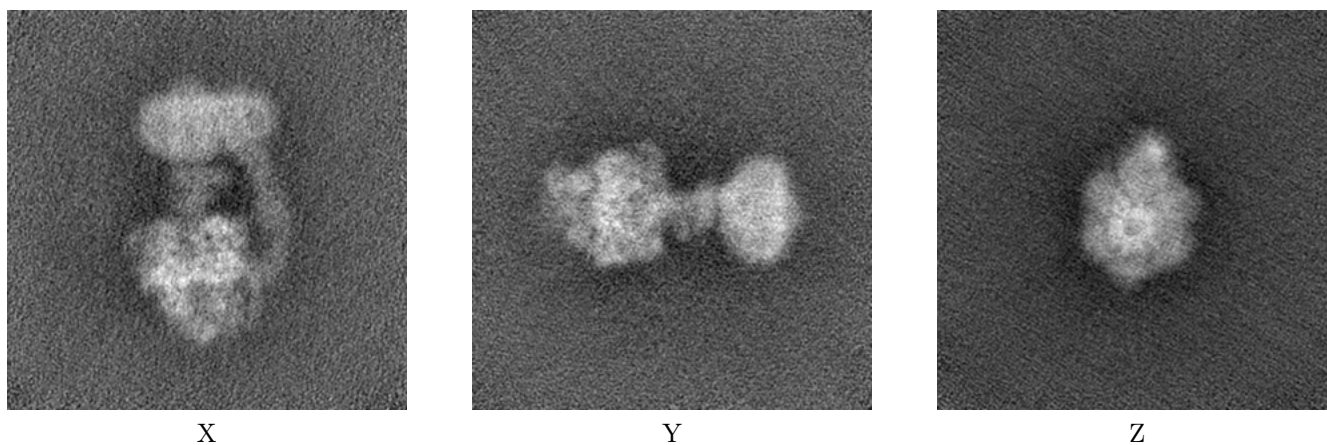
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



6.1.2 Raw map



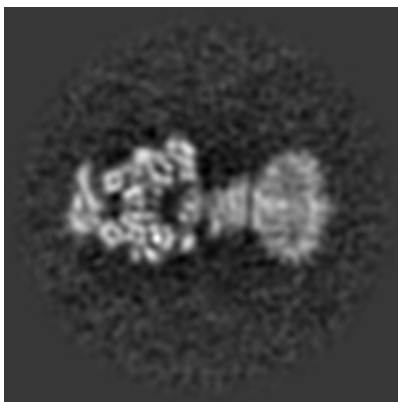
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

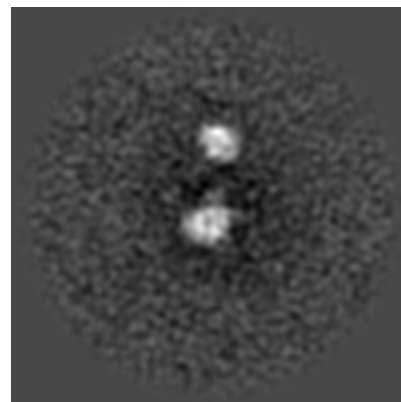
6.2.1 Primary map



X Index: 128



Y Index: 128

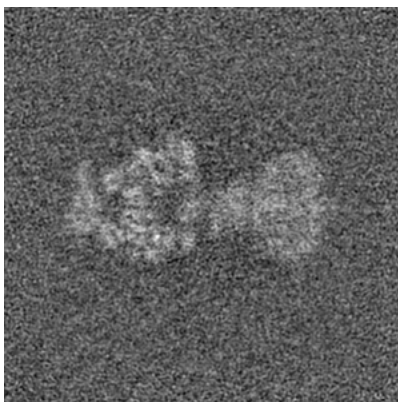


Z Index: 128

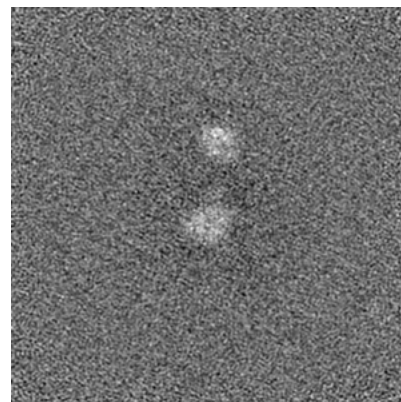
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

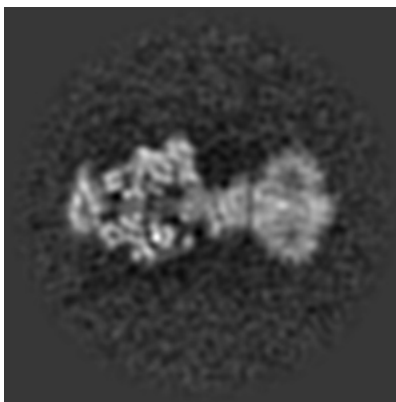
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

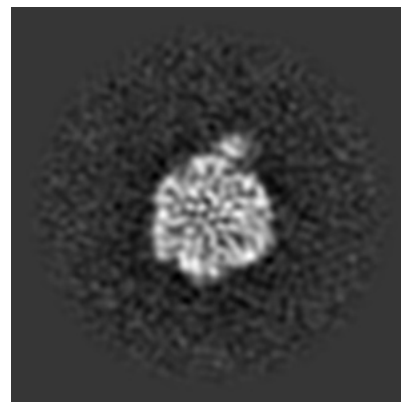
6.3.1 Primary map



X Index: 129

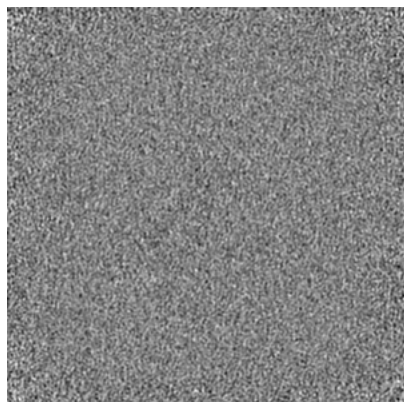


Y Index: 126

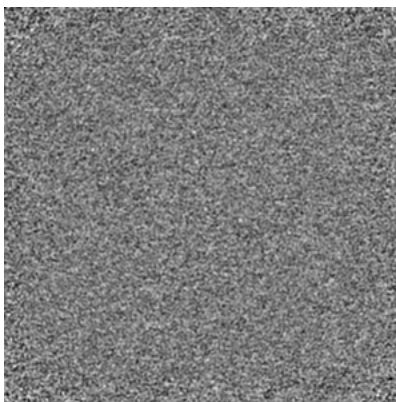


Z Index: 85

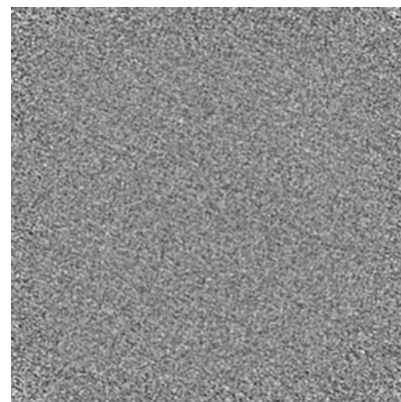
6.3.2 Raw map



X Index: 0



Y Index: 0

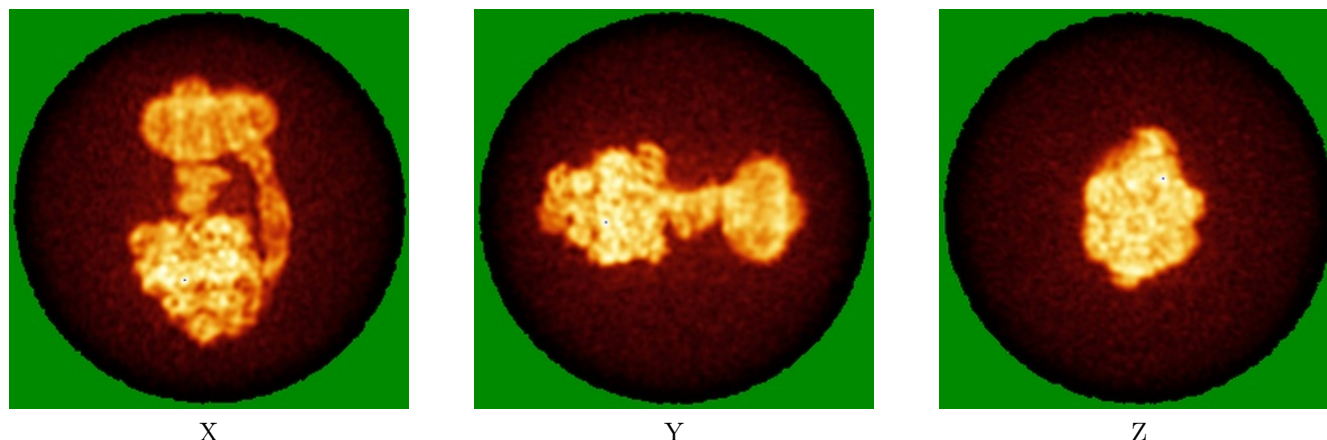


Z Index: 0

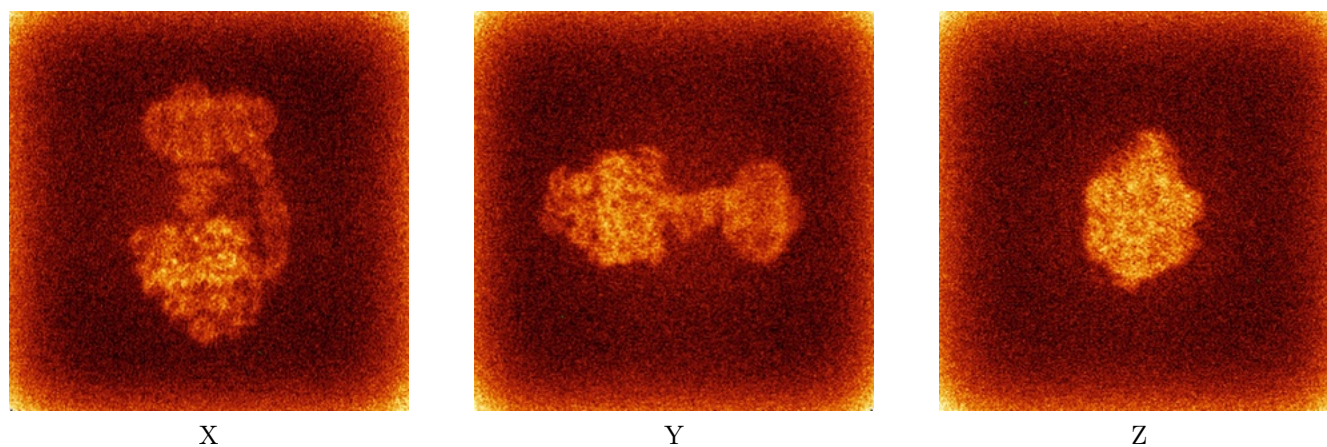
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



6.4.2 Raw map



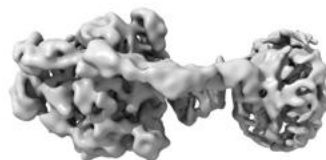
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



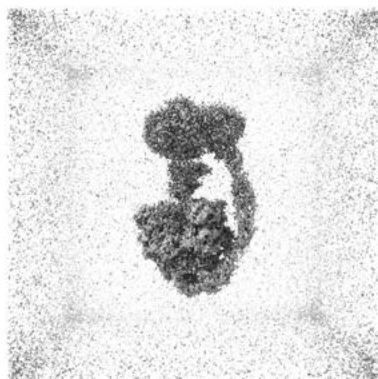
Y



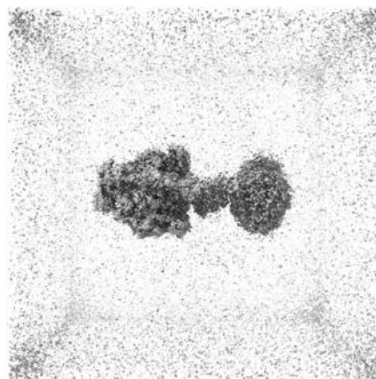
Z

The images above show the 3D surface view of the map at the recommended contour level 0.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

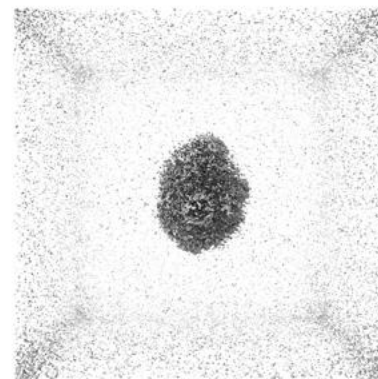
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

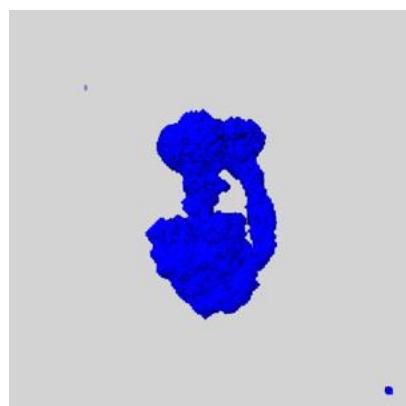
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

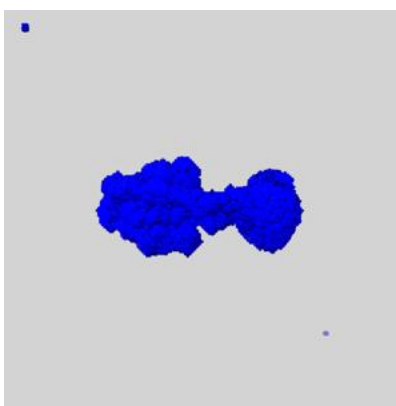
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

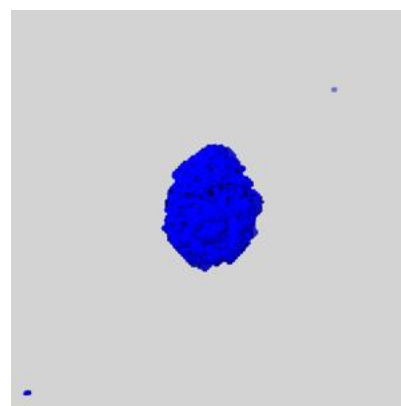
6.6.1 emd_25957_msk_1.map [i](#)



X



Y

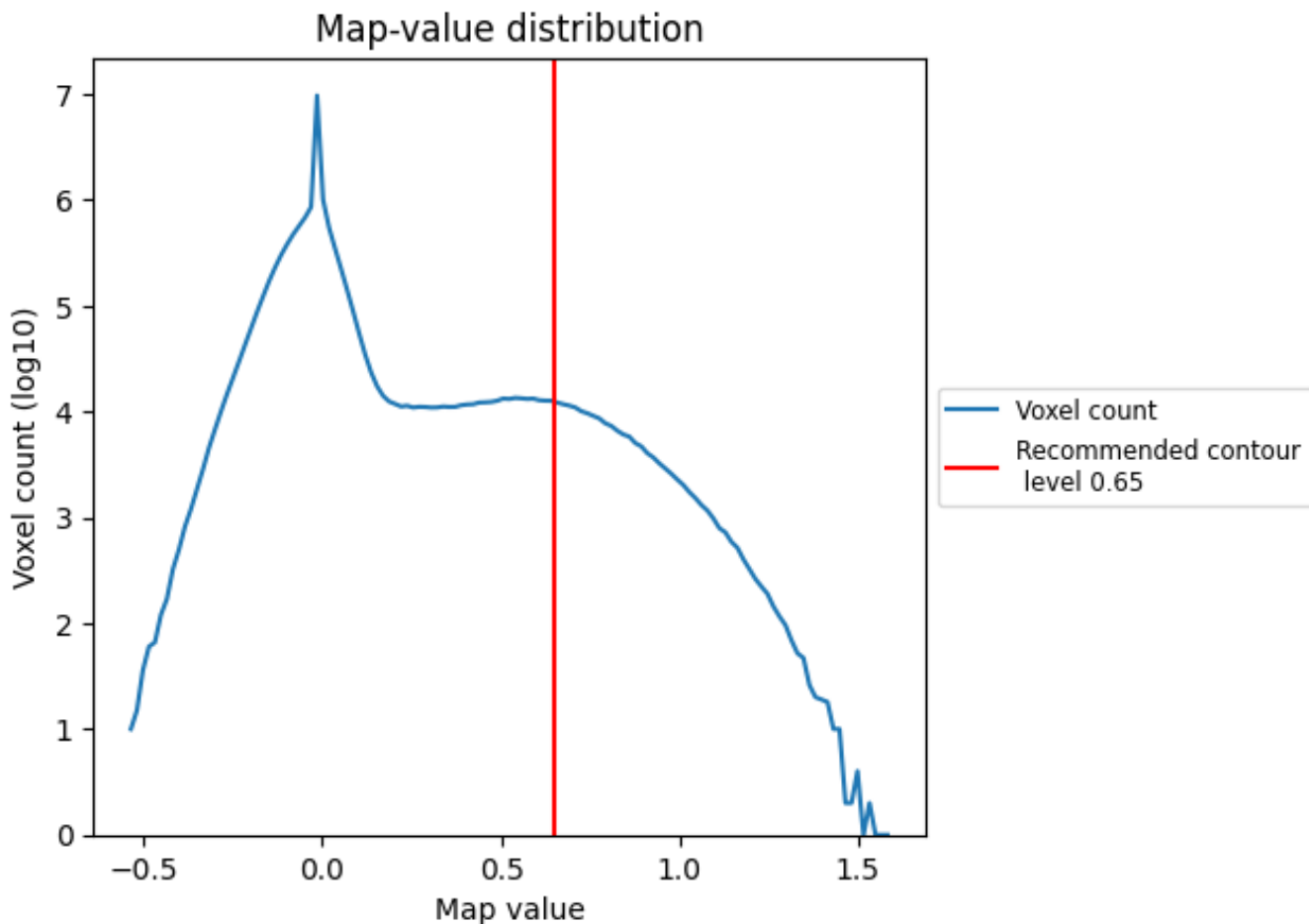


Z

7 Map analysis [i](#)

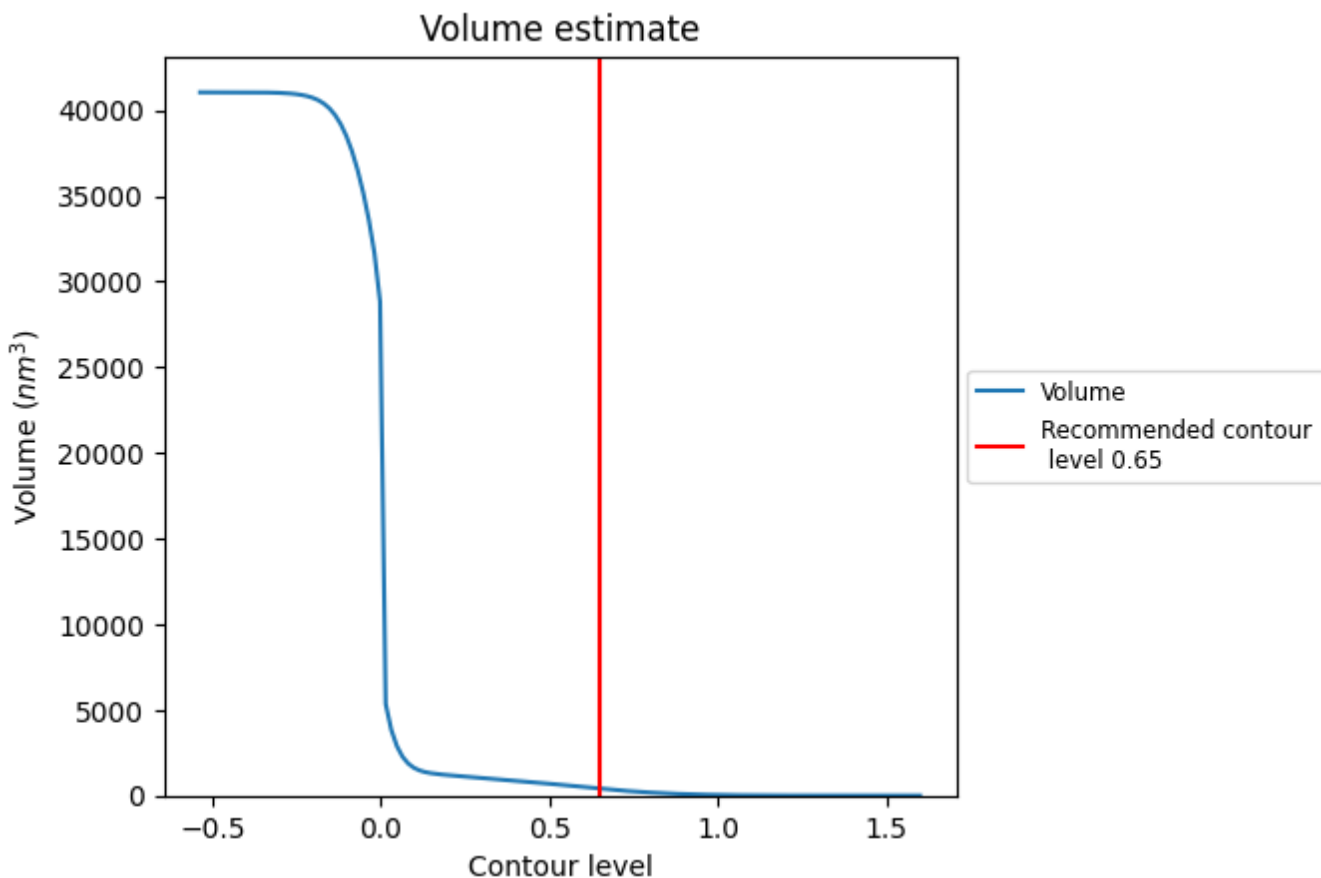
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

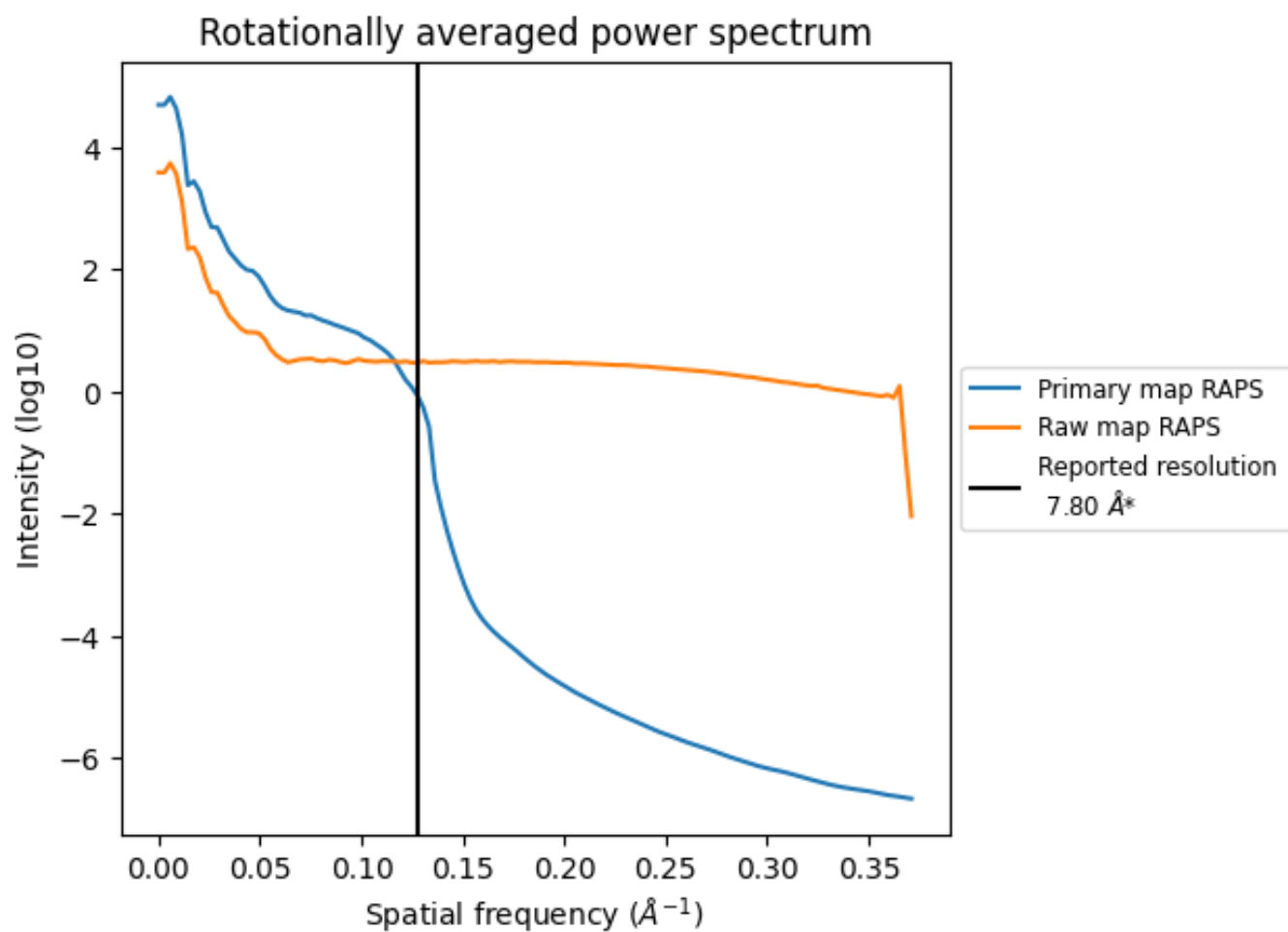
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404 nm³; this corresponds to an approximate mass of 365 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

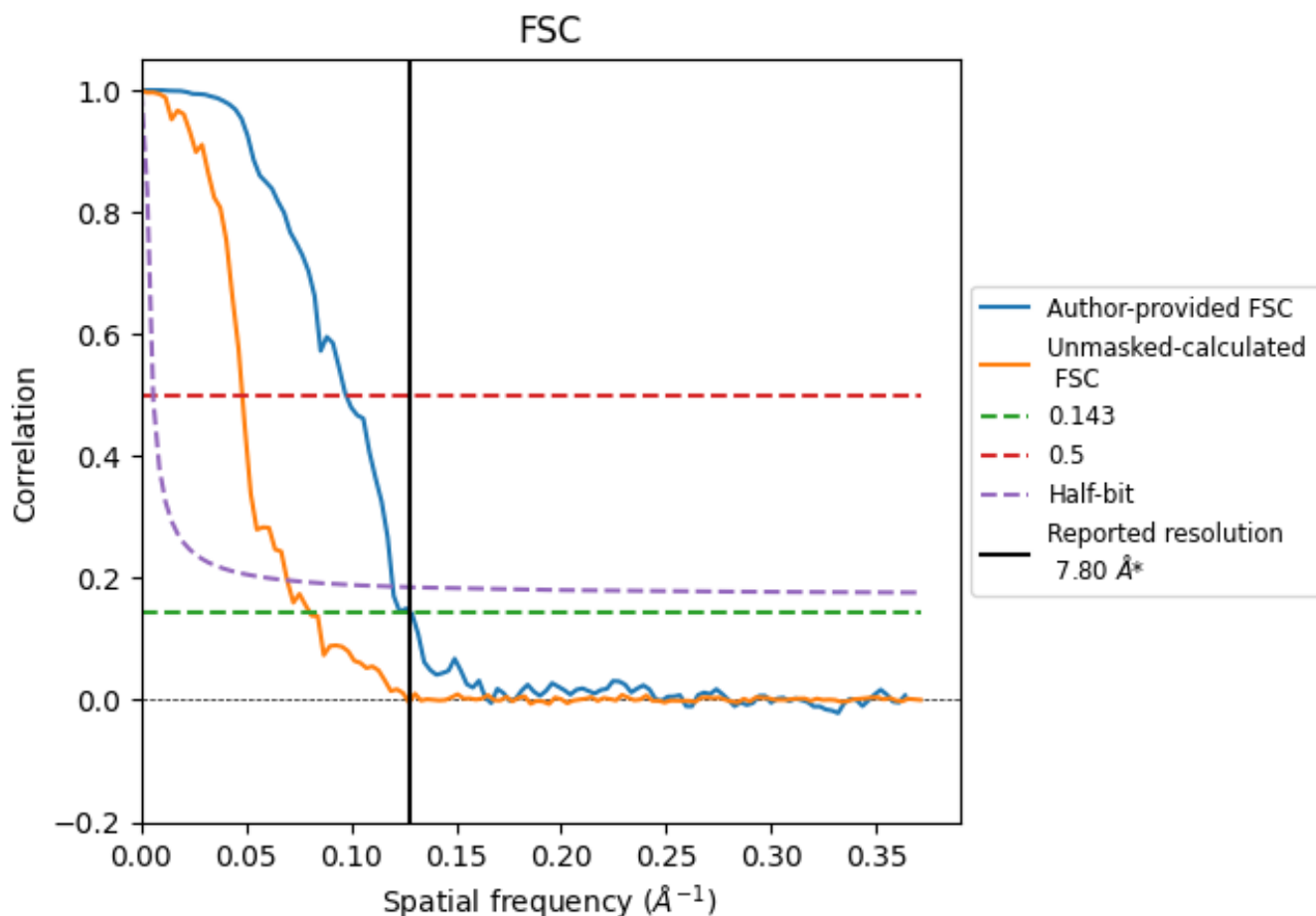


*Reported resolution corresponds to spatial frequency of 0.128 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.128 Å⁻¹

8.2 Resolution estimates

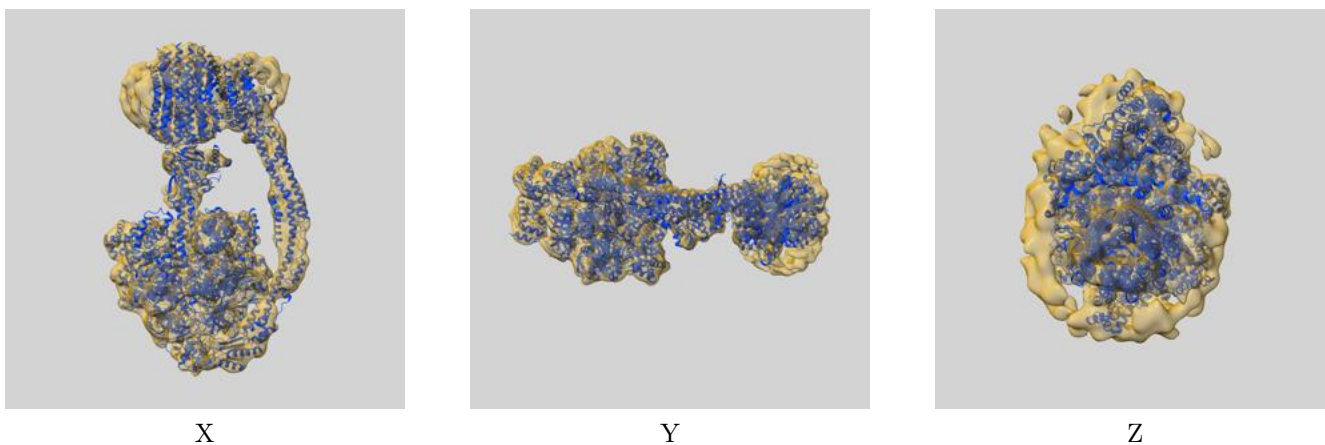
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.80	-	-
Author-provided FSC curve	7.79	10.25	8.35
Unmasked-calculated*	12.44	20.79	14.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 12.44 differs from the reported value 7.8 by more than 10 %

9 Map-model fit [i](#)

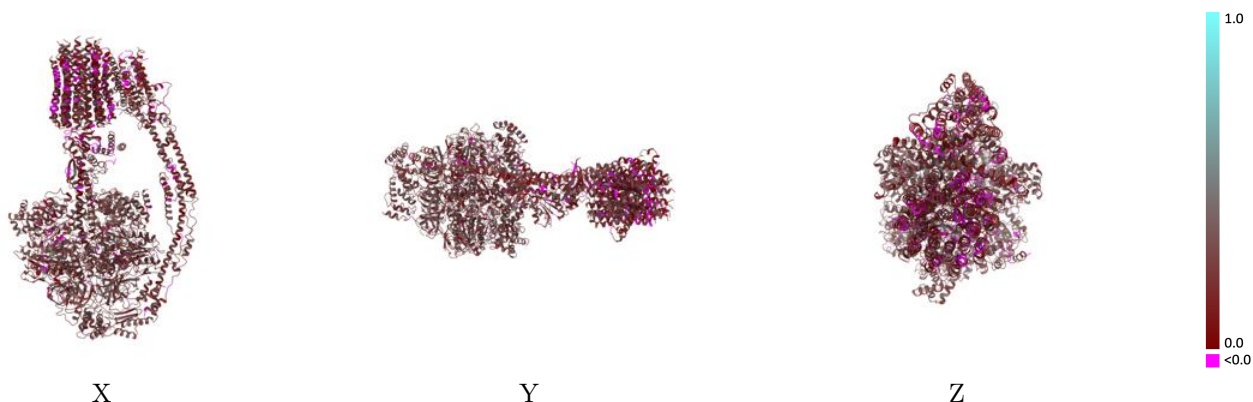
This section contains information regarding the fit between EMDB map EMD-25957 and PDB model 7TK5. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



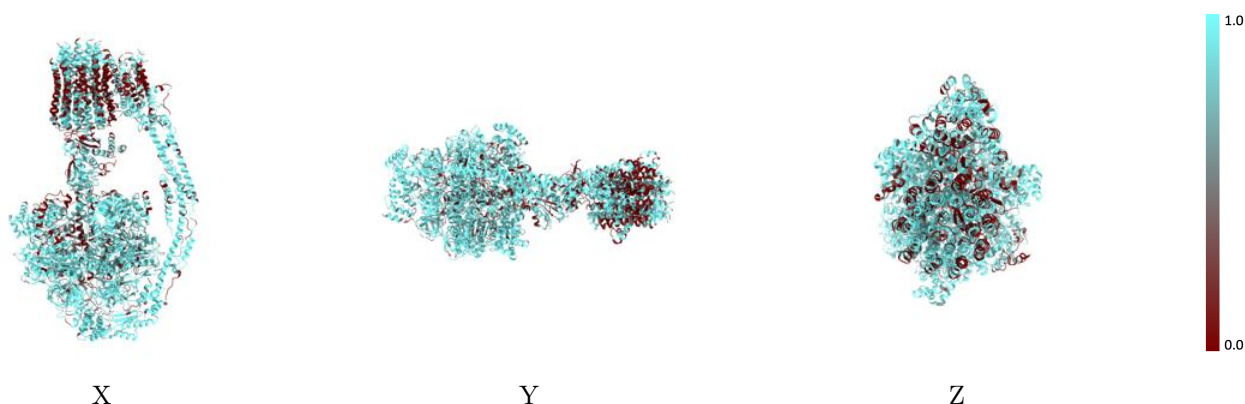
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



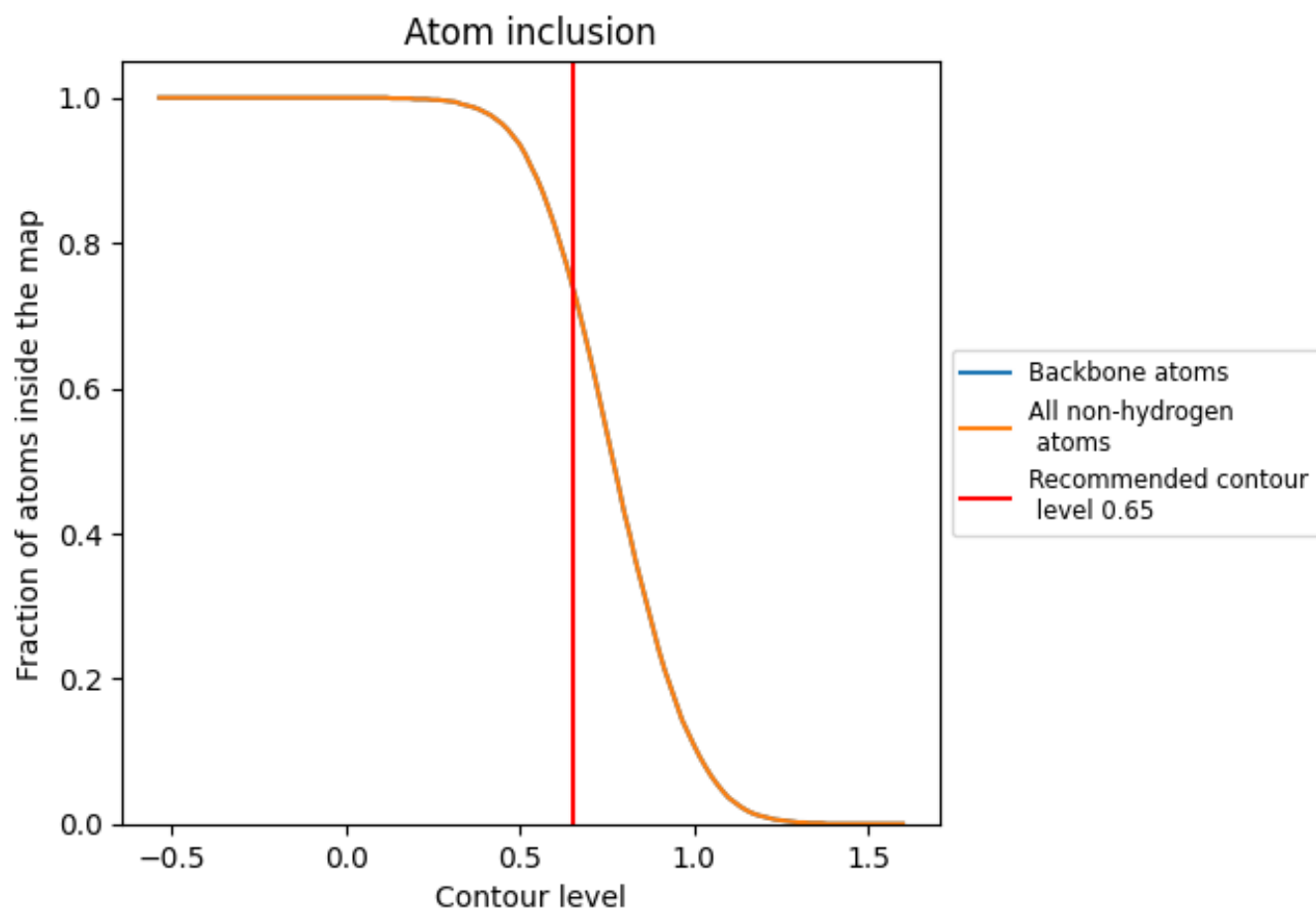
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.65).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7420	 0.2110
0	 0.5170	 0.1570
1	 0.5300	 0.1600
2	 0.4870	 0.0910
3	 0.6320	 0.1980
4	 0.5230	 0.1400
5	 0.5200	 0.1150
6	 0.6790	 0.1760
7	 0.6920	 0.1620
8	 0.5600	 0.1250
9	 0.6010	 0.1320
A	 0.8320	 0.2520
B	 0.8470	 0.2310
C	 0.8430	 0.2490
D	 0.7740	 0.2400
E	 0.7220	 0.2200
F	 0.8430	 0.2420
G	 0.6750	 0.1910
H	 0.4470	 0.1130
I	 0.4400	 0.1370
O	 0.9080	 0.2470
T	 0.5560	 0.1950
U	 0.9050	 0.2280
V	 0.8250	 0.2090
W	 0.6240	 0.1450
X	 0.5520	 0.1490
Y	 0.5950	 0.1350
Z	 0.5860	 0.1290

