



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:04 AM UTC

PDB ID : 1YKP / pdb_00001ykp
Title : Protocatechuate 3,4-Dioxygenase Y408H mutant bound to DHB
Authors : Brown, C.K.; Ohlendorf, D.H.
Deposited on : 2005-01-18
Resolution : 2.41 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

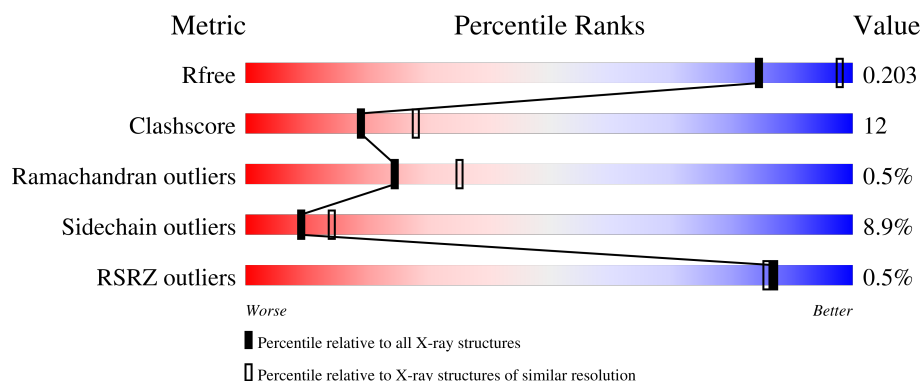
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	200	32% 54% 12% .
1	C	200	2% 31% 54% 14% .
1	E	200	36% 51% 11% .
1	G	200	% 34% 50% 14% .
1	I	200	34% 52% 12% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	200	
2	B	238	
2	D	238	
2	F	238	
2	H	238	
2	J	238	
2	L	238	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CME	F	429	-	X	-	-
2	CME	H	429	-	X	-	-
2	CME	L	429	-	X	-	-
3	DHB	A	550	-	-	X	-
3	DHB	H	3550	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21546 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Protocatechuate 3,4-dioxygenase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	C	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	E	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	G	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	I	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	K	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			

- Molecule 2 is a protein called Protocatechuate 3,4-dioxygenase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	D	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	F	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	H	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	J	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	L	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			

There are 12 discrepancies between the modelled and reference sequences:

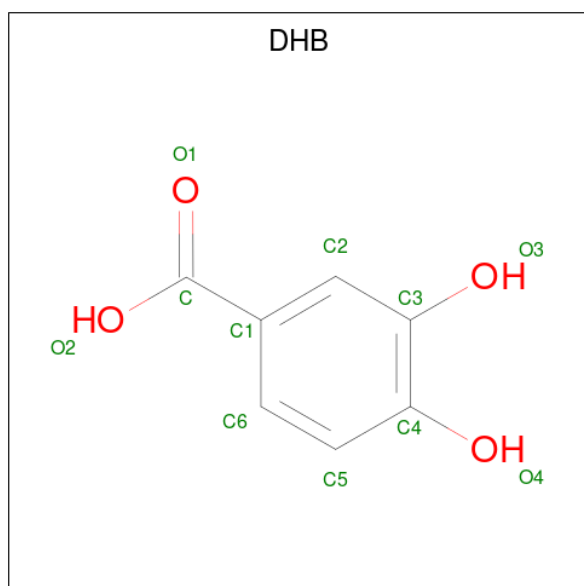
Chain	Residue	Modelled	Actual	Comment	Reference
B	408	HIS	TYR	engineered mutation	UNP P00437

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	429	CME	CYS	modified residue	UNP P00437
D	408	HIS	TYR	engineered mutation	UNP P00437
D	429	CME	CYS	modified residue	UNP P00437
F	408	HIS	TYR	engineered mutation	UNP P00437
F	429	CME	CYS	modified residue	UNP P00437
H	408	HIS	TYR	engineered mutation	UNP P00437
H	429	CME	CYS	modified residue	UNP P00437
J	408	HIS	TYR	engineered mutation	UNP P00437
J	429	CME	CYS	modified residue	UNP P00437
L	408	HIS	TYR	engineered mutation	UNP P00437
L	429	CME	CYS	modified residue	UNP P00437

- Molecule 3 is 3,4-DIHYDROXYBENZOIC ACID (CCD ID: DHB) (formula: $C_7H_6O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	7	4		
3	D	1	Total	C	O	0	0
			11	7	4		
3	F	1	Total	C	O	0	0
			11	7	4		
3	H	1	Total	C	O	0	0
			11	7	4		
3	J	1	Total	C	O	0	0
			11	7	4		
3	L	1	Total	C	O	0	0
			11	7	4		

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Fe 1 1	0	0
4	D	1	Total Fe 1 1	0	0
4	F	1	Total Fe 1 1	0	0
4	H	1	Total Fe 1 1	0	0
4	J	1	Total Fe 1 1	0	0
4	L	1	Total Fe 1 1	0	0

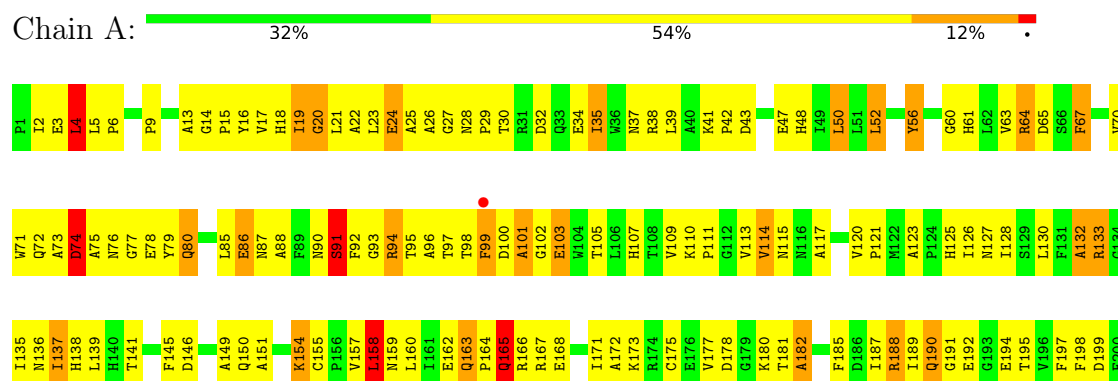
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	47	Total O 47 47	0	0
5	B	83	Total O 83 83	0	0
5	C	45	Total O 45 45	0	0
5	D	87	Total O 87 87	0	0
5	E	49	Total O 49 49	0	0
5	F	82	Total O 82 82	0	0
5	G	49	Total O 49 49	0	0
5	H	83	Total O 83 83	0	0
5	I	46	Total O 46 46	0	0
5	J	85	Total O 85 85	0	0
5	K	43	Total O 43 43	0	0
5	L	87	Total O 87 87	0	0

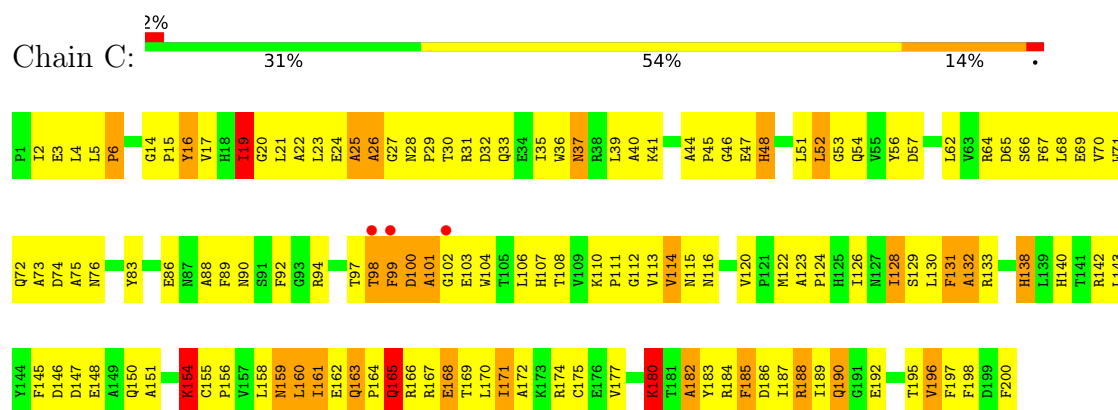
3 Residue-property plots

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

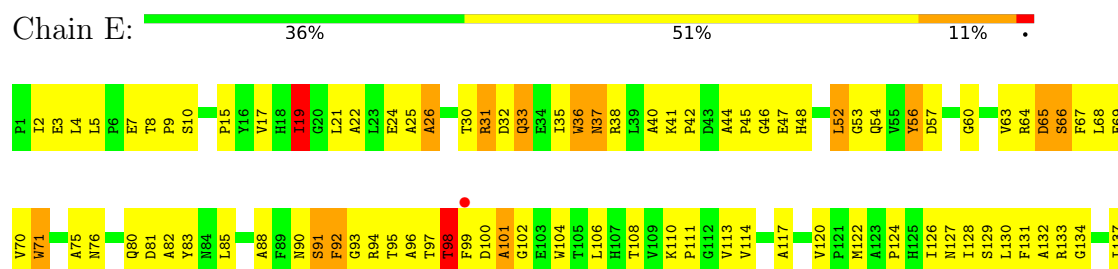
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain





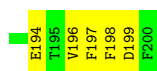
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



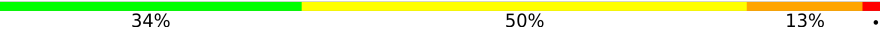
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

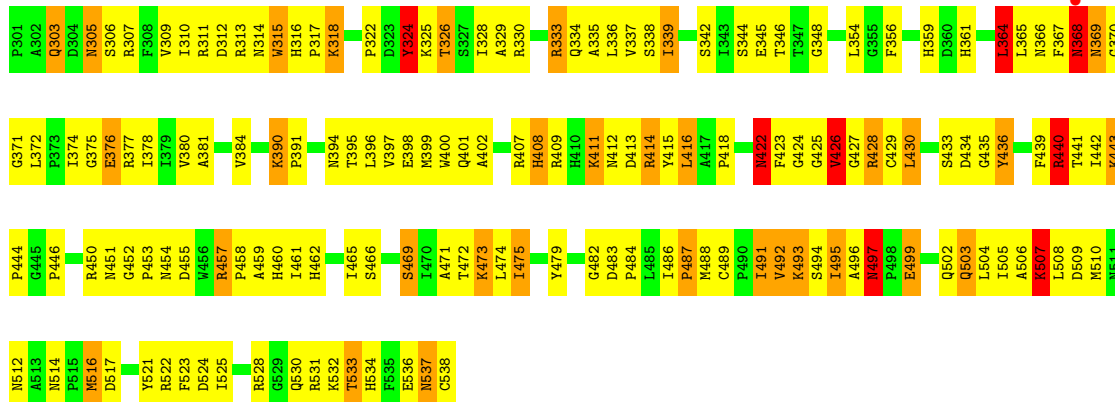


• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

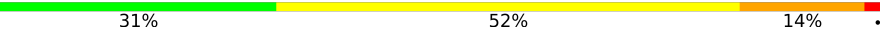


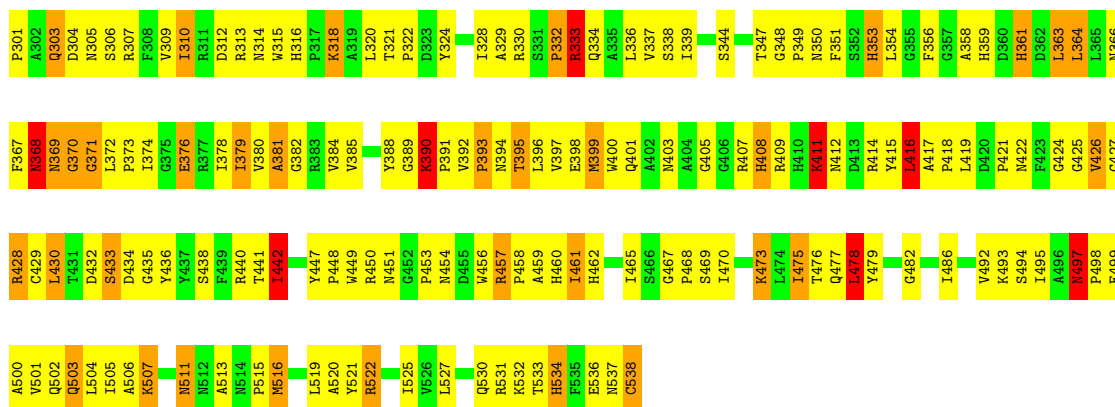
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain B:  34% 50% 13% .



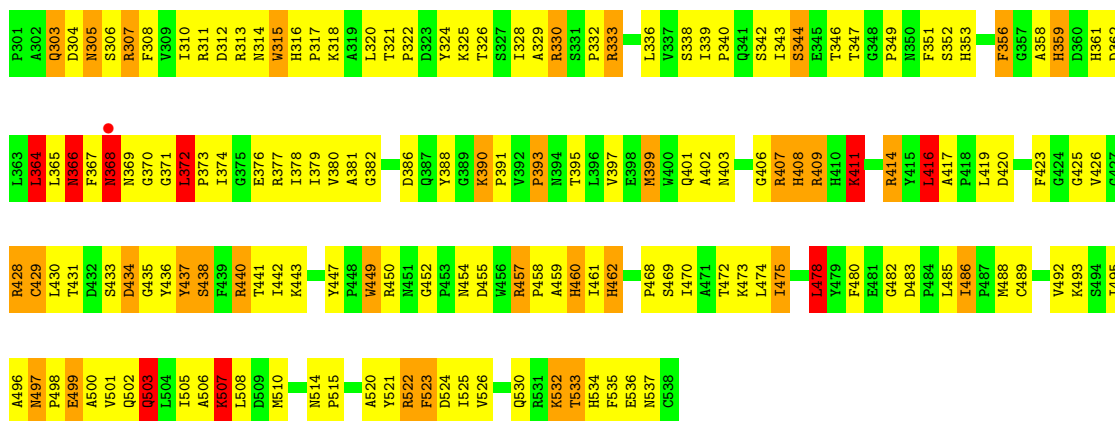
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain D:  31% 52% 14% .

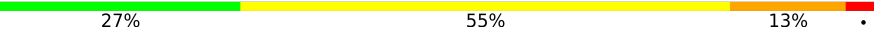


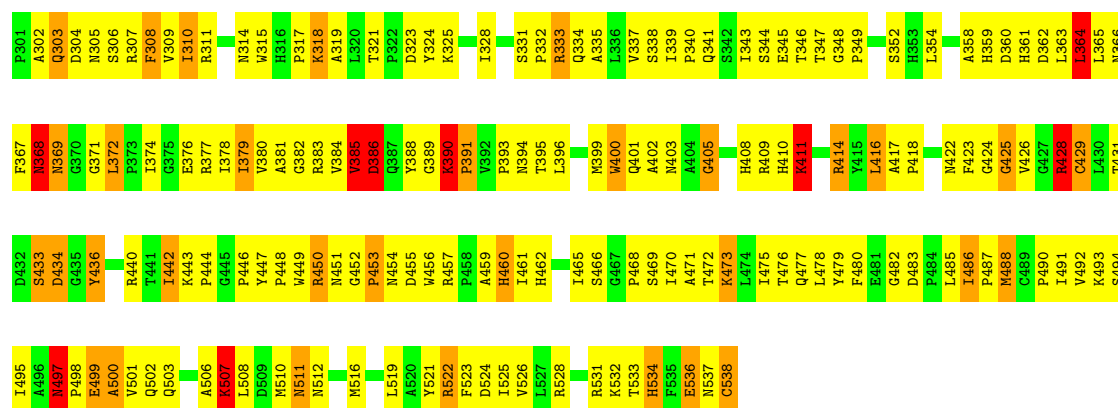
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain F:  33% 49% 14% .

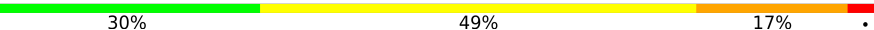


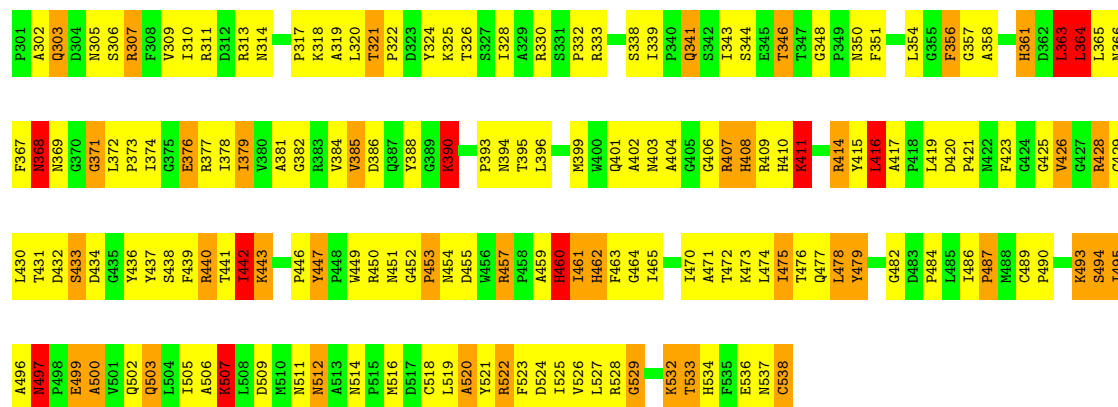
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain H:  27% 55% 13% .



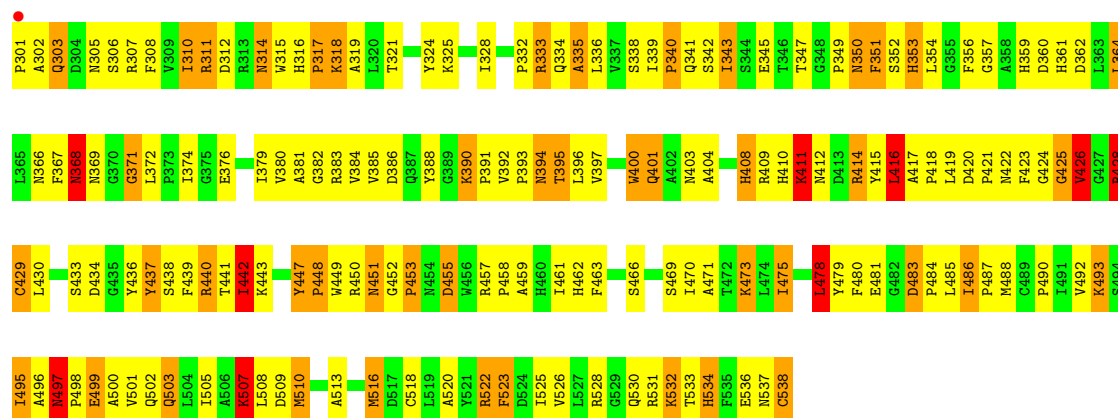
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain J:  30% 49% 17% .



• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain L:  29% 48% 19% .



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.19Å 127.97Å 134.18Å 90.00° 97.68° 90.00°	Depositor
Resolution (Å)	30.37 – 2.41 30.37 – 2.41	Depositor EDS
% Data completeness (in resolution range)	72.4 (30.37-2.41) 72.6 (30.37-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.145 , 0.211 0.144 , 0.203	Depositor DCC
R_{free} test set	1950 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21546	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FE, CME, DHB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.92	150/1611 (9.3%)	2.12	68/2195 (3.1%)
1	C	2.97	160/1611 (9.9%)	2.30	82/2195 (3.7%)
1	E	2.92	150/1611 (9.3%)	2.16	57/2195 (2.6%)
1	G	2.97	164/1611 (10.2%)	2.18	68/2195 (3.1%)
1	I	2.96	146/1611 (9.1%)	2.17	59/2195 (2.7%)
1	K	3.22	176/1611 (10.9%)	2.21	74/2195 (3.4%)
2	B	2.95	168/1922 (8.7%)	2.19	84/2615 (3.2%)
2	D	2.97	184/1922 (9.6%)	2.18	67/2615 (2.6%)
2	F	2.89	160/1922 (8.3%)	2.18	80/2615 (3.1%)
2	H	2.91	162/1922 (8.4%)	2.20	80/2615 (3.1%)
2	J	3.02	185/1922 (9.6%)	2.21	95/2615 (3.6%)
2	L	3.05	175/1922 (9.1%)	2.22	99/2615 (3.8%)
All	All	2.98	1980/21198 (9.3%)	2.19	913/28860 (3.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	7
1	E	0	5
1	G	0	6
1	I	0	4
1	K	0	9
2	B	0	9
2	D	0	6
2	F	0	6
2	H	0	5
2	J	0	8

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	6
All	All	0	75

All (1980) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	532	LYS	CA-CB	22.14	1.90	1.53
1	K	121	PRO	C-O	20.52	1.48	1.23
2	H	303	GLN	CA-CB	20.13	1.84	1.53
1	A	101	ALA	CA-CB	19.33	1.77	1.52
2	J	303	GLN	CA-CB	18.32	1.82	1.53
2	D	303	GLN	CA-CB	17.49	1.80	1.53
2	L	303	GLN	CA-CB	16.75	1.79	1.53
2	B	303	GLN	CA-CB	16.56	1.82	1.53
2	L	403	ASN	C-O	15.51	1.39	1.23
2	F	303	GLN	CA-CB	15.28	1.80	1.53
2	J	409	ARG	CA-C	14.77	1.72	1.52
2	H	381	ALA	CA-CB	-14.75	1.28	1.54
2	F	532	LYS	CA-CB	14.56	1.76	1.53
2	J	532	LYS	CA-CB	14.50	1.76	1.53
1	C	98	THR	N-CA	13.73	1.63	1.45
2	D	390	LYS	CA-C	-13.65	1.37	1.53
1	E	149	ALA	CA-CB	-13.54	1.30	1.53
2	L	516	MET	SD-CE	12.53	2.10	1.79
2	J	368	ASN	N-CA	12.44	1.62	1.46
2	B	324	TYR	CA-C	12.43	1.69	1.52
2	D	310	ILE	C-O	12.38	1.38	1.24
2	H	461	ILE	CA-CB	-12.36	1.39	1.54
2	D	525	ILE	CA-CB	-12.33	1.39	1.54
1	C	100	ASP	N-CA	12.30	1.60	1.46
2	B	486	ILE	CA-CB	-11.95	1.47	1.54
2	H	507	LYS	CE-NZ	11.85	1.84	1.49
1	C	107	HIS	C-O	-11.76	1.10	1.24
2	L	532	LYS	CA-C	11.75	1.68	1.52
2	J	403	ASN	C-O	11.69	1.38	1.23
1	C	88	ALA	CA-C	11.54	1.68	1.52
2	H	405	GLY	C-O	11.53	1.39	1.23
2	D	500	ALA	CA-CB	-11.38	1.34	1.53
2	H	337	VAL	N-CA	11.29	1.60	1.46
2	H	417	ALA	CA-CB	-11.29	1.38	1.53
1	E	189	ILE	N-CA	-11.20	1.32	1.46
2	F	532	LYS	CA-C	11.20	1.68	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	101	ALA	C-N	11.10	1.48	1.33
1	K	89	PHE	C-O	11.06	1.36	1.24
1	I	199	ASP	C-O	11.06	1.36	1.23
2	J	384	VAL	CA-CB	11.04	1.67	1.54
1	E	122	MET	SD-CE	-10.98	1.52	1.79
1	E	46	GLY	C-O	-10.97	1.13	1.23
2	L	369	ASN	C-O	10.95	1.36	1.23
2	L	448	PRO	C-O	10.92	1.35	1.23
2	H	385	VAL	C-O	10.90	1.35	1.23
1	E	46	GLY	CA-C	-10.88	1.40	1.52
1	C	47	GLU	C-O	-10.84	1.10	1.24
1	A	103	GLU	C-O	-10.78	1.10	1.23
2	L	508	LEU	C-O	-10.78	1.10	1.23
1	K	44	ALA	CA-CB	10.73	1.68	1.53
1	C	98	THR	CA-C	10.73	1.66	1.52
2	J	475	ILE	C-O	10.71	1.34	1.24
1	K	173	LYS	CA-CB	10.70	1.66	1.53
2	D	366	ASN	C-O	-10.67	1.10	1.24
2	F	339	ILE	CA-CB	10.59	1.66	1.55
2	D	306	SER	C-O	-10.58	1.10	1.23
1	K	73	ALA	CA-C	10.58	1.66	1.52
2	J	419	LEU	C-O	10.50	1.38	1.23
1	I	189	ILE	CA-CB	-10.50	1.39	1.54
1	I	180	LYS	CA-C	10.49	1.65	1.52
2	J	496	ALA	CA-CB	10.45	1.69	1.53
1	K	40	ALA	C-O	10.43	1.36	1.23
2	B	303	GLN	CA-C	10.37	1.65	1.52
1	G	101	ALA	CA-CB	10.34	1.65	1.52
2	L	475	ILE	C-O	10.29	1.35	1.24
2	L	525	ILE	CA-C	10.20	1.65	1.52
2	H	389	GLY	C-O	-10.15	1.11	1.24
1	I	161	ILE	CA-C	10.15	1.64	1.52
2	H	380	VAL	C-O	-10.14	1.13	1.24
1	K	180	LYS	CA-C	10.13	1.65	1.52
1	I	97	THR	C-O	10.13	1.36	1.24
1	I	135	ILE	CA-CB	10.12	1.65	1.53
2	B	488	MET	SD-CE	-10.11	1.54	1.79
2	D	380	VAL	CA-CB	10.11	1.67	1.54
1	A	111	PRO	C-O	-10.07	1.12	1.23
1	C	172	ALA	CA-C	10.05	1.65	1.52
2	H	403	ASN	C-O	10.04	1.35	1.23
2	L	426	VAL	CB-CG2	-10.03	1.19	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	333	ARG	CZ-NH2	10.00	1.46	1.33
2	B	415	TYR	CA-C	9.98	1.65	1.52
1	E	137	ILE	C-O	9.97	1.33	1.24
1	C	94	ARG	C-O	-9.96	1.11	1.23
2	L	347	THR	CA-C	9.88	1.65	1.52
1	K	71	TRP	C-O	9.86	1.34	1.23
2	D	507	LYS	CE-NZ	9.85	1.78	1.49
2	B	509	ASP	C-O	9.83	1.35	1.23
2	H	532	LYS	CA-CB	9.82	1.69	1.53
1	C	35	ILE	CA-CB	-9.81	1.42	1.53
2	J	414	ARG	NE-CZ	9.80	1.43	1.33
1	K	181	THR	C-O	9.80	1.35	1.23
1	I	98	THR	N-CA	9.79	1.58	1.45
2	L	488	MET	SD-CE	-9.78	1.55	1.79
2	J	357	GLY	C-O	9.77	1.35	1.23
2	F	500	ALA	CA-CB	-9.74	1.37	1.53
1	E	189	ILE	CA-C	-9.72	1.40	1.52
1	K	64	ARG	CZ-NH1	9.72	1.46	1.32
2	L	420	ASP	C-O	9.70	1.35	1.24
2	L	303	GLN	CA-C	9.69	1.64	1.52
2	B	492	VAL	C-O	-9.68	1.13	1.24
2	H	532	LYS	CA-C	9.67	1.65	1.52
2	B	409	ARG	CA-C	9.67	1.64	1.53
1	A	198	PHE	C-O	-9.66	1.11	1.23
1	C	100	ASP	CA-C	9.64	1.64	1.52
1	A	136	ASN	CA-C	-9.62	1.39	1.52
1	E	98	THR	N-CA	9.61	1.57	1.45
2	F	532	LYS	N-CA	9.60	1.58	1.45
2	D	417	ALA	CA-CB	-9.56	1.40	1.53
2	H	378	ILE	C-O	-9.52	1.13	1.23
2	L	400	TRP	CA-C	-9.52	1.40	1.52
2	L	507	LYS	CE-NZ	9.51	1.77	1.49
1	K	57	ASP	C-O	9.49	1.34	1.23
1	G	88	ALA	CA-CB	-9.45	1.38	1.53
1	K	47	GLU	CD-OE2	9.45	1.43	1.25
2	D	392	VAL	CA-CB	9.43	1.66	1.54
2	J	390	LYS	CG-CD	9.43	1.80	1.52
2	B	315	TRP	CA-C	9.42	1.65	1.52
1	A	17	VAL	CA-C	9.41	1.65	1.52
1	G	188	ARG	C-O	9.40	1.34	1.24
2	B	337	VAL	C-O	9.39	1.33	1.24
1	G	36	TRP	CA-C	9.38	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	144	TYR	C-O	9.38	1.36	1.23
2	D	368	ASN	C-O	9.38	1.35	1.24
2	J	354	LEU	C-O	9.37	1.35	1.23
1	E	173	LYS	CA-CB	9.37	1.66	1.53
2	B	536	GLU	C-O	9.37	1.35	1.24
1	E	94	ARG	C-O	-9.35	1.12	1.23
1	E	96	ALA	CA-CB	-9.34	1.38	1.53
2	L	525	ILE	CA-CB	-9.34	1.42	1.54
2	H	354	LEU	C-O	9.32	1.35	1.23
1	K	45	PRO	C-O	9.31	1.34	1.23
1	E	98	THR	CA-C	9.31	1.64	1.52
1	C	100	ASP	CB-CG	9.28	1.75	1.52
2	D	492	VAL	C-O	-9.27	1.12	1.24
2	B	510	MET	SD-CE	-9.26	1.56	1.79
1	K	33	GLN	CA-C	9.24	1.64	1.52
1	C	102	GLY	CA-C	9.23	1.64	1.51
2	F	525	ILE	CA-CB	-9.22	1.41	1.55
1	I	116	ASN	CA-C	9.21	1.66	1.53
1	I	169	THR	C-O	-9.20	1.12	1.24
1	G	65	ASP	C-O	9.20	1.35	1.24
1	G	16	TYR	C-O	9.20	1.36	1.24
2	F	368	ASN	CA-C	9.19	1.65	1.52
2	J	396	LEU	C-O	9.19	1.35	1.24
2	F	461	ILE	C-O	-9.18	1.15	1.24
1	K	7	GLU	CA-C	9.17	1.64	1.52
2	J	309	VAL	CA-CB	9.16	1.63	1.54
1	A	163	GLN	CG-CD	9.14	1.75	1.52
1	A	185	PHE	C-O	-9.14	1.13	1.23
2	B	532	LYS	C-O	9.14	1.35	1.23
1	K	177	VAL	CA-CB	9.12	1.66	1.53
1	I	74	ASP	C-O	9.12	1.35	1.23
2	J	537	ASN	CA-C	9.09	1.65	1.53
2	L	423	PHE	C-O	9.08	1.34	1.23
1	A	79	TYR	CA-C	-9.08	1.41	1.52
2	F	378	ILE	N-CA	-9.08	1.35	1.46
1	G	98	THR	N-CA	9.07	1.59	1.46
2	B	495	ILE	C-O	-9.07	1.14	1.24
2	J	426	VAL	N-CA	9.06	1.56	1.46
2	B	381	ALA	CA-CB	-9.05	1.37	1.53
2	L	333	ARG	CZ-NH1	9.04	1.45	1.32
2	J	318	LYS	C-O	9.01	1.35	1.23
1	C	64	ARG	C-O	-9.00	1.12	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	475	ILE	CA-CB	-9.00	1.43	1.54
2	B	523	PHE	CA-C	9.00	1.62	1.53
2	H	488	MET	SD-CE	-8.98	1.57	1.79
2	L	352	SER	C-O	8.97	1.35	1.24
1	G	132	ALA	CA-CB	-8.95	1.38	1.53
2	J	462	HIS	N-CA	8.95	1.56	1.46
1	A	60	GLY	C-O	-8.93	1.11	1.24
2	D	516	MET	SD-CE	8.92	2.01	1.79
2	B	328	ILE	C-O	8.91	1.33	1.24
2	L	532	LYS	C-O	8.90	1.34	1.23
1	G	122	MET	SD-CE	-8.89	1.57	1.79
1	I	98	THR	CA-C	8.88	1.63	1.52
1	K	188	ARG	CA-C	8.87	1.63	1.52
1	C	188	ARG	CZ-NH1	8.86	1.45	1.32
1	A	126	ILE	C-O	-8.84	1.15	1.24
1	G	55	VAL	CA-CB	-8.82	1.43	1.54
2	D	390	LYS	CG-CD	8.82	1.78	1.52
1	A	93	GLY	C-O	8.79	1.32	1.23
2	L	486	ILE	CA-C	8.78	1.62	1.52
1	C	180	LYS	CG-CD	8.76	1.78	1.52
2	F	459	ALA	C-O	8.76	1.34	1.23
2	H	347	THR	CA-C	8.75	1.63	1.52
1	K	82	ALA	CA-CB	8.74	1.63	1.52
2	D	486	ILE	CA-CB	-8.73	1.43	1.54
1	K	163	GLN	CG-CD	8.73	1.73	1.52
2	L	453	PRO	C-O	-8.72	1.13	1.24
1	K	41	LYS	CA-C	8.71	1.64	1.53
1	K	80	GLN	C-O	8.70	1.35	1.23
1	K	45	PRO	CA-C	8.70	1.63	1.52
1	K	47	GLU	CD-OE1	8.70	1.41	1.25
1	C	69	GLU	C-O	8.70	1.35	1.24
2	J	438	SER	C-O	8.70	1.34	1.23
2	H	494	SER	CA-C	8.69	1.64	1.52
1	K	143	LEU	C-O	8.69	1.34	1.23
1	C	56	TYR	C-O	-8.68	1.13	1.23
1	G	154	LYS	CD-CE	8.68	1.78	1.52
2	J	434	ASP	CG-OD2	8.66	1.41	1.25
1	K	78	GLU	CD-OE1	8.66	1.41	1.25
1	G	98	THR	CA-C	8.65	1.65	1.53
2	H	443	LYS	C-O	-8.65	1.13	1.24
2	H	499	GLU	CA-C	-8.65	1.40	1.52
1	K	123	ALA	CA-C	8.65	1.63	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	309	VAL	CA-CB	8.64	1.63	1.54
1	K	13	ALA	CA-CB	-8.64	1.38	1.53
1	A	150	GLN	CA-C	-8.63	1.42	1.52
2	B	434	ASP	N-CA	-8.61	1.35	1.46
1	E	8	THR	CA-CB	-8.61	1.41	1.53
2	B	532	LYS	CA-CB	8.61	1.67	1.53
1	K	88	ALA	CA-CB	8.61	1.66	1.53
2	D	461	ILE	CA-CB	-8.61	1.42	1.54
1	G	56	TYR	CA-C	-8.59	1.42	1.52
2	B	507	LYS	CD-CE	8.59	1.78	1.52
1	I	88	ALA	CA-C	8.58	1.63	1.52
2	F	368	ASN	CA-CB	8.57	1.68	1.53
2	F	523	PHE	C-O	-8.57	1.14	1.24
1	C	39	LEU	CA-C	-8.56	1.40	1.52
1	K	109	VAL	CA-CB	8.56	1.66	1.54
1	A	149	ALA	CA-CB	-8.55	1.39	1.53
2	L	371	GLY	C-O	8.55	1.32	1.23
2	B	493	LYS	CA-C	8.54	1.64	1.52
2	F	520	ALA	CA-C	-8.53	1.42	1.52
2	D	536	GLU	C-O	8.53	1.34	1.23
2	F	366	ASN	C-O	-8.52	1.13	1.24
2	B	397	VAL	C-O	-8.51	1.14	1.24
1	I	64	ARG	CZ-NH1	8.51	1.44	1.32
1	A	64	ARG	CZ-NH1	8.50	1.44	1.32
2	J	434	ASP	CG-OD1	8.50	1.41	1.25
2	F	502	GLN	C-O	-8.49	1.13	1.24
1	A	101	ALA	C-N	8.49	1.44	1.33
1	E	113	VAL	CA-CB	8.48	1.63	1.54
1	E	150	GLN	CA-C	-8.48	1.42	1.52
1	A	172	ALA	CA-C	8.48	1.63	1.52
1	G	64	ARG	NE-CZ	8.47	1.42	1.33
1	G	100	ASP	CA-C	8.47	1.63	1.52
2	D	376	GLU	CD-OE2	8.47	1.41	1.25
1	K	155	CYS	C-O	8.46	1.35	1.24
2	F	486	ILE	C-O	-8.46	1.17	1.24
2	F	382	GLY	CA-C	-8.45	1.43	1.52
1	A	177	VAL	C-O	8.44	1.34	1.24
1	K	98	THR	CA-C	8.43	1.63	1.52
2	D	537	ASN	N-CA	8.43	1.59	1.46
2	J	461	ILE	N-CA	8.43	1.56	1.46
2	L	324	TYR	CD1-CE1	8.42	1.64	1.38
2	B	461	ILE	CA-CB	-8.42	1.44	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	128	ILE	C-O	8.42	1.33	1.24
1	K	171	ILE	N-CA	8.41	1.56	1.46
2	J	390	LYS	CD-CE	8.41	1.77	1.52
2	D	428	ARG	CA-C	-8.41	1.35	1.52
1	C	151	ALA	CA-C	8.39	1.63	1.52
2	F	478	LEU	CA-C	8.36	1.63	1.52
2	F	336	LEU	C-O	8.35	1.33	1.23
2	D	537	ASN	CA-CB	8.34	1.66	1.53
1	I	145	PHE	C-O	8.34	1.34	1.24
2	D	492	VAL	CA-C	-8.34	1.41	1.52
1	C	98	THR	CA-CB	8.33	1.67	1.53
2	L	502	GLN	C-O	-8.33	1.13	1.24
2	L	368	ASN	CA-C	8.32	1.64	1.52
1	K	113	VAL	CA-C	8.32	1.64	1.52
1	A	97	THR	C-O	8.32	1.34	1.23
1	K	163	GLN	CD-NE2	8.31	1.50	1.33
2	D	395	THR	CA-CB	-8.30	1.40	1.53
1	E	70	VAL	C-O	-8.29	1.15	1.23
2	J	450	ARG	CZ-NH1	8.29	1.44	1.32
1	C	126	ILE	CA-CB	-8.28	1.44	1.54
2	J	328	ILE	CA-CB	8.26	1.64	1.54
1	G	154	LYS	CA-C	8.26	1.65	1.52
2	F	402	ALA	CA-C	8.25	1.64	1.53
1	E	47	GLU	N-CA	-8.24	1.36	1.46
1	G	7	GLU	C-O	8.24	1.34	1.23
2	J	388	TYR	CZ-OH	8.24	1.55	1.38
2	D	432	ASP	C-O	8.23	1.32	1.23
1	K	47	GLU	CA-C	8.23	1.64	1.52
1	G	189	ILE	C-O	-8.23	1.12	1.24
1	K	28	ASN	C-O	8.23	1.32	1.24
1	K	176	GLU	N-CA	8.22	1.56	1.45
2	B	369	ASN	C-O	8.21	1.35	1.23
2	D	450	ARG	CZ-NH1	8.21	1.44	1.32
1	E	8	THR	C-O	-8.20	1.14	1.24
2	L	538	CYS	CA-C	8.19	1.70	1.52
2	D	390	LYS	CD-CE	8.18	1.77	1.52
2	F	344	SER	C-O	-8.18	1.13	1.24
1	E	165	GLN	CG-CD	8.18	1.72	1.52
2	L	350	ASN	N-CA	-8.18	1.36	1.46
2	B	317	PRO	CA-C	8.18	1.63	1.52
2	L	410	HIS	CA-C	-8.17	1.41	1.52
1	E	97	THR	CB-CG2	-8.14	1.25	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	154	LYS	CD-CE	8.14	1.76	1.52
2	L	530	GLN	CA-C	-8.14	1.42	1.52
1	K	165	GLN	CG-CD	8.13	1.72	1.52
2	B	505	ILE	N-CA	8.13	1.55	1.46
1	C	106	LEU	CA-CB	-8.13	1.39	1.53
2	L	396	LEU	CA-C	8.13	1.63	1.52
1	I	192	GLU	CD-OE2	8.13	1.40	1.25
1	K	11	GLN	C-O	8.13	1.34	1.23
1	G	185	PHE	C-O	-8.12	1.14	1.23
1	G	50	LEU	CA-C	8.11	1.62	1.52
2	D	530	GLN	CA-C	8.10	1.62	1.52
2	D	434	ASP	C-O	8.10	1.34	1.24
2	D	303	GLN	CA-C	8.10	1.62	1.52
2	B	318	LYS	CE-NZ	8.10	1.73	1.49
2	B	486	ILE	CA-C	8.09	1.60	1.52
1	K	178	ASP	C-O	8.08	1.35	1.23
2	H	349	PRO	C-O	-8.07	1.14	1.23
1	E	154	LYS	CE-NZ	8.06	1.73	1.49
1	I	19	ILE	N-CA	-8.05	1.36	1.46
1	G	162	GLU	CA-C	-8.05	1.42	1.52
1	K	181	THR	CA-C	8.04	1.63	1.52
2	J	507	LYS	CD-CE	8.04	1.76	1.52
2	L	414	ARG	NE-CZ	8.03	1.41	1.33
1	G	190	GLN	N-CA	-8.02	1.35	1.45
1	C	195	THR	N-CA	-8.02	1.35	1.45
1	A	107	HIS	C-O	-8.01	1.14	1.24
2	B	368	ASN	CA-C	8.01	1.63	1.52
1	I	47	GLU	CD-OE2	8.01	1.40	1.25
1	C	138	HIS	CA-C	-8.00	1.42	1.53
2	L	459	ALA	CA-C	8.00	1.63	1.52
2	D	370	GLY	C-O	7.99	1.34	1.23
2	H	455	ASP	CA-C	-7.99	1.42	1.52
2	D	332	PRO	C-O	-7.99	1.14	1.23
2	J	516	MET	CA-C	-7.99	1.42	1.52
2	D	389	GLY	C-O	-7.99	1.13	1.24
1	I	185	PHE	CE2-CZ	7.98	1.62	1.38
1	K	129	SER	C-O	7.98	1.33	1.24
2	J	368	ASN	C-O	7.98	1.34	1.24
1	G	33	GLN	C-O	-7.98	1.14	1.24
2	B	499	GLU	CD-OE1	7.97	1.40	1.25
1	G	163	GLN	CD-OE1	7.97	1.38	1.23
2	H	414	ARG	CB-CG	7.97	1.76	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	436	TYR	C-O	-7.95	1.14	1.23
1	G	130	LEU	CA-C	7.94	1.62	1.52
2	H	390	LYS	CA-C	-7.93	1.42	1.53
1	A	94	ARG	C-O	-7.92	1.14	1.23
2	D	368	ASN	N-CA	7.91	1.56	1.46
2	F	411	LYS	CG-CD	7.91	1.76	1.52
2	H	503	GLN	CA-CB	-7.90	1.40	1.53
1	K	3	GLU	C-O	7.90	1.33	1.24
1	K	124	PRO	CA-C	7.90	1.63	1.52
2	H	343	ILE	CA-C	7.88	1.64	1.52
1	G	100	ASP	N-CA	7.87	1.55	1.46
2	B	345	GLU	CA-C	7.87	1.63	1.52
2	J	369	ASN	C-O	7.86	1.31	1.23
1	C	3	GLU	CA-C	7.84	1.62	1.52
1	A	73	ALA	CA-CB	-7.84	1.40	1.53
1	K	101	ALA	C-N	7.84	1.43	1.33
1	A	168	GLU	N-CA	-7.84	1.36	1.46
2	D	414	ARG	CA-C	7.83	1.65	1.52
2	F	473	LYS	C-O	7.83	1.33	1.23
1	C	65	ASP	CA-CB	-7.82	1.42	1.53
2	B	525	ILE	CA-CB	-7.82	1.44	1.54
2	L	451	ASN	C-O	-7.81	1.14	1.24
2	F	450	ARG	CZ-NH1	7.80	1.43	1.32
1	A	163	GLN	CA-C	-7.79	1.43	1.52
2	D	333	ARG	CZ-NH1	7.79	1.43	1.32
2	B	450	ARG	CA-C	-7.78	1.44	1.53
2	D	426	VAL	CB-CG2	-7.78	1.26	1.52
2	B	303	GLN	C-O	7.78	1.33	1.23
1	E	104	TRP	C-O	-7.78	1.14	1.23
2	L	302	ALA	CA-C	7.78	1.63	1.52
2	B	390	LYS	CD-CE	7.77	1.75	1.52
1	I	94	ARG	C-O	-7.75	1.14	1.23
2	L	436	TYR	CD2-CE2	7.75	1.61	1.38
1	C	64	ARG	CZ-NH1	7.75	1.43	1.32
1	E	117	ALA	CA-CB	-7.75	1.39	1.53
1	C	188	ARG	NE-CZ	7.75	1.41	1.33
2	L	531	ARG	CZ-NH2	7.75	1.43	1.33
1	K	97	THR	C-O	7.74	1.33	1.24
1	C	92	PHE	N-CA	-7.74	1.36	1.46
2	D	373	PRO	C-O	7.73	1.32	1.23
2	J	526	VAL	C-O	7.73	1.32	1.24
2	H	456	TRP	CA-C	-7.72	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	409	ARG	CA-C	7.72	1.62	1.53
1	C	130	LEU	C-O	7.71	1.33	1.24
1	I	198	PHE	CA-C	-7.71	1.42	1.53
2	F	507	LYS	CD-CE	7.71	1.75	1.52
1	I	144	TYR	C-O	7.71	1.33	1.23
1	A	97	THR	CA-C	7.70	1.61	1.52
1	G	65	ASP	CA-CB	-7.70	1.39	1.53
2	H	383	ARG	CZ-NH2	7.70	1.43	1.33
1	I	165	GLN	CA-CB	7.69	1.66	1.53
2	J	462	HIS	CA-CB	-7.68	1.40	1.53
2	D	538	CYS	CA-C	7.68	1.69	1.52
2	D	470	ILE	CG1-CD1	-7.67	1.21	1.51
2	H	374	ILE	CA-C	7.67	1.61	1.52
2	J	538	CYS	CA-C	7.67	1.69	1.52
2	H	459	ALA	CA-CB	-7.66	1.41	1.53
1	G	99	PHE	CD2-CE2	7.66	1.61	1.38
1	C	100	ASP	CA-CB	7.65	1.65	1.53
1	G	188	ARG	CZ-NH1	7.65	1.43	1.32
1	I	174	ARG	CZ-NH2	7.64	1.43	1.33
1	E	98	THR	CA-CB	7.64	1.65	1.53
1	E	142	ARG	CA-C	-7.64	1.43	1.52
2	H	400	TRP	C-O	-7.63	1.14	1.23
1	G	127	ASN	N-CA	7.63	1.55	1.46
1	K	98	THR	N-CA	7.60	1.55	1.45
1	I	55	VAL	CA-C	7.60	1.62	1.52
2	L	417	ALA	CA-CB	-7.58	1.40	1.53
2	F	478	LEU	C-O	-7.58	1.14	1.23
1	G	64	ARG	CA-C	-7.58	1.42	1.52
1	K	88	ALA	C-O	7.58	1.32	1.24
1	E	5	LEU	CA-C	7.58	1.60	1.53
2	L	459	ALA	N-CA	7.58	1.55	1.46
1	C	165	GLN	CG-CD	7.57	1.71	1.52
2	L	319	ALA	CA-CB	-7.57	1.41	1.53
2	H	450	ARG	CZ-NH1	7.56	1.43	1.32
1	E	108	THR	CA-C	7.55	1.62	1.53
1	G	100	ASP	CA-CB	7.55	1.65	1.53
1	I	177	VAL	CA-CB	7.54	1.64	1.54
2	H	364	LEU	CA-C	7.54	1.62	1.52
1	I	57	ASP	CA-C	-7.53	1.42	1.53
1	K	115	ASN	CG-OD1	7.53	1.37	1.23
2	L	357	GLY	C-O	7.53	1.34	1.23
2	H	442	ILE	CB-CG1	-7.52	1.38	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	450	ARG	CZ-NH2	7.52	1.43	1.33
2	L	496	ALA	C-O	-7.52	1.15	1.24
1	A	126	ILE	CA-C	7.51	1.61	1.52
1	A	13	ALA	CA-C	-7.50	1.42	1.52
1	K	27	GLY	C-O	7.50	1.34	1.23
1	K	54	GLN	C-O	7.50	1.33	1.23
1	C	100	ASP	C-O	7.49	1.32	1.24
1	I	163	GLN	C-O	-7.48	1.15	1.24
2	F	493	LYS	N-CA	-7.47	1.35	1.46
1	A	182	ALA	CA-C	-7.47	1.43	1.52
2	B	414	ARG	NE-CZ	7.46	1.41	1.33
2	H	402	ALA	CA-C	7.46	1.63	1.53
1	E	150	GLN	CD-OE1	7.46	1.37	1.23
1	E	92	PHE	N-CA	-7.46	1.36	1.45
2	L	341	GLN	N-CA	7.45	1.55	1.46
2	D	349	PRO	C-O	7.45	1.32	1.23
1	C	99	PHE	CA-C	7.43	1.62	1.52
1	G	54	GLN	CA-C	7.43	1.62	1.52
1	C	115	ASN	C-O	-7.40	1.14	1.23
2	L	340	PRO	C-O	7.39	1.32	1.23
2	D	409	ARG	CA-C	7.38	1.62	1.53
1	G	177	VAL	CA-CB	7.38	1.63	1.53
2	J	367	PHE	C-O	7.38	1.35	1.23
2	D	403	ASN	C-O	7.38	1.33	1.23
2	L	440	ARG	CZ-NH1	7.37	1.43	1.32
2	F	390	LYS	CD-CE	7.36	1.74	1.52
2	J	361	HIS	C-O	-7.36	1.13	1.24
2	L	414	ARG	CD-NE	7.36	1.56	1.46
1	G	184	ARG	N-CA	-7.36	1.37	1.46
2	B	339	ILE	CG1-CD1	7.35	1.80	1.51
1	I	126	ILE	CA-CB	-7.35	1.45	1.54
2	F	370	GLY	C-O	7.34	1.33	1.23
1	E	168	GLU	N-CA	-7.34	1.36	1.46
1	A	125	HIS	CA-C	-7.33	1.43	1.52
1	C	29	PRO	CA-C	7.32	1.61	1.52
1	A	114	VAL	CB-CG2	-7.31	1.28	1.52
1	G	17	VAL	C-O	7.31	1.33	1.24
1	E	101	ALA	C-N	7.31	1.43	1.33
1	K	128	ILE	CA-C	7.31	1.61	1.52
2	F	338	SER	C-O	-7.30	1.15	1.23
2	J	538	CYS	CB-SG	-7.30	1.57	1.81
2	D	333	ARG	C-O	-7.30	1.14	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	188	ARG	NE-CZ	7.29	1.41	1.33
2	J	482	GLY	CA-C	7.29	1.62	1.51
2	L	333	ARG	CZ-NH2	7.29	1.43	1.33
1	A	146	ASP	CA-C	-7.28	1.42	1.52
1	E	128	ILE	CA-CB	-7.28	1.45	1.54
2	D	363	LEU	CG-CD2	-7.27	1.28	1.52
2	H	501	VAL	CA-CB	-7.27	1.45	1.54
2	B	368	ASN	CA-CB	7.26	1.65	1.53
2	H	449	TRP	CZ3-CH2	7.26	1.58	1.40
2	L	499	GLU	CD-OE1	7.26	1.39	1.25
2	F	522	ARG	CA-C	7.25	1.61	1.52
2	L	534	HIS	CA-C	7.25	1.61	1.52
2	L	303	GLN	C-O	7.25	1.32	1.23
2	L	531	ARG	N-CA	7.25	1.55	1.45
2	H	536	GLU	C-O	7.25	1.32	1.23
2	L	368	ASN	C-O	7.24	1.33	1.24
2	D	403	ASN	CA-C	7.23	1.62	1.53
1	K	92	PHE	C-O	7.23	1.32	1.24
1	A	96	ALA	C-O	-7.23	1.15	1.23
2	F	469	SER	CA-C	-7.23	1.43	1.52
1	A	173	LYS	CA-CB	7.22	1.63	1.53
2	L	466	SER	C-O	7.22	1.32	1.24
2	D	462	HIS	CA-C	-7.22	1.43	1.52
1	G	153	ALA	CA-CB	-7.22	1.41	1.53
2	H	396	LEU	N-CA	-7.22	1.36	1.46
2	J	477	GLN	C-O	-7.22	1.15	1.24
1	C	147	ASP	C-O	-7.21	1.14	1.24
2	F	520	ALA	C-O	7.21	1.32	1.23
2	F	521	TYR	CA-C	-7.21	1.44	1.52
2	F	368	ASN	C-O	7.21	1.33	1.24
2	F	440	ARG	CZ-NH2	-7.21	1.24	1.33
2	J	439	PHE	C-O	7.20	1.32	1.23
1	I	120	VAL	CA-CB	-7.20	1.41	1.53
2	J	414	ARG	CD-NE	7.19	1.56	1.46
1	A	103	GLU	CA-C	-7.19	1.44	1.52
1	E	181	THR	CA-C	7.19	1.62	1.52
1	G	81	ASP	CA-C	-7.19	1.42	1.52
2	J	524	ASP	C-O	7.19	1.32	1.23
2	B	396	LEU	CA-C	7.19	1.62	1.52
1	A	187	ILE	CA-CB	-7.18	1.45	1.54
2	H	469	SER	CA-C	7.18	1.61	1.52
1	K	31	ARG	C-O	7.18	1.32	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	465	ILE	C-O	7.17	1.31	1.24
2	B	483	ASP	C-O	7.17	1.32	1.24
1	E	188	ARG	NE-CZ	7.16	1.41	1.33
1	K	57	ASP	CA-C	7.16	1.62	1.53
1	A	168	GLU	CD-OE1	7.16	1.39	1.25
1	A	47	GLU	CD-OE1	7.16	1.39	1.25
1	G	149	ALA	CA-CB	-7.16	1.40	1.53
2	L	385	VAL	C-O	7.15	1.32	1.23
1	G	99	PHE	CD1-CE1	7.15	1.60	1.38
2	B	440	ARG	CG-CD	-7.15	1.31	1.52
2	J	482	GLY	C-O	7.14	1.33	1.23
1	K	23	LEU	N-CA	7.14	1.54	1.46
1	A	13	ALA	CA-CB	-7.14	1.41	1.53
2	D	378	ILE	CA-CB	7.14	1.64	1.54
2	B	443	LYS	C-O	-7.13	1.15	1.24
2	D	416	LEU	C-O	7.13	1.32	1.24
2	D	507	LYS	CD-CE	7.13	1.73	1.52
2	F	441	THR	N-CA	-7.13	1.36	1.46
1	E	8	THR	CA-C	7.12	1.61	1.53
1	K	198	PHE	C-O	7.12	1.32	1.23
1	E	26	ALA	C-O	7.12	1.33	1.24
1	K	188	ARG	CZ-NH1	7.12	1.42	1.32
2	F	499	GLU	CA-C	-7.12	1.43	1.52
1	A	101	ALA	N-CA	7.11	1.55	1.46
1	G	38	ARG	CZ-NH1	7.11	1.42	1.32
2	J	532	LYS	CA-C	7.11	1.62	1.52
1	K	119	GLY	CA-C	7.11	1.61	1.51
2	B	444	PRO	CA-CB	-7.11	1.43	1.53
1	A	139	LEU	C-O	7.10	1.32	1.24
1	K	150	GLN	CD-OE1	7.09	1.37	1.23
1	G	87	ASN	CA-C	-7.08	1.43	1.53
2	J	479	TYR	C-O	7.08	1.32	1.23
2	L	403	ASN	CA-CB	7.07	1.64	1.53
2	B	391	PRO	C-O	7.07	1.32	1.23
2	H	431	THR	CA-CB	7.06	1.64	1.53
2	J	404	ALA	C-O	7.05	1.33	1.24
1	E	24	GLU	C-O	7.05	1.32	1.24
1	E	19	ILE	CG1-CD1	7.05	1.79	1.51
2	F	399	MET	CA-CB	-7.04	1.41	1.53
2	J	439	PHE	N-CA	-7.04	1.36	1.45
2	F	455	ASP	CA-C	-7.04	1.44	1.52
2	F	499	GLU	CD-OE1	7.04	1.38	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	503	GLN	CA-C	-7.04	1.42	1.52
2	L	362	ASP	N-CA	-7.04	1.36	1.46
2	D	460	HIS	C-O	-7.04	1.15	1.23
1	K	175	CYS	CB-SG	7.03	2.04	1.81
1	E	158	LEU	C-O	-7.03	1.15	1.24
2	F	347	THR	CA-CB	7.03	1.65	1.53
1	K	64	ARG	NE-CZ	7.03	1.40	1.33
1	G	162	GLU	CA-CB	-7.02	1.42	1.53
1	A	105	THR	C-O	-7.02	1.15	1.23
2	H	414	ARG	NE-CZ	7.02	1.40	1.33
1	A	41	LYS	CA-C	7.01	1.62	1.53
1	E	94	ARG	CA-C	-7.01	1.44	1.52
2	D	454	ASN	CA-C	-7.01	1.45	1.53
1	I	97	THR	CA-C	7.01	1.61	1.52
1	I	70	VAL	CA-C	-7.01	1.44	1.52
1	K	52	LEU	C-O	7.01	1.32	1.23
2	B	346	THR	N-CA	-7.00	1.37	1.46
1	A	100	ASP	CB-CG	7.00	1.69	1.52
2	H	331	SER	C-O	-7.00	1.14	1.25
1	A	172	ALA	CA-CB	-6.99	1.41	1.53
2	D	318	LYS	C-O	6.99	1.33	1.23
1	A	130	LEU	CA-C	6.98	1.61	1.52
1	E	7	GLU	CA-C	6.98	1.61	1.52
2	D	396	LEU	C-O	6.98	1.32	1.24
2	D	441	THR	N-CA	-6.98	1.35	1.46
2	H	384	VAL	C-O	-6.98	1.16	1.24
2	D	407	ARG	CA-C	6.97	1.61	1.52
2	F	333	ARG	CZ-NH2	6.97	1.42	1.33
2	F	369	ASN	C-O	6.97	1.32	1.24
1	A	47	GLU	CD-OE2	6.97	1.38	1.25
1	C	71	TRP	C-O	6.96	1.31	1.23
2	H	362	ASP	CA-C	6.96	1.62	1.53
2	F	374	ILE	CA-C	6.96	1.61	1.52
2	B	508	LEU	C-O	-6.96	1.15	1.23
2	J	356	PHE	N-CA	6.95	1.54	1.46
2	J	374	ILE	CA-C	6.95	1.61	1.52
1	K	50	LEU	CA-C	6.95	1.61	1.52
2	H	533	THR	N-CA	6.95	1.54	1.45
2	L	538	CYS	CB-SG	-6.95	1.58	1.81
1	C	180	LYS	C-O	-6.95	1.15	1.24
2	D	479	TYR	CA-CB	-6.95	1.43	1.53
2	D	537	ASN	CA-C	6.95	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	391	PRO	CB-CG	-6.95	1.15	1.49
2	F	321	THR	CA-CB	6.94	1.62	1.53
2	J	426	VAL	CB-CG1	6.94	1.75	1.52
1	K	150	GLN	CA-C	-6.94	1.44	1.52
2	L	481	GLU	CA-C	6.94	1.61	1.52
2	H	486	ILE	CA-C	6.94	1.60	1.52
2	B	473	LYS	CE-NZ	6.94	1.70	1.49
1	K	111	PRO	C-O	6.93	1.31	1.23
1	A	197	PHE	N-CA	6.93	1.54	1.46
2	D	380	VAL	C-O	6.93	1.31	1.24
2	L	351	PHE	CD2-CE2	6.93	1.59	1.38
2	H	323	ASP	C-O	-6.93	1.15	1.24
1	A	138	HIS	C-O	-6.93	1.14	1.23
1	C	90	ASN	CA-CB	-6.92	1.43	1.53
1	G	100	ASP	CB-CG	6.92	1.69	1.52
2	D	441	THR	CA-C	6.91	1.61	1.53
1	G	154	LYS	CE-NZ	6.91	1.70	1.49
2	B	462	HIS	CA-CB	-6.91	1.43	1.53
2	B	531	ARG	C-O	6.90	1.32	1.23
2	F	377	ARG	C-O	-6.90	1.15	1.24
1	C	66	SER	CA-C	-6.90	1.43	1.53
2	H	510	MET	C-O	-6.90	1.15	1.24
2	B	450	ARG	CZ-NH1	6.89	1.42	1.32
2	B	370	GLY	C-O	6.89	1.33	1.24
1	K	76	ASN	C-O	6.89	1.33	1.24
2	H	339	ILE	CA-CB	6.88	1.62	1.55
2	J	394	ASN	CA-CB	6.88	1.63	1.53
2	H	532	LYS	C-O	6.88	1.32	1.23
2	D	450	ARG	CZ-NH2	6.88	1.42	1.33
1	G	47	GLU	CD-OE2	6.88	1.38	1.25
1	I	183	TYR	CE1-CZ	6.87	1.54	1.38
1	G	34	GLU	C-O	6.87	1.32	1.23
1	I	45	PRO	C-O	6.87	1.31	1.23
1	G	6	PRO	C-O	-6.86	1.16	1.23
2	B	496	ALA	C-O	-6.86	1.15	1.24
1	C	19	ILE	CA-CB	6.86	1.64	1.54
2	B	450	ARG	C-O	-6.86	1.13	1.23
2	B	376	GLU	CD-OE2	6.85	1.38	1.25
2	D	368	ASN	CA-CB	6.85	1.65	1.53
2	D	505	ILE	CA-C	-6.85	1.44	1.52
1	E	174	ARG	CA-CB	-6.85	1.42	1.53
1	I	192	GLU	C-O	6.85	1.32	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	GLU	CD-OE1	6.84	1.38	1.25
2	D	318	LYS	CG-CD	6.84	1.73	1.52
2	H	306	SER	CA-C	-6.84	1.44	1.52
2	B	495	ILE	CA-CB	-6.84	1.46	1.54
1	E	83	TYR	C-O	6.84	1.32	1.24
1	C	167	ARG	CA-CB	-6.84	1.42	1.53
2	F	474	LEU	C-O	-6.84	1.15	1.23
1	I	172	ALA	CA-C	6.84	1.61	1.52
1	E	96	ALA	C-O	-6.83	1.15	1.23
2	B	473	LYS	C-O	-6.83	1.15	1.23
2	J	358	ALA	CA-CB	6.83	1.64	1.53
2	J	302	ALA	CA-C	6.83	1.61	1.52
2	J	333	ARG	CZ-NH2	6.83	1.42	1.33
1	K	161	ILE	N-CA	6.82	1.54	1.46
1	C	25	ALA	CA-C	6.82	1.61	1.52
1	A	177	VAL	CA-CB	6.82	1.63	1.54
1	E	197	PHE	CD2-CE2	6.82	1.59	1.38
1	I	108	THR	C-O	-6.82	1.16	1.23
1	K	18	HIS	CA-C	-6.81	1.44	1.52
1	G	173	LYS	C-O	-6.81	1.16	1.24
1	K	184	ARG	C-O	6.81	1.32	1.24
2	B	461	ILE	C-O	-6.80	1.16	1.24
1	C	168	GLU	C-O	6.80	1.32	1.24
1	C	198	PHE	CA-C	-6.80	1.44	1.52
2	J	440	ARG	C-O	6.80	1.31	1.24
2	H	523	PHE	CA-C	6.80	1.60	1.53
1	C	113	VAL	CA-CB	6.80	1.63	1.54
1	E	111	PRO	CA-C	-6.79	1.45	1.52
1	I	41	LYS	CA-C	6.79	1.61	1.53
2	L	414	ARG	CA-CB	6.79	1.65	1.53
2	B	440	ARG	CD-NE	-6.79	1.36	1.46
2	J	305	ASN	CA-CB	6.79	1.63	1.54
2	H	369	ASN	C-O	6.78	1.31	1.23
1	G	173	LYS	CA-CB	6.78	1.62	1.53
2	L	318	LYS	CD-CE	6.78	1.72	1.52
2	L	411	LYS	CA-C	-6.78	1.43	1.52
2	B	359	HIS	C-O	-6.78	1.14	1.24
2	F	468	PRO	C-O	-6.77	1.15	1.24
1	K	152	ASN	C-O	6.77	1.32	1.24
1	E	75	ALA	CA-CB	-6.77	1.41	1.53
2	F	352	SER	C-O	6.77	1.31	1.24
2	J	455	ASP	C-O	6.77	1.32	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	53	GLY	C-O	6.77	1.31	1.23
2	H	386	ASP	C-O	-6.77	1.16	1.23
2	B	333	ARG	N-CA	-6.76	1.37	1.46
2	H	399	MET	CA-C	-6.76	1.44	1.52
1	C	142	ARG	CG-CD	-6.76	1.32	1.52
2	B	335	ALA	CA-C	6.75	1.61	1.52
1	E	99	PHE	CD1-CE1	6.75	1.58	1.38
2	J	305	ASN	CA-C	6.75	1.61	1.52
1	K	168	GLU	CA-CB	-6.75	1.42	1.53
1	A	114	VAL	C-O	-6.75	1.17	1.24
1	A	162	GLU	CD-OE1	6.75	1.38	1.25
1	A	100	ASP	CA-CB	6.74	1.64	1.53
2	F	311	ARG	C-O	-6.74	1.14	1.23
2	L	475	ILE	CA-CB	-6.74	1.45	1.54
1	I	178	ASP	CA-C	6.74	1.61	1.53
1	A	133	ARG	CA-CB	-6.74	1.42	1.53
2	B	426	VAL	C-O	-6.74	1.17	1.24
1	A	188	ARG	CZ-NH1	6.73	1.42	1.32
2	F	312	ASP	CA-CB	-6.73	1.44	1.53
2	H	479	TYR	N-CA	6.73	1.54	1.45
1	K	82	ALA	CA-C	6.73	1.61	1.52
2	L	366	ASN	C-O	-6.73	1.15	1.24
2	B	441	THR	C-O	6.73	1.30	1.24
1	A	163	GLN	C-O	-6.72	1.15	1.24
2	H	516	MET	SD-CE	6.72	1.96	1.79
2	L	334	GLN	CD-OE1	6.72	1.36	1.23
1	C	45	PRO	C-O	-6.72	1.16	1.23
2	F	506	ALA	CA-CB	-6.71	1.42	1.53
1	C	192	GLU	CG-CD	6.71	1.68	1.52
1	E	162	GLU	N-CA	6.71	1.54	1.46
2	L	434	ASP	CG-OD1	6.71	1.38	1.25
1	G	22	ALA	CA-C	6.71	1.63	1.53
2	B	472	THR	N-CA	-6.71	1.37	1.46
2	F	414	ARG	NE-CZ	6.70	1.40	1.33
1	I	191	GLY	C-O	6.70	1.32	1.23
1	G	26	ALA	CA-CB	6.70	1.65	1.53
1	C	192	GLU	C-O	6.70	1.32	1.24
1	G	13	ALA	CA-C	-6.70	1.43	1.52
2	J	460	HIS	C-O	-6.70	1.15	1.23
1	C	89	PHE	C-O	6.69	1.31	1.23
1	C	175	CYS	CA-C	-6.69	1.44	1.53
2	H	476	THR	C-O	-6.69	1.15	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	47	GLU	CD-OE1	6.69	1.38	1.25
1	K	6	PRO	C-O	6.69	1.31	1.23
2	J	509	ASP	CG-OD2	6.69	1.38	1.25
2	L	500	ALA	CA-CB	-6.69	1.42	1.53
2	D	306	SER	CA-C	-6.68	1.44	1.52
1	G	46	GLY	CA-C	-6.68	1.45	1.52
1	G	118	ALA	CA-CB	-6.68	1.42	1.53
2	B	506	ALA	C-O	-6.67	1.15	1.23
1	I	188	ARG	C-O	6.67	1.31	1.24
2	J	533	THR	CA-C	6.67	1.61	1.52
1	K	190	GLN	CA-C	-6.67	1.44	1.52
1	I	171	ILE	CA-C	-6.67	1.44	1.52
2	H	304	ASP	CB-CG	6.66	1.68	1.52
1	K	100	ASP	C-N	6.66	1.41	1.33
2	J	377	ARG	CZ-NH2	6.66	1.42	1.33
2	J	470	ILE	CG1-CD1	-6.66	1.25	1.51
2	D	522	ARG	CA-C	6.65	1.60	1.52
2	F	315	TRP	CA-C	6.65	1.61	1.52
1	K	144	TYR	C-O	6.65	1.32	1.23
2	D	438	SER	C-O	-6.65	1.15	1.23
2	J	502	GLN	CD-NE2	6.65	1.47	1.33
1	C	2	ILE	CA-C	6.65	1.60	1.52
1	K	43	ASP	C-O	6.65	1.32	1.24
1	K	162	GLU	CG-CD	6.65	1.68	1.52
2	B	458	PRO	C-O	6.65	1.32	1.23
2	D	476	THR	N-CA	-6.65	1.35	1.46
1	I	72	GLN	CD-NE2	6.64	1.47	1.33
1	C	86	GLU	CD-OE1	6.64	1.38	1.25
2	J	368	ASN	CA-CB	6.63	1.64	1.53
1	K	168	GLU	CD-OE1	6.63	1.38	1.25
2	F	401	GLN	N-CA	-6.62	1.38	1.46
1	A	35	ILE	CA-C	-6.62	1.44	1.52
2	F	306	SER	CA-C	-6.62	1.44	1.52
1	A	64	ARG	NE-CZ	6.62	1.40	1.33
2	B	311	ARG	CZ-NH1	6.62	1.42	1.32
2	D	505	ILE	CA-CB	-6.62	1.46	1.54
2	D	324	TYR	CA-C	6.61	1.61	1.52
2	D	425	GLY	C-O	-6.61	1.17	1.24
2	F	533	THR	CA-C	6.61	1.61	1.52
2	H	426	VAL	CA-CB	-6.61	1.45	1.54
2	J	324	TYR	CA-C	6.61	1.61	1.52
2	L	336	LEU	C-O	-6.61	1.15	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	512	ASN	CG-OD1	6.61	1.36	1.23
2	B	530	GLN	N-CA	6.59	1.54	1.46
2	F	480	PHE	CD2-CE2	6.59	1.58	1.38
2	J	376	GLU	CD-OE2	6.59	1.37	1.25
2	J	306	SER	C-O	-6.59	1.16	1.23
2	L	376	GLU	CD-OE2	6.59	1.37	1.25
2	F	342	SER	CA-C	-6.58	1.44	1.52
1	I	150	GLN	C-O	6.58	1.31	1.24
2	L	536	GLU	CA-C	6.58	1.61	1.52
2	J	314	ASN	C-O	-6.58	1.15	1.24
1	G	116	ASN	N-CA	-6.58	1.38	1.46
1	G	38	ARG	NE-CZ	6.58	1.40	1.33
2	H	503	GLN	N-CA	-6.58	1.36	1.46
2	L	390	LYS	CA-C	-6.58	1.44	1.53
1	C	94	ARG	CB-CG	-6.57	1.32	1.52
2	B	376	GLU	C-O	-6.56	1.16	1.24
2	F	356	PHE	C-O	6.56	1.31	1.23
1	A	38	ARG	CZ-NH1	6.55	1.42	1.32
2	D	400	TRP	C-O	6.55	1.31	1.23
2	D	417	ALA	CA-C	6.55	1.59	1.53
2	J	373	PRO	C-O	6.55	1.31	1.23
2	B	390	LYS	CB-CG	-6.55	1.32	1.52
1	I	10	SER	CA-CB	6.55	1.63	1.53
1	E	127	ASN	C-O	-6.55	1.16	1.24
2	B	503	GLN	CA-CB	-6.54	1.42	1.53
2	L	303	GLN	N-CA	6.54	1.53	1.46
2	D	369	ASN	C-O	6.54	1.31	1.23
1	K	16	TYR	CE2-CZ	6.54	1.53	1.38
1	A	194	GLU	C-O	-6.54	1.15	1.23
1	G	81	ASP	C-O	-6.54	1.15	1.24
1	K	86	GLU	CD-OE1	6.54	1.37	1.25
2	D	534	HIS	N-CA	6.54	1.54	1.45
2	F	440	ARG	CA-CB	-6.54	1.43	1.53
2	H	368	ASN	CA-C	6.54	1.61	1.52
2	L	531	ARG	CZ-NH1	6.54	1.41	1.32
1	E	35	ILE	C-O	-6.53	1.17	1.24
1	K	116	ASN	CA-C	6.53	1.61	1.53
2	L	426	VAL	CA-CB	6.53	1.66	1.55
2	H	433	SER	N-CA	6.53	1.54	1.46
1	E	163	GLN	CG-CD	6.52	1.68	1.52
1	G	165	GLN	CD-NE2	6.52	1.47	1.33
2	B	424	GLY	CA-C	6.52	1.61	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	396	LEU	CA-C	6.52	1.60	1.52
1	A	102	GLY	N-CA	6.52	1.54	1.45
2	H	468	PRO	C-O	-6.52	1.16	1.24
1	K	197	PHE	CE1-CZ	6.52	1.58	1.38
2	J	330	ARG	N-CA	-6.51	1.39	1.46
2	L	376	GLU	CA-C	-6.51	1.44	1.52
1	K	177	VAL	C-O	6.51	1.31	1.24
2	F	493	LYS	CA-CB	-6.51	1.42	1.53
2	D	312	ASP	CA-CB	-6.51	1.44	1.52
1	K	101	ALA	C-O	6.51	1.32	1.23
2	B	411	LYS	CG-CD	6.50	1.72	1.52
1	E	94	ARG	CB-CG	-6.50	1.32	1.52
1	K	49	ILE	N-CA	6.50	1.53	1.46
2	D	408	HIS	CD2-NE2	6.50	1.45	1.37
1	A	79	TYR	C-O	-6.49	1.16	1.24
2	B	532	LYS	CA-C	6.49	1.61	1.52
2	L	414	ARG	CB-CG	6.49	1.72	1.52
2	L	526	VAL	N-CA	6.48	1.54	1.46
1	G	98	THR	CA-CB	6.48	1.63	1.53
2	J	318	LYS	CA-C	6.48	1.61	1.53
1	C	98	THR	CB-OG1	6.48	1.54	1.43
1	K	25	ALA	CA-C	6.48	1.61	1.52
2	J	527	LEU	N-CA	6.47	1.53	1.45
2	D	497	ASN	C-O	-6.47	1.16	1.24
2	F	333	ARG	CZ-NH1	6.46	1.41	1.32
1	A	25	ALA	CA-C	6.46	1.61	1.52
2	F	508	LEU	CA-CB	-6.46	1.43	1.53
2	L	305	ASN	CB-CG	6.45	1.68	1.52
2	J	536	GLU	C-O	6.45	1.31	1.24
2	F	507	LYS	CE-NZ	6.45	1.68	1.49
1	E	68	LEU	C-O	-6.45	1.16	1.23
2	H	310	ILE	CA-CB	-6.45	1.47	1.54
2	B	306	SER	CA-C	-6.44	1.45	1.52
1	I	54	GLN	N-CA	-6.44	1.38	1.45
1	K	118	ALA	CA-CB	6.44	1.64	1.53
1	C	14	GLY	C-O	6.43	1.32	1.24
2	H	466	SER	N-CA	-6.43	1.38	1.46
2	B	497	ASN	C-N	6.43	1.42	1.33
1	C	154	LYS	CE-NZ	6.43	1.68	1.49
1	G	161	ILE	C-O	-6.43	1.17	1.24
2	B	398	GLU	CA-CB	-6.42	1.43	1.53
1	C	69	GLU	N-CA	-6.42	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	427	GLY	C-O	-6.42	1.17	1.24
2	D	417	ALA	N-CA	6.42	1.53	1.45
2	B	414	ARG	CZ-NH2	6.42	1.41	1.33
1	G	59	ASN	CA-C	6.42	1.61	1.52
2	L	301	PRO	CG-CD	6.42	1.72	1.50
2	D	304	ASP	CA-CB	6.41	1.61	1.52
2	L	497	ASN	CA-C	6.41	1.59	1.52
2	D	376	GLU	CD-OE1	6.41	1.37	1.25
1	G	114	VAL	CA-CB	6.41	1.66	1.55
2	F	416	LEU	CG-CD2	6.41	1.73	1.52
2	B	374	ILE	CA-C	6.40	1.60	1.52
1	C	99	PHE	CA-CB	6.40	1.63	1.53
2	D	531	ARG	CA-CB	-6.40	1.43	1.53
1	I	122	MET	C-O	6.40	1.31	1.23
2	F	317	PRO	CA-CB	6.39	1.62	1.53
2	H	507	LYS	CD-CE	6.39	1.71	1.52
2	D	374	ILE	CA-C	6.39	1.60	1.52
1	E	91	SER	CA-C	6.39	1.61	1.52
1	E	162	GLU	C-O	-6.39	1.16	1.24
2	J	537	ASN	C-O	6.39	1.32	1.23
1	G	56	TYR	C-O	-6.39	1.15	1.23
1	I	155	CYS	CA-CB	-6.39	1.41	1.53
2	J	500	ALA	CA-CB	-6.39	1.42	1.53
2	F	414	ARG	CA-CB	6.38	1.64	1.53
1	E	144	TYR	CA-C	6.38	1.60	1.52
2	D	318	LYS	CA-C	6.38	1.61	1.53
1	E	83	TYR	N-CA	-6.38	1.38	1.46
1	I	63	VAL	CA-C	6.37	1.59	1.53
2	F	314	ASN	N-CA	-6.37	1.37	1.46
1	I	198	PHE	CD1-CE1	6.37	1.57	1.38
1	A	117	ALA	CA-CB	-6.36	1.42	1.53
2	J	525	ILE	CA-C	6.36	1.60	1.52
2	L	347	THR	C-O	6.36	1.32	1.23
1	G	3	GLU	CA-C	6.36	1.60	1.52
2	H	454	ASN	C-O	-6.36	1.16	1.23
1	I	35	ILE	CA-CB	-6.35	1.46	1.53
1	K	149	ALA	C-O	6.35	1.31	1.24
1	C	47	GLU	CD-OE2	6.35	1.37	1.25
1	E	26	ALA	CA-C	6.35	1.61	1.52
2	F	447	TYR	CA-C	6.35	1.58	1.52
2	D	414	ARG	CA-CB	6.34	1.64	1.53
2	B	441	THR	N-CA	-6.34	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	511	ASN	C-O	-6.34	1.15	1.24
2	J	437	TYR	CA-C	-6.34	1.44	1.52
2	L	420	ASP	C-N	6.34	1.43	1.33
1	A	120	VAL	CB-CG2	-6.34	1.31	1.52
2	H	323	ASP	CA-C	-6.34	1.44	1.52
1	C	76	ASN	CA-C	-6.33	1.43	1.52
2	D	367	PHE	C-O	6.33	1.31	1.23
2	D	363	LEU	N-CA	-6.33	1.37	1.46
1	G	114	VAL	C-O	-6.33	1.17	1.23
1	C	22	ALA	CA-CB	6.33	1.64	1.53
2	J	486	ILE	C-N	6.33	1.41	1.34
1	K	78	GLU	CG-CD	6.33	1.67	1.52
2	H	359	HIS	CA-CB	6.33	1.61	1.53
2	H	365	LEU	N-CA	-6.33	1.37	1.45
2	B	491	ILE	C-O	-6.32	1.16	1.24
2	L	383	ARG	CZ-NH2	6.32	1.41	1.33
2	F	430	LEU	C-O	-6.32	1.10	1.23
1	I	145	PHE	C-N	6.32	1.42	1.33
2	J	368	ASN	CB-CG	6.32	1.67	1.52
1	A	76	ASN	N-CA	-6.31	1.37	1.46
2	D	401	GLN	N-CA	6.31	1.53	1.46
1	C	169	THR	CA-C	-6.31	1.43	1.52
2	D	329	ALA	CA-C	-6.31	1.44	1.52
2	H	522	ARG	N-CA	-6.31	1.38	1.46
1	G	100	ASP	C-O	6.31	1.31	1.24
1	I	51	LEU	CA-C	-6.31	1.45	1.52
2	J	321	THR	CA-CB	6.31	1.62	1.53
1	K	116	ASN	C-O	6.31	1.32	1.23
1	E	168	GLU	CD-OE1	6.31	1.37	1.25
1	G	188	ARG	CG-CD	6.31	1.71	1.52
1	E	192	GLU	CA-C	-6.30	1.44	1.52
1	G	143	LEU	C-O	6.30	1.31	1.24
2	L	516	MET	CA-CB	6.30	1.62	1.53
2	B	338	SER	CA-CB	-6.30	1.43	1.53
1	G	102	GLY	C-O	-6.30	1.16	1.23
2	F	305	ASN	CA-C	6.29	1.60	1.52
2	J	507	LYS	CE-NZ	6.29	1.68	1.49
1	E	167	ARG	CD-NE	6.29	1.55	1.46
1	K	161	ILE	CA-CB	6.29	1.60	1.53
2	F	470	ILE	N-CA	-6.29	1.39	1.46
2	H	502	GLN	CD-OE1	6.29	1.35	1.23
2	L	443	LYS	CA-CB	-6.29	1.43	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	403	ASN	CA-C	6.29	1.60	1.53
2	F	450	ARG	C-O	-6.29	1.15	1.23
1	G	11	GLN	C-O	6.28	1.31	1.23
2	J	385	VAL	C-O	-6.28	1.17	1.24
2	D	305	ASN	CB-CG	6.27	1.67	1.52
1	A	126	ILE	CA-CB	6.27	1.63	1.54
1	C	24	GLU	CD-OE2	6.27	1.37	1.25
1	K	154	LYS	CD-CE	6.27	1.71	1.52
1	G	108	THR	CA-CB	6.27	1.62	1.53
2	B	422	ASN	CA-C	-6.26	1.44	1.52
2	J	388	TYR	CD1-CE1	6.26	1.57	1.38
1	A	26	ALA	CA-CB	6.26	1.64	1.53
1	I	98	THR	CA-CB	6.26	1.64	1.53
1	I	73	ALA	CA-CB	-6.25	1.43	1.53
2	J	401	GLN	N-CA	6.25	1.54	1.46
2	F	414	ARG	CB-CG	6.25	1.71	1.52
1	G	180	LYS	CD-CE	6.25	1.71	1.52
2	H	334	GLN	C-O	6.25	1.31	1.23
2	D	378	ILE	CA-C	6.25	1.60	1.52
2	D	504	LEU	N-CA	-6.24	1.38	1.46
2	F	310	ILE	CA-CB	6.24	1.60	1.54
2	H	501	VAL	C-O	-6.24	1.16	1.24
1	A	65	ASP	CA-C	-6.24	1.43	1.52
2	J	442	ILE	CA-C	6.24	1.60	1.52
1	K	163	GLN	CD-OE1	6.24	1.35	1.23
1	A	98	THR	N-CA	6.24	1.54	1.45
1	E	38	ARG	NE-CZ	6.24	1.40	1.33
2	F	472	THR	CB-CG2	-6.24	1.31	1.52
2	D	516	MET	CA-C	-6.24	1.43	1.52
1	G	176	GLU	CD-OE1	6.24	1.37	1.25
2	L	473	LYS	CA-CB	-6.24	1.43	1.53
2	D	320	LEU	C-O	-6.23	1.16	1.24
2	F	535	PHE	CE2-CZ	6.23	1.57	1.38
1	K	78	GLU	CD-OE2	6.23	1.37	1.25
1	G	94	ARG	CA-C	-6.23	1.45	1.52
2	F	316	HIS	CA-C	6.23	1.61	1.53
1	G	133	ARG	CB-CG	-6.23	1.33	1.52
2	J	361	HIS	N-CA	-6.23	1.37	1.46
2	F	443	LYS	C-O	-6.23	1.16	1.24
1	E	71	TRP	N-CA	-6.22	1.38	1.46
1	E	150	GLN	CD-NE2	6.22	1.46	1.33
1	I	146	ASP	CG-OD2	6.22	1.37	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	321	THR	N-CA	-6.22	1.39	1.46
2	B	324	TYR	N-CA	-6.22	1.38	1.46
1	K	199	ASP	C-O	6.22	1.31	1.23
1	K	180	LYS	CE-NZ	6.21	1.68	1.49
2	L	462	HIS	C-O	-6.21	1.16	1.23
1	E	180	LYS	CA-C	6.21	1.60	1.52
2	J	533	THR	C-O	-6.21	1.16	1.23
1	K	80	GLN	CG-CD	6.21	1.67	1.52
1	A	145	PHE	CA-C	-6.21	1.45	1.52
2	F	346	THR	C-O	-6.21	1.15	1.24
2	J	414	ARG	CZ-NH1	6.21	1.41	1.32
1	K	26	ALA	N-CA	6.21	1.54	1.46
2	B	471	ALA	CA-C	6.21	1.61	1.52
1	G	25	ALA	CA-C	6.21	1.61	1.52
1	K	177	VAL	CA-C	6.21	1.60	1.52
1	E	66	SER	N-CA	-6.20	1.38	1.45
2	D	435	GLY	C-O	-6.20	1.15	1.23
2	J	460	HIS	C-N	-6.20	1.25	1.33
2	F	325	LYS	C-O	6.19	1.31	1.24
2	L	439	PHE	CE2-CZ	6.19	1.57	1.38
2	L	354	LEU	CA-C	6.19	1.61	1.52
1	E	177	VAL	C-O	6.19	1.30	1.24
2	F	431	THR	CA-CB	6.19	1.63	1.53
2	J	471	ALA	CA-CB	6.18	1.63	1.53
2	D	382	GLY	C-N	-6.18	1.25	1.33
1	E	38	ARG	CZ-NH1	6.18	1.41	1.32
2	H	408	HIS	N-CA	6.18	1.54	1.46
1	E	90	ASN	C-O	6.18	1.31	1.24
1	K	63	VAL	N-CA	-6.18	1.39	1.46
1	G	64	ARG	C-O	-6.17	1.15	1.24
1	K	69	GLU	N-CA	-6.17	1.38	1.46
2	D	519	LEU	C-O	6.17	1.32	1.23
2	L	419	LEU	CA-CB	-6.17	1.43	1.53
2	F	426	VAL	CB-CG2	-6.17	1.32	1.52
1	I	101	ALA	C-N	6.17	1.42	1.33
1	E	108	THR	C-O	6.17	1.28	1.24
2	H	436	TYR	CD1-CE1	6.16	1.57	1.38
2	F	316	HIS	CB-CG	-6.16	1.41	1.50
2	H	492	VAL	CA-C	6.16	1.60	1.52
1	A	88	ALA	CA-C	6.16	1.60	1.52
2	B	434	ASP	CG-OD2	6.16	1.37	1.25
1	A	190	GLN	CA-C	-6.15	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	374	ILE	C-O	6.15	1.32	1.24
2	H	303	GLN	CA-C	6.15	1.60	1.52
2	D	353	HIS	CA-C	-6.15	1.44	1.52
2	J	431	THR	CA-CB	6.15	1.63	1.53
1	C	114	VAL	CA-C	-6.14	1.45	1.52
2	F	403	ASN	C-O	6.14	1.32	1.24
2	H	434	ASP	CG-OD1	6.14	1.37	1.25
1	I	188	ARG	CB-CG	-6.14	1.34	1.52
2	F	495	ILE	CG1-CD1	-6.14	1.27	1.51
1	E	192	GLU	CG-CD	6.14	1.67	1.52
2	F	397	VAL	C-O	-6.14	1.17	1.24
1	K	36	TRP	C-O	6.14	1.29	1.24
2	J	410	HIS	C-O	6.13	1.31	1.23
2	B	514	ASN	CA-C	6.13	1.59	1.52
2	B	522	ARG	N-CA	-6.13	1.38	1.46
2	B	523	PHE	N-CA	-6.13	1.39	1.46
1	I	43	ASP	CB-CG	6.13	1.67	1.52
1	C	89	PHE	N-CA	-6.13	1.38	1.46
2	L	450	ARG	CZ-NH2	6.13	1.41	1.33
1	G	180	LYS	CE-NZ	6.12	1.67	1.49
1	K	4	LEU	CA-C	6.12	1.61	1.53
1	K	66	SER	C-O	-6.12	1.15	1.23
1	C	102	GLY	N-CA	6.12	1.54	1.45
1	C	156	PRO	CA-C	6.12	1.61	1.52
1	I	154	LYS	CA-C	6.12	1.60	1.52
2	J	522	ARG	CZ-NH1	6.12	1.41	1.32
2	F	313	ARG	C-O	-6.12	1.15	1.24
1	A	162	GLU	CG-CD	6.12	1.67	1.52
1	C	180	LYS	CE-NZ	6.12	1.67	1.49
2	H	450	ARG	CZ-NH2	6.12	1.41	1.33
2	J	475	ILE	CA-C	6.12	1.59	1.52
2	B	344	SER	CA-CB	-6.11	1.43	1.53
2	F	450	ARG	CD-NE	6.11	1.54	1.46
2	J	472	THR	CA-CB	6.11	1.64	1.53
2	D	324	TYR	CZ-OH	-6.11	1.25	1.38
2	F	475	ILE	N-CA	6.11	1.53	1.46
2	H	337	VAL	CA-CB	-6.11	1.47	1.54
1	A	168	GLU	CA-CB	-6.10	1.42	1.53
2	J	402	ALA	N-CA	6.10	1.53	1.45
2	L	411	LYS	CG-CD	6.10	1.70	1.52
1	A	175	CYS	C-O	6.10	1.30	1.23
1	C	62	LEU	C-N	-6.10	1.27	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	305	ASN	CG-OD1	6.09	1.35	1.23
1	I	100	ASP	C-N	6.09	1.41	1.33
2	B	453	PRO	CA-C	6.09	1.62	1.52
1	C	185	PHE	CA-CB	-6.09	1.43	1.53
2	D	419	LEU	C-O	6.09	1.31	1.23
2	F	325	LYS	N-CA	6.09	1.53	1.46
2	H	318	LYS	CE-NZ	6.09	1.67	1.49
2	H	391	PRO	CA-C	-6.08	1.44	1.52
2	B	531	ARG	CA-C	6.08	1.60	1.52
1	A	90	ASN	CA-C	-6.08	1.45	1.52
2	H	499	GLU	CA-CB	-6.08	1.43	1.53
2	L	376	GLU	CG-CD	6.08	1.67	1.52
1	G	55	VAL	CB-CG1	-6.07	1.32	1.52
1	E	110	LYS	CD-CE	-6.07	1.34	1.52
1	I	117	ALA	N-CA	-6.07	1.39	1.46
2	B	394	ASN	CG-ND2	6.06	1.46	1.33
2	L	537	ASN	N-CA	6.06	1.55	1.46
1	I	117	ALA	CA-CB	-6.05	1.43	1.53
1	C	170	LEU	C-O	-6.05	1.16	1.24
1	C	17	VAL	CA-CB	-6.05	1.46	1.54
1	E	57	ASP	C-O	-6.05	1.16	1.23
2	H	473	LYS	CG-CD	-6.05	1.34	1.52
2	J	442	ILE	CB-CG2	6.05	1.72	1.52
1	C	162	GLU	CD-OE2	6.05	1.36	1.25
1	G	165	GLN	CG-CD	6.05	1.67	1.52
2	J	346	THR	CA-CB	-6.05	1.43	1.53
1	C	177	VAL	C-O	-6.04	1.17	1.24
1	E	198	PHE	N-CA	-6.04	1.38	1.45
1	G	48	HIS	CA-C	-6.04	1.44	1.52
1	C	190	GLN	CA-C	-6.04	1.45	1.52
1	C	97	THR	CB-CG2	-6.04	1.32	1.52
2	L	537	ASN	CG-OD1	6.04	1.35	1.23
1	C	99	PHE	CB-CG	6.04	1.64	1.50
2	H	333	ARG	CA-C	6.04	1.61	1.52
2	D	476	THR	C-O	-6.03	1.17	1.23
1	I	121	PRO	CA-C	6.03	1.60	1.52
2	J	381	ALA	CA-CB	-6.03	1.43	1.53
2	H	414	ARG	CG-CD	6.03	1.70	1.52
1	I	136	ASN	C-O	6.03	1.31	1.24
2	J	518	CYS	CA-C	6.03	1.60	1.52
2	L	381	ALA	C-O	-6.03	1.16	1.23
2	D	405	GLY	C-O	6.03	1.30	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	368	ASN	CA-CB	6.03	1.63	1.53
2	B	317	PRO	C-O	6.02	1.30	1.23
1	I	126	ILE	C-O	6.02	1.30	1.24
1	K	90	ASN	CA-C	6.02	1.59	1.52
2	F	454	ASN	CA-C	6.02	1.62	1.53
1	K	197	PHE	C-O	6.02	1.31	1.23
2	D	398	GLU	C-O	6.01	1.31	1.23
2	D	318	LYS	CD-CE	6.01	1.70	1.52
2	H	490	PRO	C-O	-6.01	1.16	1.24
1	I	43	ASP	CA-C	6.01	1.60	1.52
2	J	322	PRO	CG-CD	-6.01	1.30	1.50
1	I	142	ARG	CA-C	-6.01	1.45	1.52
2	B	502	GLN	CD-OE1	6.01	1.34	1.23
1	C	94	ARG	CA-C	-6.01	1.45	1.52
2	F	510	MET	C-O	-6.01	1.16	1.24
1	G	168	GLU	CD-OE1	6.01	1.36	1.25
1	G	188	ARG	NE-CZ	6.01	1.39	1.33
2	H	382	GLY	CA-C	-6.01	1.43	1.51
1	A	109	VAL	C-O	6.00	1.30	1.24
1	C	51	LEU	CA-C	-6.00	1.45	1.52
1	G	118	ALA	C-O	-6.00	1.16	1.24
1	I	183	TYR	CA-C	-6.00	1.45	1.52
2	F	488	MET	C-O	-6.00	1.16	1.24
1	G	23	LEU	N-CA	6.00	1.53	1.46
1	G	176	GLU	CD-OE2	6.00	1.36	1.25
2	D	414	ARG	N-CA	5.99	1.53	1.46
1	E	22	ALA	CA-CB	5.99	1.63	1.53
1	G	99	PHE	CB-CG	5.99	1.64	1.50
1	G	171	ILE	CG1-CD1	-5.99	1.28	1.51
2	B	479	TYR	N-CA	5.98	1.53	1.45
2	F	459	ALA	CA-CB	-5.98	1.43	1.53
2	D	414	ARG	NE-CZ	5.97	1.39	1.33
1	C	192	GLU	CD-OE2	5.97	1.36	1.25
2	D	469	SER	N-CA	-5.97	1.38	1.45
1	K	23	LEU	CA-CB	5.97	1.62	1.53
2	B	502	GLN	CD-NE2	5.97	1.45	1.33
1	C	168	GLU	CD-OE1	5.97	1.36	1.25
2	F	447	TYR	CB-CG	-5.96	1.38	1.51
2	L	374	ILE	CA-CB	-5.96	1.47	1.54
1	I	29	PRO	C-O	5.96	1.30	1.23
1	I	32	ASP	CG-OD2	5.96	1.36	1.25
2	J	393	PRO	C-O	-5.96	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	473	LYS	CG-CD	-5.96	1.34	1.52
1	I	35	ILE	CB-CG2	-5.96	1.32	1.52
2	B	402	ALA	N-CA	5.96	1.53	1.45
2	J	495	ILE	CA-CB	-5.95	1.47	1.53
1	K	66	SER	N-CA	-5.95	1.38	1.45
2	B	486	ILE	CB-CG2	-5.95	1.32	1.52
1	C	14	GLY	C-N	5.95	1.41	1.34
1	G	163	GLN	CG-CD	5.95	1.67	1.52
2	D	522	ARG	NE-CZ	5.95	1.39	1.33
2	D	527	LEU	CA-C	5.95	1.60	1.52
1	G	80	GLN	CD-OE1	5.94	1.34	1.23
1	G	158	LEU	C-O	-5.93	1.17	1.24
2	J	449	TRP	C-O	5.93	1.30	1.23
2	J	524	ASP	CA-CB	-5.93	1.44	1.53
1	C	47	GLU	CD-OE1	5.93	1.36	1.25
1	G	142	ARG	CA-CB	-5.93	1.42	1.53
1	E	184	ARG	CA-CB	-5.93	1.45	1.53
1	I	163	GLN	CG-CD	5.93	1.66	1.52
1	C	116	ASN	CA-C	5.93	1.61	1.53
1	G	48	HIS	C-O	-5.92	1.17	1.24
1	A	166	ARG	C-O	-5.92	1.16	1.24
2	B	396	LEU	N-CA	-5.92	1.38	1.46
1	G	92	PHE	CA-C	-5.92	1.45	1.52
2	B	378	ILE	N-CA	-5.92	1.39	1.46
2	H	339	ILE	N-CA	-5.92	1.41	1.46
1	A	180	LYS	CA-C	5.91	1.59	1.52
1	E	176	GLU	CD-OE2	5.91	1.36	1.25
2	J	333	ARG	CZ-NH1	5.91	1.41	1.32
2	F	525	ILE	N-CA	-5.91	1.39	1.46
1	K	51	LEU	C-O	5.91	1.30	1.23
1	E	65	ASP	C-O	5.91	1.29	1.24
1	G	192	GLU	CD-OE2	5.90	1.36	1.25
1	K	197	PHE	N-CA	5.90	1.53	1.45
1	I	70	VAL	C-O	-5.90	1.18	1.24
2	B	316	HIS	C-N	5.90	1.41	1.33
1	C	196	VAL	CA-C	5.90	1.59	1.52
2	H	363	LEU	N-CA	-5.90	1.38	1.46
1	K	40	ALA	N-CA	-5.90	1.38	1.46
2	H	314	ASN	C-O	-5.90	1.16	1.24
2	D	495	ILE	CA-CB	-5.89	1.47	1.53
1	K	110	LYS	CA-C	5.89	1.60	1.53
1	A	178	ASP	CB-CG	5.89	1.66	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	438	SER	CA-C	-5.89	1.45	1.52
2	H	436	TYR	CA-C	-5.89	1.45	1.52
2	D	475	ILE	CA-C	5.88	1.59	1.52
2	J	505	ILE	C-O	-5.88	1.17	1.24
2	D	502	GLN	CA-C	-5.88	1.44	1.52
2	J	351	PHE	C-O	-5.88	1.16	1.24
1	A	181	THR	CA-CB	-5.88	1.43	1.53
2	L	442	ILE	CA-C	5.88	1.59	1.52
1	C	162	GLU	CD-OE1	5.88	1.36	1.25
2	B	377	ARG	C-O	-5.88	1.16	1.23
2	B	528	ARG	CD-NE	-5.88	1.38	1.46
1	K	119	GLY	C-O	5.88	1.32	1.24
2	D	502	GLN	CD-NE2	5.87	1.45	1.33
2	F	312	ASP	N-CA	-5.87	1.38	1.46
2	J	399	MET	CA-CB	-5.87	1.42	1.54
1	G	43	ASP	CA-CB	5.87	1.59	1.53
2	J	344	SER	C-O	-5.87	1.16	1.24
2	L	471	ALA	N-CA	5.87	1.53	1.46
1	A	35	ILE	CA-CB	-5.87	1.47	1.53
2	D	361	HIS	N-CA	-5.87	1.38	1.46
2	F	318	LYS	CG-CD	5.87	1.70	1.52
1	C	112	GLY	C-O	-5.86	1.18	1.23
1	I	114	VAL	N-CA	5.86	1.52	1.46
1	A	132	ALA	CA-C	5.86	1.59	1.52
1	K	128	ILE	CA-CB	-5.86	1.47	1.54
2	L	443	LYS	N-CA	-5.86	1.38	1.45
1	I	175	CYS	C-O	5.86	1.30	1.23
2	J	476	THR	N-CA	-5.86	1.39	1.46
2	J	507	LYS	CG-CD	5.86	1.70	1.52
1	E	9	PRO	CB-CG	-5.85	1.20	1.49
2	J	411	LYS	CG-CD	5.85	1.70	1.52
2	J	502	GLN	CD-OE1	5.85	1.34	1.23
2	F	462	HIS	CA-CB	-5.85	1.44	1.53
2	L	436	TYR	CD1-CE1	5.84	1.56	1.38
2	F	330	ARG	N-CA	-5.84	1.39	1.46
2	H	428	ARG	CA-C	-5.84	1.40	1.52
1	I	197	PHE	C-O	5.84	1.31	1.24
2	B	474	LEU	N-CA	-5.84	1.39	1.46
2	B	499	GLU	C-O	-5.84	1.16	1.24
2	B	368	ASN	C-O	5.84	1.31	1.24
2	L	317	PRO	CA-C	5.84	1.60	1.52
1	A	154	LYS	CE-NZ	5.83	1.66	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	455	ASP	C-O	5.83	1.31	1.23
1	A	24	GLU	N-CA	5.83	1.53	1.46
2	B	337	VAL	N-CA	5.83	1.52	1.46
2	B	368	ASN	CG-OD1	5.83	1.34	1.23
1	C	187	ILE	CA-CB	5.83	1.61	1.54
1	I	23	LEU	N-CA	5.83	1.53	1.46
1	A	115	ASN	C-O	-5.83	1.16	1.23
1	I	116	ASN	CG-OD1	5.82	1.34	1.23
2	F	419	LEU	C-O	5.82	1.31	1.23
1	I	89	PHE	C-O	5.82	1.31	1.23
2	F	380	VAL	CA-C	5.82	1.59	1.52
2	L	488	MET	C-O	-5.82	1.16	1.24
2	D	449	TRP	CD2-CE2	5.81	1.51	1.41
2	F	336	LEU	N-CA	-5.81	1.38	1.46
2	H	317	PRO	CA-C	5.81	1.59	1.52
1	K	48	HIS	C-O	5.81	1.31	1.24
2	F	390	LYS	CE-NZ	5.81	1.66	1.49
2	B	496	ALA	CA-CB	-5.81	1.44	1.53
2	F	434	ASP	CG-OD2	5.81	1.36	1.25
2	D	392	VAL	CB-CG1	-5.81	1.33	1.52
1	K	146	ASP	C-O	5.80	1.31	1.24
2	L	354	LEU	C-O	5.80	1.31	1.23
2	J	537	ASN	CA-CB	5.80	1.62	1.53
2	L	426	VAL	CA-C	-5.80	1.45	1.52
2	H	519	LEU	CA-C	5.80	1.60	1.53
2	L	357	GLY	CA-C	5.80	1.60	1.51
2	B	335	ALA	CA-CB	5.80	1.62	1.53
1	A	34	GLU	CA-C	5.79	1.59	1.52
1	I	168	GLU	CD-OE1	5.79	1.36	1.25
2	D	434	ASP	CG-OD1	5.79	1.36	1.25
1	I	140	HIS	CA-C	-5.79	1.45	1.52
2	L	505	ILE	CA-CB	-5.79	1.47	1.53
1	A	96	ALA	CA-CB	-5.79	1.43	1.53
1	E	98	THR	C-O	5.79	1.31	1.23
2	D	522	ARG	CZ-NH2	5.78	1.41	1.33
1	I	3	GLU	CA-C	5.78	1.59	1.52
1	C	174	ARG	C-O	-5.78	1.17	1.23
1	K	28	ASN	C-N	5.77	1.41	1.33
1	C	129	SER	N-CA	5.77	1.53	1.46
2	D	465	ILE	CA-C	-5.77	1.45	1.52
1	G	66	SER	C-O	-5.77	1.16	1.23
1	K	140	HIS	N-CA	-5.77	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	183	TYR	CB-CG	-5.77	1.39	1.51
1	E	30	THR	C-O	5.77	1.31	1.23
2	H	491	ILE	C-O	-5.76	1.17	1.24
2	J	367	PHE	C-N	5.76	1.41	1.33
2	H	401	GLN	CA-C	5.76	1.59	1.52
1	G	126	ILE	CG1-CD1	-5.76	1.29	1.51
2	D	503	GLN	CA-CB	-5.76	1.43	1.53
1	C	40	ALA	CA-C	-5.75	1.45	1.52
2	D	408	HIS	CA-C	-5.75	1.45	1.52
2	D	436	TYR	CA-C	-5.75	1.45	1.52
1	C	129	SER	CA-C	-5.75	1.45	1.52
2	H	436	TYR	CD2-CE2	5.75	1.55	1.38
1	E	7	GLU	CD-OE1	5.75	1.36	1.25
1	G	171	ILE	C-O	-5.75	1.17	1.23
1	K	126	ILE	CA-CB	-5.74	1.47	1.54
1	C	103	GLU	C-O	-5.74	1.17	1.24
1	G	68	LEU	CG-CD2	-5.74	1.33	1.52
1	C	120	VAL	CA-C	5.74	1.57	1.53
1	G	73	ALA	C-O	5.74	1.31	1.23
2	J	455	ASP	CA-CB	-5.74	1.45	1.53
2	B	339	ILE	CA-CB	5.73	1.61	1.54
1	G	35	ILE	CA-CB	-5.73	1.47	1.53
2	D	399	MET	CA-CB	-5.73	1.43	1.54
1	E	69	GLU	CB-CG	-5.73	1.35	1.52
2	F	414	ARG	CD-NE	5.73	1.54	1.46
2	J	415	TYR	CA-C	5.73	1.59	1.52
1	K	26	ALA	CA-CB	5.73	1.63	1.53
1	I	180	LYS	C-O	5.72	1.30	1.24
1	G	94	ARG	CB-CG	-5.72	1.35	1.52
1	K	183	TYR	CE1-CZ	5.72	1.51	1.38
2	B	434	ASP	CA-CB	-5.72	1.44	1.53
1	C	57	ASP	C-O	-5.72	1.16	1.24
2	J	320	LEU	CA-C	5.72	1.59	1.52
1	G	67	PHE	CE2-CZ	5.72	1.55	1.38
2	L	380	VAL	N-CA	5.71	1.53	1.46
2	L	492	VAL	CA-CB	-5.71	1.47	1.54
2	D	527	LEU	N-CA	5.71	1.52	1.45
2	B	516	MET	CG-SD	5.71	1.95	1.80
2	B	342	SER	CA-CB	-5.71	1.45	1.53
2	D	475	ILE	CA-CB	-5.71	1.47	1.54
2	H	500	ALA	CA-CB	-5.71	1.44	1.53
1	I	22	ALA	CA-C	5.71	1.60	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	390	LYS	N-CA	-5.71	1.37	1.46
1	C	33	GLN	CA-C	5.70	1.59	1.52
2	B	365	LEU	C-O	-5.70	1.16	1.24
1	E	127	ASN	CA-C	-5.70	1.45	1.52
2	D	501	VAL	CA-CB	-5.70	1.47	1.54
2	D	430	LEU	C-O	-5.70	1.12	1.23
1	I	64	ARG	NE-CZ	5.70	1.39	1.33
1	A	137	ILE	CA-CB	5.70	1.65	1.55
1	C	142	ARG	C-O	5.70	1.30	1.23
2	J	493	LYS	CE-NZ	5.70	1.66	1.49
2	J	519	LEU	C-O	5.70	1.31	1.23
1	I	129	SER	CA-CB	-5.69	1.45	1.53
1	G	68	LEU	CA-C	-5.69	1.45	1.52
2	H	315	TRP	CD2-CE2	5.69	1.51	1.41
1	K	72	GLN	CD-NE2	5.69	1.45	1.33
1	K	122	MET	CA-C	-5.69	1.46	1.52
1	I	178	ASP	C-O	5.69	1.31	1.23
1	A	74	ASP	N-CA	5.68	1.53	1.46
1	C	100	ASP	C-N	5.68	1.41	1.33
2	H	424	GLY	CA-C	5.68	1.59	1.51
2	F	368	ASN	N-CA	5.68	1.53	1.46
1	C	123	ALA	C-O	-5.68	1.16	1.23
2	J	433	SER	CB-OG	5.68	1.53	1.42
1	A	28	ASN	C-O	5.68	1.29	1.24
1	G	137	ILE	C-O	-5.68	1.18	1.24
2	J	464	GLY	N-CA	-5.68	1.40	1.45
1	K	188	ARG	CZ-NH2	5.68	1.40	1.33
2	L	312	ASP	CB-CG	5.68	1.66	1.52
2	B	475	ILE	N-CA	-5.67	1.39	1.46
1	C	64	ARG	NE-CZ	5.67	1.39	1.33
2	J	537	ASN	CG-OD1	5.67	1.34	1.23
1	K	99	PHE	CD1-CE1	5.67	1.55	1.38
1	I	163	GLN	CD-OE1	5.67	1.34	1.23
1	K	24	GLU	C-O	5.67	1.30	1.24
2	B	380	VAL	C-O	5.67	1.30	1.24
1	A	99	PHE	CD2-CE2	5.66	1.55	1.38
1	I	45	PRO	CA-C	5.66	1.59	1.52
2	F	393	PRO	C-O	-5.66	1.17	1.23
1	K	108	THR	CA-C	5.66	1.59	1.53
2	B	499	GLU	CA-CB	-5.66	1.43	1.53
1	C	104	TRP	C-O	-5.66	1.16	1.23
1	E	76	ASN	CA-C	-5.66	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	537	ASN	N-CA	5.65	1.54	1.46
2	F	521	TYR	N-CA	5.65	1.52	1.45
1	K	81	ASP	C-O	5.65	1.30	1.24
2	J	441	THR	CA-CB	5.65	1.61	1.53
1	A	22	ALA	CA-CB	5.65	1.62	1.53
2	J	305	ASN	C-O	5.65	1.30	1.23
2	L	305	ASN	CA-CB	5.65	1.61	1.54
2	B	472	THR	C-O	5.65	1.31	1.24
1	E	168	GLU	CA-CB	-5.65	1.43	1.53
2	J	379	ILE	C-O	5.65	1.30	1.24
1	C	99	PHE	C-O	5.64	1.30	1.24
1	E	167	ARG	C-O	-5.64	1.17	1.24
2	H	531	ARG	CA-C	5.64	1.59	1.52
2	L	308	PHE	CD1-CE1	5.64	1.55	1.38
2	B	402	ALA	CA-C	5.64	1.60	1.53
1	C	28	ASN	C-N	5.64	1.41	1.33
1	G	151	ALA	C-O	-5.64	1.17	1.24
1	K	88	ALA	CA-C	5.64	1.59	1.52
1	I	74	ASP	CA-C	5.63	1.60	1.53
1	E	38	ARG	CG-CD	5.63	1.69	1.52
2	H	534	HIS	CA-C	5.63	1.59	1.52
1	K	122	MET	CB-CG	5.63	1.69	1.52
1	A	56	TYR	C-O	-5.62	1.16	1.24
2	J	414	ARG	CA-CB	5.62	1.63	1.53
2	H	414	ARG	CA-C	5.62	1.60	1.52
2	L	495	ILE	CA-CB	-5.62	1.47	1.53
1	A	189	ILE	CB-CG1	-5.62	1.42	1.53
1	I	119	GLY	CA-C	5.62	1.59	1.51
1	K	24	GLU	CA-C	5.62	1.59	1.52
1	C	74	ASP	CA-C	5.61	1.61	1.53
2	F	324	TYR	N-CA	-5.61	1.39	1.46
2	J	351	PHE	CA-C	-5.61	1.45	1.52
2	L	442	ILE	CG1-CD1	-5.61	1.29	1.51
1	E	69	GLU	N-CA	-5.61	1.38	1.45
1	K	165	GLN	CD-NE2	5.61	1.45	1.33
2	L	509	ASP	N-CA	5.61	1.54	1.46
2	B	414	ARG	CB-CG	5.61	1.69	1.52
1	E	185	PHE	CA-CB	-5.61	1.44	1.52
1	E	188	ARG	CB-CG	-5.61	1.35	1.52
1	K	174	ARG	CA-CB	-5.61	1.44	1.53
2	H	511	ASN	CA-C	-5.61	1.45	1.52
1	A	157	VAL	C-O	-5.61	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	108	THR	CA-C	5.61	1.59	1.52
2	H	444	PRO	CA-CB	-5.61	1.45	1.53
2	L	440	ARG	CG-CD	-5.60	1.35	1.52
2	L	368	ASN	N-CA	5.60	1.53	1.46
1	I	16	TYR	CZ-OH	5.60	1.49	1.38
2	H	492	VAL	C-O	-5.60	1.17	1.24
1	G	172	ALA	CA-CB	-5.60	1.45	1.53
1	I	125	HIS	CA-C	-5.60	1.45	1.52
2	D	397	VAL	CB-CG1	-5.59	1.34	1.52
1	G	59	ASN	CG-ND2	5.59	1.45	1.33
2	H	367	PHE	C-O	5.59	1.31	1.23
2	J	381	ALA	C-O	-5.59	1.16	1.23
1	K	173	LYS	C-O	5.59	1.30	1.24
2	F	414	ARG	CA-C	5.59	1.61	1.52
2	F	536	GLU	C-O	5.59	1.30	1.24
1	G	86	GLU	CD-OE1	5.59	1.35	1.25
2	B	503	GLN	CA-C	-5.59	1.45	1.52
1	C	41	LYS	CE-NZ	5.59	1.66	1.49
2	D	453	PRO	C-O	-5.59	1.16	1.24
2	D	520	ALA	CA-CB	-5.59	1.42	1.54
2	J	330	ARG	CA-C	5.59	1.60	1.52
1	K	87	ASN	N-CA	5.59	1.53	1.46
1	A	162	GLU	CA-C	-5.58	1.45	1.52
2	H	498	PRO	C-O	-5.58	1.16	1.24
2	H	528	ARG	CD-NE	-5.58	1.38	1.46
1	K	62	LEU	C-O	5.58	1.30	1.23
1	C	126	ILE	CG1-CD1	-5.58	1.29	1.51
2	F	376	GLU	CD-OE2	5.58	1.35	1.25
2	F	450	ARG	CZ-NH2	5.58	1.40	1.33
2	F	505	ILE	N-CA	-5.58	1.39	1.46
1	I	23	LEU	CA-C	5.58	1.60	1.52
1	I	34	GLU	CA-C	5.58	1.59	1.52
2	H	506	ALA	C-O	-5.58	1.17	1.23
2	F	317	PRO	CA-C	5.58	1.59	1.52
2	F	408	HIS	C-O	-5.58	1.17	1.23
1	K	101	ALA	N-CA	5.58	1.54	1.46
1	K	159	ASN	CG-OD1	5.57	1.34	1.23
2	B	503	GLN	N-CA	-5.57	1.38	1.46
2	B	329	ALA	CA-C	5.57	1.60	1.52
1	I	176	GLU	CD-OE1	5.57	1.35	1.25
2	J	457	ARG	CZ-NH1	5.57	1.40	1.32
2	B	459	ALA	CA-CB	-5.56	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	GLU	CA-C	5.56	1.59	1.52
2	B	430	LEU	CA-CB	-5.56	1.42	1.53
1	C	198	PHE	C-O	-5.56	1.16	1.23
1	E	152	ASN	N-CA	-5.56	1.39	1.46
1	G	9	PRO	C-O	-5.55	1.17	1.23
2	L	424	GLY	CA-C	5.55	1.59	1.51
1	I	155	CYS	CA-C	-5.55	1.45	1.52
1	I	54	GLN	CA-CB	-5.55	1.44	1.53
1	I	67	PHE	CA-C	5.55	1.59	1.52
2	F	503	GLN	CD-OE1	5.55	1.34	1.23
1	A	191	GLY	CA-C	-5.54	1.44	1.51
1	C	111	PRO	CA-C	-5.54	1.46	1.52
2	L	392	VAL	CA-C	5.54	1.58	1.52
1	G	96	ALA	CA-CB	-5.54	1.44	1.53
2	J	305	ASN	CG-OD1	5.54	1.34	1.23
2	D	328	ILE	CA-CB	-5.54	1.48	1.54
2	H	525	ILE	CB-CG2	5.54	1.70	1.52
2	B	359	HIS	CA-C	5.54	1.60	1.52
2	D	351	PHE	C-O	-5.54	1.16	1.24
2	D	411	LYS	CG-CD	5.54	1.69	1.52
1	E	167	ARG	CB-CG	-5.54	1.35	1.52
2	F	496	ALA	CA-CB	-5.54	1.44	1.53
2	B	473	LYS	CA-CB	-5.53	1.44	1.53
1	A	6	PRO	C-O	-5.53	1.17	1.23
1	I	168	GLU	CA-CB	-5.53	1.44	1.53
1	C	161	ILE	CA-C	5.53	1.59	1.53
1	G	57	ASP	C-O	-5.53	1.17	1.23
1	K	117	ALA	C-O	5.53	1.31	1.24
2	H	497	ASN	N-CA	-5.53	1.38	1.46
2	L	332	PRO	C-O	5.53	1.30	1.23
2	B	451	ASN	N-CA	-5.53	1.39	1.46
2	J	416	LEU	C-O	5.53	1.30	1.24
2	L	305	ASN	CA-C	5.53	1.60	1.52
2	L	520	ALA	C-O	5.53	1.30	1.23
1	C	6	PRO	CA-CB	-5.52	1.47	1.53
2	J	406	GLY	C-O	5.52	1.31	1.24
1	E	132	ALA	CA-CB	-5.52	1.44	1.53
2	D	493	LYS	CE-NZ	5.52	1.66	1.49
2	H	390	LYS	CE-NZ	5.52	1.66	1.49
2	B	435	GLY	C-O	-5.52	1.17	1.24
2	J	367	PHE	CA-C	5.52	1.59	1.52
1	E	171	ILE	N-CA	5.51	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	497	ASN	CG-OD1	-5.51	1.13	1.23
2	L	436	TYR	CZ-OH	5.51	1.49	1.38
1	A	159	ASN	CB-CG	5.51	1.65	1.52
1	G	154	LYS	CG-CD	5.51	1.69	1.52
2	H	334	GLN	CA-C	5.51	1.60	1.53
1	I	165	GLN	CG-CD	5.51	1.65	1.52
1	G	43	ASP	CA-C	5.51	1.61	1.52
1	K	43	ASP	CG-OD2	5.51	1.35	1.25
2	D	511	ASN	C-O	5.50	1.31	1.24
2	L	443	LYS	CE-NZ	5.50	1.65	1.49
2	L	532	LYS	N-CA	5.50	1.52	1.46
1	C	130	LEU	N-CA	-5.50	1.39	1.46
2	H	453	PRO	C-O	5.50	1.31	1.24
2	J	319	ALA	CA-C	5.50	1.59	1.52
2	D	436	TYR	CD1-CE1	5.50	1.55	1.38
2	F	443	LYS	CA-C	5.50	1.60	1.52
1	G	189	ILE	CA-C	-5.50	1.44	1.52
2	B	433	SER	CA-C	-5.50	1.45	1.52
2	D	388	TYR	CZ-OH	5.50	1.49	1.38
2	H	393	PRO	C-O	-5.50	1.17	1.23
2	B	454	ASN	CG-OD1	5.50	1.33	1.23
2	F	366	ASN	CG-OD1	5.49	1.33	1.23
1	I	161	ILE	C-O	5.49	1.30	1.23
1	I	19	ILE	C-O	5.49	1.30	1.24
2	J	314	ASN	CA-CB	-5.49	1.44	1.53
1	A	111	PRO	CA-C	-5.49	1.45	1.52
2	J	523	PHE	CA-C	-5.49	1.46	1.52
2	L	503	GLN	CA-CB	-5.48	1.44	1.53
1	G	103	GLU	CD-OE2	5.48	1.35	1.25
2	L	475	ILE	CG1-CD1	5.48	1.73	1.51
1	I	103	GLU	C-O	-5.48	1.16	1.23
2	B	368	ASN	N-CA	5.48	1.53	1.46
2	D	344	SER	C-O	-5.48	1.17	1.24
1	E	60	GLY	CA-C	-5.48	1.44	1.51
2	D	336	LEU	CA-C	5.48	1.59	1.52
2	B	415	TYR	CA-CB	5.47	1.62	1.53
2	F	436	TYR	CG-CD1	5.47	1.50	1.39
1	I	16	TYR	CE1-CZ	5.47	1.51	1.38
2	L	493	LYS	CA-C	5.47	1.60	1.52
2	B	486	ILE	CG1-CD1	-5.47	1.30	1.51
1	G	63	VAL	C-O	-5.47	1.18	1.24
2	F	364	LEU	C-O	5.47	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	16	TYR	CE1-CZ	5.47	1.51	1.38
1	K	184	ARG	CZ-NH2	5.47	1.40	1.33
2	F	524	ASP	CA-CB	-5.46	1.45	1.53
2	H	493	LYS	CE-NZ	5.46	1.65	1.49
1	C	197	PHE	N-CA	5.46	1.52	1.45
2	J	346	THR	C-O	-5.46	1.16	1.24
2	J	436	TYR	CA-C	-5.46	1.45	1.52
2	F	314	ASN	C-O	-5.46	1.17	1.24
2	H	321	THR	CA-C	5.46	1.59	1.52
1	E	169	THR	C-O	-5.46	1.17	1.24
2	D	532	LYS	N-CA	5.46	1.52	1.45
1	G	129	SER	C-O	5.46	1.30	1.24
1	G	14	GLY	C-O	5.46	1.31	1.24
1	E	100	ASP	CG-OD1	5.46	1.35	1.25
1	I	99	PHE	C-O	5.45	1.31	1.24
2	H	480	PHE	CB-CG	-5.45	1.38	1.50
1	C	31	ARG	CA-C	5.45	1.60	1.53
1	K	69	GLU	C-O	5.45	1.30	1.23
2	J	446	PRO	CA-C	-5.45	1.46	1.52
2	J	447	TYR	CE1-CZ	5.44	1.51	1.38
2	J	414	ARG	CA-C	5.44	1.59	1.52
2	D	515	PRO	C-O	-5.43	1.16	1.24
1	G	136	ASN	CA-C	-5.43	1.45	1.52
1	K	91	SER	CA-C	5.43	1.60	1.52
1	E	183	TYR	CA-CB	-5.43	1.43	1.53
1	I	86	GLU	C-O	5.43	1.31	1.24
1	E	183	TYR	N-CA	-5.43	1.39	1.46
2	J	532	LYS	N-CA	5.43	1.52	1.45
2	B	310	ILE	CA-C	5.42	1.59	1.52
1	E	145	PHE	CA-CB	-5.42	1.45	1.53
1	G	77	GLY	C-O	-5.42	1.16	1.24
2	J	506	ALA	CA-CB	-5.42	1.45	1.53
1	A	94	ARG	N-CA	-5.42	1.39	1.45
1	C	161	ILE	CA-CB	-5.42	1.47	1.53
2	F	328	ILE	N-CA	-5.42	1.40	1.46
1	I	40	ALA	CA-C	-5.42	1.46	1.52
1	I	43	ASP	CA-CB	5.42	1.62	1.53
1	K	170	LEU	CG-CD2	5.42	1.70	1.52
2	L	455	ASP	CG-OD1	5.42	1.35	1.25
1	A	9	PRO	CA-CB	-5.42	1.46	1.53
1	E	40	ALA	CA-CB	-5.42	1.45	1.53
1	I	151	ALA	N-CA	5.42	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	428	ARG	C-O	-5.41	1.12	1.23
1	I	25	ALA	CA-C	5.41	1.60	1.52
1	K	42	PRO	CA-C	5.41	1.60	1.52
1	E	186	ASP	C-O	-5.41	1.17	1.23
1	K	185	PHE	CA-CB	-5.41	1.45	1.53
1	K	165	GLN	CD-OE1	5.41	1.33	1.23
1	G	194	GLU	CA-C	5.41	1.59	1.52
2	D	337	VAL	C-O	5.40	1.31	1.24
1	K	116	ASN	N-CA	-5.40	1.39	1.45
2	L	425	GLY	C-O	5.40	1.31	1.24
2	H	537	ASN	CA-C	5.40	1.60	1.52
1	K	68	LEU	N-CA	5.40	1.52	1.46
2	F	308	PHE	C-O	-5.39	1.17	1.24
1	I	66	SER	C-O	-5.39	1.17	1.23
2	F	362	ASP	CG-OD1	5.39	1.35	1.25
2	L	500	ALA	C-O	-5.39	1.17	1.24
2	B	497	ASN	N-CA	-5.38	1.38	1.46
1	C	147	ASP	N-CA	-5.38	1.39	1.46
1	I	73	ALA	C-O	5.38	1.31	1.23
2	F	508	LEU	CB-CG	-5.38	1.42	1.53
1	A	105	THR	CA-CB	5.38	1.63	1.53
1	C	75	ALA	C-O	-5.38	1.17	1.24
1	C	197	PHE	C-O	5.38	1.30	1.23
2	D	350	ASN	CA-CB	-5.38	1.43	1.53
1	A	2	ILE	CB-CG1	-5.37	1.42	1.53
1	E	100	ASP	CB-CG	5.37	1.65	1.52
1	E	120	VAL	CB-CG2	-5.37	1.34	1.52
1	E	21	LEU	CG-CD1	-5.37	1.34	1.52
1	G	150	GLN	N-CA	-5.37	1.39	1.46
1	G	172	ALA	C-N	5.37	1.41	1.33
1	K	98	THR	CA-CB	5.37	1.62	1.53
2	J	411	LYS	CE-NZ	5.37	1.65	1.49
1	C	72	GLN	CA-C	-5.36	1.46	1.52
1	E	142	ARG	NE-CZ	5.36	1.39	1.33
1	E	45	PRO	CA-C	5.36	1.59	1.52
1	G	26	ALA	C-O	5.36	1.31	1.24
2	H	471	ALA	CA-CB	-5.36	1.44	1.53
1	C	183	TYR	CE1-CZ	5.36	1.51	1.38
1	A	167	ARG	C-O	-5.35	1.17	1.24
2	F	381	ALA	C-O	-5.35	1.17	1.23
2	F	501	VAL	C-O	-5.35	1.17	1.24
2	H	349	PRO	CA-CB	5.35	1.61	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	503	GLN	CA-CB	-5.35	1.44	1.53
2	L	479	TYR	CA-C	5.35	1.59	1.52
1	E	143	LEU	C-O	-5.35	1.17	1.24
1	A	150	GLN	CD-OE1	5.35	1.33	1.23
2	B	439	PHE	CB-CG	-5.35	1.38	1.50
1	E	183	TYR	C-O	-5.35	1.17	1.24
1	I	52	LEU	C-O	5.35	1.30	1.23
1	K	1	PRO	C-O	5.35	1.34	1.23
2	L	510	MET	CA-CB	-5.35	1.43	1.53
1	C	133	ARG	NE-CZ	5.35	1.39	1.33
1	E	7	GLU	N-CA	5.35	1.52	1.46
2	J	494	SER	CA-C	5.35	1.60	1.52
2	F	503	GLN	CB-CG	-5.34	1.36	1.52
1	K	165	GLN	C-O	5.34	1.30	1.24
2	B	414	ARG	CD-NE	5.34	1.53	1.46
2	D	318	LYS	CB-CG	5.34	1.68	1.52
1	K	143	LEU	CA-C	5.34	1.59	1.52
1	E	142	ARG	CG-CD	-5.33	1.36	1.52
1	G	178	ASP	CA-CB	5.33	1.61	1.53
2	J	499	GLU	CA-CB	-5.33	1.44	1.53
2	F	329	ALA	CA-CB	5.33	1.63	1.53
1	A	92	PHE	C-O	-5.33	1.17	1.23
2	B	411	LYS	CD-CE	5.33	1.68	1.52
2	B	492	VAL	CA-C	-5.33	1.46	1.52
1	G	45	PRO	CA-C	5.33	1.59	1.52
1	I	190	GLN	CA-C	-5.33	1.45	1.52
2	J	341	GLN	N-CA	5.33	1.52	1.46
1	E	171	ILE	C-O	-5.33	1.18	1.24
2	F	320	LEU	CG-CD1	5.33	1.70	1.52
2	J	438	SER	N-CA	5.33	1.52	1.46
2	F	358	ALA	C-O	-5.32	1.17	1.24
1	I	13	ALA	CA-CB	-5.32	1.44	1.53
1	E	82	ALA	C-O	-5.32	1.17	1.24
2	F	388	TYR	CG-CD1	5.32	1.50	1.39
1	K	79	TYR	C-O	5.32	1.30	1.23
2	L	508	LEU	CG-CD2	-5.32	1.34	1.52
1	C	154	LYS	CD-CE	5.32	1.68	1.52
2	H	319	ALA	CA-CB	-5.32	1.45	1.53
2	J	408	HIS	CA-C	-5.32	1.46	1.52
1	E	10	SER	CA-C	5.32	1.60	1.53
1	G	15	PRO	CA-C	-5.32	1.43	1.52
2	D	450	ARG	CA-C	-5.31	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	99	PHE	CA-CB	5.31	1.62	1.53
2	D	467	GLY	C-O	-5.31	1.16	1.24
1	E	69	GLU	C-O	5.31	1.30	1.23
1	C	30	THR	CA-C	5.31	1.60	1.53
1	G	151	ALA	CA-CB	-5.31	1.45	1.53
2	J	459	ALA	CA-C	5.31	1.59	1.52
1	G	110	LYS	CA-C	5.31	1.59	1.53
1	C	99	PHE	CD2-CE2	5.31	1.54	1.38
2	B	316	HIS	CB-CG	-5.30	1.42	1.50
2	D	436	TYR	CD2-CE2	5.30	1.54	1.38
1	C	44	ALA	CA-C	-5.30	1.46	1.53
1	C	46	GLY	CA-C	-5.30	1.46	1.52
2	D	458	PRO	C-O	5.30	1.30	1.23
2	F	497	ASN	C-O	-5.30	1.17	1.24
2	H	307	ARG	N-CA	5.30	1.52	1.45
1	I	146	ASP	N-CA	5.30	1.53	1.46
2	J	371	GLY	C-O	5.30	1.28	1.23
1	I	129	SER	N-CA	5.30	1.52	1.46
1	C	16	TYR	CE2-CZ	5.30	1.50	1.38
2	D	301	PRO	N-CA	5.30	1.54	1.47
2	D	457	ARG	CB-CG	-5.30	1.36	1.52
1	C	182	ALA	CA-CB	-5.29	1.44	1.54
1	A	32	ASP	CG-OD1	5.29	1.35	1.25
1	G	188	ARG	CZ-NH2	5.29	1.40	1.33
2	H	333	ARG	C-O	-5.29	1.17	1.24
2	L	428	ARG	CA-C	-5.29	1.41	1.52
2	F	332	PRO	CA-C	-5.29	1.45	1.52
1	K	194	GLU	C-O	5.29	1.30	1.23
1	A	3	GLU	CD-OE1	5.29	1.35	1.25
2	H	324	TYR	C-O	5.29	1.30	1.23
1	C	99	PHE	CD1-CE1	5.29	1.54	1.38
1	G	19	ILE	N-CA	-5.29	1.39	1.46
2	L	305	ASN	C-O	5.29	1.30	1.24
1	C	167	ARG	CA-C	-5.29	1.46	1.52
2	D	442	ILE	CA-CB	-5.29	1.48	1.54
2	F	496	ALA	C-O	-5.29	1.17	1.24
2	F	508	LEU	CG-CD2	-5.29	1.35	1.52
1	C	184	ARG	CZ-NH2	5.28	1.40	1.33
2	D	304	ASP	CB-CG	5.28	1.65	1.52
1	I	145	PHE	N-CA	5.28	1.52	1.46
1	A	110	LYS	CA-C	5.28	1.58	1.52
1	G	32	ASP	CG-OD2	5.28	1.35	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	497	ASN	C-O	-5.28	1.17	1.24
2	L	312	ASP	C-O	-5.28	1.17	1.23
1	C	198	PHE	CE2-CZ	5.28	1.54	1.38
1	K	43	ASP	CG-OD1	5.28	1.35	1.25
1	K	151	ALA	N-CA	5.28	1.52	1.46
1	E	99	PHE	N-CA	5.28	1.52	1.46
2	H	510	MET	SD-CE	5.28	1.92	1.79
1	K	165	GLN	CA-C	5.28	1.59	1.52
2	L	469	SER	CA-CB	-5.28	1.47	1.53
1	K	3	GLU	CD-OE2	5.27	1.35	1.25
1	E	110	LYS	CA-C	5.27	1.59	1.53
2	H	426	VAL	C-O	-5.27	1.18	1.24
1	I	88	ALA	C-O	5.27	1.30	1.24
1	I	99	PHE	N-CA	5.27	1.53	1.46
2	B	461	ILE	CA-C	5.27	1.59	1.52
1	A	32	ASP	CG-OD2	5.27	1.35	1.25
1	A	150	GLN	CG-CD	5.27	1.65	1.52
1	A	178	ASP	C-N	5.27	1.38	1.33
1	E	188	ARG	CZ-NH1	5.27	1.40	1.32
1	K	47	GLU	C-O	5.27	1.30	1.24
1	E	120	VAL	C-O	-5.27	1.17	1.24
1	K	91	SER	CA-CB	-5.27	1.44	1.53
1	A	110	LYS	C-N	5.27	1.40	1.33
2	H	399	MET	CA-CB	-5.27	1.44	1.53
1	E	200	PHE	CG-CD2	5.26	1.50	1.38
2	D	442	ILE	CA-C	5.26	1.58	1.52
2	F	338	SER	CB-OG	-5.26	1.31	1.42
1	G	24	GLU	N-CA	5.26	1.52	1.46
1	A	127	ASN	CA-CB	-5.26	1.45	1.53
2	F	340	PRO	CA-C	-5.26	1.45	1.52
1	G	26	ALA	CA-C	5.26	1.60	1.52
2	L	518	CYS	C-O	-5.26	1.17	1.23
1	G	70	VAL	CB-CG2	-5.26	1.35	1.52
1	G	13	ALA	CA-CB	-5.26	1.45	1.53
2	L	301	PRO	N-CA	5.25	1.54	1.47
2	F	514	ASN	CA-CB	5.25	1.61	1.52
2	L	386	ASP	CA-CB	-5.25	1.44	1.53
1	G	53	GLY	C-O	5.25	1.29	1.23
2	B	336	LEU	CG-CD2	5.25	1.69	1.52
1	K	165	GLN	CA-CB	5.25	1.61	1.53
1	A	9	PRO	C-O	5.25	1.29	1.23
1	A	195	THR	N-CA	-5.25	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	132	ALA	CA-CB	-5.25	1.45	1.53
1	G	73	ALA	CA-CB	-5.25	1.44	1.53
2	H	470	ILE	CB-CG2	5.25	1.69	1.52
1	I	129	SER	CA-C	-5.25	1.46	1.52
1	C	189	ILE	CG1-CD1	5.24	1.72	1.51
2	F	499	GLU	N-CA	-5.24	1.39	1.46
2	B	305	ASN	CA-C	5.24	1.59	1.52
1	C	72	GLN	CD-NE2	5.24	1.44	1.33
2	D	409	ARG	C-O	-5.24	1.17	1.23
1	G	107	HIS	CA-C	-5.24	1.46	1.52
1	A	19	ILE	CA-CB	5.24	1.61	1.54
2	B	368	ASN	CG-ND2	5.24	1.44	1.33
1	G	9	PRO	CA-CB	-5.24	1.46	1.53
2	J	339	ILE	CA-C	-5.23	1.47	1.52
1	A	158	LEU	CA-CB	-5.23	1.44	1.53
2	J	363	LEU	C-O	5.23	1.30	1.24
1	A	158	LEU	C-O	-5.23	1.17	1.24
1	C	14	GLY	CA-C	5.23	1.59	1.51
1	G	64	ARG	CZ-NH1	5.23	1.40	1.32
1	I	28	ASN	C-O	5.23	1.29	1.24
2	L	538	CYS	C-OXT	5.23	1.34	1.23
1	C	32	ASP	CA-CB	5.23	1.61	1.53
1	I	173	LYS	CA-CB	5.23	1.60	1.53
1	I	67	PHE	CE1-CZ	5.23	1.54	1.38
2	L	420	ASP	N-CA	-5.22	1.39	1.46
1	C	185	PHE	CB-CG	-5.22	1.38	1.50
1	G	177	VAL	C-O	5.22	1.29	1.24
2	J	527	LEU	C-O	5.22	1.30	1.23
2	L	417	ALA	N-CA	5.22	1.53	1.45
2	D	405	GLY	N-CA	-5.22	1.38	1.45
2	F	307	ARG	N-CA	-5.22	1.39	1.46
2	H	522	ARG	CB-CG	-5.22	1.36	1.52
2	B	408	HIS	CD2-NE2	5.22	1.43	1.37
1	G	183	TYR	CA-C	-5.21	1.46	1.52
2	J	423	PHE	CE1-CZ	5.21	1.54	1.38
1	A	75	ALA	CA-CB	5.21	1.62	1.53
2	D	521	TYR	CA-C	-5.21	1.46	1.52
2	H	500	ALA	C-O	-5.21	1.18	1.24
2	F	501	VAL	CA-C	-5.21	1.46	1.52
1	I	16	TYR	C-O	5.21	1.30	1.24
1	I	100	ASP	CB-CG	5.21	1.65	1.52
2	H	311	ARG	NE-CZ	5.21	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	9	PRO	CA-CB	-5.21	1.46	1.53
1	E	177	VAL	CA-CB	5.21	1.61	1.54
1	G	3	GLU	CD-OE2	5.21	1.35	1.25
1	E	24	GLU	CA-C	5.20	1.59	1.52
1	K	160	LEU	CB-CG	-5.20	1.43	1.53
2	D	427	GLY	N-CA	-5.20	1.39	1.45
2	F	390	LYS	CG-CD	5.20	1.68	1.52
1	E	163	GLN	C-O	-5.20	1.17	1.24
2	F	492	VAL	C-O	-5.20	1.17	1.24
2	F	522	ARG	CB-CG	-5.20	1.36	1.52
2	H	402	ALA	C-O	5.20	1.31	1.23
1	E	165	GLN	CD-NE2	5.20	1.44	1.33
2	B	336	LEU	N-CA	-5.20	1.39	1.46
2	D	530	GLN	C-O	-5.20	1.17	1.24
2	F	458	PRO	CA-CB	-5.20	1.46	1.53
2	J	365	LEU	CG-CD2	5.19	1.69	1.52
1	C	182	ALA	CA-C	-5.19	1.46	1.52
1	E	88	ALA	CA-CB	-5.19	1.44	1.53
2	F	530	GLN	CA-CB	-5.19	1.46	1.53
2	B	324	TYR	C-O	5.19	1.30	1.23
1	A	63	VAL	CA-C	-5.19	1.46	1.52
2	B	414	ARG	CG-CD	5.19	1.68	1.52
2	D	477	GLN	CA-C	-5.19	1.46	1.52
1	C	163	GLN	CD-OE1	5.18	1.33	1.23
1	K	99	PHE	CD2-CE2	5.18	1.54	1.38
2	L	390	LYS	CE-NZ	5.18	1.65	1.49
1	I	7	GLU	CA-C	5.18	1.59	1.52
1	I	76	ASN	C-O	5.18	1.30	1.24
2	F	369	ASN	CB-CG	-5.18	1.39	1.52
2	B	342	SER	C-N	-5.18	1.28	1.34
1	C	171	ILE	CB-CG1	5.18	1.63	1.53
2	L	328	ILE	CB-CG2	-5.18	1.35	1.52
1	K	42	PRO	N-CA	5.17	1.53	1.47
1	C	88	ALA	CA-CB	5.17	1.62	1.53
1	C	187	ILE	C-O	-5.17	1.18	1.24
1	A	78	GLU	CA-C	5.17	1.58	1.52
1	C	41	LYS	CA-C	5.17	1.59	1.53
1	E	68	LEU	CA-C	-5.17	1.46	1.52
1	I	41	LYS	CE-NZ	5.17	1.64	1.49
2	J	417	ALA	CA-C	5.17	1.59	1.53
1	A	171	ILE	CG1-CD1	-5.17	1.31	1.51
2	F	425	GLY	C-O	-5.17	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	107	HIS	CA-C	-5.16	1.46	1.52
2	J	399	MET	C-O	-5.16	1.17	1.23
2	L	380	VAL	CB-CG1	-5.16	1.35	1.52
1	A	123	ALA	CA-CB	-5.16	1.46	1.53
2	B	384	VAL	CA-CB	-5.16	1.47	1.54
2	D	382	GLY	CA-C	-5.16	1.46	1.52
2	H	368	ASN	C-O	5.16	1.30	1.24
2	L	369	ASN	C-N	5.16	1.38	1.33
1	I	8	THR	CA-C	5.16	1.58	1.53
2	L	335	ALA	CA-CB	5.16	1.61	1.53
1	E	56	TYR	CD2-CE2	5.16	1.54	1.38
2	H	345	GLU	CA-CB	-5.16	1.45	1.53
2	J	319	ALA	CA-CB	-5.16	1.45	1.53
2	J	453	PRO	CA-CB	-5.16	1.46	1.53
2	L	483	ASP	N-CA	5.16	1.53	1.46
1	E	99	PHE	CE1-CZ	5.15	1.54	1.38
1	A	181	THR	CA-C	5.15	1.59	1.52
2	J	321	THR	C-N	5.15	1.41	1.33
2	J	423	PHE	N-CA	5.15	1.52	1.46
2	J	493	LYS	CA-C	5.15	1.61	1.52
2	L	447	TYR	N-CA	-5.15	1.40	1.46
1	G	99	PHE	CE1-CZ	5.15	1.54	1.38
2	J	520	ALA	CA-C	-5.15	1.46	1.52
1	G	199	ASP	CA-CB	-5.14	1.45	1.53
1	I	17	VAL	CA-CB	-5.14	1.47	1.54
1	I	105	THR	C-O	-5.14	1.17	1.23
2	L	436	TYR	CE1-CZ	5.14	1.50	1.38
2	B	466	SER	C-O	-5.14	1.18	1.24
1	A	35	ILE	C-O	-5.14	1.18	1.24
1	A	145	PHE	C-O	-5.14	1.17	1.24
2	J	534	HIS	N-CA	-5.14	1.39	1.45
2	F	449	TRP	CD2-CE2	5.14	1.50	1.41
2	L	414	ARG	CZ-NH1	5.14	1.40	1.32
1	A	30	THR	CA-C	5.13	1.60	1.53
2	J	407	ARG	C-O	5.13	1.30	1.24
2	J	324	TYR	CA-CB	-5.13	1.46	1.52
1	K	69	GLU	CB-CG	-5.13	1.37	1.52
1	C	19	ILE	CG1-CD1	5.13	1.71	1.51
1	C	172	ALA	C-O	5.13	1.29	1.23
2	J	411	LYS	CB-CG	5.13	1.67	1.52
2	B	333	ARG	CZ-NH1	5.12	1.40	1.32
1	G	197	PHE	CD2-CE2	5.12	1.54	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	488	MET	C-O	-5.12	1.16	1.23
2	D	385	VAL	CA-C	5.12	1.58	1.52
2	D	506	ALA	CA-CB	-5.12	1.45	1.53
1	G	29	PRO	CA-C	5.12	1.59	1.52
2	L	523	PHE	CD2-CE2	5.12	1.54	1.38
2	H	338	SER	CA-C	5.12	1.59	1.52
1	A	41	LYS	C-O	5.12	1.30	1.23
2	D	460	HIS	C-N	-5.12	1.26	1.33
2	D	394	ASN	C-O	5.12	1.30	1.23
2	D	470	ILE	CA-C	5.12	1.60	1.52
1	I	47	GLU	CG-CD	5.12	1.64	1.52
1	G	16	TYR	CG-CD1	5.11	1.50	1.39
2	L	307	ARG	CD-NE	5.11	1.53	1.46
2	D	364	LEU	CG-CD2	-5.11	1.35	1.52
1	E	134	GLY	N-CA	-5.11	1.37	1.45
1	A	9	PRO	CG-CD	-5.11	1.33	1.50
1	A	188	ARG	NE-CZ	5.11	1.38	1.33
2	D	379	ILE	CA-C	5.11	1.58	1.52
1	E	128	ILE	N-CA	-5.11	1.40	1.46
1	E	110	LYS	CB-CG	5.11	1.67	1.52
2	H	308	PHE	CA-C	-5.11	1.46	1.52
1	A	168	GLU	CD-OE2	5.10	1.35	1.25
1	C	54	GLN	C-O	5.10	1.30	1.23
2	L	401	GLN	CD-OE1	5.10	1.33	1.23
2	H	524	ASP	CG-OD2	5.10	1.35	1.25
1	I	87	ASN	CG-OD1	5.10	1.33	1.23
2	J	533	THR	CA-CB	5.10	1.61	1.53
1	E	17	VAL	CB-CG1	5.10	1.69	1.52
2	L	484	PRO	CG-CD	5.10	1.68	1.50
1	I	13	ALA	N-CA	5.09	1.52	1.46
1	K	80	GLN	CD-OE1	5.09	1.33	1.23
2	F	391	PRO	C-O	-5.09	1.17	1.23
1	I	199	ASP	CA-C	-5.09	1.46	1.52
1	A	90	ASN	C-O	-5.09	1.18	1.24
1	I	75	ALA	CA-CB	-5.09	1.44	1.53
2	D	530	GLN	N-CA	-5.09	1.40	1.46
2	L	412	ASN	CB-CG	5.09	1.64	1.52
2	B	524	ASP	C-O	5.09	1.29	1.23
1	C	160	LEU	CA-CB	-5.09	1.44	1.53
2	D	424	GLY	C-N	-5.09	1.27	1.33
1	G	6	PRO	CA-C	5.09	1.59	1.52
1	G	46	GLY	C-O	-5.09	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	95	THR	CA-CB	-5.09	1.45	1.53
2	H	465	ILE	CA-CB	5.09	1.61	1.54
1	K	121	PRO	CA-C	5.08	1.58	1.52
2	J	303	GLN	N-CA	5.08	1.51	1.45
1	G	3	GLU	CD-OE1	5.08	1.35	1.25
2	H	475	ILE	CA-C	5.08	1.58	1.52
2	B	325	LYS	N-CA	-5.08	1.40	1.46
2	L	503	GLN	CD-OE1	5.08	1.33	1.23
1	I	192	GLU	CD-OE1	5.08	1.34	1.25
1	E	168	GLU	CD-OE2	5.08	1.34	1.25
1	G	97	THR	N-CA	-5.08	1.40	1.46
2	B	412	ASN	CG-ND2	5.07	1.44	1.33
2	H	341	GLN	CD-OE1	-5.07	1.14	1.23
2	J	509	ASP	CG-OD1	5.07	1.34	1.25
1	A	97	THR	CB-CG2	-5.07	1.35	1.52
1	C	68	LEU	CG-CD2	-5.07	1.35	1.52
1	C	167	ARG	C-O	-5.07	1.18	1.24
1	E	195	THR	CA-CB	-5.07	1.44	1.53
1	I	148	GLU	CD-OE1	5.07	1.34	1.25
2	D	368	ASN	CG-OD1	5.07	1.33	1.23
2	B	443	LYS	CA-C	-5.07	1.46	1.52
2	L	360	ASP	C-O	-5.07	1.17	1.24
2	L	408	HIS	N-CA	5.07	1.51	1.45
2	D	309	VAL	CA-CB	5.06	1.60	1.54
2	J	499	GLU	CD-OE1	5.06	1.34	1.25
2	J	514	ASN	CG-OD1	5.06	1.33	1.23
1	K	16	TYR	CD2-CE2	5.06	1.53	1.38
1	K	94	ARG	CZ-NH2	-5.06	1.26	1.33
2	H	532	LYS	N-CA	5.06	1.52	1.45
1	C	16	TYR	N-CA	5.06	1.52	1.46
2	D	478	LEU	CG-CD2	5.06	1.69	1.52
2	L	415	TYR	CG-CD2	5.06	1.50	1.39
1	A	74	ASP	CA-C	5.06	1.59	1.52
2	B	407	ARG	C-O	-5.06	1.17	1.24
2	J	497	ASN	CA-CB	-5.06	1.45	1.52
1	A	158	LEU	CG-CD1	-5.05	1.35	1.52
1	A	73	ALA	CA-C	5.05	1.59	1.52
2	H	423	PHE	CA-C	5.05	1.58	1.52
1	I	67	PHE	CB-CG	-5.05	1.39	1.50
2	B	434	ASP	CG-OD1	5.05	1.34	1.25
2	D	459	ALA	N-CA	5.05	1.52	1.46
2	H	537	ASN	CG-OD1	5.04	1.33	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	354	LEU	CA-C	5.04	1.59	1.52
1	E	75	ALA	CA-C	-5.04	1.45	1.52
1	G	55	VAL	C-O	-5.04	1.18	1.24
2	H	537	ASN	CA-CB	5.04	1.61	1.53
2	L	513	ALA	N-CA	5.04	1.52	1.45
2	L	485	LEU	CA-C	5.04	1.59	1.52
1	A	80	GLN	N-CA	-5.04	1.40	1.46
1	I	128	ILE	CA-C	5.04	1.58	1.52
2	B	412	ASN	CG-OD1	5.04	1.33	1.23
2	D	421	PRO	CA-C	5.04	1.59	1.52
1	K	183	TYR	C-O	5.04	1.30	1.23
1	G	179	GLY	CA-C	5.03	1.58	1.51
1	C	184	ARG	CA-C	-5.03	1.46	1.52
1	I	120	VAL	N-CA	-5.03	1.41	1.46
1	A	121	PRO	C-O	-5.03	1.18	1.23
1	A	151	ALA	CA-C	5.03	1.59	1.52
1	C	120	VAL	N-CA	5.03	1.52	1.46
2	D	503	GLN	CD-OE1	5.03	1.33	1.23
1	E	171	ILE	CG1-CD1	-5.03	1.32	1.51
1	A	115	ASN	CA-C	5.03	1.59	1.52
2	D	334	GLN	CG-CD	5.03	1.64	1.52
1	E	64	ARG	CZ-NH1	5.03	1.39	1.32
2	L	459	ALA	C-N	5.03	1.40	1.33
1	A	3	GLU	CD-OE2	5.02	1.34	1.25
1	C	160	LEU	CB-CG	-5.02	1.43	1.53
2	D	385	VAL	N-CA	5.02	1.51	1.46
1	E	129	SER	CA-C	-5.02	1.46	1.52
2	L	430	LEU	CG-CD2	5.02	1.69	1.52
2	B	399	MET	C-O	-5.02	1.17	1.23
2	L	310	ILE	CA-CB	5.02	1.60	1.54
1	A	165	GLN	CG-CD	5.02	1.64	1.52
2	J	317	PRO	N-CA	5.02	1.52	1.47
1	E	193	GLY	C-O	-5.02	1.17	1.23
1	E	174	ARG	CZ-NH2	5.02	1.40	1.33
1	G	37	ASN	N-CA	-5.02	1.39	1.46
1	K	146	ASP	CA-C	5.02	1.59	1.52
1	A	113	VAL	CA-CB	5.01	1.59	1.54
1	E	188	ARG	CD-NE	5.01	1.53	1.46
1	G	158	LEU	CA-C	5.01	1.59	1.52
1	A	20	GLY	CA-C	-5.01	1.44	1.51
1	E	47	GLU	C-O	-5.01	1.17	1.24
2	H	449	TRP	CD2-CE2	5.01	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	438	SER	CA-C	-5.01	1.46	1.52
1	E	162	GLU	CD-OE1	5.01	1.34	1.25
2	H	414	ARG	CZ-NH1	5.01	1.39	1.32
1	E	163	GLN	CD-OE1	5.01	1.33	1.23
2	L	345	GLU	CD-OE1	5.01	1.34	1.25
1	I	142	ARG	CG-CD	-5.01	1.37	1.52
1	A	50	LEU	CA-C	5.00	1.58	1.52
1	G	86	GLU	CD-OE2	5.00	1.34	1.25
1	E	166	ARG	CG-CD	-5.00	1.37	1.52
2	H	492	VAL	CB-CG2	-5.00	1.36	1.52
2	H	510	MET	CA-C	-5.00	1.45	1.52
2	J	474	LEU	CG-CD2	-5.00	1.36	1.52

All (913) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	333	ARG	NE-CZ-NH1	-13.07	108.43	121.50
1	G	37	ASN	N-CA-C	13.00	127.50	112.93
2	J	443	LYS	CA-C-N	-12.46	107.69	120.03
2	J	443	LYS	C-N-CA	-12.46	107.69	120.03
1	C	101	ALA	CA-C-O	-12.20	107.92	121.58
2	H	440	ARG	CB-CG-CD	-12.18	83.30	111.30
1	A	101	ALA	CA-C-O	-12.16	107.96	121.58
1	C	37	ASN	N-CA-C	11.79	127.17	113.02
1	I	37	ASN	N-CA-C	11.64	125.99	112.72
1	K	120	VAL	CB-CA-C	-11.52	100.23	110.94
1	K	37	ASN	N-CA-C	11.50	125.81	112.93
2	F	333	ARG	NE-CZ-NH1	-11.43	110.08	121.50
1	C	168	GLU	N-CA-C	11.33	126.25	111.75
1	C	102	GLY	CA-C-O	11.32	133.00	119.65
1	E	101	ALA	CA-C-O	-11.02	109.24	121.58
1	E	21	LEU	N-CA-C	10.64	128.88	113.02
1	C	133	ARG	NE-CZ-NH1	10.61	132.11	121.50
2	F	440	ARG	CB-CG-CD	-10.40	87.37	111.30
2	F	440	ARG	NE-CZ-NH2	-10.26	109.97	119.20
2	J	537	ASN	N-CA-C	-10.24	98.19	111.92
1	I	94	ARG	NE-CZ-NH2	-10.02	110.18	119.20
2	D	426	VAL	CB-CA-C	-9.93	95.52	110.82
2	H	537	ASN	CA-C-N	9.92	139.55	121.70
2	H	537	ASN	C-N-CA	9.92	139.55	121.70
2	D	440	ARG	CB-CG-CD	-9.79	88.79	111.30
2	D	417	ALA	CA-C-N	-9.76	110.74	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	417	ALA	C-N-CA	-9.76	110.74	120.31
2	H	538	CYS	CA-CB-SG	-9.75	91.98	114.40
1	E	37	ASN	N-CA-C	9.71	124.70	113.15
1	A	60	GLY	N-CA-C	-9.70	102.31	114.92
2	H	332	PRO	CB-CA-C	-9.66	99.37	111.64
1	C	94	ARG	NE-CZ-NH1	9.45	130.95	121.50
1	C	99	PHE	CA-C-N	9.44	133.46	120.63
1	C	99	PHE	C-N-CA	9.44	133.46	120.63
2	L	392	VAL	CA-C-N	9.41	129.35	119.85
2	L	392	VAL	C-N-CA	9.41	129.35	119.85
1	I	133	ARG	NE-CZ-NH2	-9.33	110.80	119.20
2	J	366	ASN	N-CA-C	9.28	124.43	113.20
2	B	440	ARG	NE-CZ-NH2	-9.14	110.97	119.20
2	B	367	PHE	N-CA-C	-9.13	99.89	112.12
1	K	150	GLN	CA-C-O	-9.09	110.82	120.55
1	A	138	HIS	N-CA-C	9.04	122.47	110.53
2	L	314	ASN	N-CA-C	-9.03	101.80	113.17
2	B	306	SER	N-CA-C	9.02	124.11	110.14
2	L	333	ARG	N-CA-C	-8.89	101.26	112.90
2	D	371	GLY	N-CA-C	8.87	123.70	110.75
1	K	64	ARG	NE-CZ-NH1	8.85	130.35	121.50
1	G	163	GLN	CA-C-O	8.83	125.03	119.29
2	J	428	ARG	NE-CZ-NH2	-8.80	111.28	119.20
2	L	458	PRO	CB-CA-C	-8.78	99.45	110.95
1	K	113	VAL	N-CA-C	8.71	120.72	109.30
2	J	494	SER	N-CA-C	-8.69	102.67	113.18
2	D	316	HIS	CA-C-N	-8.68	111.44	120.03
2	D	316	HIS	C-N-CA	-8.68	111.44	120.03
1	C	5	LEU	CA-C-N	-8.64	110.98	120.14
1	C	5	LEU	C-N-CA	-8.64	110.98	120.14
1	A	94	ARG	NE-CZ-NH2	-8.61	111.45	119.20
1	A	94	ARG	NE-CZ-NH1	8.60	130.10	121.50
2	H	482	GLY	N-CA-C	8.59	126.74	115.40
1	E	168	GLU	CB-CG-CD	-8.59	98.00	112.60
2	F	458	PRO	CB-CA-C	-8.59	100.04	111.12
2	B	440	ARG	CB-CG-CD	-8.56	91.60	111.30
1	G	101	ALA	CA-C-O	-8.55	112.02	120.92
1	I	5	LEU	CA-C-N	-8.55	110.76	119.99
1	I	5	LEU	C-N-CA	-8.55	110.76	119.99
2	J	367	PHE	N-CA-C	-8.50	102.84	113.55
2	H	440	ARG	NE-CZ-NH2	-8.42	111.62	119.20
2	H	442	ILE	CB-CG1-CD1	-8.41	96.14	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	451	ASN	N-CA-C	-8.41	92.89	110.80
1	K	94	ARG	NE-CZ-NH2	-8.41	111.63	119.20
1	K	168	GLU	N-CA-C	8.40	121.37	111.71
1	E	113	VAL	N-CA-C	8.37	119.76	109.30
2	H	500	ALA	N-CA-C	-8.31	102.30	111.36
1	G	138	HIS	N-CA-C	8.26	122.15	110.50
2	J	428	ARG	NE-CZ-NH1	8.23	129.73	121.50
2	H	522	ARG	NE-CZ-NH1	-8.22	113.28	121.50
1	E	36	TRP	N-CA-C	8.21	119.41	108.07
1	I	64	ARG	NE-CZ-NH1	8.19	129.69	121.50
1	C	180	LYS	CB-CA-C	8.18	125.00	109.37
1	A	100	ASP	CA-C-N	8.18	135.42	122.34
1	A	100	ASP	C-N-CA	8.18	135.42	122.34
1	A	23	LEU	N-CA-C	8.15	119.79	111.07
1	G	94	ARG	NE-CZ-NH2	-8.12	111.89	119.20
2	J	512	ASN	N-CA-C	8.10	123.21	113.16
1	A	86	GLU	N-CA-C	8.06	121.17	111.82
2	B	366	ASN	N-CA-C	8.06	121.90	112.72
2	J	378	ILE	CA-C-O	8.05	129.60	121.63
2	J	306	SER	N-CA-C	8.04	123.12	110.17
2	D	322	PRO	N-CA-C	8.04	124.29	113.84
2	J	371	GLY	N-CA-C	8.02	125.89	110.66
2	B	473	LYS	CD-CE-NZ	-7.99	86.33	111.90
1	E	33	GLN	N-CA-C	7.99	122.00	108.02
2	D	382	GLY	CA-C-O	7.98	129.73	121.35
2	D	473	LYS	CD-CE-NZ	-7.98	86.37	111.90
2	D	378	ILE	CA-C-O	7.97	129.43	120.90
2	B	537	ASN	CA-C-N	7.97	136.04	121.70
2	B	537	ASN	C-N-CA	7.97	136.04	121.70
1	C	94	ARG	NE-CZ-NH2	-7.97	112.03	119.20
2	J	440	ARG	CB-CG-CD	-7.97	92.98	111.30
1	K	102	GLY	CA-C-N	7.97	134.52	122.65
1	K	102	GLY	C-N-CA	7.97	134.52	122.65
1	K	73	ALA	N-CA-C	7.92	121.67	110.50
1	E	106	LEU	CB-CG-CD2	-7.90	87.00	110.70
2	B	415	TYR	N-CA-C	7.90	120.51	110.24
2	H	434	ASP	N-CA-CB	-7.90	98.80	110.49
2	J	416	LEU	N-CA-C	7.89	120.78	111.71
2	L	440	ARG	CB-CG-CD	-7.87	93.20	111.30
2	F	407	ARG	NE-CZ-NH2	-7.86	112.12	119.20
2	B	538	CYS	CA-CB-SG	-7.85	96.33	114.40
2	B	504	LEU	CD1-CG-CD2	-7.83	93.58	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	480	PHE	N-CA-C	7.80	121.96	109.24
2	F	333	ARG	NE-CZ-NH2	7.72	126.15	119.20
2	B	423	PHE	N-CA-C	7.70	120.95	108.41
2	L	339	ILE	CA-C-N	-7.69	112.77	120.31
2	L	339	ILE	C-N-CA	-7.69	112.77	120.31
2	D	482	GLY	N-CA-C	7.68	125.54	115.40
2	L	391	PRO	CB-CA-C	-7.68	100.92	110.98
1	E	168	GLU	N-CA-C	7.66	121.73	112.38
2	D	412	ASN	CA-C-N	-7.64	112.91	122.84
2	D	412	ASN	C-N-CA	-7.64	112.91	122.84
2	F	333	ARG	N-CA-C	-7.64	104.10	113.50
1	I	64	ARG	NE-CZ-NH2	-7.63	112.34	119.20
2	J	311	ARG	CG-CD-NE	-7.61	95.27	112.00
1	I	32	ASP	CB-CA-C	-7.60	98.95	110.88
1	I	171	ILE	N-CA-CB	-7.59	102.33	111.21
1	I	24	GLU	CA-C-N	7.59	130.77	120.38
1	I	24	GLU	C-N-CA	7.59	130.77	120.38
1	K	40	ALA	CA-C-O	7.59	129.38	120.66
2	L	367	PHE	N-CA-C	-7.56	104.03	113.55
2	L	470	ILE	N-CA-C	-7.56	101.31	111.44
2	L	522	ARG	NE-CZ-NH1	-7.55	113.95	121.50
1	E	69	GLU	N-CA-C	-7.52	97.62	109.50
2	L	461	ILE	N-CA-C	-7.51	97.31	108.12
2	L	528	ARG	NE-CZ-NH1	-7.46	114.04	121.50
1	I	86	GLU	N-CA-C	7.46	122.48	113.23
1	K	150	GLN	N-CA-CB	7.46	121.17	110.13
1	C	126	ILE	CA-CB-CG1	-7.41	97.81	110.40
1	C	48	HIS	N-CA-C	7.39	120.97	109.96
1	C	171	ILE	N-CA-C	7.37	118.43	107.15
2	J	450	ARG	NE-CZ-NH1	-7.37	114.13	121.50
1	E	81	ASP	N-CA-C	7.37	120.75	111.69
2	F	365	LEU	N-CA-C	7.36	123.81	114.31
2	B	313	ARG	N-CA-C	7.35	122.07	113.18
2	D	428	ARG	CB-CG-CD	7.34	128.19	111.30
1	E	41	LYS	N-CA-C	-7.34	99.96	110.08
2	L	411	LYS	CA-C-O	-7.33	111.81	120.10
1	C	180	LYS	N-CA-C	-7.33	97.46	109.40
2	D	321	THR	N-CA-C	-7.32	92.68	108.64
1	K	96	ALA	N-CA-C	7.31	120.32	108.76
2	L	473	LYS	CG-CD-CE	-7.31	94.48	111.30
2	D	537	ASN	N-CA-C	-7.31	102.89	112.24
1	A	103	GLU	N-CA-C	7.30	121.56	109.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	322	PRO	N-CA-C	7.29	127.49	112.47
1	C	133	ARG	NE-CZ-NH2	-7.29	112.64	119.20
1	C	148	GLU	N-CA-C	-7.28	101.56	110.88
1	G	108	THR	CA-C-O	-7.28	113.41	121.05
1	A	72	GLN	N-CA-C	7.27	120.41	108.99
1	K	64	ARG	NE-CZ-NH2	-7.26	112.67	119.20
2	B	311	ARG	CA-C-N	-7.26	112.77	122.42
2	B	311	ARG	C-N-CA	-7.26	112.77	122.42
1	G	163	GLN	N-CA-C	7.26	121.46	108.47
2	D	428	ARG	NE-CZ-NH2	-7.24	112.68	119.20
2	D	333	ARG	CG-CD-NE	-7.23	96.10	112.00
1	A	141	THR	CA-C-O	-7.22	113.71	121.36
2	D	306	SER	N-CA-C	7.22	121.27	109.72
1	E	38	ARG	NE-CZ-NH1	7.20	128.70	121.50
2	F	426	VAL	CB-CA-C	-7.20	99.17	110.69
2	H	366	ASN	N-CA-C	7.20	121.65	113.01
2	B	328	ILE	N-CA-C	7.20	117.28	110.30
1	G	70	VAL	CA-C-O	-7.20	113.50	121.92
1	I	23	LEU	N-CA-C	7.19	119.74	111.11
1	C	66	SER	N-CA-C	7.18	120.25	110.55
1	K	121	PRO	O-C-N	7.18	131.90	123.14
2	J	426	VAL	CB-CA-C	-7.17	99.78	110.82
2	D	358	ALA	N-CA-C	7.16	119.94	111.71
2	L	418	PRO	N-CA-C	7.15	121.23	111.22
1	K	163	GLN	N-CA-C	7.14	119.16	109.24
1	G	191	GLY	N-CA-C	7.12	121.86	111.24
2	J	460	HIS	N-CA-C	7.12	119.56	108.96
1	E	181	THR	CB-CA-C	-7.09	98.84	109.90
2	J	464	GLY	N-CA-C	-7.08	99.07	111.46
1	C	154	LYS	CB-CA-C	-7.06	98.79	110.72
2	L	538	CYS	CA-CB-SG	-7.02	98.26	114.40
1	K	94	ARG	NE-CZ-NH1	7.00	128.50	121.50
1	K	101	ALA	CA-C-O	-7.00	112.91	121.58
1	C	146	ASP	N-CA-C	6.99	121.07	112.54
1	C	159	ASN	N-CA-C	6.99	121.26	112.87
1	G	134	GLY	CA-C-O	-6.98	111.64	119.04
1	I	100	ASP	N-CA-C	-6.98	101.99	112.04
2	L	457	ARG	CB-CA-C	-6.98	98.47	109.42
1	C	22	ALA	N-CA-C	-6.97	95.95	110.80
2	L	492	VAL	N-CA-C	-6.96	103.88	110.42
1	E	3	GLU	CB-CA-C	-6.94	98.81	110.19
1	I	47	GLU	CA-C-O	-6.93	113.49	120.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	314	ASN	N-CA-C	-6.91	105.00	113.50
1	I	198	PHE	N-CA-C	6.90	120.67	110.46
1	K	144	TYR	CA-C-N	-6.89	112.94	122.93
1	K	144	TYR	C-N-CA	-6.89	112.94	122.93
1	C	186	ASP	CA-C-N	-6.88	114.18	123.12
1	C	186	ASP	C-N-CA	-6.88	114.18	123.12
1	I	168	GLU	N-CA-C	6.87	118.76	111.28
1	K	69	GLU	N-CA-C	-6.85	97.80	109.24
2	F	438	SER	N-CA-C	6.84	119.57	108.76
1	E	44	ALA	CA-C-N	6.84	126.82	119.78
1	E	44	ALA	C-N-CA	6.84	126.82	119.78
2	F	507	LYS	CD-CE-NZ	6.84	133.77	111.90
1	I	126	ILE	CA-C-O	-6.82	112.69	120.67
2	H	528	ARG	NE-CZ-NH1	-6.82	114.68	121.50
1	E	111	PRO	CA-C-N	-6.82	111.78	121.54
1	E	111	PRO	C-N-CA	-6.82	111.78	121.54
2	L	416	LEU	N-CA-C	6.81	119.54	111.71
2	F	452	GLY	N-CA-C	-6.80	103.73	112.10
2	D	494	SER	N-CA-C	-6.78	103.96	111.82
1	G	26	ALA	N-CA-C	-6.78	105.00	113.20
2	F	409	ARG	NE-CZ-NH1	-6.77	114.73	121.50
1	G	15	PRO	CA-C-N	-6.76	112.41	122.83
1	G	15	PRO	C-N-CA	-6.76	112.41	122.83
2	L	328	ILE	N-CA-C	6.76	117.52	110.62
2	L	416	LEU	CA-C-O	-6.76	112.46	120.10
2	D	388	TYR	N-CA-C	-6.75	104.79	113.16
1	I	101	ALA	CA-C-O	-6.75	113.46	122.51
2	H	507	LYS	CD-CE-NZ	6.75	133.50	111.90
1	G	180	LYS	CD-CE-NZ	6.75	133.49	111.90
2	D	440	ARG	NE-CZ-NH2	-6.74	113.13	119.20
1	A	95	THR	N-CA-C	-6.74	99.29	108.38
2	B	314	ASN	N-CA-C	-6.73	104.89	113.23
1	C	188	ARG	NE-CZ-NH1	6.71	128.21	121.50
2	J	452	GLY	CA-C-N	-6.71	112.72	119.56
2	J	452	GLY	C-N-CA	-6.71	112.72	119.56
2	F	505	ILE	N-CA-CB	-6.70	103.36	111.00
1	A	94	ARG	CB-CG-CD	6.70	126.71	111.30
1	G	41	LYS	N-CA-C	-6.70	101.05	110.29
2	D	451	ASN	N-CA-C	-6.69	96.54	110.80
1	G	96	ALA	N-CA-C	6.69	118.73	108.42
1	E	122	MET	N-CA-C	-6.69	100.05	110.42
2	L	422	ASN	N-CA-C	6.68	120.12	112.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	440	ARG	NE-CZ-NH1	6.68	128.18	121.50
1	E	126	ILE	CB-CG1-CD1	-6.67	99.80	113.80
2	H	450	ARG	NE-CZ-NH1	-6.67	114.83	121.50
1	K	88	ALA	O-C-N	6.67	128.94	122.07
1	C	112	GLY	CA-C-O	-6.66	114.37	122.03
1	A	64	ARG	NE-CZ-NH1	6.65	128.15	121.50
2	H	486	ILE	CA-C-N	-6.65	111.52	119.84
2	H	486	ILE	C-N-CA	-6.65	111.52	119.84
2	B	384	VAL	CB-CA-C	-6.65	101.25	110.96
1	K	100	ASP	CA-C-N	6.65	133.22	123.12
1	K	100	ASP	C-N-CA	6.65	133.22	123.12
1	A	190	GLN	CA-C-O	-6.64	113.55	120.99
1	C	56	TYR	N-CA-C	6.64	120.51	109.95
2	J	497	ASN	N-CA-CB	-6.63	100.33	110.01
2	F	305	ASN	N-CA-C	-6.62	105.12	113.72
2	F	306	SER	N-CA-C	6.62	120.31	109.85
1	E	158	LEU	N-CA-C	-6.62	104.14	111.82
1	K	81	ASP	N-CA-C	6.61	118.57	111.36
1	E	95	THR	CA-C-O	-6.60	114.36	121.36
2	J	377	ARG	NE-CZ-NH1	-6.60	114.90	121.50
2	F	359	HIS	N-CA-C	6.60	120.97	112.26
2	H	473	LYS	CD-CE-NZ	-6.59	90.81	111.90
2	L	420	ASP	CA-C-N	6.59	127.11	119.47
2	L	420	ASP	C-N-CA	6.59	127.11	119.47
2	L	473	LYS	CD-CE-NZ	-6.59	90.82	111.90
2	B	364	LEU	N-CA-C	-6.58	103.94	112.23
2	L	501	VAL	N-CA-C	-6.58	104.07	110.72
2	D	390	LYS	CG-CD-CE	6.58	126.43	111.30
1	C	166	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	A	14	GLY	CA-C-N	6.57	126.51	119.28
1	A	14	GLY	C-N-CA	6.57	126.51	119.28
2	D	318	LYS	CA-CB-CG	6.57	127.24	114.10
1	G	94	ARG	NE-CZ-NH1	6.56	128.06	121.50
2	B	452	GLY	N-CA-C	-6.56	98.96	112.34
2	B	427	GLY	CA-C-O	-6.55	115.22	121.19
2	J	441	THR	N-CA-C	6.55	116.88	108.24
2	B	354	LEU	N-CA-C	-6.54	100.80	110.48
1	G	150	GLN	CB-CG-CD	-6.54	101.48	112.60
1	K	30	THR	N-CA-C	6.54	119.38	110.55
2	H	306	SER	N-CA-C	6.53	120.17	109.72
2	D	492	VAL	N-CA-C	-6.53	103.88	111.00
2	H	483	ASP	CA-C-O	6.51	125.26	119.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LEU	N-CA-CB	-6.51	100.53	110.49
1	C	168	GLU	CB-CG-CD	-6.51	101.54	112.60
1	I	147	ASP	N-CA-C	6.51	121.37	113.17
2	B	457	ARG	CB-CA-C	-6.50	98.79	109.46
1	C	64	ARG	NE-CZ-NH1	6.49	127.99	121.50
1	A	35	ILE	N-CA-C	-6.47	97.86	107.51
1	G	114	VAL	CG1-CB-CG2	-6.47	96.56	110.80
2	B	428	ARG	NE-CZ-NH2	-6.47	113.37	119.20
2	J	356	PHE	N-CA-C	6.47	119.67	109.96
2	B	375	GLY	CA-C-O	-6.47	115.58	122.05
2	F	497	ASN	CA-C-N	-6.46	113.15	119.87
2	F	497	ASN	C-N-CA	-6.46	113.15	119.87
2	B	426	VAL	CA-C-O	-6.45	113.45	120.67
2	F	523	PHE	CA-C-O	-6.45	113.36	120.33
1	C	16	TYR	N-CA-C	6.45	120.15	112.93
1	E	22	ALA	N-CA-C	-6.44	97.08	110.80
2	B	473	LYS	CA-C-O	-6.44	114.48	121.44
1	C	128	ILE	N-CA-C	6.43	118.04	108.46
2	F	526	VAL	CA-C-O	6.43	127.07	120.39
1	A	48	HIS	CA-C-O	-6.42	113.43	120.81
2	L	440	ARG	NE-CZ-NH2	-6.41	113.43	119.20
2	L	359	HIS	N-CA-C	6.41	120.80	112.92
2	L	369	ASN	O-C-N	6.41	130.36	121.83
2	H	466	SER	N-CA-C	6.41	119.22	111.40
1	A	103	GLU	CA-C-O	-6.40	113.93	121.16
2	H	358	ALA	O-C-N	6.39	128.90	122.12
2	H	364	LEU	N-CA-C	-6.38	105.32	113.23
1	G	173	LYS	CA-C-N	6.38	130.62	121.50
1	G	173	LYS	C-N-CA	6.38	130.62	121.50
2	L	311	ARG	CB-CA-C	-6.38	99.13	109.72
1	I	24	GLU	O-C-N	6.37	128.90	122.08
2	J	377	ARG	NE-CZ-NH2	6.37	124.93	119.20
2	B	430	LEU	CB-CG-CD2	-6.37	91.59	110.70
1	C	171	ILE	CB-CG1-CD1	6.36	127.16	113.80
2	D	307	ARG	NE-CZ-NH2	-6.36	113.48	119.20
1	K	196	VAL	CB-CA-C	-6.36	102.31	111.34
2	H	426	VAL	CA-C-O	-6.34	113.57	120.67
2	F	417	ALA	N-CA-C	-6.34	101.67	109.65
1	A	168	GLU	N-CA-C	6.33	120.10	112.38
1	I	182	ALA	N-CA-C	6.32	119.03	109.23
1	A	87	ASN	CA-C-N	6.32	128.75	120.28
1	A	87	ASN	C-N-CA	6.32	128.75	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	66	SER	N-CA-CB	-6.32	101.12	110.85
2	J	415	TYR	N-CA-C	6.32	119.15	110.24
1	E	177	VAL	O-C-N	6.32	128.65	122.97
2	B	401	GLN	N-CA-C	6.31	117.82	108.60
1	E	134	GLY	CA-C-O	-6.31	112.35	119.04
2	B	538	CYS	N-CA-C	6.30	128.65	111.00
2	L	395	THR	CB-CA-C	6.30	120.90	109.37
2	L	397	VAL	CA-C-N	-6.30	112.22	122.81
2	L	397	VAL	C-N-CA	-6.30	112.22	122.81
2	F	364	LEU	CA-C-N	-6.29	112.36	122.24
2	F	364	LEU	C-N-CA	-6.29	112.36	122.24
1	I	19	ILE	CA-C-O	-6.29	113.83	120.57
2	B	325	LYS	N-CA-C	6.29	118.65	111.11
2	D	426	VAL	CA-C-O	-6.28	113.02	121.32
2	F	431	THR	CA-C-O	-6.28	114.58	121.87
1	G	171	ILE	N-CA-C	6.28	117.53	107.73
1	I	48	HIS	N-CA-C	6.28	119.38	109.96
2	J	364	LEU	N-CA-C	-6.28	104.88	112.54
2	H	310	ILE	CA-C-O	-6.28	114.46	121.36
2	J	385	VAL	CA-C-O	-6.27	114.01	121.28
2	J	438	SER	O-C-N	6.27	130.12	123.42
2	J	461	ILE	CB-CA-C	-6.26	101.36	110.63
1	K	1	PRO	N-CA-CB	6.25	109.88	103.00
2	L	526	VAL	CB-CA-C	-6.25	101.89	110.77
2	J	339	ILE	CA-C-N	-6.24	113.85	120.03
2	J	339	ILE	C-N-CA	-6.24	113.85	120.03
2	D	366	ASN	N-CA-C	6.24	120.50	113.01
2	F	372	LEU	CB-CA-C	6.24	117.35	108.68
2	F	426	VAL	CA-C-O	-6.23	114.05	121.28
1	I	21	LEU	N-CA-C	6.23	123.42	114.39
1	G	23	LEU	N-CA-C	6.22	118.06	111.28
2	F	346	THR	N-CA-C	6.20	120.55	112.92
2	B	418	PRO	N-CA-C	6.20	121.23	111.38
1	C	140	HIS	CA-C-N	-6.19	112.56	122.53
1	C	140	HIS	C-N-CA	-6.19	112.56	122.53
1	E	188	ARG	N-CA-CB	6.19	120.27	110.55
2	F	505	ILE	CB-CA-C	6.19	118.45	110.96
1	C	26	ALA	N-CA-C	-6.18	105.84	113.19
2	H	462	HIS	CA-C-O	-6.18	114.36	121.47
1	A	5	LEU	CB-CA-C	-6.18	99.92	109.62
2	F	460	HIS	CA-C-N	-6.17	114.36	122.94
2	F	460	HIS	C-N-CA	-6.17	114.36	122.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	102	GLY	N-CA-C	-6.17	107.89	114.67
1	I	81	ASP	N-CA-C	6.17	120.00	112.23
2	J	368	ASN	N-CA-CB	6.16	120.91	110.49
2	J	474	LEU	CA-C-N	-6.16	114.56	123.06
2	J	474	LEU	C-N-CA	-6.16	114.56	123.06
1	K	152	ASN	N-CA-C	6.16	117.99	111.28
1	A	39	LEU	N-CA-C	6.15	118.07	111.36
2	B	487	PRO	CB-CA-C	-6.15	103.11	111.85
1	A	21	LEU	N-CA-C	6.14	122.23	114.31
1	A	19	ILE	N-CA-C	6.13	118.76	111.09
2	B	533	THR	CA-C-O	-6.13	114.88	121.56
2	J	356	PHE	CA-C-N	-6.13	113.10	121.06
2	J	356	PHE	C-N-CA	-6.13	113.10	121.06
1	A	94	ARG	CD-NE-CZ	6.12	132.97	124.40
2	F	482	GLY	N-CA-C	6.12	123.49	115.47
1	K	175	CYS	N-CA-C	-6.12	100.74	108.45
2	H	324	TYR	N-CA-C	-6.11	97.24	107.99
1	C	110	LYS	CA-C-N	-6.11	114.33	120.31
1	C	110	LYS	C-N-CA	-6.11	114.33	120.31
1	C	184	ARG	CG-CD-NE	-6.10	98.58	112.00
1	C	98	THR	N-CA-C	6.10	119.14	109.81
2	L	525	ILE	N-CA-CB	-6.09	101.12	110.86
2	F	535	PHE	N-CA-C	6.09	119.94	111.90
2	D	438	SER	CA-C-O	-6.09	114.19	120.89
2	L	507	LYS	N-CA-C	6.09	119.74	109.76
1	K	72	GLN	N-CA-C	6.07	118.08	108.79
1	E	42	PRO	N-CA-C	6.07	121.73	113.84
1	K	141	THR	CA-C-O	-6.07	114.78	121.33
1	K	47	GLU	CA-C-N	-6.06	112.93	121.72
1	K	47	GLU	C-N-CA	-6.06	112.93	121.72
2	F	419	LEU	CA-C-O	6.06	128.17	121.56
2	D	440	ARG	NE-CZ-NH1	6.06	127.56	121.50
2	B	457	ARG	NE-CZ-NH2	-6.05	113.75	119.20
1	C	187	ILE	N-CA-C	6.05	116.57	107.80
1	I	120	VAL	N-CA-CB	-6.04	103.77	110.23
1	I	94	ARG	NE-CZ-NH1	6.04	127.54	121.50
2	D	333	ARG	NE-CZ-NH2	6.03	124.63	119.20
2	L	417	ALA	N-CA-C	-6.03	102.17	109.83
2	J	528	ARG	N-CA-C	6.03	119.11	110.24
2	B	493	LYS	CD-CE-NZ	6.03	131.19	111.90
2	F	379	ILE	CB-CG1-CD1	-6.03	101.14	113.80
1	G	65	ASP	O-C-N	6.02	129.67	122.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	PHE	CA-C-N	6.01	128.80	120.63
1	A	99	PHE	C-N-CA	6.01	128.80	120.63
2	F	322	PRO	N-CA-C	6.00	124.84	112.47
2	H	459	ALA	CA-C-N	-5.99	112.05	121.87
2	H	459	ALA	C-N-CA	-5.99	112.05	121.87
2	H	377	ARG	NE-CZ-NH1	-5.99	115.51	121.50
2	H	440	ARG	NE-CZ-NH1	5.98	127.48	121.50
2	J	414	ARG	CD-NE-CZ	5.98	132.78	124.40
1	K	114	VAL	CA-C-N	-5.98	112.40	122.92
1	K	114	VAL	C-N-CA	-5.98	112.40	122.92
2	D	347	THR	N-CA-C	-5.98	100.67	109.81
1	A	94	ARG	CA-CB-CG	5.97	126.05	114.10
1	I	66	SER	N-CA-C	5.97	119.32	110.48
1	I	78	GLU	CA-CB-CG	-5.97	102.15	114.10
1	G	173	LYS	CA-C-O	-5.97	113.65	120.58
2	H	372	LEU	CA-C-N	-5.97	114.12	120.03
2	H	372	LEU	C-N-CA	-5.97	114.12	120.03
1	A	101	ALA	CA-C-N	5.97	131.01	120.74
1	A	101	ALA	C-N-CA	5.97	131.01	120.74
2	B	465	ILE	O-C-N	-5.97	116.81	123.26
1	I	88	ALA	CA-C-N	5.96	132.39	122.73
1	I	88	ALA	C-N-CA	5.96	132.39	122.73
2	H	451	ASN	N-CA-C	-5.95	98.12	110.80
2	L	437	TYR	CA-C-O	-5.95	114.15	121.11
1	K	163	GLN	CA-C-N	-5.95	112.74	119.28
1	K	163	GLN	C-N-CA	-5.95	112.74	119.28
2	L	379	ILE	CB-CG1-CD1	-5.94	101.33	113.80
2	L	382	GLY	N-CA-C	-5.94	101.46	111.08
2	L	463	PHE	CA-C-O	-5.94	114.49	121.44
2	D	364	LEU	N-CA-C	-5.93	105.54	112.89
2	B	326	THR	OG1-CB-CG2	-5.93	97.45	109.30
2	H	394	ASN	N-CA-C	5.93	119.36	111.30
2	H	431	THR	N-CA-CB	5.92	118.73	110.26
2	B	312	ASP	CB-CG-OD1	5.92	132.01	118.40
2	H	452	GLY	CA-C-N	5.92	125.79	119.28
2	H	452	GLY	C-N-CA	5.92	125.79	119.28
2	L	374	ILE	CA-C-N	-5.92	114.70	122.63
2	L	374	ILE	C-N-CA	-5.92	114.70	122.63
1	C	73	ALA	CA-C-N	-5.92	112.39	121.74
1	C	73	ALA	C-N-CA	-5.92	112.39	121.74
2	D	348	GLY	N-CA-C	-5.91	100.28	112.34
2	B	504	LEU	N-CA-C	-5.91	105.38	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	438	SER	N-CA-CB	5.90	120.71	111.56
1	A	113	VAL	N-CA-C	5.90	116.67	109.30
2	H	372	LEU	CB-CA-C	5.89	116.87	108.68
2	J	423	PHE	N-CA-C	5.89	118.00	108.34
2	D	428	ARG	N-CA-CB	5.89	120.51	110.50
2	H	508	LEU	CD1-CG-CD2	-5.88	97.85	110.80
2	J	529	GLY	N-CA-C	5.88	118.23	111.36
2	J	379	ILE	N-CA-C	-5.87	99.96	108.89
1	I	174	ARG	CG-CD-NE	-5.87	99.08	112.00
1	A	37	ASN	N-CA-C	5.87	120.14	112.92
2	J	434	ASP	OD1-CG-OD2	5.87	136.99	122.90
2	H	346	THR	OG1-CB-CG2	5.87	121.04	109.30
2	L	353	HIS	CA-C-N	-5.86	111.73	120.94
2	L	353	HIS	C-N-CA	-5.86	111.73	120.94
2	J	449	TRP	CA-C-N	-5.86	112.96	122.34
2	J	449	TRP	C-N-CA	-5.86	112.96	122.34
1	E	93	GLY	CA-C-O	-5.86	115.29	121.56
2	J	390	LYS	CG-CD-CE	5.85	124.76	111.30
1	E	91	SER	N-CA-C	5.85	120.26	113.18
1	K	168	GLU	CA-CB-CG	-5.85	102.41	114.10
2	L	478	LEU	N-CA-C	-5.85	100.17	109.76
2	L	394	ASN	N-CA-C	5.84	119.45	111.39
2	L	440	ARG	NE-CZ-NH1	5.84	127.34	121.50
2	D	418	PRO	N-CA-C	5.84	120.44	111.57
2	B	466	SER	N-CA-C	5.83	118.52	111.40
1	C	102	GLY	CA-C-N	5.83	131.39	122.93
1	C	102	GLY	C-N-CA	5.83	131.39	122.93
2	D	493	LYS	CD-CE-NZ	5.83	130.57	111.90
2	F	416	LEU	N-CA-C	5.83	120.01	113.01
2	L	428	ARG	CD-NE-CZ	5.83	132.57	124.40
1	C	94	ARG	N-CA-CB	5.83	121.69	111.13
1	I	28	ASN	CA-C-N	-5.83	113.93	119.76
1	I	28	ASN	C-N-CA	-5.83	113.93	119.76
2	B	413	ASP	CB-CA-C	5.82	120.89	111.05
2	J	350	ASN	N-CA-C	-5.82	99.71	109.07
1	A	43	ASP	CA-C-O	5.81	127.65	120.15
1	C	94	ARG	CD-NE-CZ	5.81	132.54	124.40
2	L	390	LYS	CG-CD-CE	5.81	124.66	111.30
1	I	165	GLN	N-CA-CB	5.81	119.16	110.22
1	K	100	ASP	CA-C-O	-5.81	113.79	120.24
2	J	514	ASN	N-CA-C	-5.81	98.01	109.10
1	G	98	THR	N-CA-C	5.80	118.04	109.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	LYS	CD-CE-NZ	5.80	130.46	111.90
2	D	395	THR	CA-C-N	-5.80	114.02	122.19
2	D	395	THR	C-N-CA	-5.80	114.02	122.19
1	G	21	LEU	N-CA-C	5.80	121.92	114.56
2	L	328	ILE	CG1-CB-CG2	-5.79	93.32	110.70
1	E	124	PRO	CA-C-N	-5.79	113.10	122.36
1	E	124	PRO	C-N-CA	-5.79	113.10	122.36
1	A	56	TYR	O-C-N	-5.79	115.71	123.23
1	I	167	ARG	N-CA-C	-5.79	105.06	111.71
2	B	494	SER	N-CA-C	-5.78	105.48	112.54
1	G	56	TYR	CA-C-O	-5.78	114.57	121.11
2	F	347	THR	N-CA-C	-5.78	100.96	109.81
2	F	489	CYS	N-CA-C	5.78	116.94	109.65
2	H	483	ASP	CA-C-N	-5.77	113.73	119.56
2	H	483	ASP	C-N-CA	-5.77	113.73	119.56
2	B	326	THR	CA-C-O	-5.77	112.51	119.49
1	G	152	ASN	N-CA-C	5.77	118.34	111.71
2	L	384	VAL	N-CA-C	-5.77	99.24	107.77
2	B	311	ARG	NE-CZ-NH2	-5.76	114.01	119.20
2	F	435	GLY	CA-C-O	-5.76	112.43	119.06
1	K	163	GLN	CA-C-O	5.76	123.58	119.32
1	C	103	GLU	N-CA-CB	-5.75	101.43	110.69
2	H	352	SER	N-CA-C	5.75	118.29	111.33
2	D	450	ARG	CG-CD-NE	-5.74	99.37	112.00
1	I	151	ALA	N-CA-C	-5.74	105.03	111.28
2	L	533	THR	N-CA-C	-5.74	102.41	110.50
1	A	175	CYS	CA-CB-SG	5.74	127.59	114.40
1	E	32	ASP	O-C-N	5.74	128.20	122.12
1	E	41	LYS	CA-C-N	-5.72	113.72	119.56
1	E	41	LYS	C-N-CA	-5.72	113.72	119.56
2	L	383	ARG	CG-CD-NE	-5.72	99.40	112.00
1	C	161	ILE	CA-C-N	5.72	128.74	120.79
1	C	161	ILE	C-N-CA	5.72	128.74	120.79
2	D	369	ASN	O-C-N	5.72	129.71	122.28
2	H	363	LEU	CA-C-O	5.70	126.59	119.12
1	K	86	GLU	N-CA-C	5.70	117.57	111.36
1	A	133	ARG	NE-CZ-NH2	-5.70	114.07	119.20
1	C	114	VAL	CG1-CB-CG2	-5.70	98.26	110.80
2	J	313	ARG	CA-C-N	-5.70	112.41	122.26
2	J	313	ARG	C-N-CA	-5.70	112.41	122.26
2	D	385	VAL	CA-C-O	-5.69	115.70	121.67
1	G	172	ALA	CA-C-N	5.69	129.44	121.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	172	ALA	C-N-CA	5.69	129.44	121.24
1	K	172	ALA	CA-C-N	5.69	130.47	121.99
1	K	172	ALA	C-N-CA	5.69	130.47	121.99
1	C	88	ALA	CA-C-N	5.69	130.81	122.39
1	C	88	ALA	C-N-CA	5.69	130.81	122.39
1	C	24	GLU	O-C-N	5.69	128.01	122.09
2	L	537	ASN	CA-C-N	5.68	131.93	121.70
2	L	537	ASN	C-N-CA	5.68	131.93	121.70
1	C	138	HIS	N-CA-C	5.68	118.03	110.53
2	D	525	ILE	N-CA-CB	-5.68	100.70	111.21
2	B	338	SER	CA-C-O	-5.67	114.28	120.81
1	K	191	GLY	N-CA-C	5.67	126.63	113.18
2	L	310	ILE	CA-C-O	-5.67	113.84	120.99
2	L	487	PRO	CB-CA-C	-5.67	103.34	111.62
2	L	480	PHE	N-CA-C	5.67	118.47	109.24
2	D	324	TYR	CA-C-N	5.66	129.32	120.82
2	D	324	TYR	C-N-CA	5.66	129.32	120.82
1	I	100	ASP	CA-C-N	5.66	129.93	122.06
1	I	100	ASP	C-N-CA	5.66	129.93	122.06
2	D	428	ARG	CD-NE-CZ	5.66	132.32	124.40
1	A	92	PHE	N-CA-C	5.66	118.77	109.72
2	B	411	LYS	CB-CA-C	-5.66	100.17	110.63
1	G	28	ASN	CA-C-N	-5.66	113.94	119.76
1	G	28	ASN	C-N-CA	-5.66	113.94	119.76
1	C	54	GLN	N-CA-C	-5.65	100.76	109.52
1	C	106	LEU	CB-CG-CD2	-5.65	93.74	110.70
1	G	4	LEU	CD1-CG-CD2	5.65	123.23	110.80
2	F	473	LYS	CD-CE-NZ	-5.65	93.82	111.90
2	H	344	SER	N-CA-C	5.65	118.21	111.71
1	C	25	ALA	N-CA-C	5.65	117.44	111.28
1	K	120	VAL	N-CA-C	-5.64	103.78	108.63
2	L	452	GLY	CA-C-N	-5.64	113.86	119.56
2	L	452	GLY	C-N-CA	-5.64	113.86	119.56
2	H	497	ASN	N-CA-C	5.64	117.08	109.24
2	F	457	ARG	CB-CA-C	-5.64	100.97	109.26
1	I	165	GLN	CA-CB-CG	5.64	125.38	114.10
2	B	492	VAL	N-CA-C	-5.63	105.12	110.42
2	H	426	VAL	CB-CA-C	-5.63	101.83	110.50
2	H	348	GLY	CA-C-N	5.63	125.58	119.78
2	H	348	GLY	C-N-CA	5.63	125.58	119.78
2	B	510	MET	CA-CB-CG	5.63	125.35	114.10
2	J	333	ARG	N-CA-C	-5.62	106.77	113.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	492	VAL	CA-C-O	-5.62	114.66	121.18
2	J	307	ARG	N-CA-C	-5.62	100.62	109.50
2	H	402	ALA	N-CA-C	-5.61	103.50	110.41
1	A	86	GLU	CA-CB-CG	-5.61	102.88	114.10
2	F	414	ARG	CD-NE-CZ	5.61	132.25	124.40
1	A	102	GLY	CA-C-N	5.61	131.90	122.87
1	A	102	GLY	C-N-CA	5.61	131.90	122.87
1	I	63	VAL	CA-C-O	5.60	127.59	121.04
1	E	24	GLU	O-C-N	5.59	127.85	122.03
2	H	328	ILE	CG1-CB-CG2	-5.59	93.92	110.70
2	J	419	LEU	CA-C-O	5.59	128.37	121.99
1	C	103	GLU	N-CA-C	5.59	118.59	109.59
2	H	410	HIS	CA-C-N	5.59	132.22	121.54
2	H	410	HIS	C-N-CA	5.59	132.22	121.54
2	J	367	PHE	CA-C-N	5.59	132.22	121.54
2	J	367	PHE	C-N-CA	5.59	132.22	121.54
2	J	321	THR	N-CA-C	-5.58	95.16	108.40
2	H	321	THR	CA-C-N	5.58	126.81	119.84
2	H	321	THR	C-N-CA	5.58	126.81	119.84
1	G	86	GLU	N-CA-C	5.58	119.93	113.18
2	H	367	PHE	O-C-N	5.58	128.17	121.76
2	J	343	ILE	CA-C-N	-5.58	111.83	120.31
2	J	343	ILE	C-N-CA	-5.58	111.83	120.31
2	D	425	GLY	CA-C-O	-5.57	112.90	118.86
2	F	469	SER	CA-C-O	-5.57	115.46	121.36
2	H	418	PRO	N-CA-C	5.57	120.04	111.57
1	K	100	ASP	O-C-N	5.57	129.47	122.23
1	K	165	GLN	CA-CB-CG	5.56	125.22	114.10
1	G	72	GLN	N-CA-C	5.56	117.52	109.07
1	C	75	ALA	CA-C-O	-5.56	113.82	120.10
1	G	53	GLY	CA-C-N	-5.55	113.09	123.03
1	G	53	GLY	C-N-CA	-5.55	113.09	123.03
2	L	428	ARG	NE-CZ-NH2	-5.55	114.20	119.20
2	J	417	ALA	CA-C-N	-5.55	114.53	120.03
2	J	417	ALA	C-N-CA	-5.55	114.53	120.03
2	L	503	GLN	CB-CG-CD	-5.55	103.16	112.60
2	D	333	ARG	NH1-CZ-NH2	5.55	126.51	119.30
2	L	451	ASN	N-CA-C	-5.55	98.98	110.80
2	D	415	TYR	CB-CA-C	5.54	118.76	109.89
2	L	459	ALA	CA-C-N	-5.54	112.78	121.87
2	L	459	ALA	C-N-CA	-5.54	112.78	121.87
2	F	441	THR	CA-C-O	-5.54	115.23	121.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	473	LYS	CB-CA-C	5.54	119.12	109.65
2	L	537	ASN	CB-CA-C	-5.53	102.98	111.66
2	J	442	ILE	CB-CG1-CD1	-5.53	102.19	113.80
2	J	524	ASP	CA-C-N	-5.53	115.43	123.06
2	J	524	ASP	C-N-CA	-5.53	115.43	123.06
1	I	106	LEU	N-CA-CB	-5.52	101.25	111.13
2	H	302	ALA	N-CA-C	5.52	118.23	109.96
1	G	38	ARG	NE-CZ-NH1	5.51	127.02	121.50
2	B	483	ASP	CA-C-N	-5.51	113.94	119.56
2	B	483	ASP	C-N-CA	-5.51	113.94	119.56
1	I	9	PRO	CB-CA-C	-5.51	103.76	110.98
2	B	528	ARG	CA-C-N	-5.51	115.11	120.34
2	B	528	ARG	C-N-CA	-5.51	115.11	120.34
2	J	431	THR	N-CA-CB	5.51	118.24	110.36
2	L	443	LYS	CA-C-N	-5.51	114.58	120.03
2	L	443	LYS	C-N-CA	-5.51	114.58	120.03
2	B	436	TYR	N-CA-C	5.50	118.63	110.48
2	J	446	PRO	N-CA-C	-5.50	103.20	111.57
2	H	414	ARG	CD-NE-CZ	5.50	132.10	124.40
2	D	507	LYS	CB-CG-CD	5.50	123.95	111.30
2	B	377	ARG	NE-CZ-NH1	-5.50	116.00	121.50
2	D	367	PHE	N-CA-C	-5.50	104.21	111.96
2	D	332	PRO	CA-C-N	5.49	130.02	120.68
2	D	332	PRO	C-N-CA	5.49	130.02	120.68
2	F	473	LYS	CG-CD-CE	-5.49	98.66	111.30
2	L	412	ASN	N-CA-CB	5.49	118.44	110.47
2	L	426	VAL	O-C-N	5.49	128.88	123.00
1	A	9	PRO	CB-CA-C	-5.49	104.38	111.46
2	F	462	HIS	CA-C-O	-5.49	114.79	121.05
2	L	360	ASP	N-CA-C	5.49	118.02	111.71
2	F	496	ALA	N-CA-C	5.48	118.44	111.69
2	H	411	LYS	CB-CA-C	-5.48	99.51	110.42
2	J	407	ARG	CG-CD-NE	-5.48	99.94	112.00
2	J	432	ASP	CA-C-N	5.48	128.38	120.38
2	J	432	ASP	C-N-CA	5.48	128.38	120.38
1	G	154	LYS	CA-CB-CG	5.47	125.05	114.10
1	I	147	ASP	CA-C-O	5.47	125.76	119.35
2	L	505	ILE	N-CA-CB	-5.47	104.58	111.31
1	C	51	LEU	CA-C-N	5.47	131.54	121.85
1	C	51	LEU	C-N-CA	5.47	131.54	121.85
1	C	52	LEU	CA-CB-CG	5.47	135.46	116.30
1	K	100	ASP	CB-CA-C	-5.47	100.69	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	390	LYS	N-CA-CB	-5.47	102.23	110.32
2	L	475	ILE	CG1-CB-CG2	-5.47	94.30	110.70
2	L	409	ARG	NE-CZ-NH2	5.46	124.12	119.20
2	L	385	VAL	CA-C-O	-5.46	115.88	121.67
2	H	308	PHE	O-C-N	-5.46	116.80	123.30
1	I	94	ARG	CA-C-O	-5.46	115.05	121.44
1	A	100	ASP	O-C-N	5.46	127.92	122.03
1	E	194	GLU	CB-CA-C	-5.46	101.65	109.84
2	F	495	ILE	N-CA-C	-5.46	99.88	108.23
1	E	48	HIS	N-CA-C	5.46	118.14	109.96
1	E	66	SER	CB-CA-C	5.46	119.53	109.71
1	G	198	PHE	N-CA-C	5.45	118.15	110.14
1	C	150	GLN	N-CA-CB	5.45	118.22	110.16
1	K	11	GLN	N-CA-C	-5.45	100.89	109.50
2	H	388	TYR	N-CA-C	-5.45	106.68	113.38
1	C	123	ALA	CA-C-N	-5.45	114.10	119.93
1	C	123	ALA	C-N-CA	-5.45	114.10	119.93
2	F	351	PHE	N-CA-C	5.45	118.93	112.72
2	B	505	ILE	N-CA-C	5.45	116.23	107.73
2	B	532	LYS	N-CA-C	-5.44	102.82	110.50
1	C	100	ASP	CA-C-N	5.44	131.05	122.34
1	C	100	ASP	C-N-CA	5.44	131.05	122.34
1	K	136	ASN	O-C-N	5.44	128.97	122.27
2	F	488	MET	N-CA-CB	-5.44	102.53	110.53
2	L	343	ILE	CG1-CB-CG2	-5.44	94.39	110.70
1	A	121	PRO	N-CA-C	5.44	119.01	110.80
1	E	130	LEU	CA-C-O	5.43	126.12	120.30
2	F	495	ILE	CB-CA-C	-5.43	104.39	110.96
2	L	425	GLY	N-CA-C	5.43	123.93	115.72
1	I	108	THR	CA-C-O	-5.43	115.55	121.14
2	J	346	THR	N-CA-C	5.43	119.60	112.92
1	E	63	VAL	N-CA-C	-5.43	99.42	107.51
1	G	23	LEU	CA-C-N	5.43	127.50	120.44
1	G	23	LEU	C-N-CA	5.43	127.50	120.44
2	H	383	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	A	101	ALA	O-C-N	5.42	129.48	122.43
1	I	33	GLN	CA-C-O	-5.42	114.36	120.32
2	F	457	ARG	NH1-CZ-NH2	5.42	126.34	119.30
2	L	419	LEU	N-CA-C	-5.42	103.23	110.55
2	L	421	PRO	CA-C-N	-5.42	114.49	122.83
2	L	421	PRO	C-N-CA	-5.42	114.49	122.83
1	E	52	LEU	N-CA-C	5.41	117.29	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	492	VAL	N-CA-C	-5.41	105.45	110.53
1	E	54	GLN	CA-CB-CG	-5.41	103.29	114.10
2	B	311	ARG	N-CA-CB	5.40	117.99	109.83
2	D	416	LEU	N-CA-C	5.40	118.67	111.75
2	H	476	THR	CA-C-O	-5.40	115.64	121.36
2	B	416	LEU	N-CA-C	5.40	119.13	112.54
1	A	97	THR	N-CA-C	-5.39	101.38	109.95
2	B	505	ILE	CG1-CB-CG2	-5.39	94.53	110.70
1	A	103	GLU	CB-CA-C	-5.39	99.51	109.37
1	G	115	ASN	N-CA-C	5.39	118.45	110.48
2	H	433	SER	CA-CB-OG	-5.38	100.33	111.10
1	C	72	GLN	N-CA-C	5.38	117.44	108.99
1	E	142	ARG	NE-CZ-NH2	5.38	124.04	119.20
2	D	338	SER	CA-C-O	-5.37	114.47	120.54
1	K	96	ALA	O-C-N	-5.37	117.46	123.48
1	G	25	ALA	N-CA-C	5.37	117.89	111.71
1	A	94	ARG	CG-CD-NE	-5.37	100.19	112.00
2	J	473	LYS	CD-CE-NZ	-5.37	94.73	111.90
2	D	337	VAL	CB-CA-C	5.36	118.55	111.21
2	F	406	GLY	CA-C-O	-5.36	113.06	119.06
2	J	332	PRO	CB-CA-C	-5.36	104.37	111.23
1	K	121	PRO	CA-C-N	5.35	130.69	122.93
1	K	121	PRO	C-N-CA	5.35	130.69	122.93
2	L	404	ALA	N-CA-C	5.35	119.07	112.54
1	G	168	GLU	N-CA-C	5.35	118.90	112.38
2	J	414	ARG	NE-CZ-NH1	5.35	126.85	121.50
2	B	369	ASN	O-C-N	5.34	129.04	121.83
2	F	478	LEU	N-CA-CB	-5.34	101.57	110.23
2	D	350	ASN	N-CA-C	-5.34	100.19	108.90
2	B	482	GLY	N-CA-C	5.34	122.46	115.36
1	G	172	ALA	CA-C-O	-5.34	114.60	120.69
1	G	96	ALA	CA-C-N	-5.34	115.63	123.00
1	G	96	ALA	C-N-CA	-5.34	115.63	123.00
1	K	128	ILE	CB-CG1-CD1	-5.33	102.60	113.80
1	A	77	GLY	N-CA-C	-5.33	105.70	114.76
1	E	154	LYS	CA-CB-CG	5.32	124.73	114.10
2	J	461	ILE	CB-CG1-CD1	5.31	124.96	113.80
1	C	154	LYS	CA-CB-CG	5.31	124.72	114.10
1	G	138	HIS	CA-C-N	-5.31	114.74	122.65
1	G	138	HIS	C-N-CA	-5.31	114.74	122.65
2	H	390	LYS	CG-CD-CE	5.31	123.52	111.30
1	K	168	GLU	CB-CG-CD	-5.31	103.57	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	LYS	CB-CA-C	5.31	118.43	109.67
2	F	474	LEU	CA-C-O	-5.31	114.90	121.06
2	B	377	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	H	460	HIS	CA-C-O	-5.31	115.77	121.45
2	H	477	GLN	CA-C-O	5.31	126.43	120.70
2	B	334	GLN	O-C-N	-5.30	117.00	122.94
2	F	501	VAL	CB-CA-C	-5.30	104.91	112.22
1	K	41	LYS	CA-C-N	5.30	126.46	119.84
1	K	41	LYS	C-N-CA	5.30	126.46	119.84
2	B	313	ARG	NE-CZ-NH1	5.30	126.80	121.50
2	B	376	GLU	CA-CB-CG	-5.29	103.52	114.10
1	C	52	LEU	N-CA-C	5.29	117.30	108.99
2	J	459	ALA	CA-C-N	-5.29	113.19	121.87
2	J	459	ALA	C-N-CA	-5.29	113.19	121.87
2	L	336	LEU	N-CA-C	-5.29	102.45	110.28
1	G	9	PRO	N-CD-CG	-5.29	95.27	103.20
1	K	164	PRO	N-CA-C	5.29	120.79	113.65
2	H	522	ARG	NE-CZ-NH2	5.28	123.95	119.20
2	B	497	ASN	CB-CG-ND2	5.28	124.32	116.40
2	F	382	GLY	N-CA-C	-5.28	103.67	110.69
1	I	160	LEU	N-CA-C	-5.28	106.80	113.18
1	G	64	ARG	NE-CZ-NH1	5.27	126.77	121.50
1	G	111	PRO	N-CA-C	5.27	119.47	111.19
1	K	47	GLU	OE1-CD-OE2	5.27	135.56	122.90
2	B	334	GLN	CB-CA-C	-5.27	100.61	109.83
1	C	94	ARG	CA-CB-CG	5.27	124.64	114.10
2	B	440	ARG	N-CA-C	-5.26	101.30	109.72
1	I	168	GLU	CB-CG-CD	-5.26	103.66	112.60
1	I	170	LEU	N-CA-C	5.26	119.68	113.16
2	L	426	VAL	CB-CA-C	-5.26	102.28	110.69
1	G	23	LEU	O-C-N	5.25	127.69	122.12
2	L	368	ASN	N-CA-C	5.25	121.98	110.80
2	B	439	PHE	CA-C-N	-5.25	114.57	122.81
2	B	439	PHE	C-N-CA	-5.25	114.57	122.81
1	C	45	PRO	O-C-N	-5.25	116.61	123.06
2	F	498	PRO	CB-CG-CD	-5.25	89.31	106.10
1	A	199	ASP	N-CA-C	-5.24	100.48	109.24
1	C	145	PHE	N-CA-C	5.24	118.03	109.59
2	H	428	ARG	CD-NE-CZ	5.24	131.74	124.40
2	L	351	PHE	N-CA-C	5.24	118.49	112.57
1	G	98	THR	CA-C-O	-5.23	115.27	121.60
2	H	414	ARG	NE-CZ-NH1	5.23	126.73	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	98	THR	N-CA-C	5.23	117.82	110.14
2	H	386	ASP	O-C-N	-5.23	115.14	121.83
1	K	150	GLN	O-C-N	5.23	128.50	122.17
1	A	52	LEU	CA-CB-CG	5.23	134.59	116.30
2	B	374	ILE	O-C-N	-5.23	117.01	122.81
2	H	379	ILE	N-CA-C	-5.22	100.80	108.11
1	E	154	LYS	CD-CE-NZ	5.22	128.61	111.90
1	I	145	PHE	CA-C-O	-5.22	114.72	120.36
2	B	528	ARG	NE-CZ-NH1	-5.22	116.28	121.50
2	H	425	GLY	CA-C-O	-5.22	113.87	118.77
1	C	167	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	I	52	LEU	CA-C-N	-5.21	113.16	121.03
1	I	52	LEU	C-N-CA	-5.21	113.16	121.03
2	L	442	ILE	CA-C-O	-5.21	114.92	120.39
2	D	384	VAL	CG1-CB-CG2	-5.21	99.34	110.80
1	A	29	PRO	CA-N-CD	-5.21	104.71	112.00
2	F	310	ILE	CA-C-O	-5.21	115.19	121.28
2	L	438	SER	N-CA-C	5.21	117.17	108.99
1	G	46	GLY	CA-C-N	-5.21	115.50	122.42
1	G	46	GLY	C-N-CA	-5.21	115.50	122.42
1	I	135	ILE	CB-CG1-CD1	5.21	124.73	113.80
1	E	174	ARG	CB-CG-CD	-5.20	99.33	111.30
2	J	487	PRO	CA-C-N	-5.19	112.41	122.06
2	J	487	PRO	C-N-CA	-5.19	112.41	122.06
2	B	469	SER	CA-C-O	-5.18	115.89	121.38
1	A	67	PHE	CA-C-N	-5.18	114.53	122.62
1	A	67	PHE	C-N-CA	-5.18	114.53	122.62
2	F	473	LYS	CA-C-N	-5.18	113.74	122.29
2	F	473	LYS	C-N-CA	-5.18	113.74	122.29
1	E	106	LEU	N-CA-CB	-5.18	101.83	110.99
1	G	41	LYS	CA-C-N	5.18	125.22	119.32
1	G	41	LYS	C-N-CA	5.18	125.22	119.32
2	F	402	ALA	CA-C-N	5.17	132.66	122.73
2	F	402	ALA	C-N-CA	5.17	132.66	122.73
2	F	313	ARG	N-CA-C	5.17	119.34	113.19
2	F	374	ILE	O-C-N	-5.17	117.45	122.93
2	J	497	ASN	CB-CG-ND2	5.17	124.16	116.40
2	J	406	GLY	CA-C-N	-5.17	115.59	122.72
2	J	406	GLY	C-N-CA	-5.17	115.59	122.72
2	D	368	ASN	CA-C-O	5.17	127.90	120.51
1	E	102	GLY	CA-C-O	5.16	125.72	119.01
2	J	425	GLY	CA-C-O	-5.15	113.39	118.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	GLY	CA-C-N	-5.15	115.57	122.42
1	C	46	GLY	C-N-CA	-5.15	115.57	122.42
2	J	320	LEU	N-CA-CB	-5.15	102.87	110.49
2	L	305	ASN	N-CA-C	-5.15	107.67	114.31
1	G	37	ASN	N-CA-CB	-5.15	103.46	110.56
1	E	171	ILE	N-CA-C	5.14	115.18	107.51
1	E	113	VAL	CG1-CB-CG2	-5.14	99.49	110.80
1	A	52	LEU	CD1-CG-CD2	-5.14	99.50	110.80
2	J	368	ASN	CA-C-O	5.13	127.85	120.51
2	L	321	THR	CA-C-O	5.13	127.21	120.74
2	B	376	GLU	CA-C-O	-5.13	114.62	120.58
2	L	338	SER	CA-C-N	-5.13	114.70	122.24
2	L	338	SER	C-N-CA	-5.13	114.70	122.24
1	G	35	ILE	CG1-CB-CG2	-5.13	95.31	110.70
2	D	382	GLY	O-C-N	-5.13	119.00	123.92
2	F	423	PHE	N-CA-C	5.13	116.75	108.34
2	F	497	ASN	CA-C-O	5.13	124.32	119.76
1	I	95	THR	N-CA-C	-5.13	101.67	108.74
1	C	39	LEU	N-CA-CB	5.12	118.02	110.33
1	C	171	ILE	CA-C-O	-5.12	115.05	121.04
1	K	198	PHE	O-C-N	5.12	128.81	123.03
1	K	129	SER	CA-C-N	-5.12	115.94	123.00
1	K	129	SER	C-N-CA	-5.12	115.94	123.00
1	A	91	SER	N-CA-C	5.12	119.15	113.01
1	I	15	PRO	N-CA-C	-5.12	106.87	113.57
1	G	103	GLU	CB-CA-C	-5.11	98.21	109.56
2	J	314	ASN	N-CA-C	-5.11	107.09	113.38
2	L	301	PRO	N-CA-CB	5.11	108.62	103.00
1	E	145	PHE	CA-C-O	-5.11	114.86	120.43
2	F	470	ILE	N-CA-C	-5.11	106.13	113.07
2	F	420	ASP	N-CA-C	-5.10	99.36	109.10
2	L	302	ALA	N-CA-C	5.10	118.43	110.32
2	H	485	LEU	CD1-CG-CD2	-5.10	99.59	110.80
1	A	98	THR	CA-C-O	-5.09	115.80	121.51
2	J	464	GLY	O-C-N	-5.09	119.42	123.49
1	K	149	ALA	CA-C-N	-5.09	112.21	120.71
1	K	149	ALA	C-N-CA	-5.09	112.21	120.71
2	B	428	ARG	NE-CZ-NH1	5.09	126.59	121.50
2	F	537	ASN	N-CA-C	-5.09	104.62	111.54
1	I	72	GLN	CB-CG-CD	-5.09	103.95	112.60
1	G	150	GLN	CA-CB-CG	5.08	124.27	114.10
1	A	167	ARG	NE-CZ-NH2	5.08	123.78	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	507	LYS	CD-CE-NZ	5.08	128.17	111.90
1	K	86	GLU	CA-CB-CG	-5.08	103.93	114.10
2	H	503	GLN	N-CA-CB	-5.08	101.47	110.42
2	J	463	PHE	CA-C-O	-5.08	115.38	121.11
1	K	136	ASN	N-CA-C	5.08	117.71	111.82
1	A	171	ILE	N-CA-C	5.07	115.07	107.51
1	K	181	THR	CA-C-N	5.07	130.56	122.59
1	K	181	THR	C-N-CA	5.07	130.56	122.59
1	A	5	LEU	CA-C-O	5.07	124.52	119.75
2	L	414	ARG	CD-NE-CZ	5.07	131.50	124.40
2	L	497	ASN	N-CA-C	5.07	116.92	109.42
2	B	316	HIS	CA-C-N	-5.07	114.73	119.85
2	B	316	HIS	C-N-CA	-5.07	114.73	119.85
1	K	99	PHE	CA-C-N	5.07	129.24	120.58
1	K	99	PHE	C-N-CA	5.07	129.24	120.58
2	J	533	THR	OG1-CB-CG2	-5.06	99.17	109.30
2	F	438	SER	CA-CB-OG	-5.06	100.98	111.10
1	G	142	ARG	CB-CG-CD	-5.06	99.66	111.30
2	H	472	THR	CA-C-O	-5.06	113.58	119.14
1	E	31	ARG	NE-CZ-NH1	-5.06	116.44	121.50
2	F	367	PHE	CA-C-N	5.05	131.19	121.54
2	F	367	PHE	C-N-CA	5.05	131.19	121.54
1	G	6	PRO	CB-CA-C	-5.05	104.36	110.98
1	A	60	GLY	CA-C-O	-5.04	113.42	119.07
1	C	99	PHE	CB-CA-C	5.04	119.25	110.68
2	D	313	ARG	CB-CA-C	5.04	119.69	110.11
2	F	308	PHE	N-CA-C	5.04	117.19	109.07
1	G	149	ALA	CA-C-O	5.04	125.59	119.49
2	J	511	ASN	N-CA-C	-5.04	105.92	111.71
1	C	46	GLY	N-CA-C	-5.04	105.81	111.85
2	J	348	GLY	CA-C-N	5.04	124.80	119.76
2	J	348	GLY	C-N-CA	5.04	124.80	119.76
2	F	497	ASN	CB-CG-ND2	5.03	123.95	116.40
2	B	460	HIS	CA-C-O	-5.03	115.90	121.33
2	F	372	LEU	CA-C-O	5.03	124.86	120.19
2	L	481	GLU	N-CA-CB	-5.03	101.45	109.19
2	B	342	SER	N-CA-CB	-5.02	103.28	111.22
2	J	471	ALA	N-CA-C	-5.02	106.67	112.89
2	D	305	ASN	N-CA-C	-5.01	106.09	113.61
1	A	26	ALA	N-CA-C	-5.01	107.13	113.20
1	G	165	GLN	N-CA-C	5.01	117.47	111.71
1	E	80	GLN	CB-CG-CD	5.01	121.11	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	406	GLY	N-CA-C	-5.01	108.33	115.64
1	K	66	SER	CA-C-O	-5.01	115.90	121.81
2	H	365	LEU	N-CA-C	5.00	120.77	114.31
1	I	89	PHE	N-CA-C	5.00	117.60	109.24
1	K	106	LEU	CB-CG-CD1	5.00	125.71	110.70

There are no chirality outliers.

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	TYR	Sidechain
1	A	18	HIS	Mainchain
1	A	35	ILE	Mainchain
1	A	56	TYR	Sidechain
2	B	324	TYR	Sidechain
2	B	422	ASN	Mainchain
2	B	436	TYR	Sidechain
2	B	440	ARG	Sidechain
2	B	455	ASP	Mainchain
2	B	457	ARG	Mainchain
2	B	495	ILE	Mainchain
2	B	521	TYR	Sidechain
2	B	537	ASN	Mainchain
1	C	131	PHE	Mainchain
1	C	171	ILE	Mainchain
1	C	180	LYS	Mainchain
1	C	182	ALA	Mainchain
1	C	67	PHE	Mainchain
1	C	83	TYR	Mainchain
1	C	99	PHE	Mainchain
2	D	330	ARG	Sidechain
2	D	332	PRO	Mainchain
2	D	353	HIS	Sidechain
2	D	359	HIS	Sidechain
2	D	381	ALA	Mainchain
2	D	513	ALA	Mainchain
1	E	162	GLU	Mainchain
1	E	175	CYS	Mainchain
1	E	184	ARG	Sidechain
1	E	56	TYR	Sidechain
1	E	67	PHE	Sidechain
2	F	330	ARG	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	F	353	HIS	Sidechain
2	F	366	ASN	Mainchain
2	F	407	ARG	Sidechain
2	F	437	TYR	Sidechain
2	F	460	HIS	Sidechain
1	G	12	THR	Mainchain
1	G	144	TYR	Sidechain
1	G	16	TYR	Sidechain
1	G	184	ARG	Sidechain
1	G	188	ARG	Sidechain
1	G	56	TYR	Sidechain
2	H	340	PRO	Mainchain
2	H	386	ASP	Mainchain
2	H	436	TYR	Sidechain
2	H	450	ARG	Mainchain
2	H	457	ARG	Sidechain
1	I	13	ALA	Mainchain
1	I	146	ASP	Mainchain
1	I	198	PHE	Mainchain
1	I	35	ILE	Mainchain
2	J	341	GLN	Mainchain
2	J	346	THR	Mainchain
2	J	363	LEU	Mainchain
2	J	385	VAL	Mainchain
2	J	407	ARG	Sidechain
2	J	460	HIS	Mainchain
2	J	479	TYR	Sidechain
2	J	521	TYR	Sidechain
1	K	100	ASP	Mainchain
1	K	132	ALA	Mainchain
1	K	182	ALA	Mainchain
1	K	19	ILE	Mainchain
1	K	39	LEU	Mainchain
1	K	56	TYR	Sidechain
1	K	64	ARG	Mainchain
1	K	79	TYR	Sidechain
1	K	99	PHE	Sidechain
2	L	342	SER	Mainchain
2	L	351	PHE	Mainchain
2	L	353	HIS	Sidechain
2	L	388	TYR	Sidechain
2	L	401	GLN	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	L	510	MET	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1571	0	1499	35	0
1	C	1571	0	1499	32	0
1	E	1571	0	1499	34	0
1	G	1571	0	1499	34	1
1	I	1571	0	1499	30	0
1	K	1571	0	1499	38	0
2	B	1877	0	1823	44	0
2	D	1877	0	1822	46	0
2	F	1877	0	1822	55	0
2	H	1877	0	1823	53	0
2	J	1877	0	1822	60	0
2	L	1877	0	1822	55	0
3	A	11	0	4	7	0
3	D	11	0	4	1	0
3	F	11	0	4	1	0
3	H	11	0	4	6	0
3	J	11	0	4	3	0
3	L	11	0	4	3	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
5	A	47	0	0	0	0
5	B	83	0	0	1	0
5	C	45	0	0	0	0
5	D	87	0	0	2	0
5	E	49	0	0	0	1
5	F	82	0	0	2	0
5	G	49	0	0	0	0
5	H	83	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	46	0	0	0	0
5	J	85	0	0	6	0
5	K	43	0	0	0	0
5	L	87	0	0	2	0
All	All	21546	0	19952	480	1

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 12.

All (480) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ALA:CB	1:A:101:ALA:CA	1.77	1.62
2:B:507:LYS:CD	2:B:507:LYS:CE	1.78	1.62
1:E:154:LYS:CE	1:E:154:LYS:CD	1.76	1.61
2:F:532:LYS:CB	2:F:532:LYS:CA	1.76	1.61
2:J:390:LYS:CE	2:J:390:LYS:CD	1.77	1.60
2:H:414:ARG:CB	2:H:414:ARG:CG	1.76	1.60
2:F:303:GLN:CA	2:F:303:GLN:CB	1.80	1.60
2:J:507:LYS:CE	2:J:507:LYS:CD	1.76	1.59
1:C:180:LYS:CG	1:C:180:LYS:CD	1.78	1.59
1:A:163:GLN:CD	1:A:163:GLN:CG	1.74	1.59
1:G:154:LYS:CE	1:G:154:LYS:CD	1.78	1.58
2:J:390:LYS:CD	2:J:390:LYS:CG	1.80	1.58
2:J:532:LYS:CB	2:J:532:LYS:CA	1.76	1.58
2:J:303:GLN:CB	2:J:303:GLN:CA	1.82	1.57
2:F:411:LYS:CD	2:F:411:LYS:CG	1.76	1.57
2:F:507:LYS:CE	2:F:507:LYS:CD	1.75	1.57
2:L:429:CME:CE	2:L:429:CME:CZ	1.77	1.57
2:F:507:LYS:CE	2:F:507:LYS:NZ	1.68	1.57
1:G:180:LYS:NZ	1:G:180:LYS:CE	1.67	1.57
2:J:426:VAL:CB	2:J:426:VAL:CG1	1.75	1.56
2:B:339:ILE:CD1	2:B:339:ILE:CG1	1.80	1.56
1:C:180:LYS:CE	1:C:180:LYS:NZ	1.67	1.55
2:F:390:LYS:CD	2:F:390:LYS:CE	1.74	1.55
2:D:303:GLN:CB	2:D:303:GLN:CA	1.80	1.54
2:B:390:LYS:CE	2:B:390:LYS:CD	1.75	1.54
2:D:390:LYS:CE	2:D:390:LYS:CD	1.77	1.54
2:B:473:LYS:NZ	2:B:473:LYS:CE	1.70	1.54
1:C:100:ASP:CB	1:C:100:ASP:CG	1.75	1.54
2:H:318:LYS:NZ	2:H:318:LYS:CE	1.67	1.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:429:CME:CE	2:H:429:CME:CZ	1.79	1.54
2:L:303:GLN:CB	2:L:303:GLN:CA	1.79	1.54
2:D:390:LYS:CD	2:D:390:LYS:CG	1.78	1.53
2:J:507:LYS:CE	2:J:507:LYS:NZ	1.68	1.53
1:E:19:ILE:CD1	1:E:19:ILE:CG1	1.79	1.53
2:H:303:GLN:CB	2:H:303:GLN:CA	1.84	1.53
2:B:303:GLN:CB	2:B:303:GLN:CA	1.82	1.52
1:C:154:LYS:NZ	1:C:154:LYS:CE	1.68	1.51
1:G:154:LYS:CE	1:G:154:LYS:NZ	1.70	1.50
1:K:180:LYS:CE	1:K:180:LYS:NZ	1.68	1.50
1:E:154:LYS:CE	1:E:154:LYS:NZ	1.73	1.49
2:L:532:LYS:CB	2:L:532:LYS:CA	1.90	1.49
2:B:318:LYS:CE	2:B:318:LYS:NZ	1.73	1.48
2:D:516:MET:SD	2:D:516:MET:CE	2.01	1.48
2:D:507:LYS:CE	2:D:507:LYS:NZ	1.78	1.46
2:L:507:LYS:NZ	2:L:507:LYS:CE	1.77	1.46
1:K:175:CYS:CB	1:K:175:CYS:SG	2.04	1.45
2:H:507:LYS:CE	2:H:507:LYS:NZ	1.84	1.39
2:L:516:MET:SD	2:L:516:MET:CE	2.10	1.37
1:I:165:GLN:H	1:I:165:GLN:NE2	1.41	1.19
1:I:165:GLN:HE21	1:I:165:GLN:N	1.49	1.11
2:B:473:LYS:NZ	2:B:473:LYS:CD	2.20	1.03
2:L:416:LEU:HD23	2:L:416:LEU:H	1.23	1.03
1:K:165:GLN:H	1:K:165:GLN:NE2	1.59	1.01
1:A:165:GLN:H	1:A:165:GLN:NE2	1.61	0.98
2:F:416:LEU:H	2:F:416:LEU:HD23	1.28	0.97
1:C:165:GLN:H	1:C:165:GLN:HE21	1.02	0.97
2:H:416:LEU:HD23	2:H:416:LEU:H	1.30	0.96
2:J:368:ASN:ND2	2:J:371:GLY:H	1.66	0.92
2:B:497:ASN:HD22	2:B:499:GLU:H	1.16	0.89
1:E:165:GLN:H	1:E:165:GLN:NE2	1.71	0.88
2:B:364:LEU:HD22	2:B:440:ARG:HD3	1.55	0.88
2:L:497:ASN:ND2	2:L:499:GLU:H	1.72	0.88
2:J:408:HIS:NE2	5:J:4901:HOH:O	2.07	0.87
1:C:165:GLN:H	1:C:165:GLN:NE2	1.70	0.87
1:K:15:PRO:HD3	3:L:5550:DHB:C1	2.05	0.86
2:D:497:ASN:ND2	2:D:499:GLU:H	1.73	0.86
2:D:368:ASN:HD22	2:D:371:GLY:H	1.19	0.84
2:F:368:ASN:ND2	2:F:371:GLY:H	1.75	0.84
2:H:453:PRO:HB2	2:J:310:ILE:HD12	1.56	0.83
2:L:364:LEU:HD22	2:L:440:ARG:HD3	1.59	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLY:HA2	2:B:426:VAL:HG13	1.61	0.82
2:H:361:HIS:H	2:H:361:HIS:CD2	1.94	0.82
2:B:497:ASN:ND2	2:B:499:GLU:H	1.77	0.81
2:J:368:ASN:ND2	2:J:371:GLY:N	2.28	0.81
2:H:369:ASN:H	2:H:422:ASN:HD22	1.28	0.81
1:A:165:GLN:H	1:A:165:GLN:HE21	1.27	0.81
1:E:165:GLN:H	1:E:165:GLN:HE21	1.25	0.81
1:G:67:PHE:CZ	1:G:94:ARG:HD2	2.16	0.81
2:L:408:HIS:NE2	5:L:5901:HOH:O	2.14	0.80
2:B:473:LYS:NZ	2:B:473:LYS:HD3	1.95	0.80
2:D:368:ASN:ND2	2:D:371:GLY:H	1.80	0.80
2:J:390:LYS:HD3	5:J:4677:HOH:O	1.83	0.79
2:J:361:HIS:CD2	2:J:361:HIS:H	1.99	0.79
2:J:411:LYS:HZ2	2:J:411:LYS:H	1.31	0.76
2:L:497:ASN:HD22	2:L:499:GLU:H	1.32	0.76
2:H:411:LYS:HB2	2:H:411:LYS:HZ3	1.51	0.76
2:J:426:VAL:CG1	2:J:426:VAL:HB	2.09	0.75
1:I:20:GLY:HA2	2:J:426:VAL:HG13	1.68	0.75
1:G:38:ARG:HG3	1:G:38:ARG:HH11	1.52	0.75
1:A:101:ALA:CB	1:A:101:ALA:C	2.61	0.74
2:F:411:LYS:H	2:F:411:LYS:HZ2	1.36	0.74
2:B:473:LYS:HD3	2:B:473:LYS:HZ2	1.53	0.74
2:J:368:ASN:HD21	2:J:371:GLY:N	1.84	0.74
1:E:31:ARG:HH12	2:F:428:ARG:HG2	1.52	0.73
2:F:361:HIS:H	2:F:361:HIS:CD2	2.05	0.73
2:B:390:LYS:CD	2:B:390:LYS:NZ	2.52	0.73
1:G:67:PHE:HZ	1:G:94:ARG:HD2	1.53	0.73
1:G:15:PRO:HD3	3:H:3550:DHB:C1	2.18	0.73
2:L:416:LEU:HD23	2:L:416:LEU:N	2.02	0.72
3:A:550:DHB:O1	2:B:324:TYR:OH	2.03	0.71
2:H:369:ASN:H	2:H:422:ASN:ND2	1.87	0.71
1:K:67:PHE:HZ	1:K:94:ARG:HD2	1.56	0.71
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.57	0.70
2:D:497:ASN:HD22	2:D:498:PRO:N	1.89	0.70
1:K:67:PHE:CZ	1:K:94:ARG:HD2	2.26	0.70
2:H:368:ASN:HD22	2:H:371:GLY:H	1.39	0.70
2:B:315:TRP:HZ2	2:B:503:GLN:NE2	1.90	0.70
1:C:98:THR:N	1:C:101:ALA:O	2.26	0.69
2:D:411:LYS:HB2	2:D:411:LYS:NZ	2.07	0.69
1:K:165:GLN:H	1:K:165:GLN:HE21	1.40	0.69
1:E:25:ALA:HB1	1:E:98:THR:HG21	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:ASN:HD22	2:B:499:GLU:N	1.91	0.68
1:E:19:ILE:CD1	1:E:19:ILE:HG21	2.24	0.68
2:J:426:VAL:CG1	2:J:426:VAL:CA	2.69	0.68
2:L:361:HIS:CD2	2:L:361:HIS:H	2.10	0.68
2:H:416:LEU:HD23	2:H:416:LEU:N	2.07	0.68
1:K:69:GLU:OE1	1:K:94:ARG:HD3	1.95	0.67
2:L:497:ASN:HD22	2:L:497:ASN:C	2.03	0.67
2:D:369:ASN:H	2:D:422:ASN:HD22	1.43	0.67
1:E:19:ILE:CD1	1:E:19:ILE:CB	2.71	0.67
2:D:497:ASN:HD22	2:D:497:ASN:C	2.03	0.66
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.30	0.66
2:L:429:CME:CZ	2:L:429:CME:SD	2.83	0.66
1:A:15:PRO:HD3	3:A:550:DHB:C1	2.26	0.66
2:L:497:ASN:HD22	2:L:499:GLU:N	1.93	0.66
2:H:447:TYR:OH	3:H:3550:DHB:O4	2.14	0.66
2:J:390:LYS:CD	2:J:390:LYS:CB	2.72	0.66
2:H:318:LYS:NZ	2:H:318:LYS:CD	2.59	0.66
2:H:361:HIS:H	2:H:361:HIS:HD2	1.44	0.65
1:A:165:GLN:HE21	1:A:165:GLN:N	1.95	0.65
2:B:408:HIS:NE2	5:B:901:HOH:O	2.15	0.65
1:I:165:GLN:NE2	1:I:165:GLN:N	2.21	0.64
1:A:132:ALA:HB3	1:A:135:ILE:HD12	1.78	0.64
2:J:411:LYS:H	2:J:411:LYS:NZ	1.96	0.64
1:K:98:THR:N	1:K:101:ALA:O	2.27	0.64
2:F:359:HIS:O	2:F:366:ASN:HB3	1.98	0.64
2:J:368:ASN:HD22	2:J:371:GLY:H	1.45	0.64
1:I:165:GLN:H	1:I:165:GLN:HE21	0.73	0.64
2:L:364:LEU:HD22	2:L:440:ARG:CD	2.29	0.63
2:D:361:HIS:H	2:D:361:HIS:CD2	2.16	0.63
1:I:98:THR:N	1:I:101:ALA:O	2.28	0.63
1:E:31:ARG:NH1	2:F:428:ARG:HG2	2.13	0.63
2:F:507:LYS:CE	2:F:507:LYS:CG	2.72	0.63
1:E:19:ILE:CD1	1:E:19:ILE:CG2	2.77	0.63
1:G:80:GLN:O	1:G:91:SER:HB2	1.98	0.62
1:K:143:LEU:C	1:K:143:LEU:HD23	2.24	0.62
1:E:98:THR:N	1:E:101:ALA:O	2.30	0.61
1:K:25:ALA:HB1	1:K:98:THR:HG21	1.82	0.61
2:L:356:PHE:CE1	2:L:428:ARG:HD3	2.35	0.61
2:F:478:LEU:C	2:F:478:LEU:HD23	2.26	0.61
2:J:497:ASN:HD22	2:J:499:GLU:H	1.48	0.61
2:H:390:LYS:HD3	5:H:3677:HOH:O	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:453:PRO:CB	2:J:310:ILE:HD12	2.30	0.60
1:A:15:PRO:HG3	1:A:133:ARG:HD2	1.83	0.60
1:G:70:VAL:HG11	1:G:106:LEU:HD21	1.83	0.60
2:B:361:HIS:CD2	2:B:361:HIS:H	2.20	0.59
2:D:497:ASN:HD22	2:D:499:GLU:H	1.50	0.59
2:D:411:LYS:H	2:D:411:LYS:HZ2	1.50	0.59
2:B:507:LYS:CE	2:B:507:LYS:CG	2.77	0.59
2:H:497:ASN:HD22	2:H:499:GLU:H	1.49	0.59
2:L:497:ASN:ND2	2:L:499:GLU:N	2.47	0.59
2:H:536:GLU:C	2:H:538:CYS:H	2.09	0.58
2:F:497:ASN:ND2	2:F:499:GLU:H	2.01	0.58
2:B:369:ASN:H	2:B:422:ASN:HD22	1.51	0.58
1:G:155:CYS:HB3	1:G:158:LEU:HB2	1.85	0.58
1:K:15:PRO:HD3	3:L:5550:DHB:C6	2.34	0.58
1:A:101:ALA:CB	1:A:101:ALA:O	2.52	0.57
2:F:497:ASN:HD22	2:F:499:GLU:H	1.52	0.57
2:H:385:VAL:O	2:H:526:VAL:HA	2.04	0.57
2:H:368:ASN:ND2	2:H:371:GLY:H	2.01	0.57
2:F:416:LEU:HD23	2:F:416:LEU:N	2.10	0.57
2:F:409:ARG:NH1	2:F:409:ARG:HG3	2.20	0.57
2:J:497:ASN:ND2	2:J:499:GLU:H	2.03	0.57
1:E:19:ILE:HG21	1:E:19:ILE:HD13	1.87	0.56
1:E:15:PRO:HD3	3:F:2550:DHB:C1	2.35	0.56
1:K:143:LEU:HD23	1:K:144:TYR:N	2.20	0.56
2:J:447:TYR:OH	3:J:4550:DHB:O4	2.24	0.56
2:F:356:PHE:CE1	2:F:428:ARG:HD3	2.41	0.55
2:F:356:PHE:CD1	2:F:428:ARG:HD3	2.41	0.55
1:A:24:GLU:O	1:A:27:GLY:N	2.39	0.55
1:K:41:LYS:HB2	1:K:88:ALA:O	2.06	0.55
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.06	0.55
1:I:70:VAL:HG12	1:I:128:ILE:HG12	1.88	0.55
1:K:20:GLY:HA2	2:L:426:VAL:HG13	1.89	0.55
1:A:15:PRO:HD3	3:A:550:DHB:C6	2.37	0.54
1:G:165:GLN:H	1:G:165:GLN:HE21	1.54	0.54
2:B:497:ASN:ND2	2:B:499:GLU:N	2.53	0.54
1:C:20:GLY:HA2	2:D:426:VAL:HG13	1.89	0.54
1:I:161:ILE:O	1:I:167:ARG:NH2	2.41	0.54
2:J:376:GLU:O	2:J:442:ILE:HA	2.08	0.54
2:F:361:HIS:H	2:F:361:HIS:HD2	1.52	0.53
1:K:70:VAL:HG11	1:K:106:LEU:HD21	1.90	0.53
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:PRO:HD3	3:H:3550:DHB:C2	2.38	0.53
1:E:143:LEU:HD12	1:E:185:PHE:CD2	2.42	0.53
1:I:114:VAL:HG23	1:I:122:MET:HE3	1.91	0.53
1:I:132:ALA:HB3	1:I:135:ILE:HD12	1.89	0.53
2:J:497:ASN:HD22	2:J:497:ASN:C	2.16	0.53
2:L:497:ASN:HD22	2:L:498:PRO:N	2.07	0.53
1:A:15:PRO:CD	3:A:550:DHB:C6	2.87	0.53
2:F:315:TRP:HZ2	2:F:503:GLN:HE22	1.57	0.53
1:I:35:ILE:HG21	1:I:92:PHE:HE2	1.74	0.53
2:B:315:TRP:HZ2	2:B:503:GLN:HE21	1.56	0.52
1:C:20:GLY:O	1:C:21:LEU:HD23	2.09	0.52
1:E:36:TRP:CG	1:E:37:ASN:H	2.26	0.52
1:G:143:LEU:C	1:G:143:LEU:HD23	2.33	0.52
1:I:133:ARG:HG3	2:J:326:THR:HG21	1.91	0.52
2:J:379:ILE:O	2:J:520:ALA:HA	2.09	0.52
1:K:145:PHE:N	1:K:145:PHE:CD1	2.77	0.52
2:L:483:ASP:HB3	2:L:486:ILE:HG13	1.91	0.52
2:J:453:PRO:HB2	2:L:310:ILE:HD12	1.91	0.52
2:D:368:ASN:HD22	2:D:371:GLY:N	1.99	0.52
1:G:110:LYS:NZ	1:G:147:ASP:OD1	2.36	0.52
1:I:65:ASP:OD2	1:I:133:ARG:HD3	2.10	0.52
2:J:376:GLU:OE1	2:J:443:LYS:HD3	2.09	0.52
2:H:361:HIS:CD2	2:H:361:HIS:N	2.69	0.52
1:I:162:GLU:O	1:I:164:PRO:HD3	2.09	0.52
1:C:15:PRO:HD3	3:D:1550:DHB:C1	2.39	0.52
2:D:497:ASN:ND2	2:D:497:ASN:C	2.68	0.52
2:L:368:ASN:ND2	2:L:371:GLY:H	2.08	0.52
2:B:305:ASN:O	2:B:533:THR:HG23	2.09	0.52
2:F:305:ASN:O	2:F:533:THR:HG23	2.10	0.52
2:D:369:ASN:H	2:D:422:ASN:ND2	2.06	0.52
2:F:416:LEU:H	2:F:416:LEU:CD2	2.12	0.51
2:F:449:TRP:N	2:F:449:TRP:CD1	2.77	0.51
1:I:165:GLN:HE21	1:I:165:GLN:CA	2.23	0.51
1:C:26:ALA:O	2:D:411:LYS:NZ	2.42	0.51
2:D:356:PHE:HZ	2:D:430:LEU:HD13	1.75	0.51
1:E:154:LYS:CE	1:E:154:LYS:CG	2.80	0.51
2:B:473:LYS:CD	2:B:473:LYS:HZ2	2.05	0.51
2:D:368:ASN:ND2	2:D:370:GLY:N	2.58	0.51
2:H:411:LYS:HB2	2:H:411:LYS:NZ	2.22	0.51
2:D:408:HIS:NE2	5:D:1901:HOH:O	2.14	0.51
2:D:390:LYS:HD3	5:D:1677:HOH:O	2.08	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:516:MET:SD	2:H:448:PRO:HB2	2.51	0.51
2:F:507:LYS:CD	2:F:507:LYS:HE2	2.19	0.51
2:L:408:HIS:CD2	5:L:5901:HOH:O	2.62	0.51
2:D:448:PRO:HD3	2:D:456:TRP:CZ3	2.46	0.51
2:H:447:TYR:HB2	2:H:448:PRO:HD2	1.93	0.51
2:D:368:ASN:ND2	2:D:370:GLY:H	2.08	0.50
1:C:25:ALA:C	1:C:27:GLY:H	2.16	0.50
2:B:307:ARG:HG2	2:B:533:THR:HG22	1.93	0.50
2:H:507:LYS:O	2:H:521:TYR:HA	2.11	0.50
2:J:416:LEU:HD23	2:J:416:LEU:H	1.77	0.50
1:G:31:ARG:NH1	2:H:428:ARG:HG2	2.26	0.50
1:E:143:LEU:HD23	1:E:143:LEU:C	2.37	0.50
2:F:409:ARG:HG3	2:F:409:ARG:HH11	1.77	0.50
2:J:484:PRO:O	2:J:487:PRO:HD2	2.12	0.50
2:D:303:GLN:CB	2:D:303:GLN:N	2.65	0.50
1:E:33:GLN:HG2	1:E:85:LEU:HD12	1.92	0.50
1:G:165:GLN:H	1:G:165:GLN:NE2	2.09	0.50
2:D:416:LEU:H	2:D:416:LEU:HD23	1.76	0.49
2:F:303:GLN:CB	2:F:303:GLN:C	2.78	0.49
1:E:25:ALA:HB1	1:E:98:THR:CG2	2.41	0.49
2:L:497:ASN:ND2	2:L:497:ASN:C	2.70	0.49
1:G:132:ALA:O	1:G:135:ILE:HB	2.12	0.49
2:B:376:GLU:HG2	2:H:446:PRO:HD2	1.95	0.49
2:L:400:TRP:HA	2:L:425:GLY:O	2.12	0.49
2:H:495:ILE:HG21	2:H:500:ALA:HB3	1.94	0.49
2:D:399:MET:HE2	2:D:461:ILE:HG21	1.94	0.49
1:K:147:ASP:OD2	1:K:174:ARG:NH1	2.46	0.48
2:D:376:GLU:O	2:D:442:ILE:HA	2.13	0.48
1:K:15:PRO:CD	3:L:5550:DHB:C6	2.92	0.48
1:A:163:GLN:CD	1:A:163:GLN:CB	2.75	0.48
2:F:478:LEU:HD23	2:F:478:LEU:O	2.13	0.48
2:H:411:LYS:HZ3	2:H:411:LYS:CB	2.21	0.48
1:E:160:LEU:HD23	1:E:160:LEU:HA	1.67	0.48
2:H:364:LEU:HD11	2:H:442:ILE:HG23	1.96	0.48
1:C:16:TYR:HB3	1:C:19:ILE:HD13	1.95	0.48
2:F:315:TRP:HZ2	2:F:503:GLN:NE2	2.11	0.48
2:H:486:ILE:HG22	2:H:487:PRO:N	2.27	0.48
2:J:382:GLY:HA2	2:J:522:ARG:HE	1.79	0.48
1:C:26:ALA:C	2:D:411:LYS:HZ1	2.21	0.48
2:F:409:ARG:HH11	2:F:409:ARG:CG	2.26	0.48
1:E:164:PRO:HD2	1:E:165:GLN:HE22	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:408:HIS:CD2	5:J:4901:HOH:O	2.60	0.47
2:L:316:HIS:HB3	2:L:317:PRO:HD2	1.96	0.47
2:B:326:THR:HG22	2:B:330:ARG:HD2	1.96	0.47
2:L:361:HIS:CD2	2:L:361:HIS:N	2.80	0.47
1:I:123:ALA:O	1:I:124:PRO:C	2.53	0.47
1:K:160:LEU:HD11	2:L:340:PRO:HD3	1.96	0.47
2:L:356:PHE:HE1	2:L:428:ARG:HD3	1.79	0.47
2:L:356:PHE:CD1	2:L:428:ARG:HD3	2.50	0.47
1:G:14:GLY:HA2	3:H:3550:DHB:H2	1.96	0.47
1:I:67:PHE:HZ	1:I:94:ARG:HD2	1.78	0.47
1:A:15:PRO:CG	3:A:550:DHB:C6	2.92	0.47
2:F:326:THR:O	2:F:326:THR:HG22	2.14	0.47
1:C:131:PHE:O	1:C:132:ALA:HB2	2.15	0.47
1:G:133:ARG:HB2	3:H:3550:DHB:O1	2.15	0.47
2:H:429:CME:CZ	2:H:429:CME:SD	3.02	0.47
2:J:321:THR:HG21	2:J:494:SER:HB2	1.97	0.47
2:J:376:GLU:HB3	5:J:4665:HOH:O	2.14	0.47
2:H:310:ILE:HD12	2:L:453:PRO:HB2	1.96	0.47
1:G:38:ARG:HG3	1:G:38:ARG:NH1	2.23	0.47
1:K:144:TYR:CZ	1:K:158:LEU:HD22	2.50	0.47
2:L:522:ARG:HH11	2:L:522:ARG:HD3	1.44	0.47
1:C:23:LEU:HD12	1:C:23:LEU:N	2.30	0.46
1:G:25:ALA:HB1	1:G:98:THR:HG21	1.97	0.46
1:A:70:VAL:HG12	1:A:128:ILE:HG12	1.97	0.46
2:D:315:TRP:HZ2	2:D:503:GLN:NE2	2.13	0.46
1:E:184:ARG:HG3	1:E:184:ARG:HH11	1.80	0.46
2:J:426:VAL:CG1	2:J:426:VAL:CG2	2.78	0.46
1:E:92:PHE:CG	2:F:349:PRO:HG3	2.50	0.46
1:E:184:ARG:HG3	1:E:184:ARG:NH1	2.29	0.46
1:K:131:PHE:CZ	2:L:473:LYS:HE2	2.50	0.46
2:H:325:LYS:HE2	5:J:4727:HOH:O	2.15	0.46
2:J:478:LEU:HD23	2:J:478:LEU:C	2.41	0.46
2:B:369:ASN:H	2:B:422:ASN:ND2	2.14	0.46
2:D:356:PHE:CZ	2:D:430:LEU:HD13	2.50	0.46
2:F:361:HIS:ND1	2:F:429:CME:HZ2	2.31	0.46
2:F:408:HIS:NE2	5:F:2901:HOH:O	2.23	0.46
1:I:85:LEU:HD23	1:I:85:LEU:HA	1.71	0.46
2:L:411:LYS:HZ3	2:L:411:LYS:H	1.64	0.46
2:L:437:TYR:OH	2:L:523:PHE:HB3	2.16	0.46
2:B:356:PHE:CE2	2:B:430:LEU:HD22	2.51	0.46
2:B:484:PRO:O	2:B:487:PRO:HD2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:GLN:HG3	2:D:333:ARG:HG2	1.97	0.46
1:K:20:GLY:O	1:K:21:LEU:HD23	2.16	0.46
1:K:36:TRP:CG	1:K:37:ASN:H	2.34	0.46
1:K:160:LEU:HD23	1:K:160:LEU:HA	1.78	0.46
2:L:315:TRP:HZ2	2:L:503:GLN:NE2	2.13	0.46
1:E:71:TRP:HA	1:E:91:SER:O	2.16	0.46
1:K:190:GLN:HG3	2:L:333:ARG:HG2	1.98	0.46
2:H:386:ASP:OD2	2:H:386:ASP:C	2.59	0.45
2:J:307:ARG:HG2	2:J:533:THR:HG22	1.98	0.45
2:B:491:ILE:HG21	2:B:491:ILE:HD13	1.76	0.45
1:C:114:VAL:HG23	1:C:122:MET:CE	2.46	0.45
1:C:143:LEU:HD23	1:C:143:LEU:C	2.41	0.45
2:H:308:PHE:O	2:H:309:VAL:C	2.56	0.45
2:B:517:ASP:OD1	2:B:517:ASP:C	2.59	0.45
1:C:160:LEU:HD23	1:C:160:LEU:HA	1.69	0.45
2:D:393:PRO:HB3	2:D:433:SER:O	2.16	0.45
1:I:58:GLY:HA3	1:I:190:GLN:OE1	2.16	0.45
2:J:495:ILE:HG21	2:J:500:ALA:HB3	1.99	0.45
2:B:364:LEU:HD22	2:B:440:ARG:CD	2.35	0.45
1:C:36:TRP:CG	1:C:37:ASN:H	2.34	0.45
2:H:405:GLY:HA3	5:H:950:HOH:O	2.16	0.45
2:L:449:TRP:N	2:L:449:TRP:CD1	2.84	0.45
1:C:36:TRP:CD1	1:C:37:ASN:H	2.34	0.45
2:H:364:LEU:CD1	2:H:442:ILE:HG23	2.46	0.45
1:K:53:GLY:HA3	1:K:185:PHE:O	2.17	0.45
2:L:516:MET:HB3	2:L:516:MET:HE3	1.99	0.45
1:I:143:LEU:C	1:I:143:LEU:HD23	2.42	0.45
1:K:131:PHE:CD2	1:K:138:HIS:HB3	2.52	0.45
1:C:161:ILE:HD13	1:C:196:VAL:HG21	1.99	0.45
2:D:379:ILE:HG21	2:D:379:ILE:HD13	1.69	0.45
1:E:131:PHE:CD2	2:F:475:ILE:HD12	2.52	0.45
1:E:167:ARG:O	1:E:171:ILE:HD12	2.16	0.45
2:D:363:LEU:HD12	2:D:363:LEU:N	2.31	0.44
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.53	0.44
2:F:390:LYS:HD3	5:F:2677:HOH:O	2.17	0.44
2:F:532:LYS:CB	2:F:532:LYS:C	2.84	0.44
1:I:19:ILE:HG22	1:I:26:ALA:HB1	1.98	0.44
1:K:64:ARG:NH1	1:K:99:PHE:O	2.51	0.44
2:J:356:PHE:HZ	2:J:430:LEU:HD13	1.82	0.44
2:L:441:THR:OG1	2:L:442:ILE:N	2.50	0.44
2:F:368:ASN:ND2	2:F:371:GLY:N	2.56	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:511:ASN:ND2	2:D:511:ASN:H	2.15	0.44
1:G:70:VAL:HG21	1:G:106:LEU:HD21	2.00	0.44
1:A:61:HIS:ND1	1:C:163:GLN:HG3	2.33	0.43
1:G:177:VAL:O	1:G:180:LYS:HB3	2.16	0.43
2:J:361:HIS:CD2	2:J:361:HIS:N	2.72	0.43
2:J:532:LYS:CB	2:J:532:LYS:C	2.82	0.43
2:B:348:GLY:HA3	2:B:469:SER:HA	2.00	0.43
1:C:53:GLY:HA3	1:C:185:PHE:O	2.18	0.43
2:F:304:ASP:OD1	2:F:307:ARG:NH1	2.40	0.43
2:H:333:ARG:HD3	2:H:333:ARG:HA	1.74	0.43
1:K:26:ALA:O	2:L:411:LYS:NZ	2.51	0.43
2:F:343:ILE:HG23	2:F:344:SER:N	2.32	0.43
2:B:489:CYS:SG	2:B:492:VAL:HG23	2.58	0.43
2:J:363:LEU:N	2:J:363:LEU:HD12	2.34	0.43
2:J:532:LYS:CB	2:J:532:LYS:HA	2.19	0.43
1:C:155:CYS:O	1:C:159:ASN:ND2	2.51	0.43
2:F:364:LEU:HD22	2:F:440:ARG:HG2	2.00	0.43
1:G:25:ALA:C	1:G:27:GLY:H	2.27	0.43
1:G:98:THR:N	1:G:101:ALA:O	2.47	0.43
2:H:442:ILE:C	2:H:442:ILE:HD12	2.44	0.43
1:K:35:ILE:HG22	1:K:94:ARG:HG3	2.01	0.43
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.89	0.43
1:C:70:VAL:HG12	1:C:128:ILE:HG12	2.00	0.43
2:H:497:ASN:ND2	2:H:499:GLU:H	2.14	0.43
1:I:67:PHE:CZ	1:I:94:ARG:HD2	2.54	0.43
1:I:26:ALA:O	2:J:411:LYS:NZ	2.49	0.43
1:I:115:ASN:HA	1:I:121:PRO:HA	2.01	0.43
2:J:460:HIS:ND1	2:J:460:HIS:N	2.67	0.43
1:A:15:PRO:HD3	3:A:550:DHB:C2	2.48	0.43
2:J:338:SER:HB2	5:J:3694:HOH:O	2.18	0.43
1:A:160:LEU:HD23	1:A:160:LEU:HA	1.75	0.43
2:B:400:TRP:HA	2:B:425:GLY:O	2.18	0.43
1:I:133:ARG:HB2	3:J:4550:DHB:O1	2.19	0.43
1:A:64:ARG:NH1	1:A:99:PHE:O	2.51	0.42
1:A:155:CYS:HB3	1:A:158:LEU:HB2	2.01	0.42
1:C:48:HIS:CD2	1:C:48:HIS:N	2.86	0.42
1:G:113:VAL:HG22	1:G:124:PRO:HD3	2.00	0.42
2:H:460:HIS:ND1	2:H:460:HIS:N	2.67	0.42
2:J:386:ASP:HB2	2:J:529:GLY:HA2	2.00	0.42
2:D:376:GLU:H	2:D:376:GLU:HG3	1.67	0.42
1:I:178:ASP:C	1:I:180:LYS:H	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:361:HIS:H	2:J:361:HIS:HD2	1.58	0.42
2:D:411:LYS:HB2	2:D:411:LYS:HZ3	1.83	0.42
2:B:318:LYS:NZ	2:B:318:LYS:CD	2.73	0.42
2:B:333:ARG:HD3	2:B:333:ARG:HA	1.81	0.42
1:E:92:PHE:CD1	2:F:349:PRO:HG3	2.53	0.42
2:J:356:PHE:CZ	2:J:430:LEU:HD13	2.54	0.42
2:J:364:LEU:HD22	2:J:440:ARG:HG2	2.01	0.42
1:A:4:LEU:HD12	1:A:4:LEU:HA	1.83	0.42
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.55	0.42
2:J:442:ILE:H	2:J:442:ILE:HG13	1.72	0.42
2:F:437:TYR:OH	2:F:523:PHE:HB3	2.20	0.42
1:G:31:ARG:HH12	2:H:428:ARG:HG2	1.84	0.42
2:H:379:ILE:HD13	2:H:379:ILE:HG21	1.79	0.42
2:J:489:CYS:HA	2:J:490:PRO:HD3	1.84	0.42
1:K:51:LEU:HD23	1:K:51:LEU:HA	1.91	0.42
2:L:314:ASN:OD1	2:L:318:LYS:HE2	2.20	0.42
2:L:411:LYS:H	2:L:411:LYS:NZ	2.18	0.42
1:A:165:GLN:NE2	1:A:165:GLN:N	2.44	0.42
1:I:157:VAL:O	1:I:160:LEU:HB2	2.20	0.42
1:I:160:LEU:HA	1:I:160:LEU:HD23	1.79	0.42
2:D:478:LEU:C	2:D:478:LEU:HD23	2.45	0.41
1:E:26:ALA:O	2:F:411:LYS:NZ	2.46	0.41
1:G:67:PHE:CE1	1:G:94:ARG:HD2	2.53	0.41
2:J:325:LYS:HG2	2:L:335:ALA:HB1	2.02	0.41
2:L:447:TYR:HA	2:L:448:PRO:HD3	1.94	0.41
1:G:15:PRO:CD	3:H:3550:DHB:C2	2.98	0.41
1:A:165:GLN:H	1:A:165:GLN:CD	2.23	0.41
1:C:98:THR:O	1:C:101:ALA:O	2.38	0.41
2:F:372:LEU:HA	2:F:373:PRO:HD3	1.84	0.41
2:F:411:LYS:CG	2:F:411:LYS:CE	2.86	0.41
1:G:163:GLN:O	1:G:164:PRO:C	2.63	0.41
1:A:15:PRO:HG2	3:A:550:DHB:C6	2.50	0.41
1:A:190:GLN:HG3	2:B:333:ARG:HG2	2.01	0.41
1:G:52:LEU:CD2	1:G:184:ARG:NH1	2.83	0.41
2:J:461:ILE:HG22	2:J:462:HIS:O	2.20	0.41
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.69	0.41
2:B:446:PRO:HD2	2:H:376:GLU:HG2	2.02	0.41
2:H:335:ALA:HB1	2:L:325:LYS:HG2	2.02	0.41
1:I:131:PHE:CD2	1:I:138:HIS:HB3	2.55	0.41
1:K:72:GLN:O	1:K:72:GLN:HG3	2.19	0.41
1:K:125:HIS:HA	1:K:143:LEU:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:TRP:CZ3	1:A:91:SER:HB3	2.54	0.41
2:H:495:ILE:CG2	2:H:500:ALA:HB3	2.50	0.41
1:C:138:HIS:ND1	1:C:138:HIS:N	2.68	0.41
1:C:200:PHE:HB3	2:D:339:ILE:HG13	2.02	0.41
1:G:189:ILE:HD13	1:G:189:ILE:HG21	1.82	0.41
2:J:497:ASN:ND2	2:J:497:ASN:C	2.79	0.41
1:K:50:LEU:O	1:K:182:ALA:HA	2.21	0.41
1:A:50:LEU:O	1:A:182:ALA:HA	2.20	0.41
2:B:390:LYS:CE	2:B:390:LYS:CG	2.87	0.41
2:D:314:ASN:OD1	2:D:318:LYS:HE2	2.21	0.41
1:E:2:ILE:HD13	1:E:2:ILE:HA	1.84	0.41
2:F:399:MET:HA	2:F:462:HIS:O	2.21	0.41
2:F:411:LYS:H	2:F:411:LYS:NZ	2.12	0.41
2:F:437:TYR:O	2:F:438:SER:HB3	2.21	0.41
2:H:486:ILE:O	2:H:488:MET:N	2.54	0.41
2:H:522:ARG:HH11	2:H:522:ARG:HD3	1.67	0.41
1:A:74:ASP:C	1:A:74:ASP:OD1	2.64	0.41
2:F:411:LYS:O	2:F:414:ARG:NH1	2.40	0.41
2:F:485:LEU:HD23	2:F:485:LEU:HA	1.91	0.41
2:H:400:TRP:HA	2:H:425:GLY:O	2.21	0.41
1:I:15:PRO:HD3	3:J:4550:DHB:C1	2.51	0.41
2:L:478:LEU:HD12	2:L:523:PHE:CD2	2.56	0.41
2:D:381:ALA:O	2:D:522:ARG:HA	2.21	0.40
2:J:454:ASN:HB2	2:L:310:ILE:HG13	2.03	0.40
1:K:36:TRP:CD1	1:K:37:ASN:H	2.39	0.40
2:B:368:ASN:HD22	2:B:371:GLY:H	1.70	0.40
1:K:92:PHE:CG	2:L:349:PRO:HG3	2.57	0.40
2:L:451:ASN:HB3	2:L:455:ASP:OD2	2.20	0.40
2:D:411:LYS:NZ	2:D:411:LYS:H	2.18	0.40
2:F:386:ASP:OD2	2:F:386:ASP:C	2.64	0.40
2:H:360:ASP:OD2	2:H:428:ARG:HD2	2.21	0.40
2:J:420:ASP:HA	2:J:421:PRO:HD2	1.86	0.40
1:K:92:PHE:CD1	2:L:349:PRO:HG3	2.56	0.40
2:L:311:ARG:HH11	2:L:311:ARG:HD2	1.65	0.40
2:L:516:MET:CE	2:L:516:MET:HB3	2.51	0.40
2:L:303:GLN:CB	2:L:303:GLN:C	2.84	0.40
1:A:80:GLN:O	1:A:91:SER:HB2	2.20	0.40
2:D:408:HIS:HE1	2:D:447:TYR:CZ	2.38	0.40
2:F:483:ASP:HB3	2:F:486:ILE:HG13	2.04	0.40
1:G:51:LEU:HA	1:G:51:LEU:HD23	1.74	0.40
1:G:163:GLN:HA	1:G:164:PRO:HD2	1.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:GLN:CD	5:E:2951:HOH:O[3_445]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/200 (99%)	186 (94%)	11 (6%)	1 (0%)	24	35
1	C	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
1	E	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	G	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	I	198/200 (99%)	187 (94%)	10 (5%)	1 (0%)	24	35
1	K	198/200 (99%)	189 (96%)	7 (4%)	2 (1%)	12	18
2	B	235/238 (99%)	223 (95%)	10 (4%)	2 (1%)	14	20
2	D	235/238 (99%)	225 (96%)	9 (4%)	1 (0%)	30	42
2	F	235/238 (99%)	226 (96%)	8 (3%)	1 (0%)	30	42
2	H	235/238 (99%)	223 (95%)	11 (5%)	1 (0%)	30	42
2	J	235/238 (99%)	222 (94%)	12 (5%)	1 (0%)	30	42
2	L	235/238 (99%)	218 (93%)	15 (6%)	2 (1%)	14	20
All	All	2598/2628 (99%)	2467 (95%)	119 (5%)	12 (0%)	24	35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	368	ASN
2	D	368	ASN
2	F	368	ASN
2	H	368	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	368	ASN
2	L	368	ASN
2	B	493	LYS
2	L	493	LYS
1	A	74	ASP
1	I	132	ALA
1	K	179	GLY
1	K	42	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/163 (99%)	148 (91%)	14 (9%)	10	15
1	C	162/163 (99%)	150 (93%)	12 (7%)	13	20
1	E	162/163 (99%)	150 (93%)	12 (7%)	13	20
1	G	162/163 (99%)	150 (93%)	12 (7%)	13	20
1	I	162/163 (99%)	151 (93%)	11 (7%)	14	24
1	K	162/163 (99%)	146 (90%)	16 (10%)	7	11
2	B	199/201 (99%)	184 (92%)	15 (8%)	12	20
2	D	199/201 (99%)	177 (89%)	22 (11%)	6	8
2	F	199/201 (99%)	181 (91%)	18 (9%)	9	14
2	H	199/201 (99%)	181 (91%)	18 (9%)	9	14
2	J	199/201 (99%)	180 (90%)	19 (10%)	8	12
2	L	199/201 (99%)	175 (88%)	24 (12%)	5	6
All	All	2166/2184 (99%)	1973 (91%)	193 (9%)	9	14

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	42	PRO
1	A	52	LEU
1	A	86	GLU
1	A	91	SER
1	A	103	GLU
1	A	114	VAL
1	A	137	ILE
1	A	154	LYS
1	A	158	LEU
1	A	165	GLN
1	A	188	ARG
1	A	192	GLU
2	B	364	LEU
2	B	372	LEU
2	B	395	THR
2	B	411	LYS
2	B	414	ARG
2	B	416	LEU
2	B	426	VAL
2	B	428	ARG
2	B	442	ILE
2	B	443	LYS
2	B	475	ILE
2	B	497	ASN
2	B	507	LYS
2	B	512	ASN
2	B	534	HIS
1	C	4	LEU
1	C	6	PRO
1	C	19	ILE
1	C	52	LEU
1	C	124	PRO
1	C	154	LYS
1	C	158	LEU
1	C	164	PRO
1	C	165	GLN
1	C	168	GLU
1	C	180	LYS
1	C	188	ARG
2	D	310	ILE
2	D	333	ARG
2	D	364	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	368	ASN
2	D	372	LEU
2	D	390	LYS
2	D	393	PRO
2	D	395	THR
2	D	411	LYS
2	D	416	LEU
2	D	428	ARG
2	D	433	SER
2	D	442	ILE
2	D	457	ARG
2	D	468	PRO
2	D	473	LYS
2	D	475	ILE
2	D	478	LEU
2	D	497	ASN
2	D	533	THR
2	D	534	HIS
2	D	538	CYS
1	E	4	LEU
1	E	19	ILE
1	E	52	LEU
1	E	66	SER
1	E	98	THR
1	E	114	VAL
1	E	158	LEU
1	E	165	GLN
1	E	171	ILE
1	E	177	VAL
1	E	188	ARG
1	E	192	GLU
2	F	333	ARG
2	F	364	LEU
2	F	372	LEU
2	F	393	PRO
2	F	395	THR
2	F	411	LYS
2	F	416	LEU
2	F	428	ARG
2	F	433	SER
2	F	434	ASP
2	F	442	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	457	ARG
2	F	478	LEU
2	F	503	GLN
2	F	507	LYS
2	F	515	PRO
2	F	522	ARG
2	F	534	HIS
1	G	4	LEU
1	G	19	ILE
1	G	36	TRP
1	G	38	ARG
1	G	52	LEU
1	G	66	SER
1	G	86	GLU
1	G	91	SER
1	G	94	ARG
1	G	98	THR
1	G	158	LEU
1	G	165	GLN
2	H	364	LEU
2	H	368	ASN
2	H	372	LEU
2	H	385	VAL
2	H	390	LYS
2	H	391	PRO
2	H	395	THR
2	H	411	LYS
2	H	416	LEU
2	H	428	ARG
2	H	433	SER
2	H	434	ASP
2	H	473	LYS
2	H	478	LEU
2	H	497	ASN
2	H	507	LYS
2	H	511	ASN
2	H	534	HIS
1	I	4	LEU
1	I	19	ILE
1	I	38	ARG
1	I	42	PRO
1	I	52	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	94	ARG
1	I	100	ASP
1	I	165	GLN
1	I	168	GLU
1	I	180	LYS
1	I	192	GLU
2	J	364	LEU
2	J	372	LEU
2	J	390	LYS
2	J	395	THR
2	J	411	LYS
2	J	414	ARG
2	J	416	LEU
2	J	428	ARG
2	J	433	SER
2	J	442	ILE
2	J	457	ARG
2	J	475	ILE
2	J	478	LEU
2	J	493	LYS
2	J	497	ASN
2	J	503	GLN
2	J	507	LYS
2	J	512	ASN
2	J	538	CYS
1	K	4	LEU
1	K	19	ILE
1	K	42	PRO
1	K	52	LEU
1	K	66	SER
1	K	76	ASN
1	K	80	GLN
1	K	94	ARG
1	K	103	GLU
1	K	106	LEU
1	K	114	VAL
1	K	122	MET
1	K	133	ARG
1	K	158	LEU
1	K	165	GLN
1	K	171	ILE
2	L	306	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	343	ILE
2	L	350	ASN
2	L	364	LEU
2	L	372	LEU
2	L	390	LYS
2	L	393	PRO
2	L	394	ASN
2	L	395	THR
2	L	411	LYS
2	L	414	ARG
2	L	416	LEU
2	L	426	VAL
2	L	428	ARG
2	L	433	SER
2	L	442	ILE
2	L	475	ILE
2	L	478	LEU
2	L	490	PRO
2	L	495	ILE
2	L	497	ASN
2	L	507	LYS
2	L	534	HIS
2	L	538	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	59	ASN
1	A	136	ASN
1	A	140	HIS
1	A	163	GLN
1	A	165	GLN
2	B	305	ASN
2	B	314	ASN
2	B	361	HIS
2	B	368	ASN
2	B	369	ASN
2	B	412	ASN
2	B	422	ASN
2	B	497	ASN
2	B	503	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	512	ASN
1	C	59	ASN
1	C	107	HIS
1	C	163	GLN
1	C	165	GLN
2	D	305	ASN
2	D	334	GLN
2	D	361	HIS
2	D	368	ASN
2	D	369	ASN
2	D	412	ASN
2	D	422	ASN
2	D	497	ASN
2	D	503	GLN
2	D	511	ASN
1	E	107	HIS
1	E	136	ASN
1	E	163	GLN
1	E	165	GLN
2	F	334	GLN
2	F	359	HIS
2	F	361	HIS
2	F	368	ASN
2	F	369	ASN
2	F	394	ASN
2	F	497	ASN
2	F	503	GLN
1	G	11	GLN
1	G	163	GLN
1	G	165	GLN
2	H	361	HIS
2	H	368	ASN
2	H	412	ASN
2	H	422	ASN
2	H	497	ASN
2	H	503	GLN
1	I	11	GLN
1	I	115	ASN
1	I	127	ASN
1	I	165	GLN
2	J	305	ASN
2	J	361	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	368	ASN
2	J	369	ASN
2	J	412	ASN
2	J	422	ASN
2	J	497	ASN
2	J	503	GLN
2	J	530	GLN
1	K	127	ASN
1	K	165	GLN
2	L	305	ASN
2	L	361	HIS
2	L	368	ASN
2	L	394	ASN
2	L	412	ASN
2	L	497	ASN
2	L	503	GLN
2	L	530	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CME	F	429	2	8,9,10	3.51	5 (62%)	6,9,11	2.24	3 (50%)
2	CME	J	429	2	8,9,10	2.04	4 (50%)	6,9,11	1.94	2 (33%)
2	CME	H	429	2	8,9,10	3.05	5 (62%)	6,9,11	1.84	3 (50%)
2	CME	L	429	2	8,9,10	2.23	3 (37%)	6,9,11	2.45	4 (66%)
2	CME	B	429	2	8,9,10	2.06	3 (37%)	6,9,11	2.79	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CME	D	429	2	8,9,10	2.43	3 (37%)	6,9,11	2.18	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CME	F	429	2	-	3/5/8/10	-
2	CME	J	429	2	-	4/5/8/10	-
2	CME	H	429	2	-	5/5/8/10	-
2	CME	L	429	2	-	4/5/8/10	-
2	CME	B	429	2	-	4/5/8/10	-
2	CME	D	429	2	-	4/5/8/10	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	429	CME	CB-SG	-7.69	1.56	1.81
2	D	429	CME	CB-SG	-5.22	1.64	1.81
2	H	429	CME	CB-SG	-4.72	1.65	1.81
2	H	429	CME	CE-CZ	4.42	1.79	1.50
2	L	429	CME	CE-CZ	4.12	1.77	1.50
2	H	429	CME	CE-SD	3.94	1.98	1.82
2	F	429	CME	CA-N	-3.92	1.37	1.48
2	B	429	CME	CB-SG	-3.76	1.69	1.81
2	F	429	CME	CB-CA	-3.65	1.44	1.53
2	J	429	CME	CB-SG	-3.57	1.69	1.81
2	L	429	CME	CB-SG	-3.05	1.71	1.81
2	H	429	CME	O-C	2.91	1.31	1.20
2	D	429	CME	CA-N	-2.83	1.40	1.48
2	B	429	CME	CE-SD	2.66	1.93	1.82
2	J	429	CME	O-C	2.35	1.28	1.20
2	B	429	CME	CE-CZ	2.33	1.65	1.50
2	J	429	CME	CE-CZ	2.29	1.65	1.50
2	D	429	CME	CB-CA	-2.24	1.47	1.53
2	F	429	CME	CE-SD	2.20	1.91	1.82
2	J	429	CME	CB-CA	-2.17	1.47	1.53
2	F	429	CME	CE-CZ	2.15	1.64	1.50
2	H	429	CME	CB-CA	-2.14	1.47	1.53
2	L	429	CME	O-C	2.11	1.28	1.20

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	429	CME	CB-SG-SD	5.76	118.76	103.86
2	F	429	CME	CE-SD-SG	4.24	122.06	103.46
2	D	429	CME	OH-CZ-CE	3.57	124.75	110.82
2	L	429	CME	CZ-CE-SD	-3.45	101.84	113.39
2	D	429	CME	CE-SD-SG	3.21	117.56	103.46
2	J	429	CME	OH-CZ-CE	3.18	123.22	110.82
2	L	429	CME	CE-SD-SG	3.07	116.95	103.46
2	B	429	CME	OH-CZ-CE	2.84	121.92	110.82
2	H	429	CME	OH-CZ-CE	2.82	121.81	110.82
2	L	429	CME	OH-CZ-CE	2.70	121.35	110.82
2	L	429	CME	CB-SG-SD	-2.52	97.33	103.86
2	F	429	CME	OH-CZ-CE	2.46	120.42	110.82
2	H	429	CME	CE-SD-SG	2.37	113.87	103.46
2	H	429	CME	CZ-CE-SD	-2.13	106.25	113.39
2	J	429	CME	CZ-CE-SD	-2.06	106.51	113.39
2	F	429	CME	CZ-CE-SD	-2.05	106.54	113.39

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	429	CME	SD-CE-CZ-OH
2	D	429	CME	N-CA-CB-SG
2	F	429	CME	N-CA-CB-SG
2	F	429	CME	CE-SD-SG-CB
2	H	429	CME	N-CA-CB-SG
2	J	429	CME	N-CA-CB-SG
2	L	429	CME	N-CA-CB-SG
2	D	429	CME	CE-SD-SG-CB
2	H	429	CME	CE-SD-SG-CB
2	D	429	CME	SD-CE-CZ-OH
2	F	429	CME	SD-CE-CZ-OH
2	J	429	CME	SD-CE-CZ-OH
2	L	429	CME	SD-CE-CZ-OH
2	L	429	CME	CE-SD-SG-CB
2	J	429	CME	CE-SD-SG-CB
2	H	429	CME	SD-CE-CZ-OH
2	B	429	CME	N-CA-CB-SG
2	B	429	CME	CE-SD-SG-CB
2	B	429	CME	CZ-CE-SD-SG
2	D	429	CME	CZ-CE-SD-SG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	429	CME	CZ-CE-SD-SG
2	J	429	CME	CZ-CE-SD-SG
2	L	429	CME	CZ-CE-SD-SG
2	H	429	CME	CA-CB-SG-SD

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	429	CME	1	0
2	H	429	CME	2	0
2	L	429	CME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	DHB	A	550	4	11,11,11	1.12	0	15,15,15	0.92	1 (6%)
3	DHB	L	5550	4	11,11,11	0.98	0	15,15,15	0.86	1 (6%)
3	DHB	J	4550	4	11,11,11	0.89	0	15,15,15	0.86	1 (6%)
3	DHB	D	1550	4	11,11,11	0.96	0	15,15,15	0.88	1 (6%)
3	DHB	H	3550	4	11,11,11	1.04	0	15,15,15	0.82	1 (6%)
3	DHB	F	2550	4	11,11,11	1.25	1 (9%)	15,15,15	0.88	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DHB	A	550	4	-	0/4/4/4	0/1/1/1
3	DHB	L	5550	4	-	0/4/4/4	0/1/1/1
3	DHB	J	4550	4	-	0/4/4/4	0/1/1/1
3	DHB	D	1550	4	-	0/4/4/4	0/1/1/1
3	DHB	H	3550	4	-	0/4/4/4	0/1/1/1
3	DHB	F	2550	4	-	0/4/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2550	DHB	C4-C3	-2.15	1.36	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1550	DHB	O2-C-C1	2.43	121.08	114.84
3	A	550	DHB	O2-C-C1	2.38	120.94	114.84
3	F	2550	DHB	O2-C-C1	2.36	120.90	114.84
3	L	5550	DHB	O2-C-C1	2.35	120.87	114.84
3	J	4550	DHB	O2-C-C1	2.32	120.79	114.84
3	H	3550	DHB	O2-C-C1	2.19	120.45	114.84
3	F	2550	DHB	O2-C-O1	-2.06	118.91	123.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	550	DHB	7	0
3	L	5550	DHB	3	0
3	J	4550	DHB	3	0
3	D	1550	DHB	1	0
3	H	3550	DHB	6	0
3	F	2550	DHB	1	0

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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	200/200 (100%)	-0.76	1 (0%) 87 86	9, 24, 57, 73	0
1	C	200/200 (100%)	-0.68	3 (1%) 72 69	8, 25, 57, 72	0
1	E	200/200 (100%)	-0.69	1 (0%) 87 86	7, 27, 57, 73	0
1	G	200/200 (100%)	-0.70	2 (1%) 79 77	8, 26, 58, 73	0
1	I	200/200 (100%)	-0.64	1 (0%) 87 86	9, 28, 59, 73	0
1	K	200/200 (100%)	-0.51	2 (1%) 79 77	12, 30, 59, 73	0
2	B	237/238 (99%)	-0.88	1 (0%) 88 87	9, 19, 48, 68	0
2	D	237/238 (99%)	-0.90	0 100 100	8, 19, 48, 68	0
2	F	237/238 (99%)	-0.90	1 (0%) 88 87	8, 19, 48, 67	0
2	H	237/238 (99%)	-0.91	0 100 100	9, 19, 48, 65	0
2	J	237/238 (99%)	-0.81	0 100 100	11, 22, 49, 68	0
2	L	237/238 (99%)	-0.84	1 (0%) 88 87	12, 21, 50, 68	0
All	All	2622/2628 (99%)	-0.78	13 (0%) 87 86	7, 23, 56, 73	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	99	PHE	4.2
1	C	98	THR	3.5
1	E	99	PHE	3.3
1	A	99	PHE	2.8
1	C	99	PHE	2.6
2	L	301	PRO	2.5
1	C	102	GLY	2.5
2	B	368	ASN	2.4
1	G	101	ALA	2.3
1	K	101	ALA	2.3
2	F	368	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	101	ALA	2.2
1	K	99	PHE	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CME	L	429	10/11	0.95	0.10	25,34,55,57	0
2	CME	H	429	10/11	0.96	0.08	23,31,52,52	0
2	CME	J	429	10/11	0.96	0.08	26,33,55,57	0
2	CME	F	429	10/11	0.96	0.10	23,31,53,56	0
2	CME	B	429	10/11	0.97	0.07	22,30,52,55	0
2	CME	D	429	10/11	0.97	0.08	23,32,55,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DHB	D	1550	11/11	0.86	0.21	77,78,79,79	0
3	DHB	L	5550	11/11	0.87	0.24	86,87,88,88	0
3	DHB	F	2550	11/11	0.89	0.27	102,102,103,103	0
3	DHB	A	550	11/11	0.89	0.26	86,88,88,89	0
3	DHB	J	4550	11/11	0.90	0.28	103,105,106,106	0
3	DHB	H	3550	11/11	0.92	0.25	100,101,101,102	0
4	FE	J	4600	1/1	0.94	0.08	67,67,67,67	0
4	FE	H	3600	1/1	0.95	0.07	63,63,63,63	0
4	FE	B	600	1/1	0.96	0.05	62,62,62,62	0
4	FE	D	1600	1/1	0.97	0.04	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FE	L	5600	1/1	0.97	0.04	63,63,63,63	0
4	FE	F	2600	1/1	0.98	0.03	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.