



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:13 PM UTC

PDB ID : 1YKL / pdb_00001ykl
Title : Protocatechuate 3,4-Dioxygenase Y408C mutant bound to DHB
Authors : Brown, C.K.; Ohlendorf, D.H.
Deposited on : 2005-01-18
Resolution : 2.25 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

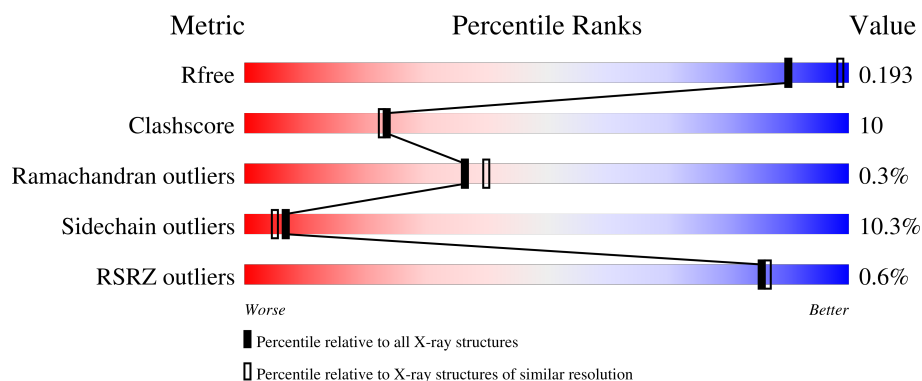
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



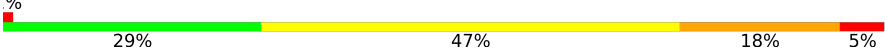
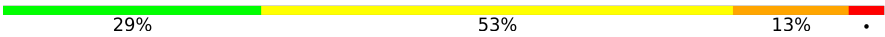
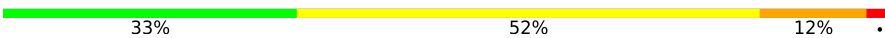
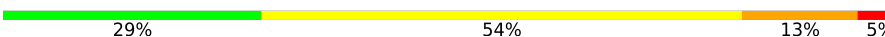
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	39% 50% 11%
1	C	200	36% 50% 12%
1	E	200	35% 44% 18%
1	G	200	40% 46% 11%
1	I	200	36% 48% 14%

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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
4	DHB	F	2550	-	-	X	-
4	DHB	L	5550	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21744 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	1	0
			1875	1185	343	337	10			
2	D	238	Total	C	N	O	S	0	1	0
			1875	1185	343	337	10			
2	F	238	Total	C	N	O	S	0	1	0
			1875	1185	343	337	10			
2	H	238	Total	C	N	O	S	0	1	0
			1875	1185	343	337	10			
2	J	238	Total	C	N	O	S	0	1	0
			1875	1185	343	337	10			
2	L	238	Total	C	N	O	S	0	1	0
			1875	1185	343	337	10			

There are 6 discrepancies between the modelled and reference sequences:

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

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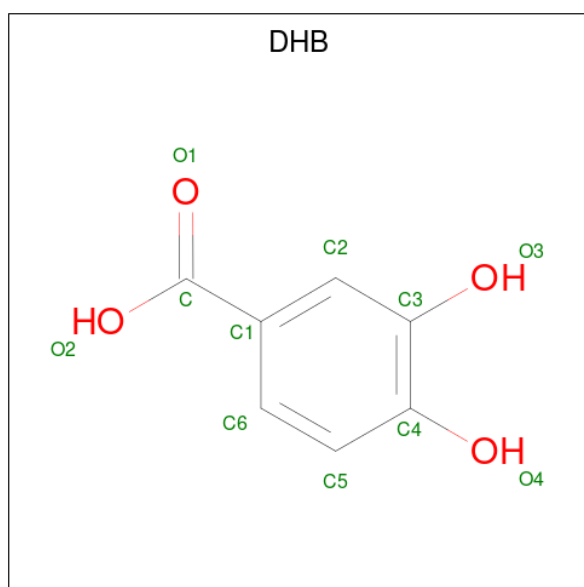
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Chain	Residue	Modelled	Actual	Comment	Reference
D	408	CYS	TYR	engineered mutation	UNP P00437
F	408	CYS	TYR	engineered mutation	UNP P00437
H	408	CYS	TYR	engineered mutation	UNP P00437
J	408	CYS	TYR	engineered mutation	UNP P00437
L	408	CYS	TYR	engineered mutation	UNP P00437

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 4 is 3,4-DIHYDROXYBENZOIC ACID (CCD ID: DHB) (formula: C₇H₆O₄).



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

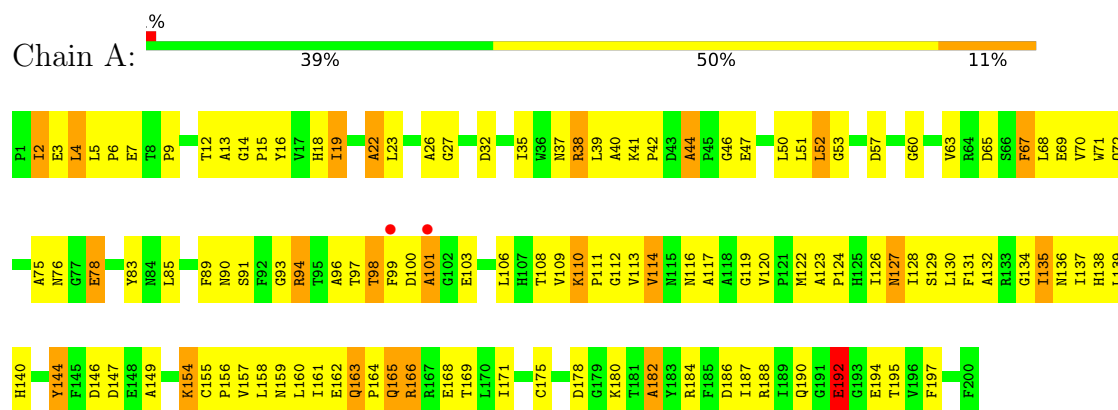
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	51	Total O 51 51	0	0
5	B	111	Total O 111 111	0	0
5	C	49	Total O 49 49	0	0
5	D	122	Total O 122 122	0	0
5	E	54	Total O 54 54	0	0
5	F	113	Total O 113 113	0	0
5	G	52	Total O 52 52	0	0
5	H	108	Total O 108 108	0	0
5	I	55	Total O 55 55	0	0
5	J	115	Total O 115 115	0	0
5	K	48	Total O 48 48	0	0
5	L	118	Total O 118 118	0	0

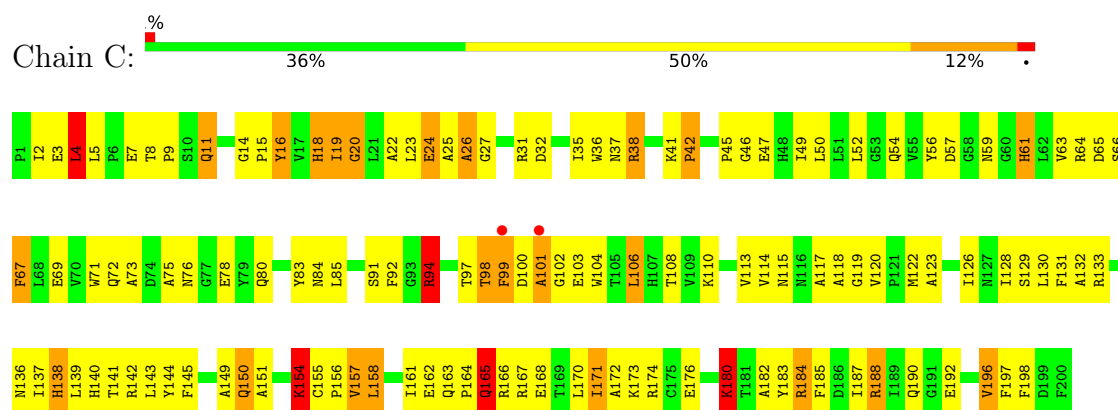
3 Residue-property plots

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.

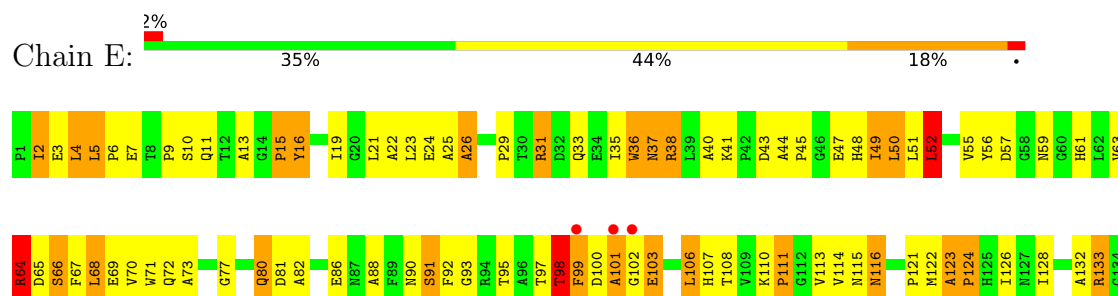
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



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

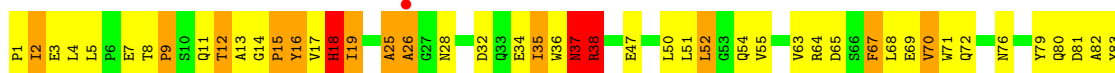


- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

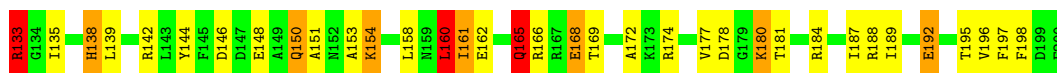
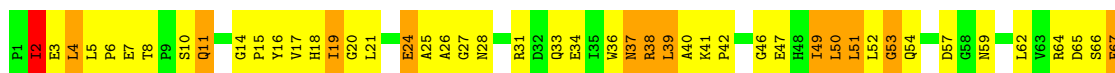




• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



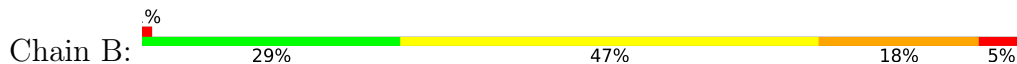
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

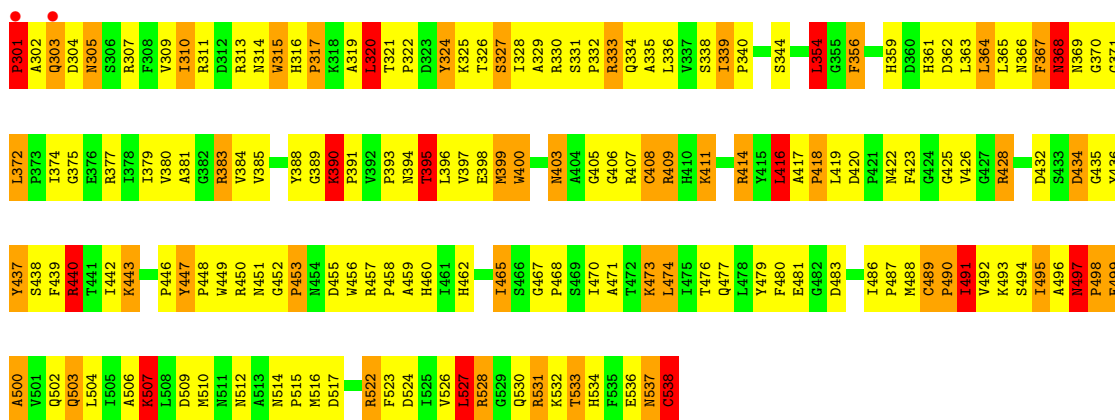


• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

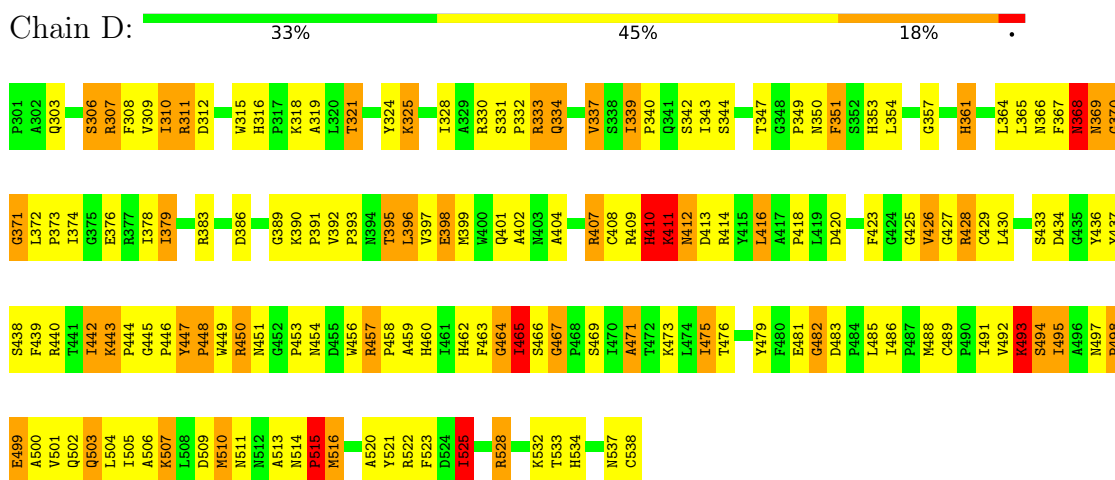


• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

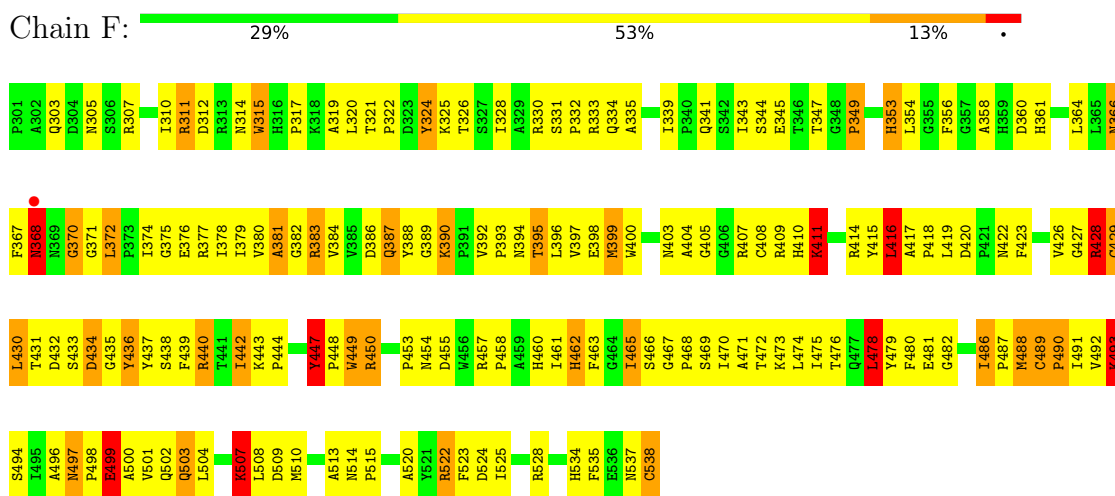




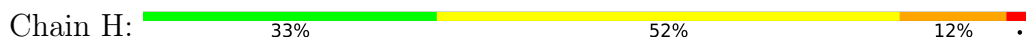
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

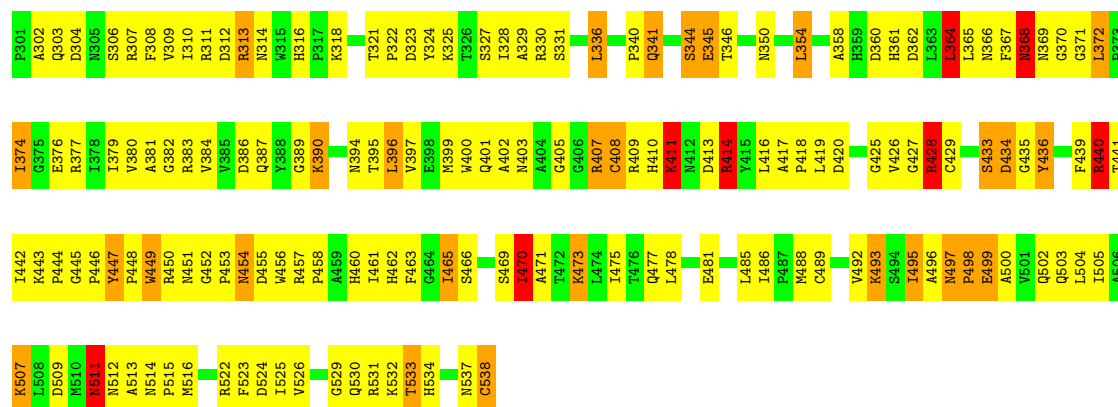


• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



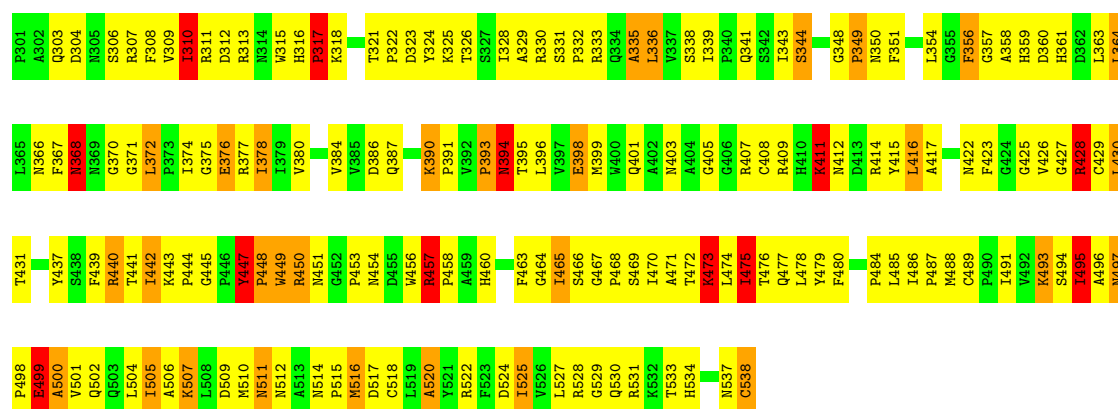
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain





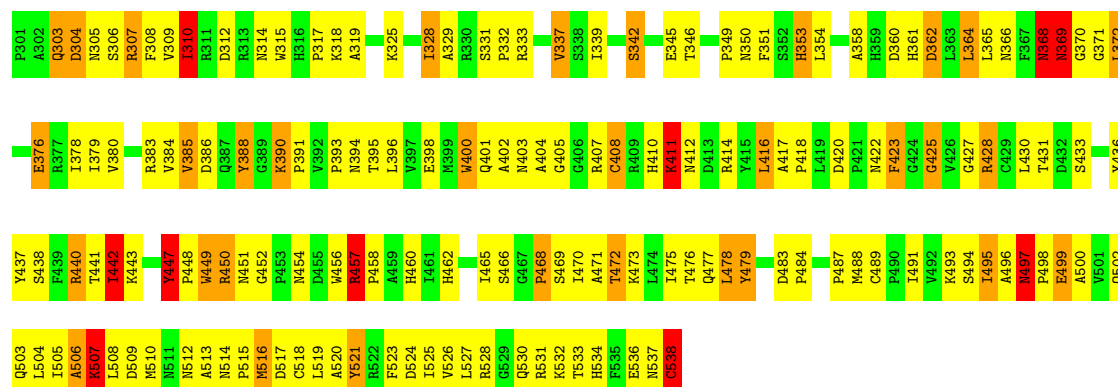
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain J: 29% 54% 13% 5%



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

Chain L: 32% 50% 13% .



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.70Å 127.20Å 133.90Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	25.64 – 2.25 25.64 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.64-2.25) 99.4 (25.64-2.25)	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}	0.158 , 0.199 0.158 , 0.193	Depositor DCC
R_{free} test set	1950 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21744	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: DHB, FE

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	2.67	114/1611 (7.1%)	2.00	53/2195 (2.4%)
1	C	2.82	118/1611 (7.3%)	2.05	55/2195 (2.5%)
1	E	2.80	128/1611 (7.9%)	2.12	55/2195 (2.5%)
1	G	2.79	117/1611 (7.3%)	2.11	61/2195 (2.8%)
1	I	2.70	109/1611 (6.8%)	2.06	55/2195 (2.5%)
1	K	2.84	126/1611 (7.8%)	2.08	61/2195 (2.8%)
2	B	2.98	177/1930 (9.2%)	2.19	86/2627 (3.3%)
2	D	2.87	158/1930 (8.2%)	2.21	86/2627 (3.3%)
2	F	2.86	163/1930 (8.4%)	2.22	96/2627 (3.7%)
2	H	2.88	161/1930 (8.3%)	2.20	85/2627 (3.2%)
2	J	2.77	141/1930 (7.3%)	2.16	91/2627 (3.5%)
2	L	2.79	148/1930 (7.7%)	2.15	84/2627 (3.2%)
All	All	2.82	1660/21246 (7.8%)	2.14	868/28932 (3.0%)

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	7
1	C	0	10
1	E	0	4
1	G	0	7
1	I	0	7
1	K	0	6
2	B	0	10
2	D	0	15
2	F	0	6
2	H	0	10
2	J	0	16

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	18
All	All	0	116

All (1660) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	303	GLN	CA-CB	18.81	1.86	1.53
2	J	486	ILE	CA-CB	-18.08	1.45	1.54
2	J	423	PHE	C-O	15.81	1.41	1.24
2	J	409	ARG	CA-C	15.02	1.70	1.53
2	D	510	MET	SD-CE	14.97	2.17	1.79
1	G	122	MET	SD-CE	-14.68	1.42	1.79
2	H	475	ILE	CG1-CD1	-14.54	0.95	1.51
2	B	331	SER	CA-C	-14.22	1.41	1.52
2	L	303	GLN	CA-CB	12.78	1.75	1.53
1	K	49	ILE	C-O	12.61	1.38	1.23
2	D	505	ILE	CA-CB	-12.45	1.39	1.53
2	L	380	VAL	CA-CB	12.40	1.70	1.53
2	B	486	ILE	CA-CB	-12.35	1.48	1.54
1	C	71	TRP	C-O	12.30	1.37	1.23
2	D	507	LYS	CE-NZ	12.14	1.85	1.49
1	C	136	ASN	C-O	12.13	1.38	1.24
1	K	149	ALA	CA-CB	12.10	1.72	1.53
2	H	321	THR	C-O	11.86	1.37	1.24
2	F	426	VAL	C-O	11.68	1.35	1.24
2	D	486	ILE	CA-CB	11.67	1.59	1.54
2	B	502	GLN	CD-OE1	11.65	1.45	1.23
1	A	63	VAL	CA-CB	-11.60	1.40	1.53
2	L	513	ALA	CA-CB	-11.57	1.33	1.53
2	H	354	LEU	C-O	11.56	1.38	1.23
1	E	11	GLN	N-CA	11.41	1.60	1.45
1	E	73	ALA	CA-CB	-11.32	1.35	1.53
2	B	488	MET	SD-CE	-11.28	1.51	1.79
2	B	495	ILE	CG1-CD1	-11.28	1.07	1.51
1	C	98	THR	N-CA	11.21	1.59	1.45
2	J	516	MET	SD-CE	-11.16	1.51	1.79
2	B	303	GLN	CA-C	11.14	1.66	1.52
2	D	409	ARG	CA-C	11.05	1.65	1.53
2	H	374	ILE	CA-C	10.97	1.66	1.52
2	L	402	ALA	CA-CB	10.80	1.68	1.53
2	F	460	HIS	CA-C	-10.76	1.39	1.52
1	G	2	ILE	CG1-CD1	-10.74	1.09	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	461	ILE	C-O	10.72	1.35	1.24
2	D	366	ASN	C-O	-10.69	1.09	1.24
2	L	418	PRO	CA-C	-10.68	1.41	1.52
1	A	114	VAL	C-O	10.65	1.34	1.24
1	K	13	ALA	C-O	10.59	1.38	1.24
1	G	161	ILE	C-O	-10.57	1.12	1.23
1	K	108	THR	CA-CB	10.57	1.67	1.54
1	I	105	THR	CA-CB	10.55	1.72	1.53
2	F	524	ASP	C-O	-10.47	1.11	1.23
1	G	132	ALA	C-O	10.45	1.34	1.23
1	C	184	ARG	N-CA	-10.41	1.33	1.46
2	B	394	ASN	C-O	-10.35	1.11	1.23
2	H	303	GLN	CA-CB	10.32	1.71	1.53
2	F	303	GLN	CA-CB	10.29	1.71	1.53
1	I	93	GLY	C-O	10.25	1.34	1.23
2	B	451	ASN	CA-C	10.25	1.58	1.52
2	L	404	ALA	CA-CB	-10.24	1.35	1.53
1	E	35	ILE	CA-CB	-10.13	1.42	1.54
2	L	369	ASN	C-O	10.12	1.36	1.24
1	G	130	LEU	C-O	10.11	1.36	1.24
1	E	2	ILE	CG1-CD1	-10.10	1.12	1.51
2	F	430	LEU	C-O	-10.08	1.11	1.23
2	D	439	PHE	CA-C	-10.06	1.40	1.52
1	A	129	SER	N-CA	-10.04	1.33	1.46
2	F	415	TYR	CA-C	10.01	1.65	1.52
2	B	365	LEU	C-O	-10.00	1.11	1.24
1	G	173	LYS	CA-CB	9.99	1.66	1.53
2	L	385	VAL	C-O	9.98	1.36	1.23
2	D	407	ARG	N-CA	9.97	1.58	1.46
1	G	137	ILE	N-CA	-9.95	1.34	1.46
1	G	108	THR	CA-CB	9.88	1.66	1.54
1	C	97	THR	C-O	9.87	1.35	1.23
1	K	52	LEU	C-O	9.87	1.35	1.23
2	H	377	ARG	C-O	9.87	1.35	1.24
2	L	354	LEU	C-O	9.84	1.36	1.23
2	B	335	ALA	CA-C	9.80	1.66	1.53
2	B	327	SER	N-CA	-9.80	1.34	1.46
1	E	183	TYR	C-O	-9.77	1.12	1.23
1	C	122	MET	SD-CE	-9.77	1.55	1.79
2	B	530	GLN	C-O	-9.71	1.12	1.24
1	K	111	PRO	C-O	9.71	1.34	1.23
2	D	453	PRO	CA-CB	-9.66	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	430	LEU	C-O	-9.64	1.12	1.24
2	B	434	ASP	N-CA	-9.60	1.33	1.46
1	E	90	ASN	C-O	9.60	1.36	1.24
2	F	454	ASN	C-O	-9.60	1.12	1.23
1	E	158	LEU	C-O	-9.58	1.12	1.24
2	H	329	ALA	CA-CB	-9.58	1.36	1.53
2	H	514	ASN	C-O	-9.55	1.12	1.24
2	F	331	SER	C-O	-9.53	1.11	1.24
2	F	500	ALA	CA-CB	-9.52	1.37	1.53
1	I	189	ILE	CA-CB	-9.50	1.42	1.54
2	F	349	PRO	CA-C	-9.48	1.40	1.52
1	C	35	ILE	CA-CB	-9.47	1.42	1.53
2	H	358	ALA	CA-CB	9.42	1.69	1.53
2	D	443	LYS	CA-C	9.42	1.64	1.52
2	D	368	ASN	CA-CB	9.40	1.69	1.53
2	L	530	GLN	N-CA	9.35	1.57	1.46
1	G	144	TYR	CA-C	9.33	1.64	1.52
1	E	108	THR	CA-CB	9.33	1.62	1.54
2	L	454	ASN	C-O	-9.28	1.14	1.23
2	L	531	ARG	CZ-NH1	9.28	1.45	1.32
2	B	506	ALA	CA-CB	-9.25	1.37	1.53
2	J	326	THR	C-O	-9.23	1.12	1.24
2	B	507	LYS	CE-NZ	9.19	1.76	1.49
2	H	428	ARG	CB-CG	-9.19	1.24	1.52
2	L	519	LEU	CA-CB	9.18	1.66	1.53
2	B	326	THR	N-CA	9.15	1.57	1.46
2	F	344	SER	C-O	-9.12	1.13	1.24
2	L	507	LYS	CE-NZ	9.10	1.76	1.49
1	C	98	THR	CA-C	9.09	1.63	1.52
2	B	309	VAL	CA-CB	9.09	1.63	1.54
2	B	537	ASN	CA-C	9.06	1.65	1.53
1	K	17	VAL	C-O	9.04	1.34	1.24
2	L	448	PRO	C-O	-9.04	1.14	1.23
1	C	100	ASP	CA-C	9.04	1.64	1.52
2	L	314	ASN	C-O	-9.03	1.12	1.24
1	C	66	SER	CB-OG	-9.03	1.24	1.42
2	H	379	ILE	CA-C	9.03	1.63	1.52
2	B	363	LEU	C-O	-9.01	1.12	1.24
2	B	320	LEU	N-CA	8.98	1.57	1.46
2	L	339	ILE	C-O	8.97	1.35	1.24
1	I	126	ILE	C-O	-8.97	1.14	1.24
2	H	450	ARG	CZ-NH2	8.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	303	GLN	CA-CB	8.94	1.69	1.53
2	J	329	ALA	CA-CB	-8.93	1.38	1.53
2	B	492	VAL	C-O	-8.93	1.14	1.24
2	J	323	ASP	CA-C	8.90	1.64	1.52
2	J	491	ILE	N-CA	8.88	1.57	1.46
2	L	532	LYS	CA-CB	8.87	1.67	1.53
2	H	471	ALA	N-CA	8.87	1.57	1.46
2	F	332	PRO	C-O	8.87	1.33	1.23
2	L	394	ASN	CA-C	-8.84	1.41	1.53
2	D	469	SER	C-O	-8.83	1.13	1.23
1	A	138	HIS	C-O	-8.81	1.13	1.23
2	F	387	GLN	C-O	-8.81	1.12	1.24
1	G	79	TYR	CA-C	8.81	1.63	1.52
2	D	306	SER	C-O	-8.80	1.12	1.24
2	F	507	LYS	CE-NZ	8.79	1.75	1.49
2	L	479	TYR	C-O	8.77	1.35	1.23
1	G	188	ARG	CZ-NH1	8.76	1.45	1.32
2	H	523	PHE	CA-C	8.76	1.64	1.53
1	E	128	ILE	CA-C	8.74	1.62	1.52
1	K	68	LEU	CA-C	-8.74	1.41	1.52
2	H	346	THR	CA-CB	-8.72	1.38	1.53
2	D	501	VAL	C-O	-8.67	1.13	1.24
2	D	378	ILE	CA-CB	8.67	1.67	1.55
2	B	499	GLU	CD-OE1	8.65	1.41	1.25
1	C	133	ARG	CA-C	8.64	1.64	1.52
1	I	6	PRO	CA-C	8.63	1.63	1.52
2	J	475	ILE	CA-C	8.63	1.62	1.52
2	F	390	LYS	CG-CD	8.63	1.78	1.52
1	I	138	HIS	C-O	-8.62	1.13	1.23
2	H	426	VAL	CA-CB	-8.60	1.43	1.54
1	A	41	LYS	CA-C	8.60	1.64	1.53
1	C	118	ALA	CA-CB	8.59	1.66	1.53
2	B	330	ARG	CZ-NH2	-8.59	1.22	1.33
1	C	100	ASP	CB-CG	8.58	1.73	1.52
2	F	523	PHE	CA-C	8.58	1.62	1.52
2	D	309	VAL	CA-CB	8.57	1.64	1.54
2	J	310	ILE	N-CA	-8.55	1.35	1.46
2	F	379	ILE	CA-C	8.55	1.63	1.52
2	J	403	ASN	C-O	8.55	1.33	1.23
1	K	168	GLU	CD-OE2	8.54	1.41	1.25
2	F	397	VAL	C-O	-8.53	1.14	1.24
2	B	462	HIS	C-O	-8.52	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	454	ASN	C-O	-8.49	1.11	1.23
1	C	73	ALA	CA-CB	-8.48	1.39	1.53
2	J	429	CYS	N-CA	8.47	1.55	1.46
2	F	396	LEU	C-O	8.45	1.34	1.24
2	H	531	ARG	CA-C	8.44	1.63	1.52
1	K	196	VAL	C-O	8.43	1.35	1.24
2	F	317	PRO	CA-C	8.42	1.63	1.52
1	G	100	ASP	N-CA	8.42	1.56	1.46
2	D	442	ILE	C-O	-8.41	1.13	1.23
1	I	108	THR	CA-CB	8.39	1.65	1.54
2	B	457	ARG	CD-NE	8.39	1.57	1.46
2	D	520	ALA	CA-CB	-8.39	1.38	1.54
2	H	341	GLN	C-O	-8.39	1.13	1.24
1	C	172	ALA	CA-C	8.38	1.63	1.52
2	H	475	ILE	CA-CB	8.37	1.65	1.54
1	C	120	VAL	CA-C	8.37	1.59	1.53
2	F	486	ILE	CA-CB	-8.37	1.49	1.54
2	D	337	VAL	C-O	8.35	1.33	1.24
2	B	526	VAL	N-CA	-8.34	1.36	1.46
2	D	495	ILE	CA-CB	8.34	1.63	1.53
1	I	59	ASN	CA-C	8.34	1.64	1.52
1	E	123	ALA	CA-C	8.32	1.63	1.53
1	A	35	ILE	C-O	-8.30	1.15	1.24
2	L	436	TYR	CA-C	-8.30	1.42	1.52
1	A	154	LYS	CE-NZ	8.29	1.74	1.49
2	J	475	ILE	C-O	8.29	1.32	1.24
1	E	13	ALA	N-CA	8.27	1.56	1.46
1	E	172	ALA	CA-C	8.27	1.63	1.52
2	L	502	GLN	CD-OE1	8.27	1.39	1.23
1	K	151	ALA	C-O	8.26	1.33	1.24
2	D	495	ILE	C-O	-8.26	1.14	1.23
2	J	520	ALA	C-O	8.24	1.33	1.23
2	J	437	TYR	C-O	8.24	1.34	1.23
1	C	130	LEU	CA-C	8.24	1.62	1.52
2	F	520	ALA	CA-CB	-8.22	1.37	1.53
2	D	350	ASN	CA-C	8.21	1.62	1.52
2	H	401	GLN	CA-C	8.21	1.62	1.52
2	L	407	ARG	CA-C	8.21	1.63	1.52
2	B	442	ILE	N-CA	-8.21	1.36	1.46
2	F	378	ILE	CA-CB	8.20	1.66	1.54
1	K	51	LEU	N-CA	8.20	1.55	1.46
1	A	13	ALA	CA-CB	-8.19	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	448	PRO	CA-C	-8.18	1.42	1.52
1	I	97	THR	C-O	8.18	1.33	1.24
2	J	368	ASN	N-CA	8.18	1.56	1.46
1	I	62	LEU	C-O	8.17	1.33	1.23
2	D	319	ALA	CA-C	8.17	1.63	1.52
1	C	101	ALA	C-N	8.16	1.43	1.33
2	F	503	GLN	CD-OE1	8.14	1.39	1.23
1	E	47	GLU	CD-OE1	8.14	1.40	1.25
2	H	475	ILE	C-O	8.14	1.33	1.24
2	D	513	ALA	N-CA	-8.13	1.35	1.45
1	I	41	LYS	CA-C	8.12	1.63	1.53
2	J	311	ARG	N-CA	-8.12	1.36	1.46
2	F	319	ALA	C-O	-8.12	1.14	1.24
2	F	375	GLY	C-O	-8.12	1.12	1.23
2	L	495	ILE	CA-CB	8.10	1.62	1.53
2	F	486	ILE	C-O	-8.10	1.17	1.24
2	J	506	ALA	CA-CB	-8.10	1.41	1.53
1	C	61	HIS	C-O	-8.09	1.13	1.23
2	J	471	ALA	CA-C	8.09	1.63	1.52
2	B	398	GLU	C-O	8.08	1.34	1.24
2	D	500	ALA	CA-C	-8.08	1.41	1.52
2	L	396	LEU	CA-C	8.04	1.63	1.52
2	L	431	THR	CA-C	8.04	1.63	1.52
2	H	396	LEU	CG-CD1	8.03	1.79	1.52
1	E	197	PHE	CA-C	8.02	1.62	1.52
2	F	394	ASN	C-O	-8.02	1.13	1.23
2	B	329	ALA	CA-CB	-8.01	1.39	1.53
1	I	126	ILE	CA-C	8.01	1.62	1.52
2	L	505	ILE	C-O	-8.00	1.15	1.24
1	G	5	LEU	CA-C	7.99	1.61	1.53
1	G	154	LYS	CD-CE	7.99	1.76	1.52
1	K	114	VAL	CA-CB	7.99	1.66	1.54
2	J	396	LEU	C-O	7.99	1.33	1.24
1	G	25	ALA	CA-CB	7.97	1.65	1.53
1	A	101	ALA	C-N	7.96	1.44	1.33
1	G	128	ILE	C-O	7.96	1.32	1.24
2	F	525	ILE	C-O	-7.96	1.16	1.24
1	A	113	VAL	CA-CB	7.95	1.64	1.54
1	C	157	VAL	CA-C	-7.95	1.42	1.52
1	I	17	VAL	CA-CB	-7.95	1.43	1.54
1	K	146	ASP	C-O	7.94	1.34	1.24
2	B	465	ILE	CA-CB	7.94	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	15	PRO	C-O	-7.94	1.14	1.24
1	A	163	GLN	CG-CD	7.93	1.71	1.52
1	E	138	HIS	N-CA	-7.92	1.36	1.46
1	G	141	THR	CA-C	-7.92	1.42	1.52
2	J	368	ASN	CA-CB	7.91	1.66	1.53
1	I	107	HIS	C-O	7.91	1.33	1.24
1	E	11	GLN	CD-NE2	-7.90	1.16	1.33
1	E	116	ASN	C-O	7.88	1.32	1.23
2	L	351	PHE	CD2-CE2	7.88	1.62	1.38
2	B	515	PRO	C-O	-7.88	1.14	1.23
2	F	490	PRO	C-O	-7.88	1.14	1.24
2	F	311	ARG	CA-CB	-7.86	1.41	1.53
2	D	369	ASN	C-O	7.86	1.32	1.24
2	F	522	ARG	C-O	7.86	1.33	1.24
2	H	402	ALA	CA-CB	7.86	1.64	1.53
1	G	133	ARG	CA-C	7.85	1.62	1.52
2	D	321	THR	CA-CB	7.83	1.62	1.53
1	A	190	GLN	C-O	-7.80	1.13	1.23
1	K	136	ASN	C-O	-7.79	1.14	1.24
2	J	308	PHE	C-O	7.77	1.33	1.24
1	E	35	ILE	C-O	-7.76	1.15	1.24
2	H	502	GLN	CD-OE1	7.76	1.38	1.23
2	D	331	SER	CA-C	-7.76	1.45	1.52
2	H	380	VAL	CA-CB	7.76	1.64	1.54
2	L	517	ASP	CA-C	7.76	1.63	1.52
1	K	8	THR	CA-CB	-7.76	1.42	1.53
1	C	183	TYR	C-O	-7.75	1.14	1.23
2	D	451	ASN	CA-C	7.74	1.56	1.52
1	A	149	ALA	N-CA	-7.73	1.36	1.46
2	H	303	GLN	CA-C	7.72	1.61	1.52
1	E	163	GLN	CD-OE1	7.72	1.38	1.23
1	E	188	ARG	NE-CZ	7.72	1.41	1.33
2	L	477	GLN	C-O	7.71	1.33	1.23
2	L	395	THR	C-O	7.71	1.33	1.23
1	A	98	THR	N-CA	7.70	1.55	1.45
1	G	117	ALA	C-O	-7.70	1.14	1.24
2	B	446	PRO	CA-C	-7.70	1.44	1.52
1	I	3	GLU	CA-C	7.70	1.61	1.52
1	C	117	ALA	CA-CB	-7.70	1.40	1.53
2	F	514	ASN	N-CA	-7.69	1.36	1.46
1	K	138	HIS	N-CA	-7.68	1.36	1.46
2	F	399	MET	N-CA	-7.67	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	ALA	CA-CB	7.67	1.66	1.52
2	B	403	ASN	C-O	7.67	1.32	1.23
1	K	184	ARG	C-O	-7.66	1.15	1.24
1	G	128	ILE	CA-C	7.66	1.61	1.52
2	H	500	ALA	C-O	-7.66	1.14	1.24
1	G	171	ILE	CG1-CD1	-7.66	1.21	1.51
2	F	429	CYS	N-CA	7.66	1.55	1.46
2	B	423	PHE	C-O	-7.65	1.15	1.24
2	J	321	THR	CA-CB	7.65	1.63	1.53
2	L	516	MET	CG-SD	7.64	1.99	1.80
2	J	447	TYR	CA-C	-7.63	1.45	1.52
2	F	305	ASN	CA-C	7.61	1.62	1.52
1	G	98	THR	N-CA	7.60	1.55	1.45
1	A	57	ASP	CA-CB	7.59	1.64	1.53
1	G	76	ASN	CG-OD1	7.59	1.38	1.23
2	D	465	ILE	C-O	7.58	1.31	1.24
1	I	104	TRP	C-O	7.58	1.33	1.23
2	B	383	ARG	C-O	7.57	1.33	1.23
1	A	155	CYS	C-O	-7.57	1.14	1.24
2	H	384	VAL	CA-C	7.56	1.62	1.52
2	D	318	LYS	C-O	7.56	1.34	1.23
1	E	192	GLU	CG-CD	7.56	1.71	1.52
2	J	522	ARG	C-O	7.56	1.33	1.24
2	L	351	PHE	C-O	7.53	1.33	1.24
2	L	383	ARG	CZ-NH1	7.52	1.43	1.32
2	D	465	ILE	CG1-CD1	-7.52	1.22	1.51
2	J	514	ASN	C-O	-7.52	1.14	1.24
2	J	516	MET	N-CA	7.51	1.56	1.46
2	H	465	ILE	CA-CB	7.51	1.64	1.54
2	L	319	ALA	CA-CB	-7.51	1.41	1.53
1	A	71	TRP	N-CA	-7.50	1.36	1.46
2	D	436	TYR	N-CA	7.50	1.54	1.45
1	C	192	GLU	CD-OE2	7.49	1.39	1.25
1	G	63	VAL	CA-CB	7.48	1.61	1.53
1	A	154	LYS	CD-CE	7.48	1.74	1.52
2	L	314	ASN	CB-CG	7.48	1.70	1.52
1	C	75	ALA	C-O	-7.48	1.14	1.24
1	K	47	GLU	CA-C	7.47	1.62	1.52
2	F	465	ILE	C-O	-7.47	1.16	1.24
2	F	333	ARG	CZ-NH2	7.46	1.43	1.33
2	H	311	ARG	CA-CB	-7.46	1.41	1.53
1	C	114	VAL	C-O	7.45	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	123	ALA	C-O	-7.45	1.14	1.23
2	F	499	GLU	CD-OE1	7.45	1.39	1.25
1	C	64	ARG	CZ-NH1	7.45	1.43	1.32
1	C	110	LYS	CA-C	7.45	1.61	1.52
1	A	112	GLY	C-O	-7.44	1.17	1.23
2	B	311	ARG	C-O	7.44	1.33	1.23
1	A	116	ASN	C-O	7.43	1.33	1.24
2	H	402	ALA	C-O	7.43	1.33	1.23
1	A	159	ASN	C-O	-7.43	1.14	1.24
1	I	180	LYS	CA-C	7.43	1.62	1.52
2	B	476	THR	CA-CB	7.43	1.63	1.53
2	B	359	HIS	C-O	-7.42	1.14	1.24
1	C	7	GLU	C-O	7.41	1.33	1.23
2	D	344	SER	C-O	-7.40	1.15	1.24
2	B	536	GLU	CA-C	7.40	1.62	1.52
1	G	92	PHE	CA-C	-7.39	1.43	1.52
2	H	481	GLU	C-O	7.39	1.32	1.23
2	H	310	ILE	N-CA	-7.38	1.36	1.46
1	K	126	ILE	CA-C	7.38	1.61	1.52
1	C	100	ASP	C-O	7.37	1.32	1.24
2	H	488	MET	SD-CE	-7.37	1.61	1.79
2	J	476	THR	N-CA	-7.37	1.36	1.46
1	C	187	ILE	CA-CB	7.36	1.63	1.54
2	B	309	VAL	N-CA	7.36	1.54	1.46
1	I	89	PHE	C-O	7.35	1.32	1.23
1	I	7	GLU	CD-OE2	7.35	1.39	1.25
1	I	70	VAL	CA-C	-7.35	1.43	1.52
2	B	336	LEU	C-O	7.35	1.32	1.23
2	L	488	MET	SD-CE	-7.34	1.61	1.79
2	D	537	ASN	N-CA	7.33	1.57	1.46
2	D	532	LYS	CA-CB	7.33	1.65	1.53
1	K	146	ASP	N-CA	7.32	1.55	1.46
2	J	527	LEU	N-CA	7.31	1.54	1.45
1	G	9	PRO	CG-CD	7.30	1.75	1.50
2	J	501	VAL	C-O	-7.29	1.15	1.24
1	G	101	ALA	CA-CB	7.28	1.62	1.52
1	A	186	ASP	C-O	-7.26	1.15	1.23
2	J	390	LYS	CG-CD	7.26	1.74	1.52
2	H	493	LYS	C-O	-7.26	1.14	1.24
2	B	532	LYS	N-CA	7.25	1.55	1.45
1	C	154	LYS	CA-C	7.25	1.62	1.52
2	D	473	LYS	C-O	7.25	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4	LEU	C-O	-7.24	1.14	1.23
2	H	340	PRO	CA-C	7.23	1.61	1.52
1	G	110	LYS	C-O	-7.23	1.15	1.24
2	L	403	ASN	C-O	7.22	1.32	1.23
2	D	437	TYR	CA-C	-7.21	1.43	1.52
1	A	22	ALA	CA-CB	-7.20	1.47	1.53
2	F	525	ILE	CA-C	-7.20	1.44	1.52
1	I	15	PRO	C-O	-7.19	1.15	1.24
1	C	100	ASP	N-CA	7.19	1.54	1.46
1	I	127	ASN	C-O	7.19	1.32	1.24
2	D	492	VAL	C-O	-7.19	1.16	1.24
2	F	417	ALA	C-O	7.19	1.33	1.24
2	L	478	LEU	CA-C	7.19	1.61	1.52
2	D	426	VAL	CB-CG2	-7.18	1.28	1.52
1	G	132	ALA	CA-CB	-7.18	1.39	1.53
1	I	79	TYR	CA-C	-7.18	1.44	1.52
2	J	511	ASN	C-O	-7.18	1.15	1.24
2	L	414	ARG	NE-CZ	7.17	1.41	1.33
1	E	182	ALA	CA-CB	-7.17	1.37	1.53
2	J	447	TYR	CE1-CZ	7.17	1.55	1.38
1	K	64	ARG	CZ-NH1	7.17	1.42	1.32
2	B	481	GLU	C-O	-7.15	1.15	1.23
2	D	368	ASN	N-CA	7.15	1.55	1.46
2	H	407	ARG	CA-CB	7.15	1.63	1.53
2	F	339	ILE	CA-C	7.15	1.59	1.52
1	K	168	GLU	CD-OE1	7.15	1.39	1.25
1	G	108	THR	CA-C	7.13	1.61	1.53
1	C	50	LEU	C-O	7.13	1.32	1.24
2	B	489	CYS	CB-SG	7.13	2.04	1.81
2	F	376	GLU	N-CA	-7.13	1.37	1.46
1	C	196	VAL	N-CA	-7.13	1.37	1.46
2	F	515	PRO	C-O	-7.13	1.13	1.23
1	C	94	ARG	N-CA	-7.12	1.36	1.45
1	E	150	GLN	CD-OE1	7.12	1.37	1.23
1	A	157	VAL	CB-CG2	-7.12	1.29	1.52
1	E	162	GLU	CA-C	-7.11	1.43	1.52
2	H	308	PHE	CA-C	-7.11	1.43	1.52
1	G	54	GLN	CD-OE1	7.11	1.37	1.23
1	K	42	PRO	N-CA	7.11	1.56	1.47
2	B	468	PRO	C-O	-7.11	1.14	1.24
1	K	100	ASP	N-CA	7.10	1.55	1.46
2	F	303	GLN	CA-C	7.10	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	455	ASP	N-CA	-7.10	1.36	1.46
2	L	528	ARG	CA-C	-7.10	1.43	1.52
2	D	514	ASN	C-O	-7.10	1.15	1.24
2	H	444	PRO	CA-C	-7.09	1.43	1.52
2	J	368	ASN	CB-CG	7.08	1.69	1.52
1	C	154	LYS	CE-NZ	7.08	1.70	1.49
1	C	142	ARG	N-CA	7.07	1.54	1.46
2	J	493	LYS	CE-NZ	7.07	1.70	1.49
1	I	100	ASP	CA-C	7.07	1.61	1.52
1	G	131	PHE	C-O	-7.06	1.15	1.24
1	G	126	ILE	CA-CB	7.05	1.63	1.54
2	B	380	VAL	CA-C	7.05	1.61	1.52
1	G	72	GLN	N-CA	7.05	1.54	1.45
1	C	5	LEU	CA-C	7.05	1.60	1.53
2	D	514	ASN	N-CA	-7.05	1.37	1.46
2	L	329	ALA	CA-CB	-7.05	1.41	1.53
2	J	477	GLN	CD-OE1	7.05	1.36	1.23
2	F	400	TRP	CA-C	7.04	1.61	1.52
1	A	178	ASP	CA-CB	7.03	1.63	1.53
1	C	92	PHE	N-CA	-7.03	1.37	1.45
2	H	486	ILE	C-O	-7.03	1.18	1.24
1	A	47	GLU	CD-OE2	7.02	1.38	1.25
2	L	328	ILE	CG1-CD1	-7.02	1.24	1.51
2	H	526	VAL	CA-CB	6.99	1.62	1.54
1	E	38	ARG	NE-CZ	6.99	1.40	1.33
1	E	157	VAL	CB-CG1	6.99	1.75	1.52
2	L	496	ALA	CA-CB	6.99	1.64	1.53
2	L	370	GLY	C-O	6.99	1.33	1.23
1	E	80	GLN	CD-OE1	6.98	1.36	1.23
1	A	2	ILE	CA-CB	6.98	1.62	1.53
1	E	31	ARG	CA-C	6.98	1.63	1.53
1	E	115	ASN	CA-C	6.98	1.62	1.53
1	E	189	ILE	CA-C	-6.98	1.43	1.52
2	B	530	GLN	CA-C	-6.97	1.44	1.52
2	F	450	ARG	CG-CD	6.97	1.73	1.52
2	B	407	ARG	CA-C	6.97	1.61	1.52
1	G	114	VAL	CA-CB	6.96	1.66	1.54
2	B	369	ASN	C-O	6.96	1.32	1.24
2	F	489	CYS	C-O	-6.96	1.15	1.24
2	L	402	ALA	C-O	-6.96	1.14	1.23
1	I	146	ASP	CG-OD2	6.96	1.38	1.25
1	I	97	THR	CA-C	6.95	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	133	ARG	NE-CZ	6.95	1.40	1.33
1	E	66	SER	CB-OG	-6.95	1.28	1.42
1	I	51	LEU	CA-C	-6.94	1.44	1.52
2	B	324	TYR	CA-C	6.94	1.61	1.53
1	K	7	GLU	CA-C	6.93	1.61	1.52
2	J	431	THR	CA-CB	6.93	1.64	1.53
2	J	457	ARG	CZ-NH2	6.93	1.42	1.33
1	K	90	ASN	CA-C	6.93	1.60	1.52
2	L	310	ILE	C-O	6.93	1.30	1.24
1	C	161	ILE	CA-CB	-6.92	1.46	1.54
1	E	111	PRO	C-O	-6.92	1.16	1.23
2	H	312	ASP	CA-CB	-6.92	1.44	1.52
1	K	43	ASP	C-O	6.92	1.33	1.23
2	B	405	GLY	C-O	6.92	1.29	1.24
2	L	451	ASN	N-CA	-6.92	1.37	1.46
1	G	197	PHE	CA-C	-6.90	1.44	1.52
2	H	399	MET	N-CA	6.88	1.54	1.45
2	D	500	ALA	CA-CB	-6.88	1.42	1.53
2	F	503	GLN	CA-C	-6.88	1.43	1.52
2	F	436	TYR	C-O	-6.88	1.15	1.23
2	L	383	ARG	CZ-NH2	6.88	1.42	1.33
2	H	507	LYS	CD-CE	6.87	1.73	1.52
2	L	496	ALA	C-O	-6.87	1.15	1.24
2	L	391	PRO	C-O	-6.87	1.15	1.23
2	H	389	GLY	C-O	-6.87	1.14	1.23
2	D	532	LYS	CA-C	6.86	1.61	1.52
1	C	154	LYS	CD-CE	6.86	1.73	1.52
2	B	453	PRO	C-O	6.85	1.32	1.24
1	G	173	LYS	C-O	-6.85	1.15	1.24
2	L	447	TYR	CE1-CZ	6.85	1.54	1.38
1	E	36	TRP	C-O	-6.84	1.16	1.23
2	D	503	GLN	CA-CB	-6.84	1.41	1.53
1	G	117	ALA	CA-C	-6.84	1.43	1.52
2	H	354	LEU	CA-C	6.84	1.61	1.52
1	K	131	PHE	N-CA	6.84	1.54	1.45
1	E	95	THR	CA-CB	6.83	1.64	1.53
1	A	101	ALA	C-O	6.83	1.31	1.23
2	H	327	SER	CA-C	6.83	1.62	1.52
2	H	330	ARG	CZ-NH2	6.82	1.42	1.33
1	I	187	ILE	CG1-CD1	-6.82	1.25	1.51
1	A	123	ALA	CA-CB	-6.81	1.42	1.53
1	G	101	ALA	CA-C	6.80	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	47	GLU	CD-OE2	6.80	1.38	1.25
2	F	537	ASN	N-CA	6.80	1.57	1.46
2	D	450	ARG	CZ-NH1	6.79	1.42	1.32
2	F	384	VAL	N-CA	-6.79	1.38	1.46
2	B	459	ALA	CA-CB	-6.79	1.42	1.53
2	B	489	CYS	C-O	-6.79	1.15	1.24
1	K	174	ARG	CZ-NH1	6.79	1.42	1.32
1	C	151	ALA	CA-CB	6.79	1.64	1.53
2	F	454	ASN	CA-C	6.79	1.63	1.53
2	H	513	ALA	N-CA	-6.79	1.37	1.46
2	H	312	ASP	C-O	6.79	1.32	1.23
2	H	436	TYR	CA-C	-6.79	1.43	1.52
2	L	472	THR	CB-CG2	-6.78	1.30	1.52
1	G	165	GLN	CG-CD	6.78	1.69	1.52
1	E	178	ASP	C-O	6.78	1.31	1.23
2	B	523	PHE	C-O	6.78	1.32	1.23
1	K	121	PRO	C-O	6.78	1.31	1.23
1	E	15	PRO	C-O	-6.77	1.15	1.24
2	H	515	PRO	CA-C	6.77	1.60	1.52
1	I	117	ALA	CA-C	-6.77	1.43	1.52
1	I	181	THR	CA-C	-6.77	1.44	1.52
1	E	26	ALA	CA-CB	6.77	1.65	1.53
1	G	142	ARG	N-CA	6.77	1.54	1.45
1	G	188	ARG	NE-CZ	6.77	1.40	1.33
1	C	11	GLN	C-O	6.76	1.32	1.23
2	L	502	GLN	CA-C	-6.76	1.43	1.52
1	E	47	GLU	C-O	-6.75	1.15	1.23
1	E	174	ARG	N-CA	6.75	1.54	1.46
1	G	67	PHE	CA-C	6.75	1.60	1.52
1	K	46	GLY	CA-C	-6.75	1.45	1.52
2	J	372	LEU	CA-CB	-6.74	1.43	1.53
2	J	506	ALA	C-O	6.74	1.32	1.23
2	H	381	ALA	CA-CB	-6.73	1.41	1.54
1	C	133	ARG	CB-CG	-6.73	1.32	1.52
1	I	71	TRP	C-O	6.73	1.31	1.23
2	H	505	ILE	CG1-CD1	-6.73	1.25	1.51
1	K	74	ASP	C-O	6.72	1.31	1.23
2	F	374	ILE	CA-C	6.72	1.61	1.52
2	F	416	LEU	CA-CB	6.72	1.65	1.53
1	E	121	PRO	CA-C	6.71	1.61	1.52
2	D	379	ILE	CA-C	6.71	1.60	1.52
1	I	53	GLY	C-O	6.71	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	40	ALA	C-O	6.70	1.32	1.24
1	K	15	PRO	C-O	-6.70	1.15	1.24
1	K	128	ILE	CA-C	6.70	1.60	1.52
2	F	493	LYS	CG-CD	6.70	1.72	1.52
1	C	14	GLY	CA-C	6.69	1.61	1.51
1	E	188	ARG	CD-NE	6.68	1.55	1.46
2	L	337	VAL	CB-CG1	6.68	1.74	1.52
2	L	417	ALA	N-CA	6.68	1.54	1.45
1	A	100	ASP	N-CA	6.68	1.54	1.46
2	L	379	ILE	CA-C	6.68	1.60	1.52
1	K	181	THR	C-O	6.68	1.31	1.23
2	L	385	VAL	CA-C	6.68	1.62	1.53
1	G	155	CYS	C-O	-6.67	1.15	1.24
2	D	404	ALA	CA-CB	6.67	1.64	1.53
2	D	525	ILE	CA-CB	6.67	1.62	1.54
1	I	68	LEU	C-O	6.66	1.32	1.23
1	E	144	TYR	CA-C	6.66	1.60	1.52
1	K	133	ARG	CZ-NH2	6.66	1.42	1.33
1	E	185	PHE	N-CA	-6.65	1.38	1.47
2	J	450	ARG	CZ-NH1	6.65	1.42	1.32
2	H	304	ASP	CA-C	6.65	1.61	1.53
1	E	133	ARG	CA-C	6.64	1.60	1.52
2	J	525	ILE	CA-C	6.64	1.60	1.52
2	L	457	ARG	CZ-NH1	6.64	1.42	1.32
2	B	453	PRO	CG-CD	6.63	1.73	1.50
2	H	533	THR	CA-C	6.63	1.61	1.52
1	I	82	ALA	CA-CB	6.63	1.64	1.53
1	E	184	ARG	N-CA	-6.62	1.38	1.45
2	B	383	ARG	CZ-NH2	6.62	1.42	1.33
2	H	532	LYS	CA-CB	6.62	1.64	1.53
1	A	119	GLY	C-O	6.62	1.32	1.24
2	J	386	ASP	CA-C	6.62	1.62	1.53
2	J	423	PHE	N-CA	6.62	1.54	1.46
2	L	378	ILE	CA-CB	6.61	1.66	1.55
1	I	67	PHE	CD1-CE1	6.60	1.58	1.38
1	C	150	GLN	CD-OE1	6.60	1.36	1.23
2	B	359	HIS	CA-CB	6.60	1.62	1.53
2	H	358	ALA	CA-C	-6.59	1.43	1.52
2	J	531	ARG	CZ-NH1	6.59	1.42	1.32
2	J	486	ILE	C-N	6.59	1.40	1.33
2	D	414	ARG	CZ-NH1	6.59	1.42	1.32
2	D	389	GLY	C-O	-6.58	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	510	MET	SD-CE	-6.58	1.63	1.79
1	G	82	ALA	C-O	-6.58	1.15	1.23
2	H	417	ALA	CA-C	6.57	1.60	1.53
1	E	86	GLU	C-O	6.56	1.32	1.24
2	L	418	PRO	C-O	-6.56	1.15	1.23
2	H	460	HIS	CA-CB	-6.56	1.42	1.53
2	H	465	ILE	CG1-CD1	-6.56	1.26	1.51
1	A	51	LEU	N-CA	6.55	1.54	1.46
1	K	41	LYS	CA-C	6.55	1.61	1.53
1	A	40	ALA	CA-CB	-6.55	1.43	1.53
2	H	382	GLY	C-O	-6.55	1.15	1.23
1	K	5	LEU	C-O	6.54	1.32	1.24
2	D	434	ASP	CA-C	-6.54	1.44	1.52
1	I	21	LEU	C-O	6.54	1.32	1.24
2	F	407	ARG	CA-C	6.54	1.61	1.52
2	J	333	ARG	CZ-NH1	6.54	1.42	1.32
1	A	136	ASN	CA-C	-6.54	1.44	1.52
1	E	93	GLY	C-O	6.54	1.30	1.23
2	F	457	ARG	CZ-NH1	6.54	1.41	1.32
1	E	67	PHE	CD1-CE1	6.53	1.58	1.38
1	G	108	THR	C-O	-6.53	1.19	1.24
2	H	505	ILE	CA-C	6.52	1.60	1.52
1	I	154	LYS	CE-NZ	6.52	1.68	1.49
2	L	531	ARG	CZ-NH2	6.52	1.42	1.33
1	C	123	ALA	CA-CB	-6.51	1.43	1.53
1	A	124	PRO	C-O	6.51	1.31	1.23
2	D	308	PHE	CA-C	6.51	1.60	1.52
1	G	118	ALA	C-O	-6.51	1.15	1.24
2	L	319	ALA	CA-C	6.50	1.61	1.52
2	B	397	VAL	CA-CB	6.50	1.62	1.54
1	I	116	ASN	CA-C	6.49	1.62	1.53
1	E	70	VAL	C-O	-6.49	1.17	1.24
2	J	339	ILE	N-CA	6.49	1.54	1.46
2	L	304	ASP	CA-C	6.48	1.60	1.53
1	C	188	ARG	CA-C	6.48	1.60	1.52
2	D	460	HIS	N-CA	6.48	1.53	1.46
2	L	537	ASN	N-CA	6.48	1.56	1.46
2	J	303	GLN	CA-CB	6.48	1.69	1.53
2	B	397	VAL	CB-CG2	-6.46	1.31	1.52
1	I	120	VAL	CA-C	-6.46	1.46	1.52
1	K	178	ASP	C-O	6.46	1.32	1.23
2	L	462	HIS	CA-CB	-6.46	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	428	ARG	C-O	-6.46	1.16	1.23
2	H	436	TYR	C-O	-6.46	1.16	1.23
2	J	528	ARG	C-O	-6.46	1.15	1.23
1	A	126	ILE	CA-C	6.45	1.60	1.52
1	A	128	ILE	C-N	6.45	1.42	1.33
1	K	84	ASN	N-CA	6.45	1.53	1.46
2	B	377	ARG	CZ-NH1	6.45	1.41	1.32
2	D	374	ILE	CA-C	6.45	1.60	1.52
2	B	399	MET	C-O	-6.44	1.16	1.23
2	D	337	VAL	CA-CB	-6.44	1.46	1.54
2	D	340	PRO	N-CA	6.44	1.54	1.47
1	C	162	GLU	C-O	-6.44	1.16	1.24
1	E	101	ALA	CA-CB	6.44	1.63	1.52
1	C	115	ASN	C-O	-6.43	1.15	1.23
1	I	68	LEU	CG-CD2	-6.43	1.31	1.52
1	E	50	LEU	CA-C	6.43	1.60	1.52
2	F	381	ALA	CA-CB	-6.43	1.41	1.54
2	J	517	ASP	C-O	6.42	1.32	1.24
1	E	41	LYS	C-O	6.42	1.31	1.23
2	J	367	PHE	N-CA	-6.42	1.37	1.46
2	H	368	ASN	N-CA	6.42	1.54	1.46
2	D	339	ILE	CA-CB	6.41	1.65	1.54
2	B	462	HIS	CA-CB	-6.41	1.43	1.53
1	E	150	GLN	CA-C	-6.41	1.44	1.52
1	K	116	ASN	N-CA	-6.40	1.38	1.46
2	D	379	ILE	CG1-CD1	-6.40	1.26	1.51
1	G	35	ILE	CG1-CD1	-6.40	1.26	1.51
1	C	173	LYS	CA-C	-6.40	1.45	1.52
1	C	188	ARG	CZ-NH1	6.39	1.41	1.32
2	F	450	ARG	CZ-NH2	6.39	1.41	1.33
2	J	460	HIS	C-O	6.39	1.31	1.23
2	D	330	ARG	CZ-NH2	6.39	1.41	1.33
2	B	500	ALA	CA-CB	-6.38	1.43	1.53
2	F	461	ILE	CA-C	-6.38	1.44	1.52
1	K	78	GLU	C-O	6.37	1.31	1.23
2	J	357	GLY	CA-C	6.37	1.57	1.52
2	B	409	ARG	N-CA	6.36	1.54	1.46
2	D	493	LYS	CE-NZ	6.36	1.68	1.49
2	D	332	PRO	C-O	6.36	1.31	1.23
2	L	305	ASN	CA-C	6.36	1.61	1.52
1	C	100	ASP	CA-CB	6.36	1.63	1.53
1	A	96	ALA	C-O	-6.36	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	398	GLU	C-O	6.36	1.32	1.24
2	F	423	PHE	C-O	6.36	1.31	1.23
2	B	440	ARG	CZ-NH1	6.35	1.41	1.32
1	C	166	ARG	CD-NE	-6.35	1.37	1.46
2	H	454	ASN	C-O	-6.35	1.17	1.23
2	B	368	ASN	CB-CG	6.35	1.68	1.52
2	H	478	LEU	CA-CB	-6.35	1.44	1.53
1	G	129	SER	N-CA	-6.34	1.38	1.46
1	C	168	GLU	CD-OE1	6.34	1.37	1.25
2	L	388	TYR	CD2-CE2	6.34	1.57	1.38
1	E	9	PRO	CG-CD	6.34	1.72	1.50
2	L	471	ALA	N-CA	6.34	1.54	1.46
1	E	72	GLN	CD-OE1	6.34	1.35	1.23
2	B	498	PRO	C-O	6.34	1.32	1.24
1	G	109	VAL	CA-C	6.34	1.60	1.52
2	J	386	ASP	N-CA	-6.34	1.38	1.45
1	K	112	GLY	C-O	-6.33	1.15	1.23
2	F	368	ASN	CA-CB	6.33	1.64	1.53
1	A	108	THR	CA-CB	6.33	1.64	1.53
2	F	457	ARG	CA-C	6.33	1.60	1.52
2	F	434	ASP	C-O	-6.33	1.15	1.24
1	G	16	TYR	CE2-CZ	6.33	1.53	1.38
2	F	492	VAL	CA-C	6.32	1.61	1.52
2	B	384	VAL	C-O	6.32	1.31	1.24
2	D	407	ARG	CA-C	6.32	1.61	1.52
2	J	378	ILE	CA-CB	6.31	1.64	1.55
2	B	388	TYR	CA-C	6.31	1.61	1.52
1	K	78	GLU	CD-OE1	6.31	1.37	1.25
2	F	450	ARG	NE-CZ	6.31	1.40	1.33
2	J	378	ILE	CG1-CD1	6.30	1.76	1.51
2	D	383	ARG	CB-CG	-6.30	1.33	1.52
1	K	117	ALA	CA-C	-6.30	1.44	1.52
2	L	346	THR	CA-C	-6.30	1.43	1.52
1	A	99	PHE	CB-CG	6.29	1.65	1.50
1	E	70	VAL	CA-CB	-6.29	1.45	1.55
2	J	372	LEU	CA-C	-6.29	1.44	1.52
2	H	311	ARG	C-O	-6.28	1.15	1.23
1	K	59	ASN	C-O	6.28	1.32	1.24
1	E	82	ALA	CA-CB	6.27	1.60	1.52
1	K	150	GLN	CD-OE1	6.27	1.35	1.23
1	G	129	SER	C-O	6.27	1.31	1.24
2	L	450	ARG	CZ-NH2	6.27	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	318	LYS	CA-C	6.27	1.61	1.53
2	H	396	LEU	C-O	6.27	1.31	1.24
2	D	333	ARG	CZ-NH2	6.26	1.41	1.33
1	K	106	LEU	CA-C	6.26	1.60	1.52
2	B	537	ASN	CG-OD1	6.26	1.35	1.23
2	J	377	ARG	CZ-NH2	6.26	1.41	1.33
1	K	200	PHE	CE2-CZ	6.26	1.57	1.38
2	L	442	ILE	CA-C	6.26	1.59	1.52
2	B	301	PRO	C-O	6.26	1.36	1.23
2	B	304	ASP	CA-C	6.26	1.60	1.53
1	I	38	ARG	CZ-NH1	6.26	1.41	1.32
2	F	432	ASP	C-O	-6.25	1.16	1.24
1	K	16	TYR	CA-CB	6.25	1.61	1.53
2	J	374	ILE	C-O	6.25	1.32	1.24
2	L	506	ALA	CA-C	-6.25	1.45	1.52
2	F	450	ARG	CZ-NH1	6.24	1.41	1.32
1	K	171	ILE	C-O	-6.24	1.17	1.24
2	L	472	THR	CA-CB	6.24	1.64	1.53
2	H	511	ASN	C-O	-6.24	1.15	1.24
2	B	394	ASN	CA-CB	6.24	1.63	1.53
2	H	514	ASN	CG-OD1	6.24	1.35	1.23
2	J	335	ALA	CA-CB	6.24	1.63	1.53
1	K	88	ALA	C-O	6.24	1.31	1.24
1	A	72	GLN	C-O	6.23	1.31	1.23
2	H	336	LEU	CA-CB	6.23	1.62	1.53
1	E	44	ALA	C-O	6.23	1.31	1.23
2	J	488	MET	C-O	6.23	1.32	1.23
1	I	101	ALA	CA-CB	6.22	1.62	1.53
2	L	390	LYS	CG-CD	6.22	1.71	1.52
2	F	341	GLN	CA-C	-6.22	1.45	1.52
1	G	80	GLN	CG-CD	6.22	1.67	1.52
2	B	315	TRP	CZ2-CH2	6.22	1.49	1.37
2	B	447	TYR	C-O	-6.21	1.16	1.24
2	J	303	GLN	CA-C	6.21	1.60	1.52
2	D	325	LYS	CE-NZ	-6.21	1.30	1.49
2	F	314	ASN	CG-OD1	6.21	1.35	1.23
1	C	185	PHE	N-CA	-6.21	1.38	1.46
1	C	122	MET	C-O	-6.21	1.16	1.23
2	F	522	ARG	N-CA	-6.20	1.38	1.46
2	J	311	ARG	CZ-NH1	-6.20	1.24	1.32
1	K	32	ASP	CA-C	-6.20	1.45	1.52
1	A	192	GLU	CB-CG	6.20	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	439	PHE	CA-C	-6.20	1.45	1.52
2	H	377	ARG	CB-CG	6.20	1.71	1.52
1	E	40	ALA	CA-C	-6.19	1.45	1.52
1	K	127	ASN	CA-C	6.19	1.60	1.52
2	D	482	GLY	C-O	-6.19	1.15	1.24
2	F	319	ALA	CA-CB	6.19	1.63	1.53
2	J	448	PRO	CB-CG	6.18	1.80	1.49
2	D	500	ALA	N-CA	6.18	1.54	1.46
2	F	522	ARG	CG-CD	-6.18	1.33	1.52
2	F	520	ALA	C-O	6.17	1.31	1.23
1	G	64	ARG	CZ-NH1	6.17	1.41	1.32
2	J	354	LEU	C-O	6.17	1.31	1.23
2	D	379	ILE	CA-CB	6.16	1.62	1.54
1	E	162	GLU	C-O	-6.16	1.17	1.24
2	L	475	ILE	C-O	6.16	1.30	1.24
1	A	94	ARG	CD-NE	-6.16	1.37	1.46
1	I	122	MET	SD-CE	-6.16	1.64	1.79
2	J	439	PHE	N-CA	-6.16	1.38	1.45
2	H	328	ILE	CA-CB	-6.16	1.46	1.54
2	F	381	ALA	N-CA	6.15	1.53	1.45
1	G	189	ILE	CA-C	-6.15	1.44	1.52
2	F	471	ALA	N-CA	6.15	1.54	1.46
2	F	383	ARG	CB-CG	-6.14	1.34	1.52
2	F	437	TYR	C-O	6.14	1.31	1.23
1	E	161	ILE	C-O	6.14	1.30	1.24
2	J	312	ASP	C-O	6.14	1.31	1.23
1	G	165	GLN	CD-NE2	6.14	1.46	1.33
1	I	192	GLU	CG-CD	6.14	1.67	1.52
2	H	323	ASP	CA-C	6.13	1.61	1.52
2	F	334	GLN	CA-C	6.13	1.61	1.53
2	J	414	ARG	CZ-NH1	6.13	1.41	1.32
1	K	73	ALA	N-CA	6.13	1.53	1.45
2	B	523	PHE	CA-C	6.13	1.59	1.53
1	G	176	GLU	CG-CD	6.13	1.67	1.52
1	I	16	TYR	C-O	6.13	1.32	1.24
1	G	130	LEU	CA-C	6.13	1.60	1.52
2	D	503	GLN	CD-OE1	6.12	1.35	1.23
2	D	396	LEU	CA-C	6.12	1.60	1.52
2	H	379	ILE	CG1-CD1	-6.12	1.27	1.51
1	E	95	THR	N-CA	-6.12	1.37	1.46
2	B	524	ASP	CA-CB	-6.12	1.44	1.53
2	J	401	GLN	CD-NE2	6.12	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	LEU	N-CA	6.11	1.53	1.45
1	G	106	LEU	C-O	6.11	1.31	1.23
2	J	367	PHE	CA-C	6.11	1.60	1.52
2	L	380	VAL	C-O	-6.11	1.17	1.24
1	K	188	ARG	CZ-NH1	6.11	1.41	1.32
1	G	120	VAL	C-O	-6.10	1.16	1.24
1	A	110	LYS	CA-C	6.10	1.59	1.52
1	G	188	ARG	CA-C	6.09	1.60	1.52
2	F	320	LEU	CA-C	6.09	1.60	1.52
2	F	419	LEU	C-O	6.09	1.31	1.23
1	K	105	THR	C-O	6.09	1.31	1.23
1	C	83	TYR	CZ-OH	-6.08	1.25	1.38
2	B	414	ARG	NE-CZ	6.08	1.39	1.33
1	G	87	ASN	CA-C	-6.08	1.45	1.52
1	A	194	GLU	C-O	-6.08	1.16	1.23
1	K	86	GLU	CD-OE2	6.08	1.36	1.25
1	E	122	MET	C-O	-6.08	1.16	1.23
1	E	197	PHE	N-CA	-6.08	1.38	1.45
2	H	502	GLN	CD-NE2	6.08	1.46	1.33
2	B	302	ALA	CA-C	6.08	1.60	1.52
1	E	38	ARG	CD-NE	6.08	1.54	1.46
1	K	151	ALA	CA-C	6.08	1.60	1.52
1	I	139	LEU	CA-C	6.08	1.60	1.52
2	B	422	ASN	C-O	6.07	1.32	1.24
1	I	46	GLY	C-O	6.07	1.29	1.23
1	E	82	ALA	C-O	-6.07	1.16	1.23
1	I	28	ASN	C-N	6.07	1.41	1.33
2	H	443	LYS	C-O	-6.07	1.16	1.24
2	L	527	LEU	C-O	-6.07	1.16	1.23
1	A	192	GLU	CG-CD	6.07	1.67	1.52
1	G	52	LEU	C-O	-6.06	1.16	1.23
2	J	512	ASN	CA-C	6.06	1.61	1.52
2	F	367	PHE	N-CA	-6.06	1.38	1.46
2	L	388	TYR	N-CA	6.06	1.54	1.46
1	A	117	ALA	CA-CB	-6.05	1.43	1.53
2	J	331	SER	N-CA	6.05	1.54	1.45
1	K	8	THR	CA-C	6.05	1.59	1.53
2	B	379	ILE	C-O	6.05	1.31	1.24
1	A	171	ILE	CG1-CD1	-6.04	1.28	1.51
2	D	521	TYR	N-CA	-6.04	1.38	1.46
1	E	66	SER	C-O	-6.04	1.16	1.23
1	E	103	GLU	N-CA	-6.04	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	197	PHE	CB-CG	-6.04	1.36	1.50
2	F	358	ALA	CA-CB	6.04	1.63	1.53
1	K	88	ALA	CA-C	6.04	1.60	1.52
1	K	77	GLY	CA-C	6.04	1.58	1.51
2	H	516	MET	CA-CB	6.04	1.63	1.53
1	A	168	GLU	CD-OE1	6.04	1.36	1.25
1	I	142	ARG	CZ-NH1	6.04	1.41	1.32
1	I	150	GLN	CG-CD	6.04	1.67	1.52
2	J	474	LEU	C-O	6.04	1.31	1.23
2	L	423	PHE	C-O	6.04	1.30	1.23
1	E	6	PRO	C-O	-6.03	1.17	1.23
2	F	450	ARG	CD-NE	6.03	1.54	1.46
1	I	94	ARG	CA-C	-6.02	1.45	1.52
2	L	507	LYS	CD-CE	6.02	1.70	1.52
2	D	506	ALA	CA-CB	-6.02	1.43	1.53
1	I	129	SER	N-CA	-6.02	1.38	1.46
2	B	385	VAL	CB-CG1	6.02	1.72	1.52
2	D	357	GLY	C-O	6.02	1.31	1.23
2	F	368	ASN	N-CA	6.01	1.53	1.46
2	B	483	ASP	CA-CB	6.01	1.63	1.53
2	L	328	ILE	C-O	-6.01	1.17	1.24
1	G	130	LEU	CG-CD2	6.01	1.72	1.52
2	L	466	SER	N-CA	6.01	1.53	1.46
1	G	151	ALA	CA-C	6.00	1.60	1.52
1	A	182	ALA	CA-C	-6.00	1.45	1.52
2	F	384	VAL	C-N	6.00	1.41	1.33
1	I	192	GLU	CD-OE2	6.00	1.36	1.25
1	C	180	LYS	CE-NZ	6.00	1.67	1.49
1	E	174	ARG	CZ-NH1	6.00	1.41	1.32
2	F	312	ASP	N-CA	-6.00	1.39	1.46
1	E	38	ARG	CA-C	-5.99	1.44	1.53
1	E	101	ALA	C-N	5.99	1.41	1.33
1	A	97	THR	CA-C	5.99	1.60	1.52
1	K	163	GLN	CD-NE2	5.99	1.45	1.33
2	B	473	LYS	CA-C	-5.99	1.45	1.52
2	H	498	PRO	CB-CG	5.99	1.79	1.49
1	K	162	GLU	CG-CD	5.99	1.67	1.52
2	H	471	ALA	CA-CB	-5.99	1.43	1.53
2	B	333	ARG	CZ-NH1	5.99	1.41	1.32
1	K	173	LYS	CA-CB	5.98	1.61	1.53
2	B	458	PRO	CA-C	-5.98	1.46	1.52
2	D	340	PRO	CA-C	5.97	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	100	ASP	CA-C	5.97	1.60	1.52
2	H	462	HIS	CA-CB	-5.97	1.44	1.53
2	J	309	VAL	CA-C	5.97	1.60	1.52
2	D	414	ARG	CD-NE	5.97	1.54	1.46
1	I	197	PHE	N-CA	5.97	1.53	1.45
1	I	11	GLN	C-O	5.96	1.31	1.23
2	F	457	ARG	C-O	5.96	1.32	1.24
2	J	454	ASN	CA-CB	5.96	1.59	1.53
2	L	408[A]	CYS	CA-C	5.96	1.60	1.52
2	L	408[B]	CYS	CA-C	5.96	1.60	1.52
2	L	521	TYR	C-O	5.96	1.31	1.23
1	C	129	SER	CA-C	-5.95	1.45	1.52
1	C	197	PHE	N-CA	-5.95	1.38	1.45
2	B	310	ILE	C-O	-5.95	1.18	1.24
1	C	57	ASP	CA-CB	5.95	1.62	1.53
2	D	475	ILE	C-O	5.95	1.30	1.24
2	J	304	ASP	CA-C	5.95	1.60	1.52
2	B	440	ARG	C-O	5.94	1.31	1.23
1	C	16	TYR	CZ-OH	5.94	1.50	1.38
1	E	49	ILE	C-O	-5.94	1.17	1.23
1	K	57	ASP	CA-C	5.94	1.61	1.53
1	E	171	ILE	C-O	5.94	1.30	1.24
2	B	356	PHE	CA-C	-5.93	1.45	1.52
1	I	123	ALA	CA-CB	-5.93	1.43	1.53
2	H	321	THR	CA-CB	5.93	1.60	1.53
2	B	434	ASP	CG-OD1	5.93	1.36	1.25
2	F	347	THR	CB-OG1	5.93	1.53	1.43
1	K	98	THR	CA-CB	5.93	1.62	1.53
2	D	515	PRO	CA-C	-5.93	1.44	1.52
1	C	128	ILE	C-O	-5.93	1.17	1.24
2	B	450	ARG	CZ-NH2	5.92	1.41	1.33
1	K	163	GLN	CD-OE1	5.92	1.34	1.23
2	B	339	ILE	CG1-CD1	5.92	1.74	1.51
2	H	428	ARG	CZ-NH2	5.92	1.41	1.33
2	D	537	ASN	CA-CB	5.92	1.62	1.53
2	J	480	PHE	CA-C	-5.91	1.45	1.52
2	B	527	LEU	C-O	5.91	1.31	1.23
1	C	155	CYS	C-O	-5.91	1.16	1.24
2	H	397	VAL	CA-C	5.91	1.59	1.52
2	H	505	ILE	C-O	-5.91	1.17	1.24
2	B	499	GLU	CD-OE2	5.90	1.36	1.25
2	B	398	GLU	CD-OE2	5.90	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	463	PHE	N-CA	5.90	1.53	1.46
2	H	345	GLU	N-CA	-5.90	1.38	1.46
2	H	365	LEU	CA-CB	-5.90	1.45	1.54
2	H	408[A]	CYS	N-CA	5.90	1.53	1.45
2	H	408[B]	CYS	N-CA	5.90	1.53	1.45
2	J	333	ARG	CG-CD	5.90	1.70	1.52
2	F	470	ILE	N-CA	-5.89	1.39	1.46
1	K	192	GLU	CB-CG	5.89	1.70	1.52
2	L	514	ASN	CA-C	-5.89	1.46	1.52
2	L	532	LYS	C-O	5.89	1.31	1.23
2	B	397	VAL	C-O	-5.89	1.17	1.24
1	C	63	VAL	CA-C	5.89	1.58	1.53
2	F	502	GLN	CA-C	-5.89	1.44	1.52
1	C	46	GLY	CA-C	-5.89	1.45	1.52
1	A	192	GLU	CD-OE2	5.88	1.36	1.25
2	F	449	TRP	CA-C	5.88	1.60	1.52
1	G	145	PHE	N-CA	5.88	1.53	1.46
1	A	137	ILE	CA-CB	-5.88	1.46	1.54
1	C	132	ALA	N-CA	5.88	1.53	1.46
1	G	192	GLU	CB-CG	5.88	1.70	1.52
2	H	427	GLY	CA-C	-5.88	1.46	1.52
2	J	502	GLN	CD-OE1	5.87	1.34	1.23
2	B	406	GLY	C-O	5.87	1.31	1.24
1	C	45	PRO	CA-C	5.87	1.60	1.52
2	D	386	ASP	N-CA	-5.87	1.38	1.45
1	G	68	LEU	C-O	5.87	1.30	1.24
2	D	343	ILE	N-CA	-5.87	1.38	1.46
2	B	305	ASN	N-CA	-5.86	1.38	1.46
2	D	502	GLN	CG-CD	5.86	1.66	1.52
2	J	343	ILE	CA-C	5.86	1.60	1.52
1	G	69	GLU	CB-CG	-5.86	1.34	1.52
1	A	103	GLU	C-O	-5.86	1.16	1.24
1	A	154	LYS	CG-CD	5.86	1.70	1.52
2	F	334	GLN	C-O	-5.86	1.16	1.23
2	H	475	ILE	CA-C	5.86	1.59	1.52
2	L	536	GLU	CA-C	5.86	1.60	1.52
1	G	89	PHE	C-O	5.85	1.30	1.23
1	G	91	SER	CA-C	5.85	1.60	1.52
1	I	34	GLU	CA-C	5.85	1.59	1.52
1	K	59	ASN	CG-OD1	5.85	1.34	1.23
2	L	376	GLU	CA-C	-5.85	1.45	1.52
2	B	503	GLN	CA-C	-5.85	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	72	GLN	CA-C	-5.85	1.45	1.52
2	L	538	CYS	CB-SG	-5.85	1.61	1.81
1	A	180	LYS	CA-C	5.85	1.60	1.52
2	B	451	ASN	CA-CB	-5.84	1.47	1.54
2	J	358	ALA	C-O	-5.84	1.16	1.24
1	A	184	ARG	CA-C	5.84	1.60	1.52
2	H	509	ASP	N-CA	5.84	1.54	1.46
2	L	524	ASP	CA-CB	-5.84	1.44	1.53
2	F	405	GLY	CA-C	-5.84	1.45	1.51
2	L	476	THR	CA-CB	5.84	1.63	1.53
2	B	379	ILE	CG1-CD1	-5.84	1.28	1.51
1	I	162	GLU	CD-OE1	5.84	1.36	1.25
1	K	149	ALA	C-O	5.83	1.30	1.24
1	K	182	ALA	C-O	5.83	1.31	1.23
1	I	47	GLU	CD-OE2	5.83	1.36	1.25
2	H	445	GLY	C-O	5.83	1.31	1.24
2	D	479	TYR	CE2-CZ	-5.82	1.24	1.38
1	K	79	TYR	CA-C	5.82	1.59	1.52
2	B	303	GLN	C-O	5.82	1.31	1.24
2	H	436	TYR	CD1-CE1	5.82	1.56	1.38
2	F	444	PRO	C-O	-5.82	1.17	1.23
1	K	101	ALA	C-O	5.82	1.30	1.23
2	B	435	GLY	C-O	5.81	1.31	1.24
1	K	190	GLN	C-O	-5.81	1.16	1.23
1	C	64	ARG	CD-NE	-5.81	1.38	1.46
2	H	471	ALA	CA-C	5.81	1.60	1.52
1	G	64	ARG	CA-C	-5.80	1.44	1.52
2	D	465	ILE	CB-CG1	5.80	1.65	1.53
2	D	471	ALA	C-O	-5.80	1.16	1.24
1	A	166	ARG	C-O	-5.80	1.16	1.24
1	E	98	THR	C-O	5.80	1.32	1.23
1	C	185	PHE	CE2-CZ	-5.80	1.21	1.38
2	H	327	SER	C-O	-5.80	1.16	1.24
1	C	149	ALA	C-O	-5.80	1.16	1.24
2	D	390	LYS	CG-CD	5.80	1.69	1.52
2	J	450	ARG	N-CA	-5.79	1.39	1.46
2	F	470	ILE	C-N	5.79	1.42	1.33
2	H	425	GLY	C-O	-5.79	1.16	1.24
1	G	116	ASN	CA-CB	-5.79	1.44	1.53
2	J	311	ARG	CA-CB	-5.79	1.43	1.53
2	J	450	ARG	CA-CB	-5.79	1.45	1.52
1	E	40	ALA	C-O	5.78	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	383	ARG	CA-C	5.78	1.59	1.52
1	C	141	THR	N-CA	-5.78	1.38	1.45
1	E	107	HIS	N-CA	-5.78	1.39	1.46
2	H	495	ILE	CA-CB	5.78	1.61	1.53
2	H	463	PHE	CD2-CE2	5.78	1.55	1.38
1	I	7	GLU	CD-OE1	5.78	1.36	1.25
2	L	443	LYS	CA-C	5.78	1.59	1.53
1	A	130	LEU	C-O	5.78	1.31	1.24
1	A	75	ALA	N-CA	5.77	1.53	1.46
2	D	522	ARG	CZ-NH2	5.77	1.41	1.33
1	K	189	ILE	CA-CB	-5.77	1.47	1.54
1	E	71	TRP	CZ2-CH2	5.77	1.48	1.37
1	C	171	ILE	CB-CG2	-5.77	1.33	1.52
2	F	398	GLU	C-O	5.77	1.31	1.23
1	K	144	TYR	N-CA	5.77	1.52	1.45
2	H	394	ASN	CG-OD1	5.76	1.34	1.23
2	L	489	CYS	C-O	-5.76	1.16	1.24
2	J	479	TYR	C-O	5.76	1.31	1.23
1	A	197	PHE	N-CA	-5.75	1.38	1.45
1	C	158	LEU	CA-C	5.75	1.60	1.52
1	A	91	SER	CA-CB	-5.75	1.42	1.53
2	D	450	ARG	CD-NE	5.75	1.54	1.46
1	I	39	LEU	CA-C	-5.75	1.45	1.52
1	A	3	GLU	CA-C	5.75	1.59	1.52
1	E	52	LEU	C-O	-5.75	1.16	1.23
2	H	344	SER	CA-C	5.75	1.60	1.52
1	K	64	ARG	NE-CZ	5.75	1.39	1.33
2	J	343	ILE	CG1-CD1	5.75	1.74	1.51
1	K	129	SER	N-CA	5.75	1.53	1.46
2	F	331	SER	C-N	-5.74	1.25	1.33
2	F	315	TRP	CA-C	5.74	1.60	1.53
1	G	25	ALA	CA-C	5.74	1.60	1.52
2	J	441	THR	CA-CB	5.74	1.61	1.53
2	J	500	ALA	CA-CB	-5.74	1.44	1.53
1	E	45	PRO	CA-C	5.74	1.59	1.52
2	L	512	ASN	CG-OD1	5.74	1.34	1.23
2	B	368	ASN	CA-CB	5.74	1.63	1.53
1	G	127	ASN	CA-C	5.74	1.60	1.52
2	D	462	HIS	CA-C	-5.73	1.45	1.52
2	B	465	ILE	C-O	-5.72	1.18	1.24
2	H	314	ASN	CG-OD1	5.72	1.34	1.23
2	B	336	LEU	N-CA	-5.72	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	493	LYS	CA-C	5.72	1.62	1.52
1	E	168	GLU	CA-CB	-5.72	1.44	1.53
1	K	42	PRO	CB-CG	5.72	1.78	1.49
2	B	324	TYR	N-CA	-5.72	1.39	1.46
1	I	19	ILE	CA-CB	5.72	1.61	1.54
2	H	502	GLN	CA-C	-5.71	1.45	1.52
1	K	199	ASP	C-O	5.71	1.30	1.24
1	E	107	HIS	C-N	5.71	1.38	1.33
1	A	9	PRO	CA-CB	-5.71	1.45	1.53
2	J	326	THR	CA-CB	5.71	1.63	1.53
1	I	153	ALA	CA-CB	-5.70	1.43	1.53
1	E	52	LEU	N-CA	-5.70	1.38	1.45
1	E	163	GLN	C-O	-5.70	1.17	1.24
1	K	142	ARG	C-O	5.70	1.30	1.23
2	L	469	SER	CA-CB	5.70	1.63	1.53
1	C	65	ASP	CA-CB	-5.70	1.45	1.53
2	D	440	ARG	CZ-NH2	-5.70	1.26	1.33
2	J	470	ILE	C-O	5.70	1.31	1.24
2	L	398	GLU	N-CA	-5.70	1.39	1.46
1	I	151	ALA	N-CA	5.69	1.53	1.46
2	B	381	ALA	CA-C	5.69	1.59	1.52
2	D	368	ASN	CB-CG	5.69	1.66	1.52
2	F	472	THR	CA-CB	5.69	1.63	1.53
1	K	199	ASP	CA-C	5.68	1.59	1.52
1	I	47	GLU	CA-C	5.68	1.60	1.52
1	K	148	GLU	CD-OE2	5.68	1.36	1.25
2	L	449	TRP	CE3-CZ3	5.68	1.55	1.38
2	F	501	VAL	C-O	-5.68	1.16	1.24
2	D	481	GLU	N-CA	-5.67	1.38	1.46
2	J	414	ARG	NE-CZ	5.67	1.39	1.33
1	I	57	ASP	CG-OD2	5.67	1.36	1.25
1	A	4	LEU	C-O	-5.67	1.16	1.23
2	D	334	GLN	CA-C	5.67	1.61	1.53
1	A	69	GLU	N-CA	-5.67	1.38	1.46
1	A	178	ASP	CB-CG	5.67	1.66	1.52
1	C	59	ASN	C-O	5.67	1.31	1.24
2	L	333	ARG	CG-CD	5.67	1.69	1.52
1	I	41	LYS	C-O	5.66	1.30	1.23
2	F	509	ASP	C-O	-5.66	1.17	1.23
2	H	446	PRO	CA-C	-5.66	1.45	1.52
1	I	161	ILE	C-O	-5.66	1.17	1.23
1	A	6	PRO	N-CA	5.66	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	TYR	N-CA	5.66	1.53	1.45
2	F	411	LYS	CE-NZ	5.66	1.66	1.49
2	F	395	THR	CA-C	-5.66	1.45	1.52
1	C	165	GLN	N-CA	-5.66	1.39	1.46
2	F	508	LEU	CG-CD1	-5.65	1.33	1.52
1	G	165	GLN	CD-OE1	5.65	1.34	1.23
2	D	437	TYR	C-O	5.65	1.30	1.23
1	G	86	GLU	CD-OE1	5.65	1.36	1.25
2	F	535	PHE	CG-CD2	5.65	1.50	1.38
2	L	354	LEU	CA-C	5.65	1.60	1.52
2	F	461	ILE	C-O	5.65	1.29	1.24
2	B	325	LYS	CG-CD	-5.64	1.35	1.52
2	B	486	ILE	C-O	-5.64	1.19	1.24
1	E	198	PHE	CA-C	-5.64	1.46	1.52
2	J	321	THR	CB-CG2	5.64	1.71	1.52
2	H	328	ILE	CA-C	-5.64	1.45	1.52
2	J	479	TYR	N-CA	5.64	1.53	1.45
1	G	70	VAL	CA-CB	-5.64	1.47	1.54
1	I	10	SER	C-O	-5.64	1.16	1.23
2	J	357	GLY	C-O	5.64	1.31	1.23
1	E	100	ASP	C-O	5.63	1.31	1.24
1	I	14	GLY	C-O	5.63	1.31	1.24
2	B	453	PRO	N-CA	5.63	1.55	1.47
1	C	57	ASP	C-O	-5.63	1.17	1.23
1	A	113	VAL	C-O	-5.62	1.17	1.24
1	A	160	LEU	CA-CB	-5.62	1.44	1.53
2	B	507	LYS	C-O	-5.62	1.17	1.23
2	D	491	ILE	C-N	5.62	1.41	1.33
1	A	23	LEU	C-O	-5.62	1.17	1.24
2	B	377	ARG	N-CA	-5.62	1.39	1.46
2	B	339	ILE	CA-C	5.62	1.58	1.52
2	B	366	ASN	CB-CG	5.62	1.66	1.52
2	L	465	ILE	N-CA	-5.61	1.39	1.46
1	E	68	LEU	C-O	-5.61	1.16	1.23
1	G	9	PRO	CB-CG	-5.61	1.21	1.49
2	J	507	LYS	CE-NZ	5.61	1.66	1.49
2	L	386	ASP	CG-OD2	5.61	1.35	1.25
2	D	307	ARG	C-O	5.60	1.31	1.23
1	K	31	ARG	C-O	5.60	1.31	1.23
1	E	170	LEU	C-O	5.60	1.31	1.23
1	I	154	LYS	CD-CE	5.60	1.69	1.52
1	I	174	ARG	CA-CB	-5.60	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	ASP	CA-C	-5.59	1.45	1.52
2	J	414	ARG	CG-CD	5.59	1.69	1.52
2	F	334	GLN	CD-NE2	5.59	1.45	1.33
2	H	507	LYS	CE-NZ	5.59	1.66	1.49
2	L	312	ASP	CG-OD1	5.59	1.35	1.25
2	B	483	ASP	C-O	5.59	1.31	1.24
2	F	368	ASN	CB-CG	5.59	1.66	1.52
1	G	37	ASN	CG-OD1	-5.59	1.12	1.23
1	C	15	PRO	C-O	-5.58	1.17	1.24
1	C	120	VAL	CB-CG1	5.58	1.71	1.52
1	G	80	GLN	N-CA	-5.58	1.39	1.46
2	F	382	GLY	C-O	-5.58	1.16	1.23
2	B	512	ASN	CA-C	5.58	1.60	1.52
2	D	498	PRO	CA-CB	5.58	1.61	1.53
1	G	81	ASP	CA-CB	-5.58	1.43	1.53
1	I	146	ASP	CA-C	5.58	1.60	1.52
1	E	64	ARG	CZ-NH1	5.58	1.40	1.32
2	H	460	HIS	C-O	5.58	1.30	1.23
2	L	358	ALA	N-CA	5.58	1.53	1.46
2	H	409	ARG	N-CA	5.57	1.54	1.46
2	L	308	PHE	CD2-CE2	5.57	1.55	1.38
1	E	200	PHE	CG-CD1	5.57	1.50	1.38
1	I	192	GLU	C-O	5.57	1.30	1.24
1	C	36	TRP	N-CA	-5.57	1.38	1.46
2	J	524	ASP	CA-CB	-5.57	1.44	1.53
1	K	133	ARG	CA-CB	-5.57	1.44	1.53
2	H	507	LYS	CA-C	5.57	1.59	1.52
2	J	318	LYS	CA-C	5.56	1.61	1.53
2	L	319	ALA	C-O	5.56	1.30	1.24
2	F	476	THR	C-O	-5.56	1.19	1.24
2	F	447	TYR	CE1-CZ	5.56	1.51	1.38
2	H	368	ASN	CB-CG	5.56	1.66	1.52
1	I	67	PHE	C-O	5.56	1.30	1.23
2	H	368	ASN	CA-CB	5.56	1.62	1.53
2	H	466	SER	CA-C	-5.56	1.45	1.52
1	I	62	LEU	N-CA	-5.55	1.39	1.46
2	D	392	VAL	N-CA	5.55	1.53	1.46
2	H	473	LYS	C-O	-5.55	1.17	1.23
1	E	176	GLU	CD-OE2	5.55	1.35	1.25
2	J	318	LYS	CG-CD	5.55	1.69	1.52
2	B	514	ASN	C-N	5.55	1.41	1.33
1	K	121	PRO	CA-C	5.55	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	140	HIS	C-O	-5.54	1.17	1.24
2	B	471	ALA	C-O	-5.54	1.17	1.24
1	C	94	ARG	CA-C	-5.54	1.45	1.52
1	I	162	GLU	CD-OE2	5.54	1.35	1.25
1	K	43	ASP	CA-CB	5.54	1.59	1.53
1	K	97	THR	C-O	5.54	1.30	1.24
2	F	395	THR	C-O	-5.54	1.16	1.23
1	I	83	TYR	C-O	5.54	1.30	1.23
1	I	135	ILE	C-O	5.54	1.30	1.24
1	A	7	GLU	N-CA	5.53	1.52	1.45
2	F	447	TYR	CA-C	-5.53	1.46	1.52
1	K	67	PHE	C-O	-5.53	1.17	1.23
1	E	100	ASP	N-CA	5.53	1.53	1.46
1	I	64	ARG	NE-CZ	5.53	1.39	1.33
1	I	98	THR	CA-C	5.53	1.59	1.52
1	K	166	ARG	CG-CD	5.52	1.69	1.52
1	A	157	VAL	CA-C	5.52	1.60	1.52
1	A	98	THR	CA-C	5.52	1.59	1.52
1	C	173	LYS	CA-CB	5.52	1.60	1.53
1	E	150	GLN	CG-CD	5.52	1.65	1.52
1	I	174	ARG	CZ-NH2	5.51	1.40	1.33
2	H	530	GLN	N-CA	-5.51	1.39	1.46
2	J	499	GLU	CG-CD	5.51	1.65	1.52
2	D	353	HIS	CA-C	-5.51	1.45	1.52
2	B	453	PRO	CB-CG	5.51	1.77	1.49
1	C	143	LEU	CA-C	5.50	1.59	1.52
1	A	47	GLU	CG-CD	5.50	1.65	1.52
2	B	420	ASP	C-N	5.50	1.40	1.34
2	F	442	ILE	C-O	5.50	1.30	1.24
2	D	397	VAL	CA-C	5.50	1.59	1.52
2	J	470	ILE	CB-CG2	5.50	1.70	1.52
1	E	166	ARG	CZ-NH2	5.50	1.40	1.33
2	H	414	ARG	CA-CB	5.50	1.62	1.53
1	C	72	GLN	CD-NE2	5.49	1.44	1.33
1	G	168	GLU	CD-OE2	5.49	1.35	1.25
1	I	166	ARG	C-O	-5.49	1.17	1.24
1	C	149	ALA	N-CA	-5.49	1.39	1.46
2	F	513	ALA	N-CA	-5.49	1.39	1.45
1	K	65	ASP	C-O	5.49	1.32	1.24
2	F	366	ASN	CG-ND2	5.49	1.44	1.33
1	K	188	ARG	CG-CD	5.49	1.69	1.52
2	B	313	ARG	CZ-NH2	-5.49	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	369	ASN	CA-C	5.49	1.60	1.52
1	I	150	GLN	C-O	5.49	1.30	1.24
1	K	78	GLU	CD-OE2	5.48	1.35	1.25
2	D	342	SER	CA-C	5.48	1.60	1.52
2	F	387	GLN	CA-C	-5.48	1.45	1.52
1	G	83	TYR	N-CA	-5.48	1.39	1.46
2	B	460	HIS	N-CA	5.48	1.52	1.45
2	L	362	ASP	CA-C	5.48	1.59	1.52
2	D	344	SER	N-CA	-5.48	1.39	1.46
1	E	88	ALA	C-O	5.48	1.30	1.24
1	E	143	LEU	CA-C	5.48	1.59	1.52
2	F	510	MET	SD-CE	-5.48	1.65	1.79
2	H	414	ARG	CB-CG	5.48	1.68	1.52
2	F	467	GLY	C-O	5.48	1.31	1.24
2	D	411	LYS	CE-NZ	5.47	1.65	1.49
1	C	64	ARG	N-CA	-5.47	1.38	1.46
2	L	450	ARG	CZ-NH1	5.47	1.40	1.32
2	B	320	LEU	C-O	-5.47	1.16	1.23
2	J	516	MET	CG-SD	5.47	1.94	1.80
2	B	390	LYS	CG-CD	5.47	1.68	1.52
2	H	327	SER	N-CA	-5.47	1.38	1.46
2	D	414	ARG	CB-CG	5.47	1.68	1.52
2	J	476	THR	C-O	-5.47	1.17	1.23
2	B	390	LYS	CE-NZ	5.46	1.65	1.49
2	F	475	ILE	CG1-CD1	-5.46	1.30	1.51
2	B	315	TRP	CA-C	5.46	1.59	1.52
2	L	440	ARG	C-O	-5.46	1.17	1.24
1	G	114	VAL	CA-C	5.46	1.59	1.52
2	H	420	ASP	C-O	5.46	1.30	1.24
2	J	390	LYS	CE-NZ	5.46	1.65	1.49
1	K	195	THR	CA-C	-5.46	1.46	1.52
1	A	78	GLU	CD-OE2	5.45	1.35	1.25
1	G	146	ASP	C-O	-5.45	1.17	1.24
2	D	456	TRP	C-O	-5.45	1.17	1.23
2	D	465	ILE	CA-C	5.44	1.59	1.52
1	E	135	ILE	N-CA	-5.44	1.39	1.46
2	F	494	SER	N-CA	-5.44	1.38	1.46
2	F	491	ILE	CA-CB	-5.44	1.47	1.54
1	G	7	GLU	CB-CG	5.44	1.68	1.52
2	L	393	PRO	C-O	-5.44	1.17	1.23
1	C	155	CYS	CA-C	-5.44	1.46	1.52
1	A	63	VAL	CA-C	5.44	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	499	GLU	CA-CB	-5.43	1.44	1.53
2	L	408[A]	CYS	CA-CB	5.43	1.61	1.53
2	L	408[B]	CYS	CA-CB	5.43	1.61	1.53
1	K	137	ILE	CA-C	5.43	1.59	1.52
1	I	111	PRO	C-O	5.43	1.29	1.23
2	J	367	PHE	CA-CB	-5.43	1.45	1.54
1	K	46	GLY	C-O	5.43	1.28	1.23
2	B	493	LYS	CG-CD	5.43	1.68	1.52
2	F	411	LYS	N-CA	5.43	1.52	1.46
2	L	465	ILE	CB-CG1	5.43	1.64	1.53
2	L	510	MET	SD-CE	-5.43	1.66	1.79
1	E	139	LEU	C-O	-5.43	1.17	1.24
1	K	116	ASN	C-O	5.43	1.29	1.23
2	D	347	THR	CA-CB	5.42	1.62	1.53
2	D	426	VAL	C-O	5.42	1.29	1.24
1	E	38	ARG	C-O	5.42	1.30	1.23
2	F	463	PHE	N-CA	-5.42	1.39	1.45
1	G	28	ASN	C-N	5.42	1.40	1.33
2	F	384	VAL	CA-CB	5.42	1.60	1.54
1	K	128	ILE	CA-CB	-5.42	1.47	1.54
2	F	397	VAL	CA-C	5.42	1.59	1.52
2	B	462	HIS	CA-C	-5.42	1.45	1.52
2	D	516	MET	CB-CG	5.42	1.68	1.52
2	L	520	ALA	C-O	5.42	1.30	1.23
1	A	139	LEU	CG-CD2	5.41	1.70	1.52
1	I	38	ARG	C-O	5.41	1.30	1.23
2	B	533	THR	C-O	5.41	1.30	1.23
1	E	195	THR	CA-CB	-5.41	1.44	1.53
1	G	52	LEU	CG-CD2	-5.41	1.34	1.52
2	F	354	LEU	C-O	5.40	1.30	1.23
2	F	414	ARG	CA-CB	5.40	1.61	1.53
2	H	513	ALA	CA-CB	-5.40	1.44	1.53
2	L	516	MET	SD-CE	5.40	1.93	1.79
1	C	2	ILE	CA-C	5.40	1.58	1.52
2	J	315	TRP	CA-C	5.40	1.60	1.52
1	G	101	ALA	C-N	5.39	1.41	1.33
2	L	303	GLN	CA-C	5.39	1.59	1.52
1	E	16	TYR	CE2-CZ	5.39	1.51	1.38
2	J	515	PRO	CA-CB	-5.39	1.46	1.53
2	D	462	HIS	CA-CB	-5.39	1.44	1.53
2	B	504	LEU	CA-CB	-5.39	1.45	1.53
2	L	479	TYR	CD2-CE2	5.39	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	ILE	CA-C	5.39	1.58	1.52
1	C	119	GLY	N-CA	5.39	1.53	1.45
1	C	187	ILE	C-O	5.38	1.29	1.24
2	H	458	PRO	C-N	-5.38	1.26	1.33
2	J	333	ARG	CA-C	5.38	1.59	1.52
2	H	512	ASN	CA-C	5.38	1.59	1.52
2	D	354	LEU	CA-C	5.38	1.59	1.52
1	E	126	ILE	CA-C	5.38	1.59	1.52
2	J	399	MET	C-O	-5.38	1.17	1.23
1	A	71	TRP	CA-CB	5.38	1.63	1.53
1	A	195	THR	C-O	-5.38	1.17	1.23
1	K	38	ARG	CB-CG	5.37	1.68	1.52
2	L	431	THR	CA-CB	5.37	1.62	1.53
2	H	328	ILE	N-CA	-5.37	1.40	1.46
1	I	187	ILE	CA-CB	-5.37	1.48	1.54
2	J	522	ARG	CZ-NH2	5.37	1.40	1.33
2	J	312	ASP	CA-CB	-5.37	1.46	1.52
1	A	27	GLY	CA-C	5.37	1.57	1.51
2	B	479	TYR	CE1-CZ	-5.37	1.25	1.38
2	H	399	MET	C-O	-5.37	1.17	1.23
1	I	100	ASP	N-CA	5.36	1.52	1.46
1	G	34	GLU	C-O	5.36	1.30	1.23
2	L	518	CYS	N-CA	5.36	1.52	1.46
2	L	365	LEU	CA-C	-5.36	1.45	1.52
2	D	333	ARG	CD-NE	-5.36	1.38	1.46
1	A	192	GLU	CD-OE1	5.35	1.35	1.25
2	D	412	ASN	CG-OD1	5.35	1.33	1.23
1	E	61	HIS	C-O	-5.35	1.17	1.23
2	F	325	LYS	C-O	-5.35	1.17	1.24
1	G	94	ARG	CA-C	-5.35	1.46	1.52
1	E	97	THR	CB-CG2	-5.35	1.34	1.52
2	H	387	GLN	CA-C	5.35	1.60	1.52
1	A	135	ILE	CA-CB	5.35	1.60	1.53
1	K	117	ALA	N-CA	-5.35	1.39	1.46
1	C	140	HIS	CA-C	5.34	1.59	1.52
1	I	188	ARG	NE-CZ	5.34	1.39	1.33
2	D	414	ARG	CA-CB	5.34	1.61	1.53
2	B	416	LEU	C-O	5.34	1.31	1.24
2	F	370	GLY	C-O	5.34	1.31	1.24
1	E	99	PHE	CD1-CE1	5.34	1.54	1.38
1	K	135	ILE	CG1-CD1	5.34	1.72	1.51
2	L	537	ASN	CA-CB	5.33	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	PHE	N-CA	-5.33	1.39	1.46
1	C	20	GLY	C-O	-5.33	1.16	1.23
1	A	192	GLU	CA-C	5.33	1.59	1.52
1	G	171	ILE	CA-C	-5.33	1.45	1.52
2	H	498	PRO	CA-C	5.33	1.61	1.52
1	A	89	PHE	CA-C	5.33	1.59	1.52
1	A	188	ARG	CZ-NH1	5.32	1.40	1.32
2	L	310	ILE	CG1-CD1	-5.32	1.31	1.51
2	F	514	ASN	CG-OD1	5.32	1.33	1.23
2	B	362	ASP	C-O	5.32	1.29	1.23
2	J	330	ARG	CZ-NH2	5.32	1.40	1.33
2	B	458	PRO	C-O	5.31	1.30	1.23
2	F	496	ALA	C-O	-5.31	1.17	1.24
1	C	144	TYR	CA-C	5.31	1.59	1.52
2	H	364	LEU	CA-C	5.31	1.60	1.52
2	D	442	ILE	CB-CG1	-5.31	1.42	1.53
1	A	32	ASP	CG-OD1	5.30	1.35	1.25
1	C	16	TYR	CA-CB	5.30	1.61	1.53
2	J	324	TYR	C-O	5.30	1.30	1.23
2	F	389	GLY	C-O	-5.30	1.16	1.24
1	G	97	THR	CB-CG2	-5.30	1.35	1.52
2	J	530	GLN	C-O	-5.30	1.17	1.24
2	L	414	ARG	CD-NE	5.30	1.53	1.46
1	E	126	ILE	N-CA	-5.30	1.40	1.46
2	H	383	ARG	CB-CG	-5.30	1.36	1.52
2	J	448	PRO	CA-C	-5.30	1.47	1.53
1	G	85	LEU	C-O	-5.29	1.17	1.24
2	D	515	PRO	CB-CG	5.29	1.76	1.49
2	F	474	LEU	CG-CD2	-5.29	1.35	1.52
2	J	414	ARG	CD-NE	5.29	1.53	1.46
2	B	396	LEU	CG-CD2	-5.29	1.35	1.52
1	C	76	ASN	C-O	-5.29	1.17	1.24
2	B	390	LYS	CD-CE	5.29	1.68	1.52
1	I	5	LEU	C-O	5.29	1.30	1.23
1	A	127	ASN	N-CA	-5.29	1.39	1.46
1	I	15	PRO	CA-CB	5.29	1.61	1.53
2	B	397	VAL	N-CA	5.29	1.53	1.46
2	H	323	ASP	C-O	5.29	1.30	1.24
2	F	466	SER	CA-C	5.28	1.59	1.53
2	H	504	LEU	CG-CD1	-5.28	1.35	1.52
1	K	85	LEU	C-O	5.28	1.30	1.24
1	E	99	PHE	CB-CG	5.28	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	520	ALA	CA-C	-5.28	1.46	1.52
1	C	182	ALA	CA-CB	-5.28	1.44	1.53
2	D	395	THR	CA-C	-5.28	1.46	1.52
1	G	69	GLU	C-O	5.27	1.30	1.24
2	J	458	PRO	C-O	5.27	1.30	1.23
2	J	472	THR	C-O	-5.27	1.17	1.24
2	H	477	GLN	CD-OE1	5.27	1.33	1.23
2	B	379	ILE	CA-C	5.27	1.59	1.52
1	G	71	TRP	CE3-CZ3	5.27	1.54	1.38
2	H	499	GLU	CD-OE1	5.27	1.35	1.25
1	C	108	THR	CA-CB	5.27	1.60	1.53
2	F	409	ARG	CA-CB	-5.27	1.45	1.52
2	D	488	MET	C-O	-5.26	1.17	1.24
2	F	437	TYR	N-CA	-5.26	1.38	1.45
1	G	185	PHE	CA-C	-5.26	1.47	1.53
2	D	397	VAL	CB-CG2	-5.26	1.35	1.52
2	D	499	GLU	CA-C	5.26	1.60	1.52
1	I	177	VAL	CA-CB	5.26	1.61	1.54
2	B	507	LYS	CD-CE	5.26	1.68	1.52
2	D	340	PRO	CA-CB	-5.26	1.46	1.53
1	A	100	ASP	CA-CB	5.26	1.61	1.53
1	C	84	ASN	CB-CG	5.26	1.65	1.52
2	F	310	ILE	CA-C	5.26	1.61	1.53
2	J	317	PRO	CB-CG	5.26	1.75	1.49
2	J	485	LEU	C-O	-5.26	1.17	1.24
1	A	41	LYS	C-O	5.25	1.30	1.23
1	K	192	GLU	CG-CD	5.25	1.65	1.52
1	C	154	LYS	N-CA	-5.25	1.39	1.46
1	E	47	GLU	CD-OE2	5.25	1.35	1.25
1	C	3	GLU	CD-OE2	5.25	1.35	1.25
2	B	470	ILE	CA-CB	-5.25	1.47	1.54
1	C	94	ARG	CD-NE	-5.25	1.39	1.46
2	D	410	HIS	N-CA	-5.25	1.39	1.46
2	B	375	GLY	N-CA	5.24	1.50	1.45
1	C	2	ILE	CA-CB	5.24	1.60	1.54
1	K	101	ALA	CA-C	-5.24	1.46	1.53
1	A	90	ASN	CA-CB	-5.24	1.45	1.53
2	B	480	PHE	C-O	5.24	1.30	1.23
1	C	97	THR	CB-CG2	-5.24	1.35	1.52
1	C	137	ILE	CG1-CD1	5.24	1.72	1.51
2	J	411	LYS	CB-CG	5.24	1.68	1.52
1	C	99	PHE	CD1-CE1	5.24	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	350	ASN	CA-C	5.24	1.58	1.52
1	K	33	GLN	CA-C	5.23	1.59	1.52
2	B	437	TYR	C-O	5.23	1.30	1.23
1	K	98	THR	CA-C	5.23	1.60	1.53
2	D	537	ASN	CG-OD1	5.23	1.33	1.23
2	H	455	ASP	CA-CB	-5.23	1.46	1.53
2	J	450	ARG	CZ-NH2	5.23	1.40	1.33
2	B	389	GLY	C-O	-5.23	1.17	1.24
1	C	2	ILE	N-CA	-5.23	1.40	1.46
2	H	523	PHE	CA-CB	-5.23	1.44	1.53
2	H	362	ASP	CA-C	5.22	1.59	1.53
1	G	188	ARG	CZ-NH2	5.22	1.40	1.33
1	A	3	GLU	CD-OE2	5.22	1.35	1.25
2	B	317	PRO	CA-C	5.22	1.59	1.52
2	D	440	ARG	CG-CD	-5.22	1.36	1.52
1	E	45	PRO	C-O	5.22	1.30	1.23
2	D	485	LEU	CB-CG	-5.21	1.43	1.53
1	I	128	ILE	CA-CB	-5.21	1.48	1.54
2	L	317	PRO	CA-C	5.21	1.59	1.52
1	G	154	LYS	N-CA	-5.21	1.40	1.46
2	J	491	ILE	CA-C	5.21	1.60	1.52
2	H	403	ASN	C-O	5.21	1.31	1.24
1	K	86	GLU	C-O	5.21	1.30	1.24
1	E	55	VAL	N-CA	-5.21	1.40	1.46
1	G	199	ASP	N-CA	-5.21	1.39	1.46
2	H	441	THR	CA-CB	5.21	1.60	1.53
1	K	195	THR	C-O	5.20	1.30	1.23
2	L	411	LYS	CG-CD	5.20	1.68	1.52
2	H	446	PRO	C-O	-5.20	1.17	1.23
2	F	418	PRO	N-CA	-5.20	1.41	1.46
1	I	115	ASN	C-O	-5.20	1.17	1.23
2	L	438	SER	C-O	-5.20	1.17	1.23
2	L	440	ARG	CZ-NH1	5.20	1.40	1.32
1	C	19	ILE	CG1-CD1	-5.19	1.31	1.51
2	F	479	TYR	CD2-CE2	5.19	1.54	1.38
2	J	509	ASP	CG-OD2	5.19	1.35	1.25
2	L	368	ASN	CA-CB	5.19	1.62	1.53
1	E	124	PRO	CA-CB	5.19	1.60	1.53
1	A	2	ILE	CA-C	5.18	1.58	1.52
1	A	71	TRP	CE3-CZ3	5.18	1.54	1.38
2	D	522	ARG	CB-CG	-5.18	1.36	1.52
2	F	422	ASN	CA-C	5.18	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	483	ASP	C-O	5.18	1.31	1.24
2	B	409	ARG	CA-C	5.18	1.60	1.53
2	D	411	LYS	CD-CE	5.18	1.68	1.52
2	D	414	ARG	NE-CZ	5.18	1.38	1.33
2	B	395	THR	CA-C	-5.18	1.46	1.52
2	B	310	ILE	CB-CG2	5.18	1.69	1.52
1	C	47	GLU	CD-OE2	5.18	1.35	1.25
1	E	188	ARG	CG-CD	5.18	1.68	1.52
1	I	150	GLN	CB-CG	5.18	1.68	1.52
1	C	171	ILE	CG1-CD1	-5.17	1.31	1.51
2	D	414	ARG	CZ-NH2	5.17	1.40	1.33
1	K	159	ASN	CA-C	5.17	1.61	1.52
2	L	368	ASN	CG-ND2	5.17	1.44	1.33
1	C	176	GLU	C-O	-5.17	1.18	1.23
1	G	50	LEU	N-CA	-5.17	1.39	1.46
2	H	493	LYS	CA-C	5.17	1.60	1.52
2	H	493	LYS	CE-NZ	5.17	1.64	1.49
2	L	400	TRP	CA-CB	-5.17	1.44	1.53
1	I	178	ASP	C-O	5.17	1.30	1.23
2	F	311	ARG	CZ-NH2	-5.17	1.26	1.33
2	B	493	LYS	CD-CE	5.16	1.68	1.52
2	F	314	ASN	CA-CB	-5.16	1.45	1.53
2	J	409	ARG	C-O	5.16	1.29	1.23
1	G	144	TYR	C-O	-5.16	1.17	1.23
2	B	372	LEU	CA-CB	-5.16	1.46	1.53
2	B	471	ALA	CA-CB	-5.16	1.44	1.53
2	H	302	ALA	C-O	-5.16	1.17	1.23
2	H	316	HIS	C-O	5.16	1.30	1.23
2	J	475	ILE	CA-CB	-5.16	1.48	1.54
2	B	452	GLY	C-O	5.16	1.32	1.24
2	D	409	ARG	CB-CG	-5.16	1.36	1.52
2	F	438	SER	CA-CB	-5.16	1.44	1.53
2	B	509	ASP	C-O	5.15	1.29	1.23
1	G	47	GLU	CD-OE2	5.15	1.35	1.25
2	D	361	HIS	N-CA	-5.15	1.39	1.46
1	E	186	ASP	N-CA	-5.15	1.39	1.45
1	E	188	ARG	CZ-NH1	5.15	1.40	1.32
2	D	483	ASP	CA-C	-5.15	1.46	1.53
2	F	478	LEU	N-CA	-5.15	1.39	1.46
1	E	198	PHE	CD1-CE1	5.15	1.54	1.38
1	K	192	GLU	CD-OE2	5.15	1.35	1.25
2	D	505	ILE	C-O	-5.15	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	161	ILE	CB-CG2	5.15	1.69	1.52
2	D	413	ASP	CA-C	-5.14	1.46	1.52
1	I	162	GLU	C-O	-5.14	1.17	1.24
2	J	495	ILE	CG1-CD1	-5.14	1.31	1.51
1	K	161	ILE	C-O	-5.14	1.18	1.24
1	A	3	GLU	N-CA	5.14	1.52	1.46
1	A	14	GLY	N-CA	5.14	1.51	1.44
1	A	187	ILE	CB-CG2	5.14	1.69	1.52
2	F	380	VAL	CA-CB	-5.14	1.47	1.53
2	F	499	GLU	CG-CD	5.14	1.64	1.52
2	H	368	ASN	CA-C	5.14	1.59	1.52
2	J	522	ARG	CB-CG	-5.14	1.37	1.52
1	K	123	ALA	CA-C	5.14	1.59	1.53
1	A	113	VAL	N-CA	-5.14	1.40	1.46
2	L	430	LEU	CA-CB	-5.14	1.45	1.53
2	B	490	PRO	CG-CD	-5.13	1.33	1.50
2	F	319	ALA	N-CA	5.13	1.52	1.46
2	H	309	VAL	CB-CG1	5.13	1.69	1.52
1	K	47	GLU	CD-OE1	5.13	1.35	1.25
2	F	390	LYS	C-O	-5.13	1.17	1.24
1	I	16	TYR	CZ-OH	5.13	1.48	1.38
2	J	465	ILE	N-CA	5.13	1.52	1.46
1	K	96	ALA	CA-CB	5.13	1.62	1.53
2	L	510	MET	C-O	-5.13	1.17	1.24
2	B	502	GLN	CD-NE2	5.13	1.44	1.33
1	I	114	VAL	CA-C	-5.13	1.46	1.52
2	D	491	ILE	CG1-CD1	5.13	1.71	1.51
1	E	100	ASP	CA-C	5.13	1.59	1.52
1	E	175	CYS	C-O	5.13	1.28	1.24
1	K	25	ALA	CA-C	5.13	1.59	1.52
2	H	452	GLY	C-O	5.12	1.30	1.24
1	K	153	ALA	N-CA	5.12	1.52	1.46
2	D	533	THR	CA-C	5.12	1.60	1.53
2	B	400	TRP	N-CA	5.12	1.52	1.45
2	J	485	LEU	CA-C	5.12	1.59	1.52
2	L	475	ILE	N-CA	5.12	1.52	1.46
2	D	397	VAL	CB-CG1	-5.12	1.35	1.52
1	E	3	GLU	CD-OE2	5.12	1.35	1.25
1	E	113	VAL	N-CA	-5.12	1.40	1.46
1	A	131	PHE	C-O	-5.11	1.17	1.23
2	B	436	TYR	CA-C	-5.11	1.45	1.53
2	D	469	SER	N-CA	-5.11	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	476	THR	CB-CG2	-5.11	1.35	1.52
2	F	447	TYR	C-O	-5.11	1.17	1.24
2	J	530	GLN	CD-OE1	5.11	1.33	1.23
1	A	91	SER	CA-C	5.11	1.59	1.52
1	C	8	THR	N-CA	5.11	1.52	1.45
2	D	339	ILE	N-CA	5.11	1.52	1.46
1	K	168	GLU	CG-CD	5.11	1.64	1.52
2	B	320	LEU	CA-CB	5.10	1.59	1.52
2	H	434	ASP	CG-OD1	5.10	1.35	1.25
2	H	448	PRO	CA-C	-5.10	1.46	1.52
2	B	383	ARG	CB-CG	-5.10	1.37	1.52
2	B	405	GLY	CA-C	-5.10	1.46	1.51
1	G	79	TYR	CG-CD2	5.10	1.50	1.39
1	C	67	PHE	CB-CG	-5.10	1.39	1.50
2	B	321	THR	N-CA	-5.09	1.40	1.46
1	C	49	ILE	CA-C	5.09	1.58	1.52
2	H	434	ASP	CA-C	-5.09	1.46	1.52
2	J	414	ARG	CA-CB	5.09	1.61	1.53
2	D	523	PHE	N-CA	5.09	1.53	1.46
2	H	457	ARG	CA-C	5.09	1.58	1.53
2	L	365	LEU	CG-CD2	5.09	1.69	1.52
2	L	372	LEU	C-N	5.09	1.39	1.33
1	G	70	VAL	CB-CG2	-5.08	1.35	1.52
1	G	181	THR	CA-C	5.08	1.59	1.52
1	K	174	ARG	CZ-NH2	5.08	1.40	1.33
2	D	434	ASP	CG-OD2	5.08	1.35	1.25
2	H	537	ASN	CG-OD1	5.08	1.33	1.23
1	I	71	TRP	CA-C	5.08	1.58	1.52
1	E	4	LEU	CA-C	5.08	1.59	1.53
1	I	125	HIS	N-CA	5.08	1.52	1.45
2	B	322	PRO	C-O	-5.08	1.18	1.24
1	I	103	GLU	CD-OE1	5.08	1.34	1.25
2	F	420	ASP	CA-CB	5.08	1.60	1.53
1	A	111	PRO	N-CA	-5.07	1.40	1.47
2	H	420	ASP	C-N	5.07	1.40	1.33
2	J	366	ASN	C-O	-5.07	1.17	1.24
1	K	42	PRO	CA-C	5.07	1.60	1.52
1	I	90	ASN	N-CA	5.07	1.52	1.46
1	A	96	ALA	CA-C	-5.07	1.46	1.52
2	B	460	HIS	CA-C	-5.07	1.46	1.52
2	B	516	MET	C-O	-5.07	1.16	1.24
2	L	372	LEU	N-CA	-5.07	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	390	LYS	CA-C	-5.07	1.46	1.53
2	H	456	TRP	C-O	-5.07	1.18	1.24
2	J	510	MET	N-CA	5.07	1.52	1.46
2	D	315	TRP	CA-C	5.06	1.59	1.52
2	D	450	ARG	CZ-NH2	5.06	1.40	1.33
2	D	528	ARG	CA-C	-5.06	1.46	1.52
2	D	365	LEU	CA-CB	-5.06	1.47	1.54
1	E	175	CYS	CA-CB	5.06	1.60	1.53
1	E	144	TYR	CZ-OH	5.06	1.48	1.38
2	D	509	ASP	CA-C	5.06	1.61	1.53
2	D	521	TYR	CE2-CZ	5.06	1.50	1.38
1	G	15	PRO	CA-C	-5.06	1.44	1.52
1	G	192	GLU	C-O	5.05	1.29	1.23
1	I	86	GLU	C-O	5.05	1.30	1.24
2	J	431	THR	CA-C	-5.05	1.46	1.53
2	F	354	LEU	CG-CD1	-5.05	1.35	1.52
2	H	485	LEU	C-O	-5.05	1.17	1.24
1	A	3	GLU	CG-CD	5.05	1.64	1.52
2	B	517	ASP	CG-OD2	5.05	1.34	1.25
2	H	405	GLY	C-O	5.05	1.29	1.23
2	D	370	GLY	C-O	5.04	1.30	1.23
2	F	307	ARG	CA-C	5.04	1.58	1.52
1	K	147	ASP	N-CA	-5.04	1.40	1.46
2	L	318	LYS	CE-NZ	5.04	1.64	1.49
2	B	339	ILE	CA-CB	5.04	1.60	1.54
2	B	483	ASP	CG-OD2	-5.04	1.15	1.25
2	H	428	ARG	C-O	-5.04	1.17	1.23
2	L	332	PRO	C-O	5.04	1.29	1.23
1	I	92	PHE	CG-CD2	5.04	1.49	1.38
2	L	454	ASN	CG-OD1	5.04	1.33	1.23
1	G	3	GLU	CD-OE2	5.04	1.34	1.25
1	I	165	GLN	CG-CD	5.04	1.64	1.52
2	J	380	VAL	CB-CG2	5.04	1.69	1.52
2	L	527	LEU	CA-CB	-5.04	1.45	1.53
2	H	400	TRP	N-CA	5.03	1.52	1.46
1	A	144	TYR	CZ-OH	5.03	1.48	1.38
1	C	138	HIS	N-CA	-5.03	1.39	1.46
2	L	385	VAL	CA-CB	5.03	1.62	1.54
2	F	386	ASP	N-CA	-5.03	1.39	1.45
1	I	2	ILE	CA-CB	-5.03	1.48	1.54
2	L	427	GLY	CA-C	-5.02	1.46	1.51
1	A	4	LEU	N-CA	5.02	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	GLU	C-O	5.02	1.30	1.23
2	H	532	LYS	CA-C	5.02	1.59	1.53
2	L	447	TYR	CB-CG	-5.02	1.40	1.51
1	G	117	ALA	CA-CB	-5.02	1.45	1.53
2	B	374	ILE	CA-CB	-5.02	1.48	1.54
2	F	343	ILE	C-O	-5.02	1.18	1.24
2	F	443	LYS	CE-NZ	5.02	1.64	1.49
1	A	65	ASP	C-O	-5.02	1.17	1.24
1	A	123	ALA	CA-C	-5.02	1.47	1.53
1	E	5	LEU	CG-CD1	-5.01	1.36	1.52
1	E	165	GLN	CD-NE2	5.01	1.43	1.33
2	F	377	ARG	CB-CG	5.01	1.67	1.52
2	B	319	ALA	C-O	5.01	1.30	1.24
1	E	29	PRO	CA-C	5.01	1.58	1.52
2	L	366	ASN	CA-C	-5.01	1.45	1.52
2	B	532	LYS	C-O	-5.01	1.17	1.23
1	G	178	ASP	CA-C	5.01	1.59	1.53
2	J	324	TYR	CA-CB	-5.01	1.46	1.52
1	G	32	ASP	C-O	5.01	1.29	1.24
2	J	393	PRO	C-O	-5.01	1.17	1.23
1	K	21	LEU	C-O	5.01	1.30	1.24
2	D	342	SER	CB-OG	5.00	1.52	1.42
1	E	187	ILE	CG1-CD1	-5.00	1.32	1.51
2	F	436	TYR	CG-CD1	5.00	1.49	1.39
1	K	40	ALA	CA-CB	5.00	1.62	1.53
2	D	311	ARG	CA-C	-5.00	1.46	1.52
1	E	100	ASP	CA-CB	5.00	1.62	1.53
2	J	376	GLU	CD-OE2	5.00	1.34	1.25

All (868) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	37	ASN	N-CA-C	14.92	129.43	112.57
1	I	37	ASN	N-CA-C	13.74	128.31	112.93
1	C	99	PHE	CA-C-N	13.24	138.44	120.44
1	C	99	PHE	C-N-CA	13.24	138.44	120.44
2	D	440	ARG	NE-CZ-NH2	-12.66	107.80	119.20
2	B	328	ILE	N-CA-C	12.27	122.20	110.42
2	D	440	ARG	CB-CG-CD	-12.05	83.58	111.30
2	D	340	PRO	CB-CA-C	-11.97	95.68	111.12
2	B	322	PRO	N-CA-C	11.38	129.01	113.65
1	E	37	ASN	N-CA-C	11.29	126.19	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	366	ASN	N-CA-C	11.25	126.58	113.19
2	H	538	CYS	CA-CB-SG	-11.11	88.86	114.40
2	B	538	CYS	CA-CB-SG	-10.90	89.33	114.40
2	L	371	GLY	N-CA-C	10.89	126.33	111.20
2	B	440	ARG	NE-CZ-NH2	-10.83	109.45	119.20
2	D	440	ARG	NE-CZ-NH1	10.63	132.13	121.50
2	F	322	PRO	N-CA-C	10.60	127.62	113.84
2	F	440	ARG	NE-CZ-NH2	-10.54	109.72	119.20
2	L	494	SER	N-CA-C	-10.43	100.56	113.18
2	H	427	GLY	CA-C-O	-10.41	110.50	121.63
2	H	492	VAL	N-CA-C	-10.39	100.22	110.30
1	G	94	ARG	NE-CZ-NH2	-10.36	109.88	119.20
2	J	467	GLY	CA-C-N	-10.35	108.63	120.12
2	J	467	GLY	C-N-CA	-10.35	108.63	120.12
2	D	333	ARG	NE-CZ-NH1	-10.26	111.25	121.50
2	F	467	GLY	CA-C-N	-10.24	110.39	120.83
2	F	467	GLY	C-N-CA	-10.24	110.39	120.83
2	B	452	GLY	CA-C-N	-10.07	109.39	119.56
2	B	452	GLY	C-N-CA	-10.07	109.39	119.56
2	F	339	ILE	N-CA-C	-9.95	97.77	109.01
2	B	467	GLY	CA-C-N	-9.93	107.42	119.84
2	B	467	GLY	C-N-CA	-9.93	107.42	119.84
2	L	443	LYS	CA-C-N	-9.80	110.27	120.85
2	L	443	LYS	C-N-CA	-9.80	110.27	120.85
2	B	494	SER	N-CA-C	-9.77	100.62	112.54
2	J	366	ASN	N-CA-C	9.72	124.88	112.92
2	F	328	ILE	N-CA-C	9.65	119.68	110.42
1	E	168	GLU	N-CA-C	9.64	122.80	111.71
2	F	325	LYS	N-CA-C	9.63	121.78	111.28
2	D	425	GLY	CA-C-O	-9.60	109.75	118.77
1	G	18	HIS	N-CA-C	9.56	122.71	111.71
2	D	492	VAL	N-CA-C	-9.52	101.28	110.42
1	G	173	LYS	CA-C-O	-9.49	110.67	120.54
1	A	138	HIS	N-CA-C	9.48	122.56	110.24
1	K	37	ASN	N-CA-C	9.38	124.27	113.02
2	D	467	GLY	CA-C-N	-9.29	110.01	120.04
2	D	467	GLY	C-N-CA	-9.29	110.01	120.04
2	H	440	ARG	NE-CZ-NH2	-9.21	110.91	119.20
2	B	440	ARG	CB-CG-CD	-9.19	90.17	111.30
2	H	428	ARG	CA-C-O	-9.17	111.24	121.51
1	G	9	PRO	CB-CA-C	-9.15	99.05	111.21
1	E	160	LEU	N-CA-C	-9.12	100.74	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	GLY	CA-C-N	9.10	129.34	119.87
1	A	14	GLY	C-N-CA	9.10	129.34	119.87
1	C	37	ASN	N-CA-C	9.08	123.10	112.93
2	F	440	ARG	CB-CG-CD	-9.08	90.42	111.30
1	K	81	ASP	N-CA-C	9.07	123.61	112.54
2	H	475	ILE	CA-CB-CG1	9.04	125.78	110.40
2	J	427	GLY	CA-C-O	-9.01	112.99	121.19
1	I	81	ASP	N-CA-C	8.99	122.75	111.69
2	L	420	ASP	CA-C-N	8.98	129.88	119.47
2	L	420	ASP	C-N-CA	8.98	129.88	119.47
1	I	94	ARG	CB-CG-CD	8.92	131.82	111.30
1	I	100	ASP	CA-C-N	8.91	136.33	123.14
1	I	100	ASP	C-N-CA	8.91	136.33	123.14
1	G	94	ARG	NE-CZ-NH1	8.85	130.35	121.50
2	J	367	PHE	N-CA-C	-8.78	103.15	114.04
1	K	180	LYS	N-CA-C	-8.66	92.36	110.80
2	B	315	TRP	N-CA-C	-8.65	101.17	112.68
1	E	59	ASN	N-CA-C	-8.63	102.76	113.38
2	J	489	CYS	CA-C-N	-8.63	110.76	119.56
2	J	489	CYS	C-N-CA	-8.63	110.76	119.56
2	F	438	SER	N-CA-C	8.62	122.52	108.99
2	B	495	ILE	CB-CA-C	-8.56	100.60	110.96
1	K	93	GLY	CA-C-O	-8.52	112.44	121.56
2	L	440	ARG	NE-CZ-NH2	-8.52	111.53	119.20
2	D	510	MET	CG-SD-CE	-8.52	82.17	100.90
2	F	388	TYR	N-CA-C	-8.51	102.61	113.16
1	C	101	ALA	CA-C-O	-8.49	110.67	121.11
2	J	417	ALA	N-CA-C	-8.46	98.99	109.65
2	L	440	ARG	CB-CG-CD	-8.46	91.85	111.30
2	H	440	ARG	NE-CZ-NH1	8.41	129.91	121.50
2	H	331	SER	CA-C-N	-8.34	111.42	119.85
2	H	331	SER	C-N-CA	-8.34	111.42	119.85
1	A	101	ALA	CA-C-O	-8.32	111.21	120.70
1	E	44	ALA	CA-C-N	8.31	128.81	119.92
1	E	44	ALA	C-N-CA	8.31	128.81	119.92
2	L	525	ILE	CA-C-O	-8.31	111.55	120.36
2	B	457	ARG	CA-C-N	-8.16	112.44	120.52
2	B	457	ARG	C-N-CA	-8.16	112.44	120.52
2	L	428	ARG	NE-CZ-NH2	-8.14	111.87	119.20
1	G	155	CYS	CA-C-N	-8.01	111.39	120.04
1	G	155	CYS	C-N-CA	-8.01	111.39	120.04
2	B	420	ASP	CB-CA-C	7.98	119.33	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	331	SER	CA-C-N	-7.97	111.80	119.85
2	L	331	SER	C-N-CA	-7.97	111.80	119.85
1	E	3	GLU	CB-CA-C	-7.95	97.32	110.19
2	B	380	VAL	N-CA-C	-7.92	97.02	108.11
2	J	494	SER	N-CA-C	-7.90	102.65	111.82
1	K	138	HIS	N-CA-C	7.86	121.04	110.35
2	B	434	ASP	N-CA-C	7.86	123.07	113.17
2	L	458	PRO	CB-CA-C	-7.84	101.00	111.12
2	L	538	CYS	CA-CB-SG	-7.83	96.39	114.40
2	L	493	LYS	N-CA-C	7.81	122.49	113.19
2	J	316	HIS	N-CA-C	-7.71	99.10	110.20
2	J	356	PHE	N-CA-C	7.70	122.01	109.76
1	I	146	ASP	N-CA-C	7.68	120.55	111.71
1	G	15	PRO	CA-C-N	-7.68	111.00	122.83
1	G	15	PRO	C-N-CA	-7.68	111.00	122.83
2	F	372	LEU	N-CA-C	7.68	120.89	110.29
2	D	458	PRO	N-CA-C	-7.67	100.47	111.22
2	J	412	ASN	N-CA-C	7.65	122.19	113.01
2	L	460	HIS	CA-C-N	-7.65	112.50	123.06
2	L	460	HIS	C-N-CA	-7.65	112.50	123.06
2	B	379	ILE	N-CA-C	-7.64	97.33	108.71
1	E	10	SER	N-CA-C	7.63	121.30	110.23
1	G	13	ALA	N-CA-C	-7.63	102.61	112.23
1	A	94	ARG	CB-CG-CD	7.61	128.80	111.30
2	D	473	LYS	CD-CE-NZ	-7.59	87.60	111.90
2	D	466	SER	N-CA-C	7.57	119.43	111.03
1	K	61	HIS	N-CA-C	7.51	122.07	110.20
1	I	189	ILE	CG1-CB-CG2	-7.51	88.18	110.70
2	D	392	VAL	CA-C-N	-7.50	112.96	120.31
2	D	392	VAL	C-N-CA	-7.50	112.96	120.31
2	H	452	GLY	N-CA-C	-7.50	97.05	112.34
2	F	417	ALA	N-CA-C	-7.48	98.50	109.50
1	G	157	VAL	N-CA-C	-7.48	104.49	111.45
2	F	384	VAL	CA-C-O	-7.48	112.53	120.53
1	K	94	ARG	NE-CZ-NH2	-7.48	112.47	119.20
1	G	99	PHE	CA-C-N	7.47	132.99	120.88
1	G	99	PHE	C-N-CA	7.47	132.99	120.88
2	B	372	LEU	CA-C-N	-7.47	111.93	119.92
2	B	372	LEU	C-N-CA	-7.47	111.93	119.92
2	D	451	ASN	N-CA-C	-7.44	96.69	108.30
2	H	496	ALA	N-CA-C	7.44	120.44	111.82
1	K	162	GLU	N-CA-C	7.43	119.38	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	417	ALA	N-CA-C	-7.41	100.42	109.83
2	J	375	GLY	N-CA-C	7.40	119.69	111.85
1	K	164	PRO	N-CA-C	7.39	123.63	113.65
2	J	486	ILE	CA-C-N	-7.39	112.25	120.45
2	J	486	ILE	C-N-CA	-7.39	112.25	120.45
2	F	392	VAL	CA-C-N	7.38	127.55	120.31
2	F	392	VAL	C-N-CA	7.38	127.55	120.31
2	H	486	ILE	CA-C-O	-7.37	113.75	118.69
2	H	379	ILE	CB-CA-C	-7.36	100.60	110.98
2	B	367	PHE	N-CA-C	-7.34	103.17	112.93
1	A	171	ILE	N-CA-C	7.33	118.43	107.51
2	F	426	VAL	CA-C-N	-7.32	113.82	121.35
2	F	426	VAL	C-N-CA	-7.32	113.82	121.35
1	K	120	VAL	CB-CA-C	-7.31	102.89	110.71
2	H	450	ARG	NE-CZ-NH1	-7.30	114.20	121.50
2	F	317	PRO	O-C-N	-7.30	114.34	123.10
1	K	123	ALA	CA-C-N	-7.29	112.47	119.90
1	K	123	ALA	C-N-CA	-7.29	112.47	119.90
1	I	198	PHE	N-CA-C	7.28	121.53	109.95
2	L	314	ASN	N-CA-C	-7.28	104.55	113.50
2	F	488	MET	N-CA-C	-7.27	104.44	113.38
1	E	175	CYS	N-CA-C	-7.26	98.66	108.24
2	J	377	ARG	NE-CZ-NH1	-7.26	114.24	121.50
1	A	94	ARG	NE-CZ-NH2	-7.25	112.67	119.20
2	B	366	ASN	N-CA-C	7.25	121.78	113.15
2	D	445	GLY	CA-C-N	7.23	127.40	120.31
2	D	445	GLY	C-N-CA	7.23	127.40	120.31
2	D	367	PHE	N-CA-C	-7.22	103.32	112.93
2	H	322	PRO	N-CA-C	7.22	124.28	113.81
2	H	313	ARG	N-CA-C	7.21	121.90	113.18
1	C	102	GLY	CA-C-N	7.18	133.34	122.93
1	C	102	GLY	C-N-CA	7.18	133.34	122.93
2	F	434	ASP	N-CA-C	7.15	121.72	112.92
2	B	396	LEU	N-CA-C	7.14	120.88	109.24
1	C	97	THR	N-CA-C	-7.13	98.06	109.76
2	F	460	HIS	N-CA-C	7.12	119.39	108.42
1	E	48	HIS	N-CA-C	7.10	120.95	110.30
2	L	407	ARG	N-CA-C	7.09	120.10	109.25
1	K	64	ARG	N-CA-C	7.06	121.61	112.92
1	A	175	CYS	CA-CB-SG	7.06	130.63	114.40
2	L	350	ASN	N-CA-C	-7.05	97.41	108.90
2	D	489	CYS	N-CA-C	7.04	119.85	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	ARG	CB-CG-CD	7.03	127.47	111.30
1	I	99	PHE	CA-C-N	7.02	130.18	120.63
1	I	99	PHE	C-N-CA	7.02	130.18	120.63
2	L	451	ASN	N-CA-C	-7.01	95.88	110.80
1	G	177	VAL	N-CA-C	-6.96	97.59	107.75
2	D	306	SER	CA-CB-OG	-6.95	97.19	111.10
2	F	432	ASP	CA-C-N	6.95	130.29	120.28
2	F	432	ASP	C-N-CA	6.95	130.29	120.28
1	K	49	ILE	O-C-N	6.94	130.21	122.92
2	H	365	LEU	N-CA-C	6.94	122.85	113.97
2	B	440	ARG	N-CA-C	-6.93	97.66	109.24
2	B	531	ARG	NE-CZ-NH1	-6.93	114.57	121.50
2	L	328	ILE	CA-C-O	-6.93	114.06	121.27
2	J	486	ILE	CB-CA-C	-6.92	107.13	113.70
2	D	426	VAL	CB-CA-C	-6.90	99.88	110.50
1	I	168	GLU	CB-CG-CD	-6.90	100.88	112.60
2	H	470	ILE	CB-CG1-CD1	-6.89	99.34	113.80
1	G	198	PHE	N-CA-C	6.88	120.25	110.14
2	F	436	TYR	N-CA-C	6.87	121.06	110.20
2	H	358	ALA	CA-C-O	-6.87	112.07	119.97
1	C	184	ARG	NE-CZ-NH2	-6.85	113.03	119.20
1	G	101	ALA	CA-C-O	-6.85	113.91	121.58
1	G	81	ASP	N-CA-C	6.85	121.46	113.18
1	C	188	ARG	NE-CZ-NH2	-6.83	113.05	119.20
2	D	469	SER	CA-C-O	-6.83	114.12	121.36
1	C	106	LEU	CB-CG-CD2	-6.83	90.22	110.70
2	H	372	LEU	CA-C-N	-6.82	113.28	120.03
2	H	372	LEU	C-N-CA	-6.82	113.28	120.03
1	A	155	CYS	CA-C-N	-6.79	112.81	119.87
1	A	155	CYS	C-N-CA	-6.79	112.81	119.87
1	K	160	LEU	N-CA-C	-6.79	104.00	112.90
1	G	138	HIS	N-CA-C	6.78	119.47	110.53
2	J	322	PRO	N-CA-C	6.77	123.62	113.81
1	A	46	GLY	N-CA-C	6.76	119.97	111.85
2	J	326	THR	OG1-CB-CG2	-6.76	95.79	109.30
2	D	538	CYS	CA-CB-SG	-6.75	98.86	114.40
1	K	66	SER	CA-CB-OG	-6.75	97.60	111.10
1	G	28	ASN	N-CA-C	-6.73	99.80	110.10
2	J	473	LYS	CD-CE-NZ	-6.73	90.38	111.90
2	B	330	ARG	NE-CZ-NH2	-6.72	113.15	119.20
2	B	451	ASN	N-CA-C	-6.72	97.39	108.48
1	A	99	PHE	CA-C-N	6.72	129.77	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	PHE	C-N-CA	6.72	129.77	120.63
2	D	321	THR	N-CA-C	-6.71	93.85	108.81
1	A	94	ARG	CD-NE-CZ	6.69	133.77	124.40
2	H	330	ARG	NE-CZ-NH1	-6.69	114.81	121.50
2	B	321	THR	CA-C-N	-6.67	111.94	119.28
2	B	321	THR	C-N-CA	-6.67	111.94	119.28
2	B	340	PRO	CB-CA-C	-6.66	102.70	111.23
2	H	475	ILE	CB-CG1-CD1	6.63	127.73	113.80
2	D	339	ILE	CG1-CB-CG2	-6.63	90.80	110.70
1	G	5	LEU	N-CA-C	-6.63	101.41	109.83
2	L	325	LYS	N-CA-C	6.62	120.23	111.75
2	H	367	PHE	N-CA-C	-6.62	104.13	112.93
2	B	302	ALA	N-CA-C	6.62	119.96	110.10
2	J	310	ILE	CB-CG1-CD1	-6.58	99.98	113.80
2	J	349	PRO	N-CA-C	6.58	121.40	111.14
2	D	463	PHE	CA-C-N	-6.57	117.53	122.33
2	D	463	PHE	C-N-CA	-6.57	117.53	122.33
1	E	43	ASP	N-CA-C	6.57	120.21	112.72
1	G	163	GLN	N-CA-C	6.57	117.93	109.72
1	K	177	VAL	CB-CA-C	6.57	118.38	111.09
1	K	146	ASP	N-CA-CB	6.56	121.47	110.32
1	K	163	GLN	CA-C-N	-6.56	112.07	119.28
1	K	163	GLN	C-N-CA	-6.56	112.07	119.28
2	J	496	ALA	N-CA-C	6.55	120.49	112.23
1	A	35	ILE	N-CA-C	-6.55	98.43	107.99
2	J	423	PHE	N-CA-C	6.54	119.06	108.34
1	C	123	ALA	CA-C-N	-6.54	113.03	119.76
1	C	123	ALA	C-N-CA	-6.54	113.03	119.76
1	I	105	THR	O-C-N	-6.52	115.78	123.41
2	H	411	LYS	CB-CA-C	-6.51	99.93	110.74
2	H	473	LYS	N-CA-C	6.51	119.81	110.24
2	F	524	ASP	CA-C-O	-6.51	113.58	120.80
2	J	440	ARG	CB-CG-CD	-6.49	96.38	111.30
2	H	321	THR	N-CA-C	-6.48	94.36	108.81
2	J	416	LEU	N-CA-C	6.47	120.89	113.19
2	J	440	ARG	NE-CZ-NH2	-6.47	113.38	119.20
1	A	2	ILE	CB-CA-C	-6.45	102.69	111.33
2	J	348	GLY	N-CA-C	-6.45	99.19	112.34
2	F	335	ALA	CA-C-O	-6.44	114.07	121.47
1	G	109	VAL	CA-C-O	-6.44	114.16	121.75
2	L	366	ASN	N-CA-C	6.43	120.73	113.01
2	H	457	ARG	CB-CG-CD	6.43	126.09	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	GLU	CA-CB-CG	6.43	126.95	114.10
1	G	98	THR	N-CA-C	6.42	119.58	110.14
1	G	8	THR	CA-C-N	-6.42	113.34	119.76
1	G	8	THR	C-N-CA	-6.42	113.34	119.76
1	K	52	LEU	CA-CB-CG	6.41	138.74	116.30
1	G	126	ILE	N-CA-C	-6.41	98.23	107.78
2	F	321	THR	CA-C-N	-6.41	113.03	119.56
2	F	321	THR	C-N-CA	-6.41	113.03	119.56
2	J	495	ILE	CB-CA-C	-6.40	102.83	111.15
1	K	133	ARG	N-CA-CB	-6.39	100.18	109.83
2	B	487	PRO	CA-C-N	-6.39	112.00	122.54
2	B	487	PRO	C-N-CA	-6.39	112.00	122.54
2	B	495	ILE	CG1-CB-CG2	-6.39	91.54	110.70
1	C	31	ARG	N-CA-C	-6.39	101.33	110.59
2	H	475	ILE	N-CA-C	-6.38	99.27	108.53
2	J	497	ASN	CA-C-O	6.38	123.44	119.29
1	E	184	ARG	NE-CZ-NH2	-6.38	113.46	119.20
2	F	404	ALA	N-CA-C	6.37	120.16	112.38
2	H	495	ILE	N-CA-C	-6.37	97.94	107.37
2	H	498	PRO	CB-CG-CD	-6.36	85.75	106.10
2	J	416	LEU	CA-CB-CG	6.36	138.54	116.30
2	F	430	LEU	CA-C-O	-6.35	113.62	120.92
1	A	120	VAL	N-CA-C	-6.32	100.52	107.73
1	C	136	ASN	N-CA-C	6.32	118.25	111.36
2	H	458	PRO	N-CA-C	-6.32	102.37	111.22
1	I	8	THR	CA-C-N	-6.32	113.47	119.85
1	I	8	THR	C-N-CA	-6.32	113.47	119.85
2	L	417	ALA	CA-C-N	-6.32	114.27	120.52
2	L	417	ALA	C-N-CA	-6.32	114.27	120.52
1	E	52	LEU	CA-CB-CG	6.31	138.38	116.30
2	B	528	ARG	NE-CZ-NH1	-6.29	115.20	121.50
1	E	98	THR	N-CA-C	6.29	119.01	109.95
1	E	162	GLU	CB-CA-C	-6.29	101.00	110.88
2	B	379	ILE	CB-CA-C	-6.29	102.11	110.98
2	D	438	SER	N-CA-C	6.29	119.51	108.75
1	A	94	ARG	NE-CZ-NH1	6.28	127.78	121.50
2	B	390	LYS	CB-CA-C	6.28	117.73	108.87
2	J	328	ILE	N-CA-C	6.28	116.39	110.30
1	I	142	ARG	NE-CZ-NH2	-6.28	113.55	119.20
1	A	23	LEU	N-CA-C	6.27	118.12	111.28
1	E	22	ALA	N-CA-C	-6.27	100.95	109.54
1	A	37	ASN	N-CA-C	6.26	119.86	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	443	LYS	CA-C-N	-6.26	113.84	120.03
2	B	443	LYS	C-N-CA	-6.26	113.84	120.03
1	C	19	ILE	O-C-N	6.26	128.87	121.80
2	H	435	GLY	CA-C-O	-6.26	111.50	119.13
2	D	464	GLY	CA-C-O	-6.25	114.63	120.57
2	F	418	PRO	N-CA-C	6.25	121.06	111.57
2	H	428	ARG	CD-NE-CZ	6.24	133.14	124.40
1	K	103	GLU	CA-CB-CG	6.24	126.58	114.10
1	K	120	VAL	N-CA-C	6.23	114.05	107.76
2	J	447	TYR	OH-CZ-CE2	-6.23	101.21	119.90
1	G	142	ARG	CB-CG-CD	-6.22	96.99	111.30
2	L	532	LYS	N-CA-C	-6.22	102.32	110.53
2	H	456	TRP	CA-C-N	-6.22	111.09	120.60
2	H	456	TRP	C-N-CA	-6.22	111.09	120.60
1	E	167	ARG	CA-C-N	-6.21	111.33	120.28
1	E	167	ARG	C-N-CA	-6.21	111.33	120.28
2	F	367	PHE	N-CA-C	-6.21	104.67	112.93
1	C	102	GLY	CA-C-O	6.21	126.54	119.09
2	H	505	ILE	CA-CB-CG1	6.21	120.95	110.40
2	J	375	GLY	CA-C-O	-6.20	117.31	122.33
1	K	135	ILE	N-CA-CB	-6.18	103.88	111.67
2	L	496	ALA	N-CA-C	6.18	118.99	111.82
2	F	473	LYS	CG-CD-CE	-6.17	97.11	111.30
2	H	457	ARG	N-CA-C	6.17	118.41	109.84
2	F	324	TYR	N-CA-C	-6.16	97.14	107.99
2	F	360	ASP	N-CA-C	6.16	118.79	111.71
1	K	171	ILE	CA-C-N	6.16	129.61	120.87
1	K	171	ILE	C-N-CA	6.16	129.61	120.87
2	H	330	ARG	NE-CZ-NH2	6.16	124.74	119.20
1	I	5	LEU	N-CA-C	-6.15	101.59	110.08
2	J	325	LYS	N-CA-C	6.15	118.49	111.11
2	L	460	HIS	N-CA-C	6.15	118.42	109.07
2	J	518	CYS	N-CA-C	6.14	118.64	108.99
1	G	38	ARG	CG-CD-NE	-6.14	98.49	112.00
2	H	414	ARG	CA-CB-CG	6.14	126.38	114.10
2	J	450	ARG	N-CA-C	6.13	118.82	109.62
2	H	428	ARG	N-CA-C	-6.12	100.03	109.14
1	G	19	ILE	CB-CG1-CD1	-6.11	100.97	113.80
1	C	167	ARG	NE-CZ-NH1	-6.11	115.39	121.50
1	C	120	VAL	CB-CA-C	-6.11	105.26	110.94
2	D	390	LYS	CB-CA-C	6.10	118.17	109.08
1	E	103	GLU	N-CA-C	6.10	119.41	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	472	THR	CB-CA-C	-6.10	98.01	109.72
2	L	528	ARG	NE-CZ-NH1	-6.10	115.40	121.50
2	J	502	GLN	N-CA-C	6.10	118.72	111.71
1	A	38	ARG	NE-CZ-NH2	-6.09	113.72	119.20
1	A	52	LEU	CA-CB-CG	6.09	137.63	116.30
2	H	473	LYS	CD-CE-NZ	-6.09	92.42	111.90
1	K	38	ARG	CA-CB-CG	6.09	126.28	114.10
1	I	5	LEU	CA-C-N	-6.07	113.70	120.14
1	I	5	LEU	C-N-CA	-6.07	113.70	120.14
2	L	418	PRO	N-CA-C	6.07	120.18	111.13
2	F	427	GLY	CA-C-O	-6.07	115.13	121.63
2	F	494	SER	N-CA-C	-6.07	105.73	113.01
2	L	436	TYR	N-CA-C	6.06	119.70	109.76
2	J	390	LYS	N-CA-CB	-6.06	102.11	110.29
2	J	493	LYS	CD-CE-NZ	6.06	131.29	111.90
2	B	522	ARG	NE-CZ-NH1	-6.06	115.44	121.50
1	E	80	GLN	CB-CG-CD	6.05	122.89	112.60
2	F	489	CYS	CA-C-N	6.05	125.77	119.05
2	F	489	CYS	C-N-CA	6.05	125.77	119.05
2	H	433	SER	CA-C-N	-6.05	112.99	122.49
2	H	433	SER	C-N-CA	-6.05	112.99	122.49
2	D	379	ILE	CA-CB-CG1	6.05	120.68	110.40
2	D	459	ALA	N-CA-C	-6.05	101.46	110.23
1	G	175	CYS	CA-CB-SG	6.05	128.31	114.40
1	A	42	PRO	N-CA-C	6.04	121.70	113.84
1	E	26	ALA	N-CA-C	-6.04	105.56	113.17
1	A	156	PRO	CA-C-N	-6.04	111.56	121.34
1	A	156	PRO	C-N-CA	-6.04	111.56	121.34
1	C	19	ILE	CB-CG1-CD1	-6.03	101.14	113.80
2	J	323	ASP	N-CA-CB	-6.03	100.94	110.22
2	H	377	ARG	NE-CZ-NH1	-6.03	115.47	121.50
1	G	14	GLY	CA-C-N	6.02	125.90	119.28
1	G	14	GLY	C-N-CA	6.02	125.90	119.28
2	J	310	ILE	N-CA-C	6.01	118.29	109.63
2	J	525	ILE	N-CA-C	-6.01	99.50	108.46
2	F	387	GLN	CA-C-O	-6.00	112.00	119.38
1	E	36	TRP	N-CA-C	6.00	116.00	108.45
1	K	133	ARG	NE-CZ-NH2	-5.99	113.81	119.20
2	J	332	PRO	CB-CA-C	-5.99	102.07	110.63
2	D	416	LEU	N-CA-C	5.99	120.19	113.01
2	B	338	SER	CA-C-O	-5.98	115.04	121.56
2	B	473	LYS	CB-CA-C	5.98	120.47	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	31	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	C	64	ARG	NE-CZ-NH2	-5.97	113.83	119.20
2	F	344	SER	N-CA-C	5.97	117.46	111.07
2	B	418	PRO	N-CA-C	5.96	119.56	111.22
2	B	334	GLN	O-C-N	-5.94	116.29	122.94
2	J	522	ARG	NE-CZ-NH1	-5.94	115.56	121.50
2	L	332	PRO	CB-CA-C	-5.94	103.20	110.98
2	L	497	ASN	CA-C-N	-5.93	113.57	119.56
2	L	497	ASN	C-N-CA	-5.93	113.57	119.56
1	I	133	ARG	N-CA-C	-5.93	100.83	110.20
2	B	395	THR	CA-CB-CG2	5.93	120.58	110.50
2	F	457	ARG	NH1-CZ-NH2	5.93	127.01	119.30
2	F	468	PRO	N-CA-C	5.93	120.84	114.68
2	D	537	ASN	N-CA-C	-5.92	103.07	111.24
2	H	390	LYS	N-CA-CB	-5.92	101.56	110.32
1	C	113	VAL	N-CA-C	5.92	117.72	109.55
2	F	414	ARG	N-CA-C	-5.91	105.98	112.72
1	A	94	ARG	CA-CB-CG	5.91	125.91	114.10
2	H	418	PRO	N-CA-C	5.91	120.27	111.41
2	F	375	GLY	CA-C-N	5.90	129.74	121.24
2	F	375	GLY	C-N-CA	5.90	129.74	121.24
1	G	94	ARG	CD-NE-CZ	5.90	132.66	124.40
1	A	103	GLU	CA-C-O	-5.90	114.33	120.70
1	C	140	HIS	CB-CA-C	-5.90	100.02	109.75
1	I	95	THR	CA-C-O	-5.90	114.36	121.32
2	B	460	HIS	N-CA-C	5.90	117.75	108.96
2	D	420	ASP	CA-C-N	5.90	125.52	119.56
2	D	420	ASP	C-N-CA	5.90	125.52	119.56
2	H	379	ILE	N-CA-C	-5.89	99.94	108.71
2	J	495	ILE	N-CA-CB	5.89	116.95	110.53
2	L	396	LEU	N-CA-C	5.89	119.12	109.76
2	F	457	ARG	CA-C-N	-5.88	112.48	119.84
2	F	457	ARG	C-N-CA	-5.88	112.48	119.84
1	I	195	THR	CA-C-O	-5.88	114.05	120.81
2	J	430	LEU	N-CA-CB	-5.88	100.85	110.43
1	C	104	TRP	CA-C-N	-5.88	112.69	122.21
1	C	104	TRP	C-N-CA	-5.88	112.69	122.21
2	F	371	GLY	N-CA-C	5.88	119.71	111.19
2	L	479	TYR	CA-CB-CG	-5.88	103.33	113.90
1	I	108	THR	CA-C-O	-5.87	114.64	120.80
2	J	439	PHE	CA-C-N	-5.87	114.71	122.99
2	J	439	PHE	C-N-CA	-5.87	114.71	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	69	GLU	N-CA-C	-5.87	98.31	108.69
2	D	371	GLY	N-CA-C	5.87	119.33	110.18
2	D	328	ILE	N-CA-C	5.86	116.33	110.23
2	L	420	ASP	CB-CA-C	5.86	116.68	110.17
2	L	510	MET	CA-CB-CG	5.86	125.82	114.10
1	C	80	GLN	CB-CG-CD	5.86	122.56	112.60
1	A	110	LYS	CA-C-N	5.85	125.81	119.78
1	A	110	LYS	C-N-CA	5.85	125.81	119.78
2	B	379	ILE	CA-CB-CG1	5.85	120.34	110.40
2	D	428	ARG	NE-CZ-NH2	-5.85	113.94	119.20
2	F	428	ARG	NE-CZ-NH2	-5.85	113.94	119.20
2	L	412	ASN	N-CA-C	5.85	120.03	113.01
2	D	495	ILE	CB-CG1-CD1	5.85	126.08	113.80
1	C	192	GLU	N-CA-CB	-5.85	100.61	110.49
2	F	525	ILE	CB-CG1-CD1	-5.84	101.53	113.80
2	H	367	PHE	CA-C-N	5.84	132.70	121.54
2	H	367	PHE	C-N-CA	5.84	132.70	121.54
1	E	168	GLU	CA-CB-CG	-5.84	102.41	114.10
1	G	13	ALA	CA-C-N	-5.84	112.70	121.87
1	G	13	ALA	C-N-CA	-5.84	112.70	121.87
1	G	123	ALA	CA-C-N	-5.83	113.95	119.90
1	G	123	ALA	C-N-CA	-5.83	113.95	119.90
1	K	106	LEU	CB-CG-CD2	-5.83	93.21	110.70
2	J	504	LEU	CB-CG-CD1	-5.82	93.23	110.70
2	D	333	ARG	NE-CZ-NH2	5.82	124.44	119.20
2	L	384	VAL	CA-C-O	-5.81	114.31	120.53
1	A	60	GLY	N-CA-C	-5.81	107.16	115.64
2	H	413	ASP	CA-C-N	-5.81	113.49	122.49
2	H	413	ASP	C-N-CA	-5.81	113.49	122.49
1	A	76	ASN	N-CA-CB	5.80	119.32	110.44
1	E	157	VAL	N-CA-C	-5.80	106.05	111.45
2	J	511	ASN	N-CA-C	-5.80	105.04	111.71
2	B	438	SER	O-C-N	-5.80	116.99	123.48
2	B	354	LEU	N-CA-C	-5.79	101.04	110.20
1	A	140	HIS	CB-CA-C	-5.79	100.81	110.19
2	B	491	ILE	CB-CA-C	-5.79	104.23	112.22
1	E	93	GLY	CA-C-O	-5.79	115.53	121.61
1	K	99	PHE	CA-C-N	5.78	128.50	120.29
1	K	99	PHE	C-N-CA	5.78	128.50	120.29
1	C	180	LYS	CB-CA-C	5.78	121.11	109.38
2	B	371	GLY	CA-C-O	5.78	127.39	121.21
2	D	366	ASN	N-CA-C	5.78	120.19	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	LEU	N-CA-C	5.77	118.03	111.11
2	F	465	ILE	CA-C-O	-5.77	114.21	120.67
1	G	76	ASN	CB-CG-ND2	-5.77	107.75	116.40
1	C	26	ALA	N-CA-C	-5.76	106.01	113.16
2	D	504	LEU	N-CA-C	-5.76	105.91	113.17
1	K	189	ILE	N-CA-C	5.76	116.50	110.62
2	H	449	TRP	CA-C-N	-5.76	114.25	122.77
2	H	449	TRP	C-N-CA	-5.76	114.25	122.77
2	B	460	HIS	CA-C-O	-5.75	115.29	121.45
1	E	24	GLU	CA-C-O	-5.75	114.98	120.90
2	F	400	TRP	N-CA-C	-5.75	100.56	109.24
2	H	469	SER	N-CA-C	5.75	116.99	108.60
2	H	473	LYS	CB-CA-C	5.75	118.46	109.84
2	D	515	PRO	CB-CA-C	-5.74	102.09	111.56
1	A	169	THR	N-CA-C	-5.73	105.55	112.54
1	I	104	TRP	N-CA-C	-5.73	101.72	110.14
2	F	330	ARG	NE-CZ-NH2	-5.72	114.05	119.20
2	F	448	PRO	CA-C-N	-5.72	113.21	122.36
2	F	448	PRO	C-N-CA	-5.72	113.21	122.36
2	L	452	GLY	CA-C-N	-5.72	113.86	120.04
2	L	452	GLY	C-N-CA	-5.72	113.86	120.04
1	I	2	ILE	CG1-CB-CG2	-5.72	93.55	110.70
1	C	38	ARG	N-CA-CB	-5.71	99.10	110.64
2	D	494	SER	N-CA-C	-5.71	105.58	112.54
2	B	332	PRO	N-CA-C	5.71	120.28	111.21
2	D	349	PRO	N-CA-C	5.71	120.15	111.19
2	B	481	GLU	CA-C-O	-5.70	115.25	120.95
2	H	341	GLN	CA-C-O	-5.70	113.88	120.49
2	B	530	GLN	CA-C-O	-5.70	114.21	120.36
1	K	167	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	I	113	VAL	N-CA-C	5.69	116.40	108.89
2	L	342	SER	N-CA-C	-5.69	98.67	110.80
2	L	388	TYR	CE1-CZ-OH	-5.69	102.83	119.90
1	E	138	HIS	N-CA-C	5.68	118.08	110.35
2	F	482	GLY	CA-C-O	-5.68	113.02	119.04
2	F	492	VAL	N-CA-C	-5.68	104.98	110.72
2	B	439	PHE	CA-C-N	-5.68	113.52	122.73
2	B	439	PHE	C-N-CA	-5.68	113.52	122.73
1	C	31	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	K	31	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	K	47	GLU	CA-CB-CG	-5.68	102.75	114.10
2	F	486	ILE	CA-C-N	-5.67	114.15	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	486	ILE	C-N-CA	-5.67	114.15	120.45
1	K	13	ALA	N-CA-C	-5.67	105.86	112.89
1	C	36	TRP	N-CA-C	5.67	115.89	108.07
2	J	505	ILE	N-CA-C	5.67	115.95	107.51
1	A	53	GLY	N-CA-C	5.66	119.83	110.55
2	D	398	GLU	N-CA-C	-5.65	100.58	109.50
2	J	443	LYS	CA-C-N	-5.65	114.78	120.31
2	J	443	LYS	C-N-CA	-5.65	114.78	120.31
2	D	316	HIS	N-CA-C	-5.64	101.84	110.07
2	L	384	VAL	CB-CA-C	-5.64	102.73	110.96
1	A	137	ILE	CA-C-O	-5.64	114.61	120.64
1	C	78	GLU	CA-CB-CG	-5.63	102.83	114.10
1	I	94	ARG	CA-CB-CG	5.63	125.36	114.10
1	C	174	ARG	NE-CZ-NH1	-5.63	115.87	121.50
2	H	502	GLN	CA-C-O	5.62	126.45	120.10
1	C	42	PRO	N-CA-C	5.62	121.95	113.81
1	A	160	LEU	CD1-CG-CD2	-5.62	98.44	110.80
1	E	188	ARG	NH1-CZ-NH2	-5.62	112.00	119.30
2	H	420	ASP	CA-C-N	5.62	125.29	119.56
2	H	420	ASP	C-N-CA	5.62	125.29	119.56
2	D	427	GLY	CA-C-O	-5.61	115.63	121.63
1	E	37	ASN	N-CA-CB	-5.61	102.44	110.57
2	D	493	LYS	N-CA-C	5.61	119.86	113.19
2	F	528	ARG	CA-C-O	-5.60	115.03	121.19
2	L	425	GLY	N-CA-C	5.60	124.17	115.72
2	D	447	TYR	CA-C-N	5.60	126.03	119.99
2	D	447	TYR	C-N-CA	5.60	126.03	119.99
2	L	475	ILE	N-CA-C	-5.59	100.12	108.46
2	H	324	TYR	N-CA-C	-5.59	97.47	107.98
1	C	24	GLU	N-CA-C	-5.58	104.84	111.03
2	F	486	ILE	CB-CG1-CD1	-5.58	102.09	113.80
2	L	457	ARG	CB-CA-C	-5.58	100.74	109.11
2	F	379	ILE	CB-CA-C	-5.58	103.57	111.21
2	D	357	GLY	N-CA-C	-5.58	103.98	112.51
2	D	402	ALA	N-CA-C	5.57	117.10	110.19
1	K	94	ARG	CB-CG-CD	5.57	124.12	111.30
2	B	453	PRO	N-CD-CG	-5.57	94.84	103.20
2	D	465	ILE	CA-C-N	-5.56	113.07	120.63
2	D	465	ILE	C-N-CA	-5.56	113.07	120.63
2	D	520	ALA	N-CA-C	5.56	117.63	109.24
2	F	462	HIS	CA-C-O	-5.56	114.35	120.69
1	G	199	ASP	N-CA-C	-5.56	99.96	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	367	PHE	CB-CA-C	5.55	119.03	109.15
2	B	498	PRO	N-CA-C	5.55	121.14	113.65
1	E	162	GLU	N-CA-CB	5.55	118.06	110.01
1	E	2	ILE	CB-CG1-CD1	-5.54	102.16	113.80
2	B	446	PRO	N-CA-C	-5.54	102.87	111.13
2	F	504	LEU	N-CA-C	-5.54	106.19	113.17
2	F	326	THR	N-CA-C	-5.54	105.78	112.54
2	J	464	GLY	N-CA-C	-5.54	100.06	113.18
1	K	144	TYR	CA-C-N	-5.54	114.90	122.93
1	K	144	TYR	C-N-CA	-5.54	114.90	122.93
2	F	457	ARG	NE-CZ-NH2	-5.53	114.22	119.20
2	J	445	GLY	CA-C-N	5.53	125.50	120.03
2	J	445	GLY	C-N-CA	5.53	125.50	120.03
1	K	53	GLY	N-CA-C	5.53	118.59	110.80
2	L	388	TYR	OH-CZ-CE2	5.53	136.48	119.90
2	F	428	ARG	N-CA-C	-5.53	100.90	109.24
2	L	307	ARG	N-CA-C	-5.53	100.77	109.50
2	D	446	PRO	N-CA-C	-5.52	103.18	111.57
1	G	176	GLU	CB-CG-CD	5.52	121.98	112.60
2	D	351	PHE	N-CA-C	5.51	119.11	112.93
2	F	475	ILE	CB-CA-C	-5.51	102.41	110.62
1	K	124	PRO	CA-C-O	-5.51	115.13	121.36
2	L	516	MET	N-CA-CB	5.51	121.21	112.78
1	I	139	LEU	CA-C-N	5.51	130.92	122.93
1	I	139	LEU	C-N-CA	5.51	130.92	122.93
2	J	351	PHE	N-CA-C	5.51	119.00	112.72
1	A	157	VAL	N-CA-C	-5.50	105.75	111.58
2	D	522	ARG	CA-C-N	-5.50	114.82	123.13
2	D	522	ARG	C-N-CA	-5.50	114.82	123.13
2	D	426	VAL	CA-C-O	-5.50	114.51	120.67
2	F	353	HIS	N-CA-C	5.50	119.68	112.92
2	F	500	ALA	N-CA-C	-5.50	105.30	112.23
2	D	507	LYS	CB-CG-CD	5.49	123.93	111.30
2	L	416	LEU	N-CA-C	5.49	119.69	112.89
2	L	508	LEU	CA-C-N	-5.48	114.80	123.24
2	L	508	LEU	C-N-CA	-5.48	114.80	123.24
2	F	347	THR	N-CA-C	-5.48	101.43	109.81
1	I	94	ARG	CD-NE-CZ	5.47	132.06	124.40
2	B	426	VAL	CB-CA-C	-5.47	102.08	110.50
2	L	517	ASP	N-CA-CB	-5.46	101.25	110.49
2	F	314	ASN	N-CA-C	-5.46	106.66	113.38
1	K	72	GLN	N-CA-C	5.46	117.38	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	477	GLN	CA-C-N	5.45	130.78	122.65
2	B	477	GLN	C-N-CA	5.45	130.78	122.65
2	D	331	SER	CA-C-N	-5.45	114.97	120.21
2	D	331	SER	C-N-CA	-5.45	114.97	120.21
1	E	102	GLY	CA-C-O	5.45	126.10	119.01
1	E	106	LEU	CB-CG-CD2	-5.45	94.34	110.70
1	E	133	ARG	N-CA-CB	5.45	118.36	109.69
2	B	496	ALA	N-CA-C	5.45	118.14	111.82
1	K	88	ALA	N-CA-C	-5.45	105.50	111.82
2	F	507	LYS	CB-CG-CD	-5.45	98.77	111.30
2	L	504	LEU	CA-C-N	-5.45	115.80	122.93
2	L	504	LEU	C-N-CA	-5.45	115.80	122.93
2	F	442	ILE	CG1-CB-CG2	-5.44	94.38	110.70
2	L	448	PRO	O-C-N	-5.44	116.21	123.06
1	K	133	ARG	N-CA-C	-5.44	102.34	110.23
1	K	101	ALA	CA-C-O	-5.44	112.96	120.52
1	A	15	PRO	CA-C-N	-5.43	114.13	122.60
1	A	15	PRO	C-N-CA	-5.43	114.13	122.60
1	C	162	GLU	N-CA-C	5.42	117.19	111.28
1	G	102	GLY	CA-C-N	5.42	130.72	122.65
1	G	102	GLY	C-N-CA	5.42	130.72	122.65
2	D	439	PHE	CA-C-N	-5.42	115.36	123.00
2	D	439	PHE	C-N-CA	-5.42	115.36	123.00
1	K	171	ILE	N-CA-CB	-5.42	104.84	111.67
1	A	128	ILE	CA-C-O	-5.41	114.34	120.67
1	E	57	ASP	N-CA-C	-5.41	101.44	109.94
2	D	418	PRO	N-CA-C	5.41	119.52	111.41
1	G	26	ALA	N-CA-C	-5.41	106.72	113.15
1	I	123	ALA	CA-C-N	-5.41	113.08	119.84
1	I	123	ALA	C-N-CA	-5.41	113.08	119.84
1	I	142	ARG	NE-CZ-NH1	5.41	126.91	121.50
2	D	401	GLN	N-CA-C	5.40	116.74	108.42
1	G	113	VAL	N-CA-C	5.40	116.36	108.58
2	F	433	SER	CA-C-N	-5.40	114.01	122.65
2	F	433	SER	C-N-CA	-5.40	114.01	122.65
1	A	188	ARG	CB-CG-CD	5.39	123.70	111.30
2	J	307	ARG	N-CA-C	-5.39	100.88	109.23
2	D	423	PHE	N-CA-C	5.39	117.68	108.90
2	B	474	LEU	CD1-CG-CD2	-5.38	98.95	110.80
1	A	72	GLN	N-CA-C	5.38	117.25	109.07
2	F	435	GLY	N-CA-C	-5.38	107.89	115.32
1	G	173	LYS	CA-C-N	5.38	128.74	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	173	LYS	C-N-CA	5.38	128.74	121.05
2	B	450	ARG	CA-C-O	-5.38	115.69	122.63
1	E	81	ASP	CB-CG-OD1	5.38	130.76	118.40
1	E	81	ASP	N-CA-C	5.37	119.89	113.23
2	L	328	ILE	N-CA-CB	5.37	116.47	110.51
2	L	425	GLY	CA-C-N	5.37	130.45	122.71
2	L	425	GLY	C-N-CA	5.37	130.45	122.71
1	K	149	ALA	CA-C-N	-5.37	113.56	120.65
1	K	149	ALA	C-N-CA	-5.37	113.56	120.65
2	L	345	GLU	N-CA-C	5.37	119.93	112.90
2	B	442	ILE	CB-CG1-CD1	-5.36	102.54	113.80
2	B	372	LEU	N-CA-C	5.36	117.70	110.31
2	B	438	SER	N-CA-C	5.36	117.22	108.76
1	C	117	ALA	N-CA-C	-5.36	105.55	111.71
1	I	100	ASP	O-C-N	5.36	127.81	122.03
1	K	33	GLN	N-CA-C	5.36	117.36	108.20
1	I	41	LYS	CA-CB-CG	-5.35	103.39	114.10
2	J	449	TRP	CA-C-N	-5.35	114.13	122.05
2	J	449	TRP	C-N-CA	-5.35	114.13	122.05
1	C	145	PHE	N-CA-C	5.35	117.68	109.07
1	A	9	PRO	CB-CA-C	-5.35	104.39	111.23
2	D	465	ILE	CB-CA-C	-5.34	102.53	110.33
2	L	497	ASN	N-CA-CB	-5.34	101.67	109.90
1	G	12	THR	N-CA-C	5.34	117.18	110.24
2	D	486	ILE	N-CA-C	5.34	119.34	112.67
2	B	365	LEU	CA-C-O	-5.33	112.56	118.69
1	I	192	GLU	CB-CG-CD	-5.33	103.53	112.60
2	F	398	GLU	N-CA-C	-5.33	101.08	109.50
2	J	310	ILE	CA-C-N	-5.33	113.15	120.71
2	J	310	ILE	C-N-CA	-5.33	113.15	120.71
2	J	440	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	K	174	ARG	CA-CB-CG	-5.32	103.45	114.10
2	J	517	ASP	N-CA-CB	-5.32	101.50	110.49
1	A	44	ALA	CA-C-N	-5.32	114.44	119.76
1	A	44	ALA	C-N-CA	-5.32	114.44	119.76
2	D	525	ILE	CA-C-O	-5.31	114.86	120.39
2	L	433	SER	CB-CA-C	-5.31	100.81	110.63
1	I	113	VAL	N-CA-CB	-5.30	104.75	110.53
2	L	310	ILE	CG1-CB-CG2	-5.30	94.79	110.70
2	J	470	ILE	CB-CG1-CD1	-5.30	102.67	113.80
2	L	353	HIS	CA-C-N	-5.30	112.62	120.94
2	L	353	HIS	C-N-CA	-5.30	112.62	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	CYS	CA-C-N	-5.29	114.37	119.87
1	C	155	CYS	C-N-CA	-5.29	114.37	119.87
2	H	410	HIS	CA-C-N	5.29	128.76	120.82
2	H	410	HIS	C-N-CA	5.29	128.76	120.82
1	E	101	ALA	CA-C-O	-5.29	112.30	120.81
2	H	426	VAL	CA-C-N	-5.28	115.91	121.35
2	H	426	VAL	C-N-CA	-5.28	115.91	121.35
1	K	36	TRP	CB-CA-C	5.28	120.93	110.42
2	B	497	ASN	CA-C-N	-5.28	113.47	119.28
2	B	497	ASN	C-N-CA	-5.28	113.47	119.28
2	L	422	ASN	CA-C-N	-5.28	113.29	122.37
2	L	422	ASN	C-N-CA	-5.28	113.29	122.37
2	J	475	ILE	N-CA-C	-5.28	100.88	108.48
2	L	405	GLY	O-C-N	-5.28	116.25	122.27
2	J	359	HIS	CA-CB-CG	-5.28	108.52	113.80
2	D	369	ASN	O-C-N	5.27	128.53	121.99
2	F	321	THR	N-CA-C	-5.27	97.05	108.81
2	J	428	ARG	CA-C-O	-5.27	115.44	121.40
1	G	94	ARG	CB-CG-CD	5.27	123.42	111.30
1	G	156	PRO	CA-C-N	-5.27	113.85	121.65
1	G	156	PRO	C-N-CA	-5.27	113.85	121.65
2	D	538	CYS	N-CA-C	5.27	125.75	111.00
2	B	344	SER	CA-CB-OG	-5.26	100.58	111.10
2	B	465	ILE	O-C-N	-5.26	117.52	123.20
1	I	120	VAL	CA-C-N	5.26	125.42	119.90
1	I	120	VAL	C-N-CA	5.26	125.42	119.90
1	E	108	THR	CA-C-O	-5.25	116.41	120.19
1	E	139	LEU	CB-CG-CD1	-5.25	94.94	110.70
2	H	350	ASN	N-CA-C	-5.25	99.85	108.41
1	E	56	TYR	N-CA-C	5.25	118.12	109.72
1	G	118	ALA	CA-C-N	-5.25	113.85	122.20
1	G	118	ALA	C-N-CA	-5.25	113.85	122.20
2	L	537	ASN	CA-C-N	5.25	131.15	121.70
2	L	537	ASN	C-N-CA	5.25	131.15	121.70
2	B	390	LYS	N-CA-CB	-5.25	103.21	110.29
1	I	138	HIS	N-CA-C	5.25	117.06	110.24
2	L	437	TYR	CA-C-N	-5.25	112.56	121.85
2	L	437	TYR	C-N-CA	-5.25	112.56	121.85
1	I	172	ALA	CA-C-O	-5.24	115.29	121.16
2	J	537	ASN	CA-C-N	5.24	131.13	121.70
2	J	537	ASN	C-N-CA	5.24	131.13	121.70
2	J	447	TYR	CE1-CZ-OH	5.24	135.61	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	336	LEU	CB-CA-C	-5.23	100.70	109.65
2	H	426	VAL	CA-C-O	-5.23	114.55	120.67
1	A	130	LEU	CA-C-N	5.23	131.02	122.81
1	A	130	LEU	C-N-CA	5.23	131.02	122.81
1	E	49	ILE	CA-C-O	-5.23	116.18	121.67
1	A	113	VAL	N-CA-C	5.23	116.32	109.21
1	K	120	VAL	CA-C-N	5.23	125.14	119.76
1	K	120	VAL	C-N-CA	5.23	125.14	119.76
1	I	148	GLU	CB-CA-C	-5.22	103.04	111.18
1	K	18	HIS	N-CA-C	5.22	116.65	111.07
2	B	314	ASN	N-CA-C	-5.22	106.60	113.17
1	K	97	THR	CA-C-N	-5.21	113.64	123.27
1	K	97	THR	C-N-CA	-5.21	113.64	123.27
1	A	162	GLU	CB-CA-C	-5.20	102.15	110.79
1	C	9	PRO	CB-CA-C	-5.20	104.16	110.98
1	C	126	ILE	CA-CB-CG1	-5.20	101.56	110.40
2	B	473	LYS	CD-CE-NZ	-5.20	95.26	111.90
1	E	113	VAL	N-CA-C	5.20	115.75	108.89
2	J	444	PRO	CA-C-O	-5.20	115.67	122.12
2	H	524	ASP	N-CA-CB	5.20	118.88	110.41
1	C	98	THR	N-CA-C	5.19	118.05	109.85
1	I	177	VAL	O-C-N	5.19	128.06	123.03
1	G	103	GLU	CB-CA-C	-5.19	100.77	109.48
2	L	491	ILE	N-CA-C	-5.19	105.35	111.00
1	C	24	GLU	CB-CG-CD	-5.18	103.80	112.60
1	K	100	ASP	CB-CA-C	-5.18	102.05	110.85
2	F	474	LEU	CB-CG-CD2	-5.17	95.17	110.70
2	J	468	PRO	N-CA-C	5.17	120.41	114.20
2	F	469	SER	CA-C-O	-5.17	115.75	121.28
2	D	312	ASP	CA-CB-CG	-5.17	107.43	112.60
1	E	45	PRO	CB-CA-C	-5.17	104.45	111.12
1	G	55	VAL	CG1-CB-CG2	-5.17	99.42	110.80
2	H	428	ARG	NE-CZ-NH2	-5.17	114.55	119.20
2	J	315	TRP	CA-C-N	5.17	129.30	121.03
2	J	315	TRP	C-N-CA	5.17	129.30	121.03
2	H	418	PRO	CA-C-O	-5.17	115.47	122.08
2	J	323	ASP	N-CA-C	-5.17	105.77	111.71
2	D	340	PRO	CA-C-O	-5.16	115.50	121.95
2	F	335	ALA	N-CA-C	-5.16	102.84	110.48
2	D	500	ALA	N-CA-C	-5.16	105.73	112.23
1	E	50	LEU	CD1-CG-CD2	-5.16	99.44	110.80
1	G	91	SER	N-CA-CB	-5.16	101.36	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	507	LYS	O-C-N	-5.16	117.17	123.10
1	E	23	LEU	O-C-N	5.15	127.45	122.09
1	E	52	LEU	CB-CG-CD2	-5.15	95.26	110.70
2	H	492	VAL	CA-C-O	-5.15	115.78	121.29
1	E	13	ALA	N-CA-C	-5.14	106.10	112.38
2	H	420	ASP	N-CA-C	-5.14	100.56	109.15
2	D	457	ARG	CG-CD-NE	5.14	123.31	112.00
2	F	537	ASN	CA-C-N	5.14	130.95	121.70
2	F	537	ASN	C-N-CA	5.14	130.95	121.70
2	J	497	ASN	N-CA-CB	-5.14	103.65	110.17
2	H	440	ARG	CB-CG-CD	-5.13	99.49	111.30
2	F	367	PHE	CA-C-N	5.13	131.34	121.54
2	F	367	PHE	C-N-CA	5.13	131.34	121.54
2	H	489	CYS	CA-C-N	-5.13	114.50	120.04
2	H	489	CYS	C-N-CA	-5.13	114.50	120.04
2	F	487	PRO	N-CA-C	5.13	120.76	114.35
2	J	463	PHE	CA-C-O	-5.12	114.77	120.66
2	F	403	ASN	N-CA-CB	5.12	118.33	110.49
1	I	112	GLY	CA-C-N	5.12	128.73	121.66
1	I	112	GLY	C-N-CA	5.12	128.73	121.66
2	J	390	LYS	CA-CB-CG	5.12	124.34	114.10
1	I	160	LEU	CD1-CG-CD2	-5.12	99.54	110.80
2	J	331	SER	N-CA-C	-5.12	102.27	110.10
1	C	54	GLN	CA-C-N	5.12	129.84	123.14
1	C	54	GLN	C-N-CA	5.12	129.84	123.14
1	C	158	LEU	CA-CB-CG	5.12	134.20	116.30
2	D	373	PRO	CA-C-N	-5.11	114.32	122.50
2	D	373	PRO	C-N-CA	-5.11	114.32	122.50
1	C	38	ARG	CG-CD-NE	-5.11	100.76	112.00
1	E	106	LEU	N-CA-CB	-5.11	102.02	111.52
2	H	364	LEU	CD1-CG-CD2	5.11	122.03	110.80
1	I	75	ALA	CA-C-O	-5.11	114.48	120.20
1	A	12	THR	OG1-CB-CG2	-5.11	99.09	109.30
2	D	429	CYS	N-CA-C	-5.11	101.32	109.23
2	F	515	PRO	CA-C-O	-5.10	115.76	121.32
2	F	455	ASP	CA-C-O	5.10	126.46	120.80
2	J	533	THR	CA-CB-CG2	5.10	119.17	110.50
2	D	334	GLN	N-CA-C	-5.09	102.99	110.52
2	F	390	LYS	CG-CD-CE	5.09	123.01	111.30
2	L	456	TRP	CA-C-N	-5.09	106.51	120.97
2	L	456	TRP	C-N-CA	-5.09	106.51	120.97
1	E	4	LEU	CD1-CG-CD2	5.09	122.00	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	6	PRO	CB-CA-C	-5.09	103.35	110.63
1	K	100	ASP	N-CA-CB	5.09	117.69	110.16
2	J	479	TYR	N-CA-C	-5.08	101.69	109.41
1	I	51	LEU	CA-C-N	-5.08	113.54	121.87
1	I	51	LEU	C-N-CA	-5.08	113.54	121.87
2	H	439	PHE	CA-C-N	-5.08	115.57	122.93
2	H	439	PHE	C-N-CA	-5.08	115.57	122.93
2	D	504	LEU	CA-C-O	-5.08	113.41	119.35
2	L	394	ASN	CA-C-O	-5.08	116.38	122.27
2	B	301	PRO	CA-C-N	5.07	127.97	120.82
2	B	301	PRO	C-N-CA	5.07	127.97	120.82
2	B	457	ARG	CG-CD-NE	5.07	123.16	112.00
1	G	51	LEU	O-C-N	-5.07	117.26	123.30
1	I	169	THR	CA-CB-OG1	-5.07	101.99	109.60
2	J	338	SER	CA-CB-OG	-5.07	100.96	111.10
2	J	367	PHE	CA-C-N	5.07	131.22	121.54
2	J	367	PHE	C-N-CA	5.07	131.22	121.54
1	C	154	LYS	O-C-N	-5.07	116.22	122.25
1	I	70	VAL	N-CA-C	5.07	116.59	108.89
2	H	481	GLU	O-C-N	5.07	128.78	123.11
1	I	166	ARG	CA-C-N	5.06	128.01	120.31
1	I	166	ARG	C-N-CA	5.06	128.01	120.31
2	J	367	PHE	N-CA-CB	-5.06	103.32	110.81
1	C	8	THR	OG1-CB-CG2	5.06	119.42	109.30
2	B	325	LYS	N-CA-C	5.06	119.71	111.37
1	C	115	ASN	CA-C-O	-5.06	115.75	121.72
2	H	458	PRO	CB-CA-C	-5.06	103.58	111.22
1	I	86	GLU	CA-CB-CG	-5.06	103.99	114.10
1	A	188	ARG	CA-CB-CG	-5.05	103.99	114.10
1	A	146	ASP	N-CA-C	5.05	118.70	112.54
1	E	64	ARG	CB-CA-C	-5.05	101.38	110.37
1	E	152	ASN	CA-C-N	-5.05	112.67	122.06
1	E	152	ASN	C-N-CA	-5.05	112.67	122.06
1	I	33	GLN	CA-C-O	-5.04	115.10	120.40
1	C	180	LYS	N-CA-C	-5.04	100.49	109.06
2	L	383	ARG	NE-CZ-NH1	-5.04	116.46	121.50
2	B	432	ASP	CA-C-N	5.04	127.74	120.38
2	B	432	ASP	C-N-CA	5.04	127.74	120.38
2	B	390	LYS	CA-C-N	5.04	124.94	119.85
2	B	390	LYS	C-N-CA	5.04	124.94	119.85
2	D	483	ASP	CA-C-O	5.03	123.97	119.59
1	E	33	GLN	N-CA-C	5.03	116.83	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	439	PHE	CA-C-N	-5.03	115.89	122.99
2	F	439	PHE	C-N-CA	-5.03	115.89	122.99
1	G	162	GLU	N-CA-C	5.03	117.15	111.11
2	J	495	ILE	CB-CG1-CD1	5.03	124.36	113.80
1	G	12	THR	CA-C-N	5.03	129.22	120.68
1	G	12	THR	C-N-CA	5.03	129.22	120.68
2	H	500	ALA	CA-C-O	-5.02	114.67	120.24
2	L	499	GLU	N-CA-CB	5.02	117.95	110.22
2	L	469	SER	CA-C-O	-5.02	115.91	121.28
2	J	469	SER	N-CA-C	5.01	115.92	108.60
1	A	19	ILE	CB-CG1-CD1	-5.01	103.28	113.80
1	G	171	ILE	CG1-CB-CG2	-5.01	95.67	110.70
2	H	377	ARG	CA-C-N	-5.01	115.17	122.58
2	H	377	ARG	C-N-CA	-5.01	115.17	122.58
2	L	523	PHE	CB-CA-C	5.01	117.75	110.79
2	F	345	GLU	CA-CB-CG	-5.00	104.09	114.10
1	I	114	VAL	CG1-CB-CG2	-5.00	99.79	110.80
2	F	431	THR	N-CA-C	-5.00	103.80	110.55

There are no chirality outliers.

All (116) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	GLY	Mainchain
1	A	144	TYR	Sidechain
1	A	16	TYR	Sidechain
1	A	166	ARG	Sidechain
1	A	192	GLU	Mainchain
1	A	44	ALA	Mainchain
1	A	83	TYR	Sidechain
2	B	354	LEU	Mainchain
2	B	383	ARG	Sidechain
2	B	395	THR	Mainchain
2	B	408[A]	CYS	Mainchain
2	B	409	ARG	Mainchain
2	B	437	TYR	Sidechain
2	B	440	ARG	Sidechain
2	B	465	ILE	Mainchain
2	B	527	LEU	Mainchain
2	B	531	ARG	Sidechain
1	C	138	HIS	Mainchain
1	C	139	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	C	156	PRO	Mainchain
1	C	16	TYR	Sidechain
1	C	18	HIS	Sidechain
1	C	180	LYS	Mainchain
1	C	184	ARG	Mainchain
1	C	56	TYR	Sidechain
1	C	69	GLU	Mainchain
1	C	99	PHE	Mainchain
2	D	311	ARG	Sidechain,Mainchain
2	D	324	TYR	Mainchain
2	D	325	LYS	Mainchain
2	D	334	GLN	Mainchain
2	D	351	PHE	Mainchain
2	D	391	PRO	Mainchain
2	D	407	ARG	Sidechain
2	D	410	HIS	Mainchain
2	D	467	GLY	Mainchain
2	D	471	ALA	Mainchain
2	D	493	LYS	Mainchain
2	D	511	ASN	Sidechain
2	D	525	ILE	Mainchain
2	D	528	ARG	Sidechain
1	E	16	TYR	Sidechain
1	E	166	ARG	Sidechain
1	E	64	ARG	Mainchain
1	E	99	PHE	Mainchain
2	F	353	HIS	Sidechain
2	F	366	ASN	Mainchain
2	F	430	LEU	Mainchain
2	F	440	ARG	Sidechain
2	F	447	TYR	Sidechain
2	F	465	ILE	Mainchain
1	G	1	PRO	Mainchain
1	G	18	HIS	Mainchain
1	G	184	ARG	Mainchain
1	G	187	ILE	Mainchain
1	G	37	ASN	Mainchain
1	G	38	ARG	Sidechain
1	G	96	ALA	Mainchain
2	H	313	ARG	Mainchain
2	H	336	LEU	Mainchain
2	H	341	GLN	Mainchain

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Mol	Chain	Res	Type	Group
2	H	354	LEU	Mainchain
2	H	360	ASP	Mainchain
2	H	407	ARG	Sidechain
2	H	428	ARG	Mainchain
2	H	436	TYR	Sidechain
2	H	447	TYR	Sidechain
2	H	525	ILE	Mainchain
1	I	11	GLN	Mainchain
1	I	133	ARG	Sidechain
1	I	18	HIS	Mainchain
1	I	184	ARG	Sidechain
1	I	53	GLY	Mainchain
1	I	69	GLU	Mainchain
1	I	95	THR	Mainchain
2	J	313	ARG	Sidechain
2	J	317	PRO	Mainchain
2	J	341	GLN	Mainchain
2	J	344	SER	Mainchain
2	J	384	VAL	Mainchain
2	J	391	PRO	Mainchain
2	J	407	ARG	Sidechain
2	J	415	TYR	Sidechain
2	J	447	TYR	Sidechain
2	J	451	ASN	Mainchain
2	J	466	SER	Mainchain
2	J	505	ILE	Mainchain
2	J	511	ASN	Sidechain
2	J	516	MET	Mainchain
2	J	520	ALA	Mainchain
2	J	529	GLY	Mainchain
1	K	144	TYR	Sidechain
1	K	183	TYR	Sidechain
1	K	56	TYR	Sidechain
1	K	74	ASP	Mainchain
1	K	83	TYR	Sidechain
1	K	90	ASN	Mainchain
2	L	309	VAL	Mainchain
2	L	342	SER	Mainchain
2	L	353	HIS	Sidechain
2	L	360	ASP	Mainchain
2	L	362	ASP	Mainchain
2	L	388	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	L	390	LYS	Mainchain
2	L	423	PHE	Mainchain
2	L	447	TYR	Sidechain
2	L	468	PRO	Mainchain
2	L	479	TYR	Sidechain
2	L	484	PRO	Mainchain
2	L	487	PRO	Mainchain
2	L	506	ALA	Mainchain
2	L	509	ASP	Mainchain
2	L	516	MET	Mainchain
2	L	521	TYR	Sidechain
2	L	533	THR	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	21	0
1	C	1571	0	1499	28	0
1	E	1571	0	1499	36	0
1	G	1571	0	1499	26	0
1	I	1571	0	1499	33	0
1	K	1571	0	1499	39	0
2	B	1875	0	1821	51	1
2	D	1875	0	1821	50	0
2	F	1875	0	1821	44	1
2	H	1875	0	1821	40	1
2	J	1875	0	1821	48	0
2	L	1875	0	1821	43	1
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	B	11	0	4	3	0
4	D	11	0	5	2	0
4	F	11	0	3	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	11	0	4	3	0
4	J	11	0	4	3	0
4	L	11	0	5	4	0
5	A	51	0	0	1	0
5	B	111	0	0	5	0
5	C	49	0	0	1	0
5	D	122	0	0	2	1
5	E	54	0	0	0	0
5	F	113	0	0	3	1
5	G	52	0	0	0	0
5	H	108	0	0	5	0
5	I	55	0	0	1	0
5	J	115	0	0	6	1
5	K	48	0	0	1	0
5	L	118	0	0	3	1
All	All	21744	0	19945	416	4

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 10.

All (416) 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)
2:L:337:VAL:CG1	2:L:337:VAL:CB	1.74	1.62
2:B:339:ILE:CD1	2:B:339:ILE:CG1	1.74	1.60
1:G:154:LYS:CE	1:G:154:LYS:CD	1.76	1.60
2:F:390:LYS:CD	2:F:390:LYS:CG	1.78	1.59
2:H:396:LEU:CG	2:H:396:LEU:CD1	1.79	1.59
2:J:378:ILE:CG1	2:J:378:ILE:CD1	1.76	1.58
1:E:157:VAL:CB	1:E:157:VAL:CG1	1.75	1.57
1:A:154:LYS:CE	1:A:154:LYS:CD	1.74	1.56
2:B:453:PRO:CB	2:B:453:PRO:CG	1.77	1.56
2:L:303:GLN:CB	2:L:303:GLN:CA	1.75	1.56
1:I:154:LYS:CE	1:I:154:LYS:NZ	1.68	1.55
2:J:493:LYS:CE	2:J:493:LYS:NZ	1.70	1.54
2:D:493:LYS:CE	2:D:493:LYS:NZ	1.68	1.52
2:B:303:GLN:CB	2:B:303:GLN:CA	1.86	1.51
1:C:154:LYS:NZ	1:C:154:LYS:CE	1.70	1.51
2:D:515:PRO:CG	2:D:515:PRO:CB	1.76	1.50
2:L:507:LYS:NZ	2:L:507:LYS:CE	1.76	1.49
1:A:154:LYS:CE	1:A:154:LYS:NZ	1.74	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:PRO:CG	1:G:9:PRO:CD	1.75	1.47
2:D:408[B]:CYS:CB	2:D:408[B]:CYS:SG	2.04	1.45
2:H:498:PRO:CB	2:H:498:PRO:CG	1.79	1.45
2:J:448:PRO:CG	2:J:448:PRO:CB	1.80	1.45
2:F:507:LYS:CE	2:F:507:LYS:NZ	1.75	1.44
2:B:489:CYS:CB	2:B:489:CYS:SG	2.04	1.43
2:B:507:LYS:NZ	2:B:507:LYS:CE	1.76	1.43
2:J:317:PRO:CG	2:J:317:PRO:CB	1.75	1.42
1:K:42:PRO:CG	1:K:42:PRO:CB	1.78	1.41
2:D:507:LYS:CE	2:D:507:LYS:NZ	1.85	1.38
2:D:510:MET:SD	2:D:510:MET:CE	2.17	1.31
1:K:165:GLN:H	1:K:165:GLN:NE2	1.43	1.17
2:H:364:LEU:HD22	2:H:440:ARG:HD3	1.22	1.10
1:I:165:GLN:HE21	1:I:165:GLN:N	1.49	1.09
1:I:165:GLN:H	1:I:165:GLN:NE2	1.54	1.05
2:D:368:ASN:ND2	2:D:370:GLY:H	1.59	1.01
1:E:165:GLN:H	1:E:165:GLN:HE21	1.05	1.00
1:C:165:GLN:H	1:C:165:GLN:HE21	1.04	0.93
1:K:165:GLN:HE21	1:K:165:GLN:N	1.66	0.93
2:H:368:ASN:ND2	2:H:370:GLY:H	1.68	0.93
2:B:497:ASN:C	2:B:497:ASN:HD22	1.80	0.89
1:K:165:GLN:H	1:K:165:GLN:HE21	0.89	0.88
1:E:165:GLN:H	1:E:165:GLN:NE2	1.70	0.87
1:C:26:ALA:O	2:D:411:LYS:NZ	2.06	0.87
2:F:408[A]:CYS:SG	5:F:2901:HOH:O	2.35	0.85
1:E:25:ALA:HB1	1:E:98:THR:HG21	1.61	0.83
1:I:25:ALA:HB1	1:I:98:THR:HG21	1.61	0.81
1:C:165:GLN:H	1:C:165:GLN:NE2	1.78	0.81
2:D:368:ASN:ND2	2:D:370:GLY:N	2.30	0.79
2:J:538:CYS:OXT	5:J:833:HOH:O	1.99	0.79
2:B:390:LYS:HD3	5:B:677:HOH:O	1.83	0.78
2:J:408[A]:CYS:SG	5:J:4901:HOH:O	2.42	0.76
1:E:26:ALA:O	2:F:411:LYS:NZ	2.19	0.76
2:B:497:ASN:HD22	2:B:498:PRO:N	1.84	0.76
1:C:98:THR:N	1:C:101:ALA:O	2.19	0.75
1:E:157:VAL:CG1	1:E:157:VAL:CA	2.65	0.74
2:H:408[A]:CYS:SG	5:H:3901:HOH:O	2.44	0.74
2:F:361:HIS:H	2:F:361:HIS:CD2	2.05	0.73
2:D:447:TYR:OH	4:D:1550:DHB:O4	2.07	0.73
1:A:165:GLN:H	1:A:165:GLN:NE2	1.86	0.73
1:E:165:GLN:HE21	1:E:165:GLN:N	1.85	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:510:MET:CE	2:D:510:MET:CG	2.67	0.73
2:F:497:ASN:ND2	2:F:499:GLU:H	1.87	0.72
2:L:337:VAL:CG1	2:L:337:VAL:CG2	2.67	0.72
1:K:67:PHE:HZ	1:K:94:ARG:HD2	1.55	0.72
1:G:67:PHE:CZ	1:G:94:ARG:HD2	2.25	0.71
2:H:396:LEU:CD1	2:H:396:LEU:CB	2.69	0.71
2:F:324:TYR:OH	4:F:2550:DHB:O1	2.07	0.71
1:K:165:GLN:NE2	1:K:165:GLN:N	2.28	0.70
1:I:51:LEU:HD12	1:I:106:LEU:HD23	1.73	0.69
1:K:67:PHE:CZ	1:K:94:ARG:HD2	2.28	0.69
2:L:337:VAL:CG1	2:L:337:VAL:CA	2.69	0.68
1:K:110:LYS:NZ	1:K:148:GLU:OE2	2.20	0.68
2:D:361:HIS:H	2:D:361:HIS:CD2	2.11	0.68
2:L:361:HIS:CD2	2:L:361:HIS:H	2.12	0.67
1:C:165:GLN:HE21	1:C:165:GLN:N	1.86	0.67
2:L:368:ASN:O	2:L:369:ASN:ND2	2.27	0.67
2:L:411:LYS:CE	2:L:411:LYS:H	2.08	0.67
2:H:376:GLU:OE1	5:H:3665:HOH:O	2.13	0.67
2:L:447:TYR:HE1	4:L:5550:DHB:H5	1.59	0.67
2:L:468:PRO:HD2	2:L:472:THR:HG21	1.76	0.67
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.77	0.66
1:G:154:LYS:CE	1:G:154:LYS:CG	2.71	0.66
1:K:143:LEU:C	1:K:143:LEU:HD23	2.19	0.66
2:D:368:ASN:HD21	2:D:370:GLY:H	1.40	0.66
2:H:368:ASN:ND2	2:H:370:GLY:N	2.43	0.66
2:F:368:ASN:HD22	2:F:370:GLY:H	1.44	0.66
1:C:24:GLU:O	1:C:27:GLY:N	2.24	0.65
2:B:393:PRO:O	5:B:779:HOH:O	2.12	0.65
2:B:339:ILE:CD1	2:B:339:ILE:CB	2.70	0.65
2:D:368:ASN:HD21	2:D:370:GLY:CA	2.09	0.65
2:H:325:LYS:HD3	2:J:335:ALA:HB1	1.79	0.65
2:F:497:ASN:HD22	2:F:499:GLU:H	1.45	0.64
1:K:15:PRO:HB3	1:K:133:ARG:HD2	1.78	0.64
2:H:361:HIS:H	2:H:361:HIS:CD2	2.16	0.64
1:I:54:GLN:O	5:I:4754:HOH:O	2.15	0.63
2:F:497:ASN:HD22	2:F:497:ASN:C	2.05	0.63
1:I:24:GLU:O	1:I:27:GLY:N	2.31	0.63
1:A:154:LYS:CE	1:A:154:LYS:CG	2.75	0.63
1:G:67:PHE:HZ	1:G:94:ARG:HD2	1.63	0.63
2:D:465:ILE:HG13	2:D:525:ILE:HG21	1.80	0.63
2:L:447:TYR:OH	4:L:5550:DHB:O4	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408[A]:CYS:SG	5:B:901:HOH:O	2.42	0.62
2:F:390:LYS:HD2	5:F:2677:HOH:O	1.99	0.62
2:D:416:LEU:H	2:D:416:LEU:HD23	1.64	0.62
1:I:161:ILE:HD13	1:I:196:VAL:HG21	1.82	0.62
2:H:368:ASN:HD22	2:H:370:GLY:H	1.48	0.62
2:B:361:HIS:CD2	2:B:361:HIS:H	2.16	0.61
2:D:482:GLY:O	5:D:1704:HOH:O	2.16	0.61
2:J:453:PRO:HB2	2:L:310:ILE:HG12	1.81	0.61
2:D:510:MET:CE	2:D:510:MET:HG3	2.30	0.61
2:D:447:TYR:HE1	4:D:1550:DHB:H5	1.65	0.60
1:G:165:GLN:H	1:G:165:GLN:HE21	1.49	0.60
2:J:473:LYS:NZ	5:J:4783:HOH:O	2.33	0.60
1:K:64:ARG:NH1	5:K:5903:HOH:O	2.31	0.60
1:I:94:ARG:NH2	2:J:398:GLU:OE2	2.33	0.60
1:G:70:VAL:HG11	1:G:106:LEU:HD21	1.83	0.60
1:C:67:PHE:HZ	1:C:94:ARG:HD2	1.66	0.59
2:L:376:GLU:OE1	5:L:5665:HOH:O	2.16	0.59
2:J:390:LYS:HD2	5:J:4677:HOH:O	2.02	0.59
2:H:453:PRO:HB2	2:J:310:ILE:HG12	1.84	0.59
2:D:368:ASN:HD21	2:D:370:GLY:N	1.96	0.59
2:J:497:ASN:HD22	2:J:499:GLU:H	1.51	0.59
2:B:497:ASN:ND2	2:B:499:GLU:H	2.02	0.58
2:F:447:TYR:OH	4:F:2550:DHB:O4	2.21	0.58
2:L:303:GLN:CB	2:L:303:GLN:C	2.74	0.58
1:E:157:VAL:CG1	1:E:157:VAL:HB	2.17	0.58
2:L:364:LEU:HD22	2:L:440:ARG:HD3	1.86	0.58
2:L:497:ASN:ND2	2:L:499:GLU:H	2.01	0.58
2:J:361:HIS:CD2	2:J:361:HIS:H	2.21	0.58
2:L:411:LYS:H	2:L:411:LYS:HE2	1.68	0.58
1:E:111:PRO:HD2	1:E:145:PHE:CZ	2.40	0.57
2:L:315:TRP:HZ2	2:L:503:GLN:HE21	1.53	0.57
1:E:157:VAL:CG1	1:E:157:VAL:C	2.78	0.57
2:H:411:LYS:NZ	2:H:411:LYS:H	2.03	0.56
2:L:497:ASN:C	2:L:497:ASN:HD22	2.13	0.56
2:H:429:CYS:SG	5:H:3766:HOH:O	2.19	0.56
1:K:17:VAL:CG2	1:K:21:LEU:HD12	2.35	0.56
2:L:497:ASN:HD22	2:L:498:PRO:N	2.04	0.56
2:H:396:LEU:CD1	2:H:396:LEU:CD2	2.74	0.56
1:A:26:ALA:O	2:B:411:LYS:NZ	2.36	0.55
1:E:80:GLN:O	1:E:91:SER:HB2	2.07	0.55
2:H:411:LYS:O	2:H:414:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:447:TYR:HE1	4:J:4550:DHB:H5	1.71	0.55
2:L:408[A]:CYS:SG	5:L:5901:HOH:O	2.45	0.55
2:J:368:ASN:ND2	2:J:370:GLY:H	2.05	0.55
2:H:497:ASN:C	2:H:497:ASN:HD22	2.15	0.55
2:J:364:LEU:HD22	2:J:440:ARG:HD3	1.89	0.55
2:J:495:ILE:HG21	2:J:500:ALA:HB3	1.87	0.55
2:B:367:PHE:O	2:B:368:ASN:O	2.24	0.54
2:B:364:LEU:HD22	2:B:440:ARG:HD3	1.88	0.54
1:G:165:GLN:H	1:G:165:GLN:NE2	2.06	0.54
2:F:478:LEU:C	2:F:478:LEU:HD23	2.33	0.54
2:F:368:ASN:ND2	2:F:370:GLY:H	2.05	0.54
2:H:497:ASN:HD22	2:H:499:GLU:H	1.55	0.54
2:B:310:ILE:HG13	2:F:453:PRO:HB2	1.90	0.54
2:H:345:GLU:HA	2:H:470:ILE:HD11	1.90	0.53
2:B:507:LYS:HB2	1:I:2:ILE:HD13	1.90	0.53
2:J:394:ASN:HB3	2:J:430:LEU:HD21	1.90	0.53
2:H:497:ASN:ND2	2:H:499:GLU:H	2.07	0.53
1:C:19:ILE:HG21	2:D:410:HIS:HB2	1.90	0.53
1:A:165:GLN:H	1:A:165:GLN:HE21	1.56	0.53
2:F:497:ASN:HD22	2:F:498:PRO:N	2.07	0.53
2:J:371:GLY:H	2:J:422:ASN:ND2	2.07	0.53
1:I:26:ALA:O	2:J:411:LYS:NZ	2.40	0.53
2:B:453:PRO:HB2	2:D:310:ILE:HG13	1.89	0.53
2:H:449:TRP:CD1	2:H:449:TRP:N	2.76	0.53
2:L:447:TYR:CZ	4:L:5550:DHB:O4	2.59	0.53
1:E:92:PHE:CD1	2:F:349:PRO:HG3	2.45	0.52
2:F:356:PHE:CD1	2:F:428:ARG:HD3	2.43	0.52
1:I:127:ASN:HD21	2:J:344:SER:HB3	1.74	0.52
1:A:70:VAL:HA	1:A:127:ASN:O	2.09	0.52
2:J:376:GLU:O	2:J:442:ILE:HA	2.09	0.52
2:B:315:TRP:HZ2	2:B:503:GLN:NE2	2.07	0.52
1:G:15:PRO:HD3	4:H:3550:DHB:C1	2.40	0.52
1:A:114:VAL:HG23	1:A:122:MET:HE3	1.92	0.52
1:E:15:PRO:HB3	1:E:133:ARG:HD2	1.93	0.51
2:F:449:TRP:N	2:F:449:TRP:CD1	2.78	0.51
1:I:20:GLY:HA2	2:J:426:VAL:HG13	1.93	0.51
2:D:368:ASN:HD21	2:D:370:GLY:HA2	1.74	0.51
2:F:390:LYS:CD	2:F:390:LYS:CB	2.80	0.51
2:H:386:ASP:HB2	2:H:529:GLY:HA2	1.91	0.51
2:J:497:ASN:ND2	2:J:499:GLU:H	2.07	0.51
2:B:315:TRP:HZ2	2:B:503:GLN:HE21	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:LEU:HD22	2:B:440:ARG:CD	2.40	0.51
2:J:447:TYR:CZ	4:J:4550:DHB:O4	2.64	0.51
1:K:174:ARG:HH21	1:K:181:THR:HG21	1.75	0.51
2:L:385:VAL:O	2:L:526:VAL:HA	2.11	0.51
1:A:39:LEU:HD11	1:A:93:GLY:HA3	1.93	0.50
2:B:411:LYS:HZ3	2:B:411:LYS:H	1.59	0.50
2:B:448:PRO:HD3	2:B:456:TRP:CZ3	2.45	0.50
2:B:324:TYR:OH	4:B:550:DHB:O1	2.21	0.50
1:E:110:LYS:HE3	1:E:183:TYR:OH	2.11	0.50
2:B:368:ASN:HD22	2:B:370:GLY:H	1.59	0.50
1:C:19:ILE:CG2	2:D:410:HIS:HB2	2.41	0.50
1:I:165:GLN:HE21	1:I:165:GLN:H	0.71	0.50
1:I:67:PHE:HZ	1:I:94:ARG:HD2	1.77	0.50
1:C:131:PHE:CD2	2:D:475:ILE:HD12	2.46	0.50
1:G:65:ASP:OD2	1:G:133:ARG:HD3	2.11	0.50
1:I:65:ASP:OD2	1:I:133:ARG:HD3	2.12	0.50
1:K:18:HIS:HB2	1:K:26:ALA:HB2	1.93	0.50
1:K:30:THR:HG22	1:K:34:GLU:HG3	1.93	0.50
1:A:114:VAL:HG22	5:A:680:HOH:O	2.12	0.50
2:J:448:PRO:HD3	2:J:456:TRP:CZ3	2.47	0.50
1:A:18:HIS:HA	1:A:22:ALA:HB3	1.92	0.50
1:I:39:LEU:HD11	1:I:93:GLY:HA3	1.94	0.50
1:I:131:PHE:CE2	1:I:138:HIS:HB3	2.47	0.50
2:B:400:TRP:HA	2:B:425:GLY:O	2.12	0.50
2:H:368:ASN:HD22	2:H:369:ASN:N	2.10	0.50
1:I:36:TRP:CG	1:I:37:ASN:H	2.30	0.50
1:K:195:THR:HG22	1:K:196:VAL:O	2.12	0.50
2:D:411:LYS:NZ	2:D:411:LYS:H	2.11	0.49
2:D:447:TYR:HB2	2:D:448:PRO:HD2	1.94	0.49
1:C:11:GLN:NE2	2:D:495:ILE:HD11	2.26	0.49
2:F:429:CYS:SG	5:F:2766:HOH:O	1.93	0.49
1:G:143:LEU:C	1:G:143:LEU:HD23	2.37	0.49
1:I:49:ILE:HD13	1:I:110:LYS:N	2.28	0.49
2:L:497:ASN:HD22	2:L:499:GLU:H	1.59	0.49
2:B:320:LEU:HD22	2:B:333:ARG:CZ	2.42	0.49
1:C:18:HIS:HA	1:C:22:ALA:HB3	1.93	0.49
2:H:493:LYS:C	2:H:495:ILE:H	2.20	0.49
1:C:170:LEU:HD21	1:C:196:VAL:HB	1.95	0.49
1:C:25:ALA:HB1	1:C:98:THR:HG21	1.93	0.49
1:G:131:PHE:O	1:G:132:ALA:HB2	2.12	0.49
1:K:98:THR:N	1:K:101:ALA:O	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:315:TRP:HZ2	2:F:503:GLN:NE2	2.11	0.49
2:D:368:ASN:ND2	2:D:371:GLY:H	2.10	0.49
2:H:368:ASN:HD21	2:H:370:GLY:H	1.56	0.49
1:K:92:PHE:CD1	2:L:349:PRO:HG3	2.48	0.49
1:K:145:PHE:N	1:K:145:PHE:CD1	2.80	0.49
1:I:123:ALA:HB3	1:I:144:TYR:HE2	1.78	0.48
2:D:497:ASN:C	2:D:497:ASN:HD22	2.20	0.48
1:I:123:ALA:O	1:I:124:PRO:C	2.56	0.48
2:J:360:ASP:OD2	2:J:428:ARG:HD2	2.14	0.48
2:H:390:LYS:HD2	5:H:3677:HOH:O	2.13	0.48
1:E:52:LEU:C	1:E:52:LEU:HD22	2.38	0.48
1:C:98:THR:H	1:C:101:ALA:HB3	1.78	0.48
2:F:381:ALA:O	2:F:522:ARG:HA	2.14	0.48
2:J:449:TRP:CD1	2:J:457:ARG:HG2	2.49	0.48
1:G:25:ALA:HB1	1:G:98:THR:HG21	1.96	0.48
1:K:71:TRP:CD1	2:L:470:ILE:HD13	2.49	0.47
1:K:165:GLN:H	1:K:165:GLN:CD	2.15	0.47
2:L:410:HIS:HA	2:L:411:LYS:NZ	2.29	0.47
1:G:132:ALA:HB3	1:G:135:ILE:HD12	1.95	0.47
2:B:497:ASN:C	2:B:497:ASN:ND2	2.52	0.47
1:I:98:THR:N	1:I:101:ALA:O	2.44	0.47
2:J:484:PRO:O	2:J:487:PRO:HD2	2.14	0.47
2:D:376:GLU:OE1	5:D:1665:HOH:O	2.20	0.47
1:E:15:PRO:HD3	4:F:2550:DHB:C2	2.45	0.47
1:E:15:PRO:HD3	4:F:2550:DHB:C1	2.44	0.47
2:J:350:ASN:C	2:J:350:ASN:OD1	2.58	0.47
2:J:393:PRO:O	2:J:394:ASN:C	2.57	0.47
1:C:198:PHE:HA	2:D:337:VAL:O	2.14	0.47
2:F:356:PHE:CE1	2:F:428:ARG:HD3	2.50	0.47
2:F:368:ASN:HD22	2:F:370:GLY:N	2.12	0.47
2:F:383:ARG:HG3	2:F:436:TYR:CE2	2.50	0.47
1:C:190:GLN:HG3	2:D:333:ARG:HG2	1.97	0.47
2:J:495:ILE:CG2	5:J:4698:HOH:O	2.63	0.47
1:E:132:ALA:HB3	1:E:135:ILE:HD12	1.96	0.46
1:K:84:ASN:O	1:K:90:ASN:ND2	2.39	0.46
2:D:411:LYS:H	2:D:411:LYS:CE	2.28	0.46
1:E:123:ALA:O	1:E:124:PRO:C	2.57	0.46
2:H:454:ASN:HB2	2:J:310:ILE:HD13	1.97	0.46
2:L:495:ILE:HG21	2:L:500:ALA:HB3	1.98	0.46
2:B:356:PHE:CD1	2:B:428:ARG:HD3	2.50	0.46
2:F:497:ASN:ND2	2:F:497:ASN:C	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:325:LYS:NZ	2:H:451:ASN:O	2.48	0.46
1:I:92:PHE:CD1	2:J:349:PRO:HG3	2.50	0.46
1:I:123:ALA:HB3	1:I:144:TYR:CE2	2.50	0.46
2:J:363:LEU:N	2:J:363:LEU:HD12	2.31	0.46
2:J:405:GLY:HA3	5:J:4682:HOH:O	2.16	0.46
1:C:67:PHE:CZ	1:C:94:ARG:HD2	2.50	0.46
2:J:363:LEU:HD23	2:J:425:GLY:HA2	1.97	0.46
2:F:486:ILE:HG21	2:F:486:ILE:HD13	1.76	0.45
2:J:411:LYS:NZ	2:J:411:LYS:H	2.15	0.45
2:L:441:THR:OG1	2:L:442:ILE:N	2.50	0.45
2:B:495:ILE:HG21	2:B:500:ALA:HB3	1.98	0.45
1:C:20:GLY:HA2	2:D:426:VAL:HG13	1.97	0.45
1:C:94:ARG:HH22	2:D:398:GLU:CD	2.24	0.45
2:H:368:ASN:ND2	2:H:371:GLY:H	2.14	0.45
2:B:419:LEU:HD23	2:B:419:LEU:HA	1.80	0.45
2:D:321:THR:HG21	2:D:494:SER:HB2	1.97	0.45
2:D:368:ASN:HD22	2:D:369:ASN:N	2.14	0.45
1:K:50:LEU:O	1:K:182:ALA:HA	2.17	0.45
1:G:15:PRO:HD3	4:H:3550:DHB:C2	2.47	0.45
1:K:174:ARG:HE	1:K:181:THR:CG2	2.29	0.45
2:B:489:CYS:HA	2:B:490:PRO:HD3	1.79	0.45
1:E:36:TRP:CG	1:E:37:ASN:H	2.34	0.45
2:F:480:PHE:O	2:F:481:GLU:C	2.59	0.45
2:F:458:PRO:HD3	2:F:489:CYS:HB2	1.98	0.45
2:H:411:LYS:HB2	2:H:411:LYS:HE2	1.67	0.45
2:L:447:TYR:CE1	4:L:5550:DHB:H5	2.47	0.45
1:E:64:ARG:HG2	1:E:64:ARG:HH11	1.81	0.45
1:A:39:LEU:N	1:A:39:LEU:HD12	2.31	0.45
1:K:160:LEU:HD23	1:K:160:LEU:HA	1.82	0.45
2:B:356:PHE:HD1	2:B:428:ARG:HD3	1.80	0.44
1:G:16:TYR:O	1:G:17:VAL:C	2.60	0.44
2:H:368:ASN:HD22	2:H:370:GLY:N	2.10	0.44
2:H:447:TYR:HE1	4:H:3550:DHB:H5	1.82	0.44
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.83	0.44
2:D:443:LYS:HG2	2:D:444:PRO:HD2	2.00	0.44
1:I:50:LEU:HD13	1:I:107:HIS:CE1	2.53	0.44
1:K:92:PHE:CG	2:L:349:PRO:HG3	2.52	0.44
1:I:31:ARG:NH1	2:J:428:ARG:HG2	2.32	0.44
1:I:160:LEU:HD23	1:I:160:LEU:HA	1.56	0.44
2:F:447:TYR:CZ	4:F:2550:DHB:O4	2.70	0.44
2:J:447:TYR:OH	4:J:4550:DHB:O4	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:6:PRO:HB2	2:L:503:GLN:HE22	1.83	0.44
2:L:410:HIS:HA	2:L:411:LYS:HZ1	1.83	0.44
2:B:522:ARG:NH1	5:B:716:HOH:O	2.51	0.44
2:D:449:TRP:N	2:D:449:TRP:CD1	2.86	0.44
2:L:449:TRP:CD1	2:L:449:TRP:N	2.85	0.44
1:A:50:LEU:O	1:A:182:ALA:HA	2.18	0.44
1:G:35:ILE:HG21	1:G:92:PHE:CE2	2.53	0.44
1:I:67:PHE:CZ	1:I:94:ARG:HD2	2.52	0.44
2:B:403:ASN:HB2	5:B:620:HOH:O	2.17	0.44
1:C:101:ALA:C	1:C:103:GLU:H	2.26	0.44
1:C:4:LEU:HB2	5:C:3765:HOH:O	2.17	0.43
1:E:101:ALA:C	1:E:103:GLU:H	2.23	0.43
1:K:17:VAL:HG22	1:K:21:LEU:HD12	1.99	0.43
1:K:50:LEU:HD12	1:K:106:LEU:O	2.17	0.43
1:K:9:PRO:HG2	2:L:500:ALA:HB1	2.00	0.43
2:D:465:ILE:HD13	2:D:465:ILE:N	2.34	0.43
1:E:5:LEU:O	2:F:387:GLN:HG2	2.19	0.43
2:B:447:TYR:CE1	4:B:550:DHB:H5	2.54	0.43
1:G:123:ALA:O	1:G:124:PRO:C	2.60	0.43
1:G:163:GLN:HA	1:G:164:PRO:HD2	1.97	0.43
1:A:132:ALA:HB3	1:A:135:ILE:HD12	1.99	0.43
1:K:65:ASP:OD2	1:K:133:ARG:HD3	2.19	0.43
2:L:400:TRP:HA	2:L:425:GLY:O	2.18	0.43
2:B:411:LYS:HB2	2:B:411:LYS:HE2	1.70	0.43
2:J:465:ILE:HD12	2:J:465:ILE:N	2.34	0.43
2:B:316:HIS:HB3	2:B:317:PRO:HD2	2.01	0.43
2:B:418:PRO:HG2	2:H:374:ILE:HD13	1.99	0.43
1:C:85:LEU:HA	1:C:85:LEU:HD23	1.57	0.43
2:D:396:LEU:HD12	2:D:396:LEU:HA	1.75	0.43
1:E:116:ASN:C	1:E:116:ASN:OD1	2.61	0.43
1:I:144:TYR:CE1	1:I:158:LEU:HD13	2.53	0.43
2:J:336:LEU:HD23	2:J:336:LEU:HA	1.70	0.43
2:J:497:ASN:HA	2:J:498:PRO:HD2	1.88	0.43
2:D:408[B]:CYS:SG	2:D:408[B]:CYS:CA	3.03	0.43
2:F:399:MET:HA	2:F:462:HIS:O	2.18	0.43
2:H:307:ARG:HG2	2:H:533:THR:HG22	2.01	0.43
2:L:361:HIS:H	2:L:361:HIS:HD2	1.60	0.43
1:G:125:HIS:HA	1:G:143:LEU:O	2.19	0.42
1:K:19:ILE:HG21	2:L:410:HIS:HB2	2.00	0.42
2:B:447:TYR:HE1	4:B:550:DHB:H5	1.84	0.42
2:B:449:TRP:CH2	2:B:491:ILE:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:516:MET:HE3	2:D:516:MET:HB3	1.80	0.42
2:H:419:LEU:HD23	2:H:419:LEU:HA	1.83	0.42
1:I:4:LEU:HB3	2:J:387:GLN:HB3	2.00	0.42
1:E:7:GLU:OE2	2:F:311:ARG:HG2	2.20	0.42
1:E:77:GLY:O	1:E:114:VAL:HG12	2.19	0.42
2:H:493:LYS:C	2:H:495:ILE:N	2.78	0.42
2:H:511:ASN:H	2:H:511:ASN:ND2	2.16	0.42
2:H:522:ARG:NH1	5:H:3716:HOH:O	2.52	0.42
2:L:306:SER:HB2	5:L:5818:HOH:O	2.18	0.42
1:E:170:LEU:HD21	1:E:196:VAL:HB	2.02	0.42
1:A:98:THR:N	1:A:101:ALA:O	2.53	0.42
2:D:411:LYS:HB2	2:D:411:LYS:HE2	1.64	0.42
2:F:416:LEU:C	2:F:416:LEU:HD23	2.44	0.42
1:C:163:GLN:HA	1:C:164:PRO:HD2	1.81	0.42
1:I:92:PHE:CG	2:J:349:PRO:HG3	2.54	0.42
2:B:305:ASN:O	2:B:533:THR:HG23	2.19	0.42
2:D:307:ARG:HA	2:D:307:ARG:HD3	1.82	0.42
2:F:315:TRP:HZ2	2:F:503:GLN:HE21	1.68	0.42
1:A:78:GLU:OE1	2:B:301:PRO:HG3	2.20	0.41
1:K:19:ILE:CG2	2:L:410:HIS:HB2	2.50	0.41
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.55	0.41
1:C:18:HIS:CB	1:C:26:ALA:HB2	2.50	0.41
2:F:488:MET:O	2:F:490:PRO:HD3	2.19	0.41
1:G:18:HIS:HB2	1:G:26:ALA:HB2	2.02	0.41
1:K:85:LEU:HD23	1:K:85:LEU:HA	1.49	0.41
1:K:123:ALA:HB3	1:K:144:TYR:CE2	2.55	0.41
1:E:52:LEU:HD23	1:E:103:GLU:HG2	2.02	0.41
1:E:68:LEU:HD12	1:E:68:LEU:N	2.35	0.41
1:K:158:LEU:HD12	1:K:158:LEU:HA	1.80	0.41
2:B:307:ARG:HG2	2:B:533:THR:HG22	2.03	0.41
2:D:497:ASN:HD22	2:D:498:PRO:N	2.18	0.41
2:J:356:PHE:CD1	2:J:428:ARG:HD3	2.56	0.41
2:J:475:ILE:HD13	2:J:475:ILE:HG21	1.72	0.41
1:K:170:LEU:HA	1:K:170:LEU:HD23	1.65	0.41
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.78	0.41
2:B:489:CYS:SG	2:B:489:CYS:CA	2.98	0.41
1:C:61:HIS:ND1	1:E:163:GLN:HG3	2.35	0.41
2:L:457:ARG:HH11	2:L:457:ARG:HD3	1.70	0.41
2:B:354:LEU:HD12	2:B:354:LEU:HA	1.77	0.41
2:D:411:LYS:H	2:D:411:LYS:HZ3	1.69	0.41
2:D:412:ASN:HD22	2:D:412:ASN:HA	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:PHE:CG	2:F:349:PRO:HG3	2.56	0.41
1:E:123:ALA:HB3	1:E:144:TYR:HE2	1.86	0.41
2:F:356:PHE:HD1	2:F:428:ARG:CD	2.33	0.41
2:F:356:PHE:HD1	2:F:428:ARG:HD3	1.84	0.41
1:K:72:GLN:O	1:K:72:GLN:HG3	2.21	0.41
2:L:304:ASP:OD1	2:L:307:ARG:NH1	2.41	0.41
1:E:63:VAL:HG12	1:E:66:SER:HB3	2.02	0.41
2:H:497:ASN:C	2:H:497:ASN:ND2	2.79	0.41
1:I:85:LEU:HD23	1:I:85:LEU:HA	1.71	0.41
2:B:416:LEU:HD23	2:B:416:LEU:C	2.46	0.40
1:G:35:ILE:HG21	1:G:92:PHE:HE2	1.87	0.40
1:G:36:TRP:CG	1:G:37:ASN:H	2.39	0.40
1:K:146:ASP:OD1	1:K:174:ARG:HB2	2.21	0.40
2:F:411:LYS:NZ	2:F:411:LYS:H	2.19	0.40
2:L:307:ARG:HD3	2:L:307:ARG:HA	1.63	0.40
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.90	0.40
2:B:315:TRP:CZ2	2:B:503:GLN:NE2	2.89	0.40
2:B:390:LYS:HA	2:B:391:PRO:HD3	1.88	0.40
1:C:94:ARG:NH2	2:D:398:GLU:OE2	2.54	0.40
2:F:411:LYS:HE2	2:F:411:LYS:HB2	1.77	0.40
2:F:493:LYS:HB2	2:F:493:LYS:HE2	1.89	0.40
1:G:18:HIS:CB	1:G:26:ALA:HB2	2.51	0.40
1:A:110:LYS:NZ	1:A:147:ASP:OD1	2.55	0.40
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.21	0.40
2:B:527:LEU:O	2:B:528:ARG:C	2.65	0.40
2:D:464:GLY:C	2:D:465:ILE:HD13	2.46	0.40
1:E:31:ARG:NH1	2:F:428:ARG:HG2	2.36	0.40
1:G:11:GLN:O	1:G:12:THR:C	2.63	0.40
1:G:26:ALA:O	2:H:411:LYS:NZ	2.55	0.40

All (4) 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)
2:F:538:CYS:OXT	5:D:1833:HOH:O[2_555]	1.83	0.37
2:L:538:CYS:OXT	5:J:4833:HOH:O[2_555]	1.93	0.27
2:H:538:CYS:OXT	5:F:2833:HOH:O[2_555]	2.01	0.19
2:B:538:CYS:OXT	5:L:5833:HOH:O[2_555]	2.03	0.17

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	C	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	E	198/200 (99%)	188 (95%)	10 (5%)	0	100	100
1	G	198/200 (99%)	188 (95%)	10 (5%)	0	100	100
1	I	198/200 (99%)	183 (92%)	15 (8%)	0	100	100
1	K	198/200 (99%)	180 (91%)	17 (9%)	1 (0%)	24	24
2	B	237/238 (100%)	227 (96%)	9 (4%)	1 (0%)	30	31
2	D	237/238 (100%)	222 (94%)	14 (6%)	1 (0%)	30	31
2	F	237/238 (100%)	229 (97%)	7 (3%)	1 (0%)	30	31
2	H	237/238 (100%)	225 (95%)	11 (5%)	1 (0%)	30	31
2	J	237/238 (100%)	227 (96%)	8 (3%)	2 (1%)	16	14
2	L	237/238 (100%)	221 (93%)	14 (6%)	2 (1%)	16	14
All	All	2610/2628 (99%)	2468 (95%)	133 (5%)	9 (0%)	36	40

All (9) 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
2	J	368	ASN
2	L	368	ASN
2	L	369	ASN
1	K	179	GLY
2	J	394	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/163 (99%)	151 (93%)	11 (7%)	14	14
1	C	162/163 (99%)	145 (90%)	17 (10%)	6	4
1	E	162/163 (99%)	143 (88%)	19 (12%)	5	3
1	G	162/163 (99%)	150 (93%)	12 (7%)	13	11
1	I	162/163 (99%)	145 (90%)	17 (10%)	6	4
1	K	162/163 (99%)	139 (86%)	23 (14%)	3	2
2	B	201/202 (100%)	178 (89%)	23 (11%)	5	3
2	D	201/202 (100%)	179 (89%)	22 (11%)	6	4
2	F	201/202 (100%)	183 (91%)	18 (9%)	9	7
2	H	201/202 (100%)	180 (90%)	21 (10%)	7	5
2	J	201/202 (100%)	180 (90%)	21 (10%)	7	5
2	L	201/202 (100%)	182 (90%)	19 (10%)	8	6
All	All	2178/2190 (100%)	1955 (90%)	223 (10%)	7	5

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	4	LEU
1	A	19	ILE
1	A	38	ARG
1	A	52	LEU
1	A	68	LEU
1	A	106	LEU
1	A	109	VAL
1	A	158	LEU
1	A	165	GLN
1	A	192	GLU
2	B	301	PRO
2	B	320	LEU
2	B	327	SER

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Mol	Chain	Res	Type
2	B	364	LEU
2	B	368	ASN
2	B	372	LEU
2	B	390	LYS
2	B	395	THR
2	B	399	MET
2	B	411	LYS
2	B	414	ARG
2	B	416	LEU
2	B	428	ARG
2	B	434	ASP
2	B	443	LYS
2	B	473	LYS
2	B	474	LEU
2	B	491	ILE
2	B	497	ASN
2	B	507	LYS
2	B	534	HIS
2	B	537	ASN
2	B	538	CYS
1	C	4	LEU
1	C	32	ASP
1	C	38	ARG
1	C	41	LYS
1	C	42	PRO
1	C	52	LEU
1	C	91	SER
1	C	94	ARG
1	C	106	LEU
1	C	150	GLN
1	C	154	LYS
1	C	157	VAL
1	C	158	LEU
1	C	165	GLN
1	C	171	ILE
1	C	180	LYS
1	C	188	ARG
2	D	306	SER
2	D	310	ILE
2	D	339	ILE
2	D	364	LEU
2	D	372	LEU

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Mol	Chain	Res	Type
2	D	379	ILE
2	D	393	PRO
2	D	395	THR
2	D	399	MET
2	D	411	LYS
2	D	428	ARG
2	D	433	SER
2	D	442	ILE
2	D	448	PRO
2	D	450	ARG
2	D	457	ARG
2	D	465	ILE
2	D	493	LYS
2	D	499	GLU
2	D	503	GLN
2	D	515	PRO
2	D	534	HIS
1	E	2	ILE
1	E	4	LEU
1	E	19	ILE
1	E	21	LEU
1	E	38	ARG
1	E	49	ILE
1	E	50	LEU
1	E	52	LEU
1	E	91	SER
1	E	98	THR
1	E	143	LEU
1	E	158	LEU
1	E	164	PRO
1	E	165	GLN
1	E	171	ILE
1	E	177	VAL
1	E	181	THR
1	E	188	ARG
1	E	189	ILE
2	F	364	LEU
2	F	372	LEU
2	F	393	PRO
2	F	395	THR
2	F	410	HIS
2	F	411	LYS

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Mol	Chain	Res	Type
2	F	416	LEU
2	F	428	ARG
2	F	434	ASP
2	F	442	ILE
2	F	450	ARG
2	F	478	LEU
2	F	493	LYS
2	F	497	ASN
2	F	499	GLU
2	F	507	LYS
2	F	534	HIS
2	F	538	CYS
1	G	2	ILE
1	G	4	LEU
1	G	19	ILE
1	G	38	ARG
1	G	52	LEU
1	G	94	ARG
1	G	130	LEU
1	G	133	ARG
1	G	143	LEU
1	G	154	LYS
1	G	157	VAL
1	G	165	GLN
2	H	306	SER
2	H	344	SER
2	H	364	LEU
2	H	372	LEU
2	H	395	THR
2	H	411	LYS
2	H	414	ARG
2	H	416	LEU
2	H	428	ARG
2	H	433	SER
2	H	434	ASP
2	H	440	ARG
2	H	442	ILE
2	H	465	ILE
2	H	470	ILE
2	H	473	LYS
2	H	497	ASN
2	H	503	GLN

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Mol	Chain	Res	Type
2	H	507	LYS
2	H	511	ASN
2	H	534	HIS
1	I	2	ILE
1	I	4	LEU
1	I	19	ILE
1	I	24	GLU
1	I	38	ARG
1	I	42	PRO
1	I	49	ILE
1	I	50	LEU
1	I	52	LEU
1	I	66	SER
1	I	124	PRO
1	I	150	GLN
1	I	160	LEU
1	I	165	GLN
1	I	168	GLU
1	I	180	LYS
1	I	192	GLU
2	J	306	SER
2	J	310	ILE
2	J	364	LEU
2	J	372	LEU
2	J	394	ASN
2	J	395	THR
2	J	411	LYS
2	J	416	LEU
2	J	428	ARG
2	J	442	ILE
2	J	450	ARG
2	J	457	ARG
2	J	473	LYS
2	J	475	ILE
2	J	478	LEU
2	J	495	ILE
2	J	499	GLU
2	J	507	LYS
2	J	525	ILE
2	J	534	HIS
2	J	538	CYS
1	K	4	LEU

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Mol	Chain	Res	Type
1	K	9	PRO
1	K	19	ILE
1	K	21	LEU
1	K	24	GLU
1	K	30	THR
1	K	49	ILE
1	K	52	LEU
1	K	68	LEU
1	K	78	GLU
1	K	91	SER
1	K	94	ARG
1	K	100	ASP
1	K	114	VAL
1	K	143	LEU
1	K	150	GLN
1	K	158	LEU
1	K	165	GLN
1	K	171	ILE
1	K	177	VAL
1	K	178	ASP
1	K	181	THR
1	K	188	ARG
2	L	310	ILE
2	L	328	ILE
2	L	364	LEU
2	L	368	ASN
2	L	372	LEU
2	L	401	GLN
2	L	411	LYS
2	L	416	LEU
2	L	428	ARG
2	L	442	ILE
2	L	450	ARG
2	L	457	ARG
2	L	473	LYS
2	L	478	LEU
2	L	497	ASN
2	L	507	LYS
2	L	515	PRO
2	L	534	HIS
2	L	538	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	33	GLN
1	A	61	HIS
1	A	163	GLN
1	A	165	GLN
2	B	361	HIS
2	B	368	ASN
2	B	369	ASN
2	B	412	ASN
2	B	462	HIS
2	B	497	ASN
2	B	502	GLN
2	B	530	GLN
1	C	54	GLN
1	C	107	HIS
1	C	115	ASN
1	C	136	ASN
1	C	163	GLN
1	C	165	GLN
2	D	314	ASN
2	D	361	HIS
2	D	368	ASN
2	D	412	ASN
2	D	497	ASN
2	D	503	GLN
1	E	61	HIS
1	E	163	GLN
1	E	165	GLN
2	F	314	ASN
2	F	361	HIS
2	F	368	ASN
2	F	497	ASN
2	F	503	GLN
2	F	511	ASN
2	F	530	GLN
1	G	76	ASN
1	G	127	ASN
1	G	163	GLN
1	G	165	GLN
2	H	305	ASN
2	H	359	HIS
2	H	361	HIS

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Mol	Chain	Res	Type
2	H	368	ASN
2	H	412	ASN
2	H	497	ASN
2	H	503	GLN
2	H	511	ASN
2	H	514	ASN
1	I	59	ASN
1	I	107	HIS
1	I	127	ASN
1	I	152	ASN
1	I	163	GLN
1	I	165	GLN
2	J	305	ASN
2	J	361	HIS
2	J	368	ASN
2	J	369	ASN
2	J	394	ASN
2	J	412	ASN
2	J	422	ASN
2	J	497	ASN
2	J	503	GLN
2	J	530	GLN
1	K	11	GLN
1	K	115	ASN
1	K	163	GLN
1	K	165	GLN
2	L	334	GLN
2	L	361	HIS
2	L	368	ASN
2	L	369	ASN
2	L	412	ASN
2	L	497	ASN
2	L	503	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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
4	DHB	D	1550	3	11,11,11	1.09	0	15,15,15	0.96	2 (13%)
4	DHB	J	4550	-	11,11,11	0.84	0	15,15,15	0.95	2 (13%)
4	DHB	F	2550	3	11,11,11	1.69	2 (18%)	15,15,15	1.11	0
4	DHB	B	550	3	11,11,11	1.10	0	15,15,15	0.88	1 (6%)
4	DHB	H	3550	3	11,11,11	0.98	0	15,15,15	0.82	1 (6%)
4	DHB	L	5550	3	11,11,11	0.81	0	15,15,15	0.87	1 (6%)

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
4	DHB	D	1550	3	-	0/4/4/4	0/1/1/1
4	DHB	J	4550	-	-	0/4/4/4	0/1/1/1
4	DHB	F	2550	3	-	0/4/4/4	0/1/1/1
4	DHB	B	550	3	-	0/4/4/4	0/1/1/1
4	DHB	H	3550	3	-	0/4/4/4	0/1/1/1
4	DHB	L	5550	3	-	0/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2550	DHB	C6-C1	-3.81	1.33	1.39
4	F	2550	DHB	C4-C3	2.72	1.44	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	D	1550	DHB	O2-C-C1	2.54	121.36	114.84
4	B	550	DHB	O2-C-C1	2.38	120.95	114.84
4	L	5550	DHB	O2-C-C1	2.22	120.55	114.84
4	J	4550	DHB	O2-C-C1	2.21	120.51	114.84
4	H	3550	DHB	O2-C-C1	2.21	120.50	114.84
4	J	4550	DHB	O2-C-O1	-2.19	118.64	123.35
4	D	1550	DHB	O2-C-O1	-2.18	118.66	123.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1550	DHB	2	0
4	J	4550	DHB	3	0
4	F	2550	DHB	5	0
4	B	550	DHB	3	0
4	H	3550	DHB	3	0
4	L	5550	DHB	4	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%)	-0.72	2 (1%) 79 81	18, 33, 64, 73	0
1	C	200/200 (100%)	-0.70	2 (1%) 79 81	18, 32, 64, 73	0
1	E	200/200 (100%)	-0.65	3 (1%) 72 73	18, 33, 65, 74	0
1	G	200/200 (100%)	-0.68	3 (1%) 72 73	19, 33, 66, 74	0
1	I	200/200 (100%)	-0.65	1 (0%) 87 88	19, 35, 65, 74	0
1	K	200/200 (100%)	-0.54	1 (0%) 87 88	20, 37, 67, 74	0
2	B	238/238 (100%)	-0.92	2 (0%) 82 84	15, 26, 52, 71	1 (0%)
2	D	238/238 (100%)	-0.95	0 100 100	14, 25, 52, 71	1 (0%)
2	F	238/238 (100%)	-0.96	1 (0%) 88 89	15, 26, 53, 70	1 (0%)
2	H	238/238 (100%)	-0.94	0 100 100	15, 26, 53, 69	1 (0%)
2	J	238/238 (100%)	-0.89	0 100 100	17, 28, 53, 72	1 (0%)
2	L	238/238 (100%)	-0.90	0 100 100	16, 28, 54, 71	1 (0%)
All	All	2628/2628 (100%)	-0.80	15 (0%) 85 86	14, 30, 60, 74	6 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	99	PHE	3.1
1	A	99	PHE	3.0
1	G	101	ALA	3.0
1	E	99	PHE	2.9
1	E	101	ALA	2.8
1	K	99	PHE	2.6
2	B	301	PRO	2.5
1	A	101	ALA	2.4
1	G	99	PHE	2.3
1	C	101	ALA	2.3
2	B	303	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	101	ALA	2.3
1	G	26	ALA	2.2
2	F	368	ASN	2.1
1	E	102	GLY	2.1

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

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

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(Å ²)	Q<0.9
4	DHB	H	3550	11/11	0.84	0.19	63,70,72,74	0
4	DHB	B	550	11/11	0.86	0.15	53,57,59,61	0
4	DHB	J	4550	11/11	0.86	0.16	66,67,68,68	0
4	DHB	L	5550	11/11	0.86	0.17	65,67,68,69	0
4	DHB	F	2550	11/11	0.87	0.14	52,56,58,59	0
4	DHB	D	1550	11/11	0.87	0.15	57,59,59,60	0
3	FE	J	600	1/1	0.92	0.11	93,93,93,93	0
3	FE	B	600	1/1	0.94	0.08	85,85,85,85	0
3	FE	F	600	1/1	0.95	0.06	79,79,79,79	0
3	FE	H	600	1/1	0.95	0.09	84,84,84,84	0
3	FE	D	600	1/1	0.95	0.07	81,81,81,81	0
3	FE	L	600	1/1	0.97	0.04	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.