



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:01 PM UTC

PDB ID : 9FWV / pdb_00009fwv
EMDB ID : EMD-50836
Title : Rubisco in native beta-carboxysomes
Authors : Sheng, Y.; Hardenbrook, N.; Li, K.
Deposited on : 2024-07-01
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

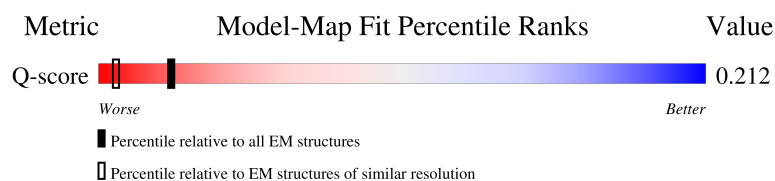
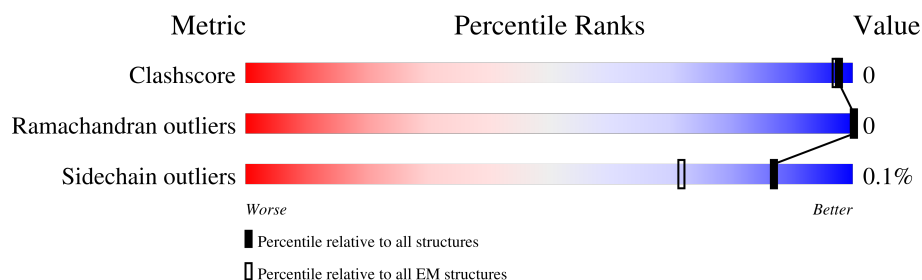
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



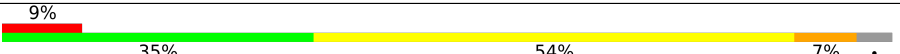
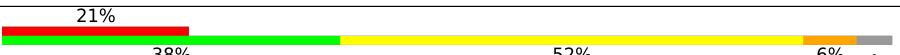
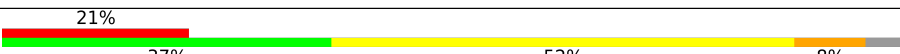
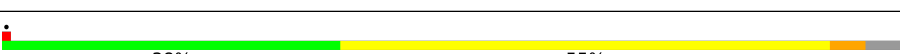
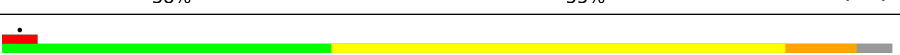
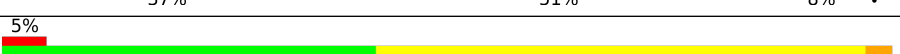
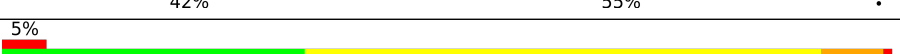
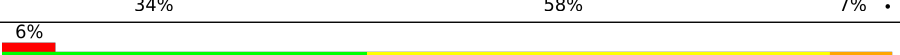
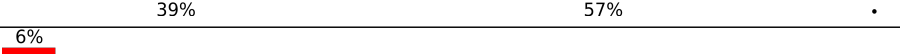
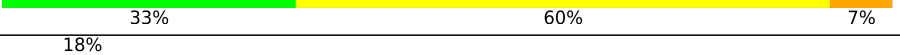
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	86	80% 38% 51% 10%
1	B	86	84% 48% 45% 7%
1	F	86	87% 41% 51% 8%
1	T	86	90% 41% 55% 5%

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Mol	Chain	Length	Quality of chain
2	C	442	
2	G	442	
2	H	442	
2	I	442	
2	J	442	
2	Q	442	
2	R	442	
2	S	442	
3	D	101	
3	E	101	
3	K	101	
3	L	101	
3	M	101	
3	N	101	
3	O	101	
3	P	101	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 36308 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Carboxysome assembly protein CcmM.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	86	Total	C	N	O	S	0	0
			697	426	132	137	2		
1	B	86	Total	C	N	O	S	0	0
			697	426	132	137	2		
1	F	86	Total	C	N	O	S	0	0
			697	426	132	137	2		
1	T	86	Total	C	N	O	S	0	0
			697	426	132	137	2		

- Molecule 2 is a protein called Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	426	Total	C	N	O	S	0	0
			3333	2114	587	615	17		
2	G	426	Total	C	N	O	S	0	0
			3333	2114	587	615	17		
2	H	426	Total	C	N	O	S	0	0
			3333	2114	587	615	17		
2	I	426	Total	C	N	O	S	0	0
			3333	2114	587	615	17		
2	J	426	Total	C	N	O	S	0	0
			3333	2114	587	615	17		
2	Q	426	Total	C	N	O	S	0	0
			3333	2114	587	615	17		
2	R	426	Total	C	N	O	S	0	0
			3333	2114	587	615	17		
2	S	426	Total	C	N	O	S	0	0
			3333	2114	587	615	17		

- Molecule 3 is a protein called Ribulose biphosphate carboxylase small subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	101	Total	C	N	O	S	0	0
			857	550	144	157	6		

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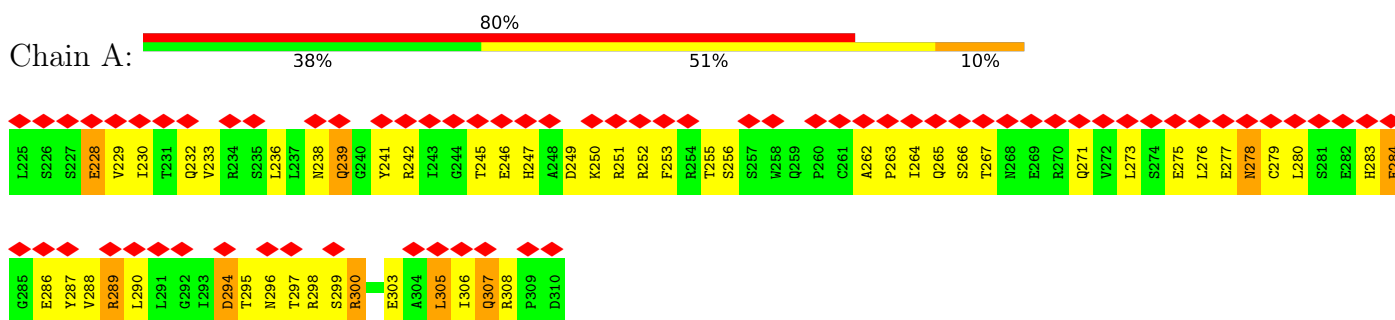
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	101	Total	C	N	O	S	0	0
			857	550	144	157	6		
3	K	101	Total	C	N	O	S	0	0
			857	550	144	157	6		
3	L	101	Total	C	N	O	S	0	0
			857	550	144	157	6		
3	M	101	Total	C	N	O	S	0	0
			857	550	144	157	6		
3	N	101	Total	C	N	O	S	0	0
			857	550	144	157	6		
3	O	101	Total	C	N	O	S	0	0
			857	550	144	157	6		
3	P	101	Total	C	N	O	S	0	0
			857	550	144	157	6		

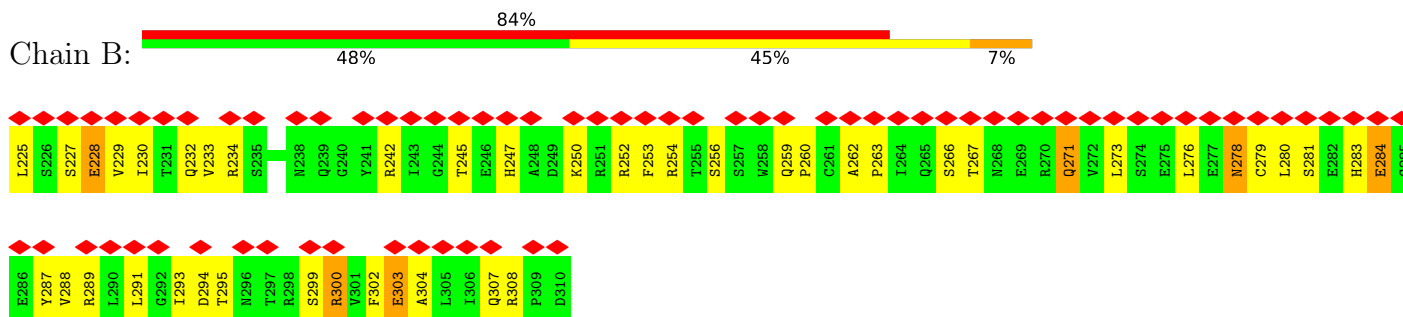
3 Residue-property plots

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 atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

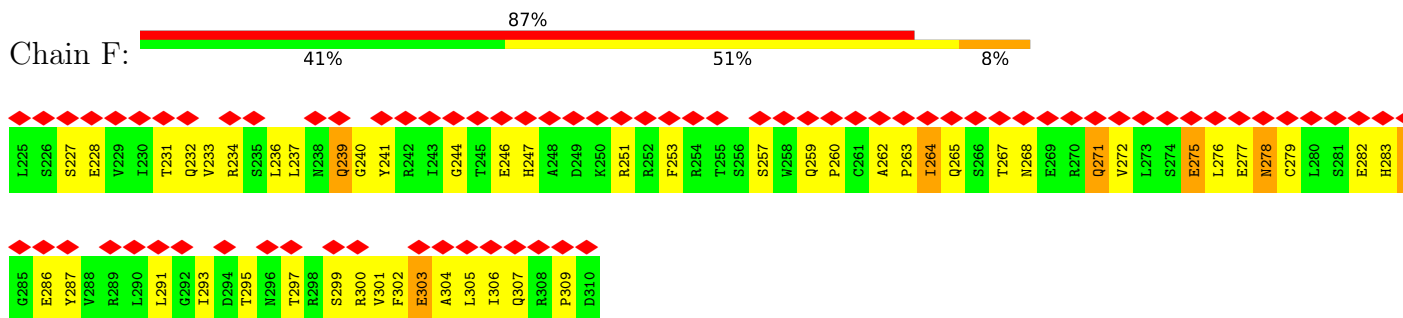
- Molecule 1: Carboxysome assembly protein CcmM



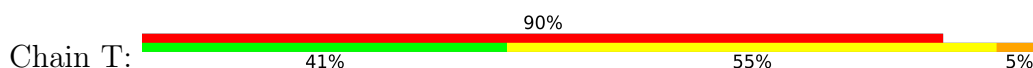
- Molecule 1: Carboxysome assembly protein CcmM

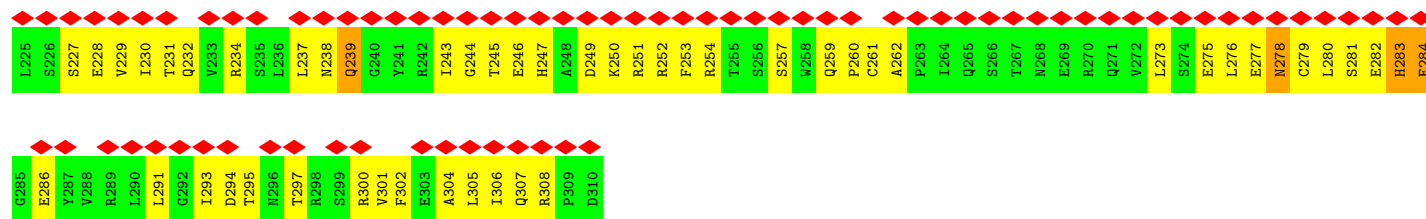


- Molecule 1: Carboxysome assembly protein CcmM

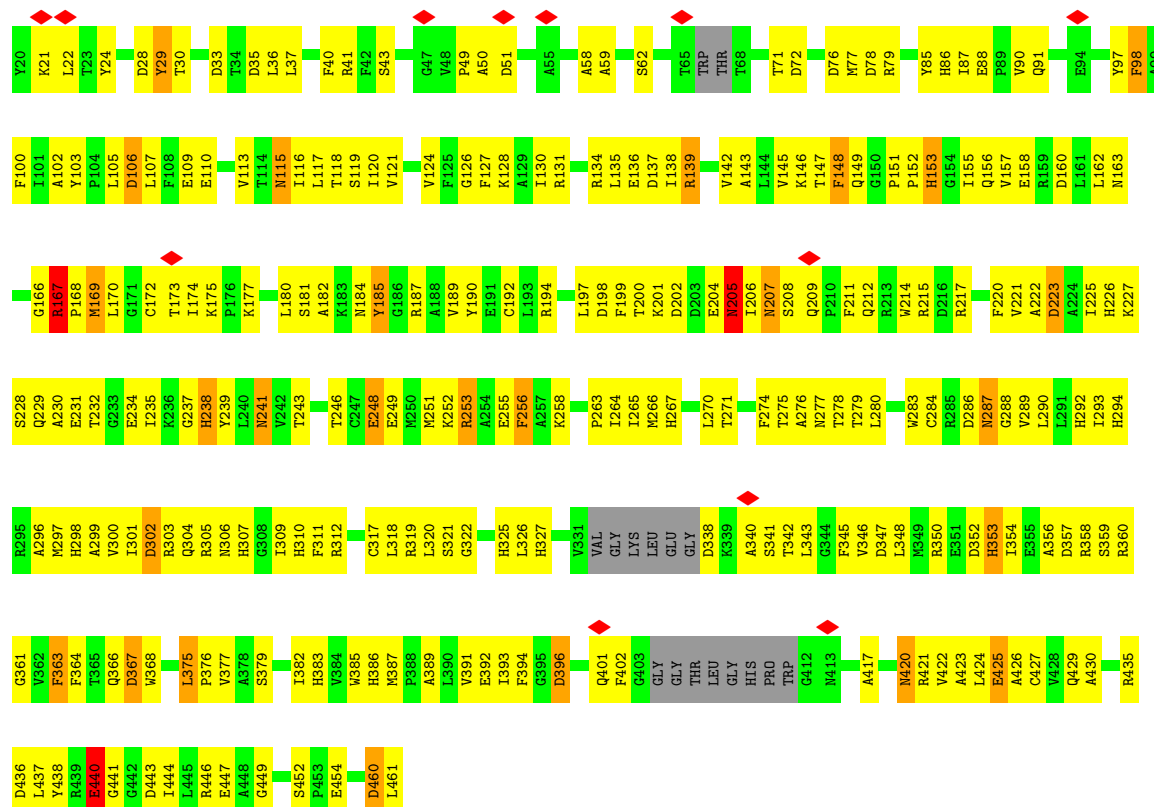


- Molecule 1: Carboxysome assembly protein CcmM

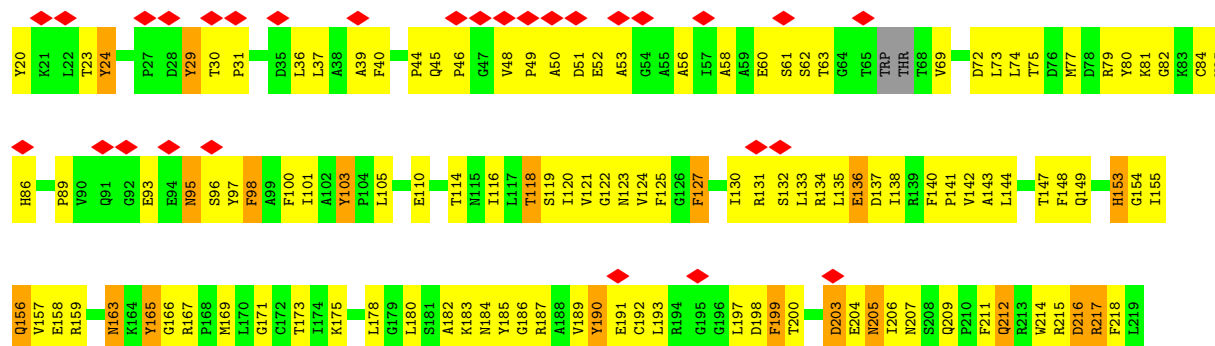


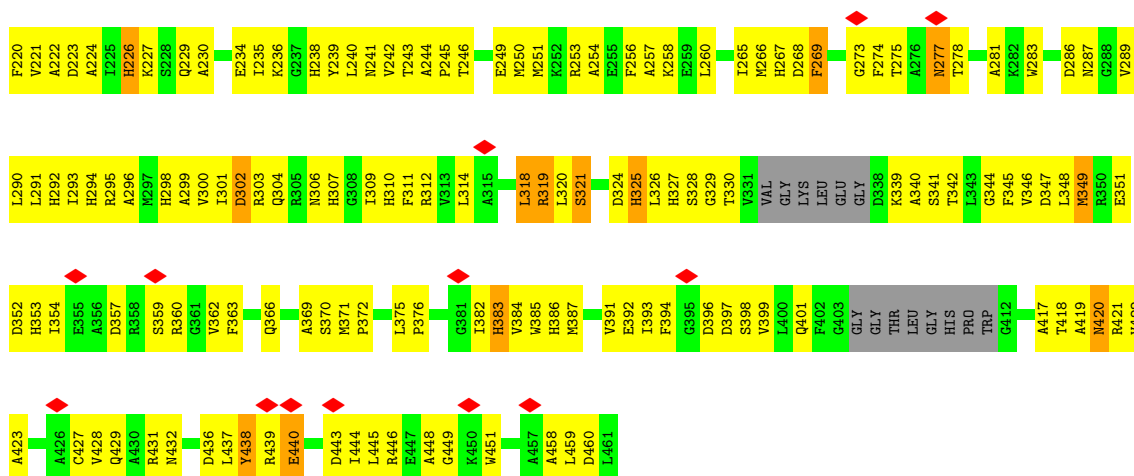


• Molecule 2: Ribulose biphosphate carboxylase large chain

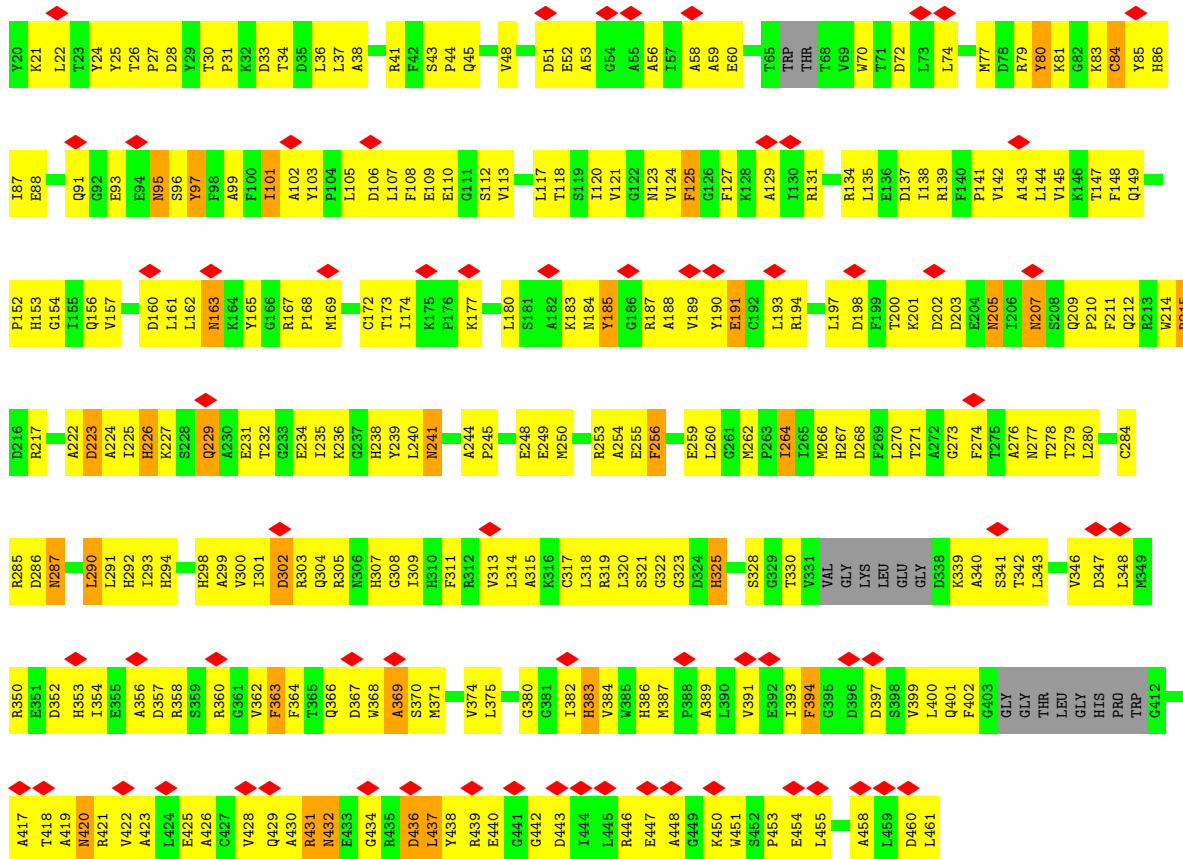


• Molecule 2: Ribulose biphosphate carboxylase large chain



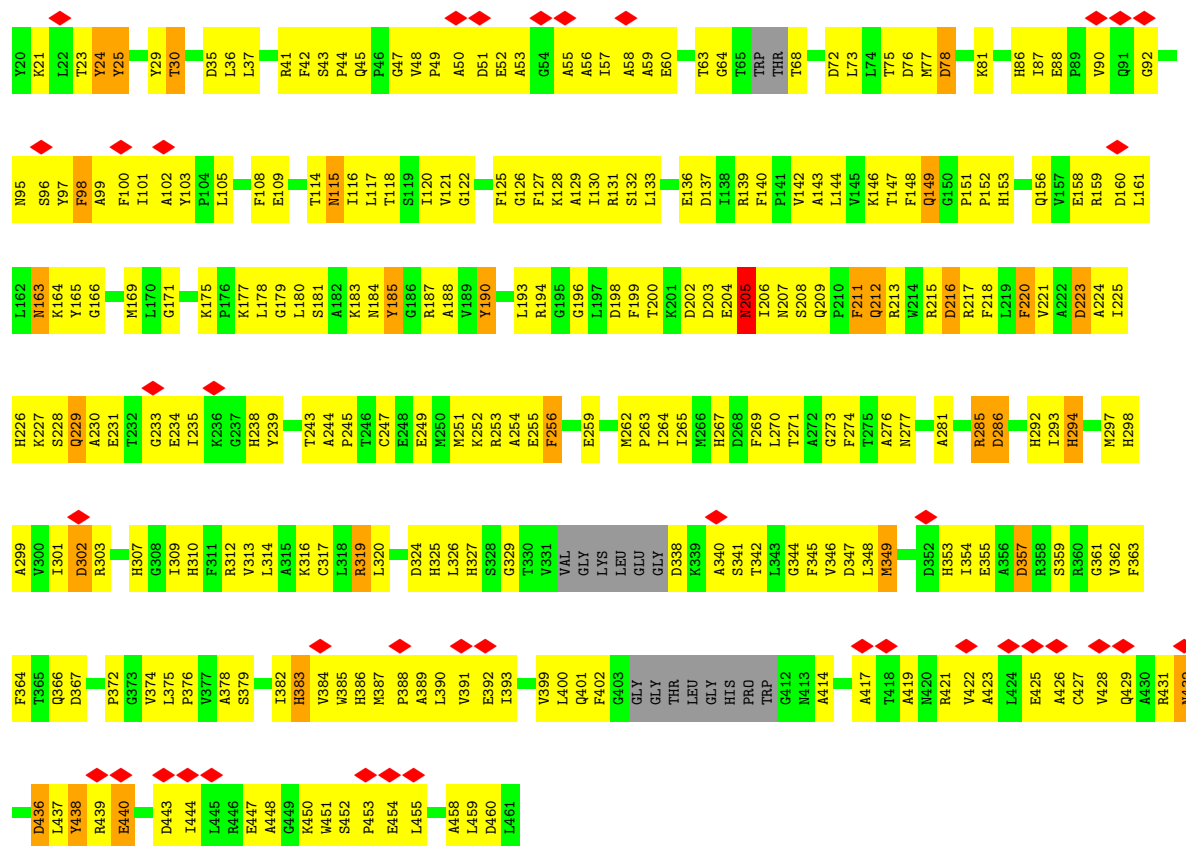


• Molecule 2: Ribulose biphosphate carboxylase large chain

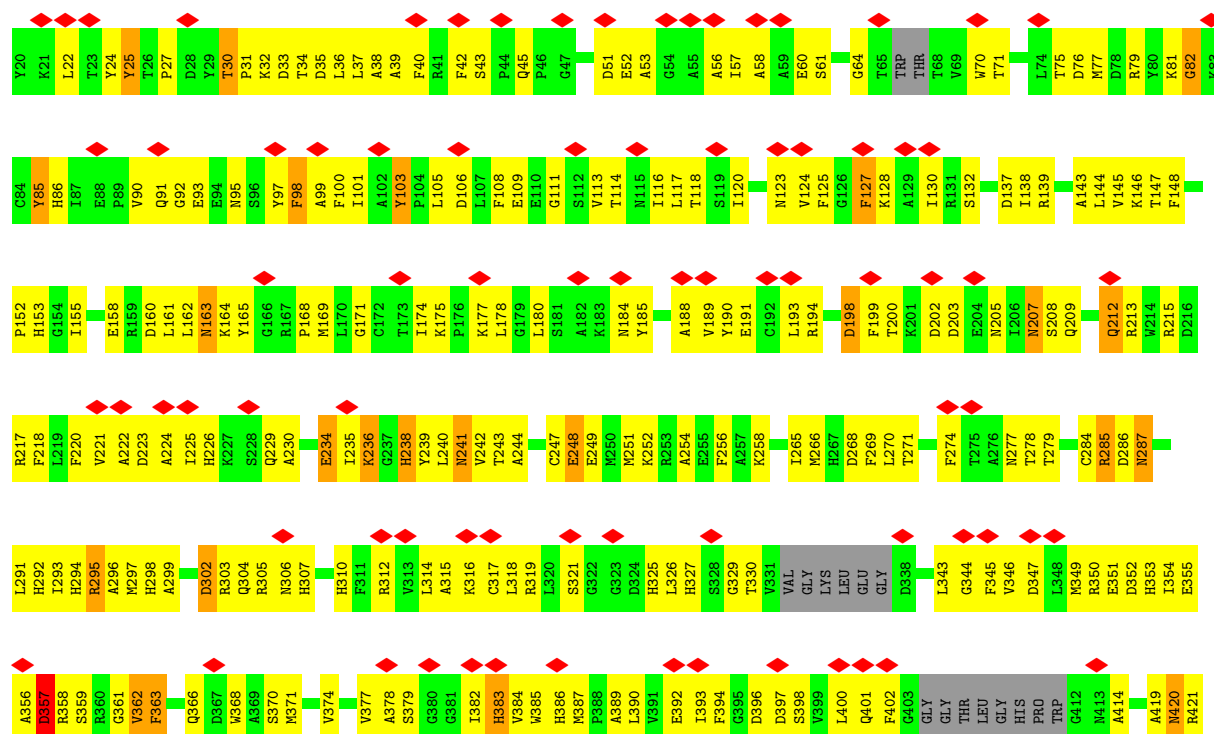


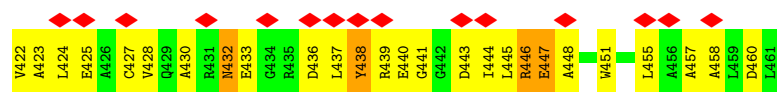
• Molecule 2: Ribulose bisphosphate carboxylase large chain



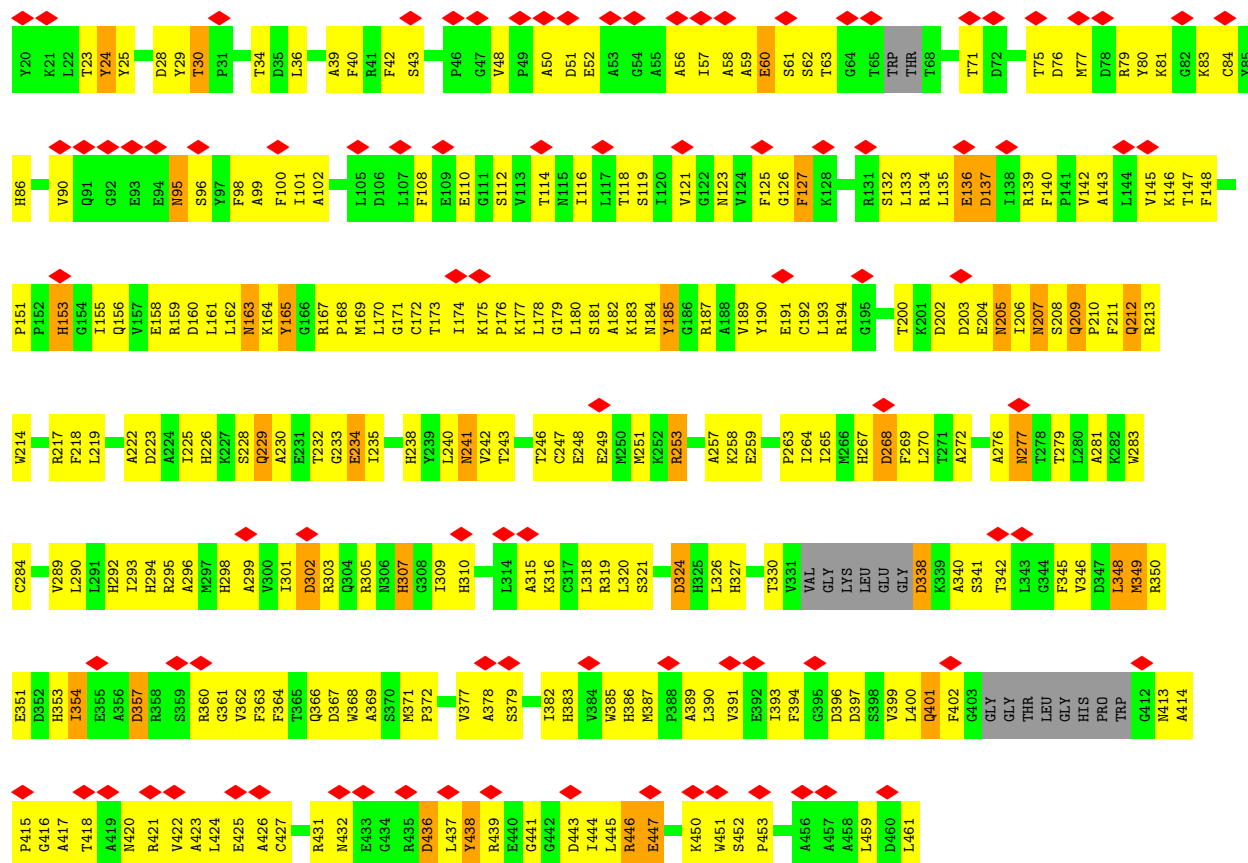


• Molecule 2: Ribulose biphosphate carboxylase large chain

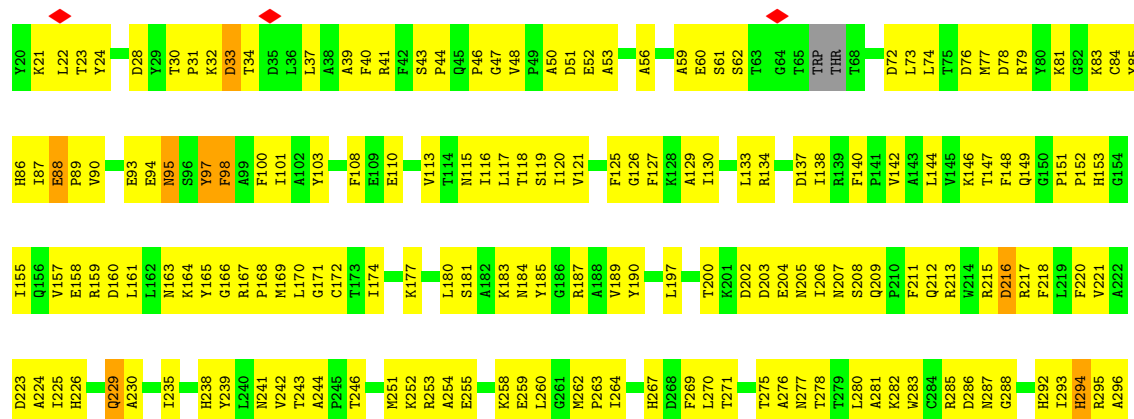


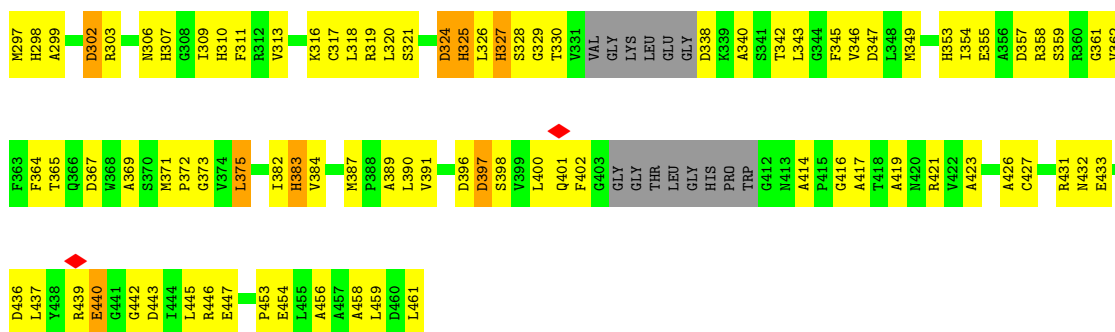


• Molecule 2: Ribulose biphosphate carboxylase large chain

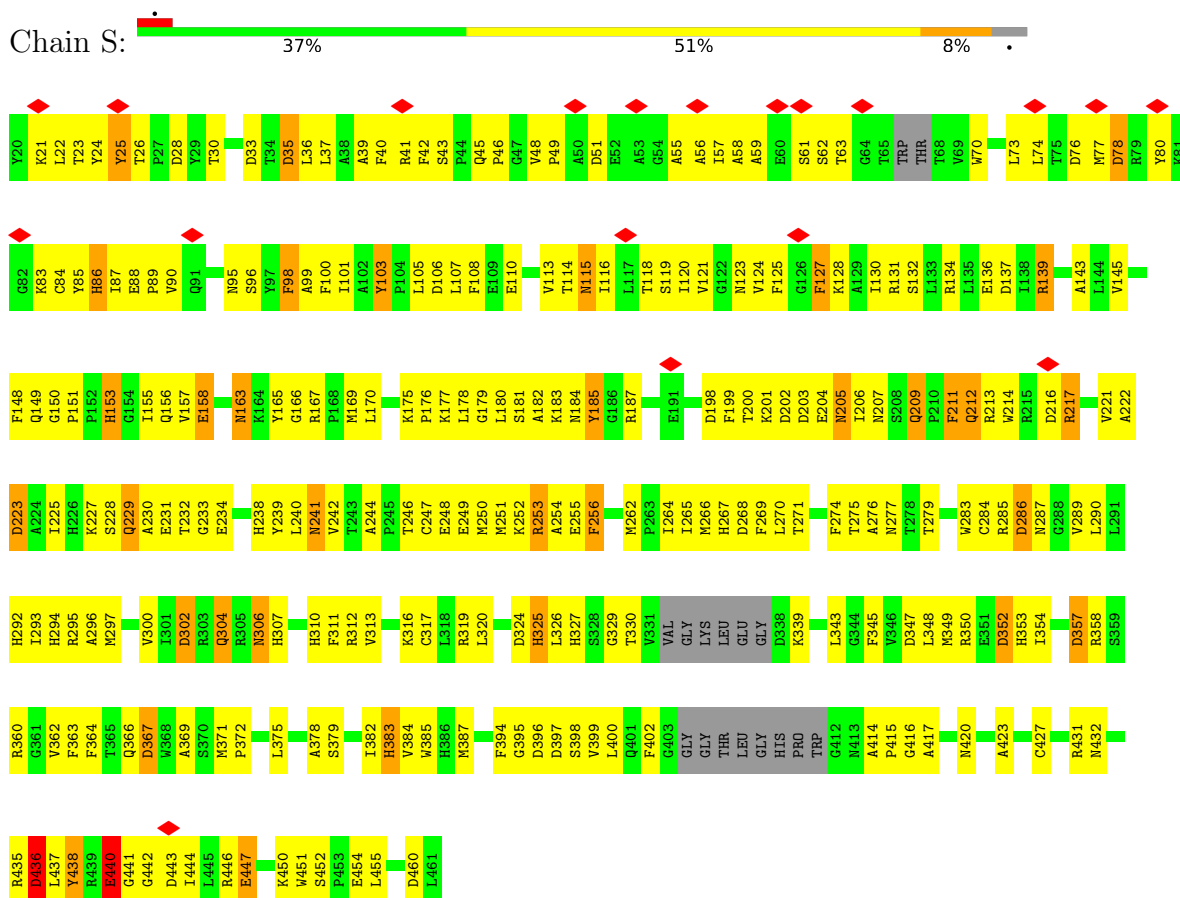


• Molecule 2: Ribulose biphosphate carboxylase large chain

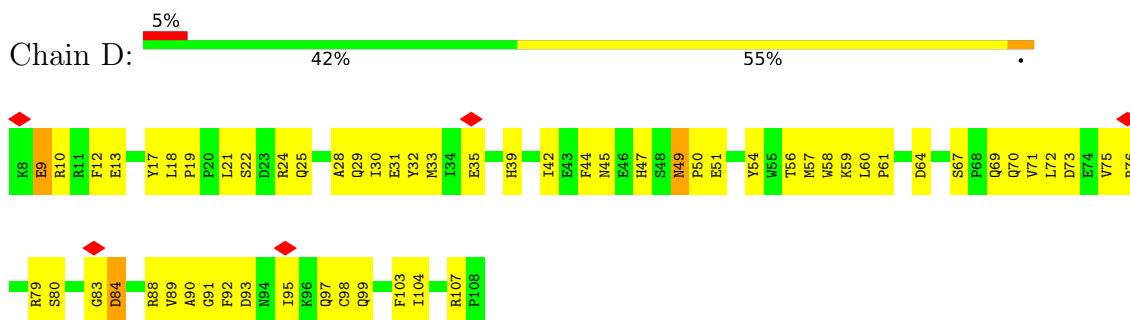




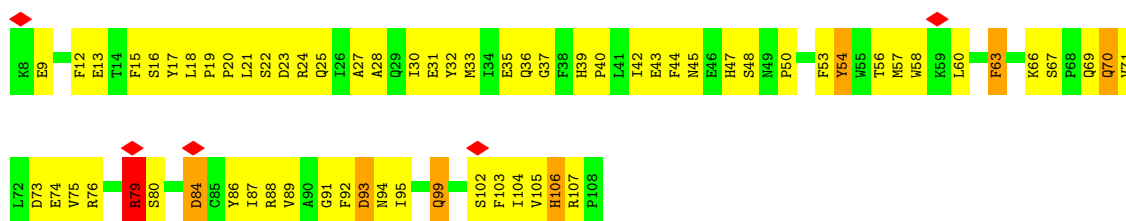
• Molecule 2: Ribulose biphosphate carboxylase large chain



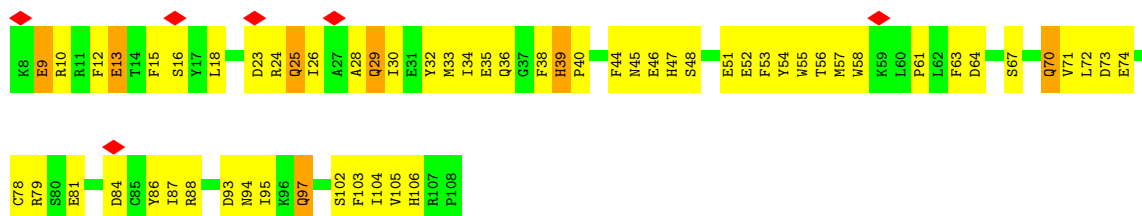
• Molecule 3: Ribulose biphosphate carboxylase small subunit



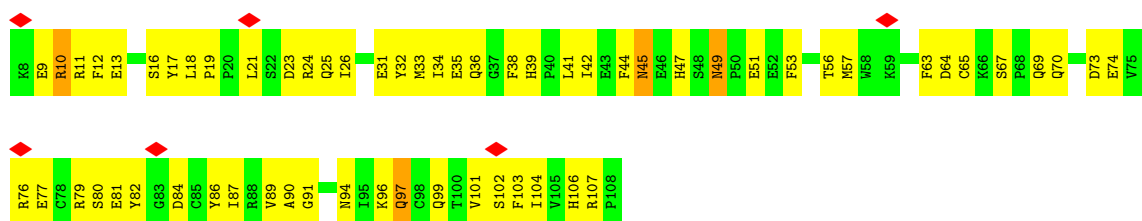
• Molecule 3: Ribulose biphosphate carboxylase small subunit



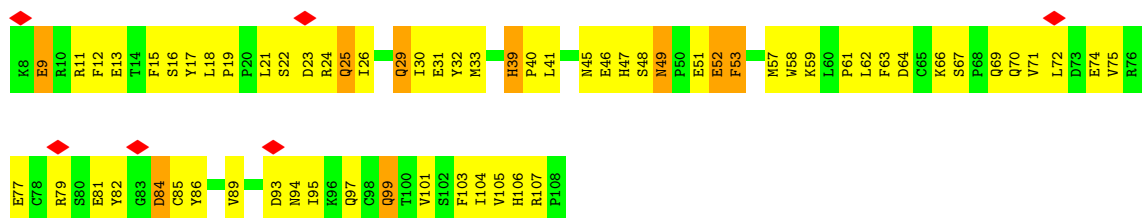
- Molecule 3: Ribulose biphosphate carboxylase small subunit



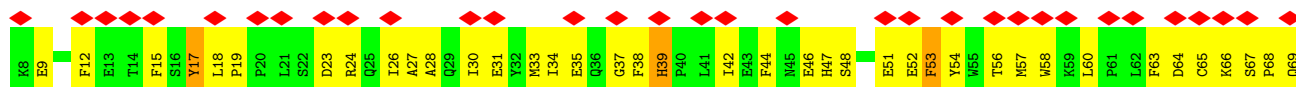
- Molecule 3: Ribulose biphosphate carboxylase small subunit

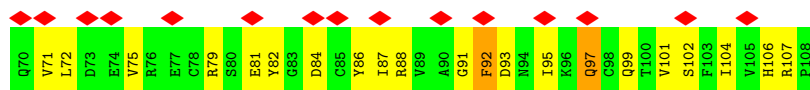


- Molecule 3: Ribulose biphosphate carboxylase small subunit

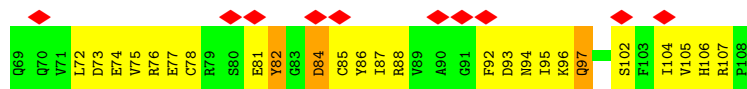


- Molecule 3: Ribulose biphosphate carboxylase small subunit

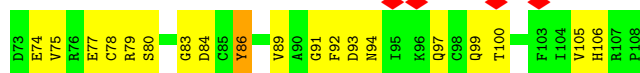




- Molecule 3: Ribulose biphosphate carboxylase small subunit



- Molecule 3: Ribulose biphosphate carboxylase small subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, D4	Depositor
Number of subtomograms used	185	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	123	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.744	Depositor
Minimum map value	-3.571	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.227	Depositor
Recommended contour level	0.311	Depositor
Map size (Å)	275.4, 275.4, 275.4	wwPDB
Map dimensions	204, 204, 204	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	2.75	48/707 (6.8%)	2.06	33/955 (3.5%)
1	B	2.74	45/707 (6.4%)	2.17	36/955 (3.8%)
1	F	2.71	41/707 (5.8%)	2.10	28/955 (2.9%)
1	T	2.92	57/707 (8.1%)	2.06	35/955 (3.7%)
2	C	2.83	258/3411 (7.6%)	2.17	178/4617 (3.9%)
2	G	2.84	265/3411 (7.8%)	2.15	191/4617 (4.1%)
2	H	2.84	240/3411 (7.0%)	2.27	202/4617 (4.4%)
2	I	2.87	275/3411 (8.1%)	2.21	193/4617 (4.2%)
2	J	2.81	233/3411 (6.8%)	2.26	181/4617 (3.9%)
2	Q	2.85	239/3411 (7.0%)	2.22	205/4617 (4.4%)
2	R	2.87	257/3411 (7.5%)	2.19	193/4617 (4.2%)
2	S	2.88	270/3411 (7.9%)	2.22	177/4617 (3.8%)
3	D	2.74	65/883 (7.4%)	2.02	36/1195 (3.0%)
3	E	2.74	63/883 (7.1%)	2.08	43/1195 (3.6%)
3	K	2.72	52/883 (5.9%)	2.18	50/1195 (4.2%)
3	L	2.73	65/883 (7.4%)	2.24	54/1195 (4.5%)
3	M	2.73	60/883 (6.8%)	2.28	58/1195 (4.9%)
3	N	2.76	56/883 (6.3%)	2.20	49/1195 (4.1%)
3	O	2.84	65/883 (7.4%)	2.16	43/1195 (3.6%)
3	P	2.64	53/883 (6.0%)	2.04	33/1195 (2.8%)
All	All	2.82	2707/37180 (7.3%)	2.19	2018/50316 (4.0%)

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	9
1	B	0	7
1	F	0	7
1	T	0	7
2	C	0	28

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	30
2	H	0	28
2	I	0	34
2	J	0	28
2	Q	0	35
2	R	0	17
2	S	0	40
3	D	0	6
3	E	0	7
3	K	0	10
3	L	0	3
3	M	0	11
3	N	0	8
3	O	0	9
3	P	0	8
All	All	0	332

All (2707) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	86	HIS	CD2-NE2	12.07	1.51	1.37
2	R	383	HIS	ND1-CE1	11.96	1.44	1.32
3	L	47	HIS	CD2-NE2	10.63	1.49	1.37
3	K	33	MET	SD-CE	-10.61	1.53	1.79
1	T	291	LEU	C-N	10.57	1.40	1.33
2	I	294	HIS	CD2-NE2	10.56	1.49	1.37
2	J	153	HIS	CD2-NE2	10.54	1.49	1.37
2	Q	298	HIS	CD2-NE2	10.50	1.49	1.37
2	J	353	HIS	CD2-NE2	10.40	1.49	1.37
2	I	226	HIS	ND1-CE1	10.34	1.42	1.32
2	I	251	MET	SD-CE	-10.34	1.53	1.79
2	H	386	HIS	ND1-CE1	10.29	1.42	1.32
3	E	57	MET	SD-CE	-10.28	1.53	1.79
2	R	383	HIS	CA-C	-10.22	1.43	1.53
2	R	327	HIS	CE1-NE2	-10.17	1.22	1.32
2	I	294	HIS	ND1-CE1	10.13	1.42	1.32
3	M	39	HIS	CE1-NE2	-10.08	1.22	1.32
2	S	88	GLU	CA-C	-10.08	1.42	1.52
3	L	106	HIS	CE1-NE2	-9.94	1.22	1.32
2	S	251	MET	SD-CE	-9.94	1.54	1.79
3	N	47	HIS	ND1-CE1	9.88	1.42	1.32
2	I	243	THR	C-N	9.87	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	292	HIS	ND1-CE1	9.68	1.42	1.32
2	R	246	THR	CA-C	9.68	1.64	1.52
3	K	48	SER	CA-C	-9.64	1.41	1.52
3	E	19	PRO	C-O	-9.56	1.16	1.25
2	R	325	HIS	CE1-NE2	-9.56	1.23	1.32
2	Q	394	PHE	CA-C	-9.52	1.42	1.52
2	G	120	ILE	CA-C	-9.49	1.41	1.52
2	I	364	PHE	CA-C	9.44	1.63	1.52
2	R	306	ASN	CA-C	9.34	1.64	1.52
2	Q	369	ALA	CA-C	-9.34	1.42	1.53
1	T	308	ARG	CA-C	-9.32	1.43	1.52
2	I	361	GLY	C-N	-9.31	1.24	1.33
3	N	64	ASP	CA-C	9.22	1.64	1.53
2	Q	40	PHE	CA-C	-9.19	1.41	1.52
1	B	271	GLN	CA-C	9.18	1.64	1.52
3	L	73	ASP	CA-C	9.16	1.64	1.52
3	E	18	LEU	CA-C	9.15	1.63	1.52
2	S	155	ILE	CA-CB	9.14	1.64	1.54
2	H	134	ARG	CA-C	-9.09	1.41	1.52
3	K	39	HIS	CE1-NE2	-9.06	1.23	1.32
2	C	292	HIS	CE1-NE2	-9.04	1.23	1.32
2	Q	307	HIS	CD2-NE2	9.04	1.47	1.37
3	M	57	MET	SD-CE	-9.03	1.56	1.79
2	S	169	MET	SD-CE	-9.03	1.56	1.79
3	N	39	HIS	CD2-NE2	9.02	1.47	1.37
2	C	294	HIS	ND1-CE1	8.98	1.41	1.32
2	H	340	ALA	CA-C	8.96	1.64	1.52
3	E	93	ASP	CA-C	-8.95	1.41	1.52
1	F	303	GLU	CA-C	8.95	1.63	1.52
1	T	251	ARG	CA-C	8.94	1.64	1.52
2	R	298	HIS	CE1-NE2	-8.92	1.23	1.32
1	A	249	ASP	CA-C	-8.88	1.41	1.53
2	G	387	MET	SD-CE	-8.87	1.57	1.79
3	O	106	HIS	CE1-NE2	8.86	1.41	1.32
2	G	299	ALA	C-N	8.84	1.43	1.33
2	G	310	HIS	CD2-NE2	8.84	1.47	1.37
1	T	247	HIS	CE1-NE2	-8.83	1.23	1.32
2	G	399	VAL	CA-C	8.82	1.63	1.52
2	I	271	THR	CA-C	-8.79	1.42	1.52
3	D	58	TRP	CA-C	-8.78	1.43	1.53
3	O	12	PHE	CA-C	-8.75	1.42	1.52
1	T	273	LEU	CA-C	-8.75	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	327	HIS	ND1-CE1	-8.73	1.23	1.32
2	H	112	SER	CA-C	8.70	1.62	1.52
2	I	417	ALA	CA-C	8.70	1.63	1.52
2	R	153	HIS	ND1-CE1	-8.69	1.23	1.32
2	R	446	ARG	CA-C	-8.69	1.42	1.52
2	S	414	ALA	N-CA	-8.68	1.38	1.46
2	Q	241	ASN	CA-C	8.68	1.64	1.52
2	Q	36	LEU	CA-C	-8.66	1.42	1.52
2	S	417	ALA	CA-C	8.66	1.63	1.52
3	E	12	PHE	CA-C	8.65	1.63	1.52
2	G	265	ILE	CA-C	8.64	1.63	1.52
3	N	69	GLN	CA-C	8.64	1.64	1.52
2	S	325	HIS	CE1-NE2	-8.64	1.24	1.32
2	Q	48	VAL	CA-C	8.63	1.60	1.53
1	F	276	LEU	CA-C	-8.61	1.41	1.52
2	S	163	ASN	CA-C	8.60	1.64	1.53
2	R	174	ILE	CA-C	-8.60	1.42	1.52
3	O	102	SER	CA-C	8.59	1.62	1.52
3	P	39	HIS	CA-C	8.59	1.62	1.52
2	S	264	ILE	CA-C	-8.58	1.41	1.52
3	N	58	TRP	CA-C	-8.58	1.43	1.53
2	C	79	ARG	CA-C	8.57	1.64	1.52
2	G	93	GLU	CA-C	-8.56	1.42	1.52
2	G	325	HIS	CE1-NE2	-8.56	1.24	1.32
2	Q	294	HIS	CE1-NE2	8.54	1.41	1.32
2	C	267	HIS	CA-C	8.54	1.62	1.52
2	Q	327	HIS	ND1-CE1	-8.54	1.24	1.32
3	O	88	ARG	CA-C	8.52	1.62	1.52
3	O	106	HIS	CA-C	-8.52	1.42	1.52
2	S	110	GLU	CA-C	-8.49	1.41	1.52
2	S	244	ALA	CA-C	8.48	1.60	1.52
2	G	268	ASP	CA-C	-8.47	1.42	1.52
2	J	353	HIS	CA-C	8.46	1.62	1.52
2	H	298	HIS	CD2-NE2	8.45	1.47	1.37
1	A	289	ARG	CA-C	8.40	1.62	1.52
2	S	37	LEU	CA-C	-8.39	1.42	1.52
2	Q	206	ILE	CA-C	-8.39	1.45	1.53
2	H	241	ASN	CA-C	-8.37	1.42	1.52
3	E	73	ASP	CA-C	8.34	1.63	1.52
2	H	250	MET	SD-CE	-8.34	1.58	1.79
2	J	43	SER	CA-C	8.33	1.62	1.52
2	H	153	HIS	CA-C	8.33	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	259	GLN	CA-C	-8.33	1.44	1.52
2	H	177	LYS	C-N	8.33	1.43	1.33
2	I	349	MET	C-N	8.33	1.44	1.33
1	B	250	LYS	CA-C	8.32	1.63	1.52
2	J	53	ALA	CA-C	8.32	1.63	1.52
2	G	223	ASP	CA-C	8.30	1.63	1.52
3	E	16	SER	CA-C	-8.30	1.42	1.52
2	H	193	LEU	CA-C	-8.28	1.42	1.52
2	R	130	ILE	CA-CB	8.28	1.64	1.53
2	S	317	CYS	C-N	-8.27	1.24	1.33
2	Q	191	GLU	C-N	-8.27	1.24	1.33
3	N	81	GLU	CA-C	8.24	1.63	1.52
2	R	353	HIS	ND1-CE1	8.23	1.40	1.32
2	I	35	ASP	CA-C	-8.22	1.42	1.53
3	L	39	HIS	ND1-CE1	8.22	1.40	1.32
2	R	361	GLY	C-N	8.21	1.41	1.33
2	H	382	ILE	C-N	8.21	1.44	1.33
2	I	140	PHE	CA-C	8.21	1.61	1.52
2	Q	294	HIS	ND1-CE1	8.20	1.40	1.32
3	M	107	ARG	CA-C	8.18	1.60	1.52
2	I	68	THR	C-N	-8.16	1.26	1.33
3	D	47	HIS	CE1-NE2	-8.16	1.24	1.32
2	H	266	MET	SD-CE	-8.16	1.59	1.79
3	N	106	HIS	CA-C	-8.16	1.42	1.52
2	Q	232	THR	CA-C	8.15	1.63	1.52
2	H	205	ASN	C-N	8.14	1.43	1.33
2	Q	167	ARG	CA-C	8.14	1.61	1.52
3	O	104	ILE	C-N	-8.13	1.25	1.33
2	C	88	GLU	C-O	-8.11	1.16	1.24
2	H	341	SER	CA-C	-8.10	1.41	1.52
2	G	159	ARG	CA-C	-8.10	1.42	1.52
2	G	155	ILE	C-O	-8.09	1.15	1.24
2	C	386	HIS	ND1-CE1	8.07	1.40	1.32
2	I	353	HIS	CD2-NE2	8.06	1.46	1.37
3	N	97	GLN	C-N	8.06	1.44	1.33
3	M	49	ASN	CA-C	-8.04	1.44	1.52
2	R	97	TYR	CA-C	8.04	1.62	1.52
2	R	241	ASN	C-N	-8.03	1.24	1.33
2	I	100	PHE	CA-C	8.03	1.61	1.52
2	J	224	ALA	CA-C	-8.02	1.42	1.52
2	R	251	MET	SD-CE	-8.02	1.59	1.79
3	L	19	PRO	CA-C	8.02	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	134	ARG	CA-C	8.01	1.61	1.52
2	C	382	ILE	CA-C	-8.00	1.42	1.52
2	R	32	LYS	CA-C	-8.00	1.42	1.52
2	R	316	LYS	CA-C	-8.00	1.42	1.52
2	C	253	ARG	CA-C	7.99	1.62	1.52
1	T	228	GLU	C-N	7.99	1.44	1.33
2	H	124	VAL	CA-C	7.98	1.62	1.52
2	H	226	HIS	ND1-CE1	-7.98	1.24	1.32
2	S	262	MET	SD-CE	-7.98	1.59	1.79
2	S	167	ARG	CA-C	7.98	1.62	1.52
1	B	289	ARG	C-O	-7.97	1.14	1.24
2	G	187	ARG	CA-C	-7.96	1.42	1.52
2	Q	165	TYR	C-N	7.96	1.43	1.33
2	J	387	MET	SD-CE	-7.96	1.59	1.79
2	C	358	ARG	C-N	7.95	1.44	1.33
3	E	27	ALA	CA-C	-7.95	1.42	1.52
3	D	57	MET	C-N	7.93	1.44	1.33
3	D	103	PHE	CA-C	-7.92	1.43	1.52
2	G	63	THR	CA-CB	-7.92	1.43	1.54
1	A	295	THR	CA-C	-7.92	1.42	1.52
2	H	28	ASP	CA-C	7.92	1.63	1.52
2	Q	310	HIS	CD2-NE2	7.92	1.46	1.37
3	P	46	GLU	CA-C	7.91	1.63	1.52
2	S	400	LEU	C-O	-7.91	1.15	1.24
2	S	214	TRP	C-O	-7.89	1.15	1.24
2	S	96	SER	CA-C	-7.89	1.42	1.52
2	I	161	LEU	CA-C	-7.88	1.42	1.52
1	T	277	GLU	CA-C	7.88	1.62	1.52
2	Q	293	ILE	C-O	-7.88	1.16	1.24
2	Q	450	LYS	CA-C	7.88	1.62	1.52
2	C	202	ASP	CA-C	-7.87	1.42	1.53
2	G	256	PHE	C-N	7.86	1.43	1.33
3	D	12	PHE	CA-C	7.86	1.62	1.52
3	D	89	VAL	CA-C	-7.86	1.43	1.52
2	G	226	HIS	CE1-NE2	-7.86	1.24	1.32
2	Q	204	GLU	CA-C	7.85	1.62	1.52
2	C	425	GLU	CA-C	-7.85	1.42	1.52
2	H	420	ASN	CA-C	7.85	1.62	1.52
2	Q	24	TYR	CA-C	-7.85	1.42	1.52
3	K	57	MET	SD-CE	-7.84	1.59	1.79
2	S	202	ASP	CA-C	-7.82	1.42	1.53
2	G	169	MET	SD-CE	-7.82	1.60	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	64	ASP	CA-C	7.81	1.62	1.53
2	C	446	ARG	C-N	7.80	1.44	1.33
2	H	169	MET	SD-CE	-7.80	1.60	1.79
2	H	81	LYS	CA-C	-7.80	1.42	1.52
2	G	309	ILE	C-O	-7.79	1.16	1.24
2	R	342	THR	CA-C	-7.79	1.43	1.52
2	H	439	ARG	CA-C	7.79	1.63	1.52
3	D	70	GLN	CA-C	7.79	1.62	1.52
2	C	214	TRP	CA-C	7.78	1.62	1.52
2	Q	90	VAL	C-O	-7.77	1.14	1.24
3	P	57	MET	C-N	7.77	1.43	1.33
2	I	231	GLU	C-O	-7.76	1.15	1.24
1	A	294	ASP	CA-C	-7.75	1.43	1.52
2	J	297	MET	SD-CE	-7.75	1.60	1.79
2	Q	174	ILE	CA-CB	7.74	1.62	1.54
2	Q	48	VAL	N-CA	-7.73	1.39	1.46
3	N	28	ALA	CA-C	-7.73	1.42	1.52
2	H	180	LEU	C-N	7.72	1.44	1.33
2	C	283	TRP	C-O	-7.72	1.15	1.24
2	H	30	THR	CA-C	7.72	1.61	1.52
2	Q	230	ALA	CA-C	7.72	1.62	1.52
3	K	34	ILE	CA-C	-7.72	1.42	1.52
2	G	130	ILE	CA-CB	7.71	1.63	1.53
2	J	138	ILE	CA-C	7.71	1.62	1.52
2	R	263	PRO	C-N	7.70	1.44	1.33
2	C	251	MET	SD-CE	-7.70	1.60	1.79
2	J	251	MET	C-N	7.70	1.44	1.33
2	Q	52	GLU	CA-C	7.70	1.62	1.52
1	T	253	PHE	C-O	-7.69	1.15	1.24
2	G	215	ARG	C-N	7.69	1.44	1.33
2	I	96	SER	CA-C	7.68	1.62	1.52
2	Q	427	CYS	C-N	-7.68	1.24	1.33
2	H	248	GLU	CA-C	7.67	1.62	1.52
1	T	281	SER	C-O	-7.67	1.15	1.24
2	R	78	ASP	CA-C	7.66	1.63	1.52
2	J	241	ASN	C-N	7.66	1.42	1.33
2	Q	310	HIS	ND1-CE1	7.65	1.40	1.32
2	Q	444	ILE	C-O	-7.65	1.15	1.24
2	I	75	THR	CA-C	7.64	1.62	1.52
2	R	264	ILE	CA-C	-7.64	1.43	1.52
2	S	119	SER	CA-C	7.64	1.62	1.52
2	Q	354	ILE	CA-C	7.63	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	166	GLY	C-N	7.63	1.41	1.33
2	H	168	PRO	N-CA	7.63	1.54	1.46
2	S	254	ALA	C-O	-7.62	1.15	1.24
2	G	142	VAL	C-N	-7.62	1.24	1.33
2	Q	160	ASP	CA-C	7.62	1.62	1.52
2	G	401	GLN	CA-C	7.62	1.61	1.52
2	G	40	PHE	CA-C	-7.61	1.43	1.52
2	S	349	MET	C-N	7.60	1.43	1.33
3	M	32	TYR	C-N	-7.60	1.24	1.33
2	S	40	PHE	CA-C	7.60	1.61	1.52
3	N	53	PHE	CA-C	7.59	1.62	1.52
3	D	72	LEU	C-O	-7.59	1.15	1.24
2	G	383	HIS	ND1-CE1	-7.58	1.25	1.32
2	R	226	HIS	CE1-NE2	7.58	1.40	1.32
3	D	51	GLU	CA-C	7.58	1.62	1.52
2	I	270	LEU	CA-C	7.58	1.62	1.52
2	J	86	HIS	CA-C	-7.58	1.43	1.52
2	J	349	MET	SD-CE	-7.58	1.60	1.79
3	K	32	TYR	CA-C	-7.58	1.42	1.52
2	J	368	TRP	CA-C	-7.58	1.43	1.52
2	G	325	HIS	CA-C	7.58	1.62	1.52
2	I	239	TYR	C-N	7.58	1.44	1.33
3	O	18	LEU	CA-C	7.58	1.62	1.52
2	C	49	PRO	C-O	-7.57	1.15	1.23
2	I	382	ILE	C-N	7.56	1.43	1.33
3	K	47	HIS	ND1-CE1	-7.56	1.25	1.32
2	H	77	MET	SD-CE	-7.56	1.60	1.79
2	J	307	HIS	CA-C	-7.56	1.43	1.52
2	R	357	ASP	CA-C	7.55	1.60	1.53
2	C	85	TYR	C-N	7.55	1.43	1.33
1	T	283	HIS	C-N	7.55	1.43	1.33
2	C	37	LEU	C-O	-7.55	1.15	1.24
2	C	222	ALA	CA-C	-7.55	1.43	1.52
3	E	19	PRO	C-N	7.55	1.42	1.33
1	B	308	ARG	N-CA	-7.54	1.39	1.45
2	C	217	ARG	C-O	-7.54	1.15	1.24
2	S	379	SER	C-O	-7.54	1.15	1.24
2	S	167	ARG	N-CA	-7.53	1.38	1.46
2	I	425	GLU	C-N	-7.53	1.24	1.33
1	A	251	ARG	N-CA	-7.52	1.37	1.46
1	T	301	VAL	C-N	7.52	1.43	1.33
3	E	48	SER	CA-C	-7.52	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	16	SER	CA-C	-7.52	1.42	1.52
2	H	120	ILE	CA-CB	7.52	1.64	1.54
2	G	135	LEU	CA-C	-7.51	1.43	1.52
2	R	37	LEU	C-N	7.51	1.43	1.33
2	G	397	ASP	C-N	-7.50	1.23	1.33
2	S	182	ALA	C-N	7.50	1.43	1.33
2	H	401	GLN	CA-C	7.50	1.62	1.52
2	R	180	LEU	CA-C	-7.50	1.43	1.52
2	R	213	ARG	CA-C	-7.50	1.43	1.52
2	J	37	LEU	C-O	-7.49	1.15	1.23
2	C	103	TYR	C-N	7.49	1.43	1.33
2	R	215	ARG	CA-C	7.49	1.62	1.52
2	I	327	HIS	ND1-CE1	7.49	1.40	1.32
2	I	348	LEU	CA-C	-7.49	1.43	1.52
2	H	450	LYS	CA-C	7.49	1.62	1.52
2	R	402	PHE	CA-C	-7.49	1.43	1.52
2	C	446	ARG	C-O	-7.48	1.15	1.24
2	I	114	THR	N-CA	-7.48	1.37	1.46
3	K	81	GLU	C-N	7.48	1.43	1.33
2	C	119	SER	CA-C	-7.48	1.43	1.52
2	J	379	SER	CA-C	-7.47	1.43	1.53
2	Q	100	PHE	C-N	7.47	1.43	1.33
2	C	181	SER	C-N	-7.47	1.24	1.33
2	I	215	ARG	C-N	7.47	1.44	1.34
2	R	88	GLU	N-CA	-7.45	1.38	1.46
3	O	38	PHE	CA-C	-7.44	1.43	1.52
2	S	23	THR	CA-C	-7.43	1.46	1.52
2	I	226	HIS	CA-C	7.43	1.62	1.52
3	N	12	PHE	C-O	-7.42	1.15	1.23
2	H	386	HIS	CD2-NE2	7.42	1.46	1.37
3	P	39	HIS	ND1-CE1	7.42	1.40	1.32
3	K	106	HIS	CA-C	7.42	1.61	1.52
2	C	24	TYR	CA-C	7.42	1.62	1.52
3	E	37	GLY	C-N	7.41	1.43	1.33
2	S	438	TYR	N-CA	-7.41	1.37	1.46
2	R	32	LYS	C-N	7.40	1.43	1.34
2	J	378	ALA	C-N	-7.40	1.24	1.33
2	I	376	PRO	C-O	-7.39	1.15	1.23
2	C	275	THR	CA-C	-7.39	1.43	1.52
2	Q	378	ALA	N-CA	7.39	1.55	1.46
1	B	281	SER	C-N	7.38	1.43	1.33
2	C	258	LYS	CA-C	-7.38	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	402	PHE	C-O	-7.38	1.15	1.24
2	J	346	VAL	CA-CB	7.38	1.63	1.54
2	R	242	VAL	N-CA	7.38	1.53	1.46
2	R	307	HIS	CE1-NE2	-7.37	1.25	1.32
2	R	275	THR	N-CA	-7.37	1.37	1.46
2	I	42	PHE	CA-C	-7.37	1.43	1.52
2	R	197	LEU	CA-C	-7.37	1.43	1.52
2	S	268	ASP	CA-C	-7.37	1.43	1.52
2	H	80	TYR	N-CA	7.36	1.54	1.46
2	J	347	ASP	C-N	7.36	1.43	1.33
2	R	303	ARG	CA-C	7.35	1.62	1.52
2	H	36	LEU	C-O	-7.34	1.15	1.23
2	Q	206	ILE	CA-CB	7.34	1.61	1.53
2	C	227	LYS	C-N	-7.34	1.24	1.33
1	F	263	PRO	C-O	7.34	1.31	1.23
2	I	169	MET	SD-CE	-7.34	1.61	1.79
2	R	211	PHE	C-N	7.33	1.43	1.33
2	Q	249	GLU	C-O	-7.33	1.15	1.24
2	Q	62	SER	CA-C	-7.32	1.45	1.52
2	Q	217	ARG	N-CA	-7.32	1.37	1.46
3	P	32	TYR	CA-C	-7.32	1.42	1.52
1	A	277	GLU	CA-C	7.32	1.62	1.52
2	J	278	THR	C-N	7.32	1.43	1.33
2	R	401	GLN	CA-C	7.32	1.61	1.52
2	S	399	VAL	C-O	-7.32	1.16	1.23
2	R	59	ALA	CA-C	-7.31	1.43	1.52
2	S	454	GLU	CA-C	7.31	1.62	1.52
2	J	319	ARG	C-N	-7.31	1.25	1.33
2	S	420	ASN	C-N	-7.31	1.24	1.33
1	T	231	THR	C-O	-7.30	1.15	1.24
3	P	72	LEU	C-N	-7.30	1.24	1.33
2	Q	140	PHE	CA-C	7.30	1.61	1.52
2	R	78	ASP	C-O	-7.30	1.15	1.24
2	S	349	MET	SD-CE	-7.30	1.61	1.79
2	S	206	ILE	C-N	7.29	1.43	1.33
1	F	240	GLY	C-N	7.29	1.43	1.33
2	C	182	ALA	CA-C	-7.29	1.43	1.52
1	B	230	ILE	CA-C	7.29	1.62	1.52
2	S	347	ASP	C-N	7.29	1.43	1.33
2	I	252	LYS	C-O	-7.29	1.15	1.24
2	H	87	ILE	CA-CB	7.28	1.63	1.54
2	C	121	VAL	CA-C	7.28	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	85	TYR	C-N	7.28	1.42	1.33
2	H	99	ALA	C-N	7.28	1.43	1.33
2	H	117	LEU	C-N	-7.27	1.24	1.33
2	J	354	ILE	CA-C	-7.27	1.43	1.52
2	I	226	HIS	CD2-NE2	7.27	1.45	1.37
2	I	25	TYR	CA-C	7.26	1.61	1.52
2	R	270	LEU	C-N	-7.26	1.24	1.33
2	C	231	GLU	CA-C	7.25	1.62	1.53
2	Q	364	PHE	C-N	7.25	1.43	1.33
1	F	305	LEU	CA-C	7.25	1.62	1.52
2	H	319	ARG	C-N	7.24	1.42	1.33
2	Q	315	ALA	C-N	7.24	1.43	1.33
2	H	353	HIS	CA-C	-7.24	1.44	1.52
2	Q	362	VAL	CA-C	7.24	1.61	1.52
2	I	52	GLU	C-N	7.24	1.43	1.33
2	I	252	LYS	CA-C	7.24	1.62	1.52
3	N	60	LEU	CA-C	7.24	1.61	1.52
2	I	327	HIS	CD2-NE2	7.23	1.45	1.37
2	S	300	VAL	CA-C	7.22	1.62	1.52
2	R	138	ILE	CA-C	7.22	1.61	1.52
3	E	104	ILE	C-N	7.22	1.40	1.33
3	O	41	LEU	CA-C	-7.21	1.44	1.52
3	O	57	MET	SD-CE	-7.21	1.61	1.79
2	I	426	ALA	CA-C	7.20	1.61	1.52
2	S	382	ILE	C-N	7.20	1.43	1.33
1	A	236	LEU	CA-C	-7.19	1.43	1.52
2	C	110	GLU	CA-C	-7.19	1.43	1.52
3	D	95	ILE	CA-C	-7.18	1.44	1.52
2	R	454	GLU	C-N	7.18	1.43	1.33
2	Q	23	THR	C-N	-7.18	1.24	1.33
2	G	287	ASN	CA-CB	-7.17	1.43	1.53
2	Q	184	ASN	N-CA	7.17	1.55	1.46
2	G	98	PHE	CA-C	7.17	1.61	1.52
2	G	158	GLU	CA-C	-7.15	1.43	1.52
2	C	228	SER	N-CA	7.15	1.54	1.46
2	R	167	ARG	C-N	-7.15	1.24	1.33
2	G	257	ALA	CA-C	7.14	1.61	1.52
1	B	267	THR	CA-C	7.14	1.62	1.52
2	C	266	MET	SD-CE	-7.14	1.61	1.79
2	C	300	VAL	CA-C	7.13	1.61	1.52
2	J	184	ASN	C-N	7.13	1.43	1.33
3	K	45	ASN	CA-C	-7.13	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	350	ARG	CA-C	7.13	1.58	1.52
2	S	41	ARG	C-N	7.12	1.42	1.33
2	S	266	MET	CA-C	-7.12	1.43	1.52
2	C	277	ASN	C-N	-7.12	1.24	1.33
3	O	87	ILE	C-O	-7.12	1.16	1.24
2	S	312	ARG	N-CA	7.12	1.55	1.46
2	G	265	ILE	C-O	-7.11	1.15	1.23
2	R	206	ILE	CA-CB	7.11	1.61	1.53
2	C	134	ARG	C-O	-7.11	1.15	1.23
2	I	198	ASP	N-CA	-7.11	1.37	1.46
2	C	302	ASP	CA-C	-7.10	1.42	1.52
2	I	163	ASN	CA-C	7.10	1.63	1.52
2	R	158	GLU	CA-C	-7.10	1.43	1.52
2	C	143	ALA	C-N	-7.10	1.24	1.34
2	G	294	HIS	ND1-CE1	7.09	1.39	1.32
3	M	81	GLU	CA-C	-7.09	1.42	1.52
3	N	38	PHE	CA-C	-7.09	1.43	1.52
2	R	456	ALA	CA-C	7.09	1.61	1.52
2	H	139	ARG	CA-CB	7.09	1.62	1.53
2	S	36	LEU	C-O	-7.08	1.15	1.24
2	C	158	GLU	CA-C	-7.08	1.43	1.52
2	J	390	LEU	C-N	7.08	1.42	1.33
2	H	394	PHE	CA-C	7.08	1.61	1.52
2	I	102	ALA	C-O	-7.08	1.15	1.23
2	I	262	MET	SD-CE	-7.08	1.61	1.79
2	I	384	VAL	CA-C	7.08	1.62	1.52
2	J	75	THR	C-N	7.07	1.43	1.33
3	L	44	PHE	C-O	-7.07	1.15	1.23
2	S	292	HIS	ND1-CE1	7.07	1.39	1.32
3	L	11	ARG	C-N	-7.07	1.24	1.33
3	O	63	PHE	CA-C	7.07	1.62	1.52
3	M	48	SER	CA-C	7.06	1.60	1.52
2	C	449	GLY	C-N	7.06	1.43	1.34
2	Q	153	HIS	CA-C	7.06	1.59	1.52
2	I	121	VAL	C-N	7.06	1.42	1.33
3	M	39	HIS	C-N	7.06	1.42	1.33
2	J	457	ALA	C-N	7.05	1.43	1.33
1	B	254	ARG	CA-C	-7.05	1.43	1.52
1	F	278	ASN	C-O	-7.05	1.15	1.24
2	C	387	MET	SD-CE	-7.05	1.61	1.79
2	H	24	TYR	C-N	-7.05	1.24	1.33
2	J	274	PHE	C-N	7.05	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	267	HIS	CD2-NE2	7.04	1.45	1.37
1	F	228	GLU	N-CA	7.04	1.55	1.46
2	H	279	THR	CA-C	-7.04	1.43	1.52
2	Q	162	LEU	C-O	-7.04	1.14	1.24
2	C	271	THR	CA-C	-7.04	1.44	1.53
3	E	105	VAL	C-O	-7.04	1.15	1.24
2	H	346	VAL	N-CA	-7.04	1.38	1.46
2	H	364	PHE	C-O	-7.04	1.15	1.23
2	S	148	PHE	C-N	-7.04	1.24	1.33
2	I	357	ASP	CA-C	-7.03	1.44	1.52
3	K	56	THR	C-N	-7.03	1.24	1.33
2	I	45	GLN	CA-C	-7.03	1.46	1.53
2	Q	211	PHE	CA-C	7.03	1.62	1.52
1	A	287	TYR	C-N	7.03	1.42	1.33
2	I	76	ASP	C-N	7.02	1.43	1.33
2	G	423	ALA	C-N	7.02	1.42	1.33
2	G	189	VAL	C-N	-7.02	1.24	1.33
3	K	12	PHE	N-CA	7.02	1.54	1.45
2	J	345	PHE	C-O	-7.02	1.15	1.24
2	G	251	MET	CA-C	-7.02	1.44	1.52
2	I	429	GLN	N-CA	7.02	1.54	1.46
2	J	85	TYR	C-N	7.01	1.42	1.33
2	R	313	VAL	C-N	-7.01	1.24	1.33
2	S	51	ASP	C-N	-7.01	1.24	1.33
2	H	240	LEU	CA-C	-7.01	1.43	1.52
2	G	431	ARG	CA-C	-7.01	1.43	1.52
2	I	164	LYS	CA-C	7.01	1.61	1.52
2	R	270	LEU	N-CA	7.01	1.54	1.46
1	T	286	GLU	C-N	7.00	1.43	1.33
2	Q	118	THR	CA-C	7.00	1.61	1.52
2	R	359	SER	N-CA	-7.00	1.37	1.46
2	C	391	VAL	C-N	-7.00	1.25	1.33
2	H	430	ALA	C-O	-7.00	1.15	1.24
3	D	58	TRP	N-CA	-6.99	1.38	1.46
2	G	342	THR	C-O	-6.99	1.16	1.24
2	Q	134	ARG	C-N	-6.99	1.24	1.33
2	S	21	LYS	C-N	6.99	1.43	1.34
2	G	211	PHE	C-N	-6.99	1.24	1.33
2	S	307	HIS	CD2-NE2	6.98	1.45	1.37
2	C	356	ALA	CA-C	-6.98	1.44	1.52
2	G	116	ILE	CA-C	-6.98	1.44	1.52
2	H	284	CYS	C-O	-6.98	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	304	GLN	CA-C	-6.98	1.43	1.53
2	J	385	TRP	C-N	-6.98	1.24	1.33
2	Q	86	HIS	ND1-CE1	6.98	1.39	1.32
2	C	297	MET	SD-CE	-6.97	1.62	1.79
1	F	247	HIS	ND1-CE1	6.97	1.39	1.32
2	R	165	TYR	C-N	6.97	1.42	1.33
2	S	436	ASP	C-O	-6.97	1.15	1.24
2	Q	248	GLU	C-N	-6.97	1.25	1.33
2	C	265	ILE	CA-CB	-6.97	1.45	1.54
2	I	281	ALA	N-CA	-6.97	1.38	1.46
2	C	192	CYS	N-CA	-6.96	1.37	1.46
2	G	119	SER	CA-C	-6.96	1.44	1.52
2	I	383	HIS	CD2-NE2	6.96	1.45	1.37
2	J	361	GLY	C-N	-6.96	1.26	1.33
2	J	298	HIS	CA-C	-6.95	1.43	1.52
2	G	118	THR	CA-C	6.95	1.61	1.52
2	G	445	LEU	C-O	-6.95	1.16	1.24
2	I	400	LEU	CA-C	-6.95	1.44	1.52
3	O	39	HIS	ND1-CE1	6.95	1.39	1.32
2	H	321	SER	N-CA	-6.94	1.38	1.46
2	I	77	MET	SD-CE	-6.94	1.62	1.79
2	I	264	ILE	CA-CB	-6.94	1.48	1.55
2	J	306	ASN	CA-C	6.94	1.62	1.52
1	B	287	TYR	C-N	6.94	1.43	1.33
2	G	394	PHE	CA-C	-6.94	1.44	1.52
2	S	187	ARG	C-N	6.94	1.42	1.33
2	Q	265	ILE	C-N	-6.94	1.24	1.33
2	S	240	LEU	CA-C	-6.94	1.44	1.52
2	Q	423	ALA	CA-C	6.93	1.62	1.52
1	T	279	CYS	C-N	-6.93	1.24	1.33
2	G	242	VAL	CA-CB	-6.93	1.46	1.54
2	G	132	SER	N-CA	6.93	1.54	1.46
2	C	87	ILE	C-N	6.93	1.40	1.33
2	C	425	GLU	N-CA	-6.93	1.38	1.46
3	E	24	ARG	N-CA	-6.93	1.38	1.46
2	G	37	LEU	CA-C	6.92	1.61	1.52
2	G	214	TRP	N-CA	-6.92	1.38	1.46
2	C	58	ALA	C-O	-6.92	1.16	1.24
2	R	165	TYR	C-O	-6.92	1.15	1.23
2	G	184	ASN	N-CA	-6.91	1.37	1.46
2	J	146	LYS	C-N	-6.91	1.24	1.34
2	G	49	PRO	C-O	-6.91	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	53	ALA	C-O	-6.91	1.16	1.24
2	G	224	ALA	CA-C	6.91	1.61	1.52
2	H	276	ALA	CA-C	6.91	1.61	1.52
2	I	346	VAL	CA-C	6.90	1.61	1.52
2	Q	242	VAL	CA-C	6.90	1.59	1.52
2	G	95	ASN	CA-C	6.89	1.63	1.52
2	R	287	ASN	CA-CB	-6.89	1.42	1.53
3	D	99	GLN	N-CA	-6.89	1.37	1.46
3	M	86	TYR	N-CA	-6.89	1.37	1.45
2	Q	377	VAL	CA-C	-6.89	1.44	1.52
2	S	149	GLN	CA-C	-6.89	1.43	1.52
2	H	315	ALA	C-N	-6.89	1.24	1.33
3	K	33	MET	N-CA	-6.88	1.38	1.46
2	G	215	ARG	N-CA	-6.88	1.37	1.46
3	M	41	LEU	CA-C	6.88	1.60	1.52
2	S	320	LEU	CA-C	-6.88	1.44	1.52
1	F	228	GLU	CA-C	6.88	1.61	1.52
2	J	229	GLN	C-N	-6.88	1.25	1.33
2	C	223	ASP	C-O	-6.87	1.16	1.24
1	T	283	HIS	ND1-CE1	6.87	1.39	1.32
2	C	279	THR	C-N	-6.87	1.24	1.33
3	E	43	GLU	C-N	6.86	1.42	1.33
2	H	235	ILE	CA-C	-6.86	1.44	1.52
2	C	417	ALA	CA-C	6.86	1.61	1.52
2	G	121	VAL	C-N	6.86	1.42	1.33
2	I	180	LEU	N-CA	6.86	1.54	1.46
3	K	58	TRP	CA-C	-6.85	1.45	1.53
2	Q	426	ALA	N-CA	-6.85	1.38	1.46
2	R	130	ILE	C-N	-6.85	1.25	1.33
2	H	330	THR	CA-C	-6.84	1.44	1.52
2	G	324	ASP	CA-C	-6.84	1.44	1.52
2	H	172	CYS	CA-C	-6.84	1.44	1.52
2	R	183	LYS	CA-C	6.84	1.61	1.52
2	C	189	VAL	CA-C	-6.84	1.45	1.52
2	J	326	LEU	CB-CG	-6.84	1.39	1.53
2	R	362	VAL	CA-C	6.84	1.59	1.53
2	S	289	VAL	CA-C	-6.83	1.44	1.52
2	H	160	ASP	CA-C	-6.83	1.44	1.52
2	S	95	ASN	CA-C	-6.83	1.43	1.53
2	C	350	ARG	CA-C	6.83	1.59	1.53
2	J	39	ALA	N-CA	-6.83	1.37	1.46
2	R	51	ASP	C-N	-6.83	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	72	ASP	CA-C	-6.83	1.44	1.52
3	L	36	GLN	CA-C	6.81	1.62	1.52
2	I	128	LYS	C-N	6.81	1.43	1.33
2	Q	269	PHE	CA-C	-6.81	1.43	1.52
2	J	316	LYS	CA-C	6.81	1.61	1.52
2	J	428	VAL	C-N	-6.81	1.25	1.33
2	R	347	ASP	C-N	6.80	1.42	1.33
2	G	191	GLU	C-N	-6.80	1.25	1.33
2	I	244	ALA	CA-C	6.80	1.58	1.52
2	I	390	LEU	N-CA	-6.80	1.38	1.46
2	C	256	PHE	N-CA	-6.80	1.38	1.46
2	S	395	GLY	C-N	6.79	1.43	1.34
2	C	271	THR	C-O	-6.79	1.16	1.24
2	S	130	ILE	CA-CB	6.79	1.62	1.54
2	G	253	ARG	CA-C	6.78	1.61	1.52
3	O	63	PHE	C-O	-6.77	1.15	1.24
2	S	230	ALA	C-O	-6.77	1.16	1.24
2	I	179	GLY	C-N	-6.77	1.24	1.33
3	E	23	ASP	C-N	6.77	1.42	1.33
2	S	276	ALA	CA-C	-6.77	1.44	1.52
2	G	199	PHE	CA-C	-6.76	1.44	1.52
2	J	325	HIS	ND1-CE1	-6.76	1.25	1.32
2	S	366	GLN	CA-C	-6.76	1.44	1.52
2	G	149	GLN	C-N	6.76	1.43	1.33
2	C	309	ILE	CA-C	6.75	1.60	1.52
2	G	197	LEU	CA-C	-6.75	1.44	1.52
2	S	286	ASP	CA-C	-6.75	1.43	1.52
2	R	226	HIS	CD2-NE2	6.75	1.45	1.37
2	C	298	HIS	CA-C	-6.75	1.44	1.52
2	H	21	LYS	CA-C	-6.75	1.44	1.52
2	H	194	ARG	N-CA	6.75	1.55	1.46
2	S	118	THR	CA-CB	-6.75	1.42	1.53
2	J	397	ASP	CA-C	6.75	1.61	1.52
2	G	45	GLN	CA-C	-6.75	1.44	1.52
2	R	125	PHE	CA-C	-6.75	1.43	1.52
2	G	63	THR	CA-C	6.74	1.61	1.52
2	I	387	MET	SD-CE	6.74	1.96	1.79
2	S	284	CYS	CA-C	6.74	1.61	1.52
2	J	100	PHE	CA-C	-6.74	1.44	1.52
2	R	61	SER	CA-C	-6.74	1.43	1.52
2	I	273	GLY	C-N	-6.74	1.24	1.33
2	J	298	HIS	C-N	-6.74	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	213	ARG	CA-CB	6.74	1.63	1.53
2	C	76	ASP	N-CA	-6.74	1.37	1.46
2	R	89	PRO	CA-C	-6.74	1.44	1.52
1	A	232	GLN	CA-C	-6.73	1.43	1.52
2	I	224	ALA	CA-C	6.73	1.61	1.52
3	K	33	MET	C-N	6.73	1.42	1.34
3	L	41	LEU	C-O	-6.73	1.16	1.24
3	L	67	SER	CA-C	-6.73	1.45	1.52
2	R	313	VAL	CA-C	-6.73	1.44	1.52
2	C	252	LYS	N-CA	-6.72	1.38	1.46
3	D	25	GLN	N-CA	6.72	1.54	1.46
2	G	311	PHE	C-N	-6.72	1.25	1.33
3	L	9	GLU	CA-C	-6.72	1.44	1.52
2	J	114	THR	C-N	-6.72	1.25	1.33
1	T	262	ALA	C-N	-6.72	1.25	1.33
2	R	389	ALA	C-N	-6.71	1.25	1.33
3	D	80	SER	CA-C	-6.71	1.44	1.52
2	J	345	PHE	C-N	6.71	1.42	1.34
2	J	438	TYR	CA-C	-6.71	1.44	1.52
2	H	144	LEU	CA-C	6.71	1.61	1.52
2	C	221	VAL	N-CA	-6.71	1.38	1.46
2	S	326	LEU	N-CA	-6.71	1.38	1.46
2	H	421	ARG	N-CA	6.71	1.54	1.46
2	J	145	VAL	CA-C	-6.70	1.44	1.52
2	J	189	VAL	C-N	-6.70	1.25	1.33
2	C	294	HIS	CE1-NE2	-6.70	1.25	1.32
2	C	312	ARG	C-O	-6.70	1.16	1.24
2	R	269	PHE	C-O	-6.70	1.16	1.24
3	L	33	MET	SD-CE	-6.70	1.62	1.79
2	H	353	HIS	N-CA	6.70	1.54	1.46
3	O	51	GLU	C-O	-6.69	1.15	1.24
1	B	302	PHE	C-N	-6.69	1.23	1.33
2	R	209	GLN	CA-C	6.69	1.60	1.53
2	S	268	ASP	N-CA	6.69	1.54	1.46
2	G	444	ILE	CA-CB	6.69	1.61	1.54
2	H	436	ASP	C-O	-6.69	1.15	1.23
2	Q	413	ASN	CA-C	-6.68	1.44	1.52
2	S	121	VAL	C-N	6.68	1.42	1.33
2	C	206	ILE	CA-CB	6.68	1.60	1.53
2	C	263	PRO	C-N	6.68	1.42	1.33
2	J	143	ALA	CA-C	-6.68	1.44	1.52
2	S	84	CYS	CA-C	6.68	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	313	VAL	C-O	-6.68	1.16	1.24
2	Q	397	ASP	C-N	6.68	1.42	1.33
2	Q	229	GLN	CA-C	-6.68	1.44	1.52
2	R	133	LEU	C-O	-6.68	1.15	1.23
2	G	80	TYR	C-N	6.67	1.42	1.33
2	S	295	ARG	CA-C	6.67	1.62	1.53
2	G	79	ARG	C-N	6.67	1.42	1.33
2	I	281	ALA	C-N	6.67	1.42	1.33
2	S	130	ILE	C-O	-6.67	1.16	1.24
2	C	221	VAL	C-O	-6.67	1.16	1.24
2	S	199	PHE	N-CA	-6.67	1.37	1.45
2	H	209	GLN	N-CA	-6.66	1.38	1.45
2	J	132	SER	C-N	6.66	1.43	1.33
2	J	143	ALA	C-O	6.66	1.31	1.24
2	Q	81	LYS	C-N	6.66	1.38	1.33
2	H	101	ILE	CA-CB	6.66	1.63	1.54
3	P	79	ARG	C-O	-6.66	1.16	1.24
2	S	90	VAL	C-O	6.66	1.31	1.24
2	R	326	LEU	CA-C	-6.66	1.45	1.52
1	B	256	SER	CA-C	6.66	1.62	1.53
2	G	30	THR	CA-C	6.66	1.59	1.52
2	J	40	PHE	CA-C	-6.65	1.44	1.52
3	L	39	HIS	CE1-NE2	-6.65	1.25	1.32
2	Q	393	ILE	C-N	6.65	1.42	1.33
2	C	277	ASN	CA-C	-6.65	1.44	1.52
2	I	115	ASN	CA-C	-6.65	1.43	1.52
2	C	387	MET	CA-C	6.64	1.61	1.52
2	G	437	LEU	CA-C	-6.64	1.44	1.52
2	J	266	MET	SD-CE	-6.64	1.62	1.79
2	H	270	LEU	CB-CG	-6.64	1.40	1.53
2	I	47	GLY	C-N	6.64	1.39	1.33
2	I	233	GLY	C-N	-6.64	1.25	1.33
2	J	57	ILE	CA-CB	6.63	1.62	1.54
1	A	230	ILE	C-O	-6.63	1.16	1.24
2	I	60	GLU	C-N	-6.63	1.25	1.33
2	C	251	MET	CA-C	-6.63	1.44	1.52
2	G	448	ALA	CA-C	6.63	1.61	1.52
2	J	97	TYR	CA-C	6.63	1.60	1.52
3	E	94	ASN	CA-C	6.63	1.61	1.52
2	I	228	SER	C-N	6.63	1.42	1.33
2	Q	269	PHE	N-CA	6.63	1.54	1.46
2	G	304	GLN	C-N	-6.62	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	101	VAL	N-CA	-6.62	1.38	1.46
2	Q	264	ILE	C-O	-6.62	1.17	1.23
2	H	33	ASP	CA-C	6.62	1.61	1.52
2	H	244	ALA	CA-CB	-6.62	1.45	1.54
2	H	152	PRO	C-N	-6.62	1.24	1.33
3	P	75	VAL	N-CA	-6.62	1.38	1.46
3	K	53	PHE	CA-C	-6.61	1.44	1.52
2	S	248	GLU	C-O	-6.61	1.16	1.24
2	R	326	LEU	C-N	6.61	1.42	1.33
2	I	139	ARG	CA-C	6.61	1.62	1.53
1	A	264	ILE	C-N	6.61	1.42	1.33
2	Q	265	ILE	C-O	-6.61	1.15	1.23
2	S	116	ILE	CA-C	-6.61	1.45	1.52
3	K	32	TYR	C-O	6.61	1.31	1.24
2	G	382	ILE	C-N	6.60	1.41	1.33
2	J	38	ALA	CA-C	6.60	1.60	1.52
2	Q	234	GLU	CA-C	-6.60	1.44	1.52
3	E	17	TYR	C-N	6.60	1.43	1.33
2	S	417	ALA	C-N	-6.59	1.25	1.33
2	S	274	PHE	CA-C	-6.59	1.44	1.52
2	H	276	ALA	C-N	-6.59	1.25	1.33
2	I	116	ILE	C-N	-6.59	1.25	1.33
2	I	142	VAL	C-N	-6.59	1.25	1.33
2	S	223	ASP	C-N	6.59	1.42	1.33
3	N	54	TYR	CA-C	-6.59	1.44	1.52
2	I	143	ALA	N-CA	-6.58	1.38	1.46
2	I	153	HIS	ND1-CE1	6.58	1.39	1.32
2	G	359	SER	C-O	6.58	1.31	1.24
2	I	244	ALA	N-CA	-6.58	1.39	1.45
2	S	46	PRO	C-O	6.58	1.31	1.23
3	P	51	GLU	CA-C	6.58	1.61	1.52
3	D	18	LEU	CA-C	-6.58	1.43	1.53
2	H	437	LEU	CA-C	-6.58	1.44	1.52
2	I	24	TYR	CA-C	6.57	1.60	1.52
2	I	129	ALA	N-CA	-6.57	1.37	1.46
2	J	302	ASP	CA-C	-6.57	1.44	1.52
3	E	54	TYR	C-O	-6.57	1.16	1.23
1	F	267	THR	CA-C	6.57	1.61	1.52
2	G	382	ILE	CA-C	-6.57	1.44	1.52
2	Q	390	LEU	C-N	6.57	1.42	1.33
2	Q	451	TRP	N-CA	-6.57	1.37	1.46
1	F	227	SER	C-N	6.57	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	149	GLN	N-CA	-6.57	1.37	1.46
2	Q	222	ALA	N-CA	6.57	1.54	1.46
2	I	221	VAL	C-O	-6.57	1.16	1.24
2	H	455	LEU	C-N	6.56	1.42	1.33
2	R	343	LEU	CA-C	6.56	1.61	1.52
2	R	369	ALA	CA-C	-6.56	1.45	1.53
2	G	23	THR	CA-C	6.56	1.61	1.52
2	H	360	ARG	N-CA	6.56	1.55	1.46
3	M	30	ILE	C-O	-6.56	1.16	1.24
2	Q	316	LYS	C-N	-6.56	1.25	1.33
2	I	194	ARG	C-N	6.55	1.41	1.33
2	R	163	ASN	N-CA	-6.55	1.38	1.46
3	N	91	GLY	C-N	6.55	1.42	1.33
1	B	234	ARG	C-O	-6.55	1.16	1.24
2	Q	228	SER	C-N	-6.55	1.25	1.33
2	R	200	THR	C-O	-6.55	1.16	1.23
2	J	437	LEU	CA-C	-6.54	1.43	1.52
2	R	346	VAL	C-N	-6.54	1.25	1.33
2	I	347	ASP	C-N	-6.54	1.25	1.33
2	R	260	LEU	C-N	6.54	1.42	1.33
1	F	257	SER	C-N	6.54	1.42	1.33
2	J	30	THR	C-N	-6.54	1.26	1.33
2	Q	217	ARG	C-O	-6.54	1.16	1.24
2	S	124	VAL	C-O	-6.54	1.16	1.24
1	T	252	ARG	CA-CB	6.54	1.63	1.53
3	P	78	CYS	C-O	-6.53	1.16	1.24
2	C	230	ALA	C-N	-6.53	1.24	1.33
2	S	103	TYR	C-N	6.53	1.42	1.33
2	S	267	HIS	N-CA	-6.53	1.38	1.46
2	I	199	PHE	CA-C	-6.53	1.44	1.52
2	S	238	HIS	ND1-CE1	-6.53	1.26	1.32
2	S	369	ALA	CA-C	-6.53	1.44	1.53
2	C	361	GLY	C-N	6.52	1.39	1.33
2	C	446	ARG	N-CA	-6.52	1.38	1.46
3	K	52	GLU	CA-CB	-6.52	1.44	1.53
2	I	399	VAL	C-N	6.52	1.42	1.33
3	K	39	HIS	CG-CD2	6.52	1.43	1.35
2	G	89	PRO	C-N	-6.52	1.25	1.33
2	S	375	LEU	CB-CG	-6.52	1.40	1.53
3	O	63	PHE	C-N	6.52	1.42	1.33
2	G	419	ALA	N-CA	-6.51	1.38	1.46
2	H	156	GLN	N-CA	6.51	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	142	VAL	C-N	-6.51	1.25	1.33
2	S	293	ILE	CA-C	-6.51	1.44	1.52
1	A	308	ARG	C-O	-6.51	1.17	1.24
2	I	292	HIS	CE1-NE2	-6.51	1.26	1.32
2	R	349	MET	SD-CE	-6.51	1.63	1.79
2	I	184	ASN	C-O	-6.51	1.15	1.24
2	C	175	LYS	CA-C	6.51	1.58	1.52
1	F	231	THR	CA-CB	-6.51	1.43	1.53
2	G	353	HIS	CD2-NE2	6.50	1.45	1.37
2	R	357	ASP	C-N	-6.50	1.25	1.33
2	I	276	ALA	N-CA	6.50	1.54	1.46
2	S	283	TRP	CA-C	-6.50	1.44	1.52
3	O	95	ILE	CA-C	-6.50	1.44	1.52
2	H	86	HIS	C-O	-6.50	1.16	1.23
2	R	90	VAL	C-N	-6.50	1.24	1.33
2	S	378	ALA	CA-C	6.49	1.60	1.52
2	R	158	GLU	C-O	6.49	1.31	1.24
2	S	76	ASP	CA-C	-6.49	1.44	1.52
2	H	22	LEU	CA-C	6.49	1.61	1.52
2	R	276	ALA	C-N	6.49	1.42	1.33
2	H	120	ILE	C-O	-6.49	1.16	1.24
2	J	315	ALA	CA-C	-6.48	1.44	1.52
3	M	69	GLN	CA-C	6.48	1.61	1.52
2	H	138	ILE	C-O	-6.47	1.16	1.23
2	S	51	ASP	CA-C	6.47	1.61	1.52
1	A	288	VAL	C-N	6.47	1.43	1.33
3	E	13	GLU	C-O	-6.47	1.16	1.24
3	O	76	ARG	CA-C	-6.47	1.44	1.52
2	Q	148	PHE	C-N	-6.47	1.24	1.33
1	B	245	THR	C-N	-6.47	1.24	1.33
2	S	238	HIS	N-CA	6.47	1.53	1.45
1	T	237	LEU	CA-CB	6.47	1.64	1.53
3	L	38	PHE	CA-CB	6.47	1.62	1.53
2	Q	206	ILE	C-N	6.47	1.42	1.33
2	R	330	THR	CA-CB	6.47	1.64	1.53
2	J	458	ALA	C-N	6.46	1.42	1.33
2	Q	354	ILE	C-O	-6.46	1.17	1.24
2	R	84	CYS	N-CA	6.46	1.54	1.46
2	H	446	ARG	C-O	-6.46	1.16	1.24
3	P	75	VAL	CA-C	6.46	1.60	1.52
3	O	10	ARG	N-CA	6.46	1.54	1.46
3	D	59	LYS	C-N	6.46	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	387	MET	C-N	6.46	1.42	1.33
2	Q	193	LEU	CA-C	-6.46	1.44	1.52
2	G	207	ASN	N-CA	-6.46	1.39	1.46
2	J	317	CYS	C-N	-6.46	1.25	1.33
3	K	9	GLU	CA-C	6.46	1.61	1.52
3	M	77	GLU	N-CA	6.46	1.54	1.46
1	T	257	SER	CA-C	-6.46	1.44	1.52
1	B	284	GLU	CA-C	-6.46	1.44	1.52
2	C	223	ASP	CA-C	6.46	1.61	1.52
2	C	386	HIS	CE1-NE2	-6.45	1.26	1.32
3	E	43	GLU	CA-C	-6.45	1.44	1.52
1	T	281	SER	N-CA	6.45	1.54	1.46
2	S	244	ALA	CA-CB	-6.45	1.46	1.53
3	O	82	TYR	CA-C	6.45	1.61	1.53
3	M	39	HIS	CG-CD2	6.45	1.43	1.35
2	R	120	ILE	C-O	6.44	1.31	1.24
2	S	28	ASP	C-O	-6.44	1.15	1.24
1	A	252	ARG	N-CA	6.44	1.54	1.46
2	H	391	VAL	CA-C	6.43	1.61	1.53
2	S	289	VAL	CA-CB	6.43	1.61	1.54
2	G	125	PHE	CA-C	-6.43	1.43	1.52
2	S	106	ASP	C-N	6.43	1.42	1.33
2	S	319	ARG	CA-C	6.43	1.61	1.52
2	I	190	TYR	C-N	-6.43	1.25	1.33
2	I	98	PHE	C-O	-6.43	1.16	1.24
2	I	262	MET	C-O	-6.43	1.16	1.24
1	T	250	LYS	C-O	-6.43	1.16	1.24
2	Q	147	THR	C-N	6.42	1.42	1.33
2	Q	263	PRO	C-N	6.42	1.42	1.33
3	D	98	CYS	CA-C	-6.42	1.44	1.52
2	S	440	GLU	CA-C	6.42	1.62	1.52
2	G	240	LEU	CA-C	-6.42	1.44	1.53
3	K	26	ILE	C-N	-6.42	1.25	1.33
2	R	83	LYS	CA-C	-6.42	1.44	1.53
3	E	107	ARG	CA-C	6.42	1.58	1.52
2	H	125	PHE	C-O	-6.42	1.16	1.24
3	N	104	ILE	CA-CB	6.42	1.60	1.54
2	C	317	CYS	C-N	-6.42	1.25	1.33
1	A	305	LEU	N-CA	-6.42	1.38	1.46
2	S	51	ASP	N-CA	-6.41	1.38	1.46
3	E	45	ASN	CA-C	-6.41	1.44	1.52
2	C	356	ALA	C-O	-6.41	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	71	VAL	CA-C	-6.41	1.44	1.52
2	R	362	VAL	C-N	-6.40	1.25	1.33
2	C	58	ALA	CA-C	-6.40	1.44	1.52
2	R	258	LYS	N-CA	-6.40	1.38	1.46
2	J	447	GLU	CA-C	-6.40	1.44	1.52
2	I	391	VAL	CA-C	6.40	1.60	1.52
2	R	157	VAL	CA-C	6.40	1.61	1.52
2	R	447	GLU	C-O	6.40	1.31	1.24
2	R	330	THR	C-O	6.39	1.31	1.23
3	K	30	ILE	C-O	-6.39	1.16	1.24
3	P	70	GLN	C-N	-6.39	1.25	1.33
2	R	187	ARG	C-N	6.39	1.42	1.33
2	S	132	SER	C-O	-6.39	1.16	1.23
2	H	222	ALA	C-O	-6.39	1.16	1.24
2	J	343	LEU	CA-C	-6.39	1.44	1.52
2	G	105	LEU	C-N	6.39	1.43	1.33
2	S	87	ILE	CA-C	-6.39	1.45	1.52
2	S	255	GLU	CA-CB	6.39	1.63	1.53
2	H	135	LEU	CA-CB	-6.39	1.45	1.53
1	T	234	ARG	CA-C	-6.39	1.44	1.52
1	T	249	ASP	CA-C	6.38	1.61	1.53
3	E	47	HIS	CD2-NE2	6.38	1.44	1.37
2	H	135	LEU	CA-C	-6.38	1.44	1.52
2	I	132	SER	CA-C	-6.38	1.44	1.52
2	I	153	HIS	CG-CD2	-6.38	1.28	1.35
3	N	19	PRO	C-O	6.38	1.31	1.24
3	P	16	SER	C-O	-6.38	1.16	1.24
2	G	444	ILE	CA-C	-6.38	1.45	1.52
2	Q	354	ILE	CB-CG1	6.38	1.66	1.53
2	I	161	LEU	N-CA	6.38	1.53	1.46
2	Q	292	HIS	C-O	-6.38	1.16	1.23
3	P	77	GLU	C-N	-6.38	1.25	1.33
2	Q	353	HIS	ND1-CE1	6.37	1.39	1.32
2	S	206	ILE	N-CA	-6.37	1.38	1.46
2	S	339	LYS	CA-C	6.37	1.61	1.52
3	E	36	GLN	C-N	6.37	1.41	1.33
2	Q	357	ASP	N-CA	6.36	1.54	1.46
2	H	106	ASP	C-N	-6.36	1.25	1.33
3	P	106	HIS	CA-C	-6.36	1.44	1.52
2	R	207	ASN	C-O	-6.36	1.16	1.24
2	Q	204	GLU	N-CA	-6.36	1.38	1.46
2	I	178	LEU	CA-C	6.36	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	33	ASP	N-CA	-6.36	1.38	1.46
3	M	70	GLN	N-CA	-6.35	1.38	1.46
2	Q	383	HIS	CE1-NE2	6.35	1.39	1.32
2	S	120	ILE	C-N	6.35	1.41	1.33
2	C	201	LYS	C-N	-6.35	1.25	1.33
2	I	310	HIS	ND1-CE1	-6.35	1.26	1.32
2	J	383	HIS	CA-C	-6.35	1.47	1.53
2	C	447	GLU	N-CA	-6.35	1.38	1.46
2	J	444	ILE	N-CA	6.35	1.54	1.46
2	G	292	HIS	CD2-NE2	6.35	1.44	1.37
2	H	203	ASP	CA-C	6.35	1.60	1.52
2	Q	305	ARG	C-O	-6.35	1.16	1.24
2	C	177	LYS	C-O	-6.34	1.16	1.24
2	H	374	VAL	N-CA	-6.34	1.38	1.46
2	J	438	TYR	C-N	-6.34	1.25	1.33
2	R	431	ARG	CA-C	-6.34	1.44	1.52
3	D	31	GLU	N-CA	6.34	1.53	1.46
2	I	130	ILE	C-N	-6.34	1.25	1.33
2	G	446	ARG	N-CA	-6.34	1.38	1.46
2	H	255	GLU	C-N	6.34	1.42	1.33
2	G	53	ALA	N-CA	-6.33	1.38	1.46
2	H	358	ARG	CA-C	-6.33	1.44	1.52
2	Q	257	ALA	C-O	-6.33	1.16	1.24
2	H	236	LYS	C-N	6.33	1.41	1.33
2	R	325	HIS	CD2-NE2	6.33	1.44	1.37
2	S	80	TYR	CA-C	6.33	1.61	1.52
2	S	99	ALA	CA-CB	-6.33	1.43	1.53
1	F	246	GLU	C-N	6.33	1.43	1.33
2	I	454	GLU	C-N	6.33	1.42	1.34
2	G	136	GLU	N-CA	-6.32	1.38	1.46
2	Q	439	ARG	C-O	-6.32	1.15	1.23
2	S	227	LYS	N-CA	-6.32	1.38	1.46
2	J	64	GLY	C-N	6.32	1.42	1.33
2	G	138	ILE	C-N	6.32	1.41	1.33
2	J	258	LYS	N-CA	6.32	1.54	1.46
2	R	202	ASP	CA-C	-6.32	1.44	1.52
2	S	178	LEU	CA-C	6.32	1.60	1.52
2	C	283	TRP	CA-C	6.31	1.60	1.52
2	C	325	HIS	CG-CD2	-6.31	1.28	1.35
3	L	84	ASP	CA-C	6.31	1.63	1.52
3	E	84	ASP	N-CA	-6.31	1.39	1.46
2	H	143	ALA	C-N	-6.31	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	56	ALA	CA-C	-6.31	1.44	1.52
2	H	212	GLN	C-O	6.31	1.31	1.23
3	L	31	GLU	CA-C	6.30	1.60	1.52
2	S	246	THR	CA-C	6.30	1.60	1.52
2	H	253	ARG	CA-C	-6.30	1.44	1.52
2	J	353	HIS	C-N	6.30	1.42	1.33
2	I	215	ARG	C-O	-6.30	1.16	1.24
3	P	35	GLU	N-CA	6.30	1.54	1.46
2	Q	189	VAL	C-O	-6.30	1.17	1.24
2	C	298	HIS	CD2-NE2	6.29	1.44	1.37
2	G	321	SER	C-O	-6.29	1.16	1.24
2	G	341	SER	C-N	6.29	1.41	1.33
2	Q	424	LEU	CB-CG	-6.29	1.40	1.53
3	D	67	SER	C-N	-6.29	1.26	1.34
2	C	393	ILE	CA-CB	6.29	1.61	1.54
3	E	87	ILE	N-CA	6.29	1.54	1.46
3	O	72	LEU	CA-CB	6.29	1.63	1.53
2	S	256	PHE	CA-C	6.29	1.61	1.52
2	Q	175	LYS	N-CA	-6.28	1.38	1.45
2	S	416	GLY	C-N	-6.28	1.25	1.33
1	B	304	ALA	N-CA	-6.28	1.39	1.46
2	C	392	GLU	CA-C	-6.28	1.44	1.52
2	I	203	ASP	C-O	6.28	1.31	1.23
2	S	30	THR	CA-C	6.28	1.59	1.52
2	C	124	VAL	CA-C	-6.28	1.44	1.52
2	J	243	THR	C-O	-6.28	1.16	1.24
2	H	232	THR	CA-C	6.28	1.61	1.52
2	S	127	PHE	N-CA	-6.28	1.38	1.46
3	O	74	GLU	C-O	6.27	1.31	1.24
3	E	106	HIS	N-CA	-6.27	1.38	1.45
2	C	29	TYR	C-O	-6.27	1.16	1.23
2	C	201	LYS	CA-C	-6.27	1.45	1.52
2	S	37	LEU	CA-CB	6.27	1.62	1.53
1	F	265	GLN	C-N	6.26	1.42	1.33
2	J	138	ILE	C-O	-6.26	1.17	1.24
2	R	85	TYR	C-N	6.26	1.41	1.33
2	S	149	GLN	N-CA	-6.26	1.38	1.46
3	D	44	PHE	C-N	-6.26	1.24	1.33
2	I	81	LYS	CA-C	-6.26	1.45	1.52
2	J	370	SER	CA-C	-6.26	1.43	1.52
3	N	17	TYR	CA-C	6.26	1.61	1.52
2	R	130	ILE	C-O	-6.26	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	266	MET	SD-CE	-6.26	1.64	1.79
2	C	383	HIS	CG-CD2	-6.26	1.28	1.35
2	G	143	ALA	CA-CB	-6.25	1.43	1.53
2	S	181	SER	CA-C	-6.25	1.45	1.52
2	H	387	MET	SD-CE	-6.25	1.64	1.79
2	S	304	GLN	C-N	-6.25	1.24	1.33
2	I	125	PHE	CA-C	-6.25	1.44	1.52
2	S	267	HIS	ND1-CE1	6.25	1.38	1.32
3	D	9	GLU	C-N	6.25	1.41	1.33
2	R	172	CYS	CA-C	-6.25	1.45	1.52
2	S	39	ALA	CA-C	-6.25	1.45	1.52
2	R	44	PRO	CA-CB	-6.24	1.45	1.53
2	I	159	ARG	C-N	6.24	1.42	1.33
2	S	62	SER	CA-C	-6.24	1.46	1.52
2	S	265	ILE	CA-CB	6.24	1.62	1.54
2	C	102	ALA	N-CA	6.24	1.53	1.46
2	J	390	LEU	CA-C	6.24	1.60	1.52
2	S	158	GLU	CA-C	-6.24	1.44	1.52
3	M	85	CYS	N-CA	6.23	1.54	1.46
2	S	118	THR	CA-C	6.23	1.60	1.52
2	H	443	ASP	CA-C	-6.23	1.45	1.52
3	D	39	HIS	CD2-NE2	6.23	1.44	1.37
3	N	47	HIS	CG-CD2	6.23	1.42	1.35
2	S	269	PHE	CA-CB	6.23	1.63	1.53
1	B	283	HIS	CD2-NE2	6.22	1.44	1.37
2	J	394	PHE	CA-C	-6.22	1.44	1.52
2	H	31	PRO	C-N	-6.22	1.25	1.33
2	S	285	ARG	C-O	6.22	1.31	1.24
3	E	21	LEU	CA-C	-6.22	1.44	1.52
2	S	78	ASP	CA-C	-6.22	1.45	1.52
2	J	296	ALA	C-O	-6.21	1.16	1.23
3	P	39	HIS	CG-ND1	-6.21	1.31	1.38
1	F	309	PRO	C-N	-6.21	1.24	1.33
2	I	310	HIS	CE1-NE2	-6.21	1.26	1.32
2	I	256	PHE	N-CA	-6.21	1.38	1.46
1	T	238	ASN	CA-CB	-6.21	1.43	1.53
3	N	67	SER	CA-C	6.20	1.58	1.52
2	R	391	VAL	C-O	-6.20	1.17	1.24
1	B	250	LYS	C-N	-6.20	1.26	1.33
2	H	368	TRP	N-CA	6.20	1.53	1.46
2	H	450	LYS	C-N	6.20	1.43	1.33
3	L	13	GLU	N-CA	-6.20	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	102	ALA	CA-C	6.20	1.60	1.52
2	Q	119	SER	N-CA	6.20	1.53	1.46
2	J	252	LYS	CA-CB	6.20	1.62	1.53
2	Q	453	PRO	C-O	-6.20	1.16	1.24
2	G	101	ILE	C-O	6.20	1.30	1.24
2	Q	402	PHE	N-CA	6.20	1.53	1.45
2	J	356	ALA	C-N	-6.19	1.25	1.33
3	M	58	TRP	CA-C	-6.19	1.46	1.53
1	T	245	THR	CA-C	6.19	1.60	1.52
2	J	238	HIS	CA-C	6.19	1.59	1.52
2	S	101	ILE	C-O	6.19	1.30	1.24
3	E	76	ARG	C-N	-6.18	1.26	1.33
2	G	376	PRO	N-CA	-6.18	1.40	1.46
3	M	89	VAL	N-CA	-6.18	1.39	1.46
2	H	254	ALA	C-N	6.18	1.41	1.33
3	K	36	GLN	CA-C	6.18	1.61	1.52
2	S	131	ARG	N-CA	-6.18	1.39	1.46
2	S	329	GLY	C-N	-6.18	1.25	1.33
2	G	205	ASN	CA-C	6.18	1.61	1.52
2	H	386	HIS	C-N	-6.18	1.26	1.33
3	M	81	GLU	C-N	6.18	1.41	1.33
1	T	305	LEU	CA-CB	6.18	1.61	1.53
2	C	78	ASP	C-O	6.18	1.31	1.24
2	C	180	LEU	C-N	6.18	1.42	1.33
2	J	128	LYS	CA-C	6.18	1.61	1.52
1	A	241	TYR	C-N	6.17	1.42	1.33
2	C	348	LEU	CA-C	-6.17	1.44	1.52
2	I	97	TYR	CA-C	-6.17	1.45	1.52
2	J	56	ALA	C-O	-6.17	1.17	1.24
2	Q	205	ASN	CA-C	6.17	1.60	1.52
2	Q	436	ASP	N-CA	6.17	1.54	1.46
2	C	115	ASN	C-N	-6.17	1.26	1.33
2	G	278	THR	N-CA	-6.17	1.38	1.46
2	I	344	GLY	C-N	6.17	1.42	1.33
2	R	166	GLY	C-N	-6.17	1.26	1.33
2	H	27	PRO	C-O	-6.17	1.16	1.24
2	H	429	GLN	C-N	-6.17	1.25	1.33
2	R	306	ASN	C-N	6.17	1.42	1.33
1	T	230	ILE	C-O	-6.17	1.17	1.24
1	A	263	PRO	CA-C	-6.17	1.44	1.52
1	A	306	ILE	N-CA	-6.17	1.38	1.46
2	G	257	ALA	N-CA	-6.17	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	276	ALA	CA-CB	-6.17	1.43	1.53
2	H	421	ARG	CA-C	-6.16	1.44	1.52
2	S	203	ASP	CA-C	-6.16	1.44	1.52
2	G	192	CYS	CA-C	-6.16	1.44	1.52
2	J	432	ASN	C-O	6.16	1.31	1.24
1	T	230	ILE	N-CA	6.16	1.53	1.46
3	D	30	ILE	CA-C	-6.16	1.45	1.52
2	I	367	ASP	CA-C	6.16	1.59	1.52
2	I	185	TYR	C-N	6.15	1.42	1.33
2	J	402	PHE	C-N	-6.15	1.24	1.33
2	H	174	ILE	N-CA	-6.15	1.39	1.46
2	Q	58	ALA	CA-C	-6.15	1.45	1.52
2	R	47	GLY	C-N	6.15	1.40	1.33
2	J	248	GLU	CA-C	6.15	1.60	1.52
1	F	303	GLU	N-CA	-6.15	1.38	1.46
2	H	348	LEU	CA-C	-6.15	1.44	1.52
3	L	103	PHE	CA-C	-6.15	1.45	1.52
2	S	203	ASP	CA-CB	6.15	1.62	1.53
3	O	68	PRO	C-N	-6.14	1.25	1.33
2	H	27	PRO	C-N	6.14	1.42	1.33
2	Q	445	LEU	CA-CB	-6.14	1.43	1.53
2	C	299	ALA	C-O	-6.14	1.16	1.24
3	N	66	LYS	CA-C	-6.14	1.44	1.52
2	S	242	VAL	C-N	-6.14	1.25	1.33
1	T	238	ASN	C-N	-6.14	1.25	1.33
3	O	60	LEU	C-N	6.14	1.41	1.33
2	I	428	VAL	CA-CB	-6.13	1.47	1.54
2	J	221	VAL	C-O	-6.13	1.17	1.24
2	R	94	GLU	CA-C	6.13	1.60	1.52
2	C	167	ARG	CA-C	-6.13	1.46	1.52
2	G	29	TYR	N-CA	6.13	1.54	1.46
2	I	422	VAL	CA-CB	6.13	1.60	1.54
2	J	208	SER	C-N	-6.13	1.25	1.33
3	M	47	HIS	ND1-CE1	6.13	1.38	1.32
2	G	73	LEU	N-CA	-6.13	1.38	1.46
2	Q	363	PHE	C-N	6.13	1.40	1.33
2	H	236	LYS	C-O	-6.12	1.16	1.23
2	H	314	LEU	C-O	-6.12	1.17	1.24
2	I	49	PRO	N-CA	-6.12	1.39	1.47
2	I	55	ALA	C-N	6.12	1.41	1.33
2	I	265	ILE	CA-C	6.12	1.60	1.52
2	J	242	VAL	N-CA	-6.12	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	445	LEU	C-N	-6.12	1.26	1.33
3	N	46	GLU	N-CA	-6.12	1.38	1.46
2	S	221	VAL	C-O	-6.12	1.16	1.24
2	C	354	ILE	C-O	-6.12	1.17	1.24
2	I	302	ASP	N-CA	6.12	1.53	1.45
2	G	238	HIS	CA-C	-6.12	1.45	1.52
2	G	293	ILE	CA-CB	6.12	1.64	1.55
2	G	256	PHE	N-CA	6.12	1.54	1.46
1	B	262	ALA	CA-C	6.11	1.59	1.53
2	C	107	LEU	C-N	6.11	1.41	1.33
1	F	295	THR	CA-C	6.11	1.60	1.52
2	Q	145	VAL	C-N	-6.11	1.24	1.33
2	R	185	TYR	C-O	-6.11	1.17	1.24
2	Q	184	ASN	CA-C	-6.11	1.44	1.52
3	D	107	ARG	N-CA	6.11	1.52	1.45
2	C	264	ILE	N-CA	-6.11	1.39	1.46
2	H	309	ILE	CA-CB	6.10	1.62	1.54
2	J	120	ILE	N-CA	-6.10	1.38	1.46
3	N	75	VAL	C-N	-6.10	1.26	1.33
2	G	326	LEU	C-N	-6.10	1.25	1.33
2	I	301	ILE	CA-C	6.09	1.60	1.53
2	G	451	TRP	C-N	-6.09	1.26	1.33
2	I	245	PRO	C-O	-6.09	1.16	1.24
2	S	143	ALA	C-N	-6.09	1.25	1.34
2	G	84	CYS	C-N	6.09	1.41	1.33
2	I	293	ILE	CA-CB	6.09	1.61	1.54
3	L	76	ARG	C-N	-6.09	1.26	1.33
2	S	120	ILE	CA-C	-6.09	1.45	1.52
3	O	13	GLU	C-O	-6.09	1.16	1.24
2	Q	151	PRO	C-N	6.09	1.41	1.33
2	S	106	ASP	N-CA	6.09	1.54	1.46
2	J	292	HIS	C-N	6.09	1.43	1.33
3	L	57	MET	N-CA	6.08	1.53	1.45
2	R	183	LYS	N-CA	-6.08	1.39	1.46
2	S	89	PRO	C-O	-6.08	1.17	1.23
2	S	139	ARG	N-CA	-6.08	1.39	1.46
2	R	302	ASP	C-N	6.08	1.42	1.33
2	C	152	PRO	C-O	-6.08	1.16	1.24
2	H	80	TYR	C-N	6.08	1.42	1.33
2	J	327	HIS	CA-C	-6.08	1.44	1.52
2	Q	132	SER	C-N	6.08	1.42	1.33
1	F	253	PHE	CA-C	6.07	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	387	MET	N-CA	-6.07	1.41	1.46
2	R	129	ALA	C-N	6.07	1.40	1.33
2	C	29	TYR	CA-C	6.07	1.60	1.52
2	J	118	THR	CA-C	6.07	1.60	1.52
2	G	446	ARG	C-O	-6.07	1.17	1.24
2	G	298	HIS	CA-C	-6.07	1.45	1.52
2	S	396	ASP	N-CA	-6.06	1.38	1.46
3	D	29	GLN	C-N	-6.06	1.26	1.33
2	R	391	VAL	CA-C	6.06	1.60	1.52
2	R	371	MET	CA-C	-6.06	1.46	1.52
3	M	53	PHE	CA-C	-6.05	1.45	1.52
2	H	267	HIS	CA-C	-6.05	1.45	1.52
3	M	84	ASP	C-N	6.05	1.42	1.33
2	G	110	GLU	C-O	-6.05	1.16	1.23
2	Q	459	LEU	CA-C	-6.05	1.44	1.52
2	G	258	LYS	C-O	-6.05	1.17	1.24
2	H	77	MET	CA-C	-6.05	1.44	1.52
3	O	49	ASN	C-N	-6.05	1.25	1.34
2	Q	420	ASN	CA-CB	-6.05	1.44	1.53
2	R	258	LYS	CA-C	6.05	1.60	1.52
2	S	270	LEU	C-N	-6.04	1.26	1.33
3	M	11	ARG	CA-C	6.04	1.62	1.53
3	N	69	GLN	N-CA	-6.04	1.38	1.46
3	P	83	GLY	C-N	6.04	1.43	1.33
1	F	260	PRO	CA-CB	6.04	1.61	1.53
2	I	117	LEU	C-O	-6.04	1.17	1.24
2	G	183	LYS	C-O	-6.04	1.17	1.24
2	S	320	LEU	N-CA	-6.04	1.39	1.46
2	R	317	CYS	C-N	6.04	1.41	1.33
2	C	298	HIS	N-CA	6.04	1.53	1.46
2	J	357	ASP	CA-C	6.04	1.59	1.52
2	I	259	GLU	N-CA	-6.03	1.38	1.46
2	I	126	GLY	C-O	-6.03	1.17	1.23
2	I	392	GLU	C-N	6.03	1.41	1.33
3	L	38	PHE	CA-C	-6.03	1.45	1.52
2	C	86	HIS	CD2-NE2	6.03	1.44	1.37
3	L	106	HIS	C-N	6.02	1.39	1.33
2	J	191	GLU	N-CA	6.02	1.53	1.46
2	S	22	LEU	C-N	6.02	1.41	1.33
3	D	75	VAL	C-N	6.02	1.41	1.33
2	H	188	ALA	CA-C	-6.02	1.45	1.52
2	Q	416	GLY	C-O	-6.02	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	232	THR	CA-C	-6.02	1.45	1.52
3	E	105	VAL	N-CA	-6.02	1.40	1.46
2	S	74	LEU	CA-C	6.02	1.61	1.52
2	H	321	SER	C-N	-6.02	1.26	1.33
2	J	424	LEU	CA-C	-6.01	1.45	1.52
2	J	265	ILE	C-O	-6.01	1.17	1.24
2	C	232	THR	C-N	6.01	1.41	1.33
2	H	368	TRP	C-N	6.01	1.42	1.33
3	L	42	ILE	CB-CG1	6.01	1.65	1.53
2	Q	290	LEU	C-N	-6.01	1.24	1.33
2	R	345	PHE	CA-C	6.01	1.60	1.52
2	H	278	THR	N-CA	-6.00	1.39	1.46
2	S	148	PHE	CA-C	6.00	1.60	1.52
3	E	102	SER	CA-C	-6.00	1.46	1.52
2	I	452	SER	C-O	-6.00	1.18	1.24
2	R	204	GLU	CA-C	6.00	1.60	1.52
2	R	221	VAL	CA-C	-6.00	1.45	1.52
2	J	117	LEU	C-O	-6.00	1.17	1.24
3	E	91	GLY	C-N	6.00	1.41	1.33
2	J	254	ALA	CA-CB	-6.00	1.44	1.53
1	T	273	LEU	C-O	6.00	1.31	1.24
2	G	293	ILE	CB-CG1	6.00	1.65	1.53
3	K	87	ILE	N-CA	-6.00	1.39	1.46
2	S	265	ILE	C-O	-6.00	1.17	1.24
3	E	31	GLU	CA-CB	-5.99	1.44	1.53
1	F	232	GLN	CA-CB	5.99	1.62	1.53
2	I	310	HIS	C-O	-5.99	1.16	1.23
3	P	60	LEU	N-CA	-5.99	1.37	1.46
3	M	61	PRO	C-N	-5.99	1.25	1.33
2	C	220	PHE	N-CA	-5.99	1.39	1.46
3	O	92	PHE	N-CA	5.99	1.53	1.46
2	Q	99	ALA	CA-C	5.99	1.60	1.53
2	I	230	ALA	N-CA	-5.99	1.39	1.46
1	A	299	SER	CA-C	-5.98	1.45	1.52
2	H	428	VAL	C-N	-5.98	1.26	1.33
3	L	82	TYR	C-N	-5.98	1.26	1.33
2	R	443	ASP	C-O	-5.98	1.17	1.24
2	G	229	GLN	CA-C	5.98	1.60	1.52
2	Q	415	PRO	C-O	-5.98	1.16	1.24
2	J	436	ASP	C-N	5.98	1.41	1.34
3	D	17	TYR	CA-C	-5.98	1.44	1.52
2	J	414	ALA	C-O	-5.98	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	284	CYS	C-N	5.98	1.41	1.33
2	G	39	ALA	N-CA	-5.98	1.38	1.46
2	S	185	TYR	C-O	-5.97	1.16	1.23
2	I	180	LEU	CA-C	-5.97	1.45	1.52
2	H	384	VAL	C-N	-5.97	1.26	1.34
2	G	56	ALA	N-CA	5.97	1.53	1.46
2	Q	276	ALA	C-O	-5.97	1.17	1.24
2	Q	432	ASN	CA-C	-5.97	1.45	1.52
2	S	225	ILE	CA-C	-5.97	1.45	1.52
2	G	81	LYS	C-N	5.97	1.38	1.33
2	H	191	GLU	N-CA	5.97	1.53	1.46
3	N	35	GLU	C-O	5.97	1.31	1.24
1	B	295	THR	C-N	5.96	1.41	1.33
2	H	448	ALA	CA-CB	-5.96	1.44	1.53
3	N	18	LEU	C-N	5.96	1.40	1.33
3	P	23	ASP	C-O	5.96	1.31	1.24
1	A	280	LEU	C-N	-5.96	1.25	1.34
2	C	368	TRP	CA-C	-5.96	1.45	1.52
2	H	431	ARG	N-CA	5.96	1.53	1.46
3	O	78	CYS	C-N	5.96	1.41	1.33
2	Q	202	ASP	C-O	-5.96	1.16	1.23
2	G	189	VAL	CA-CB	5.96	1.60	1.54
3	L	24	ARG	CA-C	5.96	1.60	1.52
2	I	299	ALA	N-CA	-5.96	1.38	1.46
2	Q	267	HIS	CD2-NE2	5.95	1.44	1.37
3	P	58	TRP	N-CA	-5.95	1.39	1.46
2	Q	23	THR	N-CA	5.95	1.53	1.46
2	Q	77	MET	SD-CE	5.95	1.94	1.79
2	H	25	TYR	C-O	-5.95	1.17	1.24
2	Q	238	HIS	C-O	-5.95	1.16	1.23
2	R	357	ASP	N-CA	-5.95	1.39	1.46
2	I	265	ILE	C-N	-5.95	1.25	1.33
2	C	36	LEU	N-CA	-5.95	1.38	1.46
2	C	294	HIS	CD2-NE2	5.95	1.44	1.37
2	R	113	VAL	C-N	-5.95	1.26	1.33
2	S	394	PHE	N-CA	-5.95	1.38	1.46
2	H	131	ARG	CA-CB	5.94	1.62	1.53
2	I	77	MET	N-CA	-5.94	1.39	1.46
1	B	288	VAL	C-O	5.94	1.29	1.24
3	D	33	MET	N-CA	-5.94	1.39	1.46
2	G	45	GLN	C-N	5.94	1.41	1.33
3	K	28	ALA	CA-CB	-5.94	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	70	TRP	N-CA	5.94	1.53	1.46
2	H	200	THR	CA-C	-5.94	1.45	1.52
3	L	18	LEU	C-O	-5.94	1.16	1.23
2	R	146	LYS	CA-C	5.94	1.60	1.52
2	G	103	TYR	CA-C	5.94	1.59	1.52
2	I	52	GLU	N-CA	-5.94	1.39	1.46
2	J	153	HIS	C-O	-5.94	1.16	1.24
2	R	212	GLN	N-CA	-5.94	1.39	1.46
2	C	296	ALA	CA-C	5.94	1.60	1.52
2	C	391	VAL	N-CA	5.93	1.53	1.46
2	H	38	ALA	CA-C	-5.93	1.45	1.52
1	T	306	ILE	C-N	-5.93	1.26	1.33
2	J	207	ASN	N-CA	-5.93	1.39	1.46
2	Q	422	VAL	N-CA	-5.93	1.39	1.46
1	A	308	ARG	CA-C	-5.93	1.46	1.52
3	E	107	ARG	N-CA	-5.93	1.38	1.45
2	R	152	PRO	C-O	5.93	1.31	1.24
2	R	200	THR	CA-C	-5.93	1.45	1.52
2	J	124	VAL	CA-C	5.93	1.60	1.52
2	J	215	ARG	CA-C	5.93	1.60	1.52
2	S	199	PHE	CA-C	5.92	1.59	1.52
1	B	230	ILE	C-N	-5.92	1.25	1.33
2	H	367	ASP	C-N	-5.92	1.25	1.33
2	Q	127	PHE	C-O	-5.92	1.16	1.23
2	G	227	LYS	CA-C	-5.92	1.44	1.52
2	C	37	LEU	N-CA	-5.92	1.39	1.46
2	J	445	LEU	C-O	-5.92	1.17	1.24
2	C	71	THR	CA-C	5.92	1.61	1.52
2	I	313	VAL	CA-C	-5.92	1.45	1.52
3	D	24	ARG	CA-C	5.91	1.60	1.52
3	P	22	SER	C-N	-5.91	1.26	1.33
2	R	390	LEU	N-CA	5.91	1.53	1.46
2	I	209	GLN	C-O	-5.91	1.16	1.24
2	I	427	CYS	N-CA	-5.91	1.39	1.46
2	I	439	ARG	CA-C	-5.91	1.44	1.52
2	I	345	PHE	N-CA	-5.91	1.38	1.46
2	C	307	HIS	CE1-NE2	-5.91	1.26	1.32
2	J	114	THR	N-CA	5.91	1.53	1.46
3	N	57	MET	C-O	5.90	1.31	1.23
1	A	265	GLN	CA-C	-5.90	1.47	1.53
2	G	221	VAL	C-O	-5.90	1.17	1.24
2	J	191	GLU	CA-C	-5.90	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	443	ASP	N-CA	5.90	1.53	1.46
2	Q	213	ARG	N-CA	-5.90	1.38	1.46
2	R	56	ALA	N-CA	-5.90	1.39	1.46
2	C	243	THR	C-O	-5.89	1.16	1.23
2	R	207	ASN	CA-C	5.89	1.58	1.52
2	S	87	ILE	N-CA	5.89	1.52	1.46
2	S	124	VAL	CA-CB	5.89	1.61	1.54
2	S	249	GLU	C-O	-5.89	1.17	1.24
2	G	226	HIS	CD2-NE2	5.89	1.44	1.37
2	G	346	VAL	CA-C	5.89	1.59	1.52
2	J	169	MET	CA-C	-5.89	1.45	1.52
3	L	17	TYR	CA-C	5.89	1.61	1.52
2	R	419	ALA	N-CA	-5.89	1.39	1.46
1	F	293	ILE	CA-CB	5.89	1.62	1.54
2	J	25	TYR	C-N	5.89	1.41	1.33
3	O	51	GLU	CA-C	5.89	1.60	1.52
1	T	297	THR	C-N	-5.89	1.25	1.33
2	C	237	GLY	C-O	-5.89	1.18	1.24
3	O	84	ASP	C-N	-5.89	1.24	1.33
2	C	326	LEU	CA-C	-5.88	1.45	1.52
2	G	307	HIS	CD2-NE2	5.88	1.44	1.37
2	H	384	VAL	CA-CB	5.88	1.63	1.54
2	J	178	LEU	CA-CB	5.88	1.61	1.53
3	K	33	MET	CA-C	5.88	1.60	1.52
3	K	64	ASP	C-O	-5.88	1.16	1.23
2	R	218	PHE	CA-C	-5.88	1.45	1.52
3	O	37	GLY	C-N	5.88	1.41	1.33
2	S	114	THR	CA-CB	-5.88	1.44	1.53
2	C	113	VAL	N-CA	-5.88	1.39	1.46
2	G	199	PHE	N-CA	5.88	1.53	1.46
2	J	164	LYS	C-O	5.88	1.31	1.24
3	N	51	GLU	C-O	5.88	1.31	1.24
2	H	93	GLU	C-N	5.88	1.41	1.33
3	N	102	SER	C-N	-5.88	1.26	1.33
2	C	221	VAL	CA-C	5.88	1.60	1.52
2	G	386	HIS	CD2-NE2	5.88	1.44	1.37
2	J	205	ASN	CA-CB	5.88	1.62	1.53
2	Q	326	LEU	C-O	-5.88	1.17	1.23
2	R	115	ASN	C-N	5.88	1.41	1.33
1	T	293	ILE	CA-C	5.88	1.59	1.52
2	H	360	ARG	CA-C	-5.88	1.42	1.52
2	I	213	ARG	C-N	-5.87	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	24	ARG	CA-CB	5.87	1.62	1.53
3	E	99	GLN	CA-CB	-5.87	1.45	1.53
3	P	12	PHE	CA-CB	5.87	1.63	1.53
2	C	110	GLU	N-CA	5.87	1.53	1.46
1	B	276	LEU	CA-C	-5.87	1.45	1.52
2	C	173	THR	CA-C	5.87	1.60	1.52
2	C	389	ALA	C-O	-5.87	1.17	1.24
2	R	461	LEU	CB-CG	5.87	1.65	1.53
2	C	43	SER	C-O	-5.86	1.17	1.24
2	C	163	ASN	CA-C	-5.86	1.45	1.52
2	J	185	TYR	CA-C	5.86	1.60	1.52
3	K	78	CYS	C-N	5.86	1.41	1.33
3	O	25	GLN	N-CA	-5.86	1.39	1.46
2	S	207	ASN	N-CA	-5.86	1.39	1.46
2	Q	81	LYS	N-CA	5.86	1.53	1.46
2	I	459	LEU	C-O	-5.86	1.16	1.24
1	A	271	GLN	CA-C	5.86	1.60	1.52
2	C	426	ALA	C-O	-5.86	1.17	1.24
2	I	76	ASP	C-O	-5.86	1.17	1.24
3	O	94	ASN	N-CA	-5.86	1.38	1.46
2	S	222	ALA	CA-C	-5.86	1.45	1.52
2	Q	28	ASP	CA-C	5.86	1.60	1.52
3	E	92	PHE	N-CA	-5.85	1.39	1.46
3	P	33	MET	C-O	-5.85	1.17	1.24
3	P	34	ILE	CA-C	5.85	1.59	1.52
2	I	133	LEU	CA-C	5.85	1.59	1.52
2	J	445	LEU	N-CA	5.85	1.53	1.46
3	P	72	LEU	C-O	-5.85	1.17	1.24
2	S	354	ILE	CB-CG1	5.85	1.65	1.53
2	G	239	TYR	CA-CB	-5.85	1.45	1.53
2	Q	211	PHE	C-N	5.85	1.41	1.33
2	G	366	GLN	C-N	-5.85	1.25	1.33
2	I	355	GLU	CA-C	-5.85	1.45	1.52
2	S	267	HIS	CD2-NE2	5.85	1.44	1.37
2	C	394	PHE	C-O	-5.84	1.16	1.24
2	R	365	THR	C-O	-5.84	1.16	1.24
2	R	329	GLY	C-N	-5.84	1.25	1.33
2	R	443	ASP	N-CA	-5.84	1.39	1.46
2	S	234	GLU	C-N	5.84	1.39	1.33
1	A	295	THR	C-N	5.84	1.41	1.33
2	C	300	VAL	CA-CB	5.84	1.62	1.54
2	I	77	MET	CA-C	-5.84	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	320	LEU	C-N	-5.84	1.26	1.33
2	R	149	GLN	CA-C	-5.84	1.45	1.52
3	N	65	CYS	C-N	-5.84	1.25	1.33
1	A	283	HIS	C-N	5.84	1.41	1.33
2	H	109	GLU	N-CA	-5.84	1.38	1.46
2	C	190	TYR	CA-C	-5.83	1.45	1.52
2	C	226	HIS	CE1-NE2	5.83	1.38	1.32
3	L	89	VAL	CA-CB	-5.83	1.47	1.54
2	G	29	TYR	CA-C	-5.83	1.45	1.52
2	G	141	PRO	CA-CB	-5.83	1.45	1.53
1	A	245	THR	CA-C	5.83	1.59	1.52
2	H	374	VAL	CA-C	-5.83	1.45	1.52
2	S	185	TYR	C-N	5.83	1.42	1.33
2	C	354	ILE	CA-C	5.82	1.59	1.52
3	E	47	HIS	CE1-NE2	-5.82	1.26	1.32
2	H	322	GLY	CA-C	-5.82	1.48	1.52
2	J	99	ALA	CA-CB	-5.82	1.45	1.53
3	O	78	CYS	C-O	-5.82	1.17	1.24
2	R	297	MET	CA-CB	-5.82	1.46	1.54
2	S	451	TRP	C-N	-5.82	1.26	1.33
2	G	445	LEU	CA-CB	-5.82	1.44	1.53
2	I	354	ILE	N-CA	5.82	1.53	1.46
1	T	276	LEU	C-O	-5.82	1.17	1.24
2	I	286	ASP	C-O	-5.82	1.17	1.24
3	M	48	SER	C-N	-5.82	1.26	1.33
2	R	34	THR	CA-C	5.82	1.60	1.52
2	H	85	TYR	C-N	5.81	1.41	1.33
2	R	205	ASN	CA-CB	-5.81	1.43	1.53
2	R	343	LEU	C-N	5.81	1.41	1.33
3	E	99	GLN	C-O	-5.81	1.17	1.24
1	A	247	HIS	CA-C	5.81	1.59	1.52
2	C	294	HIS	CA-C	5.81	1.59	1.52
2	H	426	ALA	CA-C	-5.81	1.45	1.52
2	S	198	ASP	CA-C	-5.81	1.44	1.52
2	S	387	MET	SD-CE	-5.81	1.65	1.79
2	Q	289	VAL	C-O	-5.80	1.18	1.24
2	G	175	LYS	CA-CB	-5.80	1.45	1.53
2	H	328	SER	C-N	5.80	1.42	1.33
3	P	84	ASP	N-CA	-5.80	1.38	1.46
2	S	271	THR	C-N	-5.80	1.25	1.33
2	C	386	HIS	CD2-NE2	5.80	1.44	1.37
1	B	280	LEU	CA-C	-5.80	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	39	HIS	CD2-NE2	5.80	1.44	1.37
3	N	69	GLN	C-N	5.80	1.41	1.33
2	S	348	LEU	C-O	-5.80	1.17	1.24
2	Q	28	ASP	C-O	-5.80	1.16	1.24
2	S	375	LEU	CA-CB	5.80	1.63	1.53
2	I	269	PHE	C-O	-5.80	1.17	1.24
3	D	22	SER	N-CA	-5.79	1.38	1.45
2	J	423	ALA	C-O	5.79	1.31	1.24
2	R	306	ASN	CA-CB	-5.79	1.45	1.54
3	E	73	ASP	C-O	-5.79	1.17	1.24
2	H	402	PHE	CA-C	-5.79	1.46	1.52
2	I	193	LEU	CA-C	-5.79	1.45	1.52
3	P	61	PRO	C-N	5.79	1.42	1.33
1	F	267	THR	C-O	-5.79	1.16	1.24
2	R	79	ARG	CA-C	5.79	1.60	1.52
2	C	286	ASP	CA-C	-5.79	1.44	1.52
1	B	267	THR	C-N	5.78	1.41	1.33
2	G	45	GLN	C-O	-5.78	1.16	1.24
2	I	183	LYS	CA-C	5.78	1.60	1.52
2	I	212	GLN	N-CA	5.78	1.53	1.46
2	Q	207	ASN	CA-C	5.78	1.58	1.52
2	Q	438	TYR	CA-C	-5.78	1.44	1.52
2	S	233	GLY	C-N	-5.78	1.25	1.33
3	D	76	ARG	CA-C	-5.78	1.45	1.52
2	J	32	LYS	C-N	5.78	1.41	1.33
2	S	230	ALA	CA-C	5.78	1.60	1.52
1	T	230	ILE	C-N	5.78	1.41	1.33
2	H	273	GLY	C-N	5.77	1.41	1.33
2	J	70	TRP	CA-C	5.77	1.60	1.52
2	Q	177	LYS	CA-C	-5.77	1.44	1.52
2	R	103	TYR	CA-C	-5.77	1.45	1.52
1	B	303	GLU	N-CA	5.77	1.53	1.46
2	H	217	ARG	N-CA	-5.77	1.39	1.46
2	I	274	PHE	CA-CB	-5.77	1.44	1.53
2	C	41	ARG	C-N	-5.77	1.26	1.33
2	G	140	PHE	CA-CB	-5.77	1.45	1.53
2	G	330	THR	CA-CB	5.77	1.62	1.53
2	I	55	ALA	CA-C	-5.77	1.45	1.52
2	R	101	ILE	C-N	5.77	1.41	1.33
2	S	57	ILE	C-N	-5.77	1.26	1.33
2	S	275	THR	C-N	5.77	1.41	1.33
3	D	10	ARG	N-CA	-5.76	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	148	PHE	C-N	5.76	1.41	1.34
3	M	13	GLU	N-CA	-5.76	1.39	1.46
2	S	399	VAL	CA-C	5.76	1.59	1.52
2	C	441	GLY	C-N	-5.76	1.26	1.33
2	R	110	GLU	CA-C	5.76	1.60	1.52
2	Q	383	HIS	CG-CD2	-5.76	1.29	1.35
2	R	118	THR	C-N	5.76	1.42	1.33
2	S	86	HIS	CA-CB	-5.76	1.44	1.53
2	S	77	MET	C-O	5.76	1.31	1.24
2	R	127	PHE	CA-C	5.76	1.60	1.52
3	D	33	MET	C-N	5.75	1.40	1.33
2	S	275	THR	CA-CB	-5.75	1.44	1.53
3	L	101	VAL	CA-C	-5.75	1.45	1.52
2	I	302	ASP	CA-CB	-5.75	1.46	1.54
2	J	125	PHE	C-O	5.75	1.31	1.24
3	K	73	ASP	CA-C	-5.75	1.45	1.52
2	Q	292	HIS	CA-C	-5.75	1.45	1.52
2	R	86	HIS	CE1-NE2	5.75	1.38	1.32
2	H	28	ASP	N-CA	-5.75	1.38	1.46
3	K	71	VAL	CA-C	5.75	1.60	1.52
2	Q	432	ASN	C-O	-5.75	1.17	1.24
2	I	255	GLU	C-O	-5.75	1.17	1.24
3	N	18	LEU	CA-CB	5.75	1.61	1.53
2	R	157	VAL	CA-CB	-5.75	1.47	1.54
2	S	283	TRP	CA-CB	-5.75	1.44	1.53
2	C	246	THR	CA-CB	-5.74	1.42	1.54
2	G	422	VAL	CA-CB	5.74	1.60	1.54
2	C	107	LEU	CB-CG	5.74	1.65	1.53
2	C	383	HIS	C-N	-5.74	1.26	1.34
3	K	46	GLU	N-CA	-5.74	1.39	1.46
2	Q	29	TYR	C-O	-5.74	1.17	1.23
2	J	194	ARG	N-CA	-5.74	1.39	1.46
2	R	303	ARG	C-N	-5.74	1.25	1.33
2	S	394	PHE	CA-CB	-5.74	1.44	1.53
2	C	126	GLY	C-O	-5.74	1.16	1.23
2	C	155	ILE	C-O	-5.74	1.17	1.24
2	C	356	ALA	C-N	5.74	1.41	1.34
3	D	21	LEU	CA-CB	-5.74	1.44	1.53
2	G	173	THR	CA-C	-5.74	1.45	1.52
2	R	50	ALA	CA-C	-5.74	1.45	1.52
2	S	294	HIS	C-O	-5.74	1.16	1.23
2	G	77	MET	C-N	-5.73	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	234	GLU	CA-CB	-5.73	1.44	1.53
2	H	271	THR	CA-C	5.73	1.60	1.52
2	H	418	THR	C-O	-5.73	1.17	1.24
2	G	346	VAL	C-O	-5.73	1.17	1.24
3	K	45	ASN	C-O	-5.73	1.17	1.23
2	S	262	MET	CA-C	-5.73	1.46	1.52
2	H	400	LEU	CA-C	5.73	1.59	1.53
2	I	385	TRP	C-N	-5.73	1.26	1.33
2	S	353	HIS	N-CA	-5.73	1.39	1.46
3	P	72	LEU	N-CA	-5.72	1.39	1.46
3	E	69	GLN	N-CA	-5.72	1.39	1.46
2	I	247	CYS	N-CA	-5.72	1.39	1.46
3	E	20	PRO	C-N	5.72	1.41	1.33
2	Q	233	GLY	C-N	5.72	1.41	1.33
2	R	149	GLN	N-CA	-5.72	1.39	1.46
2	I	149	GLN	N-CA	-5.72	1.39	1.46
2	I	382	ILE	C-O	5.72	1.30	1.24
3	D	57	MET	CA-C	5.71	1.59	1.52
2	H	165	TYR	CA-C	-5.71	1.45	1.52
2	H	290	LEU	CA-C	-5.71	1.45	1.52
2	I	49	PRO	C-N	-5.71	1.26	1.33
2	Q	164	LYS	N-CA	5.71	1.53	1.46
2	Q	200	THR	CA-C	-5.71	1.46	1.52
3	L	56	THR	N-CA	-5.71	1.39	1.46
1	T	295	THR	N-CA	-5.71	1.39	1.46
1	F	306	ILE	CA-CB	-5.71	1.46	1.54
2	I	386	HIS	N-CA	5.71	1.53	1.46
3	K	106	HIS	ND1-CE1	5.71	1.38	1.32
2	C	270	LEU	CA-C	-5.71	1.44	1.52
3	M	18	LEU	C-N	5.71	1.38	1.33
2	G	82	GLY	CA-C	-5.70	1.46	1.52
2	Q	148	PHE	C-O	-5.70	1.16	1.23
2	R	397	ASP	N-CA	5.70	1.54	1.46
2	C	306	ASN	CA-CB	-5.70	1.45	1.53
2	H	110	GLU	C-N	-5.70	1.27	1.33
2	I	72	ASP	CA-C	-5.70	1.45	1.52
2	J	118	THR	CA-CB	-5.70	1.44	1.53
3	P	99	GLN	N-CA	-5.70	1.39	1.46
2	Q	125	PHE	CA-C	-5.70	1.44	1.52
2	R	226	HIS	CG-CD2	-5.70	1.29	1.35
2	S	150	GLY	C-N	5.70	1.40	1.33
2	S	213	ARG	CA-CB	5.70	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	383	HIS	CA-C	-5.70	1.46	1.53
3	N	63	PHE	C-N	5.70	1.41	1.33
2	C	312	ARG	N-CA	-5.70	1.39	1.46
1	F	233	VAL	C-N	-5.70	1.26	1.33
2	H	187	ARG	C-N	-5.70	1.26	1.33
3	D	70	GLN	N-CA	-5.69	1.39	1.46
2	Q	36	LEU	C-N	5.69	1.41	1.33
2	H	313	VAL	C-O	-5.69	1.17	1.24
2	R	23	THR	C-O	-5.69	1.15	1.23
3	M	71	VAL	C-O	5.69	1.30	1.24
3	P	49	ASN	CA-C	5.69	1.57	1.52
2	Q	302	ASP	C-O	-5.69	1.17	1.24
1	T	276	LEU	C-N	5.69	1.41	1.33
2	G	97	TYR	CA-C	5.69	1.59	1.52
2	I	297	MET	SD-CE	-5.69	1.65	1.79
2	R	212	GLN	C-N	5.69	1.41	1.33
1	T	293	ILE	C-N	-5.69	1.24	1.33
3	D	104	ILE	CA-C	-5.69	1.46	1.52
2	H	43	SER	C-O	-5.68	1.19	1.24
2	H	201	LYS	CA-C	-5.68	1.45	1.52
2	S	279	THR	CA-C	-5.68	1.45	1.52
2	C	435	ARG	C-N	5.68	1.41	1.33
2	C	340	ALA	C-N	5.68	1.41	1.33
3	D	39	HIS	CA-C	5.68	1.58	1.52
2	I	458	ALA	C-N	-5.68	1.26	1.34
2	J	92	GLY	C-N	5.68	1.40	1.33
2	Q	183	LYS	CA-C	5.68	1.60	1.52
3	M	106	HIS	ND1-CE1	-5.68	1.26	1.32
2	H	118	THR	N-CA	5.68	1.53	1.46
2	H	317	CYS	CA-C	-5.68	1.45	1.52
3	P	105	VAL	CA-C	5.68	1.59	1.52
2	Q	247	CYS	CA-C	5.68	1.60	1.52
2	S	292	HIS	CA-CB	5.68	1.62	1.53
2	C	151	PRO	CA-C	-5.67	1.48	1.52
2	C	174	ILE	CA-CB	5.67	1.60	1.54
2	G	227	LYS	C-N	5.67	1.41	1.33
2	J	371	MET	SD-CE	-5.67	1.65	1.79
2	Q	247	CYS	N-CA	-5.67	1.38	1.46
3	N	44	PHE	C-N	-5.67	1.26	1.33
2	H	278	THR	C-O	-5.67	1.17	1.24
2	C	194	ARG	C-N	5.67	1.41	1.33
2	I	314	LEU	CB-CG	5.67	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	11	ARG	CA-CB	-5.67	1.44	1.53
2	H	298	HIS	ND1-CE1	5.67	1.38	1.32
2	R	100	PHE	C-O	-5.67	1.17	1.24
2	C	33	ASP	CA-C	-5.67	1.44	1.52
2	C	454	GLU	C-N	5.67	1.41	1.34
2	G	348	LEU	C-O	-5.67	1.17	1.24
3	D	21	LEU	C-O	-5.66	1.17	1.23
2	H	227	LYS	C-N	5.66	1.41	1.33
3	O	67	SER	C-N	5.66	1.41	1.33
3	D	33	MET	C-O	-5.66	1.17	1.24
2	G	330	THR	CA-C	-5.66	1.45	1.52
2	G	348	LEU	CA-CB	5.66	1.62	1.53
2	I	98	PHE	CA-C	5.66	1.59	1.52
2	J	425	GLU	CA-C	5.66	1.60	1.52
1	A	267	THR	C-N	5.66	1.41	1.33
3	E	103	PHE	C-O	-5.66	1.17	1.23
2	R	262	MET	CA-C	-5.66	1.46	1.52
3	L	84	ASP	N-CA	-5.66	1.39	1.46
2	I	137	ASP	C-O	5.66	1.30	1.23
2	C	211	PHE	CA-C	5.65	1.60	1.52
2	C	278	THR	CA-C	5.65	1.60	1.52
2	G	49	PRO	CA-C	5.65	1.59	1.52
2	H	45	GLN	CA-C	5.65	1.60	1.52
2	H	48	VAL	CA-C	5.65	1.58	1.52
2	J	397	ASP	C-O	-5.65	1.16	1.23
2	S	153	HIS	CD2-NE2	5.65	1.44	1.37
3	E	74	GLU	CA-C	-5.65	1.45	1.52
2	G	459	LEU	CB-CG	-5.65	1.42	1.53
2	C	131	ARG	CA-C	5.65	1.60	1.52
3	E	80	SER	C-N	5.65	1.41	1.33
2	S	345	PHE	C-N	5.65	1.41	1.33
2	I	58	ALA	CA-C	-5.65	1.45	1.52
2	Q	108	PHE	C-O	5.65	1.30	1.23
2	C	105	LEU	CA-C	-5.64	1.45	1.52
2	G	171	GLY	N-CA	-5.64	1.39	1.45
2	R	454	GLU	CA-CB	5.64	1.62	1.53
2	H	161	LEU	CA-CB	-5.64	1.44	1.53
2	H	328	SER	N-CA	-5.64	1.39	1.46
2	J	430	ALA	CA-CB	-5.64	1.44	1.53
3	N	84	ASP	CA-C	-5.64	1.43	1.52
2	R	93	GLU	C-O	-5.64	1.17	1.23
2	J	249	GLU	C-O	-5.64	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	228	GLU	C-O	-5.64	1.17	1.24
3	E	39	HIS	C-N	5.64	1.40	1.33
2	S	307	HIS	CA-C	5.64	1.59	1.52
3	O	15	PHE	C-N	-5.64	1.25	1.33
3	K	61	PRO	N-CA	-5.64	1.40	1.47
3	M	62	LEU	C-N	5.64	1.43	1.33
2	Q	399	VAL	C-O	5.64	1.29	1.23
2	G	397	ASP	C-O	5.63	1.29	1.23
2	H	253	ARG	C-O	5.63	1.30	1.24
3	L	107	ARG	C-O	5.63	1.29	1.24
2	J	458	ALA	C-O	-5.63	1.17	1.24
2	R	21	LYS	CA-C	-5.63	1.45	1.52
2	R	164	LYS	CA-C	-5.63	1.46	1.52
2	C	172	CYS	CA-C	-5.63	1.46	1.52
2	G	314	LEU	CB-CG	5.63	1.64	1.53
2	J	226	HIS	CD2-NE2	5.63	1.44	1.37
2	S	292	HIS	CA-C	-5.63	1.45	1.52
2	H	371	MET	N-CA	-5.62	1.38	1.46
2	I	137	ASP	N-CA	5.62	1.52	1.46
2	J	402	PHE	CA-CB	5.62	1.61	1.53
2	S	423	ALA	C-O	-5.62	1.17	1.24
2	J	175	LYS	N-CA	-5.62	1.41	1.45
2	J	213	ARG	N-CA	-5.62	1.38	1.46
2	R	53	ALA	CA-C	5.62	1.59	1.52
3	P	43	GLU	C-O	-5.62	1.16	1.23
2	C	28	ASP	C-N	-5.62	1.26	1.33
2	S	330	THR	CA-C	-5.62	1.45	1.52
2	H	88	GLU	CA-C	-5.61	1.46	1.52
3	M	67	SER	CA-C	5.61	1.58	1.52
1	A	266	SER	N-CA	-5.61	1.39	1.46
1	A	276	LEU	CB-CG	-5.61	1.42	1.53
1	A	298	ARG	C-O	-5.61	1.16	1.23
2	G	312	ARG	C-N	-5.61	1.26	1.33
2	G	392	GLU	CA-CB	5.61	1.62	1.53
2	Q	350	ARG	C-O	5.61	1.30	1.24
2	I	298	HIS	C-N	5.61	1.41	1.34
2	J	97	TYR	N-CA	-5.61	1.38	1.45
2	C	215	ARG	N-CA	5.61	1.53	1.46
2	J	440	GLU	CA-CB	5.61	1.60	1.53
2	Q	229	GLN	N-CA	5.61	1.53	1.46
2	Q	240	LEU	CB-CG	-5.61	1.42	1.53
2	R	133	LEU	N-CA	-5.61	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	145	VAL	CA-C	-5.61	1.46	1.52
2	J	37	LEU	C-N	-5.60	1.26	1.33
2	J	91	GLN	C-N	-5.60	1.26	1.33
2	H	223	ASP	C-N	-5.60	1.25	1.33
2	Q	112	SER	CA-C	-5.60	1.45	1.53
2	R	31	PRO	C-O	5.60	1.30	1.23
2	I	131	ARG	CA-C	-5.60	1.45	1.52
2	Q	383	HIS	CD2-NE2	5.60	1.44	1.37
2	C	77	MET	SD-CE	5.60	1.93	1.79
2	J	230	ALA	N-CA	-5.60	1.39	1.46
2	J	344	GLY	C-N	5.60	1.41	1.34
2	Q	170	LEU	CA-C	-5.60	1.45	1.52
2	I	218	PHE	C-O	-5.60	1.17	1.24
2	J	222	ALA	N-CA	-5.60	1.39	1.46
2	C	423	ALA	C-N	5.59	1.40	1.33
2	G	301	ILE	CB-CG1	5.59	1.64	1.53
2	G	438	TYR	C-N	-5.59	1.26	1.33
2	I	359	SER	CA-C	-5.59	1.45	1.52
2	R	397	ASP	CA-CB	-5.59	1.45	1.52
2	S	176	PRO	C-N	5.59	1.41	1.33
2	G	396	ASP	CA-C	5.59	1.60	1.52
2	I	160	ASP	CA-C	-5.59	1.45	1.52
2	J	86	HIS	C-O	-5.59	1.17	1.23
1	F	297	THR	C-N	-5.59	1.25	1.33
2	G	23	THR	C-N	-5.59	1.26	1.33
2	H	301	ILE	CB-CG1	-5.59	1.42	1.53
2	I	187	ARG	N-CA	-5.59	1.39	1.46
2	I	327	HIS	CA-C	5.59	1.60	1.52
2	R	396	ASP	N-CA	5.59	1.53	1.46
2	S	435	ARG	N-CA	-5.59	1.39	1.46
2	I	193	LEU	CB-CG	-5.59	1.42	1.53
2	G	340	ALA	C-O	-5.59	1.17	1.24
2	S	383	HIS	N-CA	-5.59	1.38	1.46
2	C	346	VAL	C-O	-5.59	1.17	1.24
2	G	24	TYR	N-CA	5.59	1.53	1.46
2	G	329	GLY	C-N	5.59	1.41	1.33
2	H	197	LEU	C-O	-5.59	1.17	1.23
3	M	19	PRO	CA-C	5.59	1.54	1.51
2	Q	182	ALA	C-O	-5.59	1.17	1.24
2	C	147	THR	C-O	-5.58	1.17	1.24
2	G	300	VAL	N-CA	-5.58	1.38	1.46
3	K	56	THR	CA-CB	5.58	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	228	GLU	CA-CB	-5.58	1.44	1.53
2	G	249	GLU	N-CA	-5.58	1.39	1.46
3	L	77	GLU	CA-C	5.58	1.59	1.52
3	D	28	ALA	C-N	5.58	1.41	1.33
3	O	77	GLU	C-N	5.58	1.41	1.33
2	G	443	ASP	C-N	5.58	1.40	1.33
2	I	64	GLY	C-N	5.58	1.41	1.33
3	N	34	ILE	C-N	5.58	1.41	1.34
2	R	190	TYR	N-CA	5.58	1.53	1.46
2	S	83	LYS	CA-C	-5.58	1.45	1.52
2	S	182	ALA	CA-C	-5.58	1.45	1.52
2	G	273	GLY	C-N	5.57	1.41	1.33
2	J	460	ASP	CA-C	-5.57	1.45	1.52
2	Q	75	THR	N-CA	-5.57	1.39	1.45
2	I	122	GLY	C-O	-5.57	1.17	1.23
2	Q	238	HIS	C-N	5.57	1.41	1.33
2	I	249	GLU	C-N	-5.57	1.26	1.33
2	J	168	PRO	C-N	5.57	1.41	1.33
3	D	42	ILE	C-O	-5.57	1.17	1.24
2	H	86	HIS	C-N	-5.57	1.26	1.33
1	T	283	HIS	CG-CD2	-5.57	1.29	1.35
1	A	283	HIS	CA-C	5.57	1.60	1.52
3	D	61	PRO	N-CA	5.57	1.53	1.46
2	H	24	TYR	N-CA	5.57	1.52	1.46
2	H	229	GLN	CA-C	-5.57	1.45	1.52
3	K	88	ARG	C-N	5.57	1.42	1.33
2	G	458	ALA	C-N	-5.56	1.26	1.33
2	J	443	ASP	C-O	-5.56	1.17	1.24
3	M	82	TYR	CA-CB	-5.56	1.45	1.53
2	G	239	TYR	N-CA	-5.56	1.39	1.46
2	I	455	LEU	C-O	-5.56	1.17	1.24
2	Q	146	LYS	CA-C	5.56	1.60	1.52
2	S	139	ARG	C-N	-5.56	1.24	1.33
2	H	121	VAL	CA-CB	-5.56	1.48	1.54
2	J	77	MET	CA-C	-5.56	1.45	1.52
2	R	281	ALA	CA-C	-5.56	1.45	1.52
2	S	56	ALA	CA-CB	-5.56	1.44	1.53
2	C	135	LEU	CA-C	5.55	1.59	1.52
2	C	318	LEU	C-O	-5.55	1.17	1.24
2	J	103	TYR	C-O	-5.55	1.16	1.25
2	R	117	LEU	CA-CB	-5.55	1.44	1.53
2	R	129	ALA	C-O	-5.55	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	294	HIS	N-CA	-5.55	1.38	1.46
1	B	242	ARG	C-N	5.55	1.40	1.33
1	B	276	LEU	C-N	5.55	1.41	1.34
1	B	278	ASN	CA-C	5.55	1.59	1.52
1	F	278	ASN	C-N	5.55	1.41	1.33
2	Q	155	ILE	C-N	-5.55	1.26	1.33
2	C	427	CYS	CA-C	-5.55	1.45	1.52
3	E	40	PRO	C-N	-5.55	1.25	1.33
2	G	436	ASP	N-CA	-5.55	1.39	1.46
3	M	51	GLU	N-CA	-5.55	1.38	1.46
3	L	74	GLU	C-N	-5.55	1.26	1.33
2	R	163	ASN	C-N	5.55	1.41	1.33
2	R	299	ALA	C-N	5.55	1.40	1.34
2	C	319	ARG	CA-C	-5.55	1.45	1.52
3	L	107	ARG	N-CA	-5.54	1.40	1.45
2	Q	63	THR	CA-C	5.54	1.60	1.52
2	C	270	LEU	N-CA	-5.54	1.39	1.46
2	I	120	ILE	CB-CG1	5.54	1.64	1.53
2	I	151	PRO	C-N	-5.54	1.26	1.34
3	O	86	TYR	C-N	5.54	1.40	1.33
2	S	49	PRO	CA-CB	-5.54	1.46	1.53
2	J	61	SER	CA-C	5.54	1.60	1.52
2	J	389	ALA	CA-C	-5.54	1.45	1.52
3	L	74	GLU	N-CA	-5.54	1.39	1.46
2	R	161	LEU	CB-CG	-5.54	1.42	1.53
2	C	51	ASP	CA-C	5.54	1.59	1.52
2	H	231	GLU	CA-C	5.54	1.60	1.52
2	J	163	ASN	N-CA	-5.54	1.39	1.46
2	C	156	GLN	C-N	-5.54	1.27	1.33
2	H	389	ALA	CA-CB	-5.54	1.44	1.53
2	C	322	GLY	C-N	5.54	1.40	1.33
2	J	421	ARG	C-N	5.54	1.40	1.33
3	P	63	PHE	C-N	5.54	1.40	1.33
2	Q	298	HIS	CE1-NE2	5.54	1.38	1.32
2	S	148	PHE	N-CA	5.54	1.52	1.45
1	B	279	CYS	CA-C	5.53	1.59	1.52
3	D	49	ASN	C-O	5.53	1.30	1.24
2	G	310	HIS	ND1-CE1	5.53	1.38	1.32
2	R	189	VAL	CA-C	-5.53	1.46	1.52
2	H	88	GLU	C-O	-5.53	1.18	1.24
3	O	39	HIS	CD2-NE2	5.53	1.44	1.37
2	I	163	ASN	C-N	5.53	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	278	THR	C-O	-5.53	1.17	1.24
2	C	145	VAL	C-N	-5.53	1.26	1.33
2	C	200	THR	CA-C	-5.53	1.46	1.52
2	H	180	LEU	CA-C	-5.53	1.45	1.53
2	J	382	ILE	CA-C	5.53	1.59	1.52
1	B	234	ARG	CA-C	-5.53	1.45	1.52
2	J	76	ASP	CA-C	-5.53	1.47	1.53
2	I	188	ALA	C-O	-5.52	1.17	1.24
3	N	42	ILE	CA-C	-5.52	1.45	1.52
3	O	48	SER	N-CA	5.52	1.53	1.46
3	P	52	GLU	CA-C	-5.52	1.46	1.53
1	A	228	GLU	C-N	5.52	1.40	1.33
1	F	277	GLU	CA-C	5.52	1.59	1.52
2	I	43	SER	N-CA	5.52	1.52	1.46
2	J	35	ASP	N-CA	5.52	1.53	1.45
2	J	451	TRP	N-CA	5.52	1.53	1.46
2	R	414	ALA	CA-CB	-5.52	1.46	1.53
2	C	420	ASN	C-O	5.52	1.30	1.24
2	H	207	ASN	C-O	-5.52	1.16	1.24
3	L	79	ARG	CA-CB	-5.52	1.44	1.53
2	R	180	LEU	N-CA	5.52	1.52	1.46
2	S	238	HIS	CD2-NE2	5.52	1.44	1.37
2	I	208	SER	N-CA	-5.52	1.38	1.46
3	P	47	HIS	CG-CD2	5.52	1.42	1.35
2	R	76	ASP	N-CA	-5.52	1.39	1.46
1	T	246	GLU	C-O	5.52	1.30	1.23
2	I	223	ASP	C-N	5.51	1.40	1.33
2	I	326	LEU	CA-CB	-5.51	1.44	1.53
2	J	56	ALA	C-N	-5.51	1.27	1.34
2	J	321	SER	N-CA	-5.51	1.39	1.46
2	R	328	SER	N-CA	-5.51	1.40	1.46
2	S	169	MET	C-N	5.51	1.41	1.33
2	C	71	THR	C-O	-5.51	1.17	1.24
2	C	327	HIS	CD2-NE2	5.51	1.44	1.37
3	D	72	LEU	C-N	-5.51	1.26	1.33
2	I	329	GLY	C-N	-5.51	1.25	1.33
3	O	44	PHE	CA-C	5.51	1.59	1.52
2	Q	219	LEU	N-CA	-5.51	1.39	1.46
1	T	282	GLU	C-O	5.51	1.30	1.24
2	C	187	ARG	CA-C	-5.51	1.45	1.52
2	C	290	LEU	C-O	-5.51	1.16	1.23
2	G	125	PHE	N-CA	-5.51	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	45	GLN	N-CA	5.51	1.53	1.45
2	S	42	PHE	CA-C	5.51	1.59	1.52
2	S	222	ALA	N-CA	-5.51	1.39	1.46
2	H	185	TYR	CA-C	5.51	1.60	1.52
2	R	295	ARG	CA-C	5.51	1.60	1.52
2	I	366	GLN	CA-C	5.51	1.59	1.52
3	L	34	ILE	CA-C	-5.51	1.46	1.52
3	P	21	LEU	CA-C	-5.51	1.45	1.52
2	I	421	ARG	N-CA	5.50	1.52	1.46
3	K	93	ASP	N-CA	-5.50	1.39	1.46
2	Q	125	PHE	C-O	-5.50	1.17	1.24
2	R	79	ARG	C-N	5.50	1.41	1.33
2	J	148	PHE	CA-C	-5.50	1.45	1.52
2	I	169	MET	N-CA	5.50	1.52	1.45
2	Q	119	SER	C-O	5.50	1.30	1.24
1	B	242	ARG	CD-NE	5.50	1.53	1.46
1	B	273	LEU	N-CA	-5.50	1.39	1.46
2	I	116	ILE	N-CA	-5.50	1.40	1.46
2	I	349	MET	SD-CE	-5.50	1.65	1.79
2	I	414	ALA	N-CA	-5.50	1.41	1.46
2	H	52	GLU	CA-CB	5.50	1.62	1.53
2	H	454	GLU	C-O	-5.49	1.17	1.24
2	Q	136	GLU	C-N	-5.49	1.26	1.33
2	Q	443	ASP	N-CA	5.49	1.52	1.46
2	G	135	LEU	CA-CB	5.49	1.60	1.53
2	Q	29	TYR	C-N	5.49	1.43	1.33
2	C	255	GLU	N-CA	5.49	1.52	1.46
3	N	17	TYR	C-N	5.49	1.43	1.33
2	R	165	TYR	CA-C	-5.49	1.46	1.52
3	D	95	ILE	CA-CB	5.49	1.60	1.54
2	H	34	THR	N-CA	5.49	1.53	1.46
2	J	390	LEU	CA-CB	5.49	1.61	1.53
2	G	398	SER	CA-C	5.49	1.59	1.52
2	H	194	ARG	CA-C	5.49	1.60	1.52
2	Q	353	HIS	CD2-NE2	5.49	1.43	1.37
3	O	75	VAL	CA-C	5.49	1.61	1.52
2	R	255	GLU	N-CA	5.49	1.52	1.46
2	C	228	SER	CA-C	-5.48	1.45	1.52
3	D	70	GLN	C-O	-5.48	1.17	1.24
2	S	156	GLN	N-CA	-5.48	1.39	1.46
2	Q	135	LEU	C-N	-5.48	1.26	1.33
2	G	24	TYR	CA-C	-5.48	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	130	ILE	CA-CB	5.48	1.60	1.54
2	R	259	GLU	N-CA	5.48	1.53	1.46
2	G	123	ASN	C-N	-5.48	1.26	1.33
2	Q	303	ARG	C-O	5.48	1.30	1.24
2	J	123	ASN	N-CA	5.47	1.52	1.46
3	O	93	ASP	CA-CB	5.47	1.59	1.52
3	D	13	GLU	C-N	5.47	1.42	1.33
3	E	30	ILE	C-O	-5.47	1.18	1.24
2	J	292	HIS	CE1-NE2	-5.47	1.27	1.32
2	S	253	ARG	C-N	-5.47	1.27	1.33
2	H	308	GLY	C-N	5.47	1.40	1.33
3	D	60	LEU	CA-C	5.47	1.61	1.53
2	I	101	ILE	N-CA	-5.47	1.39	1.46
2	Q	342	THR	CA-CB	-5.47	1.44	1.53
2	G	186	GLY	C-N	-5.47	1.26	1.33
2	C	443	ASP	C-N	5.47	1.40	1.33
2	G	275	THR	N-CA	-5.47	1.39	1.46
2	I	255	GLU	CA-C	5.47	1.59	1.52
2	J	209	GLN	N-CA	-5.47	1.38	1.45
2	H	173	THR	CA-C	-5.46	1.45	1.52
2	H	290	LEU	C-O	5.46	1.30	1.23
1	F	283	HIS	CA-C	5.46	1.60	1.52
2	Q	101	ILE	CB-CG1	5.46	1.64	1.53
2	R	44	PRO	C-N	-5.46	1.25	1.33
2	Q	301	ILE	C-O	-5.46	1.18	1.24
2	R	254	ALA	CA-C	5.46	1.59	1.52
2	H	311	PHE	N-CA	-5.46	1.39	1.46
2	S	108	PHE	CA-C	-5.46	1.46	1.52
2	J	302	ASP	CA-CB	-5.45	1.45	1.54
1	A	294	ASP	C-O	5.45	1.30	1.24
2	G	371	MET	SD-CE	5.45	1.93	1.79
2	I	263	PRO	C-N	-5.45	1.28	1.33
2	J	377	VAL	C-O	-5.45	1.17	1.24
1	B	260	PRO	CA-CB	-5.45	1.46	1.53
2	C	194	ARG	CA-C	-5.45	1.45	1.52
2	H	383	HIS	CA-C	-5.45	1.47	1.53
3	N	52	GLU	C-O	5.45	1.30	1.23
2	Q	56	ALA	CA-C	5.45	1.59	1.52
2	Q	203	ASP	CA-CB	-5.45	1.45	1.53
2	S	319	ARG	N-CA	-5.45	1.39	1.46
2	J	85	TYR	C-O	-5.45	1.16	1.24
3	O	26	ILE	CB-CG1	-5.45	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	88	GLU	C-N	5.45	1.40	1.33
2	H	226	HIS	CG-ND1	-5.44	1.32	1.38
2	R	327	HIS	CA-CB	5.44	1.62	1.53
2	S	63	THR	C-N	-5.44	1.25	1.33
2	C	131	ARG	C-O	-5.44	1.17	1.24
2	G	236	LYS	C-O	-5.44	1.16	1.23
2	Q	281	ALA	CA-C	5.44	1.59	1.52
1	T	238	ASN	CA-C	5.44	1.59	1.52
2	G	101	ILE	CB-CG1	5.44	1.64	1.53
2	I	437	LEU	CA-C	-5.44	1.45	1.52
2	J	285	ARG	C-N	-5.44	1.26	1.33
2	J	303	ARG	CA-CB	-5.44	1.45	1.53
3	M	33	MET	CA-CB	-5.44	1.45	1.53
2	S	115	ASN	CA-CB	-5.44	1.44	1.53
2	Q	320	LEU	CA-C	-5.44	1.46	1.52
2	I	271	THR	CA-CB	5.43	1.61	1.53
2	S	180	LEU	CA-CB	5.43	1.61	1.53
2	J	239	TYR	CA-CB	5.43	1.60	1.52
2	Q	210	PRO	C-O	5.43	1.31	1.24
2	I	100	PHE	N-CA	-5.43	1.39	1.46
3	D	39	HIS	ND1-CE1	5.43	1.38	1.32
2	H	285	ARG	C-N	5.43	1.41	1.33
2	J	35	ASP	CA-CB	-5.43	1.45	1.53
2	R	400	LEU	C-N	5.42	1.40	1.33
2	I	267	HIS	CD2-NE2	5.42	1.43	1.37
2	G	369	ALA	CA-CB	-5.42	1.44	1.53
2	I	383	HIS	ND1-CE1	5.42	1.38	1.32
2	C	235	ILE	CA-CB	5.42	1.61	1.54
2	I	340	ALA	CA-C	5.42	1.59	1.52
1	A	296	ASN	CA-CB	5.41	1.61	1.53
3	E	106	HIS	CA-C	-5.41	1.46	1.52
2	J	143	ALA	N-CA	-5.41	1.40	1.46
2	R	292	HIS	CA-C	-5.41	1.46	1.52
2	S	275	THR	N-CA	5.41	1.52	1.46
2	G	460	ASP	CA-C	-5.41	1.45	1.52
2	I	357	ASP	C-N	-5.41	1.25	1.33
3	P	78	CYS	C-N	5.41	1.41	1.33
2	Q	414	ALA	CA-CB	-5.41	1.46	1.53
2	R	174	ILE	C-N	5.41	1.40	1.33
1	B	294	ASP	CA-C	-5.41	1.46	1.52
2	G	138	ILE	N-CA	-5.41	1.39	1.46
2	I	86	HIS	CE1-NE2	5.41	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	302	PHE	N-CA	-5.41	1.39	1.46
2	J	352	ASP	CA-C	5.41	1.59	1.52
3	O	46	GLU	C-N	-5.41	1.25	1.33
2	C	138	ILE	CB-CG1	5.41	1.64	1.53
3	D	99	GLN	CA-C	5.41	1.59	1.52
2	H	138	ILE	C-N	5.41	1.42	1.33
2	C	292	HIS	N-CA	-5.40	1.39	1.45
2	I	298	HIS	C-O	-5.40	1.17	1.24
2	J	226	HIS	ND1-CE1	-5.40	1.27	1.32
2	H	397	ASP	C-N	-5.40	1.26	1.33
2	J	247	CYS	CA-C	-5.40	1.45	1.52
2	J	100	PHE	C-N	-5.40	1.26	1.33
2	J	158	GLU	CA-CB	-5.40	1.45	1.53
2	J	171	GLY	C-N	-5.40	1.25	1.33
1	A	297	THR	CA-CB	-5.39	1.44	1.53
2	H	53	ALA	CA-CB	-5.39	1.45	1.53
3	N	44	PHE	C-O	-5.39	1.17	1.23
2	Q	269	PHE	C-N	5.39	1.40	1.33
2	Q	295	ARG	CA-C	5.39	1.59	1.53
2	S	455	LEU	CA-CB	-5.39	1.44	1.53
2	Q	426	ALA	CA-C	-5.39	1.45	1.52
2	C	289	VAL	C-O	-5.39	1.18	1.24
2	I	21	LYS	CA-C	-5.39	1.45	1.52
2	J	251	MET	C-O	-5.39	1.18	1.24
1	F	299	SER	C-N	5.39	1.41	1.33
2	G	318	LEU	C-O	-5.39	1.18	1.24
2	Q	284	CYS	C-O	-5.39	1.17	1.24
2	Q	348	LEU	N-CA	-5.39	1.39	1.46
2	G	125	PHE	C-O	-5.39	1.17	1.24
2	G	221	VAL	C-N	5.39	1.40	1.33
2	H	358	ARG	N-CA	5.39	1.52	1.46
2	Q	192	CYS	C-N	5.39	1.41	1.33
2	C	421	ARG	C-O	-5.39	1.17	1.24
2	I	235	ILE	N-CA	-5.39	1.39	1.46
2	Q	251	MET	CA-CB	5.39	1.61	1.53
2	Q	383	HIS	C-O	-5.39	1.15	1.23
2	Q	396	ASP	CA-C	5.39	1.60	1.52
2	S	345	PHE	CA-CB	-5.38	1.44	1.53
3	E	95	ILE	C-N	-5.38	1.26	1.33
2	J	230	ALA	C-N	-5.38	1.25	1.33
3	O	22	SER	C-N	5.38	1.41	1.33
2	R	267	HIS	CG-CD2	-5.38	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	230	ALA	C-O	5.38	1.30	1.24
3	L	49	ASN	C-N	-5.38	1.26	1.34
2	H	340	ALA	C-N	-5.38	1.26	1.34
3	K	102	SER	C-O	5.38	1.30	1.24
2	G	86	HIS	CG-CD2	-5.38	1.29	1.35
2	J	174	ILE	C-O	-5.38	1.17	1.24
2	H	139	ARG	N-CA	-5.38	1.39	1.46
2	R	445	LEU	C-O	5.38	1.30	1.24
2	S	180	LEU	CA-C	-5.38	1.45	1.52
2	G	344	GLY	C-N	5.38	1.41	1.33
2	J	82	GLY	C-N	-5.38	1.26	1.33
1	A	255	THR	CB-OG1	-5.37	1.35	1.43
2	J	90	VAL	CA-CB	-5.37	1.47	1.54
3	K	94	ASN	CA-C	-5.37	1.46	1.52
2	S	398	SER	C-N	-5.37	1.26	1.33
2	G	382	ILE	C-O	5.37	1.31	1.24
2	G	440	GLU	C-O	-5.37	1.16	1.24
3	O	33	MET	C-N	-5.37	1.27	1.33
2	Q	23	THR	C-O	-5.37	1.17	1.23
2	Q	302	ASP	C-N	-5.37	1.27	1.33
2	C	103	TYR	C-O	-5.37	1.17	1.24
3	D	47	HIS	CG-CD2	-5.37	1.29	1.35
2	Q	159	ARG	CA-C	5.37	1.59	1.52
2	G	147	THR	CA-CB	5.37	1.62	1.53
2	S	300	VAL	CA-CB	-5.37	1.46	1.54
2	C	116	ILE	CB-CG1	5.37	1.64	1.53
2	I	30	THR	CA-C	5.37	1.57	1.52
1	A	242	ARG	C-N	5.36	1.40	1.33
2	R	230	ALA	C-N	-5.36	1.27	1.33
3	N	102	SER	C-O	5.36	1.30	1.24
2	Q	187	ARG	CA-C	5.36	1.59	1.52
2	J	22	LEU	C-N	5.36	1.42	1.33
2	J	226	HIS	CA-C	-5.36	1.45	1.52
2	Q	133	LEU	CB-CG	-5.36	1.42	1.53
2	Q	183	LYS	N-CA	-5.36	1.40	1.46
2	Q	360	ARG	CA-CB	-5.36	1.45	1.53
2	G	180	LEU	C-O	-5.36	1.17	1.23
3	O	31	GLU	N-CA	-5.36	1.40	1.46
3	P	32	TYR	C-N	-5.36	1.27	1.33
2	Q	123	ASN	C-N	5.36	1.40	1.33
2	G	370	SER	N-CA	5.36	1.53	1.46
3	O	87	ILE	CA-CB	-5.36	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	180	LEU	C-O	-5.36	1.17	1.23
1	A	239	GLN	CA-C	5.35	1.60	1.52
3	M	47	HIS	CE1-NE2	5.35	1.38	1.32
2	H	458	ALA	C-O	5.35	1.30	1.24
2	I	63	THR	CA-CB	-5.35	1.46	1.54
2	I	136	GLU	C-N	-5.35	1.26	1.33
2	S	247	CYS	N-CA	-5.35	1.39	1.46
2	R	126	GLY	C-O	-5.35	1.17	1.23
2	H	107	LEU	C-N	5.35	1.40	1.33
3	K	51	GLU	CA-CB	-5.35	1.44	1.53
2	S	99	ALA	CA-C	-5.35	1.46	1.52
2	G	86	HIS	CG-ND1	-5.35	1.32	1.38
3	L	87	ILE	CA-C	5.35	1.59	1.52
3	M	107	ARG	C-O	-5.35	1.17	1.24
3	L	102	SER	N-CA	-5.34	1.40	1.46
2	C	163	ASN	C-N	5.34	1.40	1.33
2	G	229	GLN	C-N	-5.34	1.27	1.33
2	R	217	ARG	CA-C	-5.34	1.46	1.52
2	C	288	GLY	CA-C	5.34	1.57	1.51
1	F	305	LEU	C-N	-5.34	1.26	1.33
2	H	79	ARG	CA-CB	-5.34	1.45	1.53
2	H	397	ASP	C-O	5.34	1.29	1.23
2	G	310	HIS	CG-ND1	-5.34	1.32	1.38
2	I	265	ILE	C-O	-5.34	1.17	1.24
2	J	217	ARG	CA-CB	-5.34	1.45	1.53
2	Q	371	MET	SD-CE	5.34	1.93	1.79
2	R	243	THR	C-N	-5.34	1.27	1.33
2	S	137	ASP	CA-C	5.34	1.59	1.52
2	H	60	GLU	C-N	5.34	1.41	1.34
2	Q	382	ILE	C-N	5.34	1.40	1.33
2	I	99	ALA	C-N	5.34	1.40	1.33
1	B	304	ALA	CA-C	-5.33	1.46	1.52
1	T	295	THR	C-O	-5.33	1.17	1.24
2	C	127	PHE	CA-CB	-5.33	1.45	1.53
2	H	448	ALA	N-CA	5.33	1.52	1.46
3	N	56	THR	C-N	-5.33	1.26	1.33
3	P	67	SER	N-CA	-5.33	1.39	1.46
2	R	202	ASP	CG-OD1	-5.33	1.15	1.25
2	G	133	LEU	CA-C	5.33	1.59	1.52
1	A	286	GLU	C-O	-5.33	1.17	1.23
2	S	441	GLY	C-N	5.33	1.40	1.33
2	C	50	ALA	C-O	-5.33	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	109	GLU	C-N	-5.33	1.25	1.33
3	E	56	THR	C-N	-5.33	1.26	1.33
2	Q	324	ASP	CA-CB	-5.33	1.44	1.53
2	C	181	SER	C-O	-5.33	1.16	1.23
2	J	433	GLU	C-O	-5.33	1.17	1.24
3	L	90	ALA	C-N	5.33	1.40	1.32
1	F	244	GLY	C-N	5.33	1.40	1.33
2	H	420	ASN	N-CA	-5.33	1.39	1.46
2	S	214	TRP	CA-CB	-5.33	1.45	1.53
3	E	28	ALA	C-O	-5.32	1.18	1.24
2	I	309	ILE	CB-CG1	5.32	1.64	1.53
3	L	25	GLN	C-N	-5.32	1.27	1.33
2	R	281	ALA	C-O	5.32	1.30	1.24
2	S	246	THR	C-N	5.32	1.40	1.33
1	F	259	GLN	N-CA	-5.32	1.39	1.45
2	G	20	TYR	CA-C	-5.32	1.41	1.52
3	O	77	GLU	N-CA	-5.32	1.39	1.46
2	S	325	HIS	CA-C	-5.32	1.46	1.52
2	H	292	HIS	C-N	5.32	1.40	1.33
2	G	127	PHE	CA-CB	5.32	1.62	1.53
2	G	445	LEU	C-N	5.32	1.40	1.33
2	I	171	GLY	CA-C	5.32	1.56	1.51
2	J	144	LEU	CA-CB	-5.32	1.44	1.53
3	N	101	VAL	CA-C	-5.32	1.46	1.52
2	Q	357	ASP	CA-C	-5.32	1.47	1.53
2	R	358	ARG	N-CA	5.32	1.52	1.46
2	G	193	LEU	C-O	5.32	1.30	1.24
3	O	94	ASN	CA-CB	-5.32	1.44	1.53
2	H	173	THR	CA-CB	5.31	1.61	1.53
2	I	342	THR	CA-CB	-5.31	1.45	1.53
2	H	141	PRO	C-O	-5.31	1.17	1.23
3	K	95	ILE	N-CA	-5.31	1.40	1.46
3	M	106	HIS	CG-CD2	-5.31	1.30	1.35
3	O	20	PRO	N-CA	-5.31	1.40	1.47
2	Q	284	CYS	C-N	-5.31	1.27	1.33
3	L	96	LYS	C-O	-5.31	1.17	1.24
1	A	253	PHE	CA-C	-5.31	1.46	1.52
2	C	367	ASP	N-CA	-5.31	1.39	1.45
2	J	392	GLU	C-N	-5.31	1.27	1.33
3	P	10	ARG	CA-CB	5.31	1.62	1.53
3	D	107	ARG	CA-C	-5.31	1.47	1.52
2	G	148	PHE	C-O	5.31	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	294	HIS	CA-C	5.31	1.59	1.52
2	H	189	VAL	CA-CB	5.31	1.60	1.54
2	C	318	LEU	CA-CB	-5.31	1.45	1.53
3	L	96	LYS	N-CA	5.31	1.53	1.46
3	M	64	ASP	C-N	5.31	1.41	1.33
2	Q	214	TRP	C-N	5.31	1.40	1.33
2	Q	341	SER	CA-C	5.31	1.59	1.52
1	B	294	ASP	C-O	-5.30	1.17	1.24
2	I	224	ALA	C-O	-5.30	1.18	1.24
2	R	121	VAL	CA-CB	5.30	1.61	1.54
2	R	177	LYS	C-O	-5.30	1.17	1.24
1	B	291	LEU	C-N	5.30	1.41	1.33
2	G	422	VAL	C-O	-5.30	1.18	1.24
2	Q	263	PRO	C-O	-5.30	1.17	1.24
2	I	211	PHE	N-CA	-5.30	1.39	1.46
1	F	291	LEU	C-N	-5.30	1.28	1.33
2	G	236	LYS	CA-C	-5.30	1.45	1.53
1	T	261	CYS	C-N	5.30	1.41	1.33
2	H	31	PRO	C-O	-5.30	1.17	1.23
2	H	207	ASN	C-N	5.30	1.43	1.34
2	J	212	GLN	CA-C	5.30	1.58	1.53
2	G	75	THR	C-N	-5.29	1.26	1.33
2	S	296	ALA	CA-C	5.29	1.60	1.53
2	J	223	ASP	CA-C	5.29	1.59	1.52
2	C	146	LYS	CA-C	-5.29	1.45	1.52
3	P	100	THR	CA-C	5.29	1.60	1.52
2	R	253	ARG	N-CA	5.29	1.52	1.46
2	S	460	ASP	C-N	5.29	1.40	1.33
2	R	224	ALA	CA-C	5.29	1.59	1.52
2	C	430	ALA	C-O	-5.29	1.18	1.24
2	J	160	ASP	CA-C	-5.29	1.46	1.52
2	J	363	PHE	CA-C	5.29	1.60	1.52
2	J	235	ILE	CA-C	-5.29	1.46	1.52
2	C	167	ARG	C-N	5.29	1.39	1.33
2	G	289	VAL	C-N	-5.29	1.26	1.33
2	Q	181	SER	CA-C	-5.29	1.46	1.52
2	Q	207	ASN	N-CA	-5.29	1.40	1.46
2	C	177	LYS	CA-C	5.28	1.59	1.52
2	C	327	HIS	CG-CD2	-5.28	1.30	1.35
2	I	212	GLN	C-N	5.28	1.41	1.33
2	C	137	ASP	CA-C	5.28	1.58	1.52
3	O	40	PRO	C-O	5.28	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	54	TYR	CA-C	-5.28	1.46	1.52
2	R	285	ARG	N-CA	-5.28	1.40	1.46
1	T	239	GLN	C-N	5.28	1.39	1.33
3	E	60	LEU	C-N	-5.28	1.27	1.33
2	C	113	VAL	CA-C	5.28	1.59	1.52
2	R	293	ILE	C-N	-5.28	1.26	1.33
2	C	460	ASP	CA-C	5.28	1.60	1.52
2	G	278	THR	C-N	-5.28	1.26	1.33
2	H	41	ARG	CA-C	-5.28	1.46	1.52
2	I	175	LYS	CA-CB	-5.28	1.47	1.54
3	M	101	VAL	C-O	5.28	1.29	1.24
3	N	31	GLU	C-N	5.28	1.40	1.33
2	G	180	LEU	CA-C	-5.27	1.46	1.52
2	H	83	LYS	C-O	-5.27	1.17	1.24
2	Q	71	THR	CA-C	5.27	1.60	1.52
3	L	94	ASN	C-N	5.27	1.40	1.33
2	Q	58	ALA	N-CA	5.27	1.52	1.46
2	R	263	PRO	C-O	-5.27	1.17	1.24
2	R	426	ALA	C-O	-5.27	1.18	1.24
2	I	317	CYS	CA-C	-5.27	1.46	1.52
2	J	117	LEU	N-CA	-5.27	1.40	1.46
3	O	72	LEU	CA-C	-5.27	1.45	1.52
2	R	439	ARG	N-CA	5.27	1.53	1.46
2	G	383	HIS	CG-CD2	5.27	1.41	1.35
2	Q	209	GLN	N-CA	5.27	1.53	1.46
1	A	236	LEU	C-O	5.26	1.30	1.24
2	C	138	ILE	CA-C	5.26	1.58	1.52
2	G	69	VAL	CA-C	5.26	1.58	1.52
2	J	455	LEU	C-N	-5.26	1.27	1.33
3	K	55	TRP	CA-CB	-5.26	1.45	1.54
3	O	16	SER	CA-C	5.26	1.59	1.52
2	R	32	LYS	N-CA	5.26	1.52	1.46
2	S	297	MET	SD-CE	5.26	1.92	1.79
3	D	79	ARG	NE-CZ	-5.26	1.27	1.33
2	I	50	ALA	CA-C	-5.26	1.46	1.52
2	C	37	LEU	CA-C	-5.25	1.46	1.52
2	G	50	ALA	CA-C	5.25	1.59	1.52
2	G	399	VAL	CA-CB	-5.25	1.47	1.54
3	O	47	HIS	ND1-CE1	5.25	1.37	1.32
3	P	65	CYS	C-N	-5.25	1.25	1.33
2	S	279	THR	C-N	-5.25	1.26	1.33
2	H	163	ASN	C-O	-5.25	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	99	ALA	C-O	-5.25	1.17	1.24
2	R	442	GLY	C-N	5.25	1.40	1.33
2	S	181	SER	C-O	-5.25	1.17	1.23
1	F	268	ASN	C-N	5.25	1.40	1.33
3	P	60	LEU	C-N	5.25	1.40	1.33
2	Q	137	ASP	C-O	-5.25	1.17	1.23
2	R	73	LEU	CB-CG	-5.25	1.43	1.53
2	Q	114	THR	C-O	5.25	1.30	1.24
2	G	243	THR	CA-C	5.24	1.59	1.52
2	Q	123	ASN	CA-C	5.24	1.59	1.52
2	G	187	ARG	N-CA	5.24	1.52	1.46
3	E	13	GLU	CA-C	-5.24	1.45	1.52
3	L	21	LEU	CA-C	-5.24	1.46	1.52
3	O	58	TRP	C-O	-5.24	1.15	1.23
2	R	286	ASP	CA-C	-5.24	1.45	1.52
2	S	132	SER	N-CA	-5.24	1.39	1.46
3	D	29	GLN	CA-C	5.24	1.59	1.52
2	I	419	ALA	N-CA	-5.24	1.40	1.46
3	N	101	VAL	C-O	5.24	1.29	1.24
2	G	133	LEU	C-O	5.24	1.30	1.23
2	H	294	HIS	N-CA	-5.24	1.39	1.45
2	I	247	CYS	CA-C	5.24	1.60	1.52
3	N	68	PRO	CA-CB	-5.24	1.46	1.53
2	R	283	TRP	C-N	-5.24	1.27	1.33
2	R	458	ALA	C-N	5.24	1.41	1.34
2	S	96	SER	C-O	5.24	1.30	1.23
1	B	225	LEU	C-N	5.23	1.40	1.33
2	C	293	ILE	N-CA	-5.23	1.40	1.46
2	Q	212	GLN	CA-C	-5.23	1.46	1.52
2	S	105	LEU	C-O	5.23	1.30	1.24
2	I	209	GLN	CA-C	5.23	1.58	1.53
2	I	220	PHE	C-O	-5.23	1.18	1.24
2	S	107	LEU	CA-C	5.23	1.60	1.52
1	T	229	VAL	C-N	-5.23	1.27	1.33
3	M	104	ILE	C-N	-5.23	1.27	1.33
3	N	86	TYR	CA-C	5.23	1.59	1.52
1	T	280	LEU	C-N	-5.23	1.27	1.33
2	C	347	ASP	N-CA	-5.23	1.40	1.46
3	N	33	MET	SD-CE	-5.23	1.66	1.79
2	R	187	ARG	NE-CZ	-5.23	1.27	1.33
2	Q	305	ARG	CD-NE	5.23	1.53	1.46
2	R	244	ALA	CA-C	5.23	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	262	ALA	C-N	5.22	1.40	1.33
2	I	388	PRO	CA-C	5.22	1.59	1.52
2	R	296	ALA	C-N	5.22	1.40	1.33
1	T	239	GLN	CA-C	5.22	1.60	1.52
2	I	349	MET	C-O	-5.22	1.17	1.24
2	Q	425	GLU	CA-C	5.22	1.59	1.52
2	G	371	MET	CA-C	5.22	1.58	1.52
3	L	84	ASP	C-N	-5.22	1.25	1.33
2	C	267	HIS	CG-CD2	5.22	1.41	1.35
1	F	301	VAL	N-CA	5.22	1.52	1.46
2	H	212	GLN	CD-NE2	-5.22	1.22	1.33
2	S	221	VAL	N-CA	5.22	1.52	1.46
2	I	444	ILE	C-N	-5.22	1.27	1.33
3	P	53	PHE	C-O	5.22	1.30	1.24
2	R	317	CYS	N-CA	-5.22	1.40	1.46
2	R	433	GLU	C-N	5.22	1.41	1.33
2	R	440	GLU	N-CA	-5.22	1.39	1.46
2	S	110	GLU	N-CA	-5.22	1.39	1.46
2	C	91	GLN	C-N	-5.21	1.26	1.33
2	C	217	ARG	CD-NE	-5.21	1.39	1.46
2	J	190	TYR	CA-C	-5.21	1.45	1.52
2	Q	338	ASP	CG-OD1	5.21	1.35	1.25
2	S	26	THR	CB-OG1	5.21	1.52	1.43
2	S	360	ARG	CA-C	5.21	1.60	1.52
1	T	250	LYS	C-N	-5.21	1.27	1.33
2	C	118	THR	CA-CB	5.21	1.61	1.53
2	I	72	ASP	C-O	5.21	1.30	1.24
3	M	69	GLN	C-O	-5.21	1.17	1.24
3	N	88	ARG	N-CA	-5.21	1.39	1.45
2	S	231	GLU	CA-C	-5.21	1.46	1.52
3	K	102	SER	CA-C	-5.21	1.46	1.52
2	I	402	PHE	CA-C	-5.21	1.46	1.52
3	K	38	PHE	N-CA	5.21	1.52	1.46
2	C	452	SER	N-CA	-5.21	1.40	1.46
2	G	418	THR	C-O	-5.21	1.18	1.24
3	O	36	GLN	CA-C	5.21	1.59	1.52
2	R	280	LEU	C-N	5.21	1.40	1.33
2	C	225	ILE	N-CA	-5.20	1.40	1.46
2	G	250	MET	CA-C	5.20	1.59	1.52
3	N	79	ARG	N-CA	5.20	1.52	1.46
3	D	47	HIS	CA-C	5.20	1.60	1.53
3	D	84	ASP	CA-CB	-5.20	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	30	ILE	CB-CG1	5.20	1.63	1.53
2	Q	389	ALA	C-O	-5.20	1.18	1.24
3	L	13	GLU	C-O	-5.20	1.18	1.24
2	R	134	ARG	C-O	5.20	1.30	1.23
2	S	385	TRP	CA-C	5.20	1.59	1.52
2	J	202	ASP	C-O	5.20	1.30	1.23
2	R	277	ASN	C-N	-5.20	1.26	1.33
2	C	239	TYR	N-CA	-5.20	1.40	1.46
2	I	389	ALA	C-N	5.20	1.41	1.33
3	M	57	MET	CA-C	-5.20	1.46	1.52
2	R	87	ILE	C-N	5.19	1.40	1.33
2	C	305	ARG	CA-C	5.19	1.59	1.52
2	H	245	PRO	CA-C	-5.19	1.44	1.52
2	J	105	LEU	CB-CG	-5.19	1.43	1.53
2	J	444	ILE	CA-CB	5.19	1.60	1.54
3	M	17	TYR	CA-C	5.19	1.59	1.52
3	O	107	ARG	C-O	-5.19	1.17	1.24
2	C	430	ALA	CA-C	-5.19	1.46	1.52
3	O	11	ARG	CA-C	5.19	1.59	1.52
2	R	220	PHE	CA-C	-5.19	1.46	1.52
2	S	442	GLY	C-N	-5.19	1.27	1.33
2	C	72	ASP	CA-CB	-5.19	1.45	1.53
2	J	240	LEU	CG-CD1	-5.19	1.35	1.52
2	J	359	SER	CA-C	-5.19	1.45	1.52
3	K	34	ILE	CB-CG1	5.19	1.63	1.53
1	T	259	GLN	C-O	-5.19	1.17	1.24
3	E	94	ASN	CA-CB	-5.19	1.44	1.53
3	P	54	TYR	CA-C	5.19	1.59	1.52
2	I	87	ILE	C-N	5.18	1.38	1.33
3	L	86	TYR	N-CA	5.18	1.52	1.45
3	M	75	VAL	C-N	-5.18	1.27	1.33
2	R	159	ARG	N-CA	-5.18	1.40	1.46
2	G	156	GLN	CA-C	-5.18	1.46	1.52
2	G	205	ASN	C-O	-5.18	1.17	1.24
2	G	240	LEU	CA-CB	-5.18	1.45	1.53
3	M	40	PRO	C-N	5.18	1.41	1.33
2	C	130	ILE	CA-CB	5.18	1.60	1.54
2	J	71	THR	N-CA	-5.18	1.39	1.46
3	K	15	PHE	N-CA	-5.18	1.39	1.46
2	G	287	ASN	CG-ND2	-5.18	1.22	1.33
2	I	443	ASP	CA-C	5.18	1.59	1.52
2	J	113	VAL	CA-C	-5.18	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	270	LEU	C-O	5.18	1.30	1.24
2	J	443	ASP	C-N	-5.18	1.27	1.33
2	R	358	ARG	C-N	5.18	1.40	1.33
2	C	435	ARG	CD-NE	-5.18	1.39	1.46
2	G	206	ILE	CA-CB	5.18	1.59	1.53
2	R	22	LEU	CA-C	5.18	1.59	1.52
2	G	207	ASN	CG-ND2	5.18	1.44	1.33
2	Q	126	GLY	N-CA	5.18	1.51	1.45
2	R	459	LEU	C-O	5.18	1.30	1.24
1	B	229	VAL	C-N	-5.17	1.27	1.33
2	C	382	ILE	C-N	5.17	1.41	1.33
2	G	267	HIS	CE1-NE2	-5.17	1.27	1.32
2	G	320	LEU	C-N	-5.17	1.27	1.33
2	G	420	ASN	N-CA	-5.17	1.40	1.46
2	H	357	ASP	CA-C	-5.17	1.48	1.53
2	I	216	ASP	CA-C	5.17	1.59	1.52
2	S	423	ALA	C-N	5.17	1.40	1.33
2	C	394	PHE	CA-C	-5.17	1.45	1.52
2	G	244	ALA	CA-C	-5.17	1.46	1.52
1	A	247	HIS	N-CA	-5.17	1.39	1.45
2	G	190	TYR	CA-C	-5.17	1.45	1.52
2	G	235	ILE	CA-C	-5.17	1.46	1.52
2	I	183	LYS	CA-CB	5.17	1.61	1.53
2	R	160	ASP	N-CA	-5.17	1.40	1.46
2	R	278	THR	N-CA	5.17	1.52	1.46
1	T	306	ILE	CA-CB	-5.17	1.48	1.54
2	C	341	SER	C-O	-5.16	1.18	1.24
2	J	203	ASP	C-O	5.16	1.30	1.23
2	R	271	THR	CA-C	5.16	1.59	1.52
1	B	299	SER	CA-C	-5.16	1.46	1.52
2	R	170	LEU	N-CA	-5.16	1.39	1.46
2	S	46	PRO	N-CA	5.16	1.53	1.47
2	H	235	ILE	CA-CB	5.16	1.61	1.54
2	S	437	LEU	CA-CB	-5.16	1.45	1.53
3	E	44	PHE	CA-CB	5.16	1.62	1.53
2	I	92	GLY	C-N	5.16	1.40	1.33
2	S	158	GLU	C-N	-5.16	1.27	1.34
2	S	316	LYS	CA-CB	5.16	1.61	1.53
1	A	229	VAL	N-CA	5.15	1.52	1.46
1	A	286	GLU	C-N	5.15	1.40	1.33
3	K	15	PHE	C-N	5.15	1.40	1.34
2	Q	86	HIS	CB-CG	-5.15	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	307	HIS	C-O	5.15	1.29	1.23
3	K	16	SER	CA-C	-5.15	1.45	1.52
3	M	24	ARG	CD-NE	5.15	1.53	1.46
3	N	107	ARG	CA-C	5.15	1.57	1.52
3	P	46	GLU	N-CA	-5.15	1.39	1.46
2	R	346	VAL	C-O	5.15	1.30	1.24
2	H	400	LEU	CB-CG	-5.15	1.43	1.53
2	R	355	GLU	CA-C	-5.15	1.46	1.52
2	I	101	ILE	CA-CB	5.15	1.61	1.54
2	I	129	ALA	CA-C	-5.15	1.45	1.52
2	R	340	ALA	C-O	-5.15	1.18	1.24
2	I	103	TYR	C-N	-5.15	1.26	1.33
2	G	351	GLU	C-N	-5.14	1.26	1.33
2	I	194	ARG	NE-CZ	-5.14	1.27	1.33
2	I	340	ALA	N-CA	-5.14	1.40	1.46
2	C	59	ALA	CA-C	-5.14	1.46	1.52
2	G	321	SER	CA-C	5.14	1.59	1.52
2	J	93	GLU	C-N	5.14	1.41	1.33
2	C	425	GLU	C-O	-5.14	1.18	1.24
2	G	352	ASP	CA-CB	5.14	1.61	1.53
2	I	338	ASP	CG-OD1	5.14	1.35	1.25
2	I	432	ASN	N-CA	-5.14	1.40	1.46
3	L	45	ASN	C-N	-5.14	1.27	1.33
3	O	86	TYR	CA-C	-5.14	1.46	1.52
2	R	416	GLY	CA-C	5.14	1.57	1.52
2	G	427	CYS	CA-C	-5.14	1.46	1.52
2	H	33	ASP	N-CA	-5.14	1.40	1.46
2	R	453	PRO	C-N	5.14	1.41	1.33
2	S	357	ASP	CA-C	-5.14	1.47	1.53
3	D	79	ARG	CA-CB	5.13	1.61	1.53
2	G	52	GLU	C-N	-5.13	1.27	1.33
3	P	79	ARG	CA-C	5.13	1.59	1.52
2	S	181	SER	C-N	-5.13	1.27	1.33
2	H	422	VAL	CA-C	-5.13	1.46	1.52
2	Q	76	ASP	C-O	-5.13	1.17	1.23
2	S	130	ILE	CA-C	-5.13	1.46	1.52
2	I	147	THR	CA-C	5.13	1.61	1.52
2	J	441	GLY	C-O	5.13	1.30	1.23
2	H	238	HIS	C-N	5.13	1.40	1.33
2	C	136	GLU	C-N	5.13	1.39	1.33
2	C	149	GLN	C-N	5.13	1.41	1.33
2	I	374	VAL	CA-C	5.13	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	303	ARG	N-CA	-5.13	1.40	1.46
2	C	319	ARG	CD-NE	5.13	1.53	1.46
2	G	154	GLY	N-CA	5.13	1.50	1.45
2	G	293	ILE	C-O	-5.13	1.18	1.24
2	I	229	GLN	CA-C	-5.13	1.45	1.52
3	M	39	HIS	CA-C	5.13	1.59	1.52
2	S	55	ALA	C-O	-5.13	1.18	1.24
1	T	249	ASP	C-N	-5.13	1.27	1.33
3	L	53	PHE	C-O	5.12	1.30	1.24
1	B	227	SER	C-O	-5.12	1.18	1.24
1	F	264	ILE	CA-C	-5.12	1.47	1.53
2	I	383	HIS	CA-CB	5.12	1.61	1.53
2	J	168	PRO	C-O	-5.12	1.17	1.24
3	L	13	GLU	CA-C	-5.12	1.46	1.52
2	I	53	ALA	CA-C	5.12	1.59	1.52
2	I	57	ILE	C-N	-5.12	1.27	1.33
2	I	156	GLN	C-O	-5.12	1.18	1.24
2	Q	242	VAL	C-N	5.12	1.40	1.33
2	Q	438	TYR	C-N	-5.12	1.27	1.33
2	H	26	THR	CA-CB	-5.12	1.47	1.53
2	H	325	HIS	CE1-NE2	-5.12	1.27	1.32
3	M	74	GLU	C-N	5.12	1.40	1.33
2	G	175	LYS	CA-C	-5.12	1.46	1.52
2	I	249	GLU	CA-C	-5.12	1.45	1.52
3	M	72	LEU	CA-C	-5.12	1.46	1.52
2	R	184	ASN	CA-C	-5.12	1.46	1.52
2	S	362	VAL	CA-CB	5.12	1.59	1.53
2	S	431	ARG	CA-C	-5.12	1.46	1.52
3	E	93	ASP	CA-CB	-5.12	1.46	1.52
2	G	391	VAL	C-N	-5.12	1.27	1.33
2	J	213	ARG	C-N	5.12	1.40	1.33
2	Q	187	ARG	CA-CB	5.12	1.61	1.53
2	R	120	ILE	C-N	5.12	1.40	1.33
2	G	319	ARG	CA-CB	5.11	1.61	1.53
2	H	48	VAL	CA-CB	-5.11	1.47	1.54
2	H	59	ALA	C-O	-5.11	1.18	1.24
2	H	362	VAL	C-N	-5.11	1.26	1.33
2	Q	121	VAL	C-N	5.11	1.40	1.33
2	Q	168	PRO	N-CA	5.11	1.52	1.47
2	R	298	HIS	N-CA	5.11	1.52	1.46
2	G	229	GLN	N-CA	-5.11	1.40	1.46
2	S	134	ARG	CA-CB	5.11	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	250	LYS	C-O	-5.11	1.18	1.24
2	C	21	LYS	C-O	-5.11	1.18	1.24
2	G	293	ILE	N-CA	-5.11	1.40	1.46
2	J	34	THR	CA-C	5.11	1.59	1.52
3	L	32	TYR	CA-C	5.11	1.59	1.52
2	Q	401	GLN	CA-C	5.11	1.58	1.52
2	S	108	PHE	C-N	5.11	1.40	1.33
2	C	166	GLY	C-O	-5.11	1.17	1.23
2	G	119	SER	C-O	5.11	1.30	1.24
3	M	63	PHE	C-N	5.11	1.40	1.33
3	P	89	VAL	N-CA	-5.11	1.40	1.46
1	T	244	GLY	N-CA	-5.11	1.39	1.45
2	J	318	LEU	CA-C	-5.11	1.46	1.52
3	M	93	ASP	N-CA	-5.11	1.39	1.46
3	O	10	ARG	C-O	-5.11	1.17	1.23
2	Q	83	LYS	CA-CB	-5.11	1.46	1.53
2	R	367	ASP	C-N	-5.11	1.26	1.33
2	C	249	GLU	CA-C	-5.11	1.46	1.52
2	J	35	ASP	C-N	5.11	1.40	1.33
2	Q	444	ILE	CB-CG1	5.11	1.63	1.53
2	S	153	HIS	CG-ND1	-5.11	1.32	1.38
3	D	88	ARG	CA-C	-5.10	1.46	1.52
2	H	299	ALA	C-O	-5.10	1.17	1.24
2	H	307	HIS	ND1-CE1	-5.10	1.27	1.32
2	I	313	VAL	C-N	-5.10	1.27	1.33
3	P	94	ASN	C-N	-5.10	1.27	1.33
2	Q	267	HIS	CA-C	5.10	1.58	1.52
2	R	134	ARG	C-N	-5.10	1.26	1.33
2	R	148	PHE	C-O	-5.10	1.17	1.23
2	S	106	ASP	CA-C	5.10	1.59	1.52
3	E	94	ASN	N-CA	-5.10	1.40	1.46
2	J	330	THR	C-N	-5.10	1.26	1.33
3	M	13	GLU	C-O	-5.10	1.18	1.24
2	C	299	ALA	CA-C	-5.10	1.45	1.52
2	G	283	TRP	C-O	-5.10	1.18	1.24
2	I	109	GLU	C-O	-5.10	1.17	1.23
2	G	245	PRO	CA-CB	-5.10	1.46	1.53
2	I	58	ALA	C-N	-5.10	1.27	1.33
3	K	24	ARG	CA-C	5.10	1.59	1.52
3	L	35	GLU	N-CA	-5.10	1.39	1.46
2	S	24	TYR	N-CA	5.10	1.52	1.46
2	S	327	HIS	CD2-NE2	5.10	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	435	ARG	CA-CB	5.10	1.61	1.53
2	G	48	VAL	CA-C	5.10	1.57	1.53
1	A	267	THR	CA-C	5.09	1.59	1.52
2	H	184	ASN	C-N	-5.09	1.26	1.33
3	M	30	ILE	CA-CB	-5.09	1.48	1.54
2	C	59	ALA	C-O	-5.09	1.18	1.24
2	G	449	GLY	C-N	5.09	1.40	1.34
2	I	152	PRO	C-N	5.09	1.42	1.33
2	I	423	ALA	CA-C	-5.09	1.46	1.52
3	K	32	TYR	N-CA	5.09	1.52	1.46
1	T	302	PHE	N-CA	-5.09	1.39	1.45
3	D	80	SER	C-N	5.09	1.41	1.33
2	G	222	ALA	C-N	-5.09	1.27	1.33
2	H	453	PRO	N-CA	5.09	1.54	1.47
2	I	432	ASN	C-N	5.09	1.41	1.33
2	J	295	ARG	CD-NE	5.09	1.53	1.46
3	N	102	SER	CA-C	5.09	1.58	1.52
2	S	209	GLN	CD-NE2	-5.09	1.22	1.33
3	O	96	LYS	N-CA	-5.09	1.39	1.46
2	C	169	MET	SD-CE	5.09	1.92	1.79
2	C	423	ALA	CA-C	-5.09	1.46	1.52
2	C	454	GLU	CA-CB	-5.09	1.45	1.53
2	G	217	ARG	CA-C	-5.09	1.46	1.52
3	K	13	GLU	CA-C	-5.09	1.46	1.52
2	C	226	HIS	N-CA	-5.08	1.40	1.46
3	M	99	GLN	CA-C	-5.08	1.46	1.52
3	D	56	THR	C-O	-5.08	1.18	1.23
2	I	453	PRO	CA-C	-5.08	1.45	1.52
2	G	235	ILE	CB-CG1	5.08	1.63	1.53
2	I	316	LYS	C-O	-5.08	1.18	1.24
2	J	265	ILE	C-N	5.08	1.40	1.33
2	Q	57	ILE	CA-CB	5.08	1.60	1.54
3	E	66	LYS	C-N	5.08	1.39	1.33
2	H	434	GLY	C-N	-5.08	1.26	1.33
2	S	384	VAL	C-O	-5.08	1.18	1.24
2	I	285	ARG	CA-C	5.08	1.59	1.52
2	I	387	MET	CA-C	5.08	1.59	1.52
2	J	400	LEU	C-O	-5.08	1.17	1.23
2	Q	84	CYS	CA-C	-5.08	1.46	1.52
2	H	129	ALA	CA-CB	-5.07	1.45	1.53
2	I	254	ALA	C-O	5.07	1.30	1.24
3	K	9	GLU	C-N	5.07	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	372	PRO	C-N	5.07	1.40	1.33
2	I	29	TYR	CA-C	-5.07	1.46	1.52
2	S	123	ASN	C-O	-5.07	1.17	1.24
2	G	184	ASN	CA-C	5.07	1.59	1.52
2	G	428	VAL	CA-C	-5.07	1.46	1.52
2	H	163	ASN	CA-C	5.07	1.60	1.53
2	I	146	LYS	C-O	5.07	1.30	1.24
2	I	213	ARG	CA-C	5.07	1.59	1.52
3	L	31	GLU	C-O	-5.07	1.18	1.24
3	L	104	ILE	C-N	5.07	1.38	1.33
2	Q	340	ALA	CA-C	5.07	1.59	1.52
1	A	277	GLU	N-CA	-5.06	1.40	1.46
2	C	168	PRO	N-CA	-5.06	1.41	1.47
2	I	378	ALA	CA-CB	-5.06	1.45	1.53
3	N	92	PHE	N-CA	-5.06	1.40	1.46
2	R	48	VAL	C-O	5.06	1.31	1.24
2	S	371	MET	SD-CE	-5.06	1.66	1.79
2	J	265	ILE	CA-C	-5.06	1.46	1.52
2	R	108	PHE	C-O	-5.06	1.17	1.24
2	I	118	THR	CA-C	5.06	1.59	1.52
3	P	40	PRO	CA-C	5.06	1.58	1.52
2	Q	253	ARG	CA-CB	-5.06	1.45	1.53
2	C	198	ASP	C-N	5.06	1.40	1.33
3	D	83	GLY	C-N	5.06	1.40	1.33
2	G	302	ASP	CA-C	-5.06	1.45	1.52
2	R	436	ASP	CA-CB	-5.06	1.45	1.53
2	S	43	SER	C-N	-5.06	1.27	1.33
3	E	86	TYR	CA-C	-5.06	1.45	1.53
2	Q	171	GLY	C-O	-5.06	1.17	1.23
2	R	398	SER	N-CA	-5.06	1.40	1.46
2	S	58	ALA	CA-C	-5.06	1.46	1.52
2	C	134	ARG	N-CA	-5.05	1.39	1.45
2	H	260	LEU	CA-C	-5.05	1.45	1.52
2	C	87	ILE	C-O	-5.05	1.18	1.24
2	I	372	PRO	CA-CB	5.05	1.60	1.53
2	S	33	ASP	CA-CB	-5.05	1.44	1.53
2	C	86	HIS	ND1-CE1	-5.05	1.27	1.32
2	H	202	ASP	CA-C	-5.05	1.46	1.53
2	H	380	GLY	C-N	5.05	1.40	1.33
2	I	53	ALA	N-CA	-5.05	1.40	1.46
2	Q	132	SER	CA-C	-5.05	1.47	1.53
2	R	37	LEU	C-O	-5.05	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	GLN	C-O	5.05	1.29	1.23
2	C	359	SER	C-O	5.05	1.29	1.24
2	J	318	LEU	C-N	-5.05	1.27	1.33
3	L	80	SER	CA-C	-5.05	1.45	1.52
2	S	450	LYS	CA-CB	5.05	1.61	1.53
2	C	100	PHE	C-N	5.04	1.40	1.33
2	H	264	ILE	CA-C	5.04	1.58	1.52
2	H	285	ARG	C-O	-5.04	1.18	1.24
2	J	419	ALA	CA-CB	-5.04	1.45	1.53
2	S	170	LEU	C-N	-5.04	1.26	1.33
2	C	206	ILE	CB-CG1	-5.04	1.43	1.53
2	C	321	SER	CA-C	5.04	1.59	1.52
2	H	342	THR	N-CA	-5.04	1.40	1.46
2	J	325	HIS	CE1-NE2	-5.04	1.27	1.32
2	R	78	ASP	N-CA	5.04	1.52	1.46
2	R	278	THR	C-N	5.04	1.40	1.33
3	D	21	LEU	C-N	5.04	1.40	1.33
2	G	260	LEU	N-CA	5.04	1.52	1.46
2	G	214	TRP	CA-C	5.04	1.59	1.52
2	G	286	ASP	C-N	5.04	1.40	1.33
2	J	161	LEU	CA-C	-5.04	1.46	1.52
2	J	258	LYS	C-O	-5.04	1.17	1.24
2	Q	425	GLU	C-N	5.04	1.40	1.33
1	B	307	GLN	C-N	-5.04	1.26	1.32
2	G	310	HIS	C-O	5.04	1.30	1.23
1	F	233	VAL	N-CA	-5.03	1.40	1.46
2	I	363	PHE	C-O	5.03	1.30	1.24
3	P	9	GLU	N-CA	-5.03	1.40	1.46
2	G	445	LEU	CB-CG	5.03	1.63	1.53
2	H	347	ASP	C-N	-5.03	1.27	1.34
2	H	356	ALA	CA-CB	-5.03	1.45	1.53
2	S	452	SER	N-CA	-5.03	1.41	1.46
3	E	67	SER	N-CA	-5.03	1.39	1.45
2	S	80	TYR	CA-CB	-5.03	1.46	1.53
2	J	326	LEU	CA-C	-5.03	1.46	1.52
2	G	277	ASN	CA-C	-5.03	1.46	1.52
2	H	74	LEU	C-N	5.03	1.41	1.33
3	M	22	SER	C-N	5.03	1.40	1.33
1	B	266	SER	CA-C	-5.02	1.46	1.52
1	F	301	VAL	CA-CB	5.02	1.60	1.54
1	F	304	ALA	N-CA	-5.02	1.40	1.46
2	H	37	LEU	CA-C	-5.02	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	182	ALA	CA-C	5.02	1.59	1.52
2	Q	165	TYR	CA-C	-5.02	1.46	1.52
3	L	31	GLU	CA-CB	-5.02	1.45	1.53
3	N	65	CYS	CA-C	5.02	1.59	1.52
2	Q	30	THR	N-CA	-5.02	1.40	1.46
2	S	306	ASN	C-O	-5.02	1.17	1.23
3	D	91	GLY	C-N	5.02	1.40	1.33
2	G	325	HIS	CA-CB	-5.02	1.45	1.54
2	I	387	MET	N-CA	5.02	1.51	1.46
2	I	86	HIS	CB-CG	-5.02	1.43	1.50
2	H	347	ASP	CG-OD1	-5.01	1.15	1.25
2	J	284	CYS	C-O	-5.01	1.18	1.24
3	M	25	GLN	C-O	-5.01	1.17	1.24
2	Q	401	GLN	C-O	5.01	1.29	1.23
2	R	327	HIS	ND1-CE1	-5.01	1.27	1.32
3	D	56	THR	CA-C	5.01	1.59	1.53
2	C	379	SER	CA-C	5.01	1.59	1.53
2	C	437	LEU	CA-CB	-5.01	1.45	1.53
2	H	212	GLN	N-CA	-5.01	1.40	1.46
2	J	329	GLY	C-O	-5.01	1.17	1.23
2	J	436	ASP	C-O	-5.01	1.17	1.24
2	R	365	THR	CA-C	-5.01	1.46	1.52
2	G	61	SER	C-N	5.01	1.40	1.33
3	L	24	ARG	CD-NE	5.01	1.53	1.46
3	O	72	LEU	CB-CG	-5.01	1.43	1.53
2	R	22	LEU	C-N	5.01	1.40	1.33
2	R	317	CYS	C-O	5.01	1.29	1.24
2	Q	258	LYS	CA-CB	-5.01	1.45	1.53
2	Q	391	VAL	C-N	-5.01	1.27	1.33
2	Q	441	GLY	C-O	-5.01	1.17	1.23
3	E	57	MET	CA-C	-5.00	1.46	1.52
3	E	33	MET	SD-CE	-5.00	1.67	1.79
2	J	310	HIS	CA-C	-5.00	1.46	1.52
2	S	327	HIS	CG-ND1	-5.00	1.32	1.38
2	C	160	ASP	C-O	-5.00	1.18	1.24
2	J	422	VAL	C-N	-5.00	1.27	1.34
3	L	45	ASN	CA-CB	5.00	1.62	1.53
3	L	70	GLN	C-O	-5.00	1.18	1.24
3	N	24	ARG	N-CA	-5.00	1.40	1.46

All (2018) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	151	PRO	CA-C-O	-13.89	109.75	120.73
2	I	444	ILE	N-CA-C	-11.46	99.42	110.42
2	G	86	HIS	CE1-NE2-CD2	-11.22	97.78	109.00
2	C	253	ARG	N-CA-C	-11.13	99.12	111.14
1	B	228	GLU	N-CA-C	-11.10	99.26	111.36
2	J	256	PHE	N-CA-C	-11.01	99.35	111.36
2	R	157	VAL	N-CA-C	-10.98	99.63	110.72
3	L	19	PRO	O-C-N	10.80	126.28	121.31
2	C	151	PRO	O-C-N	10.79	126.22	121.15
3	L	97	GLN	OE1-CD-NE2	-10.78	111.82	122.60
2	R	229	GLN	OE1-CD-NE2	-10.75	111.85	122.60
1	B	271	GLN	OE1-CD-NE2	-10.73	111.87	122.60
2	J	212	GLN	OE1-CD-NE2	-10.69	111.92	122.60
3	O	92	PHE	CA-CB-CG	-10.68	103.12	113.80
2	Q	52	GLU	N-CA-C	-10.65	99.75	111.36
2	J	394	PHE	CA-CB-CG	10.65	124.45	113.80
2	J	185	TYR	N-CA-C	-10.63	99.66	111.14
3	D	12	PHE	CA-CB-CG	-10.51	103.29	113.80
2	C	184	ASN	OD1-CG-ND2	-10.49	112.11	122.60
3	O	97	GLN	OE1-CD-NE2	-10.47	112.13	122.60
2	S	106	ASP	N-CA-C	-10.37	100.63	113.18
1	A	236	LEU	N-CA-C	10.32	122.11	111.07
3	L	45	ASN	OD1-CG-ND2	-10.26	112.34	122.60
2	Q	116	ILE	N-CA-C	-10.25	100.79	110.42
2	I	231	GLU	N-CA-C	10.18	121.96	111.07
2	J	270	LEU	N-CA-C	10.11	121.89	111.07
2	H	432	ASN	OD1-CG-ND2	-10.07	112.53	122.60
1	F	228	GLU	N-CA-C	-10.07	100.39	111.36
3	D	97	GLN	OE1-CD-NE2	-10.00	112.60	122.60
3	E	70	GLN	N-CA-C	-9.99	100.47	111.36
2	H	277	ASN	CA-CB-CG	9.99	122.59	112.60
2	G	185	TYR	N-CA-C	-9.97	99.24	111.40
2	H	198	ASP	N-CA-C	-9.96	100.50	111.36
2	C	401	GLN	OE1-CD-NE2	-9.96	112.64	122.60
2	H	363	PHE	CA-CB-CG	-9.94	103.86	113.80
2	H	352	ASP	N-CA-C	-9.94	100.80	113.72
3	M	19	PRO	O-C-N	9.91	125.87	121.31
2	J	116	ILE	N-CA-C	-9.91	100.72	110.72
2	R	298	HIS	N-CA-C	-9.87	100.60	111.36
3	L	47	HIS	CE1-NE2-CD2	-9.85	99.16	109.00
2	R	343	LEU	N-CA-C	-9.82	99.61	111.69
2	C	256	PHE	N-CA-C	9.81	122.89	111.11
3	M	19	PRO	CA-C-O	-9.81	113.84	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	294	HIS	CE1-NE2-CD2	-9.81	99.19	109.00
2	H	185	TYR	N-CA-C	-9.79	99.65	111.69
3	N	99	GLN	OE1-CD-NE2	-9.78	112.82	122.60
3	K	26	ILE	N-CA-C	-9.78	100.65	110.62
3	L	31	GLU	N-CA-C	-9.74	100.64	111.07
2	H	217	ARG	N-CA-C	9.70	123.06	111.33
3	N	53	PHE	CA-CB-CG	-9.68	104.12	113.80
2	S	163	ASN	OD1-CG-ND2	-9.68	112.92	122.60
2	I	42	PHE	CA-CB-CG	-9.64	104.16	113.80
2	S	294	HIS	CG-CD2-NE2	9.64	116.84	107.20
2	G	292	HIS	CB-CG-CD2	-9.62	118.69	131.20
2	Q	432	ASN	OD1-CG-ND2	-9.60	113.00	122.60
1	A	239	GLN	OE1-CD-NE2	-9.59	113.01	122.60
2	G	45	GLN	OE1-CD-NE2	-9.58	113.02	122.60
3	D	99	GLN	OE1-CD-NE2	-9.53	113.07	122.60
2	H	229	GLN	OE1-CD-NE2	-9.53	113.07	122.60
3	O	63	PHE	N-CA-C	-9.53	99.97	111.69
2	C	302	ASP	CA-CB-CG	9.49	122.09	112.60
3	E	18	LEU	N-CA-C	-9.47	99.24	110.13
3	M	13	GLU	CA-C-O	-9.46	110.78	120.90
2	C	277	ASN	OD1-CG-ND2	-9.44	113.16	122.60
2	R	209	GLN	OE1-CD-NE2	9.39	132.00	122.60
2	S	238	HIS	CB-CG-CD2	-9.39	118.99	131.20
2	J	202	ASP	CA-CB-CG	9.39	121.99	112.60
2	H	160	ASP	N-CA-C	9.37	121.10	111.07
2	R	324	ASP	CA-CB-CG	9.37	121.97	112.60
2	I	115	ASN	OD1-CG-ND2	-9.36	113.24	122.60
2	I	417	ALA	N-CA-C	-9.36	101.04	111.14
2	J	248	GLU	N-CA-C	-9.34	101.06	111.14
2	G	348	LEU	N-CA-C	9.31	121.43	111.28
2	Q	294	HIS	CG-CD2-NE2	9.31	116.51	107.20
2	C	425	GLU	N-CA-C	9.30	122.37	111.02
2	I	59	ALA	CA-C-O	-9.30	111.05	120.82
2	S	118	THR	N-CA-C	-9.30	101.15	111.28
2	R	161	LEU	N-CA-C	9.29	122.25	111.11
2	H	58	ALA	N-CA-C	9.28	122.24	111.11
2	R	216	ASP	N-CA-C	-9.26	101.27	111.36
2	S	256	PHE	N-CA-C	-9.26	101.08	111.82
2	C	86	HIS	CE1-NE2-CD2	-9.25	99.75	109.00
2	H	428	VAL	N-CA-C	-9.23	101.35	110.30
3	L	19	PRO	CA-C-O	-9.22	114.26	120.90
2	G	205	ASN	N-CA-C	-9.21	101.30	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	238	HIS	CB-CG-CD2	-9.19	119.25	131.20
2	Q	345	PHE	CA-CB-CG	9.19	122.99	113.80
2	I	103	TYR	CA-C-O	-9.18	112.43	119.59
2	G	394	PHE	N-CA-C	9.17	123.07	111.24
2	G	432	ASN	CA-CB-CG	9.16	121.76	112.60
2	G	256	PHE	N-CA-C	-9.15	100.70	112.23
2	H	417	ALA	N-CA-C	-9.13	101.28	111.14
2	J	427	CYS	N-CA-C	9.12	120.83	111.07
3	O	54	TYR	CA-C-O	-9.12	110.86	121.16
2	S	268	ASP	N-CA-C	9.11	122.27	109.15
2	C	220	PHE	N-CA-C	9.10	120.81	111.07
2	I	217	ARG	N-CA-C	-9.10	101.33	111.07
2	H	287	ASN	OD1-CG-ND2	-9.10	113.50	122.60
3	O	63	PHE	CA-CB-CG	-9.07	104.73	113.80
2	S	306	ASN	OD1-CG-ND2	-9.07	113.53	122.60
3	D	69	GLN	N-CA-C	9.06	122.33	111.82
2	R	77	MET	N-CA-C	-9.05	100.25	111.11
2	H	420	ASN	N-CA-C	-9.05	101.50	111.36
3	L	47	HIS	ND1-CE1-NE2	9.04	117.44	108.40
2	R	121	VAL	CA-C-N	9.04	129.97	119.94
2	R	121	VAL	C-N-CA	9.04	129.97	119.94
2	Q	298	HIS	N-CA-C	-9.03	101.52	111.36
2	I	98	PHE	CA-CB-CG	-9.01	104.79	113.80
2	I	223	ASP	N-CA-C	-9.01	101.55	111.36
3	K	25	GLN	OE1-CD-NE2	-8.98	113.62	122.60
1	F	253	PHE	N-CA-C	8.97	121.06	111.28
2	H	226	HIS	CE1-NE2-CD2	-8.96	100.04	109.00
2	H	95	ASN	OD1-CG-ND2	-8.95	113.65	122.60
2	Q	142	VAL	N-CA-C	8.94	119.75	110.36
2	J	438	TYR	N-CA-C	8.92	121.90	111.02
3	L	49	ASN	OD1-CG-ND2	-8.91	113.69	122.60
2	S	185	TYR	N-CA-C	-8.91	99.21	112.04
2	S	438	TYR	N-CA-C	8.90	121.79	111.11
2	C	277	ASN	N-CA-C	8.88	120.58	111.07
2	H	347	ASP	N-CA-C	8.87	122.06	111.33
2	C	342	THR	N-CA-C	-8.87	101.58	111.07
2	S	216	ASP	N-CA-C	-8.85	100.81	111.69
2	H	193	LEU	N-CA-C	8.84	120.53	111.07
2	C	327	HIS	CE1-NE2-CD2	-8.83	100.17	109.00
2	Q	127	PHE	CA-CB-CG	-8.83	104.97	113.80
2	S	51	ASP	N-CA-C	8.81	120.88	111.28
3	M	29	GLN	OE1-CD-NE2	-8.81	113.79	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	437	LEU	N-CA-C	8.79	120.86	111.28
2	Q	187	ARG	N-CA-C	-8.77	100.70	111.40
2	Q	277	ASN	N-CA-C	-8.77	101.80	111.36
2	I	212	GLN	OE1-CD-NE2	-8.76	113.84	122.60
2	I	35	ASP	N-CA-C	8.74	122.07	110.53
2	J	53	ALA	N-CA-C	-8.72	101.47	110.97
2	H	367	ASP	CA-CB-CG	8.71	121.31	112.60
2	S	447	GLU	N-CA-C	-8.71	101.86	111.36
2	R	226	HIS	CE1-NE2-CD2	-8.71	100.29	109.00
2	J	189	VAL	N-CA-C	8.70	119.50	110.36
3	K	16	SER	N-CA-C	8.69	121.71	111.71
2	S	348	LEU	N-CA-C	-8.69	100.03	111.24
2	H	276	ALA	N-CA-C	8.68	120.36	111.07
2	J	215	ARG	N-CA-C	-8.67	101.78	111.14
2	G	347	ASP	N-CA-C	-8.66	101.77	111.82
2	S	229	GLN	OE1-CD-NE2	-8.66	113.94	122.60
1	B	304	ALA	N-CA-C	8.66	122.52	108.32
2	S	254	ALA	N-CA-C	8.65	121.49	111.11
3	M	94	ASN	OD1-CG-ND2	-8.64	113.96	122.60
2	G	353	HIS	CB-CG-CD2	-8.64	119.97	131.20
2	I	225	ILE	N-CA-C	-8.59	101.86	110.62
3	P	47	HIS	CB-CG-CD2	-8.59	120.04	131.20
2	G	95	ASN	OD1-CG-ND2	-8.58	114.02	122.60
2	R	277	ASN	OD1-CG-ND2	-8.55	114.05	122.60
2	H	59	ALA	N-CA-C	8.55	120.29	110.97
2	J	393	ILE	N-CA-C	8.55	118.57	110.53
2	J	287	ASN	CA-CB-CG	8.54	121.14	112.60
2	I	444	ILE	CA-C-O	-8.54	112.12	121.17
2	J	269	PHE	N-CA-C	8.53	121.65	111.33
2	R	167	ARG	N-CA-C	8.53	115.80	108.13
1	T	251	ARG	CA-C-O	-8.53	111.78	120.90
2	S	304	GLN	OE1-CD-NE2	-8.52	114.08	122.60
2	G	86	HIS	ND1-CE1-NE2	8.51	116.91	108.40
1	F	271	GLN	OE1-CD-NE2	-8.49	114.11	122.60
2	J	271	THR	N-CA-C	-8.49	102.51	113.12
2	I	63	THR	CB-CA-C	8.48	122.37	109.13
2	G	437	LEU	N-CA-C	8.45	120.48	111.28
2	H	303	ARG	N-CA-C	8.44	120.10	111.07
2	C	197	LEU	N-CA-C	8.44	122.14	110.24
2	S	454	GLU	N-CA-C	-8.43	101.32	111.69
2	H	391	VAL	N-CA-C	-8.41	100.48	112.35
2	S	242	VAL	CA-C-O	-8.41	112.06	119.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	268	ASP	N-CA-C	8.41	122.33	108.96
3	E	67	SER	CA-C-O	-8.41	111.62	120.28
3	E	32	TYR	N-CA-C	-8.39	102.09	111.07
2	Q	305	ARG	N-CA-C	8.39	120.43	111.28
1	F	232	GLN	CA-C-O	-8.39	111.92	120.90
2	H	86	HIS	CE1-NE2-CD2	-8.39	100.61	109.00
2	R	215	ARG	N-CA-C	-8.39	102.08	111.14
2	H	37	LEU	CA-C-O	-8.38	111.31	120.36
2	I	149	GLN	OE1-CD-NE2	-8.38	114.22	122.60
2	H	238	HIS	CB-CG-CD2	-8.38	120.31	131.20
2	S	294	HIS	CE1-NE2-CD2	-8.38	100.62	109.00
2	I	363	PHE	N-CA-C	8.36	121.52	111.82
3	D	31	GLU	CA-C-O	-8.36	112.23	121.00
1	T	283	HIS	CG-CD2-NE2	8.35	115.55	107.20
2	G	166	GLY	CA-C-O	8.34	127.46	119.20
2	R	130	ILE	N-CA-C	8.34	119.84	108.84
2	J	327	HIS	CG-CD2-NE2	8.33	115.53	107.20
2	I	302	ASP	CA-CB-CG	8.33	120.93	112.60
2	I	432	ASN	OD1-CG-ND2	-8.33	114.27	122.60
2	J	383	HIS	CA-C-O	-8.33	111.45	122.44
3	L	36	GLN	OE1-CD-NE2	-8.32	114.28	122.60
2	H	250	MET	N-CA-C	8.31	119.97	111.07
3	L	81	GLU	N-CA-C	-8.29	103.29	113.41
2	S	157	VAL	N-CA-C	-8.29	102.16	110.62
2	C	212	GLN	N-CA-C	8.29	122.02	108.26
2	G	89	PRO	CA-C-O	-8.29	112.00	121.36
3	O	105	VAL	N-CA-CB	-8.28	102.47	112.33
2	G	295	ARG	N-CA-C	8.26	122.70	113.21
3	L	32	TYR	N-CA-C	-8.26	102.28	111.28
2	J	327	HIS	CE1-NE2-CD2	-8.25	100.75	109.00
2	H	58	ALA	CA-C-O	8.24	129.72	120.90
3	M	26	ILE	N-CA-C	-8.24	102.51	110.42
2	S	217	ARG	CA-C-O	-8.24	112.17	120.82
3	L	18	LEU	CA-C-N	-8.22	113.66	119.66
3	L	18	LEU	C-N-CA	-8.22	113.66	119.66
2	Q	348	LEU	CA-C-O	-8.22	111.83	120.55
3	O	104	ILE	CA-C-O	-8.21	111.05	121.48
2	S	119	SER	N-CA-C	-8.20	101.61	111.69
2	G	341	SER	N-CA-C	-8.19	102.32	111.82
2	I	208	SER	CA-C-O	-8.19	112.69	121.20
2	G	118	THR	N-CA-C	-8.17	102.46	111.36
2	C	86	HIS	ND1-CE1-NE2	8.16	116.56	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	75	VAL	N-CA-C	-8.16	102.30	110.62
2	S	327	HIS	CB-CG-CD2	-8.16	120.59	131.20
2	Q	446	ARG	N-CA-C	8.16	120.97	111.02
2	J	401	GLN	OE1-CD-NE2	-8.15	114.45	122.60
2	Q	119	SER	CA-C-O	-8.14	112.27	120.82
3	E	15	PHE	CA-CB-CG	8.14	121.94	113.80
2	R	303	ARG	N-CA-C	-8.13	102.36	111.14
2	G	215	ARG	N-CA-C	-8.13	102.50	111.36
2	R	401	GLN	OE1-CD-NE2	-8.12	114.48	122.60
2	R	417	ALA	N-CA-C	-8.12	102.52	111.36
3	N	81	GLU	N-CA-C	-8.11	102.98	113.12
2	R	223	ASP	N-CA-C	-8.10	101.72	111.69
2	G	274	PHE	N-CA-C	-8.08	103.37	113.55
3	P	27	ALA	CA-C-O	8.07	129.11	120.55
3	D	76	ARG	N-CA-C	8.07	119.70	111.07
2	R	320	LEU	N-CA-C	8.05	119.69	111.07
2	C	274	PHE	CA-CB-CG	8.04	121.84	113.80
2	C	299	ALA	N-CA-C	8.02	121.03	111.33
1	F	251	ARG	CA-C-O	-8.02	112.05	120.55
2	G	205	ASN	CA-CB-CG	-8.02	104.58	112.60
2	H	127	PHE	CA-CB-CG	-8.01	105.79	113.80
2	Q	225	ILE	N-CA-C	-8.01	102.73	110.42
2	J	79	ARG	N-CA-C	8.01	120.92	111.71
2	H	86	HIS	ND1-CE1-NE2	7.99	116.39	108.40
2	S	348	LEU	CA-C-O	-7.97	112.43	120.80
2	R	321	SER	N-CA-C	7.96	119.59	111.07
2	J	145	VAL	N-CA-C	7.96	118.72	110.36
2	J	193	LEU	N-CA-C	7.95	119.58	111.07
2	Q	424	LEU	N-CA-C	-7.95	102.56	111.07
2	S	402	PHE	N-CA-C	7.95	121.42	109.25
3	E	94	ASN	CA-CB-CG	7.94	120.54	112.60
2	J	441	GLY	N-CA-C	7.94	121.71	112.50
2	Q	118	THR	N-CA-C	-7.92	102.72	111.36
3	N	39	HIS	CE1-NE2-CD2	-7.92	101.08	109.00
2	R	108	PHE	CA-CB-CG	-7.92	105.88	113.80
2	J	45	GLN	N-CA-C	-7.92	99.15	110.08
3	K	29	GLN	OE1-CD-NE2	-7.92	114.68	122.60
2	R	155	ILE	N-CA-C	-7.92	102.62	110.30
2	G	274	PHE	CA-CB-CG	-7.90	105.90	113.80
2	R	125	PHE	CA-C-O	-7.88	111.37	120.20
2	H	346	VAL	N-CA-C	7.88	118.42	110.23
2	C	287	ASN	OD1-CG-ND2	-7.87	114.73	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	244	ALA	CA-C-O	-7.87	112.99	120.94
2	R	421	ARG	N-CA-C	7.86	119.48	111.07
3	N	84	ASP	N-CA-C	7.86	122.54	113.19
2	J	160	ASP	N-CA-C	7.85	119.84	111.28
2	C	298	HIS	CB-CG-CD2	7.85	141.41	131.20
2	C	311	PHE	N-CA-C	7.85	119.83	111.28
1	F	272	VAL	N-CA-C	7.85	118.39	110.23
3	P	63	PHE	N-CA-C	-7.83	101.57	112.45
2	S	292	HIS	CA-C-O	-7.82	113.04	121.56
2	J	37	LEU	CA-C-O	-7.81	112.06	121.28
2	I	385	TRP	CA-C-O	-7.81	111.45	120.20
2	Q	204	GLU	N-CA-C	-7.81	102.85	111.36
2	S	223	ASP	N-CA-C	-7.80	102.86	111.36
2	R	95	ASN	OD1-CG-ND2	-7.80	114.80	122.60
2	G	325	HIS	CB-CG-CD2	-7.79	121.07	131.20
2	H	318	LEU	N-CA-C	7.79	119.78	111.28
2	H	163	ASN	OD1-CG-ND2	-7.78	114.82	122.60
2	R	157	VAL	CA-C-O	-7.78	112.61	120.85
3	N	64	ASP	N-CA-C	-7.77	99.88	110.68
2	H	223	ASP	CA-CB-CG	7.77	120.37	112.60
2	R	163	ASN	N-CA-C	7.76	122.46	113.38
2	J	292	HIS	CB-CG-CD2	-7.76	121.11	131.20
2	I	156	GLN	N-CA-C	7.74	119.35	111.07
2	Q	248	GLU	N-CA-C	7.73	119.78	111.36
2	G	269	PHE	CA-CB-CG	7.73	121.53	113.80
2	C	264	ILE	CA-C-O	-7.72	113.73	121.45
2	Q	223	ASP	N-CA-C	-7.72	102.94	111.36
2	C	352	ASP	N-CA-C	7.71	119.69	111.28
2	G	51	ASP	N-CA-C	7.71	119.31	111.07
2	C	353	HIS	CA-CB-CG	-7.70	106.11	113.80
3	O	36	GLN	OE1-CD-NE2	-7.70	114.91	122.60
2	R	151	PRO	N-CA-C	7.69	120.08	110.70
2	Q	133	LEU	CA-C-O	-7.69	112.13	121.36
2	I	450	LYS	N-CA-C	7.68	120.33	111.11
2	H	183	LYS	N-CA-C	7.68	120.62	111.33
2	H	369	ALA	N-CA-C	7.67	122.06	112.24
2	Q	48	VAL	N-CA-C	-7.67	98.99	107.73
2	R	127	PHE	CA-CB-CG	-7.66	106.14	113.80
2	S	363	PHE	N-CA-C	7.66	120.30	111.11
1	A	278	ASN	OD1-CG-ND2	-7.66	114.94	122.60
2	S	113	VAL	N-CA-C	-7.66	102.81	110.62
2	H	262	MET	CA-C-O	-7.66	112.14	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	157	VAL	N-CA-C	-7.65	102.99	110.72
2	G	383	HIS	CA-C-O	-7.65	112.34	122.44
2	G	157	VAL	CA-C-O	-7.64	112.76	120.85
2	S	441	GLY	N-CA-C	-7.64	103.64	112.50
3	D	59	LYS	N-CA-CB	-7.63	105.47	114.17
2	R	345	PHE	N-CA-C	-7.63	102.61	112.23
2	J	226	HIS	N-CA-C	7.63	120.27	111.11
2	G	125	PHE	N-CA-C	7.61	121.50	111.75
2	R	276	ALA	N-CA-C	-7.61	102.98	111.28
2	I	277	ASN	OD1-CG-ND2	-7.61	114.99	122.60
3	D	60	LEU	N-CA-CB	7.60	118.42	111.27
2	J	100	PHE	CA-CB-CG	7.60	121.40	113.80
2	J	127	PHE	CA-CB-CG	-7.60	106.20	113.80
3	K	63	PHE	CA-CB-CG	-7.60	106.20	113.80
2	H	256	PHE	CA-CB-CG	-7.59	106.21	113.80
2	J	385	TRP	CA-C-O	-7.59	112.50	120.55
2	H	291	LEU	CA-C-O	-7.59	112.11	120.38
2	Q	438	TYR	N-CA-C	7.59	121.46	111.75
2	I	324	ASP	N-CA-C	7.58	122.36	113.18
2	R	307	HIS	ND1-CE1-NE2	7.58	115.98	108.40
2	Q	50	ALA	N-CA-C	7.58	119.19	111.07
3	L	53	PHE	CA-C-O	-7.58	112.51	120.55
2	C	151	PRO	N-CA-CB	-7.58	99.28	103.22
3	N	19	PRO	CA-C-O	-7.58	109.58	120.56
3	M	63	PHE	CA-CB-CG	-7.57	106.23	113.80
3	D	49	ASN	CA-C-O	-7.56	112.29	119.55
2	H	117	LEU	CA-C-O	-7.56	112.88	120.82
3	L	106	HIS	CB-CG-CD2	7.54	141.01	131.20
2	H	105	LEU	N-CA-C	7.54	121.40	111.75
2	J	180	LEU	N-CA-C	7.54	120.87	110.24
2	H	180	LEU	N-CA-C	7.54	120.30	110.43
2	S	157	VAL	CA-C-O	-7.54	113.11	120.95
2	Q	139	ARG	CA-C-N	7.53	130.76	120.67
2	Q	139	ARG	C-N-CA	7.53	130.76	120.67
2	C	189	VAL	N-CA-C	7.53	118.06	110.23
2	G	86	HIS	CG-CD2-NE2	7.53	114.73	107.20
2	J	287	ASN	OD1-CG-ND2	-7.51	115.09	122.60
3	O	15	PHE	CA-CB-CG	7.51	121.31	113.80
2	H	33	ASP	CA-C-O	7.51	128.51	120.55
2	I	184	ASN	OD1-CG-ND2	-7.50	115.10	122.60
3	M	106	HIS	CE1-NE2-CD2	-7.50	101.50	109.00
2	R	238	HIS	CB-CG-CD2	-7.50	121.45	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	GLN	CA-C-O	-7.50	112.88	120.90
2	I	129	ALA	N-CA-C	7.50	121.52	112.38
3	D	64	ASP	N-CA-C	-7.49	101.21	110.65
2	R	326	LEU	N-CA-C	7.49	120.52	107.49
3	M	57	MET	N-CA-C	7.48	119.97	110.24
2	C	167	ARG	N-CA-C	7.48	120.22	108.55
2	Q	148	PHE	CA-CB-CG	-7.47	106.33	113.80
3	K	39	HIS	CA-CB-CG	-7.47	106.33	113.80
3	M	79	ARG	N-CA-C	7.47	119.42	111.28
3	D	32	TYR	CA-C-O	-7.46	112.56	120.92
2	S	311	PHE	N-CA-C	7.46	120.36	111.33
3	M	46	GLU	N-CA-C	7.46	119.41	111.28
2	C	62	SER	N-CA-C	7.46	119.49	111.36
3	N	92	PHE	CA-CB-CG	-7.46	106.34	113.80
2	S	158	GLU	N-CA-C	7.46	120.06	111.11
2	I	423	ALA	N-CA-C	-7.45	103.10	111.07
2	C	251	MET	N-CA-C	7.43	119.02	111.07
2	I	274	PHE	CA-C-O	-7.43	112.55	120.42
2	S	59	ALA	N-CA-C	7.42	119.01	111.07
2	G	420	ASN	OD1-CG-ND2	-7.42	115.18	122.60
2	Q	95	ASN	OD1-CG-ND2	-7.42	115.18	122.60
1	F	237	LEU	CA-C-N	7.42	130.22	120.28
1	F	237	LEU	C-N-CA	7.42	130.22	120.28
2	J	113	VAL	N-CA-C	7.42	118.19	110.62
1	B	253	PHE	N-CA-C	7.41	119.00	111.07
2	Q	367	ASP	N-CA-C	7.40	120.96	108.90
2	H	401	GLN	CB-CG-CD	-7.40	100.02	112.60
2	Q	399	VAL	CA-C-O	-7.40	114.31	121.63
1	T	284	GLU	N-CA-C	7.40	121.22	110.42
3	E	33	MET	N-CA-C	7.39	120.28	111.33
2	G	429	GLN	OE1-CD-NE2	-7.38	115.22	122.60
3	P	63	PHE	CA-CB-CG	-7.38	106.42	113.80
2	H	311	PHE	N-CA-C	-7.38	103.32	111.36
2	C	301	ILE	CA-C-O	-7.37	111.39	118.98
2	J	52	GLU	CA-C-N	7.37	130.38	120.65
2	J	52	GLU	C-N-CA	7.37	130.38	120.65
2	Q	341	SER	N-CA-C	-7.36	103.28	111.82
2	S	148	PHE	CA-C-N	7.36	130.47	120.38
2	S	148	PHE	C-N-CA	7.36	130.47	120.38
2	Q	212	GLN	OE1-CD-NE2	-7.36	115.24	122.60
2	J	40	PHE	CA-CB-CG	7.35	121.15	113.80
2	J	171	GLY	CA-C-O	-7.35	114.50	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	125	PHE	N-CA-C	7.35	121.16	111.75
2	J	298	HIS	N-CA-C	7.33	119.91	111.11
2	I	125	PHE	CA-CB-CG	-7.33	106.47	113.80
2	I	327	HIS	CA-CB-CG	-7.32	106.48	113.80
3	L	44	PHE	O-C-N	-7.32	115.59	123.42
3	L	80	SER	CA-C-O	-7.31	112.01	120.20
2	R	119	SER	N-CA-C	-7.31	102.29	112.45
2	C	30	THR	CA-C-O	-7.31	113.22	119.36
2	Q	238	HIS	CB-CG-ND1	7.30	133.65	122.70
2	G	349	MET	N-CA-C	7.30	121.45	112.54
1	A	232	GLN	CB-CG-CD	-7.30	100.19	112.60
2	C	301	ILE	CB-CA-C	7.29	117.80	110.65
3	O	67	SER	CA-C-O	7.29	127.79	120.28
2	H	107	LEU	N-CA-C	7.29	121.61	112.87
2	Q	29	TYR	N-CA-C	7.29	120.51	110.24
2	R	147	THR	N-CA-C	7.28	121.42	112.54
3	P	40	PRO	CB-CA-C	-7.28	102.59	111.11
3	N	71	VAL	N-CA-C	-7.28	103.69	110.53
2	C	318	LEU	CA-C-O	-7.28	113.36	121.00
2	R	375	LEU	N-CA-C	7.28	122.31	109.58
2	H	215	ARG	N-CA-C	-7.27	102.75	111.69
1	F	284	GLU	N-CA-C	7.27	121.03	110.42
2	C	446	ARG	N-CA-C	7.27	119.28	111.36
2	Q	100	PHE	N-CA-C	7.27	120.27	109.59
2	G	60	GLU	N-CA-C	7.27	119.83	111.11
2	Q	425	GLU	N-CA-C	-7.26	103.09	112.23
2	G	375	LEU	N-CA-C	7.25	118.84	109.64
2	H	77	MET	CA-C-O	-7.25	113.14	120.90
3	N	27	ALA	N-CA-C	-7.24	103.47	111.36
2	J	125	PHE	CA-C-O	-7.24	112.09	120.20
2	Q	125	PHE	N-CA-C	7.23	121.74	112.34
2	I	148	PHE	CA-CB-CG	-7.23	106.57	113.80
2	Q	346	VAL	CA-C-O	7.23	128.79	121.27
3	E	103	PHE	CA-CB-CG	7.23	121.03	113.80
3	L	91	GLY	CA-C-O	-7.22	115.31	120.94
2	S	45	GLN	OE1-CD-NE2	-7.22	115.38	122.60
2	J	70	TRP	N-CA-C	-7.21	103.42	111.71
2	C	170	LEU	CA-C-N	7.21	128.31	121.46
2	C	170	LEU	C-N-CA	7.21	128.31	121.46
2	R	238	HIS	CE1-NE2-CD2	7.21	116.21	109.00
3	K	26	ILE	CA-C-O	-7.20	113.46	120.95
3	M	12	PHE	CA-CB-CG	-7.20	106.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	359	SER	N-CA-C	7.20	119.13	111.28
2	G	131	ARG	N-CA-C	7.20	118.77	111.07
3	N	106	HIS	N-CA-C	7.20	120.63	108.90
2	I	231	GLU	O-C-N	7.19	129.48	122.07
3	M	63	PHE	N-CA-C	-7.18	104.38	113.43
2	C	304	GLN	N-CA-C	-7.18	101.03	110.43
2	S	214	TRP	N-CA-C	-7.18	103.39	111.14
1	B	287	TYR	CA-C-O	-7.16	113.79	120.95
2	J	207	ASN	N-CA-C	7.15	121.70	112.12
2	I	220	PHE	N-CA-C	7.14	119.68	111.11
2	C	287	ASN	CA-CB-CG	7.13	119.73	112.60
1	B	232	GLN	N-CA-C	7.13	119.67	111.11
2	Q	205	ASN	N-CA-C	-7.13	103.59	111.36
2	J	314	LEU	CA-C-O	-7.12	113.34	120.82
2	S	207	ASN	CA-CB-CG	-7.12	105.48	112.60
2	R	153	HIS	CB-CG-CD2	7.11	140.45	131.20
2	I	379	SER	CA-C-O	-7.11	113.82	121.14
2	I	221	VAL	N-CA-C	-7.11	103.25	111.00
2	C	307	HIS	N-CA-C	7.11	120.48	108.90
3	E	16	SER	N-CA-C	7.10	119.02	111.28
2	I	44	PRO	CA-C-N	7.10	130.80	120.51
2	I	44	PRO	C-N-CA	7.10	130.80	120.51
2	J	304	GLN	CA-C-O	-7.09	113.78	121.44
3	O	39	HIS	CA-CB-CG	-7.09	106.71	113.80
1	F	262	ALA	O-C-N	7.08	127.60	121.30
2	G	353	HIS	CB-CG-ND1	7.08	133.32	122.70
2	S	327	HIS	CB-CG-ND1	7.08	133.31	122.70
2	Q	383	HIS	CA-C-O	-7.08	113.19	122.03
3	E	22	SER	N-CA-C	-7.07	99.41	110.36
3	E	107	ARG	CA-C-O	-7.07	112.48	120.46
2	C	366	GLN	OE1-CD-NE2	-7.06	115.54	122.60
1	F	232	GLN	N-CA-C	7.05	119.57	111.11
2	J	307	HIS	N-CA-C	7.05	119.97	108.55
2	R	225	ILE	N-CA-C	-7.05	103.65	110.42
2	S	40	PHE	CA-CB-CG	-7.05	106.75	113.80
2	Q	24	TYR	N-CA-C	7.05	118.96	111.28
2	S	347	ASP	N-CA-C	-7.04	103.95	112.54
2	Q	153	HIS	CB-CG-CD2	7.04	140.35	131.20
1	B	273	LEU	N-CA-C	7.03	119.84	111.33
2	H	238	HIS	CE1-NE2-CD2	7.03	116.03	109.00
2	C	303	ARG	N-CA-C	7.03	118.59	111.07
2	R	423	ALA	N-CA-C	-7.03	103.62	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	148	PHE	CA-CB-CG	-7.03	106.77	113.80
2	Q	363	PHE	CA-CB-CG	7.03	120.83	113.80
2	S	372	PRO	N-CA-C	7.03	122.10	111.14
2	H	72	ASP	N-CA-C	7.02	118.62	110.97
2	R	137	ASP	CA-CB-CG	7.01	119.61	112.60
2	C	148	PHE	CA-CB-CG	-7.01	106.79	113.80
2	I	185	TYR	N-CA-C	-7.00	103.58	111.14
2	C	115	ASN	OD1-CG-ND2	-7.00	115.60	122.60
2	S	312	ARG	CA-C-O	-7.00	113.07	120.63
1	T	239	GLN	OE1-CD-NE2	-7.00	115.60	122.60
2	I	42	PHE	N-CA-C	7.00	120.95	109.06
3	D	71	VAL	CA-C-O	-6.99	113.44	120.85
2	J	362	VAL	N-CA-CB	-6.99	105.28	112.06
2	S	444	ILE	N-CA-C	-6.99	103.52	110.30
3	D	95	ILE	N-CA-C	6.99	117.08	110.30
3	L	64	ASP	CA-CB-CG	-6.99	105.61	112.60
3	M	12	PHE	CA-C-N	6.98	129.97	120.54
3	M	12	PHE	C-N-CA	6.98	129.97	120.54
2	Q	318	LEU	CA-C-O	-6.98	113.49	120.82
2	H	135	LEU	N-CA-C	6.98	119.20	109.15
2	C	41	ARG	CA-C-O	-6.97	112.83	120.43
2	G	61	SER	N-CA-C	6.97	121.62	113.18
2	S	23	THR	N-CA-C	6.97	121.68	112.13
3	N	79	ARG	N-CA-C	6.97	119.52	111.02
2	H	274	PHE	N-CA-C	6.96	118.76	111.03
2	C	342	THR	CA-C-O	-6.96	113.51	120.82
2	Q	421	ARG	N-CA-C	6.96	119.46	111.11
1	A	284	GLU	N-CA-C	6.95	120.09	110.35
3	E	75	VAL	N-CA-C	6.95	117.66	110.36
2	Q	444	ILE	N-CA-CB	-6.95	102.42	110.55
2	C	270	LEU	N-CA-C	6.94	120.64	111.75
2	I	51	ASP	N-CA-C	6.93	118.84	111.28
3	E	71	VAL	N-CA-C	-6.93	103.55	110.62
2	H	201	LYS	N-CA-C	6.93	119.87	108.99
3	N	82	TYR	CA-C-N	6.93	129.02	120.22
3	N	82	TYR	C-N-CA	6.93	129.02	120.22
3	P	17	TYR	N-CA-C	6.92	119.70	111.33
2	C	255	GLU	N-CA-C	6.91	118.47	111.07
2	Q	119	SER	N-CA-C	-6.91	103.67	111.07
2	R	120	ILE	CA-C-O	-6.91	114.09	121.27
2	J	198	ASP	N-CA-C	-6.90	102.10	112.04
2	H	84	CYS	CA-C-O	-6.90	113.74	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	241	ASN	CA-CB-CG	6.90	119.50	112.60
2	G	36	LEU	CA-C-O	-6.89	113.41	120.71
2	J	139	ARG	CA-C-O	-6.89	113.21	120.58
3	M	59	LYS	CA-C-O	-6.88	112.12	119.00
2	S	325	HIS	CE1-NE2-CD2	6.88	115.88	109.00
2	G	250	MET	N-CA-C	-6.88	103.71	111.07
1	F	251	ARG	N-CA-C	6.88	118.78	111.28
3	M	86	TYR	N-CA-C	-6.87	99.11	110.17
2	H	253	ARG	N-CA-C	6.87	118.77	111.28
3	N	15	PHE	CA-C-O	-6.86	112.50	121.08
2	R	340	ALA	N-CA-C	6.86	118.41	111.07
3	D	9	GLU	CB-CG-CD	6.85	124.24	112.60
2	R	310	HIS	CA-C-O	-6.85	113.14	121.36
2	H	160	ASP	CA-CB-CG	6.84	119.44	112.60
2	G	325	HIS	CA-CB-CG	6.84	120.64	113.80
2	C	306	ASN	N-CA-C	6.83	121.60	111.96
2	R	30	THR	N-CA-C	-6.83	98.98	109.64
3	M	45	ASN	CA-CB-CG	6.83	119.43	112.60
2	Q	145	VAL	O-C-N	6.82	128.76	121.94
3	E	53	PHE	CA-CB-CG	6.82	120.62	113.80
2	H	209	GLN	CA-C-O	-6.82	113.98	119.71
2	C	200	THR	CA-C-O	-6.81	113.14	121.11
2	C	422	VAL	CA-C-O	-6.81	113.97	121.05
2	G	444	ILE	N-CA-CB	-6.81	102.95	110.51
3	M	16	SER	N-CA-C	6.80	119.56	111.33
1	T	232	GLN	N-CA-C	6.80	122.59	111.37
1	T	282	GLU	CA-C-O	-6.80	112.41	120.10
2	R	225	ILE	CA-C-O	-6.80	113.96	121.17
2	S	270	LEU	N-CA-C	6.80	119.27	111.11
2	Q	383	HIS	CE1-NE2-CD2	-6.79	102.20	109.00
2	C	274	PHE	N-CA-C	6.79	122.58	111.37
2	I	341	SER	N-CA-C	-6.79	103.94	111.82
2	C	292	HIS	CB-CG-ND1	6.79	132.89	122.70
2	Q	185	TYR	N-CA-C	-6.79	103.11	111.40
2	G	58	ALA	N-CA-C	-6.79	103.88	111.28
2	J	279	THR	N-CA-C	6.78	119.25	111.11
2	Q	437	LEU	N-CA-C	6.77	122.54	111.37
2	J	220	PHE	N-CA-C	6.77	118.73	111.36
3	N	95	ILE	N-CA-C	-6.76	104.17	110.53
1	B	247	HIS	CA-CB-CG	6.76	120.56	113.80
2	C	320	LEU	N-CA-C	6.75	122.51	111.37
2	J	299	ALA	N-CA-C	6.75	120.39	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	190	TYR	O-C-N	6.75	129.87	122.11
2	H	44	PRO	N-CA-C	6.74	121.26	110.40
2	C	298	HIS	CB-CG-ND1	-6.74	112.59	122.70
2	I	310	HIS	CB-CG-CD2	6.74	139.96	131.20
2	Q	145	VAL	CA-C-O	-6.74	114.26	121.27
1	T	252	ARG	N-CA-C	-6.74	104.02	111.36
2	R	365	THR	CA-C-O	-6.73	113.00	120.60
2	S	262	MET	N-CA-C	-6.73	101.17	109.65
2	S	187	ARG	N-CA-C	-6.73	104.03	111.36
2	I	385	TRP	N-CA-C	6.72	120.35	111.75
2	Q	327	HIS	CE1-NE2-CD2	-6.72	102.28	109.00
2	H	56	ALA	CA-C-O	-6.71	113.77	120.82
2	C	425	GLU	CA-C-N	6.71	129.16	120.44
2	C	425	GLU	C-N-CA	6.71	129.16	120.44
3	D	12	PHE	N-CA-C	-6.71	98.87	109.07
2	I	88	GLU	CA-C-O	-6.71	114.33	120.50
2	I	359	SER	N-CA-C	6.71	118.25	111.07
1	T	297	THR	N-CA-C	6.71	119.60	111.82
2	Q	108	PHE	CA-C-O	-6.71	113.58	121.16
1	T	300	ARG	CA-C-N	6.70	129.82	121.85
1	T	300	ARG	C-N-CA	6.70	129.82	121.85
3	E	9	GLU	CA-C-N	6.70	130.22	120.71
3	E	9	GLU	C-N-CA	6.70	130.22	120.71
3	M	93	ASP	CA-CB-CG	6.70	119.30	112.60
2	R	375	LEU	CA-C-O	-6.70	112.95	119.51
2	G	166	GLY	N-CA-C	6.69	123.92	115.42
2	J	401	GLN	CB-CG-CD	-6.69	101.22	112.60
2	C	460	ASP	N-CA-C	-6.69	104.38	112.54
2	C	438	TYR	N-CA-C	6.68	118.56	111.28
2	C	199	PHE	CA-CB-CG	-6.68	107.12	113.80
2	I	207	ASN	OD1-CG-ND2	-6.68	115.92	122.60
2	Q	382	ILE	CA-C-N	-6.68	113.01	122.63
2	Q	382	ILE	C-N-CA	-6.68	113.01	122.63
2	G	182	ALA	N-CA-C	-6.67	103.94	111.07
2	J	422	VAL	O-C-N	6.67	128.45	121.91
2	Q	451	TRP	N-CA-C	6.67	121.27	113.20
2	R	242	VAL	N-CA-C	6.67	118.56	112.43
2	J	394	PHE	N-CA-C	6.67	121.41	113.28
3	O	12	PHE	N-CA-C	6.66	120.54	109.95
2	C	180	LEU	N-CA-C	6.66	120.14	110.42
2	Q	393	ILE	CA-C-O	-6.66	114.11	121.17
2	G	306	ASN	CA-C-O	-6.66	111.73	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	303	ARG	N-CA-C	6.65	119.38	111.33
2	G	116	ILE	N-CA-CB	-6.64	103.38	110.62
2	J	71	THR	N-CA-C	6.64	119.35	111.71
2	J	226	HIS	CE1-NE2-CD2	-6.64	102.36	109.00
1	B	233	VAL	N-CA-C	6.64	117.43	110.72
2	H	259	GLU	N-CA-C	6.64	120.97	112.34
2	S	221	VAL	N-CA-C	-6.64	104.01	110.72
2	H	190	TYR	CA-C-O	-6.64	113.49	120.92
2	S	414	ALA	CA-C-O	-6.64	112.23	118.73
2	C	185	TYR	N-CA-C	6.63	119.11	111.02
2	Q	423	ALA	N-CA-C	6.63	119.35	111.33
2	S	250	MET	N-CA-C	-6.63	104.05	111.28
2	G	417	ALA	N-CA-C	-6.63	103.98	111.07
2	S	437	LEU	N-CA-C	6.63	118.16	111.07
2	C	342	THR	CA-C-N	6.62	129.69	120.29
2	C	342	THR	C-N-CA	6.62	129.69	120.29
2	G	292	HIS	CA-CB-CG	6.62	120.42	113.80
3	E	105	VAL	N-CA-CB	-6.62	104.46	112.33
2	H	393	ILE	N-CA-C	6.61	117.36	110.62
2	H	134	ARG	N-CA-C	6.60	120.28	109.06
2	J	438	TYR	O-C-N	6.60	129.14	122.08
2	R	181	SER	CA-C-O	-6.60	114.02	121.81
1	A	273	LEU	O-C-N	6.59	129.11	122.12
3	P	31	GLU	CA-C-O	-6.59	113.54	120.92
2	G	122	GLY	O-C-N	6.59	128.58	122.19
3	K	39	HIS	CA-C-O	-6.59	113.90	119.76
2	C	286	ASP	N-CA-C	6.58	120.41	112.38
2	Q	447	GLU	CB-CG-CD	6.58	123.78	112.60
2	S	225	ILE	CA-C-O	-6.58	114.11	120.95
2	S	277	ASN	OD1-CG-ND2	-6.58	116.02	122.60
2	Q	421	ARG	CA-C-N	6.58	128.85	120.56
2	Q	421	ARG	C-N-CA	6.58	128.85	120.56
2	R	383	HIS	CG-CD2-NE2	6.58	113.78	107.20
2	J	188	ALA	N-CA-C	6.58	118.11	111.07
1	A	253	PHE	N-CA-C	6.57	118.10	111.07
3	O	45	ASN	OD1-CG-ND2	-6.57	116.03	122.60
2	H	102	ALA	N-CA-C	6.57	120.57	110.20
2	S	241	ASN	OD1-CG-ND2	-6.57	116.03	122.60
2	Q	277	ASN	CA-C-O	-6.56	113.46	120.42
2	G	175	LYS	CA-C-O	-6.56	112.60	120.41
2	H	52	GLU	N-CA-C	-6.56	103.62	111.69
2	H	319	ARG	N-CA-C	-6.56	104.06	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	63	PHE	N-CA-C	-6.56	103.40	111.40
2	C	58	ALA	N-CA-C	6.55	118.08	111.07
2	H	249	GLU	CA-C-N	6.54	128.94	120.44
2	H	249	GLU	C-N-CA	6.54	128.94	120.44
2	G	226	HIS	CB-CG-ND1	-6.54	112.90	122.70
1	A	228	GLU	N-CA-C	-6.53	103.66	111.69
2	C	204	GLU	CA-C-O	-6.53	112.89	120.20
2	G	167	ARG	N-CA-C	6.53	120.68	109.06
2	S	379	SER	CA-C-O	-6.52	113.62	121.32
2	G	89	PRO	CA-C-N	6.52	129.84	120.98
2	G	89	PRO	C-N-CA	6.52	129.84	120.98
3	L	67	SER	O-C-N	-6.52	116.19	121.80
3	P	47	HIS	N-CA-C	-6.51	99.65	108.24
3	L	23	ASP	N-CA-C	-6.51	104.18	111.28
2	H	28	ASP	N-CA-C	-6.51	104.97	113.17
2	Q	351	GLU	CB-CG-CD	6.50	123.66	112.60
2	G	281	ALA	O-C-N	6.50	128.77	122.07
3	D	67	SER	N-CA-C	6.50	118.91	110.40
2	I	436	ASP	CA-C-O	6.50	128.35	120.62
2	J	351	GLU	CA-C-O	-6.50	113.48	121.67
2	C	363	PHE	CA-C-O	-6.49	112.77	120.10
2	G	127	PHE	CA-CB-CG	-6.49	107.31	113.80
2	I	327	HIS	N-CA-C	-6.49	100.30	109.96
2	J	98	PHE	N-CA-C	6.48	119.40	107.99
2	J	70	TRP	CA-C-O	-6.48	112.78	120.10
2	Q	50	ALA	CA-C-O	6.48	127.63	120.82
2	S	330	THR	N-CA-C	6.48	118.34	111.28
2	C	237	GLY	O-C-N	-6.48	118.35	123.27
2	H	184	ASN	CB-CG-ND2	6.48	126.12	116.40
2	S	302	ASP	CA-CB-CG	6.47	119.07	112.60
2	H	348	LEU	CA-C-O	-6.46	112.80	120.10
2	C	327	HIS	ND1-CE1-NE2	6.46	114.86	108.40
2	C	420	ASN	CB-CG-ND2	-6.46	106.72	116.40
2	J	251	MET	N-CA-C	-6.46	104.16	111.07
2	I	243	THR	CA-C-O	6.46	126.95	120.88
2	I	345	PHE	N-CA-C	6.46	120.42	112.54
2	J	446	ARG	N-CA-C	6.45	118.86	111.11
2	I	364	PHE	N-CA-C	-6.45	99.24	109.23
3	K	44	PHE	CA-CB-CG	-6.45	107.35	113.80
2	R	89	PRO	N-CA-C	6.45	121.46	111.21
2	J	160	ASP	CA-CB-CG	6.44	119.04	112.60
2	S	352	ASP	CA-C-O	-6.44	114.06	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	31	PRO	N-CA-C	6.44	120.53	110.80
2	C	385	TRP	N-CA-C	6.43	119.11	111.33
2	J	244	ALA	CA-C-O	-6.43	114.27	120.64
2	G	200	THR	CB-CA-C	6.43	121.65	109.37
2	I	35	ASP	CA-CB-CG	6.43	119.03	112.60
2	I	127	PHE	N-CA-C	-6.43	101.27	110.59
2	Q	180	LEU	N-CA-C	6.43	119.69	110.24
3	L	42	ILE	CA-C-O	-6.42	113.67	120.48
2	C	40	PHE	CA-C-O	-6.42	113.38	120.38
2	I	364	PHE	CA-CB-CG	-6.42	107.38	113.80
3	O	17	TYR	N-CA-C	6.42	120.82	113.19
2	I	206	ILE	N-CA-CB	6.41	118.32	111.46
2	I	238	HIS	CB-CG-ND1	6.41	132.32	122.70
3	M	21	LEU	CA-C-O	-6.41	113.98	121.16
2	I	387	MET	CA-C-O	-6.41	112.43	118.33
2	C	391	VAL	CA-C-O	-6.41	114.28	120.95
2	H	28	ASP	CA-CB-CG	-6.41	106.19	112.60
2	I	160	ASP	N-CA-C	6.41	118.34	111.36
2	R	140	PHE	O-C-N	6.41	127.14	121.18
2	H	323	GLY	CA-C-N	6.41	128.86	120.28
2	H	323	GLY	C-N-CA	6.41	128.86	120.28
2	S	198	ASP	CA-C-O	-6.41	112.86	120.10
1	A	251	ARG	N-CA-C	6.40	117.92	111.07
3	E	44	PHE	CA-CB-CG	-6.40	107.40	113.80
1	F	307	GLN	CA-C-O	6.40	128.49	121.06
2	G	204	GLU	CB-CG-CD	6.40	123.48	112.60
2	I	151	PRO	CA-C-O	-6.40	111.28	120.56
2	Q	366	GLN	OE1-CD-NE2	-6.39	116.21	122.60
1	B	250	LYS	N-CA-C	-6.39	103.61	111.40
2	J	138	ILE	CA-C-N	-6.39	113.93	122.42
2	J	138	ILE	C-N-CA	-6.39	113.93	122.42
2	J	238	HIS	CG-CD2-NE2	-6.39	100.81	107.20
2	R	330	THR	N-CA-C	-6.39	102.84	112.04
2	S	212	GLN	CG-CD-NE2	-6.38	106.83	116.40
2	S	358	ARG	N-CA-C	6.38	119.05	111.71
2	H	419	ALA	N-CA-C	-6.38	104.33	111.28
3	E	94	ASN	OD1-CG-ND2	-6.38	116.22	122.60
2	I	440	GLU	CA-C-O	-6.38	112.10	119.56
2	Q	218	PHE	CA-CB-CG	6.37	120.17	113.80
2	G	296	ALA	N-CA-C	6.37	119.47	110.23
2	J	31	PRO	CB-CA-C	-6.37	103.66	111.11
3	K	46	GLU	N-CA-C	6.37	119.03	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	10	ARG	CA-C-O	-6.36	114.20	121.19
2	Q	229	GLN	OE1-CD-NE2	-6.35	116.25	122.60
1	T	262	ALA	CA-C-O	-6.35	113.28	119.51
2	C	292	HIS	CB-CG-CD2	-6.35	122.94	131.20
2	C	202	ASP	N-CA-C	6.35	118.75	110.43
3	D	89	VAL	N-CA-C	6.35	117.06	108.17
2	J	384	VAL	N-CA-CB	-6.35	102.53	110.47
2	J	437	LEU	N-CA-C	6.35	119.87	111.75
1	T	304	ALA	CA-C-N	-6.34	114.33	122.77
1	T	304	ALA	C-N-CA	-6.34	114.33	122.77
2	I	220	PHE	CA-CB-CG	-6.34	107.46	113.80
2	H	184	ASN	OD1-CG-ND2	-6.34	116.26	122.60
2	S	61	SER	N-CA-C	6.34	120.87	113.20
3	P	32	TYR	N-CA-C	6.34	121.83	111.37
2	R	252	LYS	N-CA-C	6.34	118.72	111.11
3	E	63	PHE	N-CA-C	6.33	121.76	111.37
2	H	24	TYR	CA-C-O	-6.33	112.28	119.95
3	L	10	ARG	N-CA-C	6.33	119.80	110.30
2	J	443	ASP	CA-C-O	-6.33	114.17	120.82
2	C	199	PHE	CA-C-O	6.33	128.22	121.45
2	G	348	LEU	O-C-N	6.33	128.83	122.12
3	M	59	LYS	N-CA-CB	-6.33	106.96	114.17
2	S	339	LYS	N-CA-C	-6.33	104.38	111.28
2	I	127	PHE	CA-C-O	-6.33	114.49	121.89
1	F	282	GLU	N-CA-C	-6.32	104.39	111.28
2	H	226	HIS	ND1-CE1-NE2	6.32	114.72	108.40
2	J	392	GLU	CA-C-N	6.32	128.65	120.56
2	J	392	GLU	C-N-CA	6.32	128.65	120.56
2	S	371	MET	CA-C-O	-6.32	114.59	119.46
2	Q	161	LEU	N-CA-C	6.32	118.69	111.11
2	I	375	LEU	N-CA-C	6.32	118.79	109.50
1	A	307	GLN	OE1-CD-NE2	-6.31	116.29	122.60
3	P	54	TYR	N-CA-C	6.31	119.53	109.24
3	K	79	ARG	N-CA-C	6.31	121.72	111.37
2	I	199	PHE	CA-CB-CG	6.31	120.11	113.80
2	R	62	SER	N-CA-C	6.31	120.57	112.12
2	I	384	VAL	CB-CA-C	-6.30	102.84	112.05
2	J	455	LEU	CA-C-O	-6.30	113.87	120.55
2	S	205	ASN	OD1-CG-ND2	-6.30	116.30	122.60
2	R	383	HIS	ND1-CE1-NE2	-6.30	102.10	108.40
2	I	58	ALA	CA-C-N	6.30	128.63	120.44
2	I	58	ALA	C-N-CA	6.30	128.63	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	191	GLU	N-CA-C	-6.30	104.30	112.23
2	R	432	ASN	CA-CB-CG	6.29	118.89	112.60
2	J	33	ASP	CA-CB-CG	-6.29	106.31	112.60
2	G	45	GLN	CB-CG-CD	-6.28	101.92	112.60
3	P	71	VAL	N-CA-C	-6.28	104.38	110.72
2	H	308	GLY	CA-C-N	-6.27	113.65	122.75
2	H	308	GLY	C-N-CA	-6.27	113.65	122.75
3	L	97	GLN	CB-CG-CD	-6.27	101.94	112.60
2	C	208	SER	CA-C-O	-6.27	114.68	121.20
2	J	327	HIS	CB-CG-ND1	6.27	132.10	122.70
2	C	343	LEU	N-CA-C	-6.26	104.53	111.36
3	E	57	MET	N-CA-C	6.26	119.33	110.50
2	Q	235	ILE	CA-C-O	-6.26	114.47	121.36
2	J	439	ARG	N-CA-C	6.26	117.77	111.07
2	R	401	GLN	N-CA-C	-6.26	100.00	109.95
2	R	98	PHE	CA-CB-CG	-6.26	107.54	113.80
2	I	160	ASP	CA-CB-CG	6.25	118.85	112.60
3	O	32	TYR	N-CA-C	-6.25	104.55	111.36
2	I	56	ALA	CA-C-N	6.25	128.66	120.60
2	I	56	ALA	C-N-CA	6.25	128.66	120.60
3	K	97	GLN	OE1-CD-NE2	-6.25	116.36	122.60
2	R	116	ILE	N-CA-C	-6.24	104.42	110.42
2	S	151	PRO	O-C-N	6.24	128.83	121.46
1	T	300	ARG	N-CA-C	-6.24	99.53	109.76
2	H	113	VAL	N-CA-CB	6.23	119.50	110.52
2	S	310	HIS	CB-CG-CD2	6.23	139.31	131.20
2	Q	379	SER	CA-C-O	-6.22	113.98	121.32
3	D	76	ARG	CA-C-O	6.22	127.35	120.82
2	Q	348	LEU	O-C-N	6.22	128.71	122.12
2	G	384	VAL	O-C-N	-6.22	115.62	121.90
2	Q	310	HIS	N-CA-C	-6.22	100.16	110.17
2	R	77	MET	CA-C-O	-6.22	114.25	120.90
2	G	372	PRO	CA-C-N	6.21	130.62	121.05
2	G	372	PRO	C-N-CA	6.21	130.62	121.05
2	J	171	GLY	O-C-N	6.21	128.26	123.23
2	I	42	PHE	CA-C-N	-6.21	114.36	123.30
2	I	42	PHE	C-N-CA	-6.21	114.36	123.30
3	P	74	GLU	N-CA-C	6.21	118.56	111.11
2	S	119	SER	CA-C-N	6.20	128.50	120.56
2	S	119	SER	C-N-CA	6.20	128.50	120.56
3	K	63	PHE	CA-C-O	6.20	127.28	119.78
2	H	370	SER	N-CA-C	6.20	122.17	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	197	LEU	CA-C-N	6.20	128.49	120.44
2	R	197	LEU	C-N-CA	6.20	128.49	120.44
2	C	264	ILE	O-C-N	6.19	129.57	122.82
2	J	32	LYS	CA-C-O	-6.19	115.06	121.87
3	D	35	GLU	N-CA-C	6.19	118.82	111.33
2	C	198	ASP	N-CA-C	-6.19	104.08	111.69
2	G	193	LEU	CA-C-O	-6.19	114.53	120.90
2	C	310	HIS	N-CA-C	-6.18	101.34	110.48
2	R	115	ASN	OD1-CG-ND2	6.18	128.78	122.60
2	H	302	ASP	CA-CB-CG	6.17	118.77	112.60
2	J	448	ALA	N-CA-C	6.17	118.81	111.71
2	Q	321	SER	N-CA-C	6.17	117.67	111.07
2	I	452	SER	CA-C-O	-6.17	114.05	120.09
1	B	271	GLN	N-CA-C	-6.16	104.65	111.36
2	I	270	LEU	N-CA-C	-6.16	104.12	111.69
2	J	60	GLU	CB-CG-CD	6.16	123.06	112.60
2	G	191	GLU	CA-C-O	-6.15	113.90	120.42
3	K	104	ILE	CA-C-N	6.15	128.97	122.14
3	K	104	ILE	C-N-CA	6.15	128.97	122.14
2	G	140	PHE	N-CA-C	6.15	117.45	109.64
3	N	39	HIS	CA-CB-CG	-6.14	107.66	113.80
3	E	37	GLY	CA-C-N	-6.14	114.45	123.05
3	E	37	GLY	C-N-CA	-6.14	114.45	123.05
2	H	224	ALA	N-CA-C	-6.14	104.14	111.69
2	S	447	GLU	CA-C-O	-6.14	113.91	120.42
2	G	218	PHE	CA-C-O	-6.13	114.34	120.90
2	S	313	VAL	O-C-N	6.13	127.92	121.91
2	J	35	ASP	CA-C-N	-6.13	114.36	123.00
2	J	35	ASP	C-N-CA	-6.13	114.36	123.00
2	J	137	ASP	CA-C-O	-6.13	114.47	121.40
3	K	53	PHE	CA-C-O	-6.13	113.92	120.42
2	C	319	ARG	O-C-N	-6.13	115.63	122.12
2	C	200	THR	CB-CA-C	6.12	122.17	109.38
2	G	327	HIS	CB-CG-CD2	6.12	139.16	131.20
2	H	45	GLN	N-CA-C	-6.12	101.21	110.39
2	Q	213	ARG	N-CA-C	6.12	119.10	110.23
2	R	171	GLY	CA-C-O	-6.12	116.17	120.94
2	R	294	HIS	N-CA-C	6.12	119.86	110.20
2	I	181	SER	CA-C-O	-6.11	114.90	121.56
2	I	238	HIS	CB-CG-CD2	-6.11	123.25	131.20
2	J	177	LYS	CA-C-O	-6.11	113.19	120.10
2	Q	203	ASP	N-CA-C	-6.11	100.94	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	443	ASP	CA-C-N	6.11	128.25	120.56
2	H	443	ASP	C-N-CA	6.11	128.25	120.56
2	S	252	LYS	CA-C-O	6.10	127.02	120.55
2	Q	36	LEU	CA-C-O	-6.10	114.08	121.28
2	G	144	LEU	N-CA-C	6.10	118.00	111.36
3	O	84	ASP	CA-C-O	-6.10	112.09	119.59
2	J	51	ASP	N-CA-C	6.09	117.92	111.28
2	R	238	HIS	CG-CD2-NE2	-6.09	101.11	107.20
2	J	396	ASP	N-CA-C	6.09	121.36	111.37
3	P	31	GLU	O-C-N	6.09	129.12	122.11
3	L	65	CYS	O-C-N	-6.09	116.28	123.22
2	S	120	ILE	N-CA-C	-6.09	104.81	110.53
3	M	17	TYR	CA-C-O	-6.09	111.14	119.05
2	R	120	ILE	O-C-N	6.09	128.03	121.94
2	S	372	PRO	CA-C-O	-6.09	114.40	121.34
2	H	43	SER	CA-C-N	-6.08	114.47	120.98
2	H	43	SER	C-N-CA	-6.08	114.47	120.98
2	I	56	ALA	CA-C-O	-6.08	114.44	120.82
3	N	44	PHE	CA-C-O	-6.08	114.76	121.33
2	R	419	ALA	N-CA-C	-6.08	104.73	111.36
2	G	246	THR	CA-C-N	6.08	128.74	120.54
2	G	246	THR	C-N-CA	6.08	128.74	120.54
2	R	205	ASN	CA-C-N	-6.08	114.78	122.43
2	R	205	ASN	C-N-CA	-6.08	114.78	122.43
2	H	202	ASP	CA-C-O	-6.07	114.83	121.87
3	E	15	PHE	CA-C-N	6.07	128.42	120.28
3	E	15	PHE	C-N-CA	6.07	128.42	120.28
2	S	264	ILE	N-CA-C	6.07	116.36	108.35
2	C	199	PHE	N-CA-C	-6.07	99.92	108.96
2	G	292	HIS	CG-CD2-NE2	-6.07	101.13	107.20
2	H	109	GLU	N-CA-C	-6.07	99.81	109.76
2	Q	267	HIS	CE1-NE2-CD2	-6.07	102.93	109.00
2	R	260	LEU	N-CA-C	6.06	120.36	113.15
2	R	293	ILE	CA-C-N	6.05	130.08	121.42
2	R	293	ILE	C-N-CA	6.05	130.08	121.42
2	H	293	ILE	CA-C-O	-6.05	114.10	120.39
3	K	30	ILE	O-C-N	6.05	127.74	121.87
2	Q	277	ASN	OD1-CG-ND2	-6.05	116.55	122.60
2	H	401	GLN	N-CA-C	-6.05	99.84	109.76
2	S	256	PHE	CA-C-O	-6.05	113.02	119.97
1	B	242	ARG	N-CA-C	-6.04	102.73	110.53
2	G	339	LYS	N-CA-C	6.04	121.34	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	52	GLU	N-CA-C	-6.04	104.26	111.69
2	J	363	PHE	CA-CB-CG	-6.04	107.76	113.80
3	N	12	PHE	CA-C-O	6.04	127.78	121.38
3	M	39	HIS	CB-CG-CD2	-6.03	123.36	131.20
2	C	402	PHE	CA-CB-CG	6.03	119.83	113.80
2	Q	361	GLY	N-CA-C	6.03	123.37	115.47
2	H	30	THR	CA-C-N	-6.03	113.55	119.76
2	H	30	THR	C-N-CA	-6.03	113.55	119.76
2	I	140	PHE	O-C-N	6.03	126.44	121.31
2	G	100	PHE	CA-C-O	-6.03	113.91	120.36
2	Q	270	LEU	O-C-N	6.03	128.54	122.03
3	E	50	PRO	N-CA-C	6.02	121.90	113.53
2	R	325	HIS	CA-C-N	6.02	130.55	121.40
2	R	325	HIS	C-N-CA	6.02	130.55	121.40
2	C	424	LEU	CA-C-O	-6.02	114.46	120.90
2	C	364	PHE	CA-CB-CG	-6.02	107.78	113.80
2	J	350	ARG	N-CA-C	-6.02	104.06	112.12
1	T	254	ARG	N-CA-C	6.02	118.61	111.33
1	F	236	LEU	N-CA-C	6.01	117.50	111.07
3	E	99	GLN	OE1-CD-NE2	-6.01	116.59	122.60
2	Q	386	HIS	CA-C-N	6.01	128.32	120.26
2	Q	386	HIS	C-N-CA	6.01	128.32	120.26
2	R	364	PHE	CA-CB-CG	6.01	119.81	113.80
2	J	327	HIS	CA-CB-CG	6.01	119.81	113.80
2	Q	208	SER	CA-C-O	-6.01	114.19	120.32
2	J	35	ASP	CA-CB-CG	6.01	118.61	112.60
2	J	428	VAL	N-CA-C	6.01	121.83	109.34
3	O	28	ALA	N-CA-C	6.01	117.91	111.36
1	A	262	ALA	CA-C-N	-6.00	113.58	119.76
1	A	262	ALA	C-N-CA	-6.00	113.58	119.76
2	H	30	THR	CA-C-O	-6.00	114.84	119.46
2	J	152	PRO	N-CA-C	6.00	121.44	113.57
2	Q	98	PHE	CA-CB-CG	-6.00	107.80	113.80
2	Q	413	ASN	CA-C-O	-6.00	115.02	121.38
2	H	241	ASN	OD1-CG-ND2	-6.00	116.60	122.60
2	Q	143	ALA	CA-C-O	6.00	126.91	120.55
2	R	113	VAL	N-CA-CB	6.00	117.17	110.51
2	R	311	PHE	N-CA-C	6.00	117.82	111.28
2	S	209	GLN	CG-CD-NE2	-6.00	107.41	116.40
2	R	432	ASN	CB-CG-ND2	5.99	125.39	116.40
2	H	363	PHE	N-CA-C	5.99	119.85	112.54
2	S	200	THR	N-CA-CB	-5.99	101.78	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	200	THR	CB-CA-C	5.99	121.28	109.66
2	I	393	ILE	CB-CA-C	5.99	119.54	111.88
2	G	327	HIS	CB-CG-ND1	-5.98	113.73	122.70
2	S	417	ALA	CA-C-O	-5.98	114.55	120.82
2	G	439	ARG	CA-C-O	5.97	126.75	120.42
3	M	106	HIS	ND1-CE1-NE2	5.96	114.36	108.40
2	Q	423	ALA	O-C-N	5.96	128.44	122.12
2	C	364	PHE	N-CA-C	-5.96	99.99	109.23
3	N	19	PRO	CA-C-N	5.96	127.29	119.84
3	N	19	PRO	C-N-CA	5.96	127.29	119.84
2	G	393	ILE	CA-C-N	5.96	130.53	120.88
2	G	393	ILE	C-N-CA	5.96	130.53	120.88
2	J	398	SER	CA-CB-OG	-5.96	99.18	111.10
1	B	234	ARG	N-CA-C	5.96	121.14	111.37
2	Q	207	ASN	CA-CB-CG	-5.96	106.64	112.60
2	I	281	ALA	O-C-N	5.95	128.28	122.09
2	H	287	ASN	N-CA-C	5.95	121.27	113.30
2	I	29	TYR	N-CA-C	5.95	118.63	110.24
3	O	93	ASP	CA-C-O	-5.95	114.92	121.58
2	C	107	LEU	N-CA-C	-5.95	105.28	112.54
2	J	419	ALA	N-CA-C	-5.95	104.70	111.07
2	S	167	ARG	CA-C-O	-5.95	114.61	120.26
2	I	190	TYR	N-CA-C	5.94	118.24	111.11
2	R	31	PRO	CA-C-N	5.94	129.72	120.75
2	R	31	PRO	C-N-CA	5.94	129.72	120.75
1	A	273	LEU	CA-C-O	-5.94	114.25	120.55
2	G	98	PHE	CA-C-O	-5.94	114.00	120.36
2	I	198	ASP	O-C-N	5.94	128.42	122.12
2	I	401	GLN	CA-C-N	5.94	130.57	122.19
2	I	401	GLN	C-N-CA	5.94	130.57	122.19
2	J	58	ALA	N-CA-C	5.94	117.43	111.07
2	J	191	GLU	O-C-N	5.94	128.19	122.07
2	H	317	CYS	N-CA-C	5.94	117.75	111.28
2	R	387	MET	CA-C-O	-5.94	112.58	118.34
2	H	70	TRP	N-CA-C	-5.93	104.89	111.71
3	M	53	PHE	CA-C-N	-5.93	114.04	122.94
3	M	53	PHE	C-N-CA	-5.93	114.04	122.94
2	Q	270	LEU	CA-C-O	-5.93	114.79	120.90
2	G	226	HIS	CB-CG-CD2	5.93	138.91	131.20
2	J	35	ASP	O-C-N	5.93	129.68	122.68
1	T	278	ASN	OD1-CG-ND2	-5.93	116.67	122.60
2	C	377	VAL	CA-C-O	-5.93	114.08	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	70	GLN	CG-CD-NE2	5.93	125.29	116.40
3	O	72	LEU	N-CA-C	5.93	118.22	111.11
2	H	279	THR	CA-CB-OG1	-5.92	100.72	109.60
2	H	109	GLU	CA-C-N	5.92	129.78	121.02
2	H	109	GLU	C-N-CA	5.92	129.78	121.02
2	H	238	HIS	CA-CB-CG	5.92	119.72	113.80
3	N	31	GLU	CA-C-O	-5.92	114.56	121.07
2	R	61	SER	N-CA-C	5.91	120.22	112.89
2	C	278	THR	N-CA-C	-5.91	104.84	111.28
2	C	440	GLU	CB-CG-CD	-5.91	102.55	112.60
2	H	356	ALA	N-CA-C	-5.91	101.29	110.10
2	J	420	ASN	CA-C-N	5.91	128.12	120.44
2	J	420	ASN	C-N-CA	5.91	128.12	120.44
2	Q	241	ASN	N-CA-C	-5.91	101.53	110.28
2	S	166	GLY	N-CA-C	5.91	124.00	114.90
2	R	427	CYS	O-C-N	5.91	128.16	122.07
2	J	111	GLY	N-CA-C	5.91	123.21	115.47
3	L	44	PHE	CA-CB-CG	-5.91	107.89	113.80
2	J	270	LEU	O-C-N	5.90	128.15	122.07
3	N	28	ALA	O-C-N	-5.90	115.86	122.12
2	J	85	TYR	N-CA-C	5.90	120.64	113.38
1	T	243	ILE	CB-CA-C	5.90	119.78	110.81
2	H	262	MET	O-C-N	5.90	127.18	121.28
2	G	294	HIS	N-CA-C	5.90	119.33	109.95
1	B	252	ARG	CA-C-O	5.89	126.80	120.55
2	H	120	ILE	O-C-N	5.89	127.90	121.83
2	G	220	PHE	CA-CB-CG	5.89	119.69	113.80
2	R	402	PHE	CA-CB-CG	5.89	119.69	113.80
2	Q	371	MET	CA-C-O	-5.89	114.96	119.32
3	D	64	ASP	CA-C-N	5.89	130.25	122.30
3	D	64	ASP	C-N-CA	5.89	130.25	122.30
2	I	384	VAL	CA-C-O	-5.89	114.22	120.64
2	Q	177	LYS	CA-C-O	-5.89	113.45	120.10
2	H	305	ARG	N-CA-C	5.88	120.32	113.20
2	J	256	PHE	CA-C-O	-5.88	114.18	120.42
2	Q	189	VAL	N-CA-C	5.88	116.54	110.36
1	A	279	CYS	CA-C-O	5.88	126.78	120.55
2	C	248	GLU	CB-CG-CD	5.88	122.60	112.60
2	J	218	PHE	CA-CB-CG	5.88	119.68	113.80
2	H	37	LEU	CD1-CG-CD2	5.88	123.74	110.80
2	C	90	VAL	N-CA-CB	5.88	117.12	110.72
2	I	215	ARG	N-CA-C	-5.88	104.95	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	238	HIS	N-CA-C	-5.88	99.07	109.06
2	S	125	PHE	CA-C-O	-5.88	113.62	120.20
2	R	309	ILE	O-C-N	-5.88	117.15	123.14
3	P	26	ILE	N-CA-C	-5.87	104.63	110.62
3	N	60	LEU	CB-CA-C	-5.87	103.60	110.76
2	S	353	HIS	CB-CG-CD2	5.87	138.83	131.20
2	S	293	ILE	CB-CA-C	5.87	119.31	110.63
2	S	460	ASP	N-CA-C	-5.87	105.38	112.54
3	E	75	VAL	CB-CA-C	5.87	119.39	111.88
1	A	266	SER	CA-C-O	-5.86	113.33	120.54
2	G	329	GLY	CA-C-O	5.86	126.28	122.23
2	H	83	LYS	CA-C-O	-5.86	114.09	120.36
3	P	94	ASN	CA-CB-CG	-5.86	106.74	112.60
2	C	280	LEU	CA-C-N	5.86	128.13	120.28
2	C	280	LEU	C-N-CA	5.86	128.13	120.28
1	T	283	HIS	CE1-NE2-CD2	-5.86	103.14	109.00
2	C	429	GLN	O-C-N	5.86	128.10	122.07
2	R	318	LEU	CA-C-O	-5.86	114.87	120.90
2	I	256	PHE	N-CA-C	-5.85	104.85	112.23
2	Q	243	THR	CA-CB-OG1	-5.85	100.82	109.60
2	R	81	LYS	N-CA-C	5.85	119.62	110.32
2	C	220	PHE	O-C-N	5.85	128.09	122.07
2	C	294	HIS	CA-CB-CG	5.85	119.65	113.80
2	I	417	ALA	CA-C-O	-5.85	114.67	120.70
2	Q	153	HIS	ND1-CG-CD2	-5.85	100.25	106.10
2	I	105	LEU	CA-C-O	-5.85	112.42	119.49
2	Q	383	HIS	N-CA-C	5.85	119.17	111.28
2	C	241	ASN	OD1-CG-ND2	-5.84	116.76	122.60
3	K	16	SER	CA-C-O	5.84	126.70	120.10
2	S	357	ASP	O-C-N	-5.84	116.80	123.40
2	Q	43	SER	CA-C-N	5.83	125.77	119.76
2	Q	43	SER	C-N-CA	5.83	125.77	119.76
2	I	310	HIS	N-CA-C	-5.83	101.85	110.48
1	A	294	ASP	CA-C-O	-5.83	114.48	120.54
2	I	285	ARG	O-C-N	5.83	128.15	122.09
2	Q	61	SER	N-CA-C	5.83	121.30	113.72
2	C	376	PRO	N-CA-C	-5.83	102.71	111.57
3	K	39	HIS	ND1-CG-CD2	-5.83	100.27	106.10
2	R	327	HIS	CA-CB-CG	-5.83	107.97	113.80
2	J	225	ILE	CA-C-O	-5.82	115.00	121.17
2	S	216	ASP	CA-CB-CG	-5.82	106.78	112.60
3	O	65	CYS	N-CA-C	5.82	118.69	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	79	ARG	CA-C-O	-5.82	112.74	119.61
2	C	98	PHE	CA-CB-CG	-5.82	107.98	113.80
2	R	167	ARG	CA-C-O	-5.82	115.13	120.13
1	B	293	ILE	O-C-N	-5.81	116.92	123.20
2	Q	235	ILE	O-C-N	5.81	128.79	122.63
2	H	51	ASP	N-CA-C	5.81	118.39	111.71
2	Q	349	MET	CA-C-O	-5.81	112.11	119.31
1	T	305	LEU	N-CA-C	-5.81	99.27	108.73
2	G	153	HIS	CB-CG-ND1	-5.80	113.99	122.70
2	G	311	PHE	CA-CB-CG	-5.80	108.00	113.80
2	H	341	SER	N-CA-C	5.80	119.18	111.75
2	G	304	GLN	N-CA-C	-5.80	99.73	108.96
2	R	354	ILE	N-CA-CB	-5.80	102.70	112.44
2	C	375	LEU	N-CA-C	5.79	116.95	109.65
3	L	44	PHE	CA-C-O	5.79	127.43	121.23
2	H	225	ILE	CA-C-O	-5.79	114.62	121.05
2	Q	264	ILE	CA-C-O	-5.79	115.14	121.28
2	Q	298	HIS	ND1-CG-CD2	5.79	111.89	106.10
2	S	184	ASN	CA-CB-CG	-5.79	106.81	112.60
2	H	137	ASP	CA-C-O	-5.79	115.08	121.33
2	Q	305	ARG	O-C-N	5.79	128.25	122.12
1	F	286	GLU	CB-CG-CD	-5.79	102.77	112.60
3	P	27	ALA	N-CA-C	5.79	117.59	111.28
2	R	41	ARG	O-C-N	-5.79	116.42	122.96
3	E	32	TYR	CA-C-O	-5.78	114.75	120.82
2	J	305	ARG	CA-C-O	-5.78	112.44	119.43
2	I	97	TYR	N-CA-C	-5.78	100.35	108.96
2	Q	165	TYR	CA-C-O	5.78	127.76	121.06
3	O	19	PRO	CA-C-O	-5.78	112.18	120.56
3	P	69	GLN	CB-CG-CD	-5.78	102.78	112.60
2	S	417	ALA	N-CA-C	-5.78	104.89	111.07
2	J	243	THR	CB-CA-C	-5.77	101.85	110.16
3	M	95	ILE	N-CA-CB	5.77	117.30	110.55
2	Q	163	ASN	CB-CG-ND2	-5.77	107.74	116.40
2	Q	320	LEU	N-CA-C	5.77	117.25	111.07
3	K	13	GLU	N-CA-C	5.77	117.65	111.36
2	I	329	GLY	N-CA-C	-5.77	105.35	112.33
3	K	78	CYS	CA-C-O	-5.77	114.31	120.42
3	L	69	GLN	N-CA-C	-5.77	105.13	111.82
2	G	74	LEU	N-CA-CB	-5.77	102.11	110.47
2	J	32	LYS	CA-C-N	5.77	128.01	120.28
2	J	32	LYS	C-N-CA	5.77	128.01	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	97	GLN	OE1-CD-NE2	-5.77	116.83	122.60
2	R	275	THR	CA-C-N	5.77	128.01	120.28
2	R	275	THR	C-N-CA	5.77	128.01	120.28
2	C	234	GLU	CB-CG-CD	5.77	122.40	112.60
1	T	227	SER	O-C-N	-5.76	116.14	122.07
2	I	108	PHE	N-CA-C	-5.76	100.40	109.50
2	S	383	HIS	CA-C-O	-5.76	114.83	122.03
2	G	303	ARG	N-CA-C	5.76	119.40	112.38
2	Q	42	PHE	N-CA-C	-5.76	100.02	109.40
2	Q	267	HIS	CA-C-N	5.75	130.06	121.72
2	Q	267	HIS	C-N-CA	5.75	130.06	121.72
2	G	342	THR	CA-C-O	5.75	127.40	121.07
2	H	342	THR	CA-C-O	5.75	126.86	120.82
2	J	226	HIS	ND1-CE1-NE2	5.75	114.15	108.40
2	J	294	HIS	N-CA-C	5.75	118.94	109.85
2	C	317	CYS	N-CA-C	5.75	117.22	111.07
3	D	84	ASP	CA-C-O	-5.75	112.73	120.15
2	C	207	ASN	N-CA-C	5.75	119.82	112.12
2	Q	268	ASP	N-CA-C	5.75	118.04	109.25
2	S	58	ALA	CA-C-O	-5.75	114.79	120.82
2	S	304	GLN	N-CA-CB	5.75	118.42	109.97
2	G	251	MET	CA-C-O	-5.75	114.97	121.00
2	S	274	PHE	CA-C-O	-5.75	113.06	119.67
3	M	48	SER	CA-CB-OG	-5.74	99.61	111.10
2	R	46	PRO	CB-CA-C	5.74	118.87	111.46
2	R	202	ASP	CA-CB-CG	5.74	118.34	112.60
2	Q	452	SER	O-C-N	5.74	126.67	121.04
2	H	203	ASP	N-CA-C	-5.74	100.32	109.96
2	I	422	VAL	N-CA-C	-5.74	104.26	110.23
3	M	13	GLU	O-C-N	5.74	128.06	122.09
2	Q	181	SER	CA-C-O	-5.73	115.47	121.55
2	Q	205	ASN	CA-C-O	-5.73	114.35	120.42
3	K	18	LEU	N-CA-C	-5.73	102.69	110.36
2	J	286	ASP	N-CA-C	5.72	119.78	112.34
2	C	139	ARG	CB-CA-C	-5.72	101.53	110.74
3	L	26	ILE	N-CA-CB	-5.72	103.86	110.55
2	Q	418	THR	CA-C-O	-5.72	114.81	120.82
2	G	137	ASP	CA-CB-CG	5.72	118.32	112.60
3	D	71	VAL	CB-CA-C	-5.72	104.33	112.22
3	P	15	PHE	N-CA-C	5.72	120.07	113.38
2	Q	158	GLU	O-C-N	5.72	128.20	122.08
2	R	31	PRO	CB-CA-C	-5.72	104.54	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	34	ILE	O-C-N	-5.72	116.29	121.89
2	H	240	LEU	CA-C-O	-5.71	114.50	121.36
2	G	348	LEU	CA-C-O	-5.71	114.49	120.55
2	S	350	ARG	CB-CA-C	-5.71	101.80	110.83
3	O	73	ASP	CA-CB-CG	-5.71	106.89	112.60
2	S	88	GLU	O-C-N	-5.71	117.83	121.88
2	J	229	GLN	N-CA-C	5.71	118.28	111.71
2	J	198	ASP	CA-C-O	-5.71	113.18	120.31
2	R	447	GLU	N-CA-CB	5.71	118.51	110.12
1	B	307	GLN	CB-CG-CD	5.70	122.30	112.60
2	Q	385	TRP	N-CA-C	5.70	119.98	113.19
2	R	51	ASP	CA-CB-CG	5.70	118.30	112.60
2	C	162	LEU	N-CA-C	5.70	119.33	112.38
1	F	278	ASN	OD1-CG-ND2	-5.70	116.90	122.60
2	J	147	THR	CA-C-O	5.70	126.58	120.20
3	N	46	GLU	N-CA-C	5.70	119.33	112.38
2	R	205	ASN	N-CA-C	-5.70	105.21	111.82
2	H	343	LEU	N-CA-C	-5.70	105.07	111.28
3	O	62	LEU	N-CA-CB	-5.70	102.88	110.57
2	G	238	HIS	N-CA-C	5.70	119.10	109.76
1	A	307	GLN	CB-CG-CD	5.70	122.28	112.60
2	R	432	ASN	OD1-CG-ND2	-5.70	116.90	122.60
3	L	57	MET	N-CA-C	-5.69	102.06	110.48
3	D	90	ALA	N-CA-C	5.69	119.00	109.95
3	E	74	GLU	N-CA-C	5.69	117.48	111.28
2	C	142	VAL	N-CA-C	5.69	117.11	110.62
2	H	399	VAL	N-CA-C	-5.69	100.14	108.11
2	S	441	GLY	CA-C-N	-5.69	113.67	119.98
2	S	441	GLY	C-N-CA	-5.69	113.67	119.98
3	O	36	GLN	CB-CG-CD	5.69	122.27	112.60
2	I	48	VAL	N-CA-C	-5.68	101.25	107.73
2	Q	136	GLU	N-CA-C	-5.68	105.12	112.68
2	Q	330	THR	N-CA-C	5.68	117.55	111.36
2	C	345	PHE	CA-CB-CG	5.68	119.48	113.80
3	E	87	ILE	N-CA-C	-5.68	100.49	108.27
1	F	239	GLN	OE1-CD-NE2	-5.68	116.92	122.60
2	I	57	ILE	N-CA-C	-5.67	104.40	110.36
2	R	51	ASP	N-CA-C	5.67	117.47	111.28
1	T	276	LEU	N-CA-C	5.67	117.47	111.28
2	S	454	GLU	CA-C-O	-5.67	113.94	120.24
1	A	250	LYS	CA-C-N	5.67	127.81	120.44
1	A	250	LYS	C-N-CA	5.67	127.81	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	PRO	CB-CA-C	-5.67	103.97	111.23
2	H	354	ILE	CB-CA-C	5.67	118.82	110.77
3	L	53	PHE	O-C-N	5.67	128.13	122.12
2	H	212	GLN	CB-CA-C	-5.67	102.91	110.79
2	G	122	GLY	CA-C-O	-5.67	114.66	120.66
3	L	64	ASP	N-CA-C	-5.67	102.81	110.68
2	R	159	ARG	CA-C-N	5.66	127.80	120.44
2	R	159	ARG	C-N-CA	5.66	127.80	120.44
2	G	439	ARG	N-CA-C	5.66	117.53	111.36
2	J	361	GLY	N-CA-C	5.66	123.06	115.59
2	S	211	PHE	CA-CB-CG	-5.66	108.14	113.80
2	R	238	HIS	CA-CB-CG	5.66	119.46	113.80
3	D	72	LEU	N-CA-C	5.66	117.90	111.11
2	H	271	THR	N-CA-C	-5.66	104.59	112.45
2	R	56	ALA	CA-C-N	5.66	128.18	120.77
2	R	56	ALA	C-N-CA	5.66	128.18	120.77
2	G	101	ILE	N-CA-C	-5.65	99.98	108.12
2	G	302	ASP	CA-CB-CG	5.65	118.25	112.60
2	G	326	LEU	N-CA-C	5.65	116.99	108.46
2	I	41	ARG	N-CA-C	-5.65	100.08	109.46
2	S	179	GLY	O-C-N	-5.65	116.77	122.65
2	Q	364	PHE	N-CA-C	-5.65	101.33	108.45
2	Q	431	ARG	O-C-N	5.65	127.89	122.07
1	A	233	VAL	CA-C-N	5.65	128.16	120.54
1	A	233	VAL	C-N-CA	5.65	128.16	120.54
2	I	196	GLY	CA-C-N	5.65	128.85	120.95
2	I	196	GLY	C-N-CA	5.65	128.85	120.95
2	I	348	LEU	N-CA-CB	5.65	118.20	110.01
2	C	177	LYS	CA-C-O	-5.64	114.86	121.07
2	H	79	ARG	O-C-N	5.64	128.10	122.12
2	I	37	LEU	N-CA-C	-5.64	100.20	109.40
3	O	95	ILE	N-CA-C	5.64	116.30	110.82
2	I	431	ARG	CA-C-O	-5.64	113.73	120.10
2	Q	378	ALA	CA-C-O	-5.64	114.54	120.80
1	F	283	HIS	CB-CA-C	-5.63	101.83	111.46
2	R	345	PHE	CA-CB-CG	5.63	119.44	113.80
3	N	39	HIS	CB-CG-CD2	-5.63	123.88	131.20
2	R	121	VAL	O-C-N	-5.63	115.53	122.57
1	A	238	ASN	N-CA-C	5.63	117.42	111.28
1	F	287	TYR	N-CA-C	5.63	118.52	110.24
2	J	226	HIS	CB-CA-C	-5.63	101.80	110.81
3	K	106	HIS	CE1-NE2-CD2	-5.63	103.37	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	74	GLU	N-CA-C	5.63	118.14	111.33
2	Q	34	THR	N-CA-C	5.63	120.14	113.16
2	S	149	GLN	N-CA-C	5.63	118.14	111.33
2	J	384	VAL	CA-C-N	5.63	127.82	120.28
2	J	384	VAL	C-N-CA	5.63	127.82	120.28
2	S	80	TYR	CA-C-O	-5.63	113.89	120.53
2	G	163	ASN	CB-CG-ND2	-5.63	107.96	116.40
2	G	203	ASP	N-CA-C	-5.63	102.69	110.35
2	G	178	LEU	N-CA-C	-5.62	100.93	108.86
2	I	24	TYR	CB-CA-C	-5.62	101.63	110.85
3	M	15	PHE	CA-C-N	5.62	128.08	120.38
3	M	15	PHE	C-N-CA	5.62	128.08	120.38
2	R	283	TRP	N-CA-C	-5.62	105.06	111.07
2	H	280	LEU	CD1-CG-CD2	5.62	123.16	110.80
2	J	291	LEU	CA-C-O	-5.62	113.34	120.20
3	O	85	CYS	CA-C-N	5.62	128.82	120.90
3	O	85	CYS	C-N-CA	5.62	128.82	120.90
2	I	36	LEU	CA-C-N	-5.62	114.52	122.94
2	I	36	LEU	C-N-CA	-5.62	114.52	122.94
3	L	99	GLN	CB-CA-C	5.62	117.87	110.06
2	S	114	THR	N-CA-C	-5.62	105.06	111.07
2	S	372	PRO	CB-CA-C	-5.62	104.22	111.46
2	S	205	ASN	CA-CB-CG	-5.61	106.99	112.60
2	S	293	ILE	CA-C-O	-5.61	114.50	120.39
2	H	320	LEU	N-CA-C	5.61	117.87	111.02
3	P	86	TYR	N-CA-C	-5.61	101.14	110.17
2	H	180	LEU	CD1-CG-CD2	-5.61	98.46	110.80
3	M	39	HIS	CA-CB-CG	-5.61	108.19	113.80
2	I	383	HIS	CA-C-O	-5.61	115.02	122.03
2	R	39	ALA	CA-C-O	-5.61	114.15	120.43
2	I	249	GLU	N-CA-C	5.60	120.62	111.37
2	J	53	ALA	CA-C-O	-5.60	115.12	121.00
2	R	30	THR	CA-C-O	-5.60	112.72	119.67
2	J	81	LYS	N-CA-C	-5.60	101.42	110.32
3	K	74	GLU	CA-C-O	5.60	126.89	120.90
2	H	287	ASN	CA-CB-CG	5.60	118.20	112.60
2	R	267	HIS	CA-C-O	-5.59	115.08	121.40
2	G	369	ALA	CA-C-O	-5.59	115.35	121.84
2	Q	246	THR	N-CA-CB	-5.59	101.82	111.55
2	J	430	ALA	N-CA-C	-5.59	105.10	111.14
3	D	99	GLN	CG-CD-NE2	5.59	124.78	116.40
2	J	52	GLU	N-CA-C	-5.59	104.82	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	24	TYR	O-C-N	5.59	128.76	122.22
2	H	101	ILE	CB-CA-C	5.59	118.48	110.33
3	P	80	SER	N-CA-C	-5.59	105.09	111.07
2	R	327	HIS	ND1-CG-CD2	-5.59	100.51	106.10
2	C	128	LYS	N-CA-C	5.58	117.17	111.14
2	G	401	GLN	CB-CG-CD	-5.58	103.11	112.60
3	K	71	VAL	CB-CA-C	-5.58	104.76	112.24
2	G	217	ARG	N-CA-C	5.58	117.83	111.02
3	N	38	PHE	CA-CB-CG	5.58	119.38	113.80
2	S	120	ILE	N-CA-CB	5.58	117.71	110.57
2	Q	371	MET	O-C-N	5.58	126.48	121.35
3	K	105	VAL	N-CA-C	5.58	119.10	113.47
2	C	205	ASN	CA-C-N	-5.58	116.18	122.93
2	C	205	ASN	C-N-CA	-5.58	116.18	122.93
2	H	106	ASP	CA-C-O	-5.57	112.75	119.49
2	C	116	ILE	CB-CG1-CD1	5.57	125.50	113.80
1	B	287	TYR	O-C-N	5.57	129.35	123.11
2	J	374	VAL	CA-C-N	-5.57	113.14	121.83
2	J	374	VAL	C-N-CA	-5.57	113.14	121.83
2	S	182	ALA	CA-C-N	-5.57	113.20	120.44
2	S	182	ALA	C-N-CA	-5.57	113.20	120.44
2	S	228	SER	CA-C-O	-5.57	114.94	120.90
2	H	238	HIS	ND1-CE1-NE2	-5.57	102.83	108.40
2	H	45	GLN	OE1-CD-NE2	5.57	128.17	122.60
2	H	209	GLN	OE1-CD-NE2	5.57	128.17	122.60
3	D	71	VAL	N-CA-C	-5.56	105.10	110.72
2	J	312	ARG	CA-C-O	-5.56	114.98	120.82
3	L	25	GLN	O-C-N	5.56	127.80	122.07
3	E	79	ARG	CA-C-N	5.56	127.67	120.44
3	E	79	ARG	C-N-CA	5.56	127.67	120.44
2	G	62	SER	O-C-N	5.56	128.93	122.09
3	O	75	VAL	N-CA-C	-5.56	103.99	111.44
1	F	302	PHE	CA-C-N	5.56	130.83	122.99
1	F	302	PHE	C-N-CA	5.56	130.83	122.99
2	G	387	MET	CA-C-O	-5.56	113.28	118.73
2	C	417	ALA	N-CA-C	-5.56	105.14	111.14
2	G	114	THR	CA-C-N	5.56	127.73	120.28
2	G	114	THR	C-N-CA	5.56	127.73	120.28
2	G	116	ILE	N-CA-C	5.56	115.69	110.30
2	G	73	LEU	CD1-CG-CD2	5.56	123.03	110.80
2	Q	156	GLN	OE1-CD-NE2	-5.56	117.04	122.60
2	H	197	LEU	N-CA-CB	-5.55	101.58	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	31	PRO	N-CA-CB	-5.55	98.75	103.36
2	R	117	LEU	N-CA-C	-5.55	105.31	111.36
2	R	125	PHE	N-CA-C	5.55	118.85	111.75
2	G	165	TYR	N-CA-C	-5.55	100.64	109.07
2	G	383	HIS	CA-C-N	5.55	129.72	120.62
2	G	383	HIS	C-N-CA	5.55	129.72	120.62
2	R	212	GLN	CB-CG-CD	-5.55	103.17	112.60
1	A	271	GLN	N-CA-C	-5.54	105.15	111.14
2	I	244	ALA	CA-C-O	-5.54	115.40	120.50
2	C	360	ARG	CA-C-N	5.54	129.88	120.91
2	C	360	ARG	C-N-CA	5.54	129.88	120.91
2	I	427	CYS	N-CA-C	5.54	117.40	111.36
2	J	419	ALA	CA-C-O	-5.54	115.00	120.82
2	H	163	ASN	CA-CB-CG	5.54	118.14	112.60
2	Q	417	ALA	N-CA-C	-5.54	105.25	111.28
2	C	79	ARG	CA-C-O	-5.53	112.79	119.49
2	G	327	HIS	CE1-NE2-CD2	-5.53	103.47	109.00
2	H	268	ASP	CA-CB-CG	5.53	118.13	112.60
2	R	293	ILE	CB-CA-C	5.53	118.63	110.77
2	R	417	ALA	CA-C-O	-5.53	114.56	120.42
2	C	119	SER	CA-C-N	-5.53	113.48	120.56
2	C	119	SER	C-N-CA	-5.53	113.48	120.56
2	I	256	PHE	CA-CB-CG	-5.53	108.27	113.80
2	Q	309	ILE	N-CA-C	-5.53	99.72	108.90
2	G	212	GLN	OE1-CD-NE2	-5.53	117.07	122.60
2	G	292	HIS	O-C-N	-5.53	116.71	122.96
2	G	216	ASP	N-CA-C	-5.53	105.34	111.36
2	R	28	ASP	N-CA-CB	-5.53	102.53	110.65
2	G	125	PHE	CA-CB-CG	-5.52	108.28	113.80
1	B	253	PHE	CA-C-N	5.52	127.99	120.54
1	B	253	PHE	C-N-CA	5.52	127.99	120.54
2	I	367	ASP	CA-C-N	-5.52	113.84	122.73
2	I	367	ASP	C-N-CA	-5.52	113.84	122.73
2	G	277	ASN	OD1-CG-ND2	-5.52	117.08	122.60
2	I	277	ASN	CB-CG-ND2	5.52	124.68	116.40
2	S	384	VAL	CA-C-O	-5.52	114.63	120.64
3	D	35	GLU	CB-CG-CD	5.52	121.98	112.60
3	N	31	GLU	O-C-N	5.52	127.98	122.08
2	J	298	HIS	CB-CG-CD2	-5.51	124.03	131.20
2	S	206	ILE	CA-C-O	-5.51	114.59	121.04
1	A	232	GLN	N-CA-C	5.51	120.41	111.37
1	B	293	ILE	CA-C-O	5.51	126.20	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	58	TRP	CB-CA-C	5.51	118.61	111.50
2	G	31	PRO	CA-C-O	-5.51	115.06	121.34
2	S	43	SER	CA-C-O	-5.51	114.69	120.09
3	L	91	GLY	O-C-N	5.51	127.90	123.49
2	S	249	GLU	CB-CG-CD	5.51	121.97	112.60
2	S	80	TYR	N-CA-C	-5.51	103.96	111.56
3	E	88	ARG	O-C-N	5.50	129.22	122.84
2	J	234	GLU	CB-CG-CD	-5.50	103.25	112.60
2	Q	39	ALA	CA-C-N	5.50	130.75	122.99
2	Q	39	ALA	C-N-CA	5.50	130.75	122.99
2	G	148	PHE	N-CA-C	-5.50	101.87	110.17
2	S	327	HIS	N-CA-C	-5.50	102.14	110.28
2	C	147	THR	N-CA-C	5.50	118.03	111.71
3	L	12	PHE	CA-CB-CG	-5.50	108.30	113.80
3	M	105	VAL	N-CA-CB	-5.50	105.02	112.16
2	Q	173	THR	N-CA-C	-5.50	100.22	109.07
2	Q	135	LEU	CA-C-O	-5.49	114.39	120.60
2	Q	368	TRP	N-CA-C	5.49	120.26	113.50
2	S	438	TYR	O-C-N	5.49	127.80	122.09
2	I	402	PHE	CA-CB-CG	5.49	119.29	113.80
3	L	106	HIS	CB-CG-ND1	-5.49	114.46	122.70
2	J	220	PHE	CA-C-O	5.49	126.24	120.42
3	O	81	GLU	N-CA-C	-5.49	106.71	113.41
3	P	31	GLU	N-CA-C	5.49	120.43	111.37
1	T	237	LEU	N-CA-C	5.49	118.02	111.71
1	B	289	ARG	N-CA-C	-5.49	99.49	108.76
3	K	32	TYR	CA-C-O	-5.49	114.78	120.92
3	M	18	LEU	CD1-CG-CD2	5.49	122.87	110.80
2	G	292	HIS	CB-CG-ND1	5.48	130.93	122.70
1	T	295	THR	N-CA-C	5.48	117.26	111.28
2	G	363	PHE	CA-C-O	-5.48	112.65	119.28
2	C	90	VAL	CB-CA-C	5.48	117.71	110.91
2	Q	420	ASN	N-CA-C	-5.48	102.39	111.37
2	H	72	ASP	CB-CA-C	-5.48	102.52	110.96
2	J	230	ALA	N-CA-C	5.48	116.93	111.07
2	J	400	LEU	CA-C-O	-5.48	114.36	120.66
2	C	177	LYS	O-C-N	5.47	127.94	122.08
3	N	87	ILE	N-CA-C	-5.47	100.42	108.85
2	R	129	ALA	N-CA-C	5.47	119.06	112.38
2	J	125	PHE	CA-CB-CG	5.47	119.27	113.80
2	I	59	ALA	O-C-N	5.47	127.70	122.07
2	I	422	VAL	CA-C-O	-5.47	115.72	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	GLN	OE1-CD-NE2	-5.46	117.14	122.60
2	G	124	VAL	CA-C-N	5.46	128.35	120.38
2	G	124	VAL	C-N-CA	5.46	128.35	120.38
3	N	99	GLN	N-CA-C	5.46	117.37	108.63
3	P	59	LYS	CA-C-O	-5.46	111.90	119.16
3	E	31	GLU	CA-C-O	-5.46	114.63	121.02
2	Q	59	ALA	N-CA-C	5.46	116.91	111.07
2	G	147	THR	CB-CA-C	-5.46	100.97	110.09
1	T	277	GLU	N-CA-C	-5.46	105.41	111.36
1	F	260	PRO	CB-CA-C	-5.46	104.42	111.46
2	I	325	HIS	CE1-NE2-CD2	5.45	114.45	109.00
2	I	386	HIS	CA-C-O	-5.45	112.67	119.38
2	H	26	THR	O-C-N	5.45	126.24	121.17
2	Q	80	TYR	N-CA-C	-5.45	102.26	110.06
2	Q	170	LEU	CD1-CG-CD2	5.45	122.79	110.80
2	Q	265	ILE	O-C-N	5.45	129.00	122.95
2	Q	296	ALA	CA-C-O	-5.45	115.19	121.19
2	S	227	LYS	N-CA-CB	5.45	118.22	110.16
1	B	252	ARG	N-CA-CB	5.45	118.12	110.12
2	H	30	THR	O-C-N	5.44	125.94	121.31
2	H	174	ILE	N-CA-CB	5.44	117.20	111.00
2	H	248	GLU	CB-CA-C	-5.44	102.34	110.88
2	H	294	HIS	CA-C-O	-5.44	114.83	121.36
2	I	190	TYR	N-CA-CB	5.44	118.05	109.94
3	O	47	HIS	CE1-NE2-CD2	-5.44	103.56	109.00
2	J	155	ILE	N-CA-C	-5.44	105.31	110.42
3	N	33	MET	CB-CA-C	-5.44	101.71	110.74
2	I	48	VAL	CA-C-O	-5.44	114.40	119.62
2	H	389	ALA	CA-C-O	-5.43	114.79	120.55
2	H	125	PHE	N-CA-C	5.43	118.70	111.75
2	R	24	TYR	CA-C-O	-5.43	112.71	119.18
2	C	157	VAL	N-CA-C	-5.43	105.32	110.42
2	C	241	ASN	CB-CG-ND2	-5.43	108.26	116.40
2	R	56	ALA	N-CA-C	5.43	116.88	111.07
2	Q	416	GLY	CA-C-N	5.43	127.55	120.28
2	Q	416	GLY	C-N-CA	5.43	127.55	120.28
3	O	35	GLU	CA-C-O	-5.42	114.12	120.20
2	Q	292	HIS	CA-C-N	5.42	130.48	122.94
2	Q	292	HIS	C-N-CA	5.42	130.48	122.94
2	C	425	GLU	CA-C-O	5.42	127.03	121.07
2	C	175	LYS	O-C-N	5.42	125.78	121.55
2	C	256	PHE	N-CA-CB	5.42	118.02	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	302	ASP	O-C-N	-5.42	116.36	122.10
2	I	175	LYS	CA-C-O	-5.42	115.08	120.66
2	Q	178	LEU	N-CA-C	-5.42	100.89	108.96
2	S	286	ASP	N-CA-C	5.42	117.89	111.33
1	F	263	PRO	CB-CA-C	-5.42	104.01	111.21
2	H	238	HIS	CB-CG-ND1	5.42	130.82	122.70
2	J	162	LEU	CA-C-N	-5.42	115.27	124.31
2	J	162	LEU	C-N-CA	-5.42	115.27	124.31
2	R	401	GLN	CB-CG-CD	-5.42	103.39	112.60
1	B	232	GLN	CB-CG-CD	-5.42	103.39	112.60
2	C	59	ALA	N-CA-C	5.42	117.26	111.36
2	S	343	LEU	CD1-CG-CD2	-5.42	98.89	110.80
1	B	263	PRO	CB-CA-C	-5.41	104.48	111.46
2	G	267	HIS	CA-C-N	5.41	129.61	122.30
2	G	267	HIS	C-N-CA	5.41	129.61	122.30
2	G	393	ILE	CB-CA-C	5.41	119.69	112.22
2	I	438	TYR	N-CA-C	5.41	120.25	111.37
3	L	63	PHE	CA-C-O	-5.41	114.68	120.42
2	Q	327	HIS	ND1-CE1-NE2	5.41	113.81	108.40
2	G	291	LEU	CA-C-O	5.41	126.17	120.33
2	H	249	GLU	O-C-N	-5.41	115.89	122.22
2	G	309	ILE	CA-C-O	5.41	126.73	120.67
3	N	24	ARG	CA-C-N	5.41	127.53	120.28
3	N	24	ARG	C-N-CA	5.41	127.53	120.28
2	S	175	LYS	CA-C-O	-5.41	114.35	120.46
3	L	35	GLU	CA-C-N	-5.41	114.00	122.65
3	L	35	GLU	C-N-CA	-5.41	114.00	122.65
2	Q	51	ASP	N-CA-C	5.41	117.17	111.28
2	R	242	VAL	N-CA-CB	-5.41	105.13	112.16
2	G	354	ILE	N-CA-C	-5.41	100.05	108.81
2	G	243	THR	N-CA-C	-5.41	102.05	110.10
2	S	415	PRO	CA-C-N	-5.40	113.98	119.98
2	S	415	PRO	C-N-CA	-5.40	113.98	119.98
3	E	95	ILE	N-CA-CB	5.40	116.51	110.62
3	M	52	GLU	CB-CA-C	5.40	119.42	110.78
1	T	239	GLN	N-CA-C	5.40	119.35	112.87
2	R	382	ILE	CA-C-O	-5.40	114.74	120.14
3	M	57	MET	O-C-N	-5.40	115.91	122.82
2	R	62	SER	CA-C-N	5.39	130.33	122.08
2	R	62	SER	C-N-CA	5.39	130.33	122.08
2	H	391	VAL	CB-CA-C	-5.39	104.05	111.65
3	D	92	PHE	CA-CB-CG	5.39	119.19	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	208	SER	N-CA-C	5.39	118.93	111.71
2	R	253	ARG	N-CA-C	-5.39	105.49	111.36
1	T	228	GLU	N-CA-C	-5.39	105.31	111.07
3	N	72	LEU	CD1-CG-CD2	-5.38	98.95	110.80
2	G	155	ILE	O-C-N	5.38	127.19	121.91
2	Q	253	ARG	N-CA-CB	5.38	117.81	110.01
2	S	24	TYR	CA-C-O	-5.38	114.02	120.10
2	G	345	PHE	CA-C-N	5.38	127.54	120.60
2	G	345	PHE	C-N-CA	5.38	127.54	120.60
2	I	21	LYS	CA-C-O	5.38	126.44	120.63
3	N	63	PHE	CA-CB-CG	-5.38	108.42	113.80
2	H	120	ILE	CA-C-O	-5.38	115.15	120.85
2	I	285	ARG	N-CA-C	5.38	117.56	111.11
2	I	276	ALA	CA-C-N	-5.38	113.45	120.44
2	I	276	ALA	C-N-CA	-5.38	113.45	120.44
3	L	26	ILE	N-CA-C	-5.38	105.26	110.42
2	I	206	ILE	CB-CG1-CD1	5.38	125.09	113.80
2	J	144	LEU	N-CA-C	-5.38	105.46	112.23
2	C	444	ILE	N-CA-CB	-5.37	104.55	110.51
2	H	167	ARG	N-CA-CB	5.37	116.32	111.27
2	Q	169	MET	CA-C-N	-5.37	114.47	122.74
2	Q	169	MET	C-N-CA	-5.37	114.47	122.74
2	Q	401	GLN	CG-CD-NE2	-5.37	108.34	116.40
2	S	73	LEU	N-CA-CB	-5.37	102.22	110.44
2	H	442	GLY	N-CA-C	5.37	119.17	112.73
2	H	202	ASP	N-CA-C	5.37	117.61	110.53
2	I	50	ALA	N-CA-C	5.37	117.13	111.28
2	R	197	LEU	N-CA-CB	-5.37	101.72	109.83
3	L	19	PRO	N-CA-CB	-5.37	100.18	103.19
2	G	318	LEU	CD1-CG-CD2	5.37	122.60	110.80
2	J	199	PHE	N-CA-C	-5.37	101.14	109.14
2	Q	326	LEU	N-CA-C	5.37	118.14	108.48
2	G	324	ASP	N-CA-C	5.36	117.20	111.36
3	L	99	GLN	N-CA-C	5.36	118.34	110.30
2	I	431	ARG	N-CA-C	-5.36	105.54	111.71
2	R	89	PRO	CB-CA-C	5.36	118.09	111.23
3	D	9	GLU	CB-CA-C	-5.36	102.09	110.94
2	H	147	THR	N-CA-C	5.36	117.12	111.28
2	S	307	HIS	N-CA-C	-5.36	99.87	108.55
1	T	293	ILE	N-CA-CB	5.36	118.81	111.41
2	J	385	TRP	N-CA-C	5.36	117.12	111.28
2	I	211	PHE	CA-C-N	-5.36	115.45	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	211	PHE	C-N-CA	-5.36	115.45	123.00
3	K	70	GLN	OE1-CD-NE2	-5.36	117.24	122.60
3	N	47	HIS	N-CA-C	-5.36	101.32	108.34
2	S	35	ASP	CA-C-O	-5.36	115.11	121.16
2	S	100	PHE	CA-C-N	5.36	130.39	122.94
2	S	100	PHE	C-N-CA	5.36	130.39	122.94
2	C	163	ASN	CA-CB-CG	5.36	117.95	112.60
2	Q	346	VAL	N-CA-C	5.36	115.98	110.36
1	T	252	ARG	CA-C-O	-5.35	114.75	120.42
3	D	45	ASN	OD1-CG-ND2	5.35	127.95	122.60
2	G	221	VAL	CA-C-N	-5.35	113.48	120.44
2	G	221	VAL	C-N-CA	-5.35	113.48	120.44
2	I	73	LEU	CD1-CG-CD2	5.35	122.57	110.80
3	M	39	HIS	CB-CG-ND1	5.35	130.73	122.70
2	G	362	VAL	N-CA-C	-5.35	100.18	107.99
2	I	326	LEU	CA-C-O	-5.35	114.12	120.43
2	J	294	HIS	CA-C-O	-5.35	115.20	121.46
1	A	299	SER	CA-C-N	-5.35	115.62	123.00
1	A	299	SER	C-N-CA	-5.35	115.62	123.00
3	O	43	GLU	CA-C-O	-5.35	114.86	121.06
2	S	427	CYS	N-CA-C	5.35	117.11	111.28
2	G	290	LEU	N-CA-C	5.34	117.19	110.24
2	H	460	ASP	N-CA-C	5.34	118.59	111.75
1	T	301	VAL	CA-C-O	-5.34	114.20	118.90
2	I	443	ASP	CA-C-N	5.34	127.29	120.56
2	I	443	ASP	C-N-CA	5.34	127.29	120.56
2	H	197	LEU	N-CA-C	5.34	117.97	109.96
2	G	371	MET	CA-C-O	-5.34	115.01	119.76
2	Q	143	ALA	O-C-N	-5.34	116.46	122.12
2	C	396	ASP	CA-CB-CG	-5.34	107.26	112.60
1	F	247	HIS	N-CA-C	-5.34	101.07	109.50
2	Q	310	HIS	CA-CB-CG	-5.34	108.46	113.80
2	H	423	ALA	N-CA-C	-5.33	105.47	111.28
2	I	227	LYS	CG-CD-CE	5.33	123.57	111.30
2	R	309	ILE	N-CA-C	-5.33	100.80	108.53
2	C	22	LEU	CA-C-O	-5.33	112.12	119.05
3	L	36	GLN	CB-CA-C	-5.33	101.55	110.56
2	J	293	ILE	CB-CG1-CD1	5.33	124.99	113.80
2	G	239	TYR	CA-C-O	-5.33	114.28	120.62
3	O	104	ILE	O-C-N	5.32	128.76	122.69
2	S	253	ARG	CA-C-N	5.32	127.73	120.54
2	S	253	ARG	C-N-CA	5.32	127.73	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	184	ASN	CA-CB-CG	-5.32	107.28	112.60
2	C	356	ALA	O-C-N	-5.32	116.33	122.87
3	O	31	GLU	N-CA-C	-5.32	105.38	111.07
2	R	342	THR	CA-CB-OG1	5.32	117.58	109.60
1	B	283	HIS	CE1-NE2-CD2	-5.32	103.68	109.00
2	R	168	PRO	CB-CA-C	5.32	117.94	110.60
2	R	319	ARG	O-C-N	-5.32	116.48	122.12
2	G	391	VAL	O-C-N	-5.32	116.70	121.91
2	R	116	ILE	O-C-N	-5.32	116.70	121.91
2	R	138	ILE	O-C-N	5.32	128.69	123.00
2	I	102	ALA	CA-C-N	5.31	129.68	122.56
2	I	102	ALA	C-N-CA	5.31	129.68	122.56
2	J	291	LEU	CD1-CG-CD2	-5.31	99.11	110.80
2	Q	202	ASP	N-CA-C	-5.31	103.38	110.55
2	H	97	TYR	N-CA-CB	-5.31	103.28	111.46
2	I	319	ARG	CA-C-O	-5.31	114.10	120.10
2	Q	194	ARG	N-CA-CB	5.31	117.93	110.12
2	S	181	SER	N-CA-C	-5.31	103.12	110.35
1	A	245	THR	N-CA-C	-5.31	101.00	109.23
3	M	45	ASN	OD1-CG-ND2	-5.31	117.29	122.60
3	P	39	HIS	CA-C-N	5.31	126.13	120.13
3	P	39	HIS	C-N-CA	5.31	126.13	120.13
2	Q	96	SER	CA-C-O	-5.31	114.59	120.38
2	R	282	LYS	N-CA-CB	5.31	117.70	110.01
3	D	13	GLU	N-CA-C	5.31	120.07	111.37
2	I	139	ARG	CB-CA-C	-5.30	102.71	111.51
2	S	255	GLU	CA-C-O	-5.30	114.93	120.55
2	H	217	ARG	CB-CA-C	-5.30	101.67	110.68
2	J	108	PHE	N-CA-C	-5.30	101.01	109.23
2	S	61	SER	CA-CB-OG	-5.30	100.50	111.10
2	J	242	VAL	CB-CA-C	-5.30	105.12	111.85
3	L	39	HIS	N-CA-C	-5.30	102.50	110.24
3	M	57	MET	CA-C-N	5.30	130.03	122.08
3	M	57	MET	C-N-CA	5.30	130.03	122.08
2	R	203	ASP	N-CA-C	-5.30	102.44	110.28
2	I	78	ASP	CA-CB-CG	5.29	117.89	112.60
2	S	239	TYR	CA-C-N	5.29	129.46	122.42
2	S	239	TYR	C-N-CA	5.29	129.46	122.42
2	C	214	TRP	N-CA-C	-5.29	105.20	110.97
2	S	206	ILE	CA-C-N	-5.29	114.02	122.17
2	S	206	ILE	C-N-CA	-5.29	114.02	122.17
2	H	33	ASP	CA-CB-CG	-5.29	107.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	354	ILE	CA-CB-CG1	5.29	119.40	110.40
2	H	461	LEU	CD1-CG-CD2	5.29	122.44	110.80
2	G	100	PHE	CA-C-N	-5.29	115.64	122.99
2	G	100	PHE	C-N-CA	-5.29	115.64	122.99
2	G	398	SER	CA-C-N	-5.29	115.10	122.71
2	G	398	SER	C-N-CA	-5.29	115.10	122.71
2	I	353	HIS	O-C-N	5.28	129.49	123.31
2	R	189	VAL	CB-CA-C	5.28	118.64	111.88
2	R	230	ALA	CA-C-N	5.28	127.31	120.44
2	R	230	ALA	C-N-CA	5.28	127.31	120.44
2	R	205	ASN	CA-C-O	-5.28	113.90	119.97
2	R	343	LEU	N-CA-CB	5.28	118.07	110.20
2	S	294	HIS	CB-CG-ND1	5.28	130.62	122.70
3	E	42	ILE	CA-C-O	-5.28	114.85	120.39
2	H	286	ASP	CA-C-O	5.28	125.87	119.38
3	E	25	GLN	CA-C-N	5.28	127.21	120.56
3	E	25	GLN	C-N-CA	5.28	127.21	120.56
2	G	401	GLN	N-CA-C	-5.28	100.43	109.24
2	H	368	TRP	CA-C-N	-5.28	114.75	122.40
2	H	368	TRP	C-N-CA	-5.28	114.75	122.40
2	J	355	GLU	N-CA-C	-5.28	102.94	110.59
3	K	30	ILE	CA-C-O	-5.28	115.46	120.95
2	R	120	ILE	N-CA-C	-5.28	104.82	110.36
2	S	294	HIS	ND1-CG-CD2	-5.28	100.82	106.10
2	Q	164	LYS	CG-CD-CE	5.28	123.43	111.30
2	C	115	ASN	N-CA-CB	5.27	117.87	110.12
2	G	154	GLY	N-CA-C	5.27	119.32	112.68
2	I	238	HIS	ND1-CE1-NE2	-5.27	103.13	108.40
2	C	461	LEU	CD1-CG-CD2	5.27	122.39	110.80
2	R	144	LEU	N-CA-CB	5.27	118.45	110.28
1	B	250	LYS	CB-CA-C	-5.27	101.94	110.79
2	C	292	HIS	CA-CB-CG	5.27	119.07	113.80
2	G	326	LEU	CA-C-N	5.27	128.35	120.87
2	G	326	LEU	C-N-CA	5.27	128.35	120.87
2	R	397	ASP	N-CA-CB	-5.27	103.00	110.58
2	S	375	LEU	N-CA-CB	5.27	117.40	110.29
2	C	280	LEU	O-C-N	-5.27	116.15	122.15
2	I	44	PRO	O-C-N	-5.27	116.48	123.01
3	K	97	GLN	CA-C-O	-5.27	114.45	120.98
3	L	79	ARG	CB-CA-C	-5.26	101.90	110.85
2	Q	400	LEU	CA-C-N	-5.26	113.54	121.86
2	Q	400	LEU	C-N-CA	-5.26	113.54	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	220	PHE	N-CA-CB	5.26	117.64	110.01
2	I	233	GLY	CA-C-N	5.26	130.19	122.77
2	I	233	GLY	C-N-CA	5.26	130.19	122.77
2	S	48	VAL	CA-C-O	-5.26	116.05	119.15
2	S	222	ALA	CA-C-O	-5.26	115.30	120.82
2	S	297	MET	N-CA-C	5.26	118.69	111.54
2	I	298	HIS	N-CA-C	-5.26	105.72	111.82
3	L	10	ARG	CA-C-O	-5.26	115.12	120.80
3	N	63	PHE	CA-C-O	5.26	126.18	120.55
2	G	385	TRP	N-CA-C	5.26	119.45	113.19
2	H	157	VAL	CA-C-O	-5.26	115.48	120.95
3	N	44	PHE	CA-CB-CG	5.26	119.06	113.80
2	Q	153	HIS	CB-CG-ND1	-5.26	114.81	122.70
2	C	120	ILE	O-C-N	5.25	127.36	121.90
2	C	401	GLN	CB-CG-CD	-5.25	103.67	112.60
2	C	401	GLN	N-CA-C	-5.25	102.28	110.42
2	I	277	ASN	CA-CB-CG	5.25	117.85	112.60
2	Q	459	LEU	CD1-CG-CD2	5.25	122.36	110.80
2	S	200	THR	CB-CA-C	5.25	119.71	110.36
2	I	194	ARG	N-CA-C	-5.25	105.67	111.71
2	G	206	ILE	CB-CA-C	5.25	117.07	111.35
3	P	77	GLU	N-CA-C	5.25	117.41	111.11
2	R	159	ARG	N-CA-CB	5.25	117.83	110.12
2	S	446	ARG	CA-C-O	-5.25	114.86	120.42
2	G	301	ILE	O-C-N	-5.25	116.01	122.57
2	H	154	GLY	N-CA-C	5.25	121.78	112.02
2	J	42	PHE	N-CA-C	-5.25	101.39	109.52
2	C	149	GLN	N-CA-C	5.25	118.94	112.54
2	J	118	THR	CA-C-O	-5.25	115.31	120.82
1	B	247	HIS	N-CA-C	-5.24	101.10	109.23
2	R	119	SER	CA-C-O	-5.24	113.61	120.00
3	M	64	ASP	CB-CA-C	-5.24	104.56	111.74
3	M	79	ARG	N-CA-CB	5.24	117.82	110.12
3	D	70	GLN	OE1-CD-NE2	5.24	127.84	122.60
2	R	369	ALA	N-CA-C	-5.24	104.21	111.28
3	K	95	ILE	N-CA-C	-5.23	105.61	110.53
2	R	384	VAL	CA-C-O	-5.23	114.94	120.64
2	C	363	PHE	CA-CB-CG	-5.23	108.57	113.80
2	C	117	LEU	O-C-N	-5.23	116.58	122.12
3	K	67	SER	N-CA-C	5.23	116.99	109.04
3	K	97	GLN	N-CA-C	-5.23	104.91	111.92
2	Q	101	ILE	CA-C-O	-5.23	115.01	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	208	SER	N-CA-C	5.23	118.72	111.71
2	C	342	THR	CB-CA-C	5.23	119.09	110.88
2	C	359	SER	CA-CB-OG	5.23	121.56	111.10
2	G	97	TYR	N-CA-C	-5.23	101.12	109.07
2	H	210	PRO	CB-CA-C	-5.23	103.55	112.64
3	N	26	ILE	N-CA-C	-5.23	105.29	110.62
2	Q	60	GLU	CB-CG-CD	5.23	121.48	112.60
2	I	205	ASN	CA-CB-CG	-5.22	107.38	112.60
3	K	15	PHE	N-CA-C	5.22	121.66	113.72
2	G	399	VAL	N-CA-C	-5.22	100.72	108.45
3	K	40	PRO	CB-CA-C	-5.22	104.39	111.12
2	R	288	GLY	N-CA-C	5.22	122.94	114.90
2	G	383	HIS	ND1-CG-CD2	-5.22	100.88	106.10
2	H	145	VAL	N-CA-C	5.22	120.20	109.34
2	I	198	ASP	CA-C-O	-5.22	115.02	120.55
2	G	100	PHE	CA-CB-CG	-5.22	108.58	113.80
1	A	305	LEU	CD1-CG-CD2	5.22	122.28	110.80
2	C	238	HIS	CA-C-N	5.22	130.08	122.41
2	C	238	HIS	C-N-CA	5.22	130.08	122.41
2	G	184	ASN	N-CA-CB	5.22	117.89	110.06
3	M	39	HIS	CA-C-O	-5.22	115.38	119.66
2	R	347	ASP	N-CA-C	-5.22	105.59	111.28
2	I	303	ARG	O-C-N	5.21	127.65	122.12
2	I	23	THR	N-CA-C	5.21	119.77	113.41
2	I	90	VAL	CA-C-O	-5.21	114.82	120.71
1	F	279	CYS	CA-C-N	5.21	127.21	120.44
1	F	279	CYS	C-N-CA	5.21	127.21	120.44
2	G	96	SER	CA-C-O	-5.21	114.73	120.36
2	H	148	PHE	CA-CB-CG	-5.21	108.59	113.80
2	J	314	LEU	N-CA-CB	-5.21	102.46	110.01
2	C	376	PRO	CB-CA-C	-5.21	103.41	110.60
2	I	147	THR	N-CA-C	5.21	119.39	113.19
3	K	47	HIS	ND1-CE1-NE2	5.21	113.61	108.40
1	B	276	LEU	N-CA-C	5.21	116.95	111.28
1	A	273	LEU	CD1-CG-CD2	-5.20	99.35	110.80
2	I	59	ALA	CA-C-N	-5.20	113.55	120.63
2	I	59	ALA	C-N-CA	-5.20	113.55	120.63
2	Q	267	HIS	ND1-CE1-NE2	5.20	113.60	108.40
3	L	12	PHE	CA-C-O	-5.20	115.88	121.45
3	P	12	PHE	N-CA-CB	-5.20	102.62	111.31
2	R	43	SER	CA-C-O	-5.20	114.81	119.59
2	J	148	PHE	CA-CB-CG	5.20	119.00	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	21	LEU	O-C-N	5.20	129.23	122.89
2	R	316	LYS	N-CA-C	-5.20	104.68	111.02
1	B	287	TYR	N-CA-C	5.20	118.01	110.42
2	G	246	THR	CA-C-O	5.20	127.09	121.06
1	T	279	CYS	N-CA-C	5.20	116.63	111.07
2	Q	207	ASN	CB-CA-C	-5.19	101.85	110.37
2	R	302	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	290	LEU	N-CA-C	-5.19	102.37	110.42
3	O	26	ILE	N-CA-C	-5.19	105.32	110.62
2	G	72	ASP	O-C-N	-5.19	116.62	122.12
3	M	103	PHE	CA-C-N	5.19	127.65	120.49
3	M	103	PHE	C-N-CA	5.19	127.65	120.49
2	G	278	THR	OG1-CB-CG2	5.19	119.68	109.30
2	H	293	ILE	O-C-N	5.19	128.70	123.20
2	R	60	GLU	CA-C-N	5.19	130.22	121.14
2	R	60	GLU	C-N-CA	5.19	130.22	121.14
1	B	228	GLU	O-C-N	-5.19	116.23	122.15
2	C	107	LEU	CD1-CG-CD2	5.19	122.21	110.80
2	H	25	TYR	CA-C-O	-5.19	114.73	120.33
2	I	206	ILE	CA-C-O	-5.19	114.15	120.69
3	N	101	VAL	CA-C-O	-5.19	114.86	120.36
1	B	304	ALA	CA-C-O	-5.19	113.81	120.14
2	C	256	PHE	CA-C-O	5.19	126.45	120.90
2	G	209	GLN	N-CA-C	5.19	121.27	109.81
2	R	197	LEU	N-CA-C	5.19	117.75	110.23
2	R	282	LYS	N-CA-C	5.19	116.62	111.07
3	O	19	PRO	O-C-N	5.18	127.58	121.46
2	I	363	PHE	CA-C-O	-5.18	114.01	119.97
2	Q	372	PRO	CA-C-N	5.18	129.03	121.05
2	Q	372	PRO	C-N-CA	5.18	129.03	121.05
3	P	71	VAL	CB-CA-C	-5.18	105.07	112.22
2	C	118	THR	OG1-CB-CG2	5.18	119.66	109.30
2	S	201	LYS	N-CA-C	5.18	117.86	109.06
2	G	185	TYR	CA-C-O	-5.18	115.01	120.55
2	R	367	ASP	CA-C-O	-5.18	114.71	120.66
2	S	367	ASP	CA-CB-CG	5.18	117.78	112.60
2	C	97	TYR	CA-C-N	5.17	129.65	122.77
2	C	97	TYR	C-N-CA	5.17	129.65	122.77
2	H	362	VAL	N-CA-C	-5.17	99.23	107.15
2	S	145	VAL	CB-CA-C	5.17	118.32	111.70
3	K	48	SER	N-CA-C	5.17	116.75	107.80
2	C	103	TYR	CA-C-O	5.17	124.83	119.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	209	GLN	N-CA-C	5.17	117.03	109.84
3	N	48	SER	N-CA-C	5.17	118.48	107.67
2	S	287	ASN	CA-CB-CG	-5.17	107.43	112.60
2	C	185	TYR	O-C-N	5.17	127.61	122.08
2	G	254	ALA	N-CA-C	5.17	116.60	111.07
2	G	140	PHE	CA-C-O	-5.17	114.80	120.17
3	E	89	VAL	CB-CA-C	-5.17	102.99	110.63
2	H	301	ILE	CB-CG1-CD1	5.17	124.65	113.80
3	O	18	LEU	CD1-CG-CD2	5.17	122.16	110.80
2	H	375	LEU	N-CA-C	5.16	119.98	109.60
2	S	364	PHE	CA-C-O	-5.16	114.76	121.73
2	Q	90	VAL	O-C-N	5.16	128.24	122.61
3	K	74	GLU	N-CA-CB	5.16	117.63	109.94
3	N	39	HIS	CG-CD2-NE2	5.16	112.36	107.20
3	P	91	GLY	O-C-N	5.16	129.41	122.70
2	Q	176	PRO	N-CD-CG	-5.16	97.61	103.80
2	R	243	THR	CA-CB-OG1	5.16	117.34	109.60
2	Q	452	SER	CA-CB-OG	-5.16	100.79	111.10
3	M	9	GLU	CB-CG-CD	5.15	121.36	112.60
2	C	209	GLN	CA-C-O	-5.15	114.87	120.69
2	S	177	LYS	CG-CD-CE	5.15	123.15	111.30
3	K	86	TYR	CA-C-O	-5.15	115.95	121.56
2	Q	461	LEU	CD1-CG-CD2	5.15	122.13	110.80
2	I	451	TRP	N-CA-C	5.15	119.55	113.16
2	J	36	LEU	N-CA-C	-5.15	100.02	108.41
3	M	39	HIS	ND1-CG-CD2	-5.15	100.95	106.10
2	G	401	GLN	CA-C-O	-5.15	114.74	120.66
2	H	53	ALA	N-CA-C	-5.15	105.56	111.07
2	C	98	PHE	O-C-N	-5.15	117.35	123.22
2	C	35	ASP	CA-CB-CG	5.14	117.74	112.60
2	I	379	SER	O-C-N	5.14	129.37	122.73
2	I	139	ARG	CA-CB-CG	-5.14	103.81	114.10
2	R	238	HIS	CB-CG-ND1	5.14	130.41	122.70
2	H	185	TYR	CA-C-O	-5.14	114.54	120.24
2	J	185	TYR	O-C-N	-5.14	116.54	122.09
3	L	36	GLN	CG-CD-NE2	5.14	124.11	116.40
2	Q	172	CYS	CA-C-N	-5.14	115.91	123.00
2	Q	172	CYS	C-N-CA	-5.14	115.91	123.00
2	R	437	LEU	N-CA-CB	-5.14	102.54	110.20
2	H	370	SER	CA-CB-OG	-5.14	100.82	111.10
3	E	35	GLU	N-CA-CB	5.14	117.67	110.12
2	G	149	GLN	N-CA-C	-5.14	105.31	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	368	TRP	N-CA-C	5.14	120.67	113.02
2	S	86	HIS	CB-CA-C	5.14	118.26	109.99
2	S	153	HIS	CB-CG-ND1	-5.14	115.00	122.70
3	O	87	ILE	O-C-N	-5.13	117.65	123.20
2	Q	279	THR	CB-CA-C	-5.13	102.27	110.79
2	C	153	HIS	CE1-NE2-CD2	5.13	114.13	109.00
2	C	276	ALA	CA-C-N	5.13	127.11	120.44
2	C	276	ALA	C-N-CA	5.13	127.11	120.44
2	J	236	LYS	CA-C-N	5.13	130.14	121.47
2	J	236	LYS	C-N-CA	5.13	130.14	121.47
3	M	94	ASN	N-CA-C	5.13	116.95	111.36
2	C	363	PHE	N-CA-C	5.13	117.61	111.71
2	G	46	PRO	CB-CA-C	5.13	118.07	111.46
3	K	106	HIS	CG-CD2-NE2	5.13	112.33	107.20
2	R	85	TYR	CB-CA-C	-5.13	101.50	110.17
2	S	118	THR	CB-CA-C	-5.13	102.28	110.79
2	H	339	LYS	CA-CB-CG	-5.12	103.85	114.10
2	H	442	GLY	CA-C-N	5.12	127.41	120.44
2	H	442	GLY	C-N-CA	5.12	127.41	120.44
2	I	448	ALA	CA-C-N	5.12	126.73	120.22
2	I	448	ALA	C-N-CA	5.12	126.73	120.22
3	L	76	ARG	CB-CG-CD	5.12	123.08	111.30
2	Q	353	HIS	CB-CG-CD2	-5.12	124.54	131.20
2	R	40	PHE	CA-C-O	-5.12	115.02	120.40
2	G	397	ASP	N-CA-C	5.12	117.53	109.39
2	I	41	ARG	CB-CA-C	-5.12	101.40	109.80
2	S	290	LEU	CA-C-O	-5.12	115.98	121.56
2	C	36	LEU	CA-C-O	-5.12	114.64	120.32
2	G	100	PHE	O-C-N	5.12	129.06	123.22
2	J	347	ASP	N-CA-C	-5.12	105.39	111.69
2	J	358	ARG	N-CA-C	5.12	119.82	111.37
1	B	245	THR	CA-C-O	-5.12	115.12	121.11
2	I	133	LEU	CA-C-N	-5.12	113.73	122.33
2	I	133	LEU	C-N-CA	-5.12	113.73	122.33
2	I	177	LYS	CA-C-O	-5.12	113.30	119.49
1	B	232	GLN	O-C-N	5.12	127.41	122.09
1	T	257	SER	N-CA-C	5.12	117.58	109.24
2	G	191	GLU	CA-CB-CG	-5.11	103.87	114.10
2	I	294	HIS	CA-CB-CG	5.11	118.91	113.80
2	J	202	ASP	CA-C-O	-5.11	116.13	121.55
2	J	292	HIS	ND1-CE1-NE2	-5.11	103.29	108.40
2	G	171	GLY	CA-C-O	-5.11	117.12	121.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	286	ASP	CA-CB-CG	5.11	117.71	112.60
2	J	109	GLU	N-CA-C	-5.11	102.19	110.32
2	S	310	HIS	CA-C-N	5.11	127.38	120.38
2	S	310	HIS	C-N-CA	5.11	127.38	120.38
2	S	204	GLU	O-C-N	-5.11	116.71	122.12
2	I	144	LEU	CA-C-O	-5.10	114.33	120.10
2	H	350	ARG	CB-CA-C	-5.10	102.00	110.37
2	Q	415	PRO	CA-C-N	5.10	125.60	119.94
2	Q	415	PRO	C-N-CA	5.10	125.60	119.94
1	A	246	GLU	CA-C-O	-5.10	114.48	120.60
2	C	190	TYR	CA-C-O	-5.10	115.05	121.02
2	C	387	MET	CA-C-O	-5.10	113.39	118.34
3	K	72	LEU	N-CA-C	5.10	117.50	111.33
2	Q	194	ARG	CB-CA-C	-5.10	102.33	110.79
2	Q	205	ASN	CA-CB-CG	-5.10	107.50	112.60
2	Q	251	MET	N-CA-C	5.10	117.23	111.11
2	R	115	ASN	CB-CG-ND2	-5.10	108.75	116.40
2	S	371	MET	O-C-N	5.10	125.64	121.31
1	T	250	LYS	CA-C-N	5.10	127.42	120.54
1	T	250	LYS	C-N-CA	5.10	127.42	120.54
1	F	234	ARG	CA-C-O	-5.10	115.47	120.82
2	H	429	GLN	CB-CG-CD	5.10	121.26	112.60
2	J	312	ARG	O-C-N	5.10	127.32	122.07
2	R	271	THR	N-CA-CB	5.10	117.46	110.07
2	S	360	ARG	CA-CB-CG	-5.10	103.91	114.10
2	Q	233	GLY	N-CA-C	5.09	122.93	113.76
2	J	116	ILE	O-C-N	-5.09	116.58	121.83
2	I	158	GLU	O-C-N	5.09	127.31	122.07
2	I	362	VAL	CA-C-N	5.09	128.05	120.31
2	I	362	VAL	C-N-CA	5.09	128.05	120.31
2	J	355	GLU	CA-C-O	-5.09	115.93	121.89
2	Q	318	LEU	CD1-CG-CD2	5.09	122.00	110.80
2	S	206	ILE	N-CA-CB	5.09	117.46	111.66
2	H	112	SER	CB-CA-C	-5.09	102.93	110.62
2	S	25	TYR	CB-CA-C	5.09	119.20	110.81
2	G	328	SER	CA-C-O	-5.09	113.80	119.34
2	H	108	PHE	N-CA-C	-5.09	101.56	109.14
3	K	10	ARG	O-C-N	5.08	129.12	122.87
2	J	438	TYR	CB-CA-C	5.08	119.00	110.92
3	K	35	GLU	N-CA-CB	5.08	117.59	110.12
2	R	235	ILE	CB-CA-C	5.08	119.88	111.59
2	S	128	LYS	CA-C-O	-5.08	112.61	119.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	212	GLN	CG-CD-NE2	-5.08	108.78	116.40
2	H	123	ASN	CA-C-N	5.08	127.69	120.53
2	H	123	ASN	C-N-CA	5.08	127.69	120.53
3	M	32	TYR	N-CA-C	5.08	119.75	111.37
2	G	153	HIS	CB-CG-CD2	5.08	137.80	131.20
2	C	190	TYR	N-CA-C	5.08	119.69	111.37
3	K	103	PHE	O-C-N	-5.08	117.69	123.48
1	T	260	PRO	CB-CA-C	-5.08	104.30	110.95
2	C	85	TYR	N-CA-CB	-5.07	102.95	110.61
2	G	234	GLU	N-CA-C	5.07	118.08	109.76
2	G	310	HIS	CE1-NE2-CD2	-5.07	103.93	109.00
2	H	209	GLN	O-C-N	5.07	125.54	121.38
3	K	45	ASN	CB-CG-ND2	5.07	124.01	116.40
3	K	81	GLU	N-CA-C	-5.07	106.25	112.90
2	Q	299	ALA	CA-C-N	5.07	127.41	120.46
2	Q	299	ALA	C-N-CA	5.07	127.41	120.46
2	S	238	HIS	CB-CG-ND1	5.07	130.31	122.70
2	G	173	THR	N-CA-C	-5.07	102.01	110.17
2	I	229	GLN	CG-CD-NE2	-5.07	108.80	116.40
2	J	292	HIS	CE1-NE2-CD2	5.07	114.07	109.00
2	R	74	LEU	CD1-CG-CD2	5.07	121.95	110.80
2	H	91	GLN	O-C-N	-5.07	116.67	122.95
2	J	327	HIS	ND1-CG-CD2	-5.07	101.03	106.10
2	H	139	ARG	CB-CA-C	-5.06	102.68	110.78
2	R	271	THR	N-CA-C	-5.06	105.67	111.14
2	H	149	GLN	N-CA-C	5.06	118.92	112.34
2	R	148	PHE	CA-C-N	5.06	127.48	120.29
2	R	148	PHE	C-N-CA	5.06	127.48	120.29
2	I	438	TYR	N-CA-CB	5.06	118.32	109.72
2	Q	102	ALA	CA-C-O	-5.06	115.24	120.70
2	Q	272	ALA	N-CA-C	5.06	118.55	112.38
2	R	39	ALA	N-CA-C	5.06	117.00	108.96
2	R	373	GLY	O-C-N	5.06	127.80	122.59
2	S	251	MET	CA-C-O	-5.06	115.69	121.00
3	M	107	ARG	CA-CB-CG	-5.06	103.99	114.10
1	T	261	CYS	CA-C-O	5.06	127.72	121.60
2	R	327	HIS	CA-C-O	-5.05	115.50	121.16
2	C	443	ASP	CA-CB-CG	5.05	117.65	112.60
2	H	211	PHE	O-C-N	-5.05	115.66	122.43
2	I	166	GLY	N-CA-C	5.05	122.58	115.30
3	O	16	SER	CA-CB-OG	-5.05	100.99	111.10
2	C	356	ALA	CA-C-O	5.05	126.75	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	342	THR	N-CA-C	-5.05	104.86	111.02
2	J	194	ARG	N-CA-C	5.05	117.52	111.71
3	P	42	ILE	CA-C-O	-5.05	115.12	120.53
2	G	44	PRO	N-CA-C	5.05	119.24	111.21
3	O	47	HIS	CG-CD2-NE2	5.05	112.25	107.20
3	N	46	GLU	CA-C-N	-5.05	114.11	122.39
3	N	46	GLU	C-N-CA	-5.05	114.11	122.39
3	O	18	LEU	CA-C-N	-5.05	115.18	120.38
3	O	18	LEU	C-N-CA	-5.05	115.18	120.38
3	D	35	GLU	O-C-N	5.04	127.47	122.12
3	M	31	GLU	CA-C-O	-5.04	115.52	121.07
2	Q	346	VAL	O-C-N	-5.04	116.89	121.94
2	S	183	LYS	CA-C-O	5.04	126.12	120.82
2	G	37	LEU	N-CA-C	-5.04	101.65	109.72
3	P	23	ASP	CA-C-N	-5.04	113.89	120.44
3	P	23	ASP	C-N-CA	-5.04	113.89	120.44
2	I	68	THR	CA-C-N	5.04	128.72	121.96
2	I	68	THR	C-N-CA	5.04	128.72	121.96
2	Q	363	PHE	CA-C-N	-5.04	113.53	122.20
2	Q	363	PHE	C-N-CA	-5.04	113.53	122.20
2	R	307	HIS	CE1-NE2-CD2	-5.04	103.96	109.00
2	C	153	HIS	ND1-CE1-NE2	-5.04	103.36	108.40
3	N	39	HIS	CA-C-O	-5.04	114.88	119.62
2	Q	217	ARG	CB-CG-CD	5.04	122.89	111.30
2	H	458	ALA	CA-C-O	-5.04	115.16	120.55
2	R	223	ASP	CA-CB-CG	5.04	117.64	112.60
2	S	98	PHE	CA-C-O	-5.04	114.95	120.69
2	I	326	LEU	O-C-N	5.04	129.22	123.48
2	H	451	TRP	N-CA-C	5.04	119.27	113.18
3	K	72	LEU	O-C-N	5.04	127.46	122.12
3	M	29	GLN	O-C-N	5.04	127.89	122.15
2	R	326	LEU	CA-C-N	-5.04	113.72	120.87
2	R	326	LEU	C-N-CA	-5.04	113.72	120.87
3	D	19	PRO	CA-C-O	-5.03	113.26	120.56
1	A	276	LEU	CD1-CG-CD2	-5.03	99.73	110.80
1	B	273	LEU	CD1-CG-CD2	-5.03	99.73	110.80
2	I	366	GLN	CA-C-O	-5.03	115.22	121.11
3	L	39	HIS	CA-C-O	-5.03	115.46	120.64
2	Q	223	ASP	CA-CB-CG	-5.03	107.57	112.60
2	H	168	PRO	N-CA-C	-5.03	103.38	111.77
2	J	432	ASN	CA-CB-CG	-5.03	107.57	112.60
3	M	66	LYS	CA-C-O	-5.03	112.78	119.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	221	VAL	N-CA-C	5.02	115.74	110.62
2	Q	179	GLY	CA-C-N	-5.02	113.87	121.05
2	Q	179	GLY	C-N-CA	-5.02	113.87	121.05
2	J	269	PHE	CA-C-O	-5.02	115.21	120.63
3	N	97	GLN	N-CA-CB	-5.02	104.36	111.84
2	C	220	PHE	N-CA-CB	5.02	117.29	110.01
2	G	393	ILE	N-CA-C	5.02	115.79	110.72
2	H	300	VAL	CA-C-O	-5.02	115.73	120.95
3	M	106	HIS	CB-CG-CD2	5.02	137.72	131.20
2	R	153	HIS	CB-CG-ND1	-5.02	115.17	122.70
2	S	134	ARG	CB-CA-C	5.02	118.75	111.82
1	A	256	SER	N-CA-CB	-5.02	104.81	112.28
2	I	136	GLU	CA-C-O	-5.02	114.49	120.56
3	L	51	GLU	CA-C-N	-5.02	115.88	122.85
3	L	51	GLU	C-N-CA	-5.02	115.88	122.85
3	M	39	HIS	N-CA-C	-5.02	103.45	109.72
2	Q	208	SER	O-C-N	5.02	128.43	122.21
2	Q	367	ASP	CA-CB-CG	5.02	117.62	112.60
2	R	184	ASN	OD1-CG-ND2	-5.02	117.58	122.60
2	R	270	LEU	N-CA-CB	-5.02	102.73	110.16
2	J	345	PHE	N-CA-C	5.02	117.64	111.82
3	L	25	GLN	CA-C-O	-5.02	115.55	120.82
2	Q	207	ASN	OD1-CG-ND2	-5.02	117.58	122.60
2	I	353	HIS	CA-CB-CG	-5.01	108.78	113.80
2	I	388	PRO	CB-CA-C	-5.01	104.35	112.62
2	I	329	GLY	CA-C-O	-5.01	118.56	122.52
2	H	307	HIS	ND1-CE1-NE2	5.01	113.41	108.40
3	K	16	SER	O-C-N	-5.01	116.36	122.22
3	P	71	VAL	CA-C-O	-5.01	115.54	120.85
2	S	207	ASN	CB-CA-C	-5.01	102.94	111.26
2	H	162	LEU	CA-C-N	5.01	129.66	122.40
2	H	162	LEU	C-N-CA	5.01	129.66	122.40
2	C	106	ASP	N-CA-CB	5.01	117.48	110.12
2	Q	283	TRP	O-C-N	5.01	127.43	122.12
3	E	105	VAL	CB-CA-C	5.00	116.03	110.62
2	I	179	GLY	CA-C-O	-5.00	115.21	119.56
2	J	118	THR	N-CA-C	-5.00	105.72	111.07
2	Q	161	LEU	O-C-N	5.00	127.30	122.09
3	D	50	PRO	N-CA-C	5.00	121.21	113.75
2	J	147	THR	N-CA-C	5.00	118.15	111.75
2	S	384	VAL	N-CA-CB	-5.00	102.69	110.54
2	I	277	ASN	N-CA-C	5.00	116.42	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	37	GLY	CA-C-O	-5.00	113.46	119.06

There are no chirality outliers.

All (332) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	228	GLU	Sidechain
1	A	239	GLN	Sidechain
1	A	275	GLU	Sidechain
1	A	278	ASN	Sidechain
1	A	284	GLU	Sidechain
1	A	294	ASP	Sidechain
1	A	300	ARG	Sidechain
1	A	303	GLU	Sidechain
1	A	307	GLN	Sidechain
1	B	228	GLU	Sidechain
1	B	259	GLN	Sidechain
1	B	271	GLN	Sidechain
1	B	278	ASN	Sidechain
1	B	284	GLU	Sidechain
1	B	300	ARG	Sidechain
1	B	303	GLU	Sidechain
2	C	106	ASP	Sidechain
2	C	115	ASN	Sidechain
2	C	139	ARG	Sidechain
2	C	148	PHE	Sidechain
2	C	153	HIS	Sidechain
2	C	185	TYR	Sidechain
2	C	205	ASN	Sidechain
2	C	207	ASN	Sidechain
2	C	223	ASP	Sidechain
2	C	229	GLN	Sidechain
2	C	238	HIS	Sidechain
2	C	241	ASN	Sidechain
2	C	248	GLU	Sidechain
2	C	253	ARG	Sidechain
2	C	256	PHE	Sidechain
2	C	287	ASN	Sidechain
2	C	29	TYR	Sidechain
2	C	302	ASP	Sidechain
2	C	338	ASP	Sidechain
2	C	353	HIS	Sidechain

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Mol	Chain	Res	Type	Group
2	C	357	ASP	Sidechain
2	C	363	PHE	Sidechain
2	C	367	ASP	Sidechain
2	C	396	ASP	Sidechain
2	C	420	ASN	Sidechain
2	C	440	GLU	Sidechain
2	C	460	ASP	Sidechain
2	C	98	PHE	Sidechain
3	D	49	ASN	Sidechain
3	D	54	TYR	Sidechain
3	D	73	ASP	Sidechain
3	D	84	ASP	Sidechain
3	D	9	GLU	Sidechain
3	D	93	ASP	Sidechain
3	E	54	TYR	Sidechain
3	E	63	PHE	Sidechain
3	E	70	GLN	Sidechain
3	E	79	ARG	Sidechain
3	E	84	ASP	Sidechain
3	E	93	ASP	Sidechain
3	E	99	GLN	Sidechain
1	F	239	GLN	Sidechain
1	F	241	TYR	Sidechain
1	F	271	GLN	Sidechain
1	F	275	GLU	Sidechain
1	F	278	ASN	Sidechain
1	F	284	GLU	Sidechain
1	F	303	GLU	Sidechain
2	G	103	TYR	Sidechain
2	G	127	PHE	Sidechain
2	G	136	GLU	Sidechain
2	G	153	HIS	Sidechain
2	G	156	GLN	Sidechain
2	G	163	ASN	Sidechain
2	G	165	TYR	Sidechain
2	G	190	TYR	Sidechain
2	G	198	ASP	Sidechain
2	G	199	PHE	Sidechain
2	G	203	ASP	Sidechain
2	G	205	ASN	Sidechain
2	G	212	GLN	Sidechain
2	G	216	ASP	Sidechain

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Mol	Chain	Res	Type	Group
2	G	217	ARG	Sidechain
2	G	226	HIS	Sidechain
2	G	24	TYR	Sidechain
2	G	241	ASN	Sidechain
2	G	269	PHE	Sidechain
2	G	277	ASN	Sidechain
2	G	29	TYR	Sidechain
2	G	302	ASP	Sidechain
2	G	325	HIS	Sidechain
2	G	383	HIS	Sidechain
2	G	420	ASN	Sidechain
2	G	421	ARG	Sidechain
2	G	438	TYR	Sidechain
2	G	440	GLU	Sidechain
2	G	95	ASN	Sidechain
2	G	98	PHE	Sidechain
2	H	103	TYR	Sidechain
2	H	125	PHE	Sidechain
2	H	163	ASN	Sidechain
2	H	185	TYR	Sidechain
2	H	191	GLU	Sidechain
2	H	205	ASN	Sidechain
2	H	207	ASN	Sidechain
2	H	223	ASP	Sidechain
2	H	226	HIS	Sidechain
2	H	229	GLN	Sidechain
2	H	234	GLU	Sidechain
2	H	239	TYR	Sidechain
2	H	241	ASN	Sidechain
2	H	256	PHE	Sidechain
2	H	287	ASN	Sidechain
2	H	302	ASP	Sidechain
2	H	325	HIS	Sidechain
2	H	363	PHE	Sidechain
2	H	366	GLN	Sidechain
2	H	383	HIS	Sidechain
2	H	394	PHE	Sidechain
2	H	420	ASN	Sidechain
2	H	425	GLU	Sidechain
2	H	432	ASN	Sidechain
2	H	438	TYR	Sidechain
2	H	447	GLU	Sidechain

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Mol	Chain	Res	Type	Group
2	H	80	TYR	Sidechain
2	H	95	ASN	Sidechain
2	I	115	ASN	Sidechain
2	I	149	GLN	Sidechain
2	I	163	ASN	Sidechain
2	I	165	TYR	Sidechain
2	I	185	TYR	Sidechain
2	I	190	TYR	Sidechain
2	I	202	ASP	Sidechain
2	I	205	ASN	Sidechain
2	I	211	PHE	Sidechain
2	I	212	GLN	Sidechain
2	I	216	ASP	Sidechain
2	I	220	PHE	Sidechain
2	I	223	ASP	Sidechain
2	I	229	GLN	Sidechain
2	I	234	GLU	Sidechain
2	I	24	TYR	Sidechain
2	I	25	TYR	Sidechain
2	I	256	PHE	Sidechain
2	I	285	ARG	Sidechain
2	I	286	ASP	Sidechain
2	I	294	HIS	Sidechain
2	I	302	ASP	Sidechain
2	I	312	ARG	Sidechain
2	I	357	ASP	Sidechain
2	I	383	HIS	Sidechain
2	I	432	ASN	Sidechain
2	I	436	ASP	Sidechain
2	I	438	TYR	Sidechain
2	I	440	GLU	Sidechain
2	I	447	GLU	Sidechain
2	I	460	ASP	Sidechain
2	I	78	ASP	Sidechain
2	I	95	ASN	Sidechain
2	I	98	PHE	Sidechain
2	J	103	TYR	Sidechain
2	J	106	ASP	Sidechain
2	J	127	PHE	Sidechain
2	J	163	ASN	Sidechain
2	J	165	TYR	Sidechain
2	J	198	ASP	Sidechain

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Mol	Chain	Res	Type	Group
2	J	207	ASN	Sidechain
2	J	212	GLN	Sidechain
2	J	238	HIS	Sidechain
2	J	24	TYR	Sidechain
2	J	241	ASN	Sidechain
2	J	248	GLU	Sidechain
2	J	25	TYR	Sidechain
2	J	277	ASN	Sidechain
2	J	287	ASN	Sidechain
2	J	302	ASP	Sidechain
2	J	357	ASP	Sidechain
2	J	363	PHE	Sidechain
2	J	366	GLN	Sidechain
2	J	383	HIS	Sidechain
2	J	386	HIS	Sidechain
2	J	420	ASN	Sidechain
2	J	432	ASN	Sidechain
2	J	438	TYR	Sidechain
2	J	446	ARG	Sidechain
2	J	447	GLU	Sidechain
2	J	95	ASN	Sidechain
2	J	98	PHE	Sidechain
3	K	13	GLU	Sidechain
3	K	23	ASP	Sidechain
3	K	25	GLN	Sidechain
3	K	29	GLN	Sidechain
3	K	39	HIS	Sidechain
3	K	54	TYR	Sidechain
3	K	70	GLN	Sidechain
3	K	84	ASP	Sidechain
3	K	9	GLU	Sidechain
3	K	97	GLN	Sidechain
3	L	45	ASN	Sidechain
3	L	49	ASN	Sidechain
3	L	97	GLN	Sidechain
3	M	23	ASP	Sidechain
3	M	25	GLN	Sidechain
3	M	29	GLN	Sidechain
3	M	39	HIS	Sidechain
3	M	49	ASN	Sidechain
3	M	52	GLU	Sidechain
3	M	53	PHE	Sidechain

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Mol	Chain	Res	Type	Group
3	M	84	ASP	Sidechain
3	M	9	GLU	Sidechain
3	M	97	GLN	Sidechain
3	M	99	GLN	Sidechain
3	N	17	TYR	Sidechain
3	N	23	ASP	Sidechain
3	N	39	HIS	Sidechain
3	N	53	PHE	Sidechain
3	N	9	GLU	Sidechain
3	N	92	PHE	Sidechain
3	N	93	ASP	Sidechain
3	N	97	GLN	Sidechain
3	O	12	PHE	Sidechain
3	O	13	GLU	Sidechain
3	O	23	ASP	Sidechain
3	O	36	GLN	Sidechain
3	O	54	TYR	Sidechain
3	O	82	TYR	Sidechain
3	O	84	ASP	Sidechain
3	O	9	GLU	Sidechain
3	O	97	GLN	Sidechain
3	P	17	TYR	Sidechain
3	P	23	ASP	Sidechain
3	P	32	TYR	Sidechain
3	P	53	PHE	Sidechain
3	P	86	TYR	Sidechain
3	P	92	PHE	Sidechain
3	P	93	ASP	Sidechain
3	P	97	GLN	Sidechain
2	Q	110	GLU	Sidechain
2	Q	127	PHE	Sidechain
2	Q	136	GLU	Sidechain
2	Q	137	ASP	Sidechain
2	Q	153	HIS	Sidechain
2	Q	163	ASN	Sidechain
2	Q	165	TYR	Sidechain
2	Q	185	TYR	Sidechain
2	Q	190	TYR	Sidechain
2	Q	205	ASN	Sidechain
2	Q	207	ASN	Sidechain
2	Q	209	GLN	Sidechain
2	Q	212	GLN	Sidechain

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Mol	Chain	Res	Type	Group
2	Q	226	HIS	Sidechain
2	Q	229	GLN	Sidechain
2	Q	234	GLU	Sidechain
2	Q	24	TYR	Sidechain
2	Q	241	ASN	Sidechain
2	Q	25	TYR	Sidechain
2	Q	253	ARG	Sidechain
2	Q	259	GLU	Sidechain
2	Q	268	ASP	Sidechain
2	Q	277	ASN	Sidechain
2	Q	302	ASP	Sidechain
2	Q	307	HIS	Sidechain
2	Q	324	ASP	Sidechain
2	Q	338	ASP	Sidechain
2	Q	357	ASP	Sidechain
2	Q	401	GLN	Sidechain
2	Q	436	ASP	Sidechain
2	Q	438	TYR	Sidechain
2	Q	446	ARG	Sidechain
2	Q	447	GLU	Sidechain
2	Q	60	GLU	Sidechain
2	Q	95	ASN	Sidechain
2	R	216	ASP	Sidechain
2	R	229	GLN	Sidechain
2	R	239	TYR	Sidechain
2	R	302	ASP	Sidechain
2	R	324	ASP	Sidechain
2	R	325	HIS	Sidechain
2	R	327	HIS	Sidechain
2	R	33	ASP	Sidechain
2	R	338	ASP	Sidechain
2	R	383	HIS	Sidechain
2	R	397	ASP	Sidechain
2	R	440	GLU	Sidechain
2	R	72	ASP	Sidechain
2	R	88	GLU	Sidechain
2	R	95	ASN	Sidechain
2	R	97	TYR	Sidechain
2	R	98	PHE	Sidechain
2	S	103	TYR	Sidechain
2	S	115	ASN	Sidechain
2	S	127	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	S	136	GLU	Sidechain
2	S	139	ARG	Sidechain
2	S	153	HIS	Sidechain
2	S	158	GLU	Sidechain
2	S	163	ASN	Sidechain
2	S	165	TYR	Sidechain
2	S	185	TYR	Sidechain
2	S	205	ASN	Sidechain
2	S	209	GLN	Sidechain
2	S	211	PHE	Sidechain
2	S	212	GLN	Sidechain
2	S	217	ARG	Sidechain
2	S	223	ASP	Sidechain
2	S	229	GLN	Sidechain
2	S	241	ASN	Sidechain
2	S	25	TYR	Sidechain
2	S	256	PHE	Sidechain
2	S	286	ASP	Sidechain
2	S	302	ASP	Sidechain
2	S	304	GLN	Sidechain
2	S	306	ASN	Sidechain
2	S	324	ASP	Sidechain
2	S	325	HIS	Sidechain
2	S	35	ASP	Sidechain
2	S	352	ASP	Sidechain
2	S	357	ASP	Sidechain
2	S	367	ASP	Sidechain
2	S	383	HIS	Sidechain
2	S	432	ASN	Sidechain
2	S	436	ASP	Sidechain
2	S	438	TYR	Sidechain
2	S	440	GLU	Sidechain
2	S	447	GLU	Sidechain
2	S	78	ASP	Sidechain
2	S	85	TYR	Sidechain
2	S	86	HIS	Sidechain
2	S	98	PHE	Sidechain
1	T	239	GLN	Sidechain
1	T	275	GLU	Sidechain
1	T	278	ASN	Sidechain
1	T	283	HIS	Sidechain
1	T	284	GLU	Sidechain

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Mol	Chain	Res	Type	Group
1	T	294	ASP	Sidechain
1	T	307	GLN	Sidechain

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	697	0	684	2	0
1	B	697	0	684	1	0
1	F	697	0	684	2	0
1	T	697	0	684	0	0
2	C	3333	0	3256	4	0
2	G	3333	0	3256	4	0
2	H	3333	0	3256	7	0
2	I	3333	0	3256	4	0
2	J	3333	0	3256	7	0
2	Q	3333	0	3256	3	0
2	R	3333	0	3256	1	0
2	S	3333	0	3256	4	0
3	D	857	0	810	0	0
3	E	857	0	810	1	0
3	K	857	0	810	0	0
3	L	857	0	810	1	0
3	M	857	0	810	0	0
3	N	857	0	810	0	0
3	O	857	0	810	0	0
3	P	857	0	810	0	0
All	All	36308	0	35264	36	0

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

All (36) 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:C:169:MET:HE1	2:C:375:LEU:HD13	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:318:LEU:HD12	2:G:321:SER:OG	1.91	0.71
2:Q:348:LEU:HD23	2:Q:354:ILE:HG21	1.77	0.66
2:C:167:ARG:HH11	2:C:425:GLU:HG3	1.60	0.66
1:F:300:ARG:HE	2:I:30:THR:HB	1.72	0.55
2:C:436:ASP:N	2:C:440:GLU:OE2	2.41	0.54
2:R:169:MET:HE1	2:R:375:LEU:HD13	1.90	0.53
2:H:436:ASP:N	2:H:440:GLU:OE1	2.44	0.50
2:H:142:VAL:HG13	2:H:369:ALA:HB2	1.95	0.49
2:H:264:ILE:HB	2:H:290:LEU:HB2	1.96	0.48
2:H:431:ARG:HE	2:H:437:LEU:HD11	1.79	0.47
2:S:397:ASP:N	2:S:397:ASP:OD1	2.46	0.47
2:S:436:ASP:N	2:S:440:GLU:OE2	2.48	0.47
1:B:300:ARG:HE	2:J:30:THR:HG22	1.79	0.47
2:I:319:ARG:HH11	2:I:349:MET:HA	1.80	0.46
1:A:300:ARG:HE	2:Q:30:THR:HB	1.80	0.46
2:I:253:ARG:HH11	2:I:253:ARG:HG3	1.81	0.46
2:S:253:ARG:HG3	2:S:253:ARG:HH11	1.82	0.45
3:E:79:ARG:HE	3:E:106:HIS:HB2	1.82	0.44
3:L:10:ARG:HE	2:S:232:THR:C	2.25	0.43
2:G:319:ARG:HH11	2:G:349:MET:HA	1.84	0.43
2:H:214:TRP:CE3	2:H:215:ARG:HA	2.55	0.42
2:Q:319:ARG:HH11	2:Q:349:MET:HA	1.84	0.41
2:J:234:GLU:HB2	2:J:236:LYS:NZ	2.35	0.41
2:J:27:PRO:HA	2:J:85:TYR:O	2.20	0.41
1:A:289:ARG:HG3	1:A:305:LEU:HA	2.02	0.41
2:G:357:ASP:HB3	2:G:360:ARG:HE	1.86	0.41
2:J:82:GLY:C	2:J:101:ILE:HD11	2.46	0.41
2:C:205:ASN:OD1	2:G:118:THR:HG22	2.20	0.41
2:H:96:SER:C	2:H:97:TYR:CG	2.99	0.41
2:H:84:CYS:HA	2:H:101:ILE:HA	2.03	0.40
2:J:268:ASP:OD1	2:J:268:ASP:N	2.51	0.40
1:F:264:ILE:HA	1:F:275:GLU:OE1	2.22	0.40
2:I:204:GLU:HG2	2:I:205:ASN:N	2.37	0.40
2:J:295:ARG:O	2:J:295:ARG:HG3	2.21	0.40
2:J:357:ASP:N	2:J:362:VAL:O	2.55	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	84/86 (98%)	84 (100%)	0	0	100	100
1	B	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
1	F	84/86 (98%)	84 (100%)	0	0	100	100
1	T	84/86 (98%)	84 (100%)	0	0	100	100
2	C	418/442 (95%)	415 (99%)	3 (1%)	0	100	100
2	G	418/442 (95%)	415 (99%)	3 (1%)	0	100	100
2	H	418/442 (95%)	413 (99%)	5 (1%)	0	100	100
2	I	418/442 (95%)	414 (99%)	4 (1%)	0	100	100
2	J	418/442 (95%)	414 (99%)	4 (1%)	0	100	100
2	Q	418/442 (95%)	413 (99%)	5 (1%)	0	100	100
2	R	418/442 (95%)	415 (99%)	3 (1%)	0	100	100
2	S	418/442 (95%)	415 (99%)	3 (1%)	0	100	100
3	D	99/101 (98%)	99 (100%)	0	0	100	100
3	E	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
3	K	99/101 (98%)	99 (100%)	0	0	100	100
3	L	99/101 (98%)	99 (100%)	0	0	100	100
3	M	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
3	N	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
3	O	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
3	P	99/101 (98%)	99 (100%)	0	0	100	100
All	All	4472/4688 (95%)	4436 (99%)	36 (1%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	79/79 (100%)	79 (100%)	0	100	100
1	B	79/79 (100%)	79 (100%)	0	100	100
1	F	79/79 (100%)	79 (100%)	0	100	100
1	T	79/79 (100%)	79 (100%)	0	100	100
2	C	347/358 (97%)	346 (100%)	1 (0%)	86	83
2	G	347/358 (97%)	347 (100%)	0	100	100
2	H	347/358 (97%)	347 (100%)	0	100	100
2	I	347/358 (97%)	347 (100%)	0	100	100
2	J	347/358 (97%)	345 (99%)	2 (1%)	78	79
2	Q	347/358 (97%)	347 (100%)	0	100	100
2	R	347/358 (97%)	346 (100%)	1 (0%)	86	83
2	S	347/358 (97%)	347 (100%)	0	100	100
3	D	95/95 (100%)	95 (100%)	0	100	100
3	E	95/95 (100%)	95 (100%)	0	100	100
3	K	95/95 (100%)	95 (100%)	0	100	100
3	L	95/95 (100%)	95 (100%)	0	100	100
3	M	95/95 (100%)	95 (100%)	0	100	100
3	N	95/95 (100%)	95 (100%)	0	100	100
3	O	95/95 (100%)	95 (100%)	0	100	100
3	P	95/95 (100%)	95 (100%)	0	100	100
All	All	3852/3940 (98%)	3848 (100%)	4 (0%)	87	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	167	ARG
2	J	200	THR
2	J	285	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	R	294	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	HIS
2	C	366	GLN
2	C	383	HIS
3	D	47	HIS
3	E	47	HIS
3	E	70	GLN
3	E	99	GLN
2	G	294	HIS
2	H	241	ASN
2	H	307	HIS
2	I	184	ASN
2	J	184	ASN
2	J	429	GLN
3	L	69	GLN
3	M	69	GLN
3	M	70	GLN
3	N	69	GLN
3	O	47	HIS
3	P	47	HIS
2	Q	149	GLN
2	Q	163	ASN
2	R	91	GLN
2	R	267	HIS
2	R	353	HIS
2	R	383	HIS
2	S	207	ASN
2	S	226	HIS
2	S	229	GLN
2	S	241	ASN
2	S	267	HIS
2	S	277	ASN
2	S	383	HIS
2	S	386	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

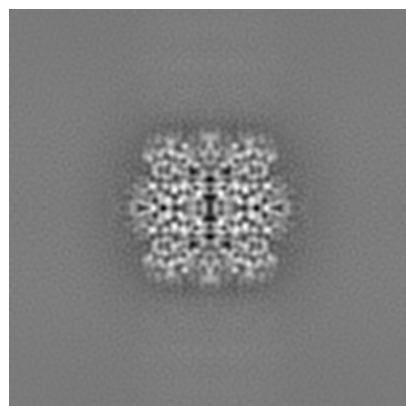
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50836. These allow visual inspection of the internal detail of the map and identification of artifacts.

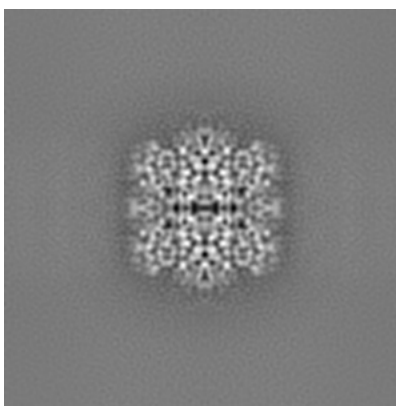
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

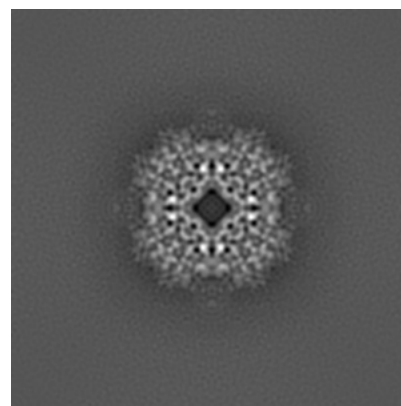
6.1.1 Primary map



X

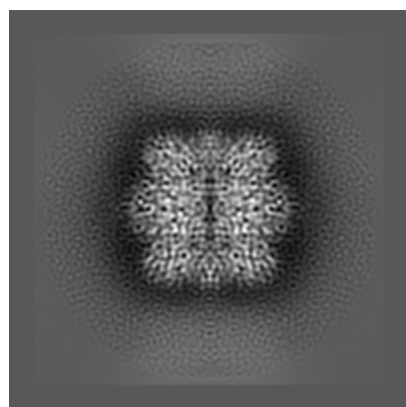


Y

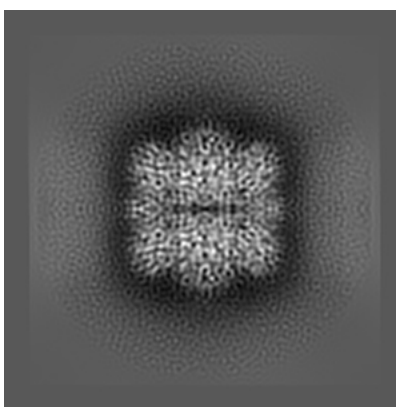


Z

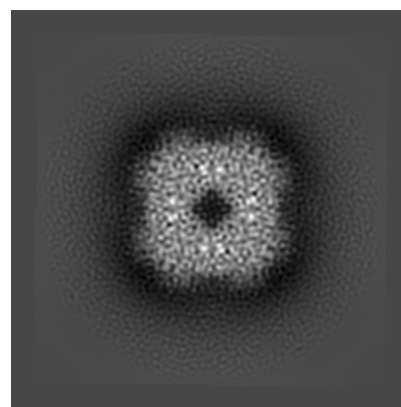
6.1.2 Raw map



X



Y

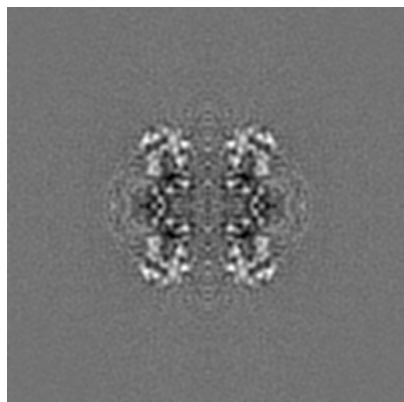


Z

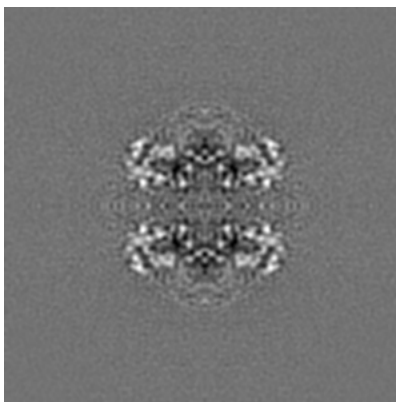
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

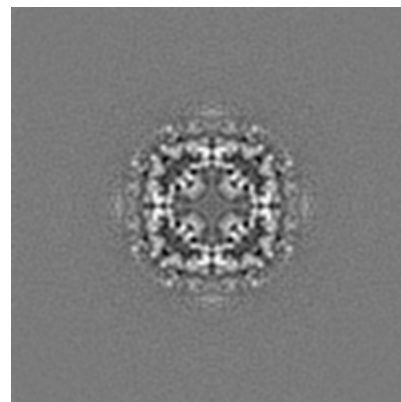
6.2.1 Primary map



X Index: 102

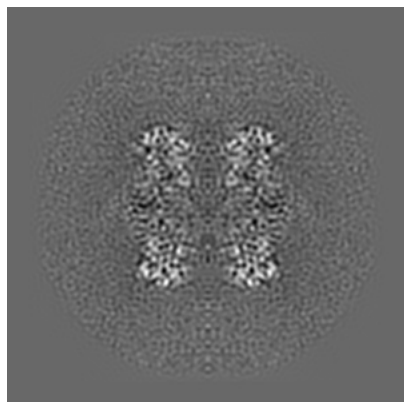


Y Index: 102

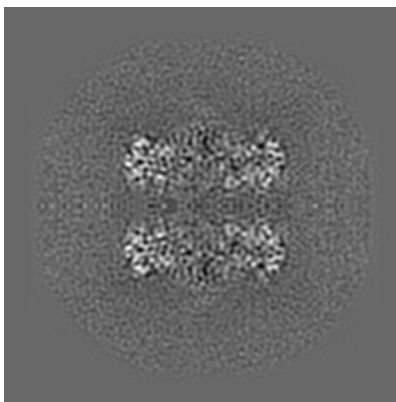


Z Index: 102

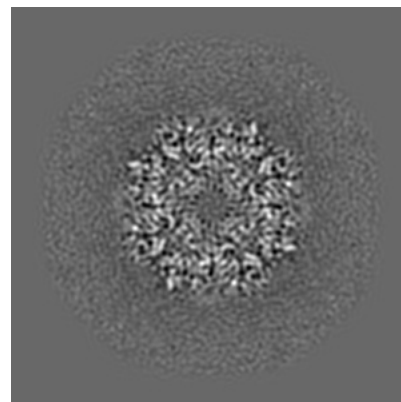
6.2.2 Raw map



X Index: 102



Y Index: 102

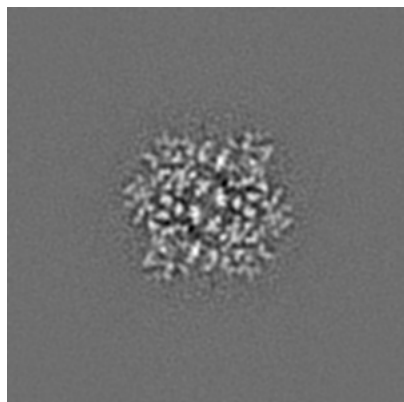


Z Index: 102

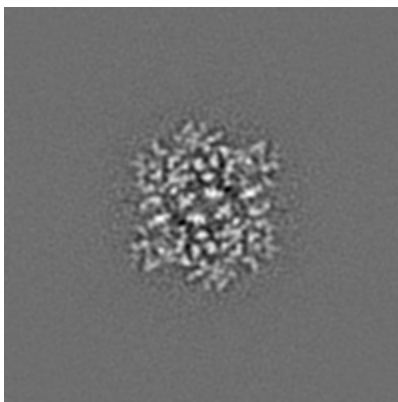
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

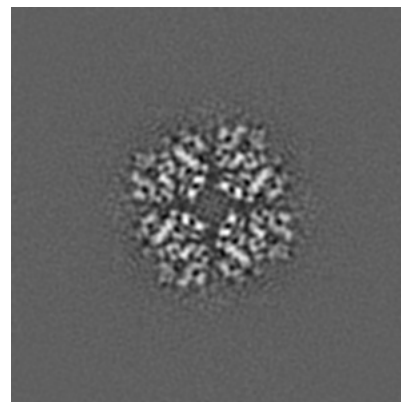
6.3.1 Primary map



X Index: 113

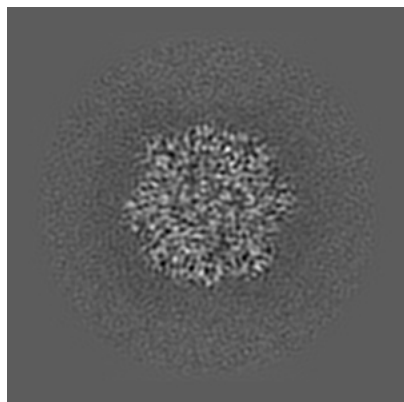


Y Index: 91

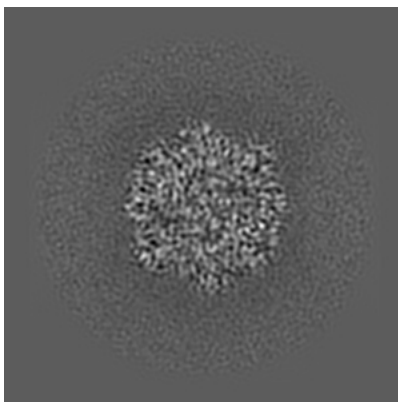


Z Index: 97

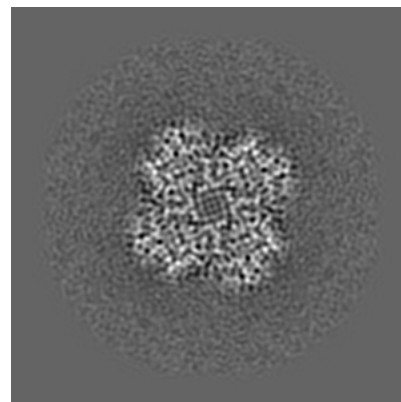
6.3.2 Raw map



X Index: 80



Y Index: 80

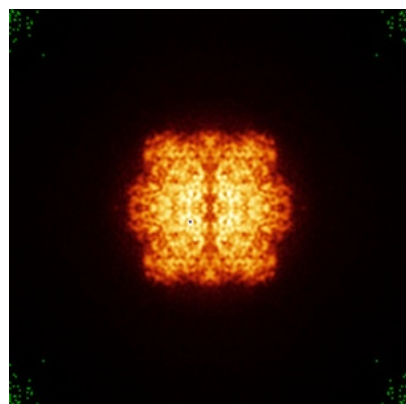


Z Index: 113

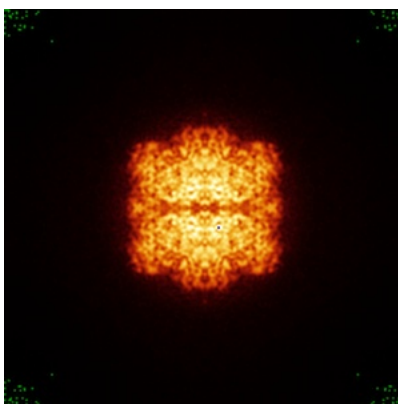
The images above show the largest variance slices of the map in three orthogonal directions.

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

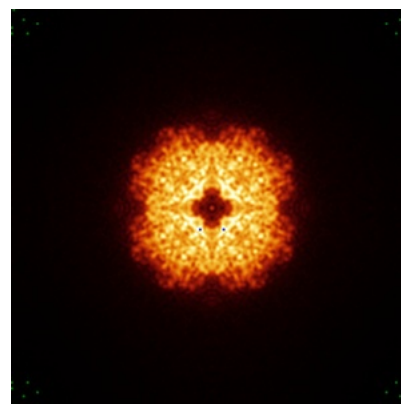
6.4.1 Primary map



X

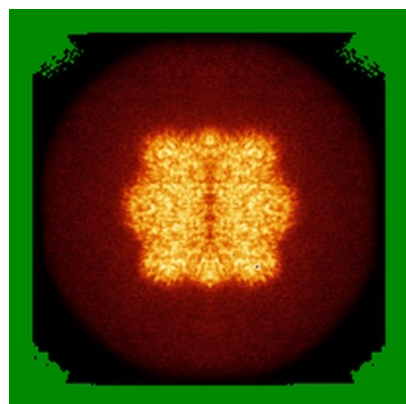


Y

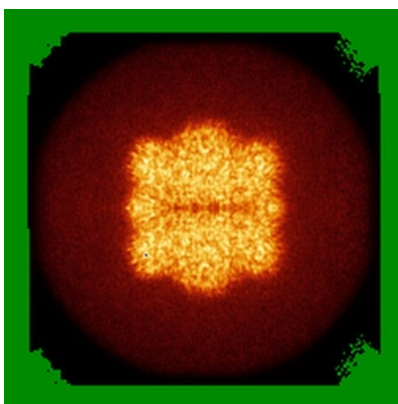


Z

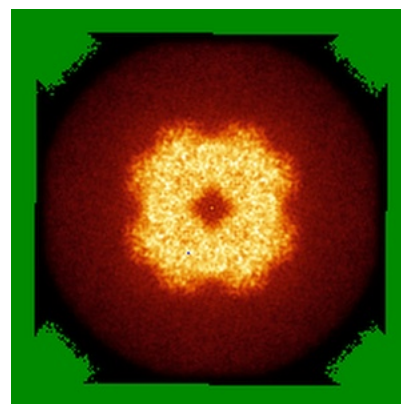
6.4.2 Raw map



X



Y

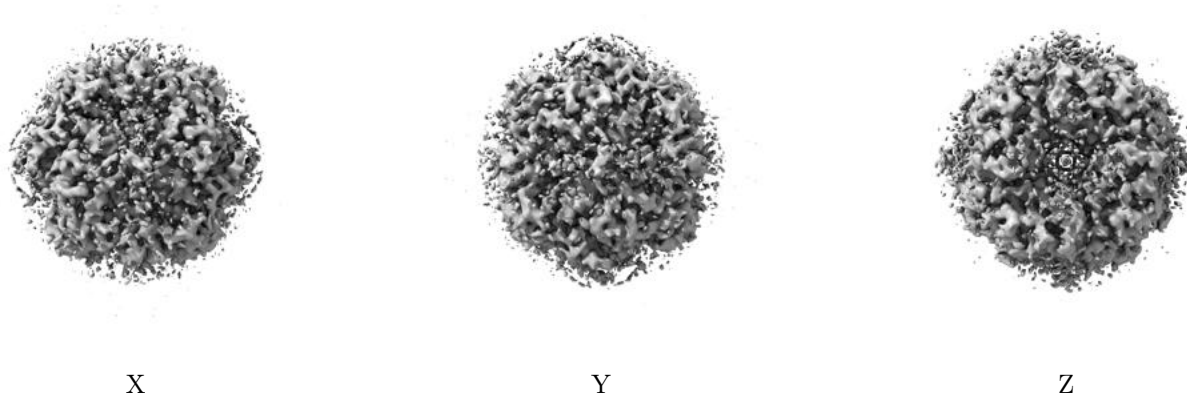


Z

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

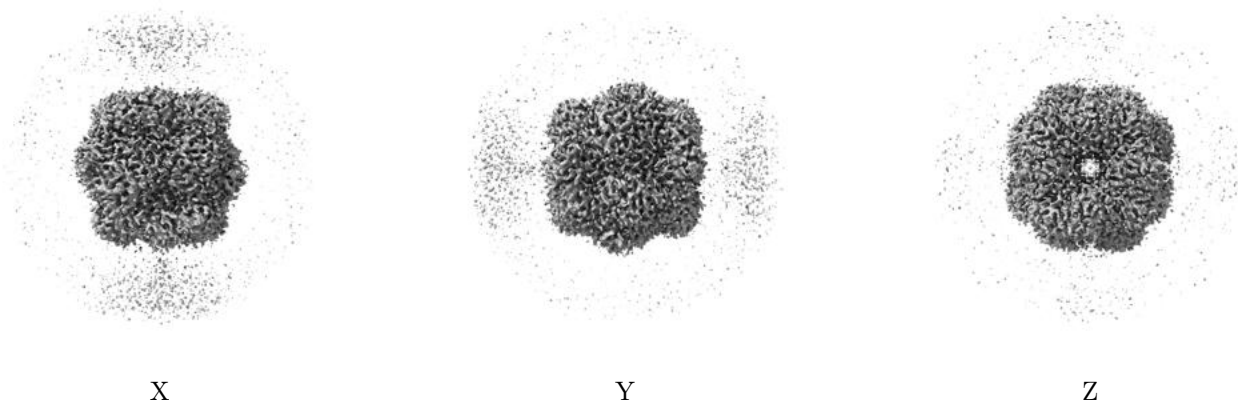
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.311. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

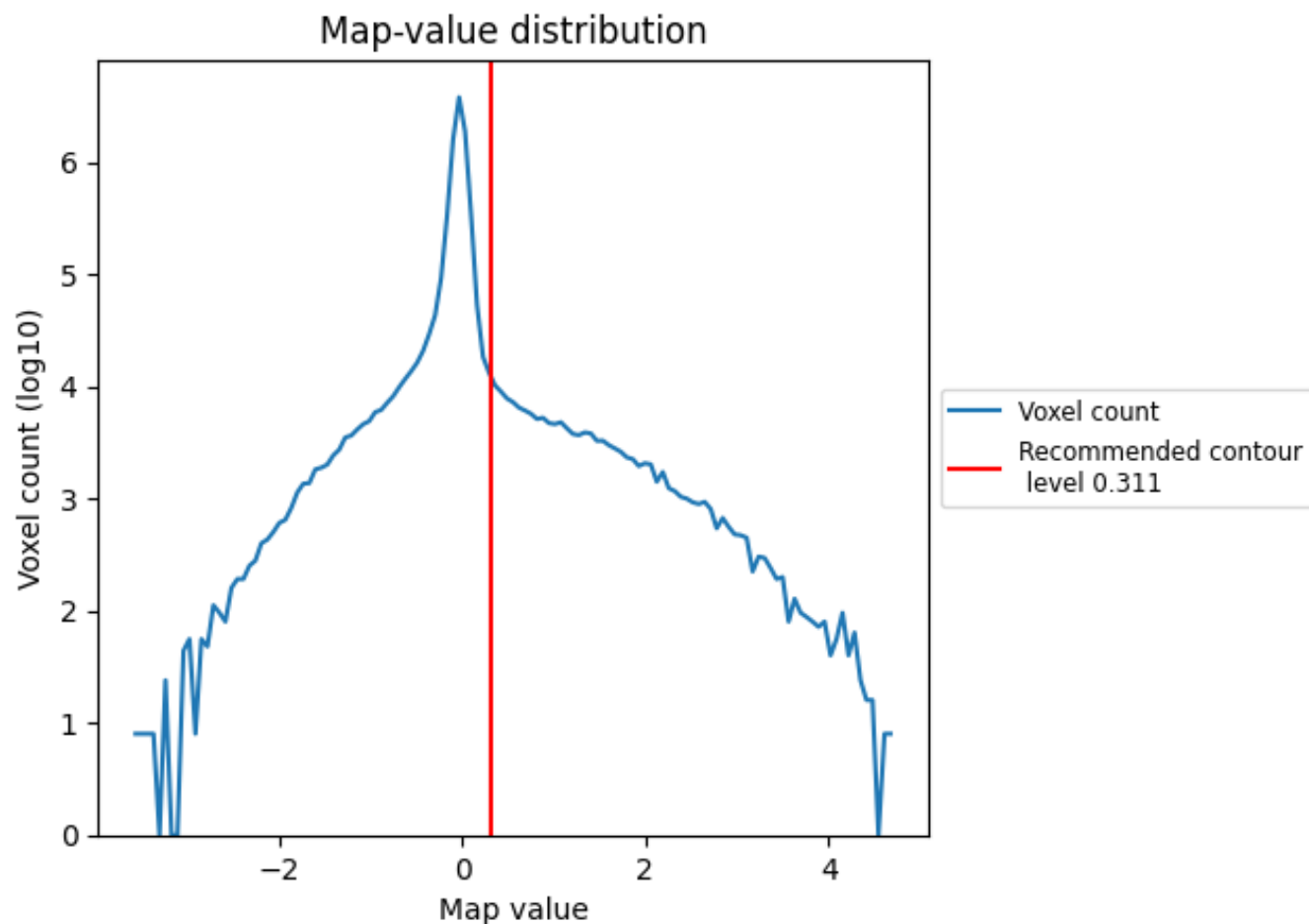
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

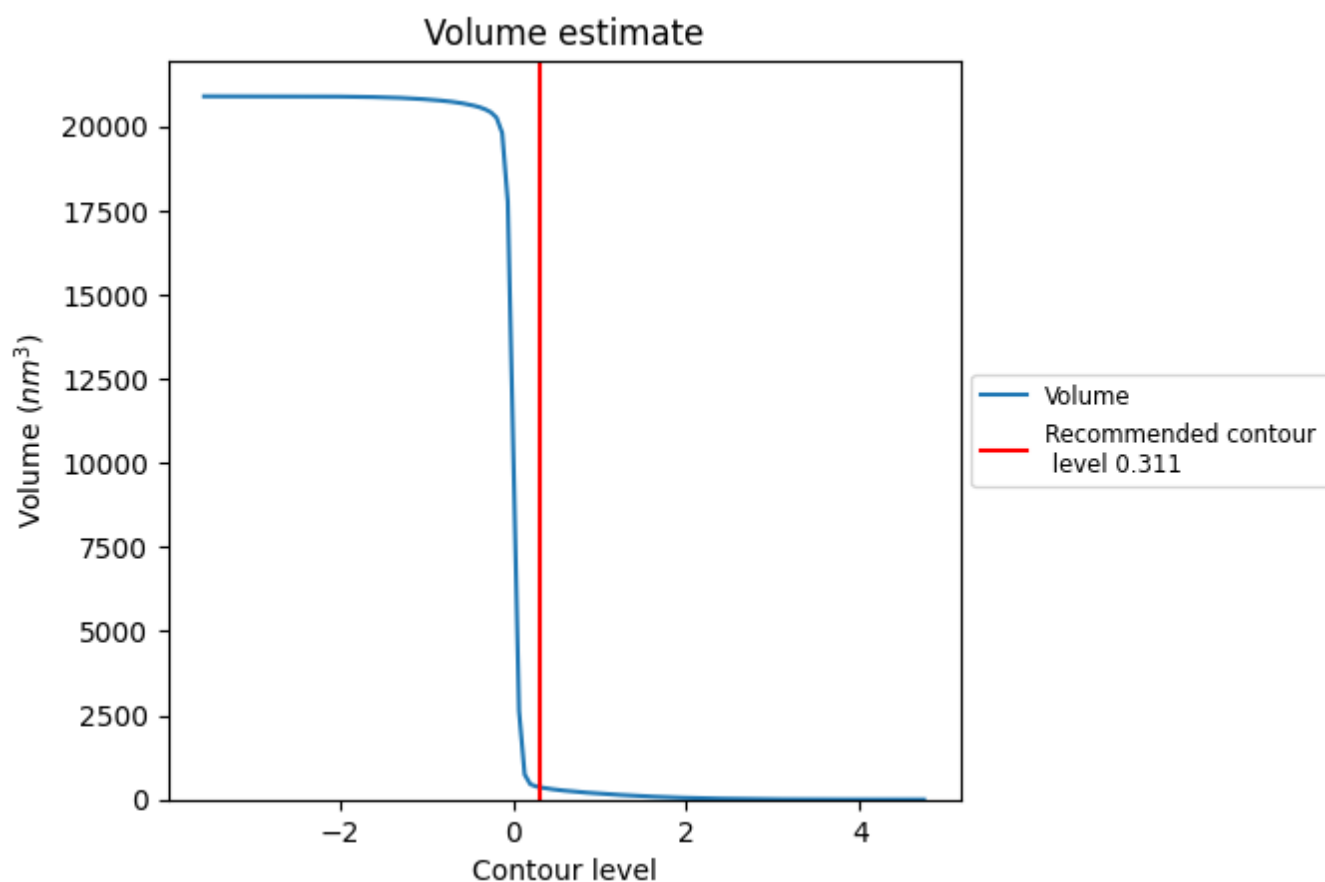
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

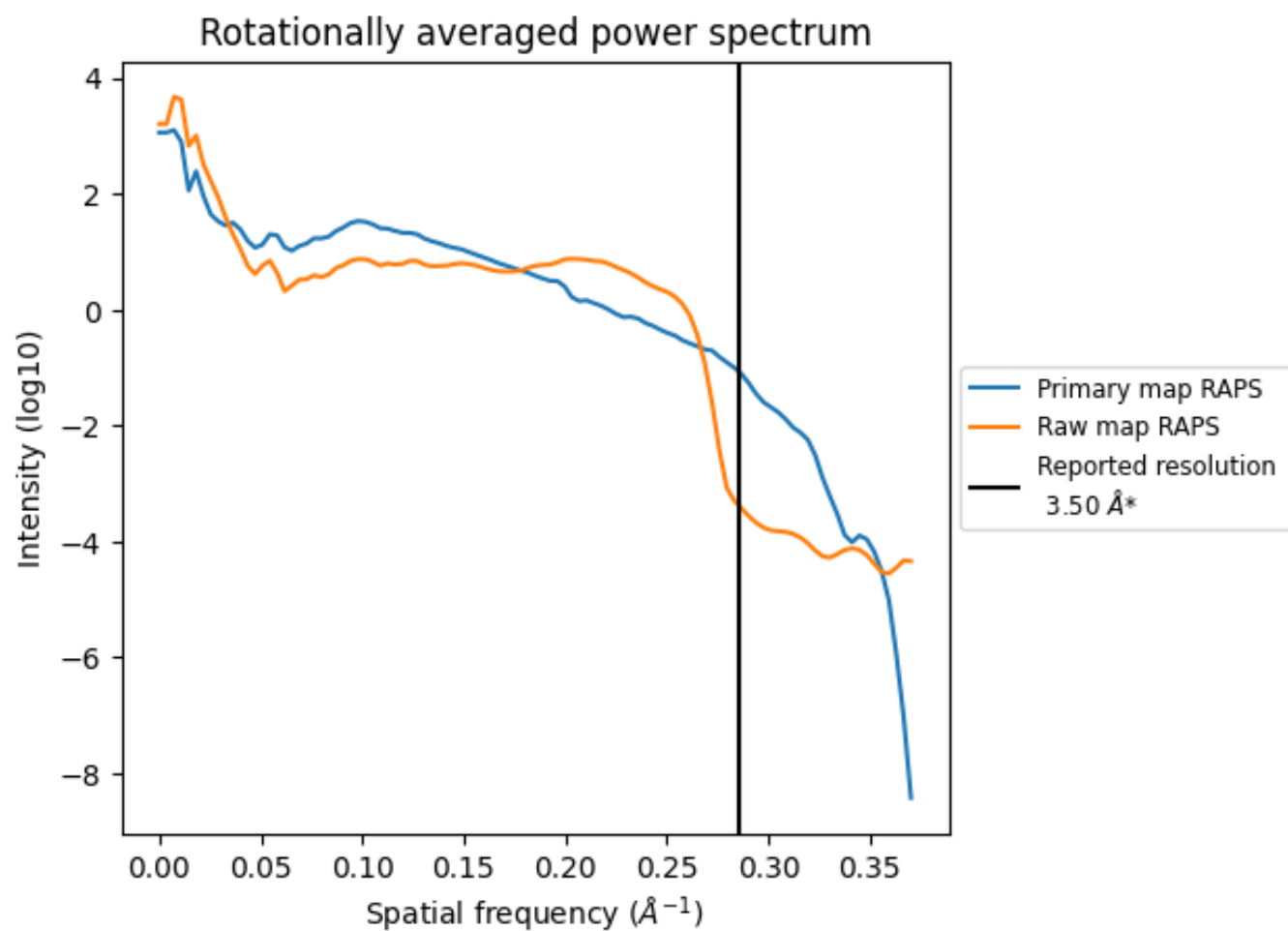
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 365 nm³; this corresponds to an approximate mass of 330 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

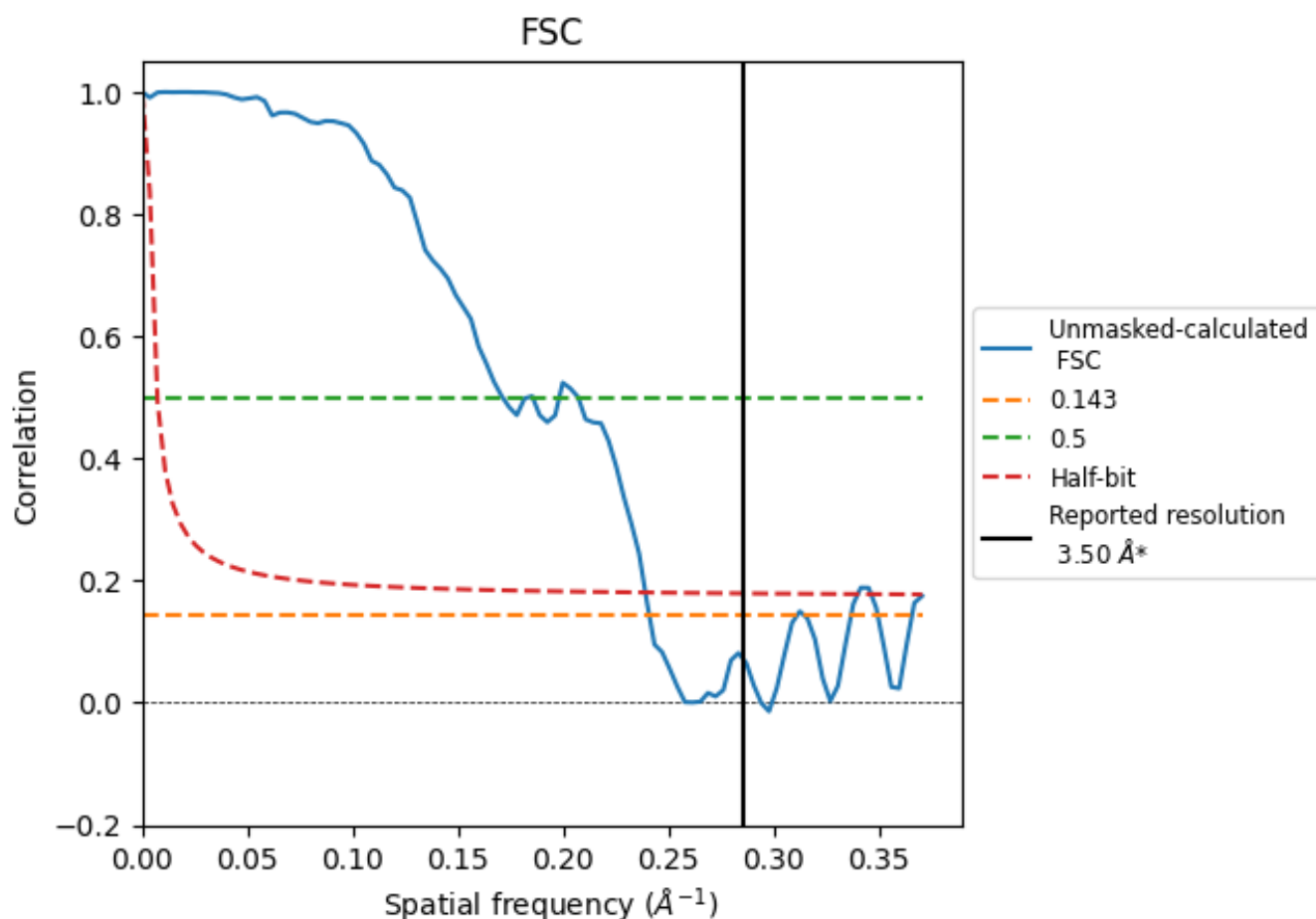


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

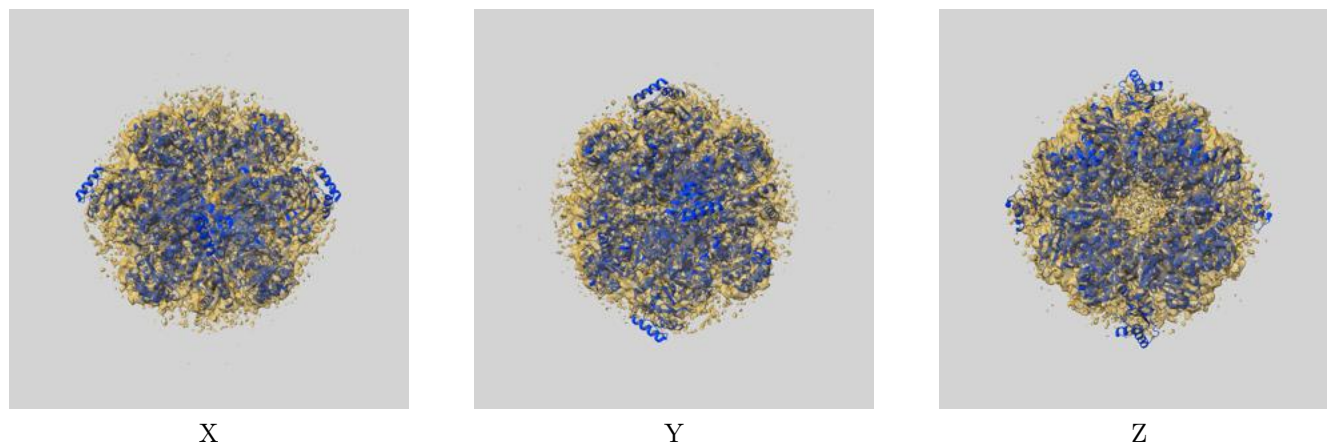
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.15	5.84	4.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

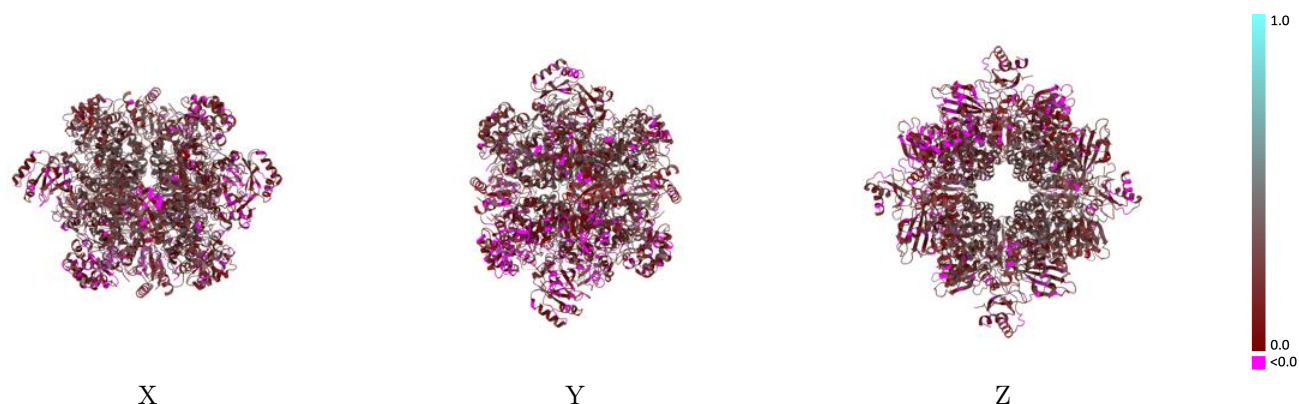
This section contains information regarding the fit between EMDB map EMD-50836 and PDB model 9FWV. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



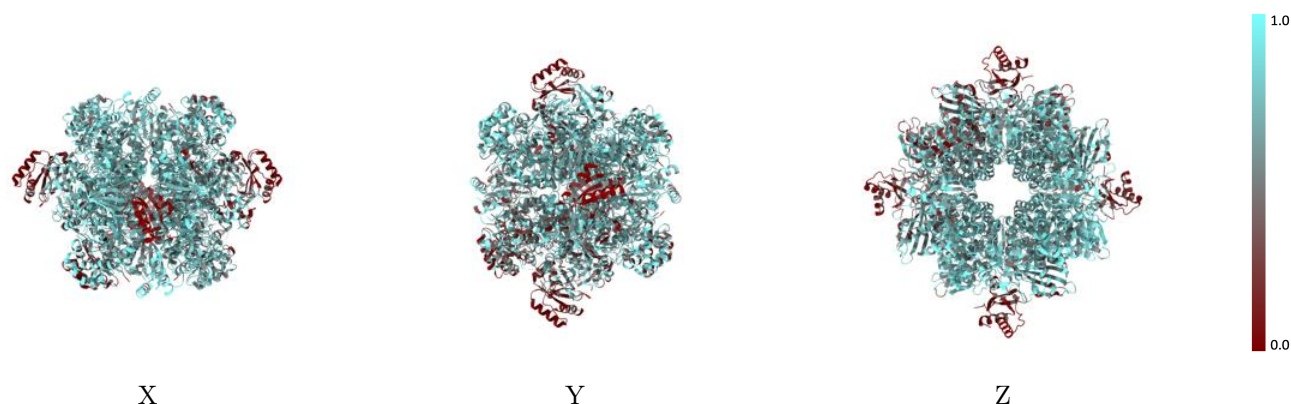
The images above show the 3D surface view of the map at the recommended contour level 0.311 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



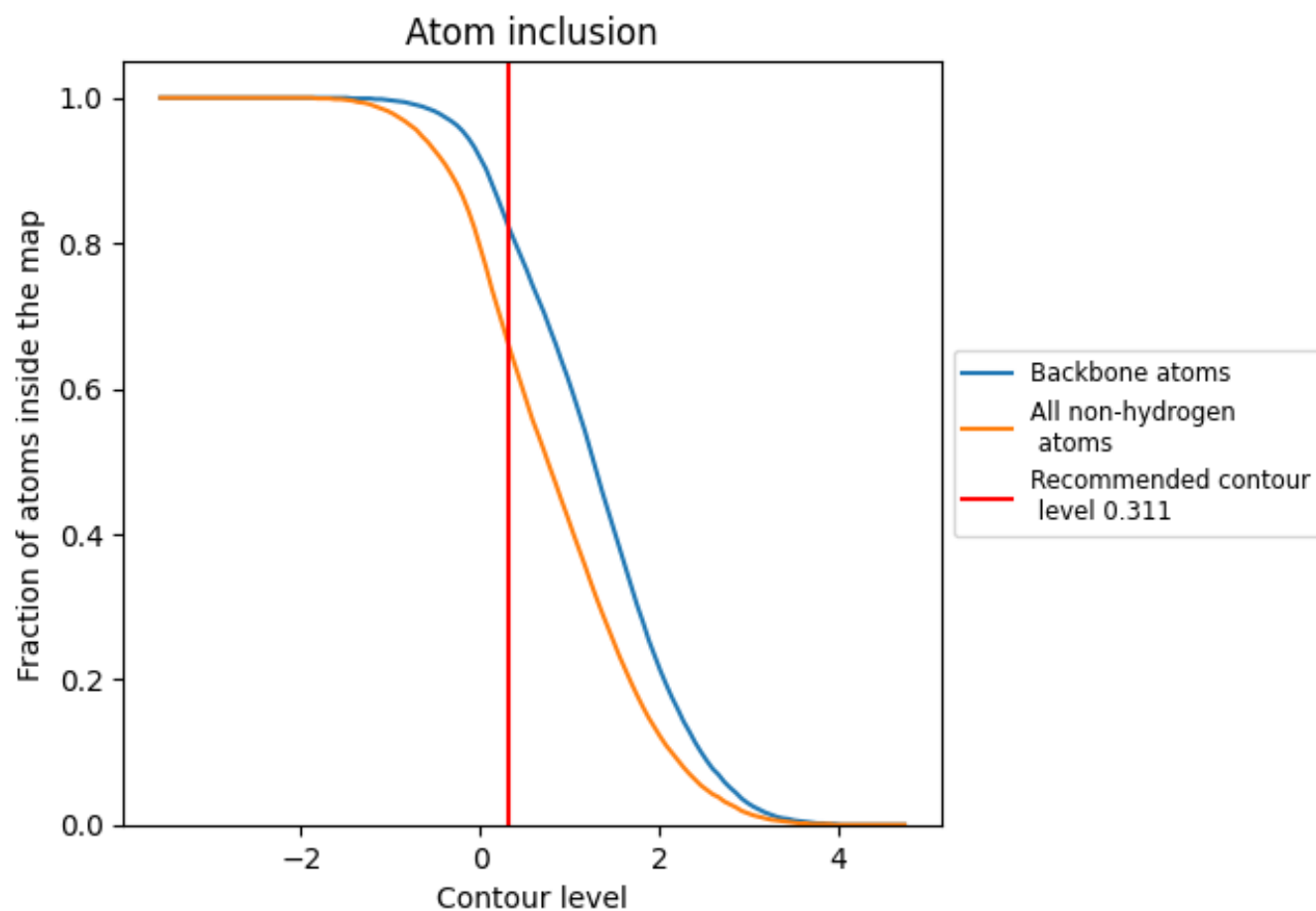
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.311).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.311) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6630	 0.2120
A	 0.1840	 0.1660
B	 0.1720	 0.1580
C	 0.7540	 0.2740
D	 0.7850	 0.2800
E	 0.7730	 0.2360
F	 0.1560	 0.1590
G	 0.7150	 0.2190
H	 0.6740	 0.1950
I	 0.7270	 0.2400
J	 0.6410	 0.1490
K	 0.7260	 0.2190
L	 0.7750	 0.2730
M	 0.7540	 0.2180
N	 0.4710	 0.0300
O	 0.5670	 0.0980
P	 0.6660	 0.1630
Q	 0.6310	 0.1570
R	 0.7710	 0.2940
S	 0.7480	 0.2590
T	 0.1620	 0.1430

