



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:36 PM UTC

PDB ID : 7PQC / pdb_00007pqc
EMDB ID : EMD-7522
Title : tau-microtubule structural ensemble based on CryoEM data
Authors : Brotzakis, Z.F.; Vendruscolo, M.
Deposited on : 2021-09-16
Resolution : 4.10 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:

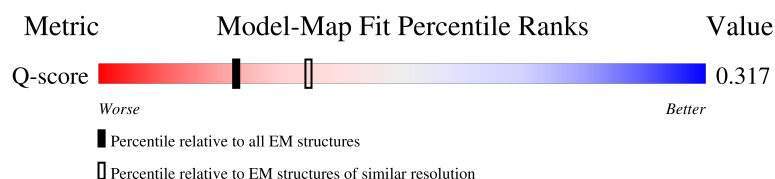
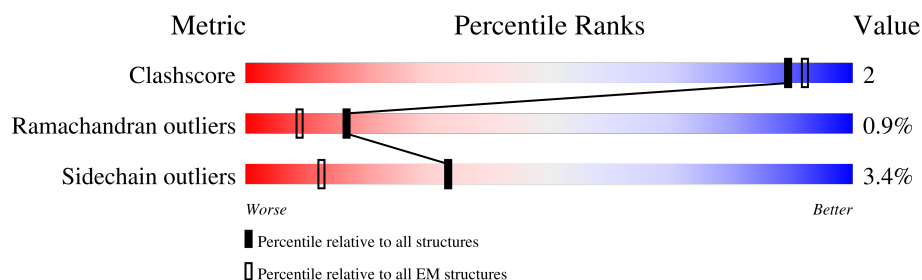
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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	445	5% 62% 35% .
1	C	445	6% 59% 39% .
1	E	445	6% 67% 31% .
1	G	445	. 62% 34% .

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Mol	Chain	Length	Quality of chain
1	I	445	5% 62% 34% .
1	K	445	6% 61% 36% .
1	M	445	6% 63% 33% .
2	B	451	7% 62% 35% .
2	D	451	8% 62% 31% 6% .
2	F	451	8% 67% 30% .
2	H	451	8% 61% 33% 5%
2	J	451	8% 65% 30% .
2	L	451	8% 61% 34% 5%
2	N	451	6% 65% 31% .
3	O	194	84% 66% 27% 6% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 51036 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 Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	445	Total	C	N	O	S	0	0
			3498	2189	595	688	26		
1	C	445	Total	C	N	O	S	0	0
			3498	2189	595	688	26		
1	E	445	Total	C	N	O	S	0	0
			3498	2189	595	688	26		
1	G	445	Total	C	N	O	S	0	0
			3498	2189	595	688	26		
1	I	445	Total	C	N	O	S	0	0
			3498	2189	595	688	26		
1	K	445	Total	C	N	O	S	0	0
			3498	2189	595	688	26		
1	M	445	Total	C	N	O	S	0	0
			3498	2189	595	688	26		

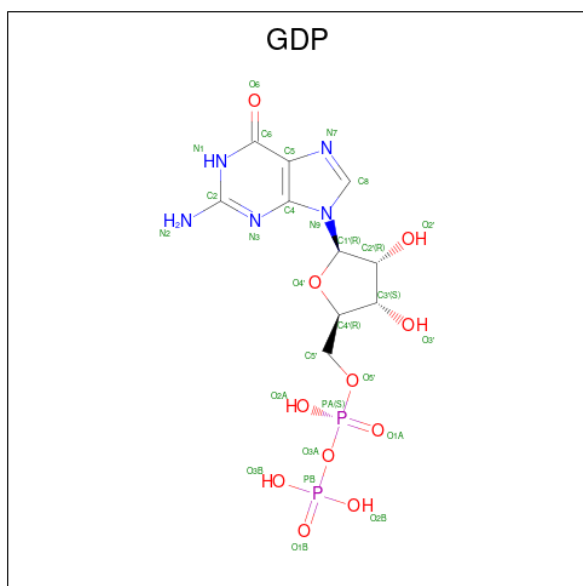
- Molecule 2 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	451	Total	C	N	O	S	0	0
			3524	2225	595	682	22		
2	D	451	Total	C	N	O	S	0	0
			3524	2225	595	682	22		
2	F	451	Total	C	N	O	S	0	0
			3524	2225	595	682	22		
2	H	451	Total	C	N	O	S	0	0
			3524	2225	595	682	22		
2	J	451	Total	C	N	O	S	0	0
			3524	2225	595	682	22		
2	L	451	Total	C	N	O	S	0	0
			3524	2225	595	682	22		
2	N	451	Total	C	N	O	S	0	0
			3524	2225	595	682	22		

- Molecule 3 is a protein called Isoform Tau-F of Microtubule-associated protein tau.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	194	Total	C	N	O	S	0	0
			1455	904	273	275	3		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	C	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	E	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	G	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	I	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	K	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	M	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	F	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	H	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	J	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	L	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	N	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	
6	D	1	Total	Mg	0
			1	1	
6	F	1	Total	Mg	0
			1	1	
6	H	1	Total	Mg	0
			1	1	

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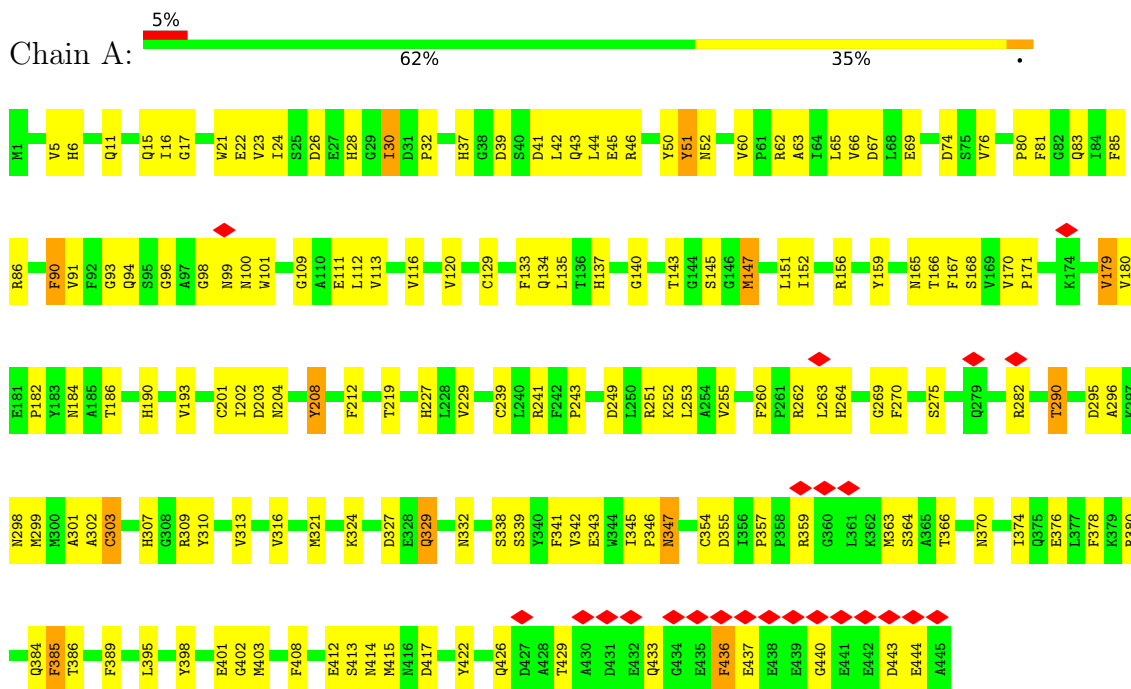
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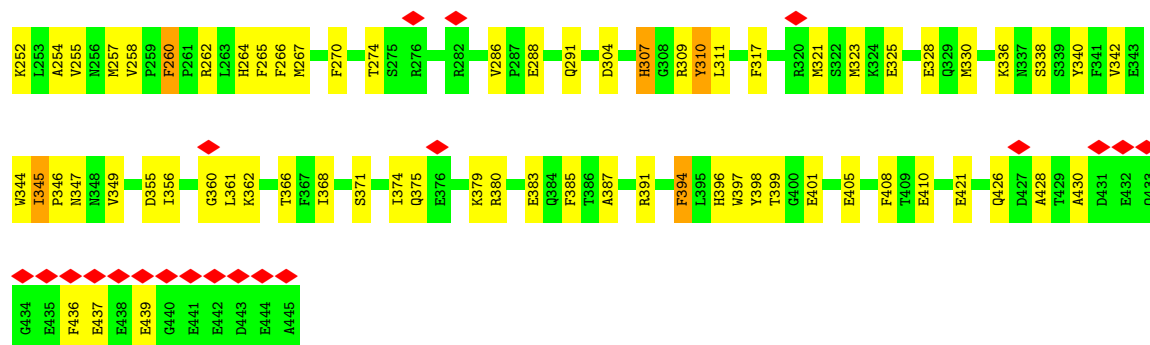
Mol	Chain	Residues	Atoms		AltConf
6	J	1	Total 1	Mg 1	0
6	L	1	Total 1	Mg 1	0
6	N	1	Total 1	Mg 1	0

3 Residue-property plots

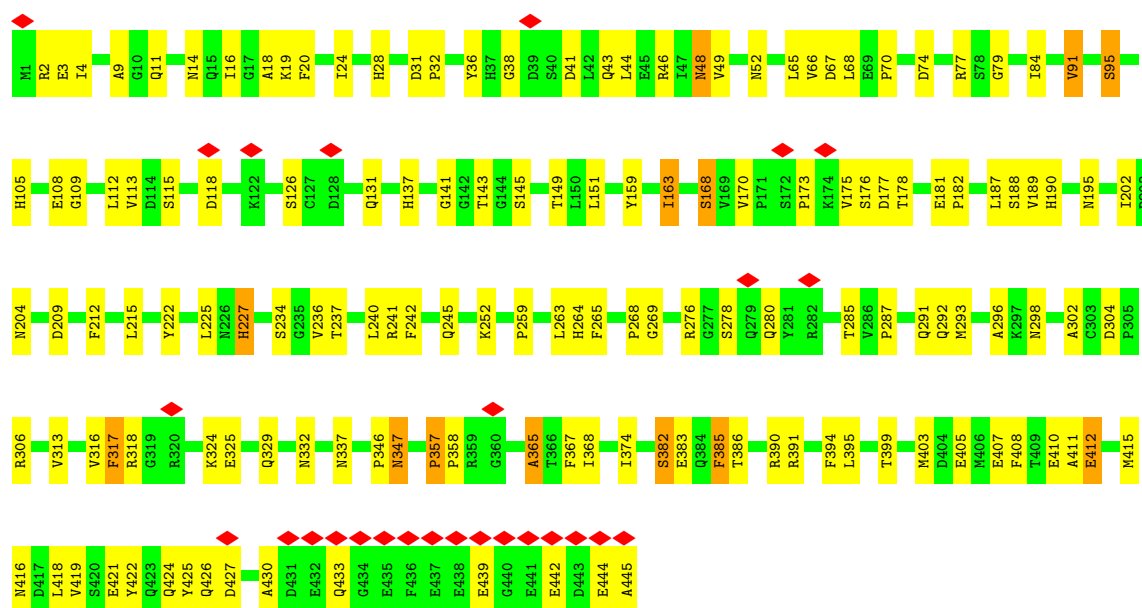
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Tubulin beta chain

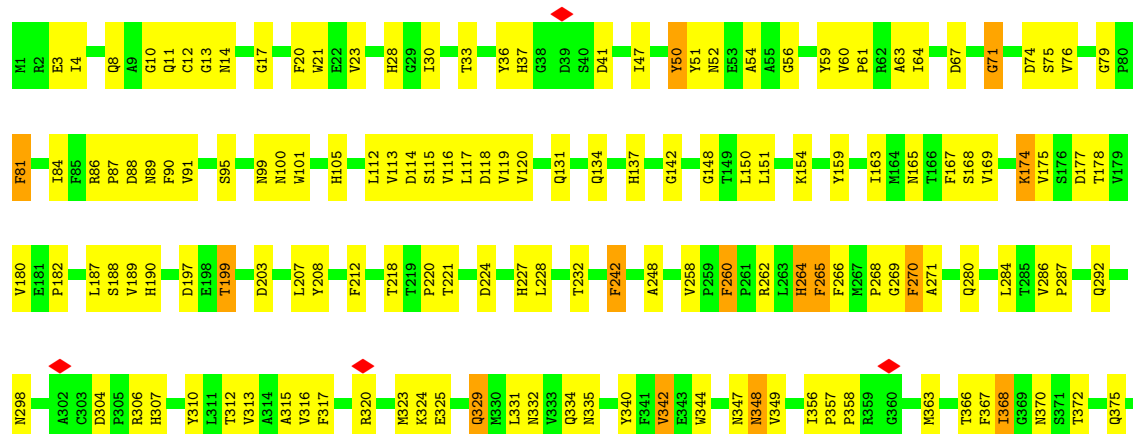


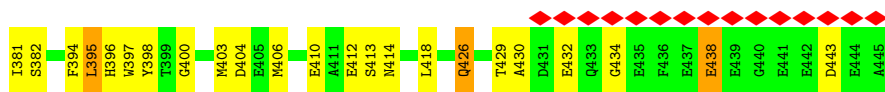


• Molecule 1: Tubulin beta chain

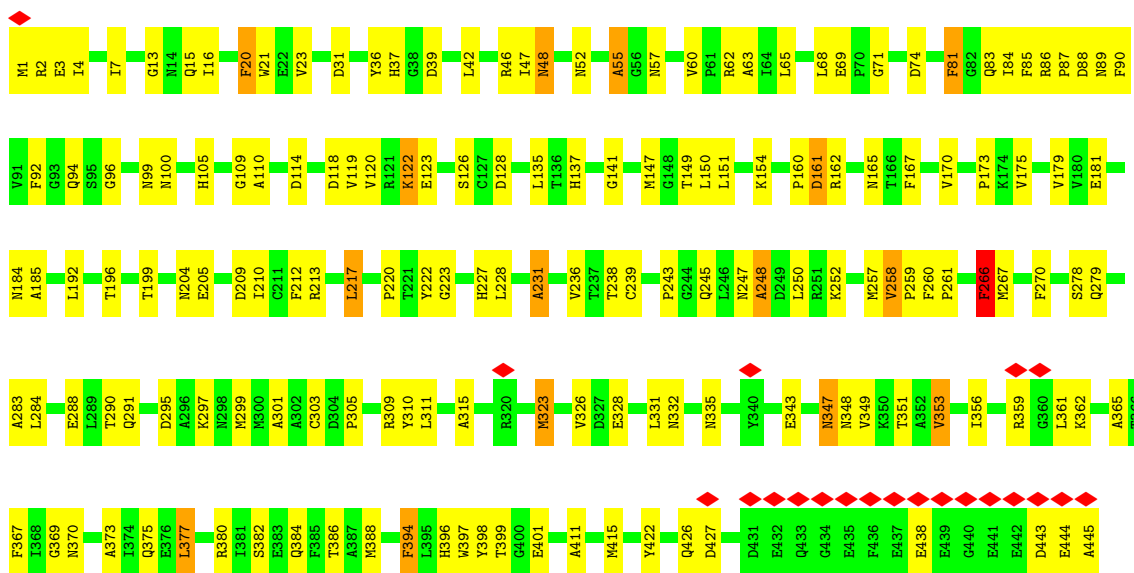


• Molecule 1: Tubulin beta chain

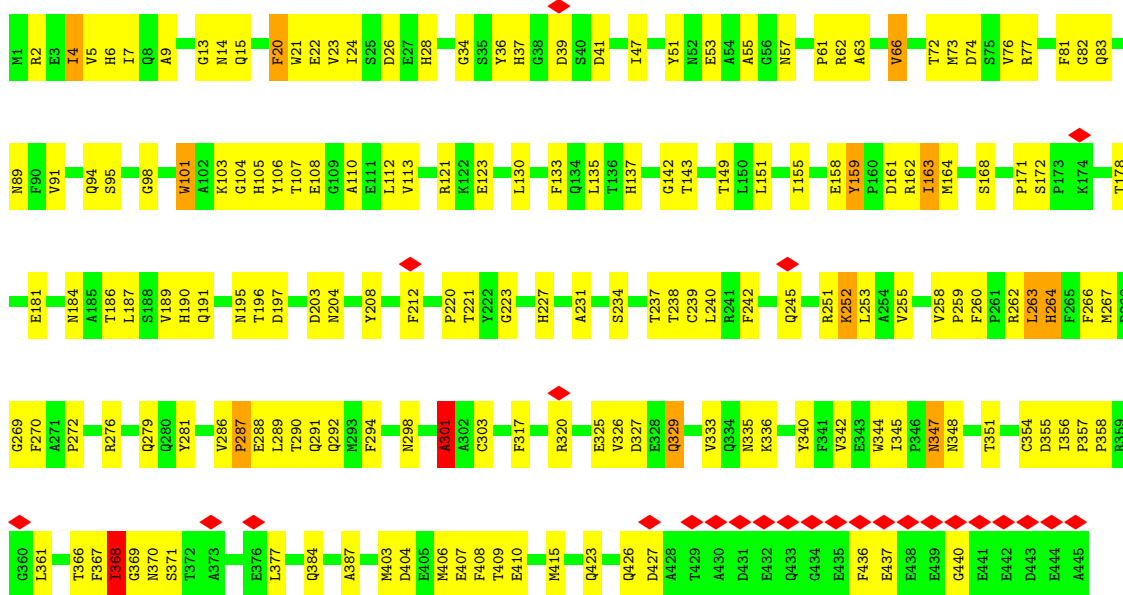




• Molecule 1: Tubulin beta chain

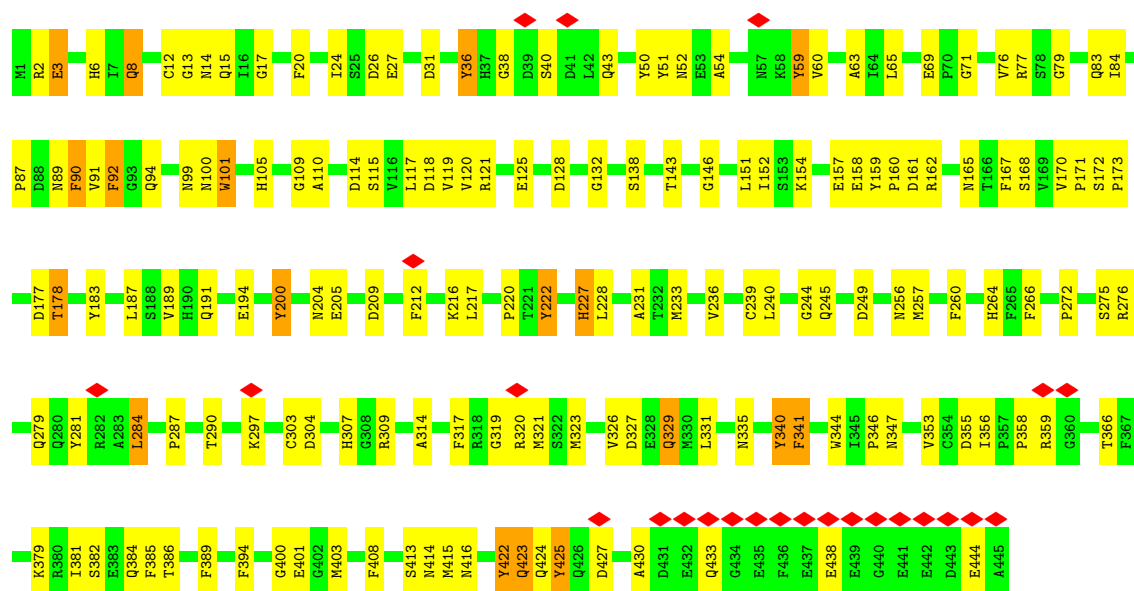


• Molecule 1: Tubulin beta chain

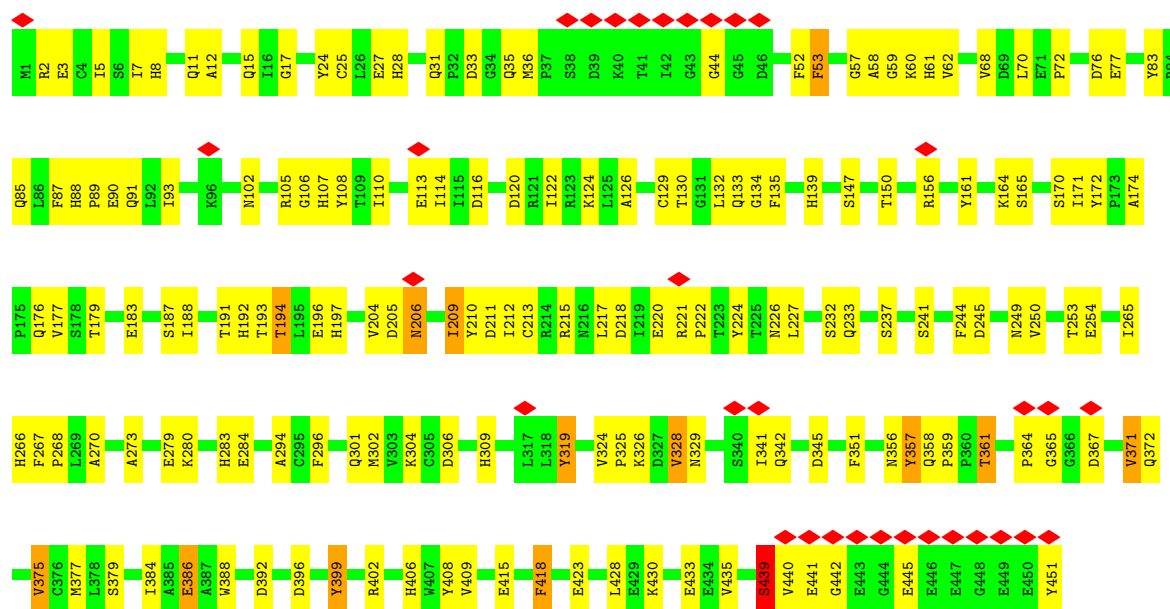


• Molecule 1: Tubulin beta chain

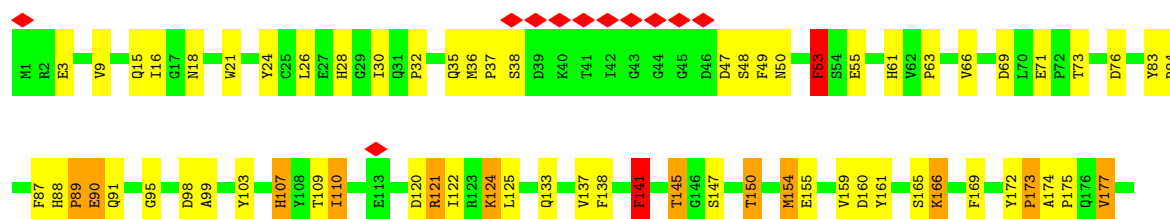


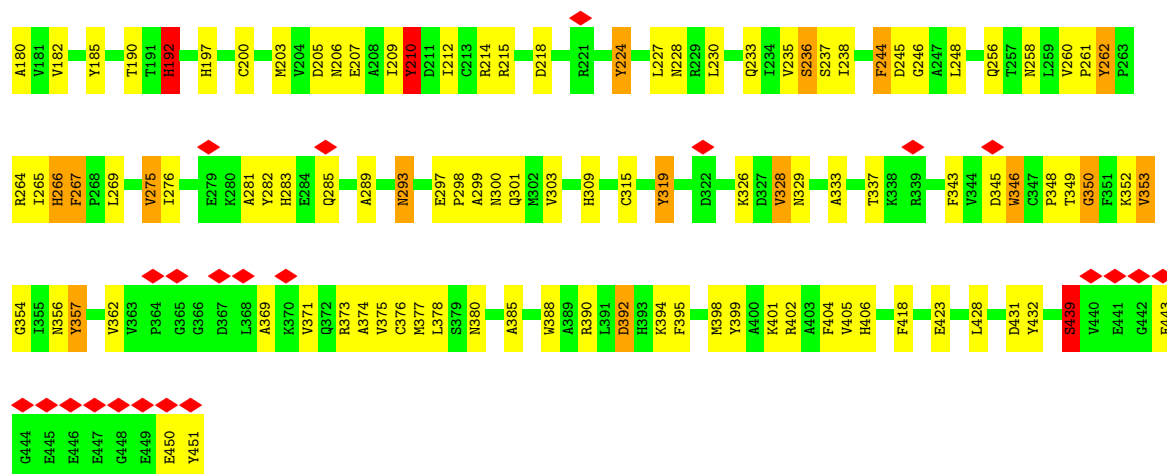


• Molecule 2: Tubulin alpha-1B chain

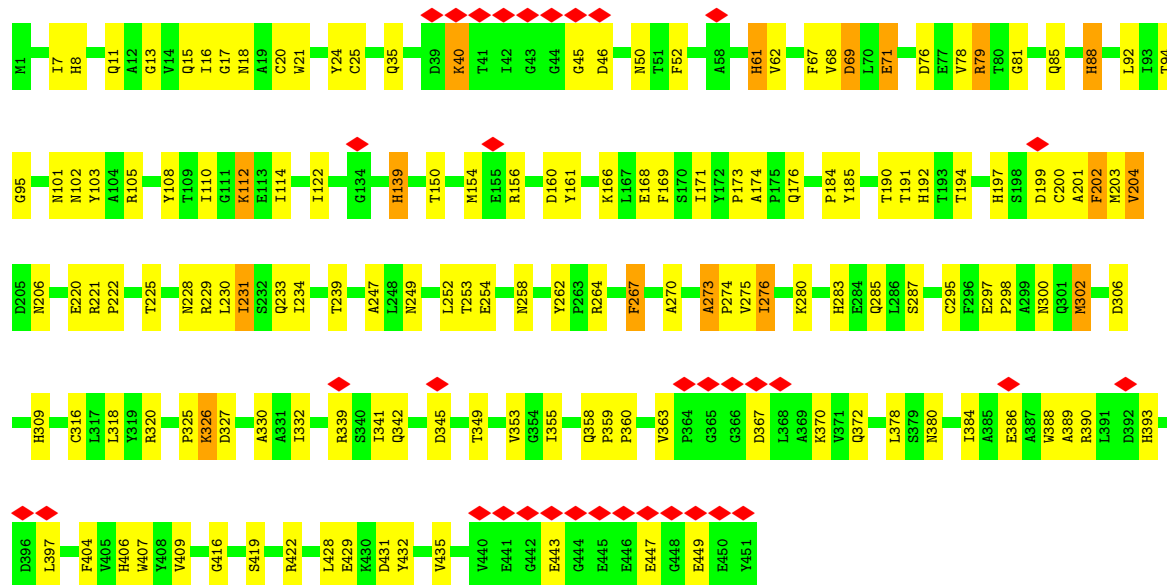


• Molecule 2: Tubulin alpha-1B chain

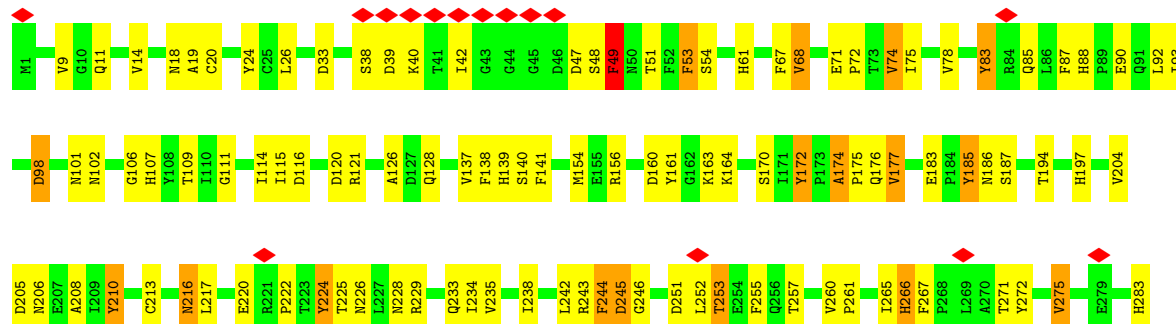


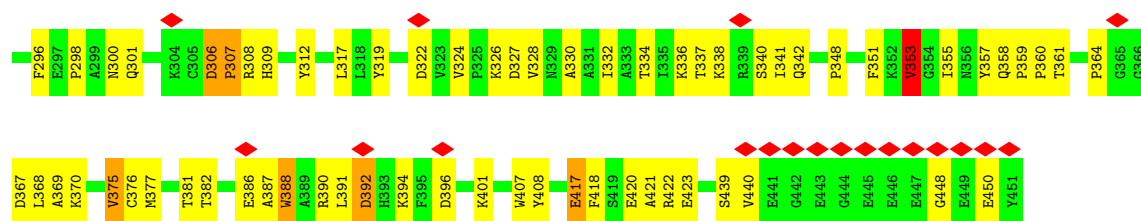


• Molecule 2: Tubulin alpha-1B chain

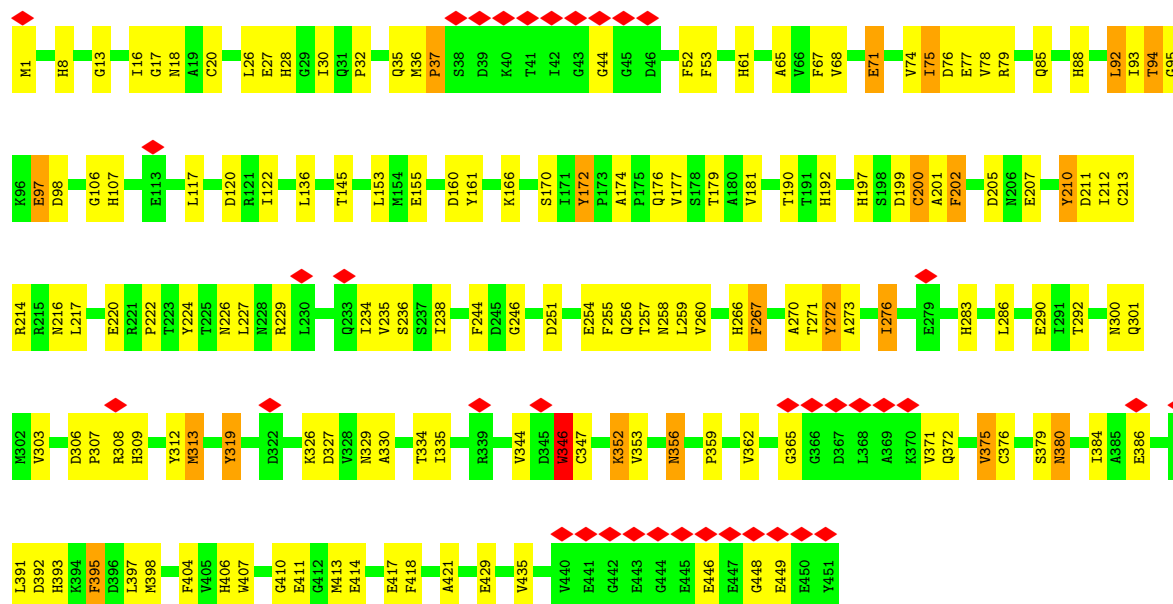


• Molecule 2: Tubulin alpha-1B chain

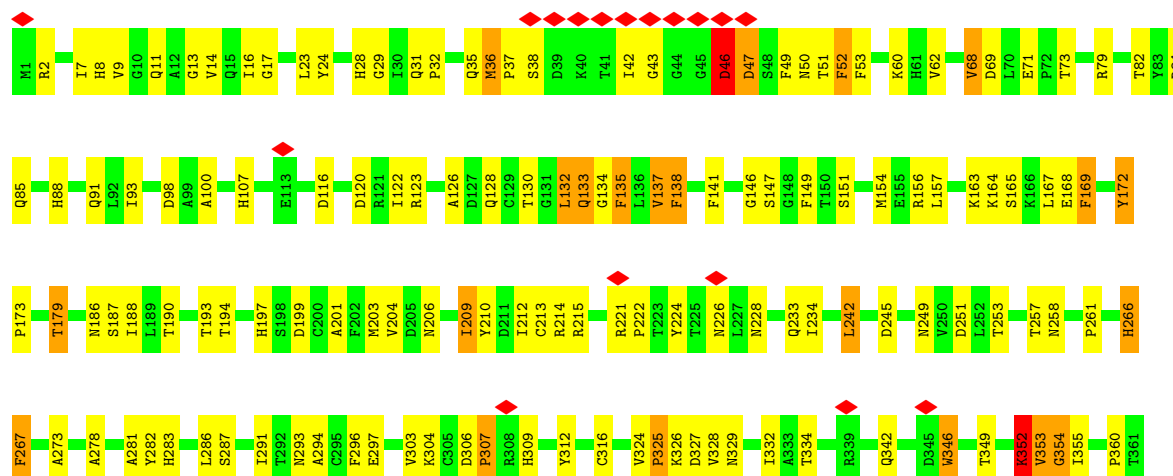


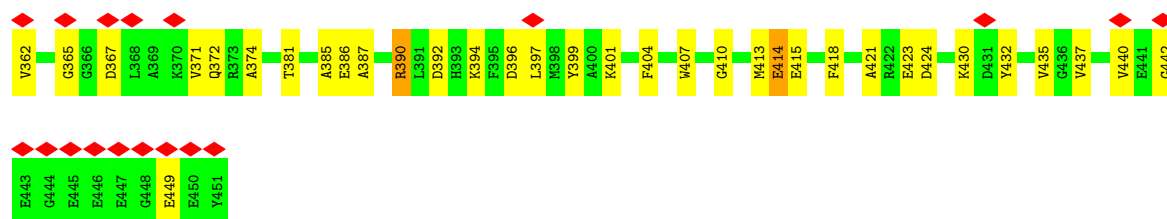


• Molecule 2: Tubulin alpha-1B chain

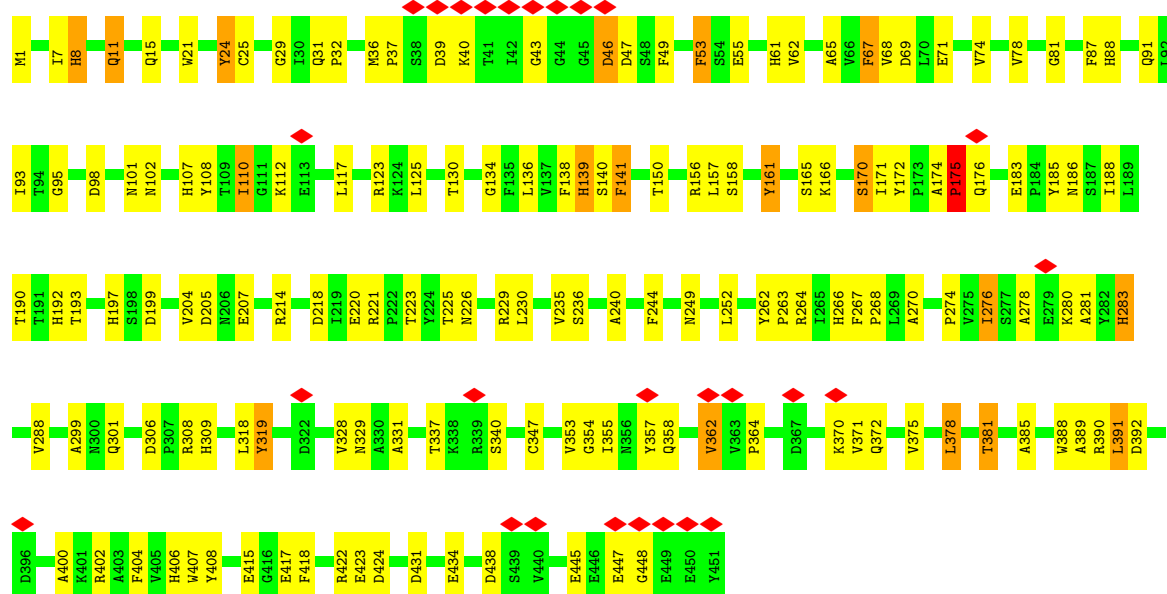


• Molecule 2: Tubulin alpha-1B chain

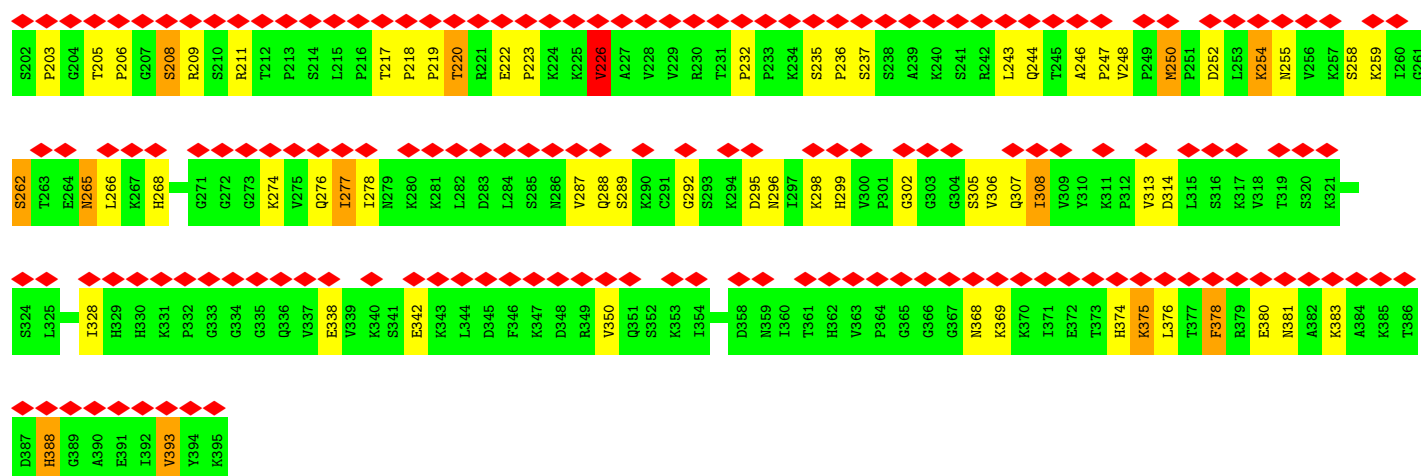
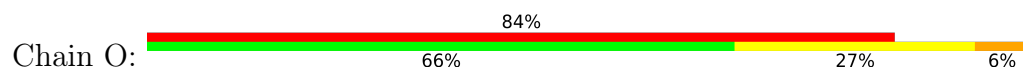




• Molecule 2: Tubulin alpha-1B chain



• Molecule 3: Isoform Tau-F of Microtubule-associated protein tau



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25963	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Images were drift-corrected using UCSF motioncorr software . CTFFIND4 was used to estimate CTFs for the drift-corrected images	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.789	Depositor
Minimum map value	-4.020	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.413	Depositor
Recommended contour level	1.26	Depositor
Map size ($\text{\AA}$)	675.84, 675.84, 675.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GDP, GTP

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	0.61	0/3574	2.38	207/4839 (4.3%)
1	C	0.60	0/3574	2.38	222/4839 (4.6%)
1	E	0.62	0/3574	2.33	181/4839 (3.7%)
1	G	0.61	0/3574	2.35	207/4839 (4.3%)
1	I	0.63	0/3574	2.32	217/4839 (4.5%)
1	K	0.63	0/3574	2.34	195/4839 (4.0%)
1	M	0.61	0/3574	2.36	195/4839 (4.0%)
2	B	0.61	1/3603 (0.0%)	2.35	213/4889 (4.4%)
2	D	0.61	0/3603	2.33	187/4889 (3.8%)
2	F	0.62	0/3603	2.33	181/4889 (3.7%)
2	H	0.62	0/3603	2.37	192/4889 (3.9%)
2	J	0.65	0/3603	2.34	194/4889 (4.0%)
2	L	0.62	0/3603	2.37	210/4889 (4.3%)
2	N	0.63	1/3603 (0.0%)	2.39	192/4889 (3.9%)
3	O	0.81	0/1483	2.25	79/1996 (4.0%)
All	All	0.63	2/51722 (0.0%)	2.35	2872/70092 (4.1%)

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	8
1	C	0	10
1	E	0	3
1	G	0	9
1	I	0	9
1	K	0	12
1	M	0	17
2	B	0	18

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	18
2	F	0	12
2	H	0	23
2	J	0	16
2	L	0	11
2	N	0	13
3	O	0	4
All	All	0	183

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	388	TRP	CZ3-CH2	6.58	1.56	1.40
2	B	388	TRP	CZ3-CH2	-5.06	1.27	1.40

All (2872) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	226	ASN	CA-CB-CG	12.89	125.49	112.60
2	F	94	THR	CA-C-N	12.45	134.68	121.48
2	F	94	THR	C-N-CA	12.45	134.68	121.48
1	C	60	VAL	CA-C-N	12.35	132.87	119.90
1	C	60	VAL	C-N-CA	12.35	132.87	119.90
1	E	347	ASN	CA-CB-CG	12.34	124.94	112.60
2	L	35	GLN	OE1-CD-NE2	-11.99	110.61	122.60
1	I	69	GLU	O-C-N	-11.86	114.12	121.71
1	G	260	PHE	CA-CB-CG	11.51	125.31	113.80
3	O	378	PHE	N-CA-C	11.49	124.55	110.41
2	B	245	ASP	CA-CB-CG	11.47	124.07	112.60
2	J	392	ASP	CA-CB-CG	11.40	124.00	112.60
2	H	301	GLN	OE1-CD-NE2	-11.32	111.28	122.60
2	B	392	ASP	CA-CB-CG	11.10	123.70	112.60
1	E	79	GLY	N-CA-C	11.04	125.68	112.10
2	J	226	ASN	CA-CB-CG	11.00	123.60	112.60
2	D	98	ASP	CA-CB-CG	11.00	123.60	112.60
3	O	288	GLN	OE1-CD-NE2	-10.96	111.64	122.60
2	L	392	ASP	CA-CB-CG	10.63	123.23	112.60
2	B	91	GLN	OE1-CD-NE2	-10.61	111.99	122.60
2	F	285	GLN	OE1-CD-NE2	-10.55	112.05	122.60
1	K	279	GLN	OE1-CD-NE2	-10.52	112.08	122.60
2	H	49	PHE	CA-CB-CG	10.49	124.29	113.80
2	B	406	HIS	CB-CG-CD2	-10.38	117.71	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	414	ASN	CA-CB-CG	-10.38	102.22	112.60
1	E	74	ASP	CA-CB-CG	-10.31	102.29	112.60
2	J	53	PHE	CA-CB-CG	10.30	124.10	113.80
1	M	356	ILE	CA-C-O	-10.25	113.38	119.12
1	K	184	ASN	OD1-CG-ND2	-10.17	112.43	122.60
1	C	73	MET	CA-C-O	-10.17	108.96	120.24
2	J	211	ASP	CA-C-O	-10.09	109.73	120.42
3	O	383	LYS	N-CA-C	10.01	123.24	110.33
2	L	397	LEU	CA-C-O	-9.85	109.31	120.24
2	D	329	ASN	OD1-CG-ND2	-9.79	112.81	122.60
2	J	71	GLU	O-C-N	-9.75	113.95	121.55
2	F	358	GLN	OE1-CD-NE2	-9.72	112.88	122.60
1	C	48	ASN	OD1-CG-ND2	-9.70	112.90	122.60
2	D	71	GLU	CB-CA-C	9.70	123.66	109.11
1	K	220	PRO	N-CA-CB	9.70	108.35	102.92
1	A	137	HIS	CA-CB-CG	9.70	123.50	113.80
2	F	11	GLN	OE1-CD-NE2	-9.69	112.91	122.60
1	A	433	GLN	OE1-CD-NE2	-9.68	112.92	122.60
1	I	258	VAL	CA-C-N	9.68	129.40	118.85
1	I	258	VAL	C-N-CA	9.68	129.40	118.85
2	B	244	PHE	N-CA-C	9.64	122.87	109.18
2	F	359	PRO	CA-C-N	9.60	129.98	119.90
2	F	359	PRO	C-N-CA	9.60	129.98	119.90
1	G	131	GLN	CG-CD-NE2	9.55	130.73	116.40
2	N	353	VAL	CA-C-N	9.55	129.30	122.33
2	N	353	VAL	C-N-CA	9.55	129.30	122.33
2	L	24	TYR	N-CA-C	9.49	122.62	111.71
3	O	307	GLN	OE1-CD-NE2	-9.47	113.12	122.60
2	H	359	PRO	N-CA-C	9.46	122.24	110.70
2	H	139	HIS	CB-CG-CD2	-9.41	118.97	131.20
2	H	358	GLN	OE1-CD-NE2	-9.32	113.28	122.60
2	H	106	GLY	CA-C-O	-9.26	110.85	120.66
1	E	84	ILE	CA-C-O	-9.25	110.26	120.25
1	E	227	HIS	CB-CG-CD2	-9.23	119.19	131.20
1	M	384	GLN	OE1-CD-NE2	-9.23	113.37	122.60
2	D	141	PHE	CA-CB-CG	9.21	123.01	113.80
2	L	88	HIS	CB-CG-CD2	-9.16	119.29	131.20
1	I	118	ASP	CA-CB-CG	9.16	121.76	112.60
1	I	290	THR	CA-C-O	-9.15	110.85	120.55
3	O	380	GLU	N-CA-C	9.15	126.00	113.37
1	M	204	ASN	CA-CB-CG	-9.14	103.46	112.60
1	I	141	GLY	CA-C-N	9.12	130.25	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	141	GLY	C-N-CA	9.12	130.25	120.03
1	K	369	GLY	CA-C-O	9.11	129.23	120.57
2	D	137	VAL	CB-CA-C	9.11	122.83	110.99
2	N	110	ILE	CA-C-N	9.08	130.06	119.98
2	N	110	ILE	C-N-CA	9.08	130.06	119.98
2	B	226	ASN	CA-CB-CG	9.08	121.68	112.60
2	N	136	LEU	CA-C-N	9.06	134.35	122.93
2	N	136	LEU	C-N-CA	9.06	134.35	122.93
1	A	378	PHE	CA-C-N	9.06	133.60	120.38
1	A	378	PHE	C-N-CA	9.06	133.60	120.38
2	N	204	VAL	O-C-N	-9.05	113.04	123.00
2	L	324	VAL	CA-C-N	9.05	128.78	119.64
2	L	324	VAL	C-N-CA	9.05	128.78	119.64
2	F	8	HIS	CB-CG-CD2	-9.04	119.44	131.20
1	I	384	GLN	OE1-CD-NE2	-9.04	113.56	122.60
2	N	423	GLU	CA-C-N	8.99	132.13	120.44
2	N	423	GLU	C-N-CA	8.99	132.13	120.44
1	E	3	GLU	CA-C-N	8.97	134.68	123.10
1	E	3	GLU	C-N-CA	8.97	134.68	123.10
2	L	193	THR	N-CA-C	8.95	121.04	111.28
1	G	307	HIS	CA-CB-CG	8.94	122.74	113.80
1	E	79	GLY	CA-C-O	-8.89	113.84	122.46
2	D	28	HIS	ND1-CE1-NE2	8.84	117.24	108.40
2	B	423	GLU	O-C-N	-8.84	112.75	122.12
1	K	258	VAL	CA-C-N	8.83	128.47	118.85
1	K	258	VAL	C-N-CA	8.83	128.47	118.85
1	C	57	ASN	OD1-CG-ND2	-8.81	113.79	122.60
1	E	11	GLN	OE1-CD-NE2	-8.79	113.81	122.60
1	K	83	GLN	CA-C-O	8.74	128.66	119.05
1	E	149	THR	N-CA-C	8.73	120.41	111.07
1	E	190	HIS	CA-CB-CG	8.72	122.52	113.80
2	H	18	ASN	N-CA-C	8.70	121.72	111.71
1	M	416	ASN	CA-CB-CG	8.68	121.28	112.60
1	E	365	ALA	CA-C-N	8.68	135.24	123.00
1	E	365	ALA	C-N-CA	8.68	135.24	123.00
1	C	249	ASP	CA-CB-CG	8.64	121.24	112.60
2	J	107	HIS	ND1-CE1-NE2	8.64	117.04	108.40
2	N	156	ARG	CD-NE-CZ	8.61	136.45	124.40
1	M	307	HIS	CA-C-N	8.61	134.15	120.55
1	M	307	HIS	C-N-CA	8.61	134.15	120.55
1	M	204	ASN	OD1-CG-ND2	-8.59	114.01	122.60
1	A	100	ASN	CA-C-N	8.57	131.97	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ASN	C-N-CA	8.57	131.97	120.65
1	G	430	ALA	CA-C-N	8.57	133.68	121.42
1	G	430	ALA	C-N-CA	8.57	133.68	121.42
2	L	367	ASP	O-C-N	-8.55	113.10	122.85
3	O	203	PRO	N-CA-CB	8.54	112.22	103.25
2	B	375	VAL	O-C-N	-8.52	113.29	123.00
2	N	31	GLN	CA-C-N	8.52	130.48	119.84
2	N	31	GLN	C-N-CA	8.52	130.48	119.84
2	B	205	ASP	CA-CB-CG	8.50	121.10	112.60
2	H	128	GLN	OE1-CD-NE2	-8.48	114.12	122.60
2	N	378	LEU	O-C-N	-8.47	113.30	123.29
1	M	160	PRO	CB-CA-C	8.46	122.03	110.52
2	J	372	GLN	OE1-CD-NE2	-8.46	114.14	122.60
1	M	245	GLN	OE1-CD-NE2	-8.45	114.15	122.60
2	F	173	PRO	N-CA-CB	8.43	112.10	103.25
1	K	292	GLN	OE1-CD-NE2	-8.42	114.18	122.60
1	K	137	HIS	CA-CB-CG	8.42	122.22	113.80
2	N	229	ARG	CD-NE-CZ	8.42	136.19	124.40
1	A	212	PHE	CA-C-O	-8.39	111.53	120.42
2	L	120	ASP	N-CA-C	-8.36	102.25	111.36
1	E	293	MET	N-CA-C	8.36	121.51	111.82
2	J	329	ASN	OD1-CG-ND2	-8.35	114.25	122.60
2	H	85	GLN	OE1-CD-NE2	-8.35	114.25	122.60
1	A	260	PHE	CA-C-N	8.32	127.98	119.82
1	A	260	PHE	C-N-CA	8.32	127.98	119.82
2	J	330	ALA	N-CA-C	8.31	119.97	111.07
2	H	387	ALA	CA-C-O	-8.30	111.62	120.42
2	N	404	PHE	CA-CB-CG	8.28	122.08	113.80
2	B	279	GLU	CA-C-O	-8.28	111.69	120.63
1	G	41	ASP	CA-C-N	8.25	131.34	120.28
1	G	41	ASP	C-N-CA	8.25	131.34	120.28
2	D	328	VAL	CA-C-N	8.25	131.54	120.65
2	D	328	VAL	C-N-CA	8.25	131.54	120.65
1	A	208	TYR	CA-C-O	-8.25	111.68	120.42
2	B	359	PRO	N-CA-CB	8.24	111.08	103.08
1	C	31	ASP	CA-CB-CG	8.24	120.84	112.60
2	D	15	GLN	OE1-CD-NE2	-8.23	114.37	122.60
1	G	23	VAL	CA-C-N	8.23	130.93	120.56
1	G	23	VAL	C-N-CA	8.23	130.93	120.56
1	A	98	GLY	O-C-N	8.22	129.17	122.51
1	G	242	PHE	CA-CB-CG	8.22	122.02	113.80
1	G	20	PHE	CA-C-O	8.20	129.43	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	206	PRO	CA-C-N	8.19	130.66	120.34
3	O	206	PRO	C-N-CA	8.19	130.66	120.34
1	I	184	ASN	N-CA-CB	-8.18	97.62	110.22
2	L	31	GLN	OE1-CD-NE2	-8.18	114.42	122.60
2	H	39	ASP	CA-CB-CG	8.18	120.78	112.60
2	F	46	ASP	CA-C-N	8.17	136.41	121.70
2	F	46	ASP	C-N-CA	8.17	136.41	121.70
1	A	249	ASP	CA-C-O	-8.17	112.89	121.55
1	M	114	ASP	CA-CB-CG	8.17	120.77	112.60
1	A	184	ASN	OD1-CG-ND2	-8.16	114.44	122.60
2	B	88	HIS	CB-CG-CD2	-8.16	120.59	131.20
2	L	435	VAL	O-C-N	-8.14	114.06	122.20
2	J	107	HIS	CE1-NE2-CD2	-8.14	100.86	109.00
2	J	18	ASN	OD1-CG-ND2	-8.13	114.47	122.60
1	A	22	GLU	CA-C-N	8.12	131.08	120.60
1	A	22	GLU	C-N-CA	8.12	131.08	120.60
2	L	46	ASP	O-C-N	-8.12	112.98	122.89
2	L	267	PHE	CA-C-N	8.12	129.98	119.84
2	L	267	PHE	C-N-CA	8.12	129.98	119.84
2	B	15	GLN	OE1-CD-NE2	-8.11	114.49	122.60
2	L	209	ILE	CA-CB-CG1	8.10	124.17	110.40
2	J	238	ILE	O-C-N	-8.10	113.69	121.87
1	I	247	ASN	CA-CB-CG	8.09	120.69	112.60
1	C	71	GLY	O-C-N	-8.08	113.47	122.28
1	A	341	PHE	CA-CB-CG	-8.07	105.73	113.80
2	B	116	ASP	N-CA-CB	-8.05	98.28	110.12
1	G	131	GLN	OE1-CD-NE2	-8.05	114.55	122.60
2	B	356	ASN	OD1-CG-ND2	-8.04	114.56	122.60
1	A	111	GLU	CA-C-N	8.04	131.38	120.44
1	A	111	GLU	C-N-CA	8.04	131.38	120.44
2	D	380	ASN	CA-CB-CG	-8.04	104.56	112.60
2	H	11	GLN	OE1-CD-NE2	-8.03	114.57	122.60
1	M	344	TRP	O-C-N	-8.02	112.11	122.37
2	H	216	ASN	CA-CB-CG	8.01	120.61	112.60
2	F	103	TYR	N-CA-C	7.99	119.62	111.07
1	K	404	ASP	CA-CB-CG	7.98	120.58	112.60
2	H	342	GLN	OE1-CD-NE2	-7.98	114.62	122.60
1	A	347	ASN	OD1-CG-ND2	-7.95	114.65	122.60
1	G	33	THR	CA-CB-CG2	7.95	124.02	110.50
2	H	358	GLN	CG-CD-NE2	7.95	128.32	116.40
1	C	230	SER	N-CA-C	7.95	119.94	111.28
1	M	54	ALA	N-CA-CB	-7.94	100.03	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	309	HIS	CB-CG-CD2	-7.94	120.88	131.20
1	E	278	SER	CA-C-N	7.93	131.96	120.38
1	E	278	SER	C-N-CA	7.93	131.96	120.38
2	B	283	HIS	N-CA-C	7.93	121.02	111.82
2	F	139	HIS	CB-CG-CD2	-7.93	120.89	131.20
1	G	227	HIS	CA-CB-CG	-7.92	105.88	113.80
1	G	79	GLY	CA-C-N	7.92	129.74	119.84
1	G	79	GLY	C-N-CA	7.92	129.74	119.84
1	M	236	VAL	CA-CB-CG1	7.91	123.85	110.40
1	M	71	GLY	N-CA-C	7.90	121.66	112.50
1	K	298	ASN	OD1-CG-ND2	-7.88	114.72	122.60
3	O	259	LYS	O-C-N	-7.88	114.43	123.42
1	K	272	PRO	CA-C-N	7.88	133.09	122.84
1	K	272	PRO	C-N-CA	7.88	133.09	122.84
1	E	426	GLN	OE1-CD-NE2	-7.88	114.72	122.60
2	B	365	GLY	CA-C-N	7.87	130.88	122.38
2	B	365	GLY	C-N-CA	7.87	130.88	122.38
1	G	329	GLN	OE1-CD-NE2	-7.87	114.73	122.60
2	J	65	ALA	CA-C-O	-7.87	112.51	121.40
2	D	276	ILE	N-CA-C	7.86	120.95	108.85
1	G	426	GLN	OE1-CD-NE2	-7.86	114.74	122.60
2	J	306	ASP	CA-C-N	7.85	127.52	119.82
2	J	306	ASP	C-N-CA	7.85	127.52	119.82
2	D	133	GLN	CA-C-O	7.85	129.05	119.79
1	C	152	ILE	CB-CA-C	7.84	122.01	111.97
1	A	15	GLN	N-CA-C	7.83	119.45	111.07
1	C	258	VAL	CA-C-N	7.83	127.49	119.19
1	C	258	VAL	C-N-CA	7.83	127.49	119.19
2	D	205	ASP	CA-CB-CG	7.82	120.42	112.60
2	J	267	PHE	CA-CB-CG	7.82	121.62	113.80
2	B	423	GLU	CA-C-O	7.82	128.84	120.55
2	H	109	THR	N-CA-C	7.81	120.69	111.71
2	B	396	ASP	CA-CB-CG	-7.80	104.80	112.60
1	K	264	HIS	CB-CG-CD2	-7.80	121.05	131.20
2	D	87	PHE	CA-CB-CG	7.80	121.60	113.80
2	H	175	PRO	N-CD-CG	7.80	114.90	103.20
1	A	426	GLN	OE1-CD-NE2	-7.80	114.80	122.60
2	F	390	ARG	N-CA-C	7.79	119.85	111.36
2	B	53	PHE	CA-CB-CG	7.79	121.59	113.80
2	N	288	VAL	O-C-N	7.79	129.52	121.89
2	L	123	ARG	CD-NE-CZ	7.79	135.30	124.40
2	D	260	VAL	CA-C-N	7.77	127.41	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	260	VAL	C-N-CA	7.77	127.41	119.56
1	A	385	PHE	O-C-N	7.76	130.07	122.07
2	J	257	THR	CA-CB-OG1	7.75	121.22	109.60
2	N	299	ALA	N-CA-C	7.75	120.81	111.82
2	J	8	HIS	CB-CG-CD2	-7.74	121.13	131.20
1	I	88	ASP	CA-CB-CG	7.74	120.34	112.60
2	D	289	ALA	CA-C-N	7.72	130.94	120.44
2	D	289	ALA	C-N-CA	7.72	130.94	120.44
2	F	367	ASP	CA-CB-CG	-7.72	104.88	112.60
2	L	261	PRO	N-CA-CB	7.72	111.35	103.25
2	N	69	ASP	OD1-CG-OD2	-7.71	104.39	122.90
2	L	126	ALA	N-CA-C	7.71	120.76	111.82
2	D	165	SER	CB-CA-C	-7.70	96.51	109.53
2	D	190	THR	CA-C-O	-7.69	112.98	120.90
2	J	300	ASN	OD1-CG-ND2	-7.69	114.91	122.60
2	H	300	ASN	OD1-CG-ND2	-7.69	114.91	122.60
2	D	28	HIS	CE1-NE2-CD2	-7.69	101.31	109.00
2	N	358	GLN	OE1-CD-NE2	-7.68	114.92	122.60
1	A	355	ASP	CA-CB-CG	7.68	120.28	112.60
2	F	61	HIS	CA-CB-CG	-7.68	106.12	113.80
2	H	14	VAL	CA-C-O	-7.68	112.71	120.85
1	M	256	ASN	OD1-CG-ND2	-7.68	114.92	122.60
1	K	260	PHE	CA-C-O	-7.67	112.74	119.72
1	K	191	GLN	OE1-CD-NE2	-7.65	114.95	122.60
2	L	116	ASP	CA-C-N	7.65	131.29	120.28
2	L	116	ASP	C-N-CA	7.65	131.29	120.28
2	F	202	PHE	CA-CB-CG	7.64	121.44	113.80
2	D	345	ASP	CA-CB-CG	-7.64	104.96	112.60
3	O	381	ASN	N-CA-C	7.64	124.08	112.54
1	C	34	GLY	CA-C-O	-7.63	110.51	119.06
2	L	346	TRP	CE2-CD2-CE3	-7.63	111.17	118.80
1	E	415	MET	CA-C-N	7.62	130.82	120.38
1	E	415	MET	C-N-CA	7.62	130.82	120.38
1	I	245	GLN	OE1-CD-NE2	-7.62	114.98	122.60
1	I	250	LEU	CA-C-N	7.62	130.80	120.44
1	I	250	LEU	C-N-CA	7.62	130.80	120.44
1	A	310	TYR	CA-C-O	-7.61	112.82	121.19
1	M	394	PHE	CA-C-N	7.61	130.48	120.28
1	M	394	PHE	C-N-CA	7.61	130.48	120.28
2	B	31	GLN	OE1-CD-NE2	-7.60	115.00	122.60
1	M	6	HIS	ND1-CG-CD2	7.60	113.70	106.10
1	G	221	THR	CA-CB-CG2	7.59	123.41	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	67	PHE	CA-CB-CG	7.59	121.39	113.80
1	M	222	TYR	CA-C-O	-7.59	112.78	120.90
2	N	378	LEU	CA-C-O	7.59	128.65	120.38
1	E	227	HIS	ND1-CE1-NE2	7.57	115.97	108.40
2	H	204	VAL	CB-CA-C	7.57	119.73	110.73
2	B	85	GLN	OE1-CD-NE2	-7.56	115.04	122.60
1	C	138	SER	CA-C-O	-7.56	112.61	121.46
3	O	296	ASN	CA-C-N	7.56	133.02	120.62
3	O	296	ASN	C-N-CA	7.56	133.02	120.62
1	A	269	GLY	O-C-N	-7.56	116.70	123.65
2	B	177	VAL	CA-CB-CG1	7.55	123.23	110.40
1	K	357	PRO	CA-C-N	7.55	127.53	119.76
1	K	357	PRO	C-N-CA	7.55	127.53	119.76
2	L	8	HIS	CB-CG-CD2	-7.55	121.39	131.20
2	N	53	PHE	CA-CB-CG	7.54	121.34	113.80
1	M	415	MET	CA-C-N	7.54	130.99	120.29
1	M	415	MET	C-N-CA	7.54	130.99	120.29
2	H	141	PHE	CA-CB-CG	7.53	121.33	113.80
1	E	367	PHE	CA-CB-CG	7.52	121.32	113.80
2	J	181	VAL	CA-C-O	-7.52	112.88	120.85
2	F	353	VAL	O-C-N	-7.51	115.07	123.18
1	A	137	HIS	N-CA-C	7.50	118.58	108.23
2	N	174	ALA	CA-C-N	7.50	129.21	119.84
2	N	174	ALA	C-N-CA	7.50	129.21	119.84
2	N	448	GLY	O-C-N	-7.49	116.55	122.99
1	G	221	THR	CA-CB-OG1	-7.48	98.37	109.60
2	H	139	HIS	ND1-CG-CD2	7.48	113.58	106.10
1	I	149	THR	CA-C-N	7.48	130.16	120.44
1	I	149	THR	C-N-CA	7.48	130.16	120.44
2	J	258	ASN	CB-CA-C	7.48	120.93	109.34
1	K	358	PRO	O-C-N	-7.47	113.99	123.03
2	N	274	PRO	N-CD-CG	7.46	112.76	103.80
2	L	362	VAL	N-CA-C	7.46	118.12	108.12
1	K	172	SER	CA-C-N	7.46	127.09	119.56
1	K	172	SER	C-N-CA	7.46	127.09	119.56
1	G	86	ARG	CA-C-N	7.45	127.32	119.05
1	G	86	ARG	C-N-CA	7.45	127.32	119.05
2	L	137	VAL	N-CA-C	7.44	117.42	106.85
1	A	28	HIS	CB-CG-CD2	-7.43	121.53	131.20
2	J	418	PHE	N-CA-C	-7.43	103.26	111.36
2	B	406	HIS	ND1-CG-CD2	7.43	113.53	106.10
1	K	227	HIS	CB-CG-CD2	-7.42	121.55	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	333	ALA	N-CA-C	7.42	119.37	111.28
1	K	369	GLY	O-C-N	-7.42	116.50	123.48
2	B	345	ASP	CA-C-O	-7.41	111.45	119.97
2	J	254	GLU	N-CA-CB	-7.40	99.67	110.47
1	G	218	THR	CA-C-N	7.39	130.58	122.74
1	G	218	THR	C-N-CA	7.39	130.58	122.74
1	M	304	ASP	CA-C-N	7.39	127.56	119.87
1	M	304	ASP	C-N-CA	7.39	127.56	119.87
1	C	330	MET	CA-C-O	7.39	128.47	119.38
1	I	48	ASN	OD1-CG-ND2	-7.39	115.21	122.60
2	F	360	PRO	N-CA-CB	7.38	109.86	103.36
1	I	347	ASN	CA-C-O	-7.38	109.95	120.51
1	K	20	PHE	O-C-N	7.38	129.76	122.09
2	L	287	SER	O-C-N	-7.38	114.28	122.84
1	M	320	ARG	N-CA-C	7.38	122.43	111.81
2	J	176	GLN	N-CA-C	-7.37	104.90	114.04
2	L	42	ILE	CA-C-N	7.37	131.85	121.09
2	L	42	ILE	C-N-CA	7.37	131.85	121.09
2	J	224	TYR	CA-CB-CG	7.37	127.16	113.90
2	F	101	ASN	CA-C-O	-7.37	111.67	120.81
2	D	107	HIS	CB-CG-CD2	-7.37	121.62	131.20
2	D	24	TYR	CA-C-O	-7.36	111.50	119.97
2	D	215	ARG	CA-C-O	-7.36	113.32	120.90
2	B	361	THR	CA-CB-CG2	7.36	123.01	110.50
2	D	177	VAL	CA-C-O	7.36	128.94	121.58
1	G	175	VAL	CA-C-O	-7.35	114.66	121.72
2	J	229	ARG	CA-C-O	-7.35	111.80	120.10
1	G	280	GLN	N-CA-C	7.35	120.16	111.71
2	N	244	PHE	CA-C-O	-7.34	113.58	121.14
1	G	8	GLN	OE1-CD-NE2	-7.34	115.26	122.60
1	K	427	ASP	CA-CB-CG	-7.34	105.26	112.60
1	M	327	ASP	CA-C-N	7.34	130.84	120.28
1	M	327	ASP	C-N-CA	7.34	130.84	120.28
1	A	67	ASP	CA-CB-CG	7.33	119.93	112.60
2	F	300	ASN	CA-CB-CG	7.32	119.92	112.60
1	M	83	GLN	OE1-CD-NE2	-7.32	115.28	122.60
1	M	368	ILE	CA-CB-CG1	7.32	122.83	110.40
2	D	309	HIS	CA-C-N	7.31	135.74	121.41
2	D	309	HIS	C-N-CA	7.31	135.74	121.41
2	N	61	HIS	ND1-CG-CD2	7.31	113.41	106.10
1	A	190	HIS	ND1-CE1-NE2	7.30	115.70	108.40
1	M	220	PRO	N-CA-CB	7.30	107.01	102.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	GLY	N-CA-C	7.30	122.57	112.57
1	I	87	PRO	N-CA-CB	7.30	111.58	103.26
2	L	193	THR	CA-CB-OG1	7.29	120.54	109.60
2	J	260	VAL	CA-C-N	7.29	126.92	119.19
2	J	260	VAL	C-N-CA	7.29	126.92	119.19
1	M	355	ASP	CB-CA-C	7.29	125.25	110.38
1	K	98	GLY	O-C-N	7.28	129.20	122.57
1	M	424	GLN	OE1-CD-NE2	-7.28	115.32	122.60
1	I	114	ASP	N-CA-C	7.28	120.14	111.33
1	E	2	ARG	CD-NE-CZ	7.27	134.58	124.40
1	E	292	GLN	OE1-CD-NE2	-7.27	115.33	122.60
1	G	117	LEU	CA-C-N	7.27	130.33	120.44
1	G	117	LEU	C-N-CA	7.27	130.33	120.44
2	B	126	ALA	CA-C-N	7.26	130.74	120.28
2	B	126	ALA	C-N-CA	7.26	130.74	120.28
1	C	61	PRO	N-CA-CB	7.26	109.75	103.36
1	G	381	ILE	CA-C-O	-7.26	113.40	120.95
2	H	120	ASP	CA-CB-CG	-7.26	105.34	112.60
2	H	233	GLN	OE1-CD-NE2	-7.26	115.34	122.60
2	L	418	PHE	O-C-N	-7.26	114.19	122.03
2	H	440	VAL	CA-CB-CG2	7.26	122.74	110.40
2	N	102	ASN	OD1-CG-ND2	-7.26	115.34	122.60
1	C	304	ASP	CA-CB-CG	7.24	119.84	112.60
2	H	102	ASN	CA-CB-CG	7.24	119.84	112.60
2	L	346	TRP	CD2-CE2-CZ2	7.24	129.64	122.40
2	H	83	TYR	N-CA-CB	-7.24	99.91	110.70
2	N	197	HIS	O-C-N	7.23	130.29	122.34
1	I	110	ALA	N-CA-C	7.23	120.02	111.71
1	M	264	HIS	CA-C-N	7.23	132.76	121.99
1	M	264	HIS	C-N-CA	7.23	132.76	121.99
1	K	83	GLN	OE1-CD-NE2	-7.22	115.38	122.60
1	I	261	PRO	N-CA-C	7.22	123.22	113.84
2	D	244	PHE	CA-CB-CG	7.21	121.01	113.80
1	M	425	TYR	N-CA-C	-7.21	106.40	114.62
2	H	176	GLN	OE1-CD-NE2	-7.21	115.39	122.60
2	F	428	LEU	N-CA-C	7.21	120.05	111.33
2	L	267	PHE	CA-CB-CG	7.20	121.00	113.80
1	C	100	ASN	CA-C-N	7.20	130.24	120.38
1	C	100	ASN	C-N-CA	7.20	130.24	120.38
1	A	414	ASN	CA-CB-CG	-7.20	105.40	112.60
1	I	266	PHE	N-CA-C	7.20	121.26	109.24
2	B	283	HIS	CB-CG-CD2	-7.19	121.85	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	258	ASN	OD1-CG-ND2	-7.19	115.41	122.60
1	G	228	LEU	CA-C-N	7.19	129.68	120.70
1	G	228	LEU	C-N-CA	7.19	129.68	120.70
2	L	273	ALA	CA-C-O	-7.18	111.89	119.50
2	J	286	LEU	N-CA-C	7.17	119.99	111.02
2	J	392	ASP	N-CA-C	7.17	118.75	111.07
2	H	360	PRO	N-CA-CB	7.17	110.78	103.25
2	J	306	ASP	O-C-N	-7.17	114.51	121.18
1	C	171	PRO	N-CA-CB	7.17	109.03	103.30
1	I	160	PRO	N-CA-C	7.16	123.22	113.98
2	H	220	GLU	N-CA-CB	-7.16	99.60	110.33
2	B	58	ALA	CA-C-N	7.15	130.91	120.11
2	B	58	ALA	C-N-CA	7.15	130.91	120.11
1	C	437	GLU	O-C-N	-7.15	115.47	123.48
1	K	26	ASP	CA-CB-CG	7.15	119.75	112.60
1	K	22	GLU	CA-C-N	7.14	129.70	120.56
1	K	22	GLU	C-N-CA	7.14	129.70	120.56
1	G	203	ASP	N-CA-CB	-7.14	99.56	110.77
2	B	441	GLU	N-CA-C	7.14	120.06	110.35
2	J	16	ILE	CA-C-N	7.13	128.04	119.99
2	J	16	ILE	C-N-CA	7.13	128.04	119.99
1	I	399	THR	CA-C-N	7.12	129.04	120.14
1	I	399	THR	C-N-CA	7.12	129.04	120.14
2	L	421	ALA	N-CA-C	-7.12	103.60	111.36
1	I	220	PRO	CA-C-O	-7.12	113.29	122.12
2	H	208	ALA	N-CA-C	7.11	118.82	111.14
1	M	172	SER	CA-C-N	7.11	127.10	119.28
1	M	172	SER	C-N-CA	7.11	127.10	119.28
1	K	123	GLU	O-C-N	-7.11	114.04	122.15
3	O	223	PRO	N-CA-CB	7.10	111.05	103.52
2	D	329	ASN	CA-C-O	-7.10	113.55	121.00
1	K	37	HIS	O-C-N	-7.10	114.99	122.30
2	D	89	PRO	CB-CA-C	-7.09	101.14	112.21
1	K	345	ILE	CA-C-O	-7.09	114.56	119.38
2	H	266	HIS	CG-CD2-NE2	-7.09	100.11	107.20
1	K	263	LEU	CB-CA-C	7.08	120.54	111.40
2	B	193	THR	O-C-N	-7.08	113.91	122.48
1	C	193	VAL	CA-CB-CG1	7.08	122.44	110.40
1	C	266	PHE	CA-CB-CG	7.07	120.87	113.80
2	D	300	ASN	CA-CB-CG	7.07	119.67	112.60
3	O	393	VAL	N-CA-C	7.06	124.02	109.34
3	O	218	PRO	N-CA-CB	7.06	109.92	103.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	394	LYS	CA-C-O	-7.05	112.13	120.10
1	M	105	HIS	CB-CG-CD2	-7.05	122.03	131.20
2	J	256	GLN	OE1-CD-NE2	-7.05	115.55	122.60
2	B	59	GLY	O-C-N	-7.04	116.80	122.51
1	C	321	MET	O-C-N	7.04	131.20	123.10
2	D	84	ARG	N-CA-C	7.04	120.76	111.75
2	J	301	GLN	OE1-CD-NE2	-7.04	115.56	122.60
2	B	17	GLY	CA-C-O	-7.03	113.91	120.80
1	K	168	SER	N-CA-C	7.03	120.19	108.73
3	O	268	HIS	CB-CG-CD2	-7.03	122.06	131.20
2	J	335	ILE	O-C-N	-7.03	115.05	121.87
1	E	212	PHE	CA-CB-CG	7.03	120.83	113.80
2	N	372	GLN	OE1-CD-NE2	-7.02	115.58	122.60
2	J	306	ASP	CB-CA-C	7.02	121.41	109.82
2	F	78	VAL	CA-C-O	-7.02	113.20	120.71
2	B	324	VAL	CB-CA-C	-7.02	103.20	110.71
2	N	240	ALA	N-CA-C	7.02	118.93	111.28
1	M	110	ALA	N-CA-C	7.02	118.93	111.28
2	F	18	ASN	CA-C-O	-7.01	113.40	120.90
2	H	334	THR	CA-CB-CG2	7.01	122.41	110.50
1	I	243	PRO	CA-C-N	7.01	129.06	120.51
1	I	243	PRO	C-N-CA	7.01	129.06	120.51
2	F	69	ASP	OD1-CG-OD2	-7.00	106.09	122.90
1	K	20	PHE	CA-C-O	-7.00	113.40	120.90
1	G	349	VAL	CA-C-N	7.00	132.59	122.85
1	G	349	VAL	C-N-CA	7.00	132.59	122.85
2	J	30	ILE	CB-CA-C	7.00	120.81	111.21
1	M	178	THR	CA-CB-CG2	7.00	122.40	110.50
2	L	133	GLN	OE1-CD-NE2	-7.00	115.60	122.60
1	I	20	PHE	CA-CB-CG	-7.00	106.81	113.80
2	F	386	GLU	CA-CB-CG	6.99	128.08	114.10
2	L	334	THR	CA-C-O	-6.99	113.48	120.82
2	N	381	THR	CA-CB-CG2	6.99	122.39	110.50
1	E	16	ILE	CB-CA-C	6.99	121.17	112.02
1	C	321	MET	N-CA-CB	-6.99	100.52	111.56
1	G	404	ASP	N-CA-CB	-6.99	99.88	111.20
2	H	245	ASP	O-C-N	-6.98	115.07	122.96
2	L	396	ASP	CA-CB-CG	6.98	119.58	112.60
2	H	309	HIS	CB-CG-CD2	-6.98	122.12	131.20
1	A	227	HIS	CA-C-N	6.98	131.29	120.82
1	A	227	HIS	C-N-CA	6.98	131.29	120.82
2	D	47	ASP	CA-CB-CG	6.98	119.58	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	61	HIS	CA-CB-CG	-6.98	106.82	113.80
1	K	72	THR	OG1-CB-CG2	-6.98	95.34	109.30
2	D	161	TYR	CA-C-N	6.97	128.92	120.13
2	D	161	TYR	C-N-CA	6.97	128.92	120.13
1	C	188	SER	N-CA-C	6.97	118.96	111.36
1	G	165	ASN	OD1-CG-ND2	-6.96	115.64	122.60
1	I	185	ALA	CA-C-N	6.96	130.18	120.29
1	I	185	ALA	C-N-CA	6.96	130.18	120.29
1	A	46	ARG	CA-C-O	-6.96	112.27	119.51
2	H	267	PHE	CA-CB-CG	6.96	120.76	113.80
1	A	159	TYR	CA-C-N	6.96	128.53	119.84
1	A	159	TYR	C-N-CA	6.96	128.53	119.84
2	J	393	HIS	CB-CG-CD2	-6.96	122.16	131.20
1	K	287	PRO	N-CA-CB	6.96	110.90	103.39
1	I	377	LEU	CA-C-N	6.95	129.90	120.44
1	I	377	LEU	C-N-CA	6.95	129.90	120.44
1	A	370	ASN	OD1-CG-ND2	-6.95	115.65	122.60
1	A	21	TRP	CA-C-O	-6.95	111.98	119.97
2	D	21	TRP	CA-C-N	6.94	130.44	120.79
2	D	21	TRP	C-N-CA	6.94	130.44	120.79
2	N	125	LEU	N-CA-CB	-6.94	99.89	110.16
1	A	260	PHE	O-C-N	-6.94	115.64	121.54
1	K	333	VAL	N-CA-CB	6.93	118.66	110.55
2	N	88	HIS	CB-CG-CD2	-6.93	122.19	131.20
2	B	266	HIS	CA-CB-CG	6.93	120.73	113.80
1	C	196	THR	CA-CB-OG1	6.93	119.99	109.60
1	K	408	PHE	CA-CB-CG	-6.92	106.88	113.80
2	L	407	TRP	CE2-CD2-CE3	-6.92	111.88	118.80
1	E	113	VAL	N-CA-C	6.92	118.51	110.62
2	D	418	PHE	CA-C-O	-6.92	113.57	120.70
2	H	330	ALA	O-C-N	-6.92	114.79	122.12
1	I	57	ASN	CA-CB-CG	6.92	119.52	112.60
1	E	182	PRO	N-CA-CB	6.92	110.51	103.25
1	K	130	LEU	O-C-N	-6.92	114.31	122.89
1	C	192	LEU	CA-C-O	-6.91	112.57	120.24
2	L	294	ALA	CA-C-N	6.91	131.66	120.60
2	L	294	ALA	C-N-CA	6.91	131.66	120.60
2	H	54	SER	N-CA-C	6.90	119.66	108.34
2	H	139	HIS	CA-C-N	6.90	132.50	122.77
2	H	139	HIS	C-N-CA	6.90	132.50	122.77
1	M	173	PRO	N-CA-CB	6.90	110.84	103.39
1	E	113	VAL	CA-CB-CG2	6.89	122.12	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ARG	CD-NE-CZ	6.89	134.05	124.40
2	F	252	LEU	N-CA-CB	-6.89	98.96	110.39
2	F	406	HIS	CB-CG-CD2	-6.88	122.25	131.20
2	F	327	ASP	CA-C-O	6.88	127.72	120.42
2	J	78	VAL	CA-CB-CG2	6.88	122.10	110.40
2	J	397	LEU	N-CA-C	6.88	118.78	111.28
2	L	251	ASP	CA-C-N	6.87	129.49	120.28
2	L	251	ASP	C-N-CA	6.87	129.49	120.28
1	A	384	GLN	OE1-CD-NE2	-6.87	115.73	122.60
1	I	120	VAL	CA-CB-CG1	6.87	122.08	110.40
1	I	151	LEU	CA-C-O	-6.87	113.14	120.42
2	N	415	GLU	CA-C-N	6.87	128.73	120.14
2	N	415	GLU	C-N-CA	6.87	128.73	120.14
1	C	206	ALA	N-CA-C	6.87	118.85	111.36
1	E	44	LEU	N-CA-C	6.87	119.79	111.82
1	G	224	ASP	CA-C-N	6.87	130.17	120.28
1	G	224	ASP	C-N-CA	6.87	130.17	120.28
2	B	106	GLY	CA-C-O	-6.87	112.74	120.09
2	J	258	ASN	OD1-CG-ND2	-6.87	115.73	122.60
2	D	233	GLN	OE1-CD-NE2	-6.86	115.75	122.60
2	J	107	HIS	CB-CG-CD2	-6.85	122.29	131.20
1	E	399	THR	O-C-N	-6.85	113.85	122.27
1	C	221	THR	O-C-N	-6.85	114.90	122.84
2	D	215	ARG	N-CA-C	6.85	118.63	111.03
1	A	165	ASN	CA-CB-CG	6.84	119.44	112.60
2	L	346	TRP	CA-C-N	6.84	129.79	122.26
2	L	346	TRP	C-N-CA	6.84	129.79	122.26
1	A	159	TYR	O-C-N	-6.84	115.03	121.05
1	E	368	ILE	CA-C-N	6.83	127.32	122.33
1	E	368	ILE	C-N-CA	6.83	127.32	122.33
2	D	76	ASP	CA-CB-CG	6.83	119.42	112.60
2	H	324	VAL	O-C-N	-6.83	115.50	121.57
1	I	351	THR	OG1-CB-CG2	-6.83	95.65	109.30
1	C	14	ASN	CA-C-N	6.82	129.98	120.29
1	C	14	ASN	C-N-CA	6.82	129.98	120.29
3	O	223	PRO	CA-N-CD	-6.82	102.45	112.00
1	C	158	GLU	N-CA-CB	-6.82	99.29	110.40
2	F	13	GLY	CA-C-N	6.81	129.28	120.56
2	F	13	GLY	C-N-CA	6.81	129.28	120.56
2	N	61	HIS	ND1-CE1-NE2	6.81	115.21	108.40
1	A	359	ARG	CA-CB-CG	6.81	127.72	114.10
1	C	260	PHE	N-CA-C	6.81	116.15	108.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	39	ASP	CA-CB-CG	6.81	119.41	112.60
1	G	115	SER	CA-C-N	6.80	129.21	120.70
1	G	115	SER	C-N-CA	6.80	129.21	120.70
2	J	44	GLY	O-C-N	-6.80	115.72	123.61
1	M	233	MET	N-CA-C	6.79	118.68	111.28
3	O	248	VAL	N-CA-C	6.79	115.29	107.89
2	B	244	PHE	O-C-N	-6.79	113.37	122.74
1	C	311	LEU	N-CA-C	6.79	119.30	111.02
2	F	17	GLY	O-C-N	-6.79	115.61	122.19
1	G	334	GLN	OE1-CD-NE2	-6.79	115.81	122.60
1	A	167	PHE	CA-CB-CG	6.78	120.58	113.80
2	B	57	GLY	CA-C-O	-6.78	116.34	122.57
2	N	214	ARG	CD-NE-CZ	6.77	133.88	124.40
1	M	381	ILE	CB-CA-C	6.77	121.31	112.24
2	N	46	ASP	CA-C-N	6.77	133.88	121.70
2	N	46	ASP	C-N-CA	6.77	133.88	121.70
1	K	371	SER	O-C-N	-6.76	115.02	123.27
2	H	121	ARG	CA-C-N	6.75	129.21	120.56
2	H	121	ARG	C-N-CA	6.75	129.21	120.56
2	F	407	TRP	N-CA-C	6.75	121.12	112.34
1	G	74	ASP	CA-C-O	-6.75	112.20	119.97
2	N	1	MET	CB-CA-C	6.75	122.93	110.10
3	O	252	ASP	CA-CB-CG	6.75	119.35	112.60
1	M	89	ASN	OD1-CG-ND2	-6.75	115.85	122.60
2	J	327	ASP	CA-C-N	6.74	129.06	120.56
2	J	327	ASP	C-N-CA	6.74	129.06	120.56
2	L	186	ASN	CA-CB-CG	6.74	119.34	112.60
1	C	121	ARG	CD-NE-CZ	6.74	133.83	124.40
2	F	397	LEU	N-CA-C	-6.73	103.41	111.69
2	L	32	PRO	N-CA-C	6.73	122.67	113.98
2	L	221	ARG	CD-NE-CZ	6.73	133.82	124.40
1	K	348	ASN	CA-CB-CG	6.73	119.33	112.60
2	B	268	PRO	N-CA-CB	6.72	109.27	103.36
1	K	108	GLU	N-CA-C	6.72	118.60	111.28
1	E	65	LEU	N-CA-C	6.71	119.87	107.99
1	I	386	THR	CA-CB-CG2	6.71	121.91	110.50
1	C	310	TYR	N-CA-CB	-6.71	98.60	109.60
2	J	61	HIS	CA-CB-CG	-6.71	107.09	113.80
1	C	37	HIS	ND1-CG-CD2	6.71	112.81	106.10
1	G	21	TRP	CZ3-CH2-CZ2	-6.71	112.78	121.50
1	I	288	GLU	CA-C-N	6.71	129.50	120.65
1	I	288	GLU	C-N-CA	6.71	129.50	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	203	MET	CA-C-N	6.70	131.88	122.23
2	F	203	MET	C-N-CA	6.70	131.88	122.23
2	B	76	ASP	N-CA-C	6.70	118.58	111.28
2	F	443	GLU	N-CA-C	6.70	118.38	108.60
1	I	69	GLU	CA-C-N	6.70	129.00	120.89
1	I	69	GLU	C-N-CA	6.70	129.00	120.89
2	F	174	ALA	CA-C-N	6.70	126.15	118.85
2	F	174	ALA	C-N-CA	6.70	126.15	118.85
1	A	30	ILE	CA-C-O	6.70	128.28	120.71
1	G	400	GLY	N-CA-C	-6.70	107.30	114.67
1	G	167	PHE	O-C-N	-6.70	114.81	122.84
1	I	328	GLU	CA-C-N	6.69	129.14	120.44
1	I	328	GLU	C-N-CA	6.69	129.14	120.44
2	H	296	PHE	CA-CB-CG	6.69	120.49	113.80
2	D	169	PHE	CA-CB-CG	6.68	120.48	113.80
1	C	71	GLY	CA-C-O	6.68	127.65	120.30
2	N	107	HIS	CB-CG-ND1	6.68	132.72	122.70
2	F	185	TYR	N-CA-C	6.68	118.64	111.36
1	I	305	PRO	N-CA-CB	6.68	109.87	103.19
2	L	36	MET	CA-C-N	6.68	126.39	119.64
2	L	36	MET	C-N-CA	6.68	126.39	119.64
1	G	207	LEU	N-CA-C	6.68	119.41	111.33
1	M	87	PRO	CA-C-N	6.68	129.89	120.28
1	M	87	PRO	C-N-CA	6.68	129.89	120.28
1	C	28	HIS	CB-CG-ND1	6.67	132.71	122.70
2	D	18	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	E	325	GLU	N-CA-C	6.67	118.63	111.36
1	C	394	PHE	CA-C-N	6.67	130.11	120.38
1	C	394	PHE	C-N-CA	6.67	130.11	120.38
2	F	388	TRP	CA-C-O	-6.67	113.77	120.90
2	H	367	ASP	N-CA-C	6.67	121.70	113.50
1	A	145	SER	N-CA-C	6.66	119.39	111.33
2	H	137	VAL	O-C-N	-6.66	115.63	123.03
1	E	77	ARG	N-CA-C	6.66	119.55	111.82
2	J	36	MET	CA-C-N	6.66	128.16	119.84
2	J	36	MET	C-N-CA	6.66	128.16	119.84
2	J	346	TRP	N-CA-CB	-6.66	100.78	110.70
1	I	311	LEU	N-CA-CB	6.66	119.63	109.98
1	M	143	THR	CA-C-N	6.65	128.46	120.14
1	M	143	THR	C-N-CA	6.65	128.46	120.14
2	B	270	ALA	CA-C-N	6.65	132.17	123.00
2	B	270	ALA	C-N-CA	6.65	132.17	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	81	PHE	CA-CB-CG	-6.65	107.15	113.80
1	G	116	VAL	CA-CB-CG2	6.65	121.70	110.40
2	L	306	ASP	CB-CA-C	6.65	116.42	110.44
1	C	201	CYS	O-C-N	-6.64	115.56	123.27
2	B	371	VAL	CA-CB-CG2	6.64	121.69	110.40
2	L	401	LYS	CA-C-N	6.64	131.79	122.36
2	L	401	LYS	C-N-CA	6.64	131.79	122.36
1	C	307	HIS	CB-CG-CD2	-6.64	122.57	131.20
2	H	266	HIS	ND1-CG-CD2	6.64	112.74	106.10
2	N	65	ALA	CA-C-O	-6.64	114.16	121.33
2	N	186	ASN	CA-C-N	6.64	129.50	120.54
2	N	186	ASN	C-N-CA	6.64	129.50	120.54
1	I	126	SER	N-CA-C	6.64	121.09	113.19
1	K	94	GLN	CG-CD-NE2	6.64	126.35	116.40
2	F	262	TYR	CA-C-O	-6.63	112.47	119.50
1	K	327	ASP	N-CA-C	6.63	118.17	111.07
1	K	260	PHE	O-C-N	6.63	129.62	121.79
2	N	98	ASP	CA-CB-CG	6.63	119.23	112.60
2	B	204	VAL	CA-C-O	-6.63	113.59	121.28
2	D	258	ASN	N-CA-CB	-6.63	101.46	110.67
1	C	167	PHE	CA-CB-CG	6.63	120.43	113.80
2	L	163	LYS	N-CA-CB	-6.62	99.40	110.39
2	L	346	TRP	CZ3-CH2-CZ2	-6.62	112.89	121.50
2	N	141	PHE	CA-CB-CG	6.62	120.42	113.80
1	E	209	ASP	CA-C-O	-6.62	114.08	120.90
1	E	280	GLN	OE1-CD-NE2	-6.62	115.98	122.60
1	A	357	PRO	CA-C-N	6.62	128.11	119.84
1	A	357	PRO	C-N-CA	6.62	128.11	119.84
1	I	90	PHE	CA-CB-CG	6.62	120.42	113.80
1	M	389	PHE	N-CA-C	6.62	118.50	111.28
3	O	266	LEU	N-CA-C	6.62	120.81	112.87
2	F	431	ASP	CA-C-O	6.61	127.57	120.10
2	B	28	HIS	ND1-CE1-NE2	6.61	115.01	108.40
2	L	346	TRP	CB-CG-CD2	6.61	136.06	126.80
2	B	31	GLN	CG-CD-NE2	6.61	126.31	116.40
1	A	417	ASP	CA-CB-CG	-6.61	105.99	112.60
1	K	13	GLY	CA-C-O	-6.61	113.94	120.75
1	A	24	ILE	CA-CB-CG2	6.61	121.73	110.50
1	M	6	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	K	137	HIS	CB-CG-CD2	-6.60	122.61	131.20
2	N	331	ALA	O-C-N	6.60	128.87	122.07
1	I	55	ALA	CA-C-N	6.60	126.25	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	55	ALA	C-N-CA	6.60	126.25	119.92
1	E	215	LEU	CA-C-N	6.60	131.76	122.46
1	E	215	LEU	C-N-CA	6.60	131.76	122.46
2	H	138	PHE	CA-C-O	-6.60	113.47	120.40
1	G	414	ASN	CA-CB-CG	6.59	119.19	112.60
2	D	214	ARG	CD-NE-CZ	6.59	133.63	124.40
1	G	178	THR	CA-CB-CG2	6.59	121.71	110.50
2	H	206	ASN	CA-CB-CG	6.59	119.19	112.60
2	D	205	ASP	O-C-N	-6.59	115.23	123.27
1	C	169	VAL	N-CA-CB	6.59	117.71	110.53
3	O	374	HIS	N-CA-C	6.59	124.83	110.80
1	E	410	GLU	N-CA-C	6.58	118.46	111.28
2	H	101	ASN	CB-CA-C	6.58	121.96	111.23
2	N	55	GLU	CA-C-O	-6.58	113.79	121.16
2	N	249	ASN	CA-CB-CG	6.58	119.18	112.60
2	D	172	TYR	CB-CG-CD2	-6.58	110.93	120.80
1	E	329	GLN	OE1-CD-NE2	-6.58	116.02	122.60
1	I	165	ASN	O-C-N	-6.58	115.53	123.29
2	D	212	ILE	CA-CB-CG2	6.58	121.68	110.50
1	E	395	LEU	CA-C-N	6.58	129.39	120.38
1	E	395	LEU	C-N-CA	6.58	129.39	120.38
2	J	202	PHE	O-C-N	6.58	130.79	123.16
2	J	17	GLY	CA-C-O	-6.57	114.28	121.05
2	J	26	LEU	CA-C-N	6.57	129.62	120.29
2	J	26	LEU	C-N-CA	6.57	129.62	120.29
2	L	418	PHE	CA-C-O	6.57	127.67	120.90
1	A	204	ASN	O-C-N	-6.57	115.15	122.12
2	D	406	HIS	CB-CG-CD2	-6.57	122.66	131.20
2	F	102	ASN	N-CA-C	6.57	120.11	109.40
1	K	325	GLU	CA-C-O	6.57	127.51	120.55
2	B	172	TYR	CA-C-O	6.57	127.86	120.97
1	A	52	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	A	171	PRO	N-CA-CB	6.57	109.14	103.36
2	F	222	PRO	O-C-N	-6.57	113.78	122.64
2	L	327	ASP	CA-C-N	6.57	128.83	120.56
2	L	327	ASP	C-N-CA	6.57	128.83	120.56
1	I	7	ILE	CA-C-N	6.56	133.36	122.33
1	I	7	ILE	C-N-CA	6.56	133.36	122.33
1	I	39	ASP	CA-C-O	6.56	125.97	119.08
2	J	92	LEU	CA-C-O	-6.56	114.23	121.58
1	K	121	ARG	CD-NE-CZ	6.56	133.59	124.40
1	I	123	GLU	N-CA-C	6.56	118.43	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	436	PHE	CA-CB-CG	6.56	120.36	113.80
2	N	392	ASP	CA-CB-CG	-6.56	106.04	112.60
2	D	214	ARG	O-C-N	6.55	129.09	122.08
1	K	340	TYR	CA-CB-CG	6.55	125.70	113.90
2	H	174	ALA	N-CA-C	6.55	118.95	109.84
1	E	382	SER	CA-C-O	-6.55	113.48	120.42
1	G	298	ASN	CA-CB-CG	6.55	119.15	112.60
2	J	276	ILE	CA-C-O	-6.55	115.14	121.63
2	N	270	ALA	N-CA-C	6.55	120.22	110.52
1	E	346	PRO	N-CA-CB	6.55	109.14	103.31
1	K	190	HIS	CB-CG-CD2	-6.55	122.69	131.20
2	J	202	PHE	CA-CB-CG	6.54	120.34	113.80
1	A	386	THR	CA-CB-CG2	6.54	121.62	110.50
1	E	20	PHE	CA-C-O	-6.54	113.90	120.90
2	N	101	ASN	OD1-CG-ND2	-6.54	116.06	122.60
1	G	30	ILE	CA-CB-CG1	6.54	121.52	110.40
2	D	177	VAL	O-C-N	-6.54	115.89	122.62
1	M	43	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	E	416	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	M	79	GLY	CA-C-N	6.53	126.29	119.76
1	M	79	GLY	C-N-CA	6.53	126.29	119.76
1	I	60	VAL	CA-CB-CG2	6.53	121.50	110.40
2	J	28	HIS	CB-CG-CD2	-6.53	122.71	131.20
2	J	359	PRO	N-CA-CB	6.53	109.41	103.08
2	N	371	VAL	O-C-N	-6.51	116.13	123.10
2	H	120	ASP	CA-C-N	6.51	130.21	120.31
2	H	120	ASP	C-N-CA	6.51	130.21	120.31
1	K	253	LEU	CA-C-N	6.51	129.84	120.79
1	K	253	LEU	C-N-CA	6.51	129.84	120.79
1	K	370	ASN	OD1-CG-ND2	-6.51	116.09	122.60
2	F	359	PRO	N-CA-CB	6.51	109.39	103.08
2	H	322	ASP	CA-CB-CG	6.51	119.11	112.60
2	L	449	GLU	CA-C-O	-6.51	112.79	120.60
2	D	38	SER	CA-C-N	6.50	130.65	121.02
2	D	38	SER	C-N-CA	6.50	130.65	121.02
2	N	204	VAL	CA-C-N	6.50	131.94	122.77
2	N	204	VAL	C-N-CA	6.50	131.94	122.77
2	N	176	GLN	OE1-CD-NE2	-6.50	116.10	122.60
2	N	140	SER	CA-C-N	6.50	128.99	120.28
2	N	140	SER	C-N-CA	6.50	128.99	120.28
2	L	210	TYR	N-CA-C	6.50	118.91	111.11
1	M	76	VAL	CA-CB-CG1	6.50	121.44	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	171	PRO	N-CA-CB	6.49	109.09	103.31
1	I	380	ARG	CD-NE-CZ	6.49	133.48	124.40
2	J	371	VAL	N-CA-C	6.49	117.95	109.58
1	G	262	ARG	CD-NE-CZ	6.48	133.48	124.40
1	M	189	VAL	N-CA-C	6.48	117.27	110.72
2	D	369	ALA	CA-C-N	6.48	130.57	121.24
2	D	369	ALA	C-N-CA	6.48	130.57	121.24
1	M	356	ILE	O-C-N	6.48	126.15	121.55
2	L	138	PHE	N-CA-C	6.47	119.45	107.99
2	H	183	GLU	CA-C-O	-6.47	112.39	118.73
1	K	5	VAL	CB-CA-C	-6.47	102.15	111.34
2	L	62	VAL	CA-C-N	6.47	126.43	119.76
2	L	62	VAL	C-N-CA	6.47	126.43	119.76
1	A	170	VAL	CA-C-N	6.47	126.69	119.90
1	A	170	VAL	C-N-CA	6.47	126.69	119.90
2	F	169	PHE	CA-CB-CG	-6.47	107.33	113.80
1	C	163	ILE	CA-C-O	-6.46	113.42	121.11
2	H	18	ASN	CA-CB-CG	6.46	119.06	112.60
2	D	154	MET	CA-C-N	6.46	128.94	120.28
2	D	154	MET	C-N-CA	6.46	128.94	120.28
1	E	18	ALA	O-C-N	-6.46	115.27	122.12
2	H	98	ASP	O-C-N	-6.46	115.06	122.68
2	J	375	VAL	O-C-N	-6.46	115.88	123.05
2	H	382	THR	OG1-CB-CG2	-6.46	96.39	109.30
2	B	406	HIS	ND1-CE1-NE2	6.46	114.86	108.40
1	E	48	ASN	CB-CG-ND2	6.46	126.08	116.40
2	H	448	GLY	N-CA-C	6.46	119.90	110.80
2	J	380	ASN	CA-C-N	6.46	132.92	121.75
2	J	380	ASN	C-N-CA	6.46	132.92	121.75
2	L	327	ASP	CA-CB-CG	6.46	119.06	112.60
2	F	358	GLN	CG-CD-NE2	6.45	126.08	116.40
1	M	8	GLN	OE1-CD-NE2	-6.45	116.15	122.60
1	E	390	ARG	CD-NE-CZ	6.45	133.43	124.40
1	M	209	ASP	CA-C-N	6.45	129.62	120.53
1	M	209	ASP	C-N-CA	6.45	129.62	120.53
2	J	172	TYR	CB-CA-C	6.45	118.48	108.61
2	D	246	GLY	CA-C-O	-6.44	114.84	121.61
1	A	91	VAL	CA-C-O	-6.44	113.75	120.51
1	E	385	PHE	CA-C-N	6.44	128.91	120.28
1	E	385	PHE	C-N-CA	6.44	128.91	120.28
2	L	371	VAL	N-CA-C	6.44	119.58	108.95
2	H	92	LEU	CA-C-N	6.44	129.13	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	92	LEU	C-N-CA	6.44	129.13	120.50
2	L	28	HIS	CA-CB-CG	-6.44	107.36	113.80
2	N	87	PHE	CA-CB-CG	6.44	120.24	113.80
2	J	448	GLY	CA-C-N	6.43	131.61	122.09
2	J	448	GLY	C-N-CA	6.43	131.61	122.09
2	B	250	VAL	CA-C-N	6.43	129.84	120.71
2	B	250	VAL	C-N-CA	6.43	129.84	120.71
1	K	317	PHE	CA-CB-CG	6.43	120.23	113.80
2	N	199	ASP	CA-CB-CG	-6.43	106.17	112.60
1	I	223	GLY	N-CA-C	-6.43	105.02	112.73
2	L	128	GLN	OE1-CD-NE2	-6.42	116.18	122.60
1	A	66	VAL	N-CA-C	6.42	117.72	108.48
2	L	69	ASP	OD1-CG-OD2	-6.42	107.50	122.90
1	C	160	PRO	CA-C-N	6.42	132.46	122.26
1	C	160	PRO	C-N-CA	6.42	132.46	122.26
1	E	269	GLY	CA-C-N	6.41	133.94	121.63
1	E	269	GLY	C-N-CA	6.41	133.94	121.63
2	F	85	GLN	OE1-CD-NE2	-6.41	116.19	122.60
2	D	450	GLU	N-CA-CB	-6.41	101.23	111.62
1	A	436	PHE	CA-CB-CG	6.41	120.21	113.80
1	E	405	GLU	O-C-N	-6.41	114.72	122.22
2	L	122	ILE	CA-C-O	-6.41	114.06	120.85
1	A	433	GLN	CG-CD-NE2	6.41	126.01	116.40
1	K	320	ARG	CA-C-O	6.40	127.21	120.36
1	M	212	PHE	N-CA-C	6.40	118.34	111.36
2	N	130	THR	N-CA-CB	6.40	120.16	110.30
2	H	74	VAL	CA-CB-CG2	6.40	121.28	110.40
1	I	238	THR	CA-C-O	-6.40	113.77	120.55
2	B	218	ASP	CA-C-N	6.40	130.37	122.37
2	B	218	ASP	C-N-CA	6.40	130.37	122.37
2	H	244	PHE	CA-CB-CG	6.39	120.19	113.80
1	I	205	GLU	N-CA-C	6.39	120.34	112.54
1	A	313	VAL	CA-CB-CG1	6.39	121.26	110.40
1	M	329	GLN	OE1-CD-NE2	-6.39	116.21	122.60
1	M	344	TRP	CA-C-O	6.39	127.45	119.59
1	M	76	VAL	CA-C-O	-6.38	113.96	121.05
1	M	205	GLU	O-C-N	6.38	130.12	122.27
1	G	13	GLY	CA-C-O	-6.38	113.28	120.30
1	I	411	ALA	N-CA-C	6.38	118.81	111.02
2	J	414	GLU	CB-CA-C	6.38	122.33	109.38
1	G	268	PRO	CB-CA-C	6.38	120.19	110.75
1	A	17	GLY	N-CA-C	6.37	120.38	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	395	PHE	CA-CB-CG	6.37	120.17	113.80
1	E	424	GLN	OE1-CD-NE2	-6.37	116.23	122.60
1	G	320	ARG	CB-CA-C	6.37	121.41	110.77
2	J	216	ASN	OD1-CG-ND2	-6.37	116.23	122.60
2	N	81	GLY	O-C-N	6.37	127.68	122.71
2	B	28	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	G	342	VAL	CA-CB-CG2	6.37	121.23	110.40
3	O	388	HIS	CA-C-N	6.37	133.16	121.70
3	O	388	HIS	C-N-CA	6.37	133.16	121.70
1	E	291	GLN	OE1-CD-NE2	-6.36	116.24	122.60
1	A	395	LEU	CA-C-N	6.36	129.44	120.28
1	A	395	LEU	C-N-CA	6.36	129.44	120.28
2	D	375	VAL	O-C-N	-6.36	116.48	123.03
1	I	343	GLU	CA-C-O	6.36	126.60	119.41
1	M	120	VAL	N-CA-CB	6.36	117.99	110.55
2	J	307	PRO	N-CA-CB	6.36	109.56	103.52
1	K	426	GLN	CG-CD-NE2	6.36	125.94	116.40
1	M	353	VAL	CA-C-O	-6.36	113.85	120.27
2	N	39	ASP	CA-CB-CG	6.36	118.96	112.60
2	D	35	GLN	OE1-CD-NE2	-6.36	116.25	122.60
2	D	266	HIS	CA-CB-CG	6.36	120.16	113.80
2	F	35	GLN	OE1-CD-NE2	-6.35	116.25	122.60
1	I	87	PRO	CA-N-CD	-6.35	103.11	112.00
2	N	67	PHE	N-CA-C	6.35	119.88	109.72
2	N	280	LYS	CB-CA-C	6.35	119.31	109.03
2	L	440	VAL	CA-C-O	-6.34	112.95	121.32
2	J	398	MET	CA-C-O	6.34	127.23	120.70
2	H	377	MET	CA-C-N	6.34	131.86	122.86
2	H	377	MET	C-N-CA	6.34	131.86	122.86
1	A	37	HIS	ND1-CG-CD2	6.34	112.44	106.10
1	K	326	VAL	CA-CB-CG1	6.34	121.17	110.40
2	B	206	ASN	N-CA-C	6.33	120.03	112.93
1	I	290	THR	O-C-N	6.33	128.83	122.12
2	J	153	LEU	CA-C-O	-6.33	113.84	120.55
2	J	380	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	K	168	SER	N-CA-CB	-6.33	100.09	110.42
3	O	250	MET	N-CA-C	6.33	117.87	109.83
1	A	147	MET	CA-C-N	6.33	128.26	120.22
1	A	147	MET	C-N-CA	6.33	128.26	120.22
1	G	395	LEU	CA-C-N	6.32	129.04	120.38
1	G	395	LEU	C-N-CA	6.32	129.04	120.38
2	N	340	SER	N-CA-C	6.31	120.55	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	369	LYS	CA-C-N	6.31	133.06	121.70
3	O	369	LYS	C-N-CA	6.31	133.06	121.70
2	J	246	GLY	CA-C-O	-6.31	114.49	121.37
2	L	222	PRO	N-CA-CB	6.31	109.18	103.19
2	L	306	ASP	CA-C-N	6.31	127.73	119.84
2	L	306	ASP	C-N-CA	6.31	127.73	119.84
1	M	231	ALA	N-CA-C	6.31	118.16	111.28
2	D	88	HIS	CA-CB-CG	6.31	120.11	113.80
1	G	332	ASN	CA-C-N	6.31	128.74	120.60
1	G	332	ASN	C-N-CA	6.31	128.74	120.60
1	E	31	ASP	N-CA-CB	-6.30	100.91	110.11
1	A	45	GLU	CA-CB-CG	6.30	126.71	114.10
2	H	139	HIS	N-CA-C	6.30	116.32	108.19
1	I	426	GLN	CA-C-N	6.30	132.44	122.61
1	I	426	GLN	C-N-CA	6.30	132.44	122.61
1	C	254	ALA	N-CA-C	6.30	118.67	111.11
2	D	197	HIS	CB-CG-CD2	-6.30	123.02	131.20
2	D	285	GLN	OE1-CD-NE2	-6.30	116.30	122.60
1	C	379	LYS	CA-C-N	6.29	128.62	120.44
1	C	379	LYS	C-N-CA	6.29	128.62	120.44
2	J	106	GLY	N-CA-C	6.29	120.83	112.77
1	C	162	ARG	O-C-N	-6.29	115.85	122.96
1	C	244	GLY	CA-C-O	-6.29	114.22	121.46
2	L	7	ILE	CB-CG1-CD1	6.29	127.02	113.80
2	D	362	VAL	CA-CB-CG1	6.29	121.09	110.40
1	A	143	THR	CA-C-N	6.29	127.09	119.99
1	A	143	THR	C-N-CA	6.29	127.09	119.99
2	F	168	GLU	CA-C-N	6.29	131.90	122.47
2	F	168	GLU	C-N-CA	6.29	131.90	122.47
2	H	88	HIS	CB-CG-CD2	-6.28	123.03	131.20
1	I	184	ASN	CA-CB-CG	6.28	118.88	112.60
1	G	52	ASN	CA-CB-CG	-6.28	106.32	112.60
3	O	287	VAL	CA-C-N	6.28	132.38	122.21
3	O	287	VAL	C-N-CA	6.28	132.38	122.21
1	E	313	VAL	CA-CB-CG2	6.27	121.06	110.40
1	K	57	ASN	CA-CB-CG	6.27	118.87	112.60
1	E	43	GLN	OE1-CD-NE2	-6.27	116.33	122.60
2	B	351	PHE	CA-C-N	6.27	132.01	122.93
2	B	351	PHE	C-N-CA	6.27	132.01	122.93
1	K	423	GLN	OE1-CD-NE2	-6.26	116.33	122.60
2	B	409	VAL	CA-CB-CG1	6.26	121.05	110.40
1	M	233	MET	CA-C-N	6.26	128.67	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	233	MET	C-N-CA	6.26	128.67	120.28
1	M	6	HIS	CG-CD2-NE2	-6.26	100.94	107.20
1	M	307	HIS	CA-CB-CG	-6.26	107.54	113.80
1	A	376	GLU	N-CA-C	6.26	120.64	113.19
2	B	440	VAL	O-C-N	-6.26	116.72	122.79
1	A	327	ASP	N-CA-C	6.25	118.18	111.36
2	L	297	GLU	CA-C-O	-6.25	113.50	120.25
1	A	171	PRO	CA-C-O	6.25	128.15	121.03
1	M	326	VAL	N-CA-C	-6.25	104.55	110.42
2	H	283	HIS	CB-CG-CD2	-6.25	123.08	131.20
1	A	16	ILE	N-CA-C	6.24	117.03	110.72
1	G	101	TRP	CE3-CZ3-CH2	-6.24	112.98	121.10
3	O	235	SER	CA-C-N	6.24	126.16	119.85
3	O	235	SER	C-N-CA	6.24	126.16	119.85
1	E	118	ASP	CA-C-N	6.24	129.01	120.46
1	E	118	ASP	C-N-CA	6.24	129.01	120.46
1	K	76	VAL	CG1-CB-CG2	-6.24	97.07	110.80
1	M	413	SER	CA-C-N	6.24	131.29	120.68
1	M	413	SER	C-N-CA	6.24	131.29	120.68
2	H	390	ARG	CA-C-O	-6.24	113.31	120.24
1	C	238	THR	N-CA-C	6.24	120.09	112.23
2	J	200	CYS	CA-C-O	6.24	128.06	121.33
2	F	17	GLY	CA-C-N	6.23	128.96	120.54
2	F	17	GLY	C-N-CA	6.23	128.96	120.54
1	K	62	ARG	CA-C-N	6.23	129.61	120.82
1	K	62	ARG	C-N-CA	6.23	129.61	120.82
1	G	175	VAL	CA-CB-CG1	6.23	121.00	110.40
2	L	53	PHE	CA-CB-CG	6.23	120.03	113.80
1	A	186	THR	CA-C-N	6.23	131.23	120.58
1	A	186	THR	C-N-CA	6.23	131.23	120.58
1	C	33	THR	CA-C-N	6.23	133.33	122.05
1	C	33	THR	C-N-CA	6.23	133.33	122.05
1	C	137	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	K	91	VAL	N-CA-C	6.23	112.88	106.21
2	L	146	GLY	CA-C-N	6.23	133.44	121.54
2	L	146	GLY	C-N-CA	6.23	133.44	121.54
3	O	265	ASN	OD1-CG-ND2	-6.23	116.37	122.60
2	F	419	SER	N-CA-C	-6.23	104.41	111.14
1	M	379	LYS	O-C-N	6.22	129.50	122.22
1	A	156	ARG	N-CA-CB	-6.22	100.64	110.28
1	G	306	ARG	CD-NE-CZ	6.22	133.11	124.40
2	L	84	ARG	O-C-N	-6.22	115.11	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	52	PHE	CA-CB-CG	6.22	120.02	113.80
1	G	220	PRO	O-C-N	6.21	129.62	123.03
1	M	40	SER	CA-C-N	6.21	129.45	120.38
1	M	40	SER	C-N-CA	6.21	129.45	120.38
2	H	61	HIS	CA-C-N	6.21	130.26	123.43
2	H	61	HIS	C-N-CA	6.21	130.26	123.43
2	H	107	HIS	CB-CG-CD2	-6.21	123.12	131.20
2	N	11	GLN	CA-C-O	-6.21	113.08	120.10
2	F	220	GLU	CA-C-N	6.21	131.84	123.46
2	F	220	GLU	C-N-CA	6.21	131.84	123.46
2	B	301	GLN	CB-CA-C	6.21	120.96	109.54
1	C	94	GLN	OE1-CD-NE2	-6.21	116.39	122.60
2	J	448	GLY	O-C-N	-6.21	116.12	122.70
1	I	398	TYR	CB-CA-C	6.20	120.56	110.95
2	L	354	GLY	O-C-N	6.20	129.34	123.57
2	B	284	GLU	CA-C-N	6.20	130.20	121.02
2	B	284	GLU	C-N-CA	6.20	130.20	121.02
1	E	268	PRO	CB-CA-C	6.20	119.25	110.20
2	F	252	LEU	CA-C-O	-6.20	111.76	119.38
2	H	67	PHE	CA-CB-CG	6.20	120.00	113.80
1	C	380	ARG	CA-C-N	6.19	128.94	120.46
1	C	380	ARG	C-N-CA	6.19	128.94	120.46
2	F	160	ASP	CB-CA-C	6.19	121.82	110.11
1	G	100	ASN	CA-CB-CG	6.19	118.79	112.60
1	G	269	GLY	O-C-N	-6.19	117.84	123.54
2	L	258	ASN	OD1-CG-ND2	-6.19	116.41	122.60
2	B	233	GLN	OE1-CD-NE2	-6.19	116.41	122.60
2	F	384	ILE	CA-CB-CG1	6.19	120.92	110.40
2	J	75	ILE	CB-CA-C	6.19	118.67	111.55
1	K	251	ARG	CA-C-N	6.19	129.72	120.31
1	K	251	ARG	C-N-CA	6.19	129.72	120.31
2	H	126	ALA	CA-C-N	6.19	128.57	120.28
2	H	126	ALA	C-N-CA	6.19	128.57	120.28
1	A	112	LEU	CA-C-N	6.18	129.25	120.53
1	A	112	LEU	C-N-CA	6.18	129.25	120.53
2	B	294	ALA	CA-C-O	-6.18	113.11	120.10
1	G	14	ASN	CA-CB-CG	-6.18	106.42	112.60
1	I	84	ILE	CA-C-N	6.18	129.65	120.87
1	I	84	ILE	C-N-CA	6.18	129.65	120.87
2	B	442	GLY	O-C-N	-6.18	115.69	122.24
1	M	266	PHE	CA-CB-CG	6.18	119.98	113.80
2	B	328	VAL	CA-C-N	6.18	129.06	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	328	VAL	C-N-CA	6.18	129.06	120.29
1	G	357	PRO	CA-C-N	6.17	126.12	119.76
1	G	357	PRO	C-N-CA	6.17	126.12	119.76
1	G	432	GLU	CA-C-O	-6.17	114.77	121.44
3	O	222	GLU	CA-C-N	6.17	125.73	119.19
3	O	222	GLU	C-N-CA	6.17	125.73	119.19
1	G	134	GLN	OE1-CD-NE2	-6.17	116.43	122.60
2	H	40	LYS	N-CA-C	6.17	120.98	112.90
1	C	362	LYS	CA-C-N	6.16	132.41	121.75
1	C	362	LYS	C-N-CA	6.16	132.41	121.75
1	G	174	LYS	CA-C-N	6.16	129.44	122.48
1	G	174	LYS	C-N-CA	6.16	129.44	122.48
2	H	210	TYR	O-C-N	-6.16	115.59	122.12
2	L	324	VAL	CA-CB-CG2	6.16	120.88	110.40
3	O	208	SER	CA-C-N	6.16	131.87	122.93
3	O	208	SER	C-N-CA	6.16	131.87	122.93
1	K	142	GLY	CA-C-N	6.16	131.12	120.58
1	K	142	GLY	C-N-CA	6.16	131.12	120.58
1	E	181	GLU	CA-C-O	-6.16	112.66	118.33
1	E	242	PHE	O-C-N	-6.16	117.16	121.65
1	A	76	VAL	CA-C-N	6.15	129.03	120.29
1	A	76	VAL	C-N-CA	6.15	129.03	120.29
1	C	375	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	G	88	ASP	CA-C-O	6.15	127.18	119.12
1	I	37	HIS	CA-CB-CG	-6.15	107.65	113.80
1	C	79	GLY	CA-C-N	6.15	126.09	119.76
1	C	79	GLY	C-N-CA	6.15	126.09	119.76
1	K	264	HIS	CB-CG-ND1	6.15	131.92	122.70
2	B	122	ILE	CB-CA-C	6.15	120.07	112.02
1	K	55	ALA	N-CA-C	6.15	118.95	110.35
2	D	309	HIS	ND1-CE1-NE2	6.14	114.55	108.40
1	K	195	ASN	OD1-CG-ND2	-6.14	116.45	122.60
1	A	298	ASN	OD1-CG-ND2	-6.14	116.46	122.60
1	C	184	ASN	O-C-N	-6.14	115.61	122.12
1	I	62	ARG	CB-CA-C	6.14	121.24	111.91
1	M	154	LYS	N-CA-C	6.13	117.63	111.07
2	N	406	HIS	ND1-CE1-NE2	6.13	114.53	108.40
2	H	423	GLU	CA-C-O	-6.13	114.01	120.63
1	A	354	CYS	CA-C-O	-6.13	114.06	121.05
1	K	66	VAL	N-CA-CB	-6.13	100.58	111.93
1	M	239	CYS	N-CA-C	6.13	123.86	110.80
1	C	63	ALA	CA-C-N	6.13	130.79	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	ALA	C-N-CA	6.13	130.79	123.19
1	C	430	ALA	CA-C-N	6.13	130.01	120.75
1	C	430	ALA	C-N-CA	6.13	130.01	120.75
2	B	33	ASP	CB-CG-OD2	6.13	132.50	118.40
2	F	339	ARG	O-C-N	6.13	130.35	122.39
2	H	307	PRO	N-CA-CB	6.12	109.02	103.20
2	B	215	ARG	N-CA-C	6.12	117.75	111.14
2	B	280	LYS	O-C-N	-6.12	115.17	122.15
2	F	253	THR	CA-CB-OG1	6.12	118.78	109.60
1	C	349	VAL	CA-CB-CG1	6.12	120.81	110.40
1	G	99	ASN	CA-CB-CG	6.12	118.72	112.60
2	H	417	GLU	CA-C-O	6.12	126.89	119.31
1	I	96	GLY	CA-C-N	6.11	132.13	122.11
1	I	96	GLY	C-N-CA	6.11	132.13	122.11
1	M	171	PRO	N-CA-CB	6.11	108.75	103.31
1	G	443	ASP	CA-CB-CG	-6.11	106.49	112.60
1	A	307	HIS	CB-CG-ND1	6.11	131.86	122.70
2	J	346	TRP	CB-CA-C	6.10	121.01	110.94
2	B	388	TRP	NE1-CE2-CZ2	6.10	139.25	130.10
1	E	38	GLY	O-C-N	-6.10	117.37	122.92
2	L	349	THR	O-C-N	-6.10	114.32	122.19
1	I	52	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	K	172	SER	O-C-N	-6.10	113.83	121.21
1	E	105	HIS	CE1-NE2-CD2	-6.10	102.90	109.00
2	F	280	LYS	O-C-N	-6.09	115.80	122.07
2	H	53	PHE	CA-C-N	6.09	131.36	122.77
2	H	53	PHE	C-N-CA	6.09	131.36	122.77
2	J	200	CYS	O-C-N	-6.09	116.31	123.25
2	L	47	ASP	CB-CA-C	6.09	121.67	110.10
1	K	63	ALA	CB-CA-C	6.09	119.40	109.90
2	F	81	GLY	CA-C-N	6.09	129.56	120.31
2	F	81	GLY	C-N-CA	6.09	129.56	120.31
1	G	197	ASP	CA-CB-CG	-6.09	106.51	112.60
2	L	190	THR	CA-CB-OG1	-6.09	100.47	109.60
1	I	81	PHE	CA-C-O	-6.08	111.81	120.51
2	F	233	GLN	OE1-CD-NE2	-6.08	116.52	122.60
2	H	296	PHE	CA-C-N	6.08	128.81	120.67
2	H	296	PHE	C-N-CA	6.08	128.81	120.67
2	B	179	THR	CA-CB-CG2	6.08	120.83	110.50
1	K	237	THR	O-C-N	-6.08	114.06	122.20
1	A	69	GLU	O-C-N	-6.07	117.83	121.71
2	D	423	GLU	CA-C-N	6.07	128.91	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	423	GLU	C-N-CA	6.07	128.91	120.29
1	G	28	HIS	N-CA-C	6.07	120.69	113.16
1	E	118	ASP	N-CA-CB	-6.07	101.21	110.01
1	A	190	HIS	CB-CG-CD2	-6.06	123.32	131.20
2	N	107	HIS	CG-CD2-NE2	6.06	113.26	107.20
2	F	254	GLU	N-CA-CB	-6.06	100.88	110.28
2	L	172	TYR	N-CA-C	6.06	118.27	110.39
2	F	287	SER	CA-C-N	6.06	129.03	120.42
2	F	287	SER	C-N-CA	6.06	129.03	120.42
1	G	410	GLU	CA-C-N	6.06	128.68	120.44
1	G	410	GLU	C-N-CA	6.06	128.68	120.44
1	G	356	ILE	O-C-N	-6.06	115.49	121.12
3	O	222	GLU	CB-CG-CD	6.06	122.89	112.60
2	J	380	ASN	O-C-N	-6.05	116.32	123.22
1	E	418	LEU	CA-C-N	6.05	128.41	120.60
1	E	418	LEU	C-N-CA	6.05	128.41	120.60
1	M	423	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	E	444	GLU	CB-CA-C	6.05	120.00	109.65
1	G	306	ARG	CA-C-N	6.05	130.82	120.72
1	G	306	ARG	C-N-CA	6.05	130.82	120.72
1	I	199	THR	CA-CB-CG2	6.05	120.79	110.50
2	L	93	ILE	CA-C-O	-6.05	114.86	121.28
1	M	177	ASP	CA-C-N	6.05	133.25	121.63
1	M	177	ASP	C-N-CA	6.05	133.25	121.63
1	C	197	ASP	CA-CB-CG	-6.05	106.55	112.60
1	C	356	ILE	CA-C-N	6.05	126.61	120.38
1	C	356	ILE	C-N-CA	6.05	126.61	120.38
1	C	360	GLY	O-C-N	-6.05	115.88	122.41
2	J	211	ASP	CA-CB-CG	6.04	118.64	112.60
2	H	309	HIS	ND1-CG-CD2	6.04	112.14	106.10
2	L	332	ILE	CA-C-O	-6.04	114.45	120.85
2	D	301	GLN	O-C-N	-6.04	115.89	123.01
1	C	405	GLU	CB-CG-CD	6.03	122.86	112.60
2	F	435	VAL	N-CA-C	6.03	116.79	111.90
2	H	306	ASP	CB-CA-C	6.03	119.19	109.41
2	D	173	PRO	O-C-N	-6.03	115.64	123.06
2	H	115	ILE	CA-CB-CG1	6.03	120.65	110.40
2	B	17	GLY	N-CA-C	6.03	120.19	112.83
1	I	267	MET	CA-C-O	-6.03	114.30	119.36
1	K	387	ALA	CA-C-O	-6.03	113.29	120.10
2	B	342	GLN	OE1-CD-NE2	-6.02	116.58	122.60
2	F	225	THR	CA-C-N	6.02	128.35	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	225	THR	C-N-CA	6.02	128.35	120.28
2	L	156	ARG	CA-C-O	6.02	127.11	120.90
1	M	430	ALA	N-CA-CB	-6.02	101.50	110.17
2	F	378	LEU	CA-C-O	6.02	127.69	120.28
1	G	264	HIS	CB-CG-CD2	-6.02	123.37	131.20
2	N	29	GLY	CA-C-N	6.02	128.57	120.50
2	N	29	GLY	C-N-CA	6.02	128.57	120.50
1	K	239	CYS	CA-C-O	-6.02	112.20	119.49
2	D	138	PHE	N-CA-CB	-6.02	101.10	110.55
2	L	23	LEU	N-CA-C	6.02	117.92	111.36
1	G	189	VAL	CA-C-N	6.01	128.66	120.54
1	G	189	VAL	C-N-CA	6.01	128.66	120.54
1	G	258	VAL	CA-C-N	6.01	127.36	119.84
1	G	258	VAL	C-N-CA	6.01	127.36	119.84
1	K	407	GLU	CA-CB-CG	-6.01	102.07	114.10
1	C	139	LEU	CA-C-O	6.01	126.20	119.41
2	J	254	GLU	CA-C-N	6.01	128.26	120.44
2	J	254	GLU	C-N-CA	6.01	128.26	120.44
1	G	165	ASN	O-C-N	-6.01	115.37	123.19
1	A	41	ASP	CA-C-N	6.01	130.31	120.63
1	A	41	ASP	C-N-CA	6.01	130.31	120.63
1	E	240	LEU	CD1-CG-CD2	-6.01	97.58	110.80
2	H	317	LEU	N-CA-C	-6.01	100.35	109.85
2	D	177	VAL	CA-CB-CG1	6.01	120.61	110.40
2	F	276	ILE	CA-CB-CG1	6.01	120.61	110.40
2	H	78	VAL	CA-C-N	6.01	128.93	120.28
2	H	78	VAL	C-N-CA	6.01	128.93	120.28
1	E	234	SER	CA-C-N	6.00	133.18	121.41
1	E	234	SER	C-N-CA	6.00	133.18	121.41
2	H	375	VAL	N-CA-C	6.00	116.49	108.27
2	L	294	ALA	N-CA-CB	-6.00	100.62	110.40
1	G	101	TRP	CD2-CE3-CZ3	6.00	126.40	118.60
2	J	211	ASP	O-C-N	6.00	128.99	122.15
2	N	235	VAL	N-CA-C	6.00	117.46	110.62
1	E	115	SER	CA-C-O	6.00	126.75	119.38
1	G	105	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	G	370	ASN	OD1-CG-ND2	-6.00	116.60	122.60
2	L	188	ILE	CA-C-O	-5.99	114.30	120.71
2	L	291	ILE	CA-CB-CG2	5.99	120.69	110.50
2	B	183	GLU	CA-CB-CG	5.99	126.08	114.10
2	N	230	LEU	CB-CA-C	5.99	118.73	109.03
2	J	404	PHE	N-CA-C	5.99	123.56	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	245	ASP	CA-CB-CG	5.99	118.59	112.60
2	H	381	THR	CA-CB-OG1	5.99	118.58	109.60
1	K	110	ALA	N-CA-CB	-5.99	100.14	110.32
2	D	133	GLN	OE1-CD-NE2	-5.98	116.62	122.60
1	E	287	PRO	N-CA-CB	5.98	109.91	103.33
1	K	181	GLU	CB-CG-CD	5.98	122.77	112.60
2	N	37	PRO	N-CA-C	5.98	121.62	113.84
1	I	181	GLU	CA-C-O	-5.98	112.82	118.44
2	D	293	ASN	OD1-CG-ND2	-5.97	116.62	122.60
2	F	447	GLU	CA-C-N	5.97	129.24	122.67
2	F	447	GLU	C-N-CA	5.97	129.24	122.67
2	N	175	PRO	N-CA-CB	5.97	109.52	103.25
2	J	234	ILE	CA-C-N	5.97	130.10	120.55
2	J	234	ILE	C-N-CA	5.97	130.10	120.55
2	J	308	ARG	N-CA-C	5.97	119.66	112.38
2	L	38	SER	N-CA-C	5.97	118.57	111.71
2	N	362	VAL	CA-C-O	-5.96	114.80	121.36
2	B	139	HIS	N-CA-C	5.96	115.96	108.45
2	N	138	PHE	CA-C-N	5.96	131.59	122.11
2	N	138	PHE	C-N-CA	5.96	131.59	122.11
2	N	172	TYR	CA-C-O	-5.96	114.50	120.64
2	J	313	MET	N-CA-C	5.96	122.26	114.75
1	A	260	PHE	CB-CA-C	-5.96	102.21	110.37
1	C	264	HIS	CB-CG-CD2	-5.96	123.46	131.20
2	D	49	PHE	CA-CB-CG	5.95	119.75	113.80
1	G	382	SER	N-CA-C	5.95	120.27	112.89
2	F	192	HIS	CB-CG-CD2	-5.95	123.46	131.20
1	I	147	MET	CA-C-N	5.95	126.55	119.94
1	I	147	MET	C-N-CA	5.95	126.55	119.94
1	M	51	TYR	CA-CB-CG	5.95	124.61	113.90
1	M	212	PHE	N-CA-CB	-5.95	101.35	110.16
1	A	401	GLU	CA-C-O	-5.95	113.13	119.97
2	F	297	GLU	CA-C-N	5.95	125.65	119.05
2	F	297	GLU	C-N-CA	5.95	125.65	119.05
2	F	372	GLN	OE1-CD-NE2	-5.95	116.65	122.60
2	N	62	VAL	CA-C-N	5.95	126.29	119.93
2	N	62	VAL	C-N-CA	5.95	126.29	119.93
3	O	276	GLN	OE1-CD-NE2	-5.95	116.65	122.60
1	E	433	GLN	N-CA-C	5.94	119.83	112.58
1	C	136	THR	N-CA-CB	5.94	119.88	110.55
2	F	353	VAL	CA-C-O	5.94	127.62	120.67
1	G	119	VAL	O-C-N	-5.94	116.11	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	160	ASP	CA-CB-CG	5.94	118.54	112.60
1	E	276	ARG	CA-C-O	-5.94	112.02	120.51
2	H	137	VAL	N-CA-CB	5.94	118.12	110.99
1	I	209	ASP	N-CA-C	5.94	118.54	111.71
2	J	94	THR	CA-CB-OG1	-5.94	100.69	109.60
1	C	270	PHE	CA-CB-CG	5.94	119.74	113.80
2	J	77	GLU	CA-C-N	5.93	128.16	120.56
2	J	77	GLU	C-N-CA	5.93	128.16	120.56
2	D	390	ARG	CA-C-O	-5.93	114.55	120.90
2	F	139	HIS	ND1-CG-CD2	5.93	112.03	106.10
3	O	211	ARG	CD-NE-CZ	5.93	132.70	124.40
1	A	120	VAL	CB-CA-C	-5.93	102.97	112.16
1	E	298	ASN	OD1-CG-ND2	-5.93	116.67	122.60
2	J	391	LEU	CA-C-N	5.93	128.15	120.44
2	J	391	LEU	C-N-CA	5.93	128.15	120.44
2	B	176	GLN	OE1-CD-NE2	-5.92	116.67	122.60
2	F	88	HIS	CA-CB-CG	-5.92	107.88	113.80
2	F	166	LYS	N-CA-CB	-5.92	100.64	110.47
3	O	306	VAL	O-C-N	-5.92	115.17	122.57
3	O	314	ASP	CA-CB-CG	5.92	118.52	112.60
1	C	436	PHE	O-C-N	-5.92	116.74	123.48
2	B	341	ILE	N-CA-C	-5.91	99.02	107.77
1	C	165	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	E	285	THR	CA-CB-CG2	5.91	120.55	110.50
1	E	408	PHE	O-C-N	-5.91	115.00	122.27
2	D	37	PRO	N-CA-CB	5.91	109.19	103.51
2	B	61	HIS	ND1-CG-CD2	5.91	112.01	106.10
1	M	284	LEU	N-CA-C	5.91	118.28	109.59
2	J	212	ILE	CA-C-N	5.91	128.48	120.44
2	J	212	ILE	C-N-CA	5.91	128.48	120.44
2	D	87	PHE	N-CA-C	5.91	119.20	110.46
1	G	406	MET	O-C-N	-5.91	115.86	122.12
1	I	266	PHE	O-C-N	-5.91	116.07	123.27
2	N	408	TYR	N-CA-CB	-5.91	101.85	110.47
2	H	392	ASP	CA-CB-CG	5.90	118.50	112.60
2	L	49	PHE	CA-C-N	5.90	131.97	120.99
2	L	49	PHE	C-N-CA	5.90	131.97	120.99
1	K	289	LEU	N-CA-C	-5.90	104.54	110.97
2	D	147	SER	CA-C-N	5.90	126.53	119.98
2	D	147	SER	C-N-CA	5.90	126.53	119.98
2	B	36	MET	CA-C-N	5.90	125.52	119.56
2	B	36	MET	C-N-CA	5.90	125.52	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ASP	CA-C-N	5.90	128.46	120.38
1	C	249	ASP	C-N-CA	5.90	128.46	120.38
2	B	365	GLY	O-C-N	-5.89	114.68	122.28
1	C	125	GLU	CB-CG-CD	-5.89	102.58	112.60
1	I	238	THR	N-CA-CB	5.89	118.79	110.12
1	M	279	GLN	N-CA-C	-5.89	105.35	112.54
2	B	156	ARG	CD-NE-CZ	5.89	132.65	124.40
1	A	99	ASN	OD1-CG-ND2	-5.89	116.71	122.60
2	B	237	SER	CA-C-N	5.89	130.28	120.62
2	B	237	SER	C-N-CA	5.89	130.28	120.62
2	B	364	PRO	N-CD-CG	5.89	112.03	103.20
2	B	183	GLU	O-C-N	-5.89	114.55	121.32
2	H	407	TRP	CE3-CZ3-CH2	-5.89	113.45	121.10
2	L	233	GLN	CA-C-N	5.89	127.98	120.56
2	L	233	GLN	C-N-CA	5.89	127.98	120.56
2	F	71	GLU	CA-C-N	5.88	125.36	119.24
2	F	71	GLU	C-N-CA	5.88	125.36	119.24
2	F	409	VAL	CB-CA-C	5.88	119.41	111.88
1	K	62	ARG	CB-CA-C	5.88	120.17	111.17
2	F	316	CYS	O-C-N	-5.88	116.39	123.27
2	J	32	PRO	N-CA-CB	5.88	108.94	103.41
2	J	176	GLN	CA-C-O	-5.88	111.72	119.06
1	M	152	ILE	CA-C-O	-5.88	115.16	121.27
1	E	24	ILE	CA-CB-CG2	5.87	120.49	110.50
2	L	98	ASP	CA-CB-CG	5.87	118.47	112.60
2	N	263	PRO	N-CA-CB	5.87	109.79	103.33
2	F	50	ASN	OD1-CG-ND2	-5.87	116.73	122.60
2	B	384	ILE	CA-C-N	5.87	128.95	120.38
2	B	384	ILE	C-N-CA	5.87	128.95	120.38
1	G	87	PRO	N-CA-CB	5.87	109.79	103.33
1	C	58	LYS	O-C-N	-5.87	116.09	123.01
2	H	222	PRO	N-CA-CB	5.87	108.52	103.36
2	H	186	ASN	O-C-N	-5.87	115.36	122.22
2	N	264	ARG	CD-NE-CZ	5.87	132.61	124.40
1	E	112	LEU	CA-C-N	5.86	128.80	120.53
1	E	112	LEU	C-N-CA	5.86	128.80	120.53
1	G	404	ASP	CA-C-N	5.86	128.72	120.28
1	G	404	ASP	C-N-CA	5.86	128.72	120.28
2	D	192	HIS	CB-CG-ND1	5.86	131.49	122.70
1	E	304	ASP	CB-CA-C	5.86	115.97	110.17
2	N	223	THR	CA-C-O	-5.86	115.31	121.99
1	G	414	ASN	OD1-CG-ND2	-5.86	116.74	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	388	TRP	CE3-CZ3-CH2	-5.86	113.49	121.10
2	H	260	VAL	CA-C-N	5.85	125.72	119.28
2	H	260	VAL	C-N-CA	5.85	125.72	119.28
1	G	438	GLU	CA-C-N	5.85	130.75	122.09
1	G	438	GLU	C-N-CA	5.85	130.75	122.09
2	H	172	TYR	CA-C-N	5.85	126.19	119.93
2	H	172	TYR	C-N-CA	5.85	126.19	119.93
2	L	130	THR	CA-CB-CG2	5.85	120.45	110.50
2	D	175	PRO	N-CA-CB	-5.85	97.63	103.48
2	H	116	ASP	N-CA-C	5.85	119.68	112.54
1	I	13	GLY	N-CA-C	5.85	120.90	113.24
2	J	75	ILE	CA-C-N	5.85	128.39	120.38
2	J	75	ILE	C-N-CA	5.85	128.39	120.38
1	K	6	HIS	CB-CG-CD2	-5.85	123.60	131.20
2	L	169	PHE	CA-CB-CG	5.85	119.65	113.80
2	F	325	PRO	CA-C-N	5.85	128.59	120.29
2	F	325	PRO	C-N-CA	5.85	128.59	120.29
1	G	340	TYR	N-CA-CB	5.85	119.10	110.56
1	A	212	PHE	N-CA-C	5.85	117.73	111.36
1	A	299	MET	O-C-N	-5.84	116.13	122.79
2	F	309	HIS	CB-CG-CD2	-5.84	123.60	131.20
2	N	157	LEU	CA-C-N	5.84	129.19	120.31
2	N	157	LEU	C-N-CA	5.84	129.19	120.31
2	B	415	GLU	CA-C-N	5.84	127.49	120.13
2	B	415	GLU	C-N-CA	5.84	127.49	120.13
2	H	355	ILE	CA-CB-CG1	5.84	120.33	110.40
1	I	394	PHE	CA-CB-CG	5.84	119.64	113.80
1	K	351	THR	CA-CB-CG2	5.84	120.43	110.50
1	A	440	GLY	CA-C-N	5.84	129.85	121.50
1	A	440	GLY	C-N-CA	5.84	129.85	121.50
1	G	150	LEU	CA-C-N	5.84	128.10	120.28
1	G	150	LEU	C-N-CA	5.84	128.10	120.28
1	G	331	LEU	O-C-N	-5.84	115.49	122.15
1	K	149	THR	N-CA-C	5.84	117.33	110.97
2	N	407	TRP	CG-CD2-CE3	5.84	139.74	133.90
1	E	20	PHE	O-C-N	5.84	128.16	122.09
1	K	163	ILE	CB-CA-C	5.84	120.38	111.68
1	M	355	ASP	CA-C-N	5.84	126.57	122.60
1	M	355	ASP	C-N-CA	5.84	126.57	122.60
1	M	231	ALA	O-C-N	-5.83	115.94	122.12
1	C	37	HIS	CB-CG-CD2	-5.83	123.61	131.20
2	D	236	SER	O-C-N	5.83	128.80	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	332	ILE	CA-C-N	5.83	128.90	120.38
2	F	332	ILE	C-N-CA	5.83	128.90	120.38
1	G	17	GLY	CA-C-N	5.83	128.68	120.28
1	G	17	GLY	C-N-CA	5.83	128.68	120.28
2	B	90	GLU	CA-CB-CG	-5.83	102.44	114.10
1	E	151	LEU	CA-C-O	-5.83	114.88	121.00
2	F	360	PRO	CA-N-CD	-5.83	103.84	112.00
2	N	161	TYR	N-CA-C	5.83	117.44	110.44
2	B	192	HIS	CB-CG-CD2	-5.83	123.62	131.20
2	F	154	MET	N-CA-CB	-5.83	101.35	110.44
1	I	150	LEU	CA-C-N	5.83	128.56	120.29
1	I	150	LEU	C-N-CA	5.83	128.56	120.29
2	N	385	ALA	CA-C-N	5.83	128.02	120.44
2	N	385	ALA	C-N-CA	5.83	128.02	120.44
1	C	28	HIS	CB-CG-CD2	-5.83	123.62	131.20
1	I	39	ASP	O-C-N	-5.83	115.35	122.05
1	M	249	ASP	N-CA-CB	-5.83	101.48	110.04
2	B	221	ARG	O-C-N	-5.82	116.31	121.20
1	G	418	LEU	N-CA-C	5.82	117.30	111.07
1	M	63	ALA	CB-CA-C	5.82	119.34	109.50
1	C	112	LEU	N-CA-CB	-5.82	102.19	110.81
1	I	83	GLN	N-CA-C	5.82	119.64	112.54
2	J	290	GLU	CA-C-O	-5.82	114.38	120.55
2	N	318	LEU	O-C-N	-5.82	116.58	123.22
3	O	206	PRO	N-CA-C	5.82	119.65	111.33
1	A	202	ILE	CA-CB-CG1	5.82	120.29	110.40
1	I	84	ILE	CA-C-O	5.82	126.75	120.47
1	M	50	TYR	CA-C-O	-5.82	112.50	118.90
2	D	283	HIS	CB-CG-CD2	-5.82	123.64	131.20
1	I	380	ARG	CA-C-N	5.82	128.43	120.46
1	I	380	ARG	C-N-CA	5.82	128.43	120.46
2	B	270	ALA	CB-CA-C	5.82	120.27	110.79
1	C	135	LEU	CA-C-N	5.82	131.19	123.05
1	C	135	LEU	C-N-CA	5.82	131.19	123.05
1	A	295	ASP	CA-C-N	5.81	128.34	120.38
1	A	295	ASP	C-N-CA	5.81	128.34	120.38
2	N	423	GLU	N-CA-C	5.81	118.56	111.82
2	B	61	HIS	CB-CG-CD2	-5.81	123.65	131.20
2	D	405	VAL	CG1-CB-CG2	-5.81	98.02	110.80
2	F	7	ILE	CA-CB-CG2	-5.81	100.63	110.50
1	G	37	HIS	CB-CG-CD2	-5.81	123.65	131.20
1	G	208	TYR	CA-CB-CG	5.80	124.35	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLY	O-C-N	-5.80	115.16	122.70
1	E	318	ARG	O-C-N	-5.80	116.28	123.36
2	L	52	PHE	N-CA-CB	-5.80	102.12	110.65
2	L	151	SER	CA-C-O	-5.80	114.37	120.63
1	C	55	ALA	N-CA-C	5.80	118.76	110.24
1	C	374	ILE	O-C-N	-5.80	115.32	122.57
1	G	105	HIS	N-CA-C	-5.80	104.56	111.69
2	L	296	PHE	O-C-N	-5.80	115.36	122.20
2	F	228	ASN	N-CA-C	-5.79	104.93	112.23
2	L	157	LEU	CA-C-N	5.79	131.77	120.99
2	L	157	LEU	C-N-CA	5.79	131.77	120.99
2	N	278	ALA	O-C-N	-5.79	114.72	122.43
2	B	5	ILE	CB-CA-C	5.79	118.09	110.91
1	C	123	GLU	N-CA-C	-5.79	104.96	111.28
1	C	410	GLU	CA-C-N	5.79	128.52	120.29
1	C	410	GLU	C-N-CA	5.79	128.52	120.29
1	I	260	PHE	CA-C-N	5.79	125.47	119.56
1	I	260	PHE	C-N-CA	5.79	125.47	119.56
1	A	179	VAL	CA-C-N	5.79	130.11	121.77
1	A	179	VAL	C-N-CA	5.79	130.11	121.77
1	C	201	CYS	CA-C-N	5.79	131.04	122.99
1	C	201	CYS	C-N-CA	5.79	131.04	122.99
2	L	283	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	M	275	SER	CA-CB-OG	-5.79	99.52	111.10
2	N	7	ILE	O-C-N	-5.79	116.32	123.10
2	N	225	THR	CA-C-O	-5.79	114.74	120.82
2	J	271	THR	N-CA-C	5.79	117.65	108.79
2	N	112	LYS	N-CA-C	5.79	119.81	112.87
1	A	86	ARG	CB-CA-C	5.78	119.36	109.82
1	A	166	THR	O-C-N	-5.78	116.54	123.31
1	I	375	GLN	OE1-CD-NE2	-5.78	116.82	122.60
1	M	99	ASN	N-CA-C	5.78	120.14	113.38
2	H	170	SER	CB-CA-C	5.78	119.39	110.14
1	C	356	ILE	O-C-N	-5.78	116.95	121.46
1	C	383	GLU	O-C-N	-5.78	114.72	122.23
1	G	307	HIS	ND1-CE1-NE2	5.78	114.18	108.40
1	C	190	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	M	216	LYS	CG-CD-CE	5.78	124.58	111.30
2	J	94	THR	CA-C-N	5.77	128.90	122.55
2	J	94	THR	C-N-CA	5.77	128.90	122.55
2	D	218	ASP	N-CA-C	5.77	118.23	111.02
1	I	212	PHE	CA-C-N	5.77	128.48	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	212	PHE	C-N-CA	5.77	128.48	120.29
1	I	71	GLY	CA-C-N	5.77	129.47	120.82
1	I	71	GLY	C-N-CA	5.77	129.47	120.82
2	B	164	LYS	CA-C-O	-5.76	115.01	121.81
1	C	129	CYS	CA-C-O	-5.76	112.27	120.51
2	J	95	GLY	CA-C-O	-5.76	115.87	121.92
2	L	386	GLU	CA-C-N	5.76	128.47	120.29
2	L	386	GLU	C-N-CA	5.76	128.47	120.29
2	H	228	ASN	OD1-CG-ND2	-5.76	116.84	122.60
2	D	3	GLU	O-C-N	-5.76	116.68	123.25
1	E	399	THR	CA-C-N	5.76	130.65	120.74
1	E	399	THR	C-N-CA	5.76	130.65	120.74
2	J	334	THR	CA-C-N	5.76	128.35	120.46
2	J	334	THR	C-N-CA	5.76	128.35	120.46
1	C	345	ILE	N-CA-CB	5.76	119.27	111.21
1	E	84	ILE	CA-CB-CG1	5.76	120.19	110.40
1	K	288	GLU	CA-C-N	5.76	128.25	120.65
1	K	288	GLU	C-N-CA	5.76	128.25	120.65
1	C	85	PHE	N-CA-C	5.76	118.13	110.53
1	C	405	GLU	CA-C-O	-5.76	113.60	120.10
2	D	206	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	M	43	GLN	CA-CB-CG	-5.75	102.59	114.10
1	C	158	GLU	O-C-N	-5.75	114.52	122.46
1	K	47	ILE	O-C-N	-5.75	116.25	121.89
1	I	248	ALA	N-CA-C	5.75	117.42	107.93
2	L	193	THR	OG1-CB-CG2	-5.75	97.81	109.30
1	M	422	TYR	CA-C-N	5.75	133.44	121.94
1	M	422	TYR	C-N-CA	5.75	133.44	121.94
2	B	93	ILE	CA-C-N	5.75	131.61	122.59
2	B	93	ILE	C-N-CA	5.75	131.61	122.59
2	B	445	GLU	O-C-N	-5.75	116.24	122.79
1	C	267	MET	O-C-N	-5.75	116.58	121.23
2	B	60	LYS	O-C-N	-5.75	116.26	123.27
2	H	111	GLY	N-CA-C	5.74	119.84	112.83
2	N	331	ALA	CA-C-O	-5.74	114.79	120.82
3	O	244	GLN	N-CA-C	5.74	118.91	109.72
1	C	20	PHE	CA-CB-CG	5.74	119.54	113.80
1	E	421	GLU	N-CA-C	5.74	118.28	111.33
1	I	65	LEU	N-CA-C	5.74	118.76	109.40
1	C	79	GLY	CA-C-O	-5.74	113.31	121.52
1	G	54	ALA	O-C-N	-5.74	116.61	123.27
2	H	139	HIS	CA-CB-CG	5.74	119.54	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	228	LEU	CA-C-N	5.74	128.57	120.42
1	M	228	LEU	C-N-CA	5.74	128.57	120.42
2	N	221	ARG	CA-C-O	-5.74	112.30	120.16
1	I	382	SER	CA-C-O	-5.74	114.41	120.55
2	B	72	PRO	N-CA-C	-5.74	106.06	113.57
1	C	218	THR	CA-CB-OG1	5.74	118.20	109.60
2	D	238	ILE	CA-CB-CG2	5.73	120.25	110.50
1	I	99	ASN	OD1-CG-ND2	-5.73	116.87	122.60
2	L	215	ARG	N-CA-C	5.73	120.00	112.89
2	L	329	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	K	335	ASN	CA-CB-CG	-5.73	106.87	112.60
1	C	236	VAL	CA-CB-CG1	5.73	120.14	110.40
3	O	277	ILE	O-C-N	-5.73	115.96	122.72
2	N	188	ILE	CA-CB-CG2	5.73	120.24	110.50
2	L	68	VAL	CG1-CB-CG2	-5.73	98.20	110.80
1	A	385	PHE	CA-C-O	-5.72	114.81	120.82
1	G	95	SER	CA-C-N	5.72	128.95	121.85
1	G	95	SER	C-N-CA	5.72	128.95	121.85
2	J	346	TRP	N-CA-C	5.72	119.25	112.72
2	B	217	LEU	N-CA-C	5.72	119.52	112.54
1	C	155	ILE	CA-CB-CG2	5.72	120.23	110.50
1	C	330	MET	CA-C-N	5.72	128.41	120.29
1	C	330	MET	C-N-CA	5.72	128.41	120.29
1	I	397	TRP	CA-C-N	5.72	128.41	120.63
1	I	397	TRP	C-N-CA	5.72	128.41	120.63
2	B	52	PHE	CA-CB-CG	-5.72	108.08	113.80
2	D	36	MET	CG-SD-CE	-5.72	88.31	100.90
1	A	116	VAL	O-C-N	5.72	129.39	121.84
2	B	129	CYS	CA-CB-SG	-5.72	101.24	114.40
1	A	202	ILE	CB-CA-C	5.72	119.31	110.96
1	I	63	ALA	O-C-N	5.72	129.77	123.25
1	C	274	THR	O-C-N	-5.72	116.87	123.33
1	I	161	ASP	CA-C-O	5.72	125.96	119.27
1	K	358	PRO	CA-C-N	5.72	128.21	120.38
1	K	358	PRO	C-N-CA	5.72	128.21	120.38
2	F	114	ILE	CA-C-N	5.71	128.29	120.46
2	F	114	ILE	C-N-CA	5.71	128.29	120.46
1	K	195	ASN	N-CA-CB	-5.71	103.40	111.00
2	N	276	ILE	N-CA-C	5.71	117.57	108.89
1	C	396	HIS	N-CA-C	5.71	119.06	111.75
2	D	122	ILE	N-CA-C	5.71	116.49	110.72
1	G	56	GLY	O-C-N	5.71	129.01	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	326	VAL	N-CA-CB	5.71	116.84	110.62
2	J	98	ASP	N-CA-C	5.71	118.06	110.53
2	L	17	GLY	CA-C-O	-5.71	114.23	120.40
2	L	100	ALA	CB-CA-C	5.71	119.13	111.82
2	L	213	CYS	CA-C-O	-5.71	114.83	120.82
1	K	189	VAL	CA-C-O	-5.71	115.33	121.27
1	A	444	GLU	CA-CB-CG	-5.71	102.69	114.10
2	F	20	CYS	CA-CB-SG	-5.71	101.28	114.40
2	B	280	LYS	CA-C-N	5.70	128.49	120.28
2	B	280	LYS	C-N-CA	5.70	128.49	120.28
3	O	262	SER	CA-C-N	5.70	129.73	120.60
3	O	262	SER	C-N-CA	5.70	129.73	120.60
1	A	81	PHE	CA-CB-CG	5.70	119.50	113.80
1	C	13	GLY	CA-C-O	-5.70	114.25	120.40
1	A	86	ARG	CA-C-N	5.70	125.81	119.32
1	A	86	ARG	C-N-CA	5.70	125.81	119.32
2	F	122	ILE	CA-C-N	5.69	128.38	120.29
2	F	122	ILE	C-N-CA	5.69	128.38	120.29
2	L	325	PRO	N-CD-CG	5.69	111.74	103.20
2	D	107	HIS	N-CA-C	5.69	118.34	111.40
1	M	444	GLU	CB-CA-C	5.69	119.93	109.46
1	E	143	THR	CA-C-N	5.69	126.40	120.03
1	E	143	THR	C-N-CA	5.69	126.40	120.03
2	H	213	CYS	N-CA-C	5.69	117.29	111.14
1	I	84	ILE	O-C-N	-5.69	115.37	121.80
2	J	214	ARG	CA-CB-CG	5.69	125.48	114.10
1	M	217	LEU	CA-C-N	5.69	128.47	120.28
1	M	217	LEU	C-N-CA	5.69	128.47	120.28
2	N	158	SER	N-CA-C	-5.69	105.22	111.82
2	D	145	THR	N-CA-CB	5.69	118.58	110.16
2	B	358	GLN	CB-CA-C	5.69	117.57	109.38
2	H	197	HIS	ND1-CG-CD2	5.68	111.78	106.10
1	A	343	GLU	CA-C-O	5.68	125.92	119.27
1	M	368	ILE	CA-CB-CG2	-5.68	100.84	110.50
1	A	262	ARG	O-C-N	-5.68	114.35	122.41
1	E	131	GLN	CB-CA-C	5.68	118.93	109.56
1	E	407	GLU	CB-CG-CD	5.68	122.25	112.60
2	L	135	PHE	CA-CB-CG	5.68	119.48	113.80
1	I	335	ASN	OD1-CG-ND2	-5.67	116.93	122.60
2	L	2	ARG	CA-C-O	-5.67	114.70	121.11
2	N	134	GLY	N-CA-C	5.67	118.86	110.63
2	B	114	ILE	N-CA-C	5.67	119.20	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	222	PRO	N-CA-CB	5.67	108.36	103.31
2	B	358	GLN	OE1-CD-NE2	-5.67	116.93	122.60
2	D	399	TYR	CA-C-N	5.67	129.67	120.60
2	D	399	TYR	C-N-CA	5.67	129.67	120.60
1	E	176	SER	N-CA-C	5.67	119.34	110.32
2	H	332	ILE	CB-CA-C	5.67	120.05	112.22
1	I	370	ASN	CA-CB-CG	-5.67	106.93	112.60
1	M	191	GLN	N-CA-CB	5.67	118.98	110.19
1	I	109	GLY	CA-C-N	5.67	128.44	120.28
1	I	109	GLY	C-N-CA	5.67	128.44	120.28
2	D	190	THR	CA-C-N	5.67	129.32	120.82
2	D	190	THR	C-N-CA	5.67	129.32	120.82
2	J	117	LEU	CA-C-N	5.67	127.80	120.88
2	J	117	LEU	C-N-CA	5.67	127.80	120.88
2	N	62	VAL	N-CA-C	-5.67	100.86	107.61
1	C	221	THR	N-CA-CB	-5.67	101.68	110.46
1	C	325	GLU	N-CA-C	5.67	117.45	111.28
1	G	367	PHE	CA-CB-CG	5.67	119.47	113.80
2	N	190	THR	CA-C-O	-5.67	115.05	121.00
1	E	32	PRO	N-CA-CB	5.66	108.90	103.52
1	G	154	LYS	CB-CA-C	5.66	118.12	109.34
1	C	42	LEU	CA-C-O	-5.66	113.86	120.20
2	D	228	ASN	N-CA-C	5.66	118.39	111.82
2	H	308	ARG	CD-NE-CZ	5.66	132.33	124.40
1	A	263	LEU	CA-C-N	5.66	131.38	122.49
1	A	263	LEU	C-N-CA	5.66	131.38	122.49
1	A	296	ALA	CA-C-N	5.66	133.26	121.94
1	A	296	ALA	C-N-CA	5.66	133.26	121.94
2	B	399	TYR	CA-C-N	5.66	128.43	120.28
2	B	399	TYR	C-N-CA	5.66	128.43	120.28
2	D	236	SER	N-CA-C	-5.66	105.19	111.36
1	E	419	VAL	CA-C-O	-5.66	115.39	121.27
2	J	270	ALA	N-CA-C	5.66	119.28	110.17
2	J	362	VAL	O-C-N	-5.66	116.27	122.83
1	M	227	HIS	CA-CB-CG	5.66	119.46	113.80
2	N	21	TRP	CE2-CD2-CE3	-5.66	113.14	118.80
1	I	154	LYS	N-CA-C	5.66	119.28	112.38
1	M	12	CYS	N-CA-CB	-5.66	101.77	110.20
1	M	125	GLU	CA-C-O	5.66	126.33	119.49
1	I	87	PRO	CA-C-N	5.65	128.63	120.38
1	I	87	PRO	C-N-CA	5.65	128.63	120.38
1	M	119	VAL	CA-C-N	5.65	127.68	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	119	VAL	C-N-CA	5.65	127.68	120.56
1	C	145	SER	CA-C-O	5.65	126.51	120.24
2	D	264	ARG	CD-NE-CZ	5.65	132.31	124.40
2	L	410	GLY	CA-C-N	5.65	131.83	122.73
2	L	410	GLY	C-N-CA	5.65	131.83	122.73
2	N	7	ILE	N-CA-C	5.65	115.99	107.80
1	A	90	PHE	CA-CB-CG	5.65	119.45	113.80
2	B	309	HIS	CB-CG-CD2	-5.65	123.86	131.20
2	L	179	THR	CA-C-N	5.65	133.14	123.03
2	L	179	THR	C-N-CA	5.65	133.14	123.03
2	B	72	PRO	CA-C-N	5.65	128.89	120.31
2	B	72	PRO	C-N-CA	5.65	128.89	120.31
2	D	244	PHE	CA-C-O	-5.65	115.41	121.45
1	E	31	ASP	CA-C-N	5.64	125.35	119.82
1	E	31	ASP	C-N-CA	5.64	125.35	119.82
1	E	108	GLU	CA-C-N	5.64	126.21	120.00
1	E	108	GLU	C-N-CA	5.64	126.21	120.00
1	E	411	ALA	CA-C-N	5.64	127.84	120.28
1	E	411	ALA	C-N-CA	5.64	127.84	120.28
1	I	310	TYR	CA-C-N	5.64	128.31	120.63
1	I	310	TYR	C-N-CA	5.64	128.31	120.63
2	F	206	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	G	232	THR	CA-CB-CG2	5.64	120.09	110.50
1	M	92	PHE	CA-CB-CG	5.64	119.44	113.80
2	N	93	ILE	CB-CG1-CD1	5.64	125.65	113.80
2	L	415	GLU	CA-C-N	5.64	127.19	120.14
2	L	415	GLU	C-N-CA	5.64	127.19	120.14
1	A	6	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	E	225	LEU	N-CA-C	5.64	118.36	111.82
1	G	116	VAL	N-CA-C	5.64	115.77	110.30
2	L	226	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	I	236	VAL	CA-C-N	5.64	131.05	122.37
1	I	236	VAL	C-N-CA	5.64	131.05	122.37
2	B	326	LYS	CB-CA-C	-5.63	101.10	110.68
1	C	265	PHE	CA-CB-CG	5.63	119.44	113.80
2	D	53	PHE	CA-CB-CG	5.63	119.43	113.80
1	E	445	ALA	CB-CA-C	5.63	118.95	110.50
1	G	347	ASN	CA-C-O	-5.63	115.15	122.14
2	H	224	TYR	CB-CG-CD2	-5.63	112.35	120.80
1	E	291	GLN	N-CA-C	-5.63	106.36	113.18
1	K	101	TRP	CZ3-CH2-CZ2	-5.63	114.18	121.50
2	B	172	TYR	O-C-N	-5.63	114.40	121.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	224	ASP	O-C-N	-5.63	116.17	122.03
1	I	3	GLU	CA-C-N	5.63	130.37	123.10
1	I	3	GLU	C-N-CA	5.63	130.37	123.10
1	I	332	ASN	CA-C-O	-5.63	114.45	120.42
1	K	149	THR	CA-CB-OG1	5.63	118.05	109.60
2	D	401	LYS	CA-C-N	5.63	132.29	121.54
2	D	401	LYS	C-N-CA	5.63	132.29	121.54
1	I	86	ARG	CA-C-N	5.63	125.73	119.32
1	I	86	ARG	C-N-CA	5.63	125.73	119.32
1	K	252	LYS	CA-C-O	-5.63	113.50	119.97
2	D	380	ASN	O-C-N	-5.62	116.81	123.22
2	L	31	GLN	CA-C-N	5.62	125.33	119.82
2	L	31	GLN	C-N-CA	5.62	125.33	119.82
1	A	101	TRP	O-C-N	-5.62	116.18	122.03
1	G	159	TYR	O-C-N	-5.62	116.39	121.17
2	H	242	LEU	CA-C-O	5.62	125.56	119.15
1	I	356	ILE	CA-CB-CG2	5.62	120.06	110.50
1	G	61	PRO	N-CA-CB	5.62	108.57	103.34
1	I	199	THR	O-C-N	-5.62	116.84	123.25
1	G	396	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	M	297	LYS	N-CA-C	5.62	120.00	113.20
1	A	346	PRO	CB-CA-C	5.62	116.51	111.40
2	D	197	HIS	CG-CD2-NE2	-5.62	101.58	107.20
2	L	168	GLU	N-CA-CB	5.62	118.54	110.06
1	M	346	PRO	CA-C-N	5.62	132.27	121.54
1	M	346	PRO	C-N-CA	5.62	132.27	121.54
2	D	315	CYS	CA-C-N	5.62	130.24	122.77
2	D	315	CYS	C-N-CA	5.62	130.24	122.77
1	E	14	ASN	CA-C-O	-5.62	113.15	120.00
1	G	324	LYS	N-CA-CB	-5.62	101.86	110.12
1	E	52	ASN	OD1-CG-ND2	-5.61	116.99	122.60
1	E	137	HIS	ND1-CG-CD2	5.61	111.71	106.10
2	H	275	VAL	CA-CB-CG2	5.61	119.94	110.40
2	N	328	VAL	CA-CB-CG2	5.61	119.94	110.40
1	E	415	MET	O-C-N	-5.61	116.29	122.07
1	I	373	ALA	N-CA-C	5.61	118.16	111.71
2	L	91	GLN	OE1-CD-NE2	-5.61	116.99	122.60
2	B	209	ILE	CA-C-N	5.61	127.80	120.28
2	B	209	ILE	C-N-CA	5.61	127.80	120.28
2	F	45	GLY	O-C-N	5.61	128.84	122.67
1	A	338	SER	CA-C-N	5.61	128.35	120.28
1	A	338	SER	C-N-CA	5.61	128.35	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	197	HIS	CA-CB-CG	5.61	119.41	113.80
2	D	18	ASN	CA-CB-CG	5.60	118.20	112.60
2	H	107	HIS	CB-CG-ND1	5.60	131.10	122.70
2	H	242	LEU	CA-C-N	5.60	131.03	122.24
2	H	242	LEU	C-N-CA	5.60	131.03	122.24
2	B	241	SER	N-CA-C	5.60	118.15	111.71
2	J	283	HIS	CB-CG-CD2	-5.60	123.92	131.20
2	J	97	GLU	CB-CG-CD	-5.60	103.08	112.60
2	L	414	GLU	O-C-N	-5.60	117.00	123.33
2	J	236	SER	CA-CB-OG	-5.60	99.91	111.10
2	J	271	THR	CA-C-N	5.60	131.60	122.81
2	J	271	THR	C-N-CA	5.60	131.60	122.81
2	D	159	VAL	O-C-N	5.60	129.18	121.90
1	M	91	VAL	CA-C-N	5.60	131.88	122.87
1	M	91	VAL	C-N-CA	5.60	131.88	122.87
2	H	177	VAL	CA-C-O	-5.59	115.98	121.58
1	I	295	ASP	CA-C-N	5.59	128.04	120.38
1	I	295	ASP	C-N-CA	5.59	128.04	120.38
1	I	331	LEU	O-C-N	-5.59	115.77	122.15
1	E	141	GLY	CA-C-O	-5.59	114.45	122.62
1	K	190	HIS	CB-CG-ND1	5.59	131.09	122.70
1	A	37	HIS	CA-CB-CG	-5.59	108.21	113.80
1	C	203	ASP	CA-CB-CG	5.59	118.19	112.60
1	I	295	ASP	CA-CB-CG	5.59	118.19	112.60
1	E	245	GLN	CA-C-N	5.59	131.00	122.95
1	E	245	GLN	C-N-CA	5.59	131.00	122.95
1	E	190	HIS	CB-CG-CD2	-5.59	123.94	131.20
1	K	344	TRP	CB-CG-CD2	5.59	134.62	126.80
1	G	412	GLU	N-CA-C	5.58	117.05	111.07
1	M	69	GLU	O-C-N	-5.58	118.14	121.71
1	K	53	GLU	CA-C-N	5.58	131.86	122.87
1	K	53	GLU	C-N-CA	5.58	131.86	122.87
2	H	376	CYS	N-CA-CB	-5.58	101.53	110.63
1	K	161	ASP	O-C-N	-5.58	115.61	122.25
1	G	14	ASN	O-C-N	-5.58	115.79	122.15
2	H	226	ASN	OD1-CG-ND2	-5.58	117.02	122.60
2	L	242	LEU	CA-C-O	5.58	125.80	119.27
1	E	105	HIS	ND1-CE1-NE2	5.58	113.98	108.40
1	I	236	VAL	CA-CB-CG1	5.58	119.88	110.40
2	B	187	SER	N-CA-C	5.58	117.82	111.02
2	L	283	HIS	ND1-CE1-NE2	5.58	113.98	108.40
2	L	360	PRO	O-C-N	-5.58	116.20	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	232	PRO	N-CA-CB	5.58	108.49	103.08
2	B	212	ILE	CA-C-O	5.57	126.75	120.95
2	D	166	LYS	CA-CB-CG	-5.57	102.95	114.10
2	N	117	LEU	CA-C-N	5.57	127.69	120.56
2	N	117	LEU	C-N-CA	5.57	127.69	120.56
2	D	110	ILE	CA-CB-CG1	5.57	119.87	110.40
1	A	239	CYS	CA-CB-SG	-5.57	101.59	114.40
2	B	227	LEU	CA-C-N	5.57	128.01	120.38
2	B	227	LEU	C-N-CA	5.57	128.01	120.38
1	C	113	VAL	N-CA-C	5.57	118.01	111.05
1	E	67	ASP	CA-CB-CG	5.57	118.17	112.60
1	E	91	VAL	CA-C-O	5.57	125.17	120.22
2	F	150	THR	CA-C-O	5.57	126.86	120.90
2	H	375	VAL	CG1-CB-CG2	-5.57	98.55	110.80
2	L	132	LEU	CB-CA-C	5.57	121.50	110.42
2	D	237	SER	CA-C-O	-5.57	114.06	120.24
2	H	217	LEU	CA-C-N	5.57	130.03	122.07
2	H	217	LEU	C-N-CA	5.57	130.03	122.07
1	K	345	ILE	N-CA-C	-5.57	101.82	107.89
2	B	3	GLU	N-CA-C	5.56	116.70	108.86
1	C	288	GLU	CB-CA-C	5.56	120.02	110.79
1	A	42	LEU	O-C-N	5.56	129.56	122.33
1	C	347	ASN	OD1-CG-ND2	-5.56	117.04	122.60
1	C	408	PHE	CA-CB-CG	5.56	119.36	113.80
2	F	25	CYS	N-CA-CB	-5.56	102.01	110.07
2	J	309	HIS	CB-CG-CD2	-5.56	123.97	131.20
2	J	386	GLU	N-CA-C	5.56	117.34	111.28
1	K	325	GLU	O-C-N	-5.56	116.23	122.12
2	N	107	HIS	CE1-NE2-CD2	-5.56	103.44	109.00
3	O	274	LYS	CA-C-O	5.56	127.38	120.54
2	D	159	VAL	CA-C-O	-5.56	114.35	120.96
1	C	99	ASN	CB-CG-ND2	5.56	124.73	116.40
2	B	135	PHE	N-CA-C	5.55	118.52	109.24
2	B	250	VAL	CB-CA-C	5.55	120.40	111.29
1	E	91	VAL	CG1-CB-CG2	-5.55	98.58	110.80
1	G	67	ASP	CA-CB-CG	5.55	118.15	112.60
2	L	293	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	A	282	ARG	CD-NE-CZ	5.55	132.17	124.40
2	D	356	ASN	O-C-N	-5.55	115.97	123.19
2	H	369	ALA	CA-C-O	-5.55	115.56	121.94
2	J	235	VAL	CA-C-N	5.55	127.72	120.28
2	J	235	VAL	C-N-CA	5.55	127.72	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	199	ASP	CA-C-O	-5.55	113.23	120.00
2	L	187	SER	CA-C-O	-5.55	114.64	120.63
1	C	113	VAL	CA-CB-CG2	5.55	119.83	110.40
1	G	113	VAL	CA-CB-CG2	5.55	119.83	110.40
1	A	113	VAL	CA-CB-CG1	5.55	119.83	110.40
1	K	377	LEU	CA-C-N	5.55	128.16	120.29
1	K	377	LEU	C-N-CA	5.55	128.16	120.29
2	B	283	HIS	ND1-CE1-NE2	5.54	113.94	108.40
1	C	106	TYR	N-CA-C	5.54	120.70	113.88
2	H	88	HIS	N-CA-C	5.54	117.66	109.62
2	H	266	HIS	N-CA-C	5.54	120.74	113.20
2	J	20	CYS	CA-C-N	5.54	128.73	120.31
2	J	20	CYS	C-N-CA	5.54	128.73	120.31
1	A	301	ALA	CA-C-O	-5.54	114.63	121.06
1	M	65	LEU	CB-CA-C	5.54	119.64	110.78
1	A	32	PRO	CA-C-N	5.54	129.46	120.60
1	A	32	PRO	C-N-CA	5.54	129.46	120.60
2	D	267	PHE	CA-C-N	5.54	126.01	120.14
2	D	267	PHE	C-N-CA	5.54	126.01	120.14
2	N	150	THR	N-CA-C	5.54	117.78	111.02
2	N	424	ASP	CA-CB-CG	-5.54	107.06	112.60
2	D	197	HIS	ND1-CG-CD2	5.54	111.64	106.10
2	D	439	SER	O-C-N	-5.54	115.23	122.59
2	J	362	VAL	CA-CB-CG1	5.54	119.81	110.40
1	G	358	PRO	N-CA-CB	5.54	108.24	103.31
1	I	105	HIS	CA-CB-CG	-5.54	108.26	113.80
2	F	283	HIS	CB-CG-CD2	-5.53	124.01	131.20
2	H	243	ARG	CA-C-O	-5.53	112.63	118.77
2	F	370	LYS	CA-C-N	5.53	128.87	120.13
2	F	370	LYS	C-N-CA	5.53	128.87	120.13
2	J	1	MET	CA-C-N	5.53	131.42	122.29
2	J	1	MET	C-N-CA	5.53	131.42	122.29
2	H	187	SER	O-C-N	-5.53	115.84	122.15
2	H	421	ALA	N-CA-C	5.53	117.31	111.28
2	N	61	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	A	37	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	A	364	SER	CA-C-O	-5.53	115.32	121.51
1	A	11	GLN	CA-C-N	5.53	129.11	120.82
1	A	11	GLN	C-N-CA	5.53	129.11	120.82
1	C	346	PRO	N-CD-CG	5.53	111.49	103.20
1	I	100	ASN	OD1-CG-ND2	-5.53	117.07	122.60
2	H	326	LYS	N-CA-C	5.53	118.06	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	449	GLU	CA-C-N	5.53	129.32	121.42
2	J	449	GLU	C-N-CA	5.53	129.32	121.42
1	A	32	PRO	N-CA-CB	5.52	109.05	103.25
1	E	204	ASN	CA-CB-CG	5.52	118.12	112.60
1	G	375	GLN	CA-C-N	5.52	127.68	120.28
1	G	375	GLN	C-N-CA	5.52	127.68	120.28
2	N	78	VAL	CB-CA-C	-5.52	104.68	112.14
2	D	443	GLU	CA-C-N	5.52	132.23	121.41
2	D	443	GLU	C-N-CA	5.52	132.23	121.41
1	E	304	ASP	CA-CB-CG	5.52	118.12	112.60
2	F	21	TRP	CB-CA-C	5.52	120.20	110.37
1	I	279	GLN	CA-C-O	-5.52	114.02	120.20
2	H	298	PRO	N-CA-CB	5.52	109.55	103.26
2	N	391	LEU	CA-C-O	-5.52	114.57	120.42
1	C	408	PHE	CA-C-N	5.52	128.12	120.29
1	C	408	PHE	C-N-CA	5.52	128.12	120.29
1	G	342	VAL	CB-CA-C	5.52	119.17	111.34
2	F	81	GLY	N-CA-C	5.51	120.97	111.98
1	M	152	ILE	O-C-N	5.51	127.45	121.94
1	M	317	PHE	CA-CB-CG	-5.51	108.29	113.80
2	L	107	HIS	CA-CB-CG	-5.51	108.29	113.80
2	L	165	SER	O-C-N	-5.51	116.77	123.16
1	G	142	GLY	CA-C-N	5.51	129.91	120.71
1	G	142	GLY	C-N-CA	5.51	129.91	120.71
2	B	211	ASP	N-CA-C	5.51	118.46	111.69
2	J	266	HIS	CB-CG-CD2	-5.51	124.04	131.20
2	B	326	LYS	CA-C-O	-5.50	114.69	120.63
2	B	359	PRO	N-CA-C	5.50	117.42	110.70
1	K	223	GLY	CA-C-N	5.50	129.99	120.58
1	K	223	GLY	C-N-CA	5.50	129.99	120.58
1	C	28	HIS	CA-C-N	5.50	131.45	120.77
1	C	28	HIS	C-N-CA	5.50	131.45	120.77
2	D	262	TYR	O-C-N	-5.50	118.00	121.85
2	F	79	ARG	CA-C-N	5.50	130.40	121.98
2	F	79	ARG	C-N-CA	5.50	130.40	121.98
1	I	310	TYR	CA-C-O	5.50	126.96	120.58
2	L	16	ILE	CA-CB-CG2	5.50	119.85	110.50
1	I	135	LEU	N-CA-C	5.50	117.37	108.41
1	I	248	ALA	CA-C-O	5.50	126.69	119.98
3	O	274	LYS	CA-C-N	5.50	130.37	122.45
3	O	274	LYS	C-N-CA	5.50	130.37	122.45
2	F	81	GLY	CA-C-O	-5.50	116.60	122.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	364	PRO	N-CA-CB	5.50	108.09	103.25
1	C	149	THR	N-CA-CB	5.50	118.80	110.28
2	J	407	TRP	CA-C-N	5.50	127.92	120.44
2	J	407	TRP	C-N-CA	5.50	127.92	120.44
1	K	15	GLN	CA-C-O	-5.50	114.67	120.55
1	K	121	ARG	N-CA-C	5.50	117.08	111.14
2	N	205	ASP	CA-CB-CG	5.50	118.10	112.60
1	E	264	HIS	N-CA-CB	-5.50	103.57	111.54
1	K	245	GLN	CG-CD-NE2	5.50	124.64	116.40
1	A	39	ASP	CB-CA-C	5.49	116.25	109.16
2	B	108	TYR	CA-CB-CG	5.49	123.79	113.90
1	E	357	PRO	CB-CA-C	5.49	117.62	110.92
1	G	412	GLU	O-C-N	5.49	127.73	122.07
1	I	192	LEU	CA-C-O	-5.49	115.02	120.90
2	L	91	GLN	CA-C-N	5.49	130.58	123.00
2	L	91	GLN	C-N-CA	5.49	130.58	123.00
1	M	385	PHE	CA-CB-CG	5.49	119.29	113.80
2	N	355	ILE	CA-C-O	-5.49	114.72	120.76
2	F	199	ASP	N-CA-C	5.49	118.19	111.82
1	I	204	ASN	CA-C-O	-5.49	113.65	119.97
2	D	357	TYR	CA-C-O	-5.49	113.66	119.97
1	K	4	ILE	CA-C-N	5.49	129.95	121.71
1	K	4	ILE	C-N-CA	5.49	129.95	121.71
1	M	279	GLN	CA-C-N	5.49	127.90	120.38
1	M	279	GLN	C-N-CA	5.49	127.90	120.38
2	H	114	ILE	CA-C-O	-5.49	114.61	119.38
2	H	175	PRO	CA-N-CD	-5.49	104.31	112.00
1	K	41	ASP	N-CA-CB	-5.49	100.78	110.39
2	D	385	ALA	O-C-N	-5.49	115.52	122.27
2	H	327	ASP	CA-CB-CG	5.49	118.09	112.60
1	C	45	GLU	CA-C-N	5.49	132.49	122.50
1	C	45	GLU	C-N-CA	5.49	132.49	122.50
1	E	189	VAL	CA-CB-CG1	5.49	119.72	110.40
1	I	297	LYS	CA-C-N	5.49	131.25	122.86
1	I	297	LYS	C-N-CA	5.49	131.25	122.86
2	D	209	ILE	CB-CA-C	5.48	121.14	112.26
2	J	273	ALA	CA-C-O	-5.48	114.44	119.76
1	K	231	ALA	CA-C-N	5.48	127.89	120.44
1	K	231	ALA	C-N-CA	5.48	127.89	120.44
1	E	145	SER	CA-C-N	5.48	126.03	120.00
1	E	145	SER	C-N-CA	5.48	126.03	120.00
1	I	396	HIS	O-C-N	-5.48	115.81	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	440	GLY	CA-C-O	5.48	126.51	121.58
1	A	359	ARG	CA-C-O	-5.48	114.67	120.92
2	D	392	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	303	CYS	CA-C-O	-5.48	115.75	121.99
1	C	80	PRO	O-C-N	-5.48	116.40	123.03
1	C	184	ASN	CA-CB-CG	5.48	118.08	112.60
1	E	241	ARG	CA-C-O	-5.48	112.66	119.18
1	A	342	VAL	CA-C-O	-5.48	114.80	121.04
2	F	191	THR	CA-C-N	5.48	127.62	120.28
2	F	191	THR	C-N-CA	5.48	127.62	120.28
1	E	278	SER	O-C-N	-5.47	116.26	122.23
2	F	95	GLY	O-C-N	-5.47	118.61	123.65
1	K	113	VAL	CA-C-N	5.47	128.16	120.28
1	K	113	VAL	C-N-CA	5.47	128.16	120.28
2	N	183	GLU	O-C-N	-5.47	115.02	121.32
2	L	423	GLU	O-C-N	-5.47	115.91	122.15
2	N	170	SER	CB-CA-C	5.47	120.11	109.33
1	A	11	GLN	CB-CA-C	5.47	119.62	110.92
2	H	377	MET	O-C-N	-5.47	116.60	123.27
1	M	194	GLU	OE1-CD-OE2	-5.47	109.77	122.90
1	C	168	SER	N-CA-C	5.47	118.16	109.96
1	C	266	PHE	CA-C-N	5.47	128.96	121.74
1	C	266	PHE	C-N-CA	5.47	128.96	121.74
2	D	182	VAL	N-CA-C	5.46	120.70	109.34
1	M	400	GLY	O-C-N	5.46	128.24	122.28
2	N	8	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	A	129	CYS	O-C-N	-5.46	117.02	123.41
2	D	55	GLU	O-C-N	-5.46	116.22	122.93
2	N	431	ASP	CA-C-N	5.46	127.59	120.28
2	N	431	ASP	C-N-CA	5.46	127.59	120.28
1	A	345	ILE	CB-CA-C	5.46	121.29	111.36
2	B	435	VAL	CA-CB-CG2	5.46	119.68	110.40
1	C	262	ARG	N-CA-CB	-5.46	103.64	110.90
2	N	165	SER	CA-C-O	-5.46	115.61	121.56
2	B	76	ASP	O-C-N	-5.46	116.34	122.12
2	B	197	HIS	CB-CG-CD2	-5.46	124.11	131.20
2	J	120	ASP	CB-CA-C	5.46	119.44	110.88
2	J	122	ILE	CA-C-O	-5.46	114.41	120.46
2	B	11	GLN	CB-CG-CD	5.45	121.87	112.60
1	C	355	ASP	CB-CA-C	5.45	120.62	109.55
1	M	335	ASN	OD1-CG-ND2	5.45	128.05	122.60
2	B	174	ALA	CA-C-N	5.45	126.65	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	174	ALA	C-N-CA	5.45	126.65	119.84
1	K	426	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	L	212	ILE	N-CA-C	5.45	117.86	111.05
1	C	209	ASP	CA-CB-CG	-5.45	107.15	112.60
1	M	165	ASN	O-C-N	-5.45	116.86	123.29
2	D	303	VAL	CB-CA-C	5.45	117.53	110.12
1	G	112	LEU	CA-C-N	5.45	129.07	120.47
1	G	112	LEU	C-N-CA	5.45	129.07	120.47
2	F	197	HIS	CB-CG-CD2	-5.44	124.12	131.20
3	O	305	SER	O-C-N	-5.44	116.83	123.36
2	F	92	LEU	CA-C-O	5.44	128.33	121.58
1	E	95	SER	CA-C-N	5.44	128.60	121.85
1	E	95	SER	C-N-CA	5.44	128.60	121.85
1	A	113	VAL	N-CA-C	5.44	116.82	110.62
1	I	137	HIS	N-CA-C	5.44	117.45	109.24
1	K	336	LYS	CA-C-N	5.44	131.65	122.79
1	K	336	LYS	C-N-CA	5.44	131.65	122.79
1	M	118	ASP	CA-CB-CG	-5.44	107.16	112.60
3	O	299	HIS	CB-CG-CD2	-5.44	124.13	131.20
2	B	110	ILE	CA-CB-CG1	5.44	119.64	110.40
2	B	384	ILE	O-C-N	-5.44	115.48	122.22
2	D	375	VAL	CA-C-O	5.44	125.63	120.25
1	C	338	SER	N-CA-C	5.43	117.96	111.71
1	C	342	VAL	CA-CB-CG2	-5.43	101.16	110.40
2	F	62	VAL	CA-C-O	-5.43	115.69	119.38
2	H	33	ASP	CA-C-N	5.43	133.08	121.18
2	H	33	ASP	C-N-CA	5.43	133.08	121.18
1	K	89	ASN	CA-CB-CG	5.43	118.03	112.60
2	L	374	ALA	CA-C-O	-5.43	115.42	121.23
1	C	115	SER	CA-C-N	5.43	127.90	120.46
1	C	115	SER	C-N-CA	5.43	127.90	120.46
1	M	340	TYR	CB-CG-CD2	-5.43	112.65	120.80
2	B	147	SER	N-CA-CB	-5.43	101.31	110.49
2	F	228	ASN	CA-CB-CG	5.43	118.03	112.60
1	G	323	MET	CA-C-O	-5.43	115.12	120.82
2	H	257	THR	N-CA-C	5.43	118.70	111.75
1	K	415	MET	N-CA-C	-5.43	105.28	111.14
1	M	13	GLY	CA-C-O	-5.43	115.48	120.80
2	N	24	TYR	CA-CB-CG	5.43	123.67	113.90
1	C	34	GLY	CA-C-N	-5.43	113.35	120.95
1	C	34	GLY	C-N-CA	-5.43	113.35	120.95
2	J	35	GLN	CA-C-N	5.43	128.82	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	35	GLN	C-N-CA	5.43	128.82	122.85
2	N	418	PHE	N-CA-C	5.43	117.20	111.28
1	A	100	ASN	CA-C-O	5.43	126.34	120.32
1	C	42	LEU	O-C-N	5.43	128.39	122.20
1	E	234	SER	CA-C-O	-5.43	115.31	120.90
1	G	76	VAL	O-C-N	5.43	127.42	121.83
2	L	68	VAL	CA-CB-CG1	5.43	119.63	110.40
2	D	50	ASN	OD1-CG-ND2	-5.42	117.18	122.60
2	F	345	ASP	CA-CB-CG	5.42	118.02	112.60
1	I	323	MET	CA-C-N	5.42	128.33	120.79
1	I	323	MET	C-N-CA	5.42	128.33	120.79
2	J	201	ALA	N-CA-CB	-5.42	103.34	111.64
1	K	196	THR	CA-C-N	5.42	131.80	122.09
1	K	196	THR	C-N-CA	5.42	131.80	122.09
2	F	280	LYS	CA-C-N	5.42	129.36	120.63
2	F	280	LYS	C-N-CA	5.42	129.36	120.63
1	K	367	PHE	CA-C-O	-5.42	115.03	121.16
2	D	192	HIS	CB-CG-CD2	-5.42	124.16	131.20
2	D	349	THR	CA-CB-CG2	5.42	119.71	110.50
2	N	337	THR	CA-CB-OG1	-5.42	101.47	109.60
2	B	433	GLU	N-CA-CB	-5.42	102.21	110.33
1	C	60	VAL	CG1-CB-CG2	5.42	122.72	110.80
1	I	266	PHE	CA-C-N	5.42	131.18	121.76
1	I	266	PHE	C-N-CA	5.42	131.18	121.76
1	K	105	HIS	N-CA-C	5.42	118.10	111.82
2	B	44	GLY	CA-C-O	5.41	127.36	121.02
1	C	291	GLN	OE1-CD-NE2	-5.41	117.19	122.60
2	J	65	ALA	N-CA-CB	-5.41	102.27	111.69
2	J	85	GLN	CA-C-N	5.41	128.31	120.79
2	J	85	GLN	C-N-CA	5.41	128.31	120.79
2	L	283	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	M	90	PHE	CA-CB-CG	5.41	119.21	113.80
2	N	67	PHE	CA-C-N	5.41	129.21	121.96
2	N	67	PHE	C-N-CA	5.41	129.21	121.96
1	A	83	GLN	OE1-CD-NE2	-5.41	117.19	122.60
1	A	403	MET	N-CA-C	5.41	118.49	110.48
1	K	77	ARG	CA-C-N	5.41	128.07	120.28
1	K	77	ARG	C-N-CA	5.41	128.07	120.28
2	L	214	ARG	CD-NE-CZ	5.41	131.98	124.40
1	K	255	VAL	N-CA-C	5.41	118.64	111.17
2	L	437	VAL	N-CA-C	5.41	116.56	109.58
2	D	406	HIS	CA-CB-CG	-5.41	108.39	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	HIS	N-CA-CB	-5.41	102.16	110.16
1	I	175	VAL	CA-C-N	5.41	130.61	122.99
1	I	175	VAL	C-N-CA	5.41	130.61	122.99
1	I	270	PHE	CA-C-O	5.41	126.42	120.31
1	E	265	PHE	CA-CB-CG	5.40	119.20	113.80
2	B	402	ARG	N-CA-C	-5.40	105.32	112.24
1	E	337	ASN	CA-C-N	5.40	128.27	120.38
1	E	337	ASN	C-N-CA	5.40	128.27	120.38
1	G	325	GLU	CB-CG-CD	5.40	121.78	112.60
2	J	429	GLU	N-CA-C	5.40	117.17	111.28
2	D	353	VAL	N-CA-C	5.40	116.36	108.53
1	M	60	VAL	CB-CA-C	-5.40	101.53	111.36
1	C	439	GLU	N-CA-C	5.40	118.25	108.69
1	K	270	PHE	CA-CB-CG	5.40	119.20	113.80
1	M	244	GLY	N-CA-C	5.40	118.46	110.42
1	A	255	VAL	CA-CB-CG1	5.40	119.57	110.40
2	L	228	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	M	382	SER	N-CA-C	5.39	117.91	111.71
3	O	209	ARG	CB-CA-C	5.39	119.09	109.38
3	O	246	ALA	CA-C-N	5.39	124.91	119.19
3	O	246	ALA	C-N-CA	5.39	124.91	119.19
1	G	286	VAL	CA-C-O	-5.39	114.27	118.85
2	H	38	SER	O-C-N	-5.39	115.20	122.43
1	A	275	SER	O-C-N	-5.39	116.44	122.75
1	G	329	GLN	CA-C-N	5.39	127.50	120.28
1	G	329	GLN	C-N-CA	5.39	127.50	120.28
2	H	139	HIS	CG-CD2-NE2	-5.39	101.81	107.20
1	I	92	PHE	CA-CB-CG	-5.39	108.41	113.80
1	K	98	GLY	CA-C-N	5.39	132.85	123.91
1	K	98	GLY	C-N-CA	5.39	132.85	123.91
2	B	87	PHE	CD1-CG-CD2	5.38	126.68	118.60
1	A	171	PRO	O-C-N	-5.38	117.07	123.10
2	B	406	HIS	CA-CB-CG	5.38	119.18	113.80
1	E	313	VAL	CA-C-O	-5.38	114.88	120.64
1	I	137	HIS	CA-CB-CG	5.38	119.18	113.80
2	B	105	ARG	CA-C-N	5.38	127.12	120.34
2	B	105	ARG	C-N-CA	5.38	127.12	120.34
1	C	138	SER	N-CA-C	5.38	118.35	109.85
2	H	368	LEU	N-CA-C	5.38	118.42	110.46
1	M	17	GLY	O-C-N	-5.38	117.03	122.19
1	E	41	ASP	CA-CB-CG	5.38	117.98	112.60
2	F	355	ILE	CA-C-N	5.38	130.57	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	355	ILE	C-N-CA	5.38	130.57	122.99
2	L	73	THR	N-CA-C	5.38	119.95	112.90
1	C	221	THR	OG1-CB-CG2	5.38	120.05	109.30
2	F	204	VAL	CA-C-O	-5.38	115.65	121.19
1	G	180	VAL	CA-CB-CG2	5.38	119.54	110.40
2	J	76	ASP	N-CA-CB	-5.38	101.99	110.06
2	L	88	HIS	CB-CG-ND1	5.38	130.76	122.70
1	M	276	ARG	CA-C-N	5.38	131.95	121.41
1	M	276	ARG	C-N-CA	5.38	131.95	121.41
2	L	43	GLY	CA-C-N	5.38	129.36	121.67
2	L	43	GLY	C-N-CA	5.38	129.36	121.67
1	K	112	LEU	CA-C-N	5.37	127.53	120.60
1	K	112	LEU	C-N-CA	5.37	127.53	120.60
3	O	258	SER	N-CA-CB	-5.37	102.58	110.26
1	A	219	THR	CB-CA-C	5.37	117.98	111.11
1	E	79	GLY	CA-C-N	5.37	125.13	119.76
1	E	79	GLY	C-N-CA	5.37	125.13	119.76
1	E	439	GLU	N-CA-CB	-5.37	102.44	110.17
2	F	171	ILE	CA-CB-CG1	5.37	119.53	110.40
1	G	349	VAL	N-CA-C	5.37	115.63	108.11
2	H	156	ARG	N-CA-C	5.37	119.92	112.45
2	H	369	ALA	CA-C-N	5.37	129.76	122.19
2	H	369	ALA	C-N-CA	5.37	129.76	122.19
2	L	281	ALA	N-CA-CB	-5.37	101.65	110.14
2	D	15	GLN	CG-CD-NE2	5.37	124.45	116.40
2	L	122	ILE	CA-CB-CG1	5.37	119.53	110.40
1	C	94	GLN	CB-CA-C	5.37	119.66	110.85
1	C	421	GLU	CA-C-O	-5.37	114.03	120.10
2	D	99	ALA	N-CA-C	-5.37	106.57	113.01
1	E	415	MET	N-CA-C	5.37	116.81	111.07
1	I	377	LEU	N-CA-C	-5.37	105.33	111.07
1	A	134	GLN	OE1-CD-NE2	-5.37	117.23	122.60
2	J	413	MET	CA-C-N	5.37	131.60	122.37
2	J	413	MET	C-N-CA	5.37	131.60	122.37
1	A	6	HIS	CB-CA-C	5.37	118.72	110.14
2	F	61	HIS	CA-C-N	5.37	129.33	123.43
2	F	61	HIS	C-N-CA	5.37	129.33	123.43
1	A	429	THR	CA-C-N	5.36	129.98	121.99
1	A	429	THR	C-N-CA	5.36	129.98	121.99
2	J	258	ASN	N-CA-CB	-5.36	102.62	110.40
1	E	316	VAL	CA-CB-CG2	5.36	119.52	110.40
2	J	292	THR	CA-CB-CG2	5.36	119.61	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	212	PHE	N-CA-C	5.36	118.28	111.69
1	K	184	ASN	CA-C-O	-5.36	114.84	120.63
2	L	372	GLN	CA-C-O	5.36	125.76	119.06
1	E	337	ASN	N-CA-C	5.36	118.95	111.56
1	K	358	PRO	CB-CA-C	5.36	118.37	111.46
2	L	13	GLY	CA-C-O	-5.36	114.98	120.66
1	E	374	ILE	CB-CG1-CD1	5.35	125.04	113.80
1	A	437	GLU	N-CA-C	5.35	117.97	109.24
2	B	89	PRO	CA-C-O	-5.35	112.16	118.90
2	B	107	HIS	CA-CB-CG	-5.35	108.45	113.80
2	L	407	TRP	CD2-CE3-CZ3	5.35	125.56	118.60
1	G	3	GLU	O-C-N	-5.35	117.06	123.27
1	A	310	TYR	O-C-N	5.35	129.45	122.87
1	E	195	ASN	OD1-CG-ND2	-5.35	117.25	122.60
2	H	54	SER	N-CA-CB	-5.35	102.38	110.77
1	C	162	ARG	CA-C-O	5.35	127.62	121.47
1	C	426	GLN	CA-CB-CG	5.35	124.79	114.10
2	J	406	HIS	CA-C-N	5.35	127.71	120.44
2	J	406	HIS	C-N-CA	5.35	127.71	120.44
1	I	16	ILE	CA-C-O	-5.34	115.39	120.95
1	I	347	ASN	CA-C-N	5.34	131.75	121.54
1	I	347	ASN	C-N-CA	5.34	131.75	121.54
1	M	358	PRO	N-CA-CB	5.34	108.41	103.39
2	N	186	ASN	CA-CB-CG	-5.34	107.25	112.60
2	N	197	HIS	CA-C-O	-5.34	112.84	118.77
1	I	445	ALA	CB-CA-C	5.34	118.52	110.50
2	L	14	VAL	CA-C-N	5.34	128.43	120.31
2	L	14	VAL	C-N-CA	5.34	128.43	120.31
2	L	282	TYR	CA-C-N	5.34	130.25	122.08
2	L	282	TYR	C-N-CA	5.34	130.25	122.08
1	M	100	ASN	N-CA-CB	-5.34	101.55	110.37
2	N	49	PHE	CA-C-N	5.34	129.23	120.63
2	N	49	PHE	C-N-CA	5.34	129.23	120.63
2	N	21	TRP	NE1-CE2-CD2	-5.34	100.46	107.40
1	M	260	PHE	CA-C-O	-5.34	115.35	120.64
2	N	438	ASP	CA-CB-CG	-5.34	107.26	112.60
2	L	328	VAL	CA-C-N	5.34	127.74	120.54
2	L	328	VAL	C-N-CA	5.34	127.74	120.54
1	M	3	GLU	CA-CB-CG	-5.33	103.43	114.10
1	M	59	TYR	CB-CA-C	5.33	118.60	109.80
2	D	354	GLY	O-C-N	-5.33	115.77	122.70
1	A	229	VAL	N-CA-C	5.33	116.10	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	155	GLU	CB-CA-C	5.33	119.63	110.79
1	E	252	LYS	CA-C-O	-5.33	114.08	120.10
2	D	210	TYR	N-CA-C	5.33	117.16	111.36
1	E	264	HIS	N-CA-C	5.33	118.91	111.56
1	I	213	ARG	CA-C-O	-5.33	114.77	120.42
1	K	437	GLU	CB-CG-CD	5.33	121.66	112.60
2	N	281	ALA	N-CA-CB	-5.33	102.07	110.06
2	F	234	ILE	N-CA-C	-5.32	105.53	110.53
2	H	246	GLY	O-C-N	-5.32	118.92	123.23
1	I	167	PHE	N-CA-C	5.32	117.41	109.59
1	K	113	VAL	N-CA-C	5.32	115.95	110.36
1	C	255	VAL	CA-C-N	5.32	127.68	120.44
1	C	255	VAL	C-N-CA	5.32	127.68	120.44
2	D	26	LEU	CA-C-O	-5.32	114.88	120.63
1	I	388	MET	CA-C-N	5.32	127.94	120.28
1	I	388	MET	C-N-CA	5.32	127.94	120.28
2	J	94	THR	N-CA-C	5.32	118.11	109.06
2	L	442	GLY	CA-C-N	5.32	129.72	120.68
2	L	442	GLY	C-N-CA	5.32	129.72	120.68
2	N	447	GLU	N-CA-C	5.32	117.69	110.35
1	A	151	LEU	CA-C-O	-5.32	115.22	121.07
1	A	316	VAL	N-CA-C	5.32	115.43	107.51
1	C	24	ILE	CA-CB-CG1	5.32	119.44	110.40
1	E	383	GLU	CA-C-N	5.32	127.35	120.44
1	E	383	GLU	C-N-CA	5.32	127.35	120.44
1	K	368	ILE	CA-CB-CG1	5.32	119.44	110.40
1	G	304	ASP	CB-CA-C	5.32	117.03	109.38
2	N	329	ASN	CA-C-N	5.32	127.84	120.29
2	N	329	ASN	C-N-CA	5.32	127.84	120.29
2	H	234	ILE	N-CA-CB	5.31	116.41	110.62
1	A	26	ASP	N-CA-CB	-5.31	102.04	110.22
1	A	338	SER	O-C-N	-5.31	116.09	122.15
1	I	278	SER	CA-C-N	5.31	128.14	120.38
1	I	278	SER	C-N-CA	5.31	128.14	120.38
2	N	268	PRO	N-CA-CB	5.31	108.27	103.33
2	F	239	THR	CA-CB-CG2	5.31	119.53	110.50
2	N	171	ILE	O-C-N	-5.31	116.18	122.77
1	G	190	HIS	CB-CG-CD2	-5.31	124.30	131.20
2	B	211	ASP	N-CA-CB	-5.31	102.29	110.20
1	M	290	THR	CA-C-O	5.31	126.58	120.90
1	C	243	PRO	N-CA-CB	5.31	108.38	103.39
2	D	90	GLU	O-C-N	5.31	130.18	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	449	GLU	O-C-N	-5.31	116.96	122.96
2	B	113	GLU	CA-C-O	-5.30	113.87	119.97
2	D	275	VAL	CA-CB-CG2	5.30	119.42	110.40
2	F	247	ALA	CA-C-N	5.30	131.67	121.54
2	F	247	ALA	C-N-CA	5.30	131.67	121.54
1	I	301	ALA	CA-C-N	5.30	127.82	120.29
1	I	301	ALA	C-N-CA	5.30	127.82	120.29
2	N	306	ASP	O-C-N	-5.30	116.25	121.18
2	N	354	GLY	CA-C-O	-5.30	115.53	120.57
2	F	264	ARG	CA-CB-CG	-5.30	103.49	114.10
1	G	118	ASP	O-C-N	-5.30	116.36	122.09
1	K	427	ASP	CA-C-O	5.30	128.09	120.51
2	L	342	GLN	CG-CD-NE2	5.30	124.35	116.40
2	N	283	HIS	CB-CG-CD2	-5.30	124.31	131.20
2	N	406	HIS	CB-CG-CD2	-5.30	124.31	131.20
2	B	61	HIS	CG-CD2-NE2	-5.30	101.90	107.20
2	F	192	HIS	O-C-N	5.30	127.74	122.12
2	J	290	GLU	O-C-N	5.30	127.74	122.12
1	A	201	CYS	CA-C-N	5.30	130.01	123.12
1	A	201	CYS	C-N-CA	5.30	130.01	123.12
1	E	234	SER	O-C-N	5.30	127.75	122.03
1	K	406	MET	CA-C-O	5.30	125.90	119.38
1	C	157	GLU	CA-C-O	5.30	124.97	119.14
1	G	76	VAL	CA-C-O	-5.29	115.24	120.85
2	B	130	THR	CA-C-O	5.29	126.08	120.10
2	D	374	ALA	N-CA-C	5.29	116.33	108.60
1	E	137	HIS	CB-CG-CD2	-5.29	124.32	131.20
2	H	337	THR	CA-C-N	5.29	131.65	121.54
2	H	337	THR	C-N-CA	5.29	131.65	121.54
3	O	308	ILE	CA-C-N	5.29	128.31	122.22
3	O	308	ILE	C-N-CA	5.29	128.31	122.22
1	E	28	HIS	CB-CA-C	5.29	119.54	111.02
1	I	222	TYR	N-CA-C	-5.29	106.78	113.18
2	J	155	GLU	CA-C-N	5.29	129.63	120.58
2	J	155	GLU	C-N-CA	5.29	129.63	120.58
2	B	367	ASP	CA-CB-CG	5.29	117.89	112.60
2	B	418	PHE	N-CA-CB	-5.29	102.33	110.16
2	H	252	LEU	CA-C-N	5.29	131.90	122.06
2	H	252	LEU	C-N-CA	5.29	131.90	122.06
2	J	32	PRO	CA-C-N	5.29	131.26	122.54
2	J	32	PRO	C-N-CA	5.29	131.26	122.54
2	B	77	GLU	N-CA-C	5.29	118.52	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	69	ASP	O-C-N	-5.29	116.77	123.17
2	J	210	TYR	CA-C-N	5.29	127.80	120.29
2	J	210	TYR	C-N-CA	5.29	127.80	120.29
2	L	316	CYS	CA-C-N	5.29	130.45	123.00
2	L	316	CYS	C-N-CA	5.29	130.45	123.00
1	M	408	PHE	CA-CB-CG	5.29	119.08	113.80
2	D	109	THR	N-CA-C	5.28	117.72	111.33
2	F	389	ALA	N-CA-C	5.28	117.79	111.71
2	L	8	HIS	ND1-CE1-NE2	5.28	113.68	108.40
1	M	217	LEU	CD1-CG-CD2	-5.28	99.17	110.80
1	M	400	GLY	N-CA-C	5.28	120.45	113.37
1	A	63	ALA	CA-C-N	5.28	130.78	122.70
1	A	63	ALA	C-N-CA	5.28	130.78	122.70
1	A	203	ASP	O-C-N	-5.28	117.02	123.30
1	C	70	PRO	CA-C-N	5.28	126.93	120.22
1	C	70	PRO	C-N-CA	5.28	126.93	120.22
2	D	237	SER	CA-CB-OG	-5.28	100.54	111.10
1	G	30	ILE	CB-CA-C	5.28	118.02	111.15
1	G	163	ILE	CB-CA-C	5.28	118.92	111.63
1	I	31	ASP	CA-C-N	5.28	126.44	119.84
1	I	31	ASP	C-N-CA	5.28	126.44	119.84
2	N	69	ASP	CB-CG-OD1	5.28	130.55	118.40
1	E	159	TYR	CA-C-N	5.28	124.79	119.19
1	E	159	TYR	C-N-CA	5.28	124.79	119.19
2	F	190	THR	CA-C-O	-5.28	113.39	119.78
2	B	196	GLU	N-CA-CB	-5.28	101.55	110.41
1	C	221	THR	CA-C-N	5.28	127.61	120.38
1	C	221	THR	C-N-CA	5.28	127.61	120.38
2	F	156	ARG	CA-C-N	5.28	127.35	120.28
2	F	156	ARG	C-N-CA	5.28	127.35	120.28
2	H	90	GLU	N-CA-C	5.28	120.37	113.30
2	H	251	ASP	N-CA-CB	-5.28	102.81	110.36
1	K	329	GLN	OE1-CD-NE2	-5.28	117.32	122.60
3	O	375	LYS	CA-C-N	5.28	131.20	121.70
3	O	375	LYS	C-N-CA	5.28	131.20	121.70
2	F	15	GLN	OE1-CD-NE2	-5.28	117.33	122.60
2	L	407	TRP	NE1-CE2-CD2	-5.28	100.54	107.40
1	A	74	ASP	CA-C-N	5.27	128.33	120.31
1	A	74	ASP	C-N-CA	5.27	128.33	120.31
1	K	74	ASP	CA-C-O	5.27	126.90	120.31
2	L	390	ARG	O-C-N	5.27	129.90	122.41
2	L	249	ASN	OD1-CG-ND2	-5.27	117.33	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	CYS	CA-C-O	5.27	126.54	120.90
1	C	410	GLU	O-C-N	-5.27	116.14	122.15
2	F	349	THR	CB-CA-C	-5.27	104.19	110.94
2	L	430	LYS	CA-C-N	5.27	127.77	120.29
2	L	430	LYS	C-N-CA	5.27	127.77	120.29
1	M	101	TRP	CA-C-N	5.27	127.87	120.28
1	M	101	TRP	C-N-CA	5.27	127.87	120.28
1	M	159	TYR	CA-C-N	5.27	126.20	120.83
1	M	159	TYR	C-N-CA	5.27	126.20	120.83
2	N	101	ASN	CB-CG-ND2	5.27	124.30	116.40
1	A	290	THR	CA-C-O	5.27	126.00	120.42
1	C	401	GLU	CA-C-O	5.27	126.17	119.95
1	K	76	VAL	CA-CB-CG1	5.27	119.35	110.40
1	K	294	PHE	O-C-N	-5.27	115.40	122.19
1	A	193	VAL	N-CA-C	5.26	120.29	109.34
2	F	230	LEU	N-CA-CB	-5.26	102.42	110.26
1	I	279	GLN	CA-C-N	5.26	127.77	120.29
1	I	279	GLN	C-N-CA	5.26	127.77	120.29
2	N	197	HIS	CB-CG-CD2	-5.26	124.36	131.20
1	I	94	GLN	N-CA-C	5.26	117.19	110.61
2	N	364	PRO	O-C-N	-5.26	116.54	122.91
1	C	148	GLY	O-C-N	-5.26	117.09	122.19
2	N	400	ALA	CA-C-N	5.26	130.81	122.60
2	N	400	ALA	C-N-CA	5.26	130.81	122.60
2	H	164	LYS	CA-C-O	-5.26	116.09	121.87
1	C	114	ASP	CA-C-N	5.26	127.59	120.44
1	C	114	ASP	C-N-CA	5.26	127.59	120.44
1	C	394	PHE	O-C-N	-5.26	115.60	122.59
1	K	2	ARG	O-C-N	5.26	129.34	123.40
1	K	28	HIS	CB-CG-CD2	-5.26	124.37	131.20
1	K	361	LEU	N-CA-C	5.26	117.38	109.23
1	M	272	PRO	N-CA-CB	5.26	108.38	102.60
1	C	361	LEU	CA-C-O	-5.25	115.31	121.46
1	I	359	ARG	CD-NE-CZ	-5.25	117.04	124.40
1	K	269	GLY	CA-C-O	-5.25	115.64	121.37
1	M	138	SER	O-C-N	-5.25	116.34	122.96
1	E	222	TYR	CA-C-N	5.25	125.91	120.03
1	E	222	TYR	C-N-CA	5.25	125.91	120.03
2	N	388	TRP	CZ3-CH2-CZ2	-5.25	114.67	121.50
2	D	343	PHE	CA-CB-CG	-5.25	108.55	113.80
1	K	384	GLN	CA-C-O	-5.25	113.93	119.97
1	I	227	HIS	CB-CG-CD2	-5.25	124.38	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	313	VAL	CB-CA-C	5.25	120.10	110.71
2	B	188	ILE	CA-CB-CG1	5.24	119.31	110.40
1	C	89	ASN	CA-CB-CG	5.24	117.84	112.60
1	M	110	ALA	CA-C-O	-5.24	114.99	120.55
2	B	150	THR	N-CA-C	-5.24	105.57	111.28
1	C	143	THR	O-C-N	-5.24	116.03	122.11
2	D	200	CYS	O-C-N	-5.24	117.08	123.10
2	N	424	ASP	O-C-N	5.24	127.47	122.07
2	B	12	ALA	N-CA-C	5.24	116.68	110.97
1	E	412	GLU	CB-CA-C	5.24	119.48	110.79
1	G	434	GLY	CA-C-N	5.24	130.00	122.40
1	G	434	GLY	C-N-CA	5.24	130.00	122.40
1	K	227	HIS	CB-CG-ND1	5.24	130.56	122.70
1	M	329	GLN	CA-CB-CG	-5.24	103.62	114.10
2	N	25	CYS	CA-C-O	5.24	126.32	120.82
2	F	112	LYS	CG-CD-CE	5.24	123.34	111.30
2	H	163	LYS	CB-CG-CD	5.24	123.34	111.30
1	K	409	THR	CA-C-N	5.24	127.30	120.28
1	K	409	THR	C-N-CA	5.24	127.30	120.28
1	M	151	LEU	O-C-N	-5.24	115.31	122.33
1	A	94	GLN	N-CA-C	-5.24	107.56	114.31
1	A	389	PHE	CA-C-O	-5.24	114.87	120.42
1	C	385	PHE	CA-C-N	5.24	127.25	120.44
1	C	385	PHE	C-N-CA	5.24	127.25	120.44
1	E	332	ASN	N-CA-CB	-5.24	102.14	109.94
2	L	147	SER	CA-C-N	5.24	126.69	120.14
2	L	147	SER	C-N-CA	5.24	126.69	120.14
2	F	397	LEU	CA-C-N	5.23	127.56	120.44
2	F	397	LEU	C-N-CA	5.23	127.56	120.44
1	K	184	ASN	O-C-N	5.23	127.67	122.12
2	D	95	GLY	O-C-N	-5.23	118.63	122.71
1	M	344	TRP	NE1-CE2-CZ2	5.23	137.95	130.10
2	N	175	PRO	CA-N-CD	-5.23	104.68	112.00
2	B	28	HIS	ND1-CG-CD2	5.23	111.33	106.10
1	G	10	GLY	N-CA-C	-5.23	106.43	112.29
1	I	48	ASN	N-CA-C	5.23	121.94	110.80
1	C	26	ASP	N-CA-C	5.23	117.72	111.71
2	N	445	GLU	CA-C-O	-5.23	114.73	120.43
1	C	309	ARG	CA-C-N	5.23	129.81	121.66
1	C	309	ARG	C-N-CA	5.23	129.81	121.66
2	F	326	LYS	CA-C-N	5.23	127.71	120.29
2	F	326	LYS	C-N-CA	5.23	127.71	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	99	ASN	CA-CB-CG	5.23	117.83	112.60
2	B	357	TYR	CA-CB-CG	5.22	123.31	113.90
1	G	20	PHE	O-C-N	-5.22	116.69	122.07
2	B	8	HIS	CA-CB-CG	-5.22	108.58	113.80
2	B	194	THR	CA-CB-OG1	5.22	117.44	109.60
2	B	372	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	C	251	ARG	N-CA-C	5.22	117.05	111.36
2	D	405	VAL	N-CA-C	5.22	116.57	110.62
1	E	46	ARG	N-CA-CB	-5.22	103.24	111.39
2	F	422	ARG	CA-C-N	5.22	127.53	120.38
2	F	422	ARG	C-N-CA	5.22	127.53	120.38
1	I	4	ILE	CA-CB-CG2	5.22	119.38	110.50
2	B	102	ASN	CB-CA-C	5.22	118.64	110.19
2	F	16	ILE	CA-CB-CG2	5.22	119.37	110.50
1	G	266	PHE	CA-CB-CG	5.22	119.02	113.80
2	H	324	VAL	N-CA-C	5.22	114.71	108.45
1	K	221	THR	OG1-CB-CG2	-5.22	98.86	109.30
1	M	157	GLU	CA-C-N	5.22	127.28	120.28
1	M	157	GLU	C-N-CA	5.22	127.28	120.28
1	M	359	ARG	CA-C-N	5.22	130.06	122.28
1	M	359	ARG	C-N-CA	5.22	130.06	122.28
2	N	370	LYS	CA-C-O	-5.22	114.70	120.70
2	L	233	GLN	N-CA-C	-5.22	105.67	111.36
1	C	23	VAL	CB-CA-C	-5.22	105.37	111.94
1	E	227	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
2	L	51	THR	CA-CB-CG2	5.22	119.37	110.50
2	L	342	GLN	OE1-CD-NE2	-5.22	117.38	122.60
2	B	220	GLU	CA-C-N	5.21	128.38	122.59
2	B	220	GLU	C-N-CA	5.21	128.38	122.59
2	H	185	TYR	N-CA-C	5.21	116.65	111.07
1	A	62	ARG	CD-NE-CZ	5.21	131.70	124.40
2	D	431	ASP	CA-C-N	5.21	127.69	120.29
2	D	431	ASP	C-N-CA	5.21	127.69	120.29
2	N	40	LYS	N-CA-C	-5.21	105.59	112.94
3	O	205	THR	CA-C-O	-5.21	115.01	120.38
2	H	394	LYS	CA-C-O	-5.21	113.19	119.49
1	M	341	PHE	CA-CB-CG	5.21	119.01	113.80
2	B	35	GLN	O-C-N	-5.21	116.87	123.01
1	M	89	ASN	CA-CB-CG	5.21	117.81	112.60
2	N	389	ALA	CA-C-N	5.21	127.21	120.44
2	N	389	ALA	C-N-CA	5.21	127.21	120.44
2	B	386	GLU	CA-C-O	-5.21	113.98	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	GLN	CA-C-N	5.20	127.68	120.29
1	A	43	GLN	C-N-CA	5.20	127.68	120.29
1	I	396	HIS	CA-CB-CG	5.20	119.00	113.80
2	J	93	ILE	CA-C-O	5.20	126.14	120.57
2	L	85	GLN	CB-CG-CD	-5.20	103.75	112.60
2	F	306	ASP	CA-CB-CG	5.20	117.80	112.60
1	M	132	GLY	O-C-N	5.20	128.81	123.29
2	B	25	CYS	CA-CB-SG	-5.20	102.44	114.40
2	D	405	VAL	CA-CB-CG1	5.20	119.24	110.40
2	L	424	ASP	N-CA-CB	-5.20	102.22	110.28
1	M	31	ASP	CB-CA-C	5.20	117.99	109.46
1	G	21	TRP	N-CA-C	5.20	117.69	111.71
1	G	265	PHE	CA-C-O	-5.20	114.60	120.32
2	L	134	GLY	CA-C-O	-5.20	115.89	121.35
1	M	433	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	A	76	VAL	O-C-N	-5.20	116.50	121.90
1	A	260	PHE	CA-CB-CG	5.20	119.00	113.80
2	B	114	ILE	CA-CB-CG1	5.20	119.23	110.40
1	I	185	ALA	N-CA-C	5.20	116.64	110.97
2	B	134	GLY	O-C-N	5.20	129.45	122.70
1	C	397	TRP	CE2-CD2-CE3	-5.20	113.60	118.80
2	F	309	HIS	ND1-CG-CD2	5.20	111.30	106.10
2	J	176	GLN	O-C-N	5.20	128.49	122.25
2	J	244	PHE	N-CA-C	5.20	116.74	108.79
2	J	251	ASP	CB-CA-C	5.20	118.39	109.51
2	J	384	ILE	CA-CB-CG1	5.19	119.23	110.40
2	N	236	SER	N-CA-C	5.19	116.94	111.28
1	C	45	GLU	N-CA-C	5.19	117.68	111.71
2	H	261	PRO	N-CA-CB	5.19	109.00	103.39
2	L	204	VAL	CA-CB-CG1	5.19	119.23	110.40
2	L	307	PRO	N-CA-CB	5.19	108.70	103.25
1	G	91	VAL	CA-CB-CG2	5.19	119.22	110.40
1	C	355	ASP	N-CA-C	-5.19	106.80	113.23
2	D	210	TYR	CB-CA-C	-5.19	102.03	110.85
2	F	105	ARG	CA-CB-CG	-5.19	103.72	114.10
1	G	151	LEU	CB-CA-C	5.19	119.41	110.79
2	H	121	ARG	CD-NE-CZ	5.19	131.66	124.40
2	J	177	VAL	N-CA-C	5.19	116.76	108.87
1	E	332	ASN	N-CA-C	5.19	117.33	111.11
2	F	432	TYR	CA-C-O	5.19	125.35	119.18
1	G	71	GLY	CA-C-N	5.19	127.75	120.28
1	G	71	GLY	C-N-CA	5.19	127.75	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	361	THR	CA-CB-CG2	5.19	119.32	110.50
2	J	199	ASP	O-C-N	5.19	129.90	122.28
3	O	254	LYS	CA-C-N	5.19	131.07	121.94
3	O	254	LYS	C-N-CA	5.19	131.07	121.94
2	B	428	LEU	N-CA-C	5.19	117.61	111.33
1	M	79	GLY	O-C-N	-5.19	116.58	121.77
1	E	49	VAL	CG1-CB-CG2	-5.18	99.40	110.80
1	G	287	PRO	CB-CA-C	-5.18	104.54	112.11
2	N	123	ARG	CA-C-O	-5.18	114.01	119.97
2	N	417	GLU	O-C-N	-5.18	115.38	122.33
1	C	349	VAL	N-CA-C	5.18	116.77	108.89
1	G	89	ASN	CA-C-O	-5.18	113.50	119.56
1	I	57	ASN	CB-CA-C	5.18	119.68	111.23
1	M	115	SER	CA-C-N	5.18	128.46	122.35
1	M	115	SER	C-N-CA	5.18	128.46	122.35
2	H	98	ASP	CA-C-O	5.18	127.88	122.03
1	A	307	HIS	N-CA-CB	-5.18	102.03	110.42
2	B	430	LYS	N-CA-C	5.18	118.86	112.54
1	G	120	VAL	N-CA-CB	5.18	117.58	110.54
2	J	107	HIS	CB-CG-ND1	5.18	130.46	122.70
2	J	190	THR	CA-CB-CG2	5.18	119.30	110.50
2	N	107	HIS	ND1-CG-CD2	-5.18	100.92	106.10
2	B	342	GLN	N-CA-CB	-5.17	102.02	109.83
2	D	352	LYS	CB-CG-CD	5.17	123.20	111.30
2	F	45	GLY	CA-C-O	-5.17	115.85	122.01
1	G	75	SER	CA-C-N	5.17	127.77	120.42
1	G	75	SER	C-N-CA	5.17	127.77	120.42
1	I	303	CYS	CA-C-N	5.17	134.43	121.80
1	I	303	CYS	C-N-CA	5.17	134.43	121.80
1	K	197	ASP	N-CA-C	-5.17	107.10	113.41
1	M	331	LEU	CD1-CG-CD2	5.17	122.18	110.80
2	H	26	LEU	CA-C-O	-5.17	115.02	120.55
2	N	308	ARG	CA-C-N	5.17	131.46	122.56
2	N	308	ARG	C-N-CA	5.17	131.46	122.56
2	B	11	GLN	CA-CB-CG	5.17	124.44	114.10
2	D	16	ILE	N-CA-C	5.17	115.94	110.72
1	K	253	LEU	N-CA-CB	5.17	117.57	110.07
1	K	259	PRO	CA-N-CD	-5.17	104.76	112.00
1	K	303	CYS	CB-CA-C	5.17	120.95	109.94
2	B	57	GLY	CA-C-N	5.17	129.46	122.07
2	B	57	GLY	C-N-CA	5.17	129.46	122.07
1	C	255	VAL	CG1-CB-CG2	-5.17	99.43	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	258	ASN	CA-C-O	-5.17	113.73	119.67
2	J	346	TRP	CB-CG-CD1	-5.17	119.15	126.90
1	A	324	LYS	CB-CG-CD	5.17	123.18	111.30
1	E	126	SER	O-C-N	5.17	128.71	122.35
2	F	380	ASN	OD1-CG-ND2	-5.17	117.43	122.60
2	J	161	TYR	CB-CG-CD1	5.17	128.55	120.80
1	K	370	ASN	CA-C-O	-5.17	115.17	120.54
1	M	256	ASN	CB-CG-ND2	5.17	124.15	116.40
1	M	386	THR	CA-CB-CG2	5.17	119.28	110.50
1	M	416	ASN	OD1-CG-ND2	-5.17	117.44	122.60
3	O	393	VAL	CA-C-N	5.17	131.00	121.70
3	O	393	VAL	C-N-CA	5.17	131.00	121.70
2	B	27	GLU	N-CA-C	5.16	117.58	111.33
2	H	205	ASP	CA-CB-CG	5.16	117.76	112.60
2	H	338	LYS	CG-CD-CE	-5.16	99.42	111.30
2	B	213	CYS	N-CA-C	5.16	117.32	111.02
2	J	259	LEU	N-CA-C	5.16	119.63	113.23
1	I	231	ALA	O-C-N	5.16	128.03	122.15
2	N	166	LYS	CB-CG-CD	5.16	123.17	111.30
1	A	413	SER	CA-C-N	5.16	127.15	120.44
1	A	413	SER	C-N-CA	5.16	127.15	120.44
1	C	86	ARG	CB-CA-C	5.16	116.77	109.08
2	H	370	LYS	CB-CA-C	5.16	118.26	109.80
1	M	323	MET	CA-C-N	5.16	127.19	120.28
1	M	323	MET	C-N-CA	5.16	127.19	120.28
3	O	255	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	G	10	GLY	CA-C-O	5.16	125.79	122.23
1	M	27	GLU	CA-C-N	5.16	130.59	122.49
1	M	27	GLU	C-N-CA	5.16	130.59	122.49
1	A	380	ARG	CD-NE-CZ	5.16	131.62	124.40
2	D	428	LEU	N-CA-C	5.16	116.71	111.14
1	G	174	LYS	CA-C-O	-5.16	115.03	120.55
1	G	394	PHE	CA-C-N	5.16	129.39	120.58
1	G	394	PHE	C-N-CA	5.16	129.39	120.58
1	I	443	ASP	CB-CA-C	5.16	118.24	109.53
2	J	28	HIS	CB-CG-ND1	5.16	130.43	122.70
1	C	248	ALA	CA-C-O	5.15	126.27	119.98
2	F	184	PRO	N-CA-CB	5.15	109.14	103.26
2	F	285	GLN	CA-C-O	-5.15	113.59	119.41
1	I	23	VAL	CA-CB-CG1	5.15	119.16	110.40
1	I	128	ASP	O-C-N	-5.15	115.94	122.17
1	C	234	SER	CA-C-N	5.15	125.55	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	SER	C-N-CA	5.15	125.55	119.94
2	J	145	THR	N-CA-C	-5.15	105.58	111.14
2	B	105	ARG	CA-C-O	-5.15	115.42	120.82
2	F	249	ASN	CA-CB-CG	-5.15	107.45	112.60
2	L	234	ILE	CA-CB-CG1	5.15	119.15	110.40
2	N	193	THR	O-C-N	-5.15	115.94	122.17
3	O	243	LEU	CB-CA-C	5.14	118.22	109.53
1	C	307	HIS	CA-C-N	5.14	127.56	120.72
1	C	307	HIS	C-N-CA	5.14	127.56	120.72
1	G	271	ALA	CA-C-O	-5.14	114.48	120.03
1	M	438	GLU	CA-C-O	-5.14	115.09	121.06
1	C	105	HIS	ND1-CE1-NE2	5.14	113.54	108.40
2	D	246	GLY	O-C-N	5.14	129.40	123.44
1	E	302	ALA	O-C-N	-5.14	114.18	122.41
2	D	150	THR	CA-C-N	5.14	127.59	120.29
2	D	150	THR	C-N-CA	5.14	127.59	120.29
1	A	384	GLN	CA-CB-CG	5.14	124.37	114.10
2	D	235	VAL	O-C-N	-5.14	116.68	121.87
2	J	13	GLY	N-CA-C	5.14	118.46	112.50
1	K	143	THR	CA-CB-OG1	5.14	117.30	109.60
1	K	276	ARG	CA-C-O	-5.14	115.10	120.55
2	N	301	GLN	CA-C-O	5.14	126.34	120.54
1	E	170	VAL	CA-CB-CG2	5.13	119.13	110.40
2	J	329	ASN	CB-CA-C	5.13	119.08	110.92
2	N	95	GLY	O-C-N	-5.13	118.25	122.92
2	F	273	ALA	N-CA-C	5.13	114.73	108.11
1	G	131	GLN	N-CA-CB	5.13	117.51	110.07
3	O	217	THR	O-C-N	5.13	126.86	121.42
1	A	182	PRO	N-CA-CB	5.13	108.23	103.46
2	F	94	THR	N-CA-CB	-5.13	103.11	111.22
1	I	283	ALA	N-CA-CB	-5.13	101.82	110.49
2	J	272	TYR	CA-CB-CG	5.13	123.14	113.90
1	K	23	VAL	CB-CA-C	5.13	118.74	112.02
3	O	219	PRO	N-CA-C	5.13	119.30	111.34
2	J	266	HIS	N-CA-C	5.13	119.10	111.87
2	D	138	PHE	CA-CB-CG	5.13	118.93	113.80
2	H	421	ALA	CA-C-O	-5.13	115.11	120.55
1	I	137	HIS	O-C-N	-5.13	116.97	123.17
1	I	196	THR	CA-CB-OG1	5.13	117.29	109.60
1	K	240	LEU	CD1-CG-CD2	-5.13	99.52	110.80
2	N	192	HIS	N-CA-C	5.13	117.54	111.33
1	A	109	GLY	CA-C-N	5.13	127.57	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	GLY	C-N-CA	5.13	127.57	120.29
1	C	6	HIS	CB-CG-CD2	-5.13	124.54	131.20
1	C	380	ARG	CB-CA-C	5.13	118.93	110.88
1	G	426	GLN	CA-CB-CG	5.12	124.35	114.10
2	D	371	VAL	CA-CB-CG1	5.12	119.11	110.40
2	H	396	ASP	CA-C-N	5.12	127.45	120.54
2	H	396	ASP	C-N-CA	5.12	127.45	120.54
2	J	88	HIS	CA-C-N	5.12	124.73	119.05
2	J	88	HIS	C-N-CA	5.12	124.73	119.05
2	J	276	ILE	CA-CB-CG1	5.12	119.11	110.40
1	A	302	ALA	N-CA-C	5.12	118.79	112.54
2	H	115	ILE	N-CA-C	5.12	115.84	110.62
1	I	100	ASN	CA-C-O	5.12	125.86	120.54
2	F	318	LEU	CA-C-O	-5.12	115.03	120.92
2	N	318	LEU	N-CA-C	5.12	117.08	108.73
2	J	395	PHE	CA-C-O	-5.12	115.13	120.55
2	B	165	SER	CA-CB-OG	-5.12	100.87	111.10
1	G	148	GLY	CA-C-O	-5.12	115.24	120.66
1	K	184	ASN	N-CA-C	5.12	117.52	111.33
2	N	306	ASP	CA-CB-CG	5.12	117.72	112.60
3	O	368	ASN	CA-C-N	5.12	131.31	121.54
3	O	368	ASN	C-N-CA	5.12	131.31	121.54
1	E	317	PHE	CB-CA-C	5.11	118.24	109.80
1	G	90	PHE	O-C-N	-5.11	117.39	123.22
1	K	186	THR	CA-CB-CG2	5.11	119.19	110.50
2	N	91	GLN	CA-CB-CG	-5.11	103.87	114.10
2	N	434	GLU	CA-C-N	5.11	127.94	121.85
2	N	434	GLU	C-N-CA	5.11	127.94	121.85
2	L	365	GLY	CA-C-N	5.11	125.52	120.31
2	L	365	GLY	C-N-CA	5.11	125.52	120.31
2	H	75	ILE	CA-CB-CG1	5.11	119.09	110.40
1	I	173	PRO	N-CA-CB	5.11	108.61	103.25
2	J	347	CYS	N-CA-CB	-5.11	102.92	110.99
2	L	132	LEU	N-CA-CB	-5.11	101.86	110.49
2	B	232	SER	CA-C-O	-5.11	114.33	120.10
2	B	306	ASP	CA-CB-CG	5.11	117.71	112.60
1	C	286	VAL	CA-CB-CG1	5.11	119.08	110.40
1	I	284	LEU	CA-C-N	5.11	130.75	122.53
1	I	284	LEU	C-N-CA	5.11	130.75	122.53
1	G	177	ASP	CA-C-N	5.11	130.93	121.94
1	G	177	ASP	C-N-CA	5.11	130.93	121.94
2	H	128	GLN	CA-C-N	5.11	130.61	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	128	GLN	C-N-CA	5.11	130.61	122.59
2	L	29	GLY	CA-C-N	5.11	127.42	120.63
2	L	29	GLY	C-N-CA	5.11	127.42	120.63
1	C	399	THR	CB-CA-C	-5.10	102.32	110.79
1	G	224	ASP	CB-CA-C	5.10	118.82	110.96
2	H	19	ALA	CA-C-N	5.10	127.38	120.44
2	H	19	ALA	C-N-CA	5.10	127.38	120.44
2	H	243	ARG	CB-CA-C	5.10	117.59	109.02
1	K	34	GLY	N-CA-C	5.10	122.15	115.36
3	O	246	ALA	CA-C-O	-5.10	114.44	119.49
2	F	40	LYS	N-CA-CB	-5.10	101.04	110.32
1	I	74	ASP	N-CA-C	5.10	117.74	111.82
3	O	247	PRO	N-CA-CB	5.10	108.93	103.52
2	D	319	TYR	N-CA-CB	-5.10	103.10	110.70
1	E	433	GLN	CA-C-O	-5.10	114.45	120.57
2	L	165	SER	CA-C-O	5.10	126.78	120.92
2	N	319	TYR	CA-CB-CG	5.10	123.08	113.90
1	A	422	TYR	N-CA-CB	5.10	118.18	110.28
2	B	133	GLN	CB-CG-CD	-5.10	103.93	112.60
1	C	336	LYS	CA-C-N	5.10	130.49	122.49
1	C	336	LYS	C-N-CA	5.10	130.49	122.49
2	D	350	GLY	CA-C-N	5.10	130.81	122.81
2	D	350	GLY	C-N-CA	5.10	130.81	122.81
2	J	376	CYS	O-C-N	-5.10	117.00	123.17
1	K	347	ASN	N-CA-C	5.10	118.42	111.39
2	F	176	GLN	O-C-N	-5.10	115.81	122.59
2	F	231	ILE	CA-CB-CG2	5.10	119.16	110.50
1	I	261	PRO	N-CA-CB	5.10	108.58	103.48
1	K	335	ASN	OD1-CG-ND2	-5.10	117.50	122.60
2	B	132	LEU	O-C-N	-5.09	115.81	122.59
1	C	325	GLU	CA-C-O	-5.09	115.15	120.55
2	H	375	VAL	CA-CB-CG2	5.09	119.06	110.40
1	C	368	ILE	CA-CB-CG1	5.09	119.06	110.40
2	H	245	ASP	CA-C-O	5.09	127.33	121.47
1	I	252	LYS	N-CA-C	5.09	116.83	111.28
3	O	220	THR	CB-CA-C	5.09	118.44	110.19
1	A	332	ASN	CA-CB-CG	-5.09	107.51	112.60
2	L	60	LYS	N-CA-CB	-5.09	102.55	110.29
1	M	239	CYS	N-CA-CB	-5.09	101.89	110.49
2	N	139	HIS	N-CA-C	5.09	115.77	108.74
1	A	98	GLY	CA-C-O	-5.09	113.67	120.29
1	G	429	THR	N-CA-C	5.09	117.42	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	410	GLY	O-C-N	5.09	127.63	122.24
1	M	303	CYS	N-CA-CB	-5.09	101.89	110.49
1	G	316	VAL	CA-C-O	-5.09	113.37	121.36
1	C	157	GLU	O-C-N	-5.09	115.67	122.49
2	D	236	SER	CA-C-O	-5.09	115.03	120.42
1	E	105	HIS	CA-C-N	5.09	131.42	122.42
1	E	105	HIS	C-N-CA	5.09	131.42	122.42
1	G	366	THR	CA-CB-CG2	5.09	119.15	110.50
2	L	37	PRO	N-CA-CB	5.09	108.19	103.46
2	D	50	ASN	N-CA-C	5.08	118.97	112.87
1	K	203	ASP	N-CA-CB	-5.08	102.57	110.55
2	B	191	THR	CA-C-N	5.08	127.60	120.28
2	B	191	THR	C-N-CA	5.08	127.60	120.28
2	B	267	PHE	CA-C-N	5.08	125.24	119.90
2	B	267	PHE	C-N-CA	5.08	125.24	119.90
2	H	93	ILE	CA-CB-CG1	5.08	119.04	110.40
2	N	347	CYS	CA-C-N	5.08	126.19	119.84
2	N	347	CYS	C-N-CA	5.08	126.19	119.84
2	D	346	TRP	CA-CB-CG	5.08	123.25	113.60
2	F	221	ARG	N-CA-C	5.08	118.37	108.21
1	G	248	ALA	N-CA-C	5.08	118.47	107.49
1	K	344	TRP	NE1-CE2-CZ2	5.08	137.72	130.10
1	M	287	PRO	N-CD-CG	5.08	110.82	103.20
1	I	52	ASN	CA-CB-CG	5.08	117.68	112.60
2	N	140	SER	CA-C-O	-5.08	114.82	120.66
1	C	149	THR	CB-CA-C	-5.08	100.92	110.67
2	F	332	ILE	N-CA-C	-5.08	105.76	110.53
1	K	234	SER	N-CA-CB	5.08	117.51	109.94
1	A	101	TRP	CA-C-N	5.08	128.72	120.60
1	A	101	TRP	C-N-CA	5.08	128.72	120.60
2	B	161	TYR	CA-C-N	5.08	131.36	121.41
2	B	161	TYR	C-N-CA	5.08	131.36	121.41
2	B	171	ILE	N-CA-C	-5.08	102.31	109.21
2	H	253	THR	CA-CB-CG2	5.08	119.13	110.50
2	B	439	SER	N-CA-C	5.07	119.56	113.17
1	E	4	ILE	O-C-N	-5.07	117.97	123.14
1	G	60	VAL	N-CA-C	5.07	113.51	107.73
1	I	444	GLU	CA-C-N	5.07	130.83	121.70
1	I	444	GLU	C-N-CA	5.07	130.83	121.70
1	K	342	VAL	CA-CB-CG2	-5.07	101.78	110.40
2	L	278	ALA	CA-C-O	5.07	125.83	120.10
1	G	398	TYR	CA-C-O	5.07	125.50	119.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	256	GLN	N-CA-CB	-5.07	102.41	110.22
1	G	182	PRO	CA-C-N	5.07	127.03	120.44
1	G	182	PRO	C-N-CA	5.07	127.03	120.44
1	I	291	GLN	N-CA-C	5.07	118.72	112.54
1	E	151	LEU	CB-CA-C	5.07	118.77	110.96
2	J	417	GLU	CA-C-N	5.07	127.49	120.29
2	J	417	GLU	C-N-CA	5.07	127.49	120.29
2	N	61	HIS	CG-ND1-CE1	-5.07	100.68	109.30
1	E	317	PHE	CA-C-N	5.07	130.84	122.33
1	E	317	PHE	C-N-CA	5.07	130.84	122.33
2	J	356	ASN	CA-C-O	-5.07	115.23	120.70
2	L	213	CYS	CA-C-N	5.07	127.34	120.65
2	L	213	CYS	C-N-CA	5.07	127.34	120.65
1	C	328	GLU	CB-CG-CD	-5.06	103.99	112.60
1	G	335	ASN	CB-CA-C	5.06	119.83	110.56
1	G	348	ASN	CA-C-N	5.06	129.77	123.14
1	G	348	ASN	C-N-CA	5.06	129.77	123.14
1	I	353	VAL	CG1-CB-CG2	-5.06	99.66	110.80
2	B	165	SER	N-CA-C	5.06	117.03	109.59
2	D	200	CYS	CB-CA-C	-5.06	99.60	111.09
1	E	422	TYR	CA-CB-CG	5.06	123.01	113.90
1	K	107	THR	CA-CB-OG1	-5.06	102.01	109.60
1	M	94	GLN	CB-CA-C	5.06	120.49	110.42
2	J	44	GLY	CA-C-N	5.06	131.33	121.41
2	J	44	GLY	C-N-CA	5.06	131.33	121.41
1	M	14	ASN	OD1-CG-ND2	-5.06	117.54	122.60
3	O	220	THR	OG1-CB-CG2	-5.06	99.18	109.30
2	D	38	SER	O-C-N	-5.06	117.48	123.25
1	E	163	ILE	CA-C-N	5.06	130.04	122.86
1	E	163	ILE	C-N-CA	5.06	130.04	122.86
1	G	63	ALA	CA-C-O	5.06	126.48	120.66
1	I	247	ASN	CB-CG-ND2	5.06	123.98	116.40
1	K	262	ARG	CA-C-N	5.06	131.62	122.62
1	K	262	ARG	C-N-CA	5.06	131.62	122.62
2	L	82	THR	N-CA-C	5.06	117.53	111.71
1	K	103	LYS	CA-C-N	5.06	131.32	121.41
1	K	103	LYS	C-N-CA	5.06	131.32	121.41
1	I	270	PHE	N-CA-C	5.05	116.09	108.46
1	I	349	VAL	CA-CB-CG2	5.05	118.99	110.40
2	J	234	ILE	CA-CB-CG1	5.05	118.99	110.40
2	L	11	GLN	OE1-CD-NE2	-5.05	117.55	122.60
2	N	78	VAL	CA-C-O	5.05	126.20	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	269	LEU	CB-CA-C	5.05	118.75	109.46
2	L	199	ASP	N-CA-CB	5.05	118.28	110.81
1	M	173	PRO	CA-N-CD	-5.05	104.93	112.00
2	F	342	GLN	N-CA-C	5.05	116.99	108.96
1	C	174	LYS	CA-C-N	5.05	129.75	123.14
1	C	174	LYS	C-N-CA	5.05	129.75	123.14
1	K	66	VAL	O-C-N	-5.05	117.60	123.00
1	E	202	ILE	N-CA-C	5.04	115.55	108.89
1	A	80	PRO	CA-C-N	5.04	129.30	122.19
1	A	80	PRO	C-N-CA	5.04	129.30	122.19
2	D	230	LEU	CA-C-N	5.04	127.64	120.53
2	D	230	LEU	C-N-CA	5.04	127.64	120.53
2	D	377	MET	CA-C-N	5.04	130.11	123.05
2	D	377	MET	C-N-CA	5.04	130.11	123.05
2	F	429	GLU	O-C-N	5.04	127.47	122.12
2	N	91	GLN	OE1-CD-NE2	-5.04	117.56	122.60
2	H	408	TYR	O-C-N	5.04	128.78	122.23
2	H	75	ILE	CA-C-N	5.04	127.54	120.28
2	H	75	ILE	C-N-CA	5.04	127.54	120.28
3	O	226	VAL	CG1-CB-CG2	-5.04	99.71	110.80
2	B	440	VAL	CA-C-N	5.04	128.36	120.75
2	B	440	VAL	C-N-CA	5.04	128.36	120.75
2	B	254	GLU	CA-C-N	5.04	126.99	120.44
2	B	254	GLU	C-N-CA	5.04	126.99	120.44
1	K	259	PRO	N-CA-CB	5.04	109.08	103.44
2	L	167	LEU	O-C-N	-5.04	117.48	123.22
1	A	436	PHE	O-C-N	-5.03	117.51	123.25
2	B	273	ALA	N-CA-CB	-5.03	103.78	110.77
1	C	387	ALA	N-CA-C	5.03	116.77	111.28
1	G	270	PHE	O-C-N	-5.03	116.69	123.23
1	I	365	ALA	CA-C-N	5.03	129.54	122.09
1	I	365	ALA	C-N-CA	5.03	129.54	122.09
2	L	206	ASN	N-CA-C	5.03	117.66	111.82
1	A	85	PHE	CA-CB-CG	5.03	118.83	113.80
2	F	276	ILE	CB-CG1-CD1	5.03	124.37	113.80
2	H	11	GLN	CG-CD-NE2	5.03	123.95	116.40
2	B	62	VAL	CA-CB-CG1	5.03	118.95	110.40
2	B	179	THR	N-CA-C	-5.03	107.31	113.50
2	B	221	ARG	CA-C-N	5.03	124.94	119.76
2	B	221	ARG	C-N-CA	5.03	124.94	119.76
1	C	61	PRO	O-C-N	5.03	128.73	123.10
2	D	180	ALA	CA-C-O	-5.03	115.88	121.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	315	ALA	CA-C-N	5.03	129.02	122.93
1	G	315	ALA	C-N-CA	5.03	129.02	122.93
1	I	109	GLY	N-CA-C	-5.03	108.07	114.16
1	E	415	MET	N-CA-CB	-5.03	102.72	110.01
1	K	135	LEU	CA-C-N	5.03	129.09	122.30
1	K	135	LEU	C-N-CA	5.03	129.09	122.30
1	A	23	VAL	O-C-N	-5.03	116.91	121.94
2	F	320	ARG	CD-NE-CZ	5.03	131.44	124.40
2	F	330	ALA	N-CA-C	5.03	116.76	111.28
2	F	393	HIS	CA-C-N	5.03	127.27	120.38
2	F	393	HIS	C-N-CA	5.03	127.27	120.38
2	J	213	CYS	CA-CB-SG	-5.03	102.84	114.40
1	G	317	PHE	CA-CB-CG	5.03	118.83	113.80
2	H	154	MET	CA-C-N	5.03	128.64	120.60
2	H	154	MET	C-N-CA	5.03	128.64	120.60
1	M	52	ASN	CA-C-N	5.03	128.69	121.50
1	M	52	ASN	C-N-CA	5.03	128.69	121.50
2	D	373	ARG	N-CA-C	5.02	116.71	109.07
1	E	306	ARG	CD-NE-CZ	5.02	131.43	124.40
2	N	67	PHE	CA-CB-CG	5.02	118.82	113.80
1	A	208	TYR	CA-CB-CG	5.02	122.94	113.90
1	I	401	GLU	CA-C-O	5.02	126.63	120.15
1	A	299	MET	CA-C-N	5.02	131.13	121.54
1	A	299	MET	C-N-CA	5.02	131.13	121.54
1	C	250	LEU	CA-C-N	5.02	127.42	120.29
1	C	250	LEU	C-N-CA	5.02	127.42	120.29
1	E	416	ASN	O-C-N	5.02	127.44	122.12
1	G	114	ASP	N-CA-C	5.02	116.56	111.14
1	G	312	THR	CB-CA-C	-5.02	101.91	109.99
1	K	301	ALA	O-C-N	-5.02	116.38	123.11
1	M	401	GLU	N-CA-C	-5.02	107.17	113.15
1	A	386	THR	CA-CB-OG1	5.02	117.13	109.60
1	G	100	ASN	CB-CA-C	5.02	118.81	110.78
1	I	179	VAL	O-C-N	5.02	127.00	121.83
1	K	279	GLN	CG-CD-NE2	5.02	123.93	116.40
2	L	197	HIS	ND1-CG-CD2	5.02	111.12	106.10
2	N	40	LYS	CB-CA-C	5.02	119.27	110.64
1	I	210	ILE	N-CA-CB	5.02	116.99	110.57
1	K	344	TRP	CG-CD2-CE3	-5.02	128.88	133.90
2	L	360	PRO	CA-C-N	5.02	130.20	122.93
2	L	360	PRO	C-N-CA	5.02	130.20	122.93
2	B	113	GLU	N-CA-C	5.02	117.64	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	176	GLN	CA-CB-CG	-5.02	104.07	114.10
2	H	229	ARG	N-CA-CB	-5.02	102.29	110.42
2	H	101	ASN	CA-CB-CG	5.01	117.61	112.60
2	D	32	PRO	N-CA-CB	5.01	108.49	103.48
2	H	163	LYS	N-CA-C	5.01	119.12	113.15
1	I	122	LYS	CB-CG-CD	5.01	122.83	111.30
2	L	352	LYS	CA-C-O	5.01	126.83	121.16
1	M	319	GLY	O-C-N	-5.01	117.84	123.10
1	I	217	LEU	CA-C-N	5.01	131.11	121.54
1	I	217	LEU	C-N-CA	5.01	131.11	121.54
1	M	170	VAL	CA-C-N	5.01	124.92	119.76
1	M	170	VAL	C-N-CA	5.01	124.92	119.76
3	O	248	VAL	CA-C-N	5.01	126.26	120.85
3	O	248	VAL	C-N-CA	5.01	126.26	120.85
1	C	53	GLU	CA-C-O	-5.01	115.71	121.47
1	G	397	TRP	CA-CB-CG	5.01	123.12	113.60
1	M	83	GLN	CG-CD-NE2	5.01	123.92	116.40
1	A	241	ARG	N-CA-CB	5.01	117.93	110.22
1	K	21	TRP	O-C-N	-5.01	114.36	122.42
1	K	162	ARG	O-C-N	-5.01	117.45	123.06
2	L	79	ARG	CD-NE-CZ	5.01	131.41	124.40
2	N	226	ASN	CB-CA-C	5.01	120.45	109.99
1	I	46	ARG	CB-CA-C	5.00	119.13	111.02
3	O	369	LYS	O-C-N	-5.00	115.93	122.59
1	A	143	THR	CA-C-O	-5.00	114.50	120.56
1	C	155	ILE	CA-C-N	5.00	128.69	120.63
1	C	155	ILE	C-N-CA	5.00	128.69	120.63
1	I	15	GLN	OE1-CD-NE2	-5.00	117.60	122.60
1	A	28	HIS	ND1-CE1-NE2	5.00	113.40	108.40
2	B	325	PRO	N-CD-CG	5.00	110.70	103.20
1	E	386	THR	CB-CA-C	5.00	119.09	110.79
2	F	197	HIS	CA-CB-CG	-5.00	108.80	113.80
2	N	267	PHE	CA-CB-CG	5.00	118.80	113.80
3	O	236	PRO	N-CA-CB	5.00	107.98	103.33

There are no chirality outliers.

All (183) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	TYR	Sidechain
1	A	243	PRO	Mainchain
1	A	270	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	A	398	TYR	Sidechain
1	A	408	PHE	Sidechain
1	A	415	MET	Mainchain
1	A	436	PHE	Sidechain
1	A	51	TYR	Sidechain
2	B	170	SER	Peptide
2	B	209	ILE	Mainchain
2	B	210	TYR	Sidechain
2	B	224	TYR	Sidechain
2	B	24	TYR	Sidechain
2	B	249	ASN	Peptide
2	B	302	MET	Peptide,Mainchain
2	B	319	TYR	Sidechain
2	B	357	TYR	Peptide
2	B	375	VAL	Mainchain
2	B	408	TYR	Sidechain
2	B	439	SER	Peptide
2	B	451	TYR	Sidechain
2	B	53	PHE	Sidechain
2	B	68	VAL	Peptide
2	B	70	LEU	Peptide
2	B	83	TYR	Sidechain
1	C	159	TYR	Sidechain
1	C	200	TYR	Sidechain
1	C	222	TYR	Sidechain
1	C	227	HIS	Sidechain
1	C	307	HIS	Sidechain
1	C	340	TYR	Sidechain
1	C	398	TYR	Sidechain
1	C	5	VAL	Peptide
1	C	51	TYR	Peptide,Sidechain
2	D	107	HIS	Sidechain
2	D	124	LYS	Peptide
2	D	185	TYR	Sidechain
2	D	192	HIS	Sidechain
2	D	210	TYR	Sidechain
2	D	245	ASP	Mainchain
2	D	248	LEU	Peptide
2	D	267	PHE	Sidechain
2	D	282	TYR	Sidechain
2	D	293	ASN	Mainchain
2	D	299	ALA	Mainchain

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Mol	Chain	Res	Type	Group
2	D	337	THR	Mainchain
2	D	357	TYR	Sidechain
2	D	404	PHE	Sidechain
2	D	439	SER	Mainchain
2	D	451	TYR	Sidechain
2	D	53	PHE	Sidechain
2	D	83	TYR	Sidechain
1	E	168	SER	Peptide
1	E	36	TYR	Sidechain
1	E	425	TYR	Sidechain
2	F	108	TYR	Sidechain
2	F	139	HIS	Sidechain
2	F	161	TYR	Sidechain
2	F	202	PHE	Sidechain
2	F	24	TYR	Sidechain
2	F	270	ALA	Peptide
2	F	275	VAL	Mainchain
2	F	302	MET	Peptide
2	F	341	ILE	Peptide
2	F	40	LYS	Mainchain
2	F	61	HIS	Sidechain
2	F	88	HIS	Sidechain
1	G	242	PHE	Sidechain
1	G	260	PHE	Sidechain
1	G	264	HIS	Sidechain
1	G	270	PHE	Sidechain
1	G	292	GLN	Mainchain
1	G	310	TYR	Mainchain
1	G	50	TYR	Sidechain
1	G	51	TYR	Sidechain
1	G	59	TYR	Sidechain
2	H	161	TYR	Sidechain
2	H	172	TYR	Sidechain
2	H	185	TYR	Sidechain
2	H	210	TYR	Sidechain
2	H	225	THR	Mainchain
2	H	238	ILE	Mainchain
2	H	24	TYR	Mainchain
2	H	255	PHE	Sidechain
2	H	265	ILE	Peptide
2	H	272	TYR	Sidechain
2	H	312	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	H	341	ILE	Peptide
2	H	351	PHE	Sidechain
2	H	353	VAL	Peptide
2	H	357	TYR	Sidechain
2	H	391	LEU	Mainchain
2	H	418	PHE	Mainchain
2	H	48	SER	Peptide
2	H	49	PHE	Sidechain
2	H	53	PHE	Sidechain
2	H	68	VAL	Peptide
2	H	83	TYR	Sidechain
2	H	87	PHE	Mainchain
1	I	1	MET	Peptide
1	I	20	PHE	Sidechain
1	I	21	TRP	Peptide
1	I	266	PHE	Sidechain
1	I	315	ALA	Mainchain
1	I	36	TYR	Sidechain
1	I	422	TYR	Sidechain
1	I	438	GLU	Mainchain
1	I	85	PHE	Sidechain
2	J	136	LEU	Peptide
2	J	170	SER	Peptide
2	J	172	TYR	Sidechain
2	J	202	PHE	Sidechain
2	J	210	TYR	Sidechain
2	J	255	PHE	Sidechain
2	J	272	TYR	Sidechain
2	J	312	TYR	Sidechain
2	J	319	TYR	Sidechain
2	J	356	ASN	Sidechain
2	J	37	PRO	Peptide
2	J	411	GLU	Peptide
2	J	67	PHE	Mainchain,Sidechain
2	J	68	VAL	Peptide
2	J	92	LEU	Mainchain
1	K	106	TYR	Sidechain
1	K	133	PHE	Sidechain
1	K	159	TYR	Sidechain
1	K	263	LEU	Mainchain
1	K	281	TYR	Sidechain
1	K	301	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	K	347	ASN	Peptide
1	K	36	TYR	Sidechain
1	K	410	GLU	Mainchain
1	K	436	PHE	Sidechain
1	K	51	TYR	Sidechain
1	K	61	PRO	Mainchain
2	L	135	PHE	Sidechain
2	L	141	PHE	Sidechain
2	L	149	PHE	Mainchain
2	L	224	TYR	Sidechain
2	L	266	HIS	Sidechain
2	L	304	LYS	Peptide
2	L	309	HIS	Sidechain
2	L	312	TYR	Sidechain
2	L	399	TYR	Sidechain
2	L	52	PHE	Sidechain
2	L	68	VAL	Peptide
1	M	109	GLY	Mainchain
1	M	128	ASP	Peptide
1	M	183	TYR	Sidechain
1	M	200	TYR	Sidechain
1	M	222	TYR	Sidechain
1	M	227	HIS	Sidechain
1	M	26	ASP	Mainchain
1	M	281	TYR	Sidechain
1	M	309	ARG	Mainchain
1	M	321	MET	Peptide
1	M	340	TYR	Sidechain
1	M	341	PHE	Sidechain
1	M	36	TYR	Sidechain
1	M	422	TYR	Sidechain
1	M	425	TYR	Sidechain
1	M	59	TYR	Sidechain
1	M	92	PHE	Sidechain
2	N	108	TYR	Peptide,Sidechain
2	N	141	PHE	Sidechain
2	N	161	TYR	Sidechain
2	N	185	TYR	Sidechain
2	N	24	TYR	Sidechain
2	N	262	TYR	Sidechain
2	N	283	HIS	Peptide
2	N	36	MET	Peptide

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Mol	Chain	Res	Type	Group
2	N	53	PHE	Mainchain
2	N	67	PHE	Sidechain
2	N	68	VAL	Peptide
2	N	8	HIS	Sidechain
3	O	262	SER	Mainchain
3	O	277	ILE	Peptide
3	O	278	ILE	Mainchain
3	O	308	ILE	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3498	0	3342	11	0
1	C	3498	0	3342	18	0
1	E	3498	0	3342	12	0
1	G	3498	0	3342	12	0
1	I	3498	0	3342	19	0
1	K	3498	0	3342	19	0
1	M	3498	0	3342	12	0
2	B	3524	0	3409	6	0
2	D	3524	0	3409	20	0
2	F	3524	0	3409	7	0
2	H	3524	0	3409	12	0
2	J	3524	0	3409	17	0
2	L	3524	0	3409	17	0
2	N	3524	0	3409	8	0
3	O	1455	0	1526	5	0
4	A	28	0	12	0	0
4	C	28	0	12	0	0
4	E	28	0	12	0	0
4	G	28	0	12	0	0
4	I	28	0	12	0	0
4	K	28	0	12	0	0
4	M	28	0	12	0	0
5	B	32	0	12	1	0
5	D	32	0	12	0	0
5	F	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	32	0	12	1	0
5	J	32	0	12	0	0
5	L	32	0	12	1	0
5	N	32	0	12	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
6	L	1	0	0	0	0
6	N	1	0	0	0	0
All	All	51036	0	48951	184	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 2.

All (184) 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)
3:O:375:LYS:CB	3:O:376:LEU:HA	2.26	0.65
1:K:187:LEU:HD22	1:K:403:MET:HE1	1.79	0.64
1:I:257:MET:HE3	1:I:266:PHE:CE1	2.33	0.63
1:K:155:ILE:HG22	1:K:164:MET:HE1	1.82	0.62
2:L:133:GLN:HE22	2:L:242:LEU:HD21	1.65	0.62
1:M:161:ASP:CG	1:M:162:ARG:HH21	2.09	0.61
2:J:326:LYS:HE3	1:K:212:PHE:CD1	2.38	0.58
2:D:319:TYR:CE1	2:D:328:VAL:HG13	2.39	0.58
1:G:187:LEU:HD22	1:G:403:MET:HE1	1.85	0.58
1:I:257:MET:HE3	1:I:266:PHE:CD1	2.38	0.58
2:J:326:LYS:HE3	1:K:212:PHE:CG	2.39	0.57
1:A:321:MET:HE1	1:A:363:MET:HB2	1.85	0.57
1:K:20:PHE:O	1:K:24:ILE:HG22	2.05	0.57
2:D:203:MET:HE1	2:D:388:TRP:HZ2	1.69	0.57
2:H:319:TYR:CD2	2:H:375:VAL:HG22	2.39	0.57
2:D:203:MET:HE1	2:D:388:TRP:CZ2	2.39	0.57
1:I:239:CYS:CB	1:I:248:ALA:H	2.19	0.55
2:L:203:MET:HE3	2:L:267:PHE:CD1	2.41	0.55
1:C:344:TRP:HE1	1:C:428:ALA:HB3	1.71	0.55
2:D:346:TRP:CE3	1:E:391:ARG:NH2	2.74	0.55
2:L:413:MET:HG2	2:L:414:GLU:H	1.72	0.55
1:M:167:PHE:CZ	1:M:200:TYR:CE1	2.96	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:402:ARG:HH11	2:N:402:ARG:HG2	1.73	0.54
1:G:12:CYS:SG	1:G:169:VAL:HG21	2.47	0.54
1:I:170:VAL:HG21	1:I:377:LEU:HD21	1.90	0.54
1:M:77:ARG:HH22	1:M:90:PHE:HB3	1.73	0.54
1:I:161:ASP:CG	1:I:162:ARG:HH21	2.16	0.53
1:I:361:LEU:HD12	1:I:362:LYS:H	1.73	0.53
2:L:137:VAL:HG21	2:L:154:MET:CE	2.38	0.53
1:C:344:TRP:HE1	1:C:428:ALA:CB	2.22	0.53
2:J:174:ALA:HB1	2:J:207:GLU:HB2	1.90	0.52
1:K:252:LYS:HE2	5:L:501:GTP:O1G	2.09	0.52
1:C:232:THR:HG23	1:C:366:THR:CG2	2.39	0.52
1:M:20:PHE:O	1:M:24:ILE:HG22	2.09	0.52
1:K:368:ILE:HD12	1:K:368:ILE:N	2.26	0.51
1:I:2:ARG:HH11	2:J:97:GLU:HA	1.75	0.51
1:C:192:LEU:HD21	1:C:199:THR:HG21	1.93	0.51
1:K:7:ILE:HD13	1:K:151:LEU:HD21	1.92	0.51
1:E:187:LEU:HD22	1:E:403:MET:HE1	1.92	0.51
2:H:328:VAL:HG11	2:H:353:VAL:HG11	1.93	0.51
1:M:257:MET:SD	1:M:314:ALA:HB2	2.51	0.51
1:C:310:TYR:CD1	1:C:371:SER:HB2	2.46	0.51
1:G:344:TRP:CG	2:H:401:LYS:HE2	2.46	0.50
3:O:375:LYS:HB2	3:O:376:LEU:HA	1.93	0.50
1:E:19:LYS:HE2	1:E:227:HIS:HB2	1.94	0.50
2:J:344:VAL:HG21	2:J:346:TRP:CZ3	2.47	0.50
2:N:46:ASP:HA	2:N:47:ASP:C	2.37	0.50
1:C:101:TRP:HE1	1:C:188:SER:HB3	1.76	0.49
2:N:71:GLU:HG3	2:N:74:VAL:H	1.78	0.49
2:J:74:VAL:HG13	2:J:75:ILE:HG13	1.94	0.49
2:J:220:GLU:C	2:J:222:PRO:HD3	2.38	0.49
2:F:201:ALA:HB3	2:F:267:PHE:CD1	2.48	0.49
3:O:375:LYS:HB3	3:O:376:LEU:HA	1.93	0.49
2:J:319:TYR:CD2	2:J:375:VAL:HG22	2.48	0.49
2:L:133:GLN:HE22	2:L:242:LEU:CD2	2.25	0.49
1:M:121:ARG:HH21	1:M:158:GLU:CD	2.21	0.49
2:H:224:TYR:CE2	5:H:501:GTP:C5	3.01	0.48
2:L:132:LEU:O	2:L:164:LYS:HE3	2.13	0.48
1:K:242:PHE:HB3	1:K:356:ILE:HD13	1.95	0.48
2:L:137:VAL:HG21	2:L:154:MET:HE2	1.95	0.48
2:L:387:ALA:HB2	2:L:390:ARG:NH2	2.29	0.48
1:C:345:ILE:HG23	2:D:398:MET:HE2	1.96	0.48
2:L:385:ALA:HB2	2:L:432:TYR:CG	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:257:MET:HE1	1:I:369:GLY:HA2	1.95	0.47
1:G:344:TRP:CD1	1:G:344:TRP:H	2.33	0.47
1:I:42:LEU:HD12	1:I:42:LEU:H	1.79	0.47
1:M:2:ARG:H	1:M:3:GLU:CD	2.22	0.47
1:M:368:ILE:HD12	1:M:368:ILE:N	2.29	0.47
1:G:284:LEU:HG	1:G:363:MET:HG2	1.96	0.47
1:K:204:ASN:O	1:K:208:TYR:CD1	2.68	0.47
1:C:32:PRO:HA	1:C:81:PHE:CD1	2.49	0.47
1:E:236:VAL:HG13	1:E:237:THR:HG23	1.96	0.46
1:A:135:LEU:CD2	1:A:152:ILE:HD11	2.45	0.46
1:A:252:LYS:HE2	5:B:501:GTP:O1G	2.16	0.46
1:A:179:VAL:HG23	1:A:180:VAL:HG13	1.96	0.46
2:J:352:LYS:HE3	2:J:353:VAL:H	1.80	0.46
2:N:139:HIS:CE1	2:N:170:SER:HB3	2.50	0.46
1:C:46:ARG:HD2	2:D:73:THR:HG22	1.98	0.46
1:G:36:TYR:C	1:G:36:TYR:CD2	2.93	0.46
1:G:199:THR:HG21	1:G:265:PHE:CE2	2.51	0.46
2:D:174:ALA:HB3	2:D:177:VAL:O	2.16	0.46
2:B:399:TYR:CE1	2:B:418:PHE:HB3	2.51	0.45
1:C:131:GLN:HE22	1:C:249:ASP:CG	2.24	0.45
2:D:90:GLU:HB2	2:D:121:ARG:NH1	2.31	0.45
2:L:354:GLY:C	2:L:355:ILE:HD12	2.41	0.45
1:A:290:THR:HG21	1:A:329:GLN:HB3	1.97	0.45
2:F:76:ASP:HA	2:F:79:ARG:HD2	1.98	0.45
1:I:309:ARG:NH2	1:I:427:ASP:HA	2.31	0.45
2:N:319:TYR:CD2	2:N:375:VAL:HG22	2.51	0.45
1:A:303:CYS:SG	1:A:374:ILE:HA	2.56	0.45
1:I:323:MET:SD	1:I:353:VAL:HG21	2.56	0.45
1:C:323:MET:HG3	2:D:224:TYR:CG	2.52	0.45
1:E:317:PHE:CD2	1:E:365:ALA:HB2	2.51	0.45
2:D:210:TYR:CE1	2:D:227:LEU:HD11	2.52	0.45
2:F:229:ARG:NH2	2:F:363:VAL:HB	2.31	0.45
1:K:286:VAL:HB	1:K:287:PRO:HD3	1.98	0.45
1:I:228:LEU:O	1:I:231:ALA:HB3	2.17	0.45
1:E:163:ILE:H	1:E:163:ILE:HD12	1.81	0.44
1:G:284:LEU:HG	1:G:363:MET:CG	2.48	0.44
2:L:390:ARG:O	2:L:394:LYS:HE3	2.17	0.44
2:N:175:PRO:HA	2:N:390:ARG:NH1	2.32	0.44
1:M:101:TRP:NE1	1:M:146:GLY:HA2	2.33	0.44
1:A:309:ARG:NH1	1:A:339:SER:O	2.45	0.44
2:L:172:TYR:CD2	2:L:173:PRO:HD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:368:ILE:N	1:G:368:ILE:HD12	2.33	0.44
2:H:47:ASP:HB3	2:H:49:PHE:CE2	2.53	0.44
1:A:264:HIS:HD1	1:A:264:HIS:H	1.63	0.44
2:F:204:VAL:HG12	2:F:302:MET:HB3	2.00	0.44
1:M:167:PHE:CZ	1:M:200:TYR:CD1	3.06	0.44
1:M:187:LEU:HD22	1:M:403:MET:HE1	1.99	0.44
1:A:65:LEU:HD22	1:A:90:PHE:CE2	2.53	0.43
2:H:71:GLU:CD	2:H:72:PRO:HD2	2.43	0.43
2:H:417:GLU:HA	2:H:420:GLU:HB3	2.00	0.43
2:L:138:PHE:CD2	2:L:169:PHE:HB2	2.53	0.43
1:E:259:PRO:HG2	1:E:263:LEU:HD23	1.99	0.43
2:J:79:ARG:HH12	2:J:94:THR:HG21	1.82	0.43
1:C:219:THR:N	1:C:220:PRO:CD	2.80	0.43
2:B:296:PHE:HA	2:B:377:MET:HE1	2.01	0.43
2:B:319:TYR:CE1	2:B:328:VAL:HG13	2.53	0.43
2:L:46:ASP:HA	2:L:47:ASP:HB2	2.00	0.43
1:C:178:THR:HG22	1:C:180:VAL:H	1.83	0.43
2:J:205:ASP:HB3	2:J:303:VAL:HA	1.99	0.43
1:C:105:HIS:CD2	1:C:106:TYR:CE2	3.07	0.43
2:D:69:ASP:HA	2:D:145:THR:HG21	2.00	0.43
1:G:413:SER:HA	3:O:302:GLY:C	2.44	0.43
1:I:367:PHE:CD2	1:I:367:PHE:C	2.96	0.43
1:K:14:ASN:OD1	1:K:73:MET:HE1	2.19	0.43
1:K:238:THR:HG22	1:K:354:CYS:SG	2.59	0.43
1:M:36:TYR:CE1	1:M:38:GLY:HA3	2.54	0.42
2:H:336:LYS:HE3	2:H:348:PRO:O	2.18	0.42
1:E:385:PHE:CE2	1:E:412:GLU:HB2	2.55	0.42
2:F:69:ASP:C	2:F:71:GLU:H	2.28	0.42
2:N:11:GLN:HG2	2:N:15:GLN:HE21	1.84	0.42
1:C:122:LYS:HE3	1:C:126:SER:OG	2.19	0.42
2:J:79:ARG:NH1	2:J:94:THR:HG21	2.34	0.42
2:J:192:HIS:CG	2:J:421:ALA:HA	2.54	0.42
1:A:30:ILE:HD13	1:A:51:TYR:CZ	2.55	0.42
1:E:9:ALA:HA	1:E:66:VAL:O	2.20	0.42
2:F:231:ILE:HD13	2:F:231:ILE:HG21	1.78	0.42
2:D:297:GLU:HA	2:D:298:PRO:HD3	1.89	0.42
1:I:170:VAL:HG21	1:I:377:LEU:CD2	2.49	0.42
1:K:264:HIS:HA	1:K:266:PHE:CZ	2.54	0.42
1:E:68:LEU:HD21	1:E:109:GLY:HA2	2.01	0.42
1:I:119:VAL:HA	1:I:122:LYS:HE3	2.02	0.42
1:K:9:ALA:HA	1:K:66:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:ILE:CD1	2:D:53:PHE:CZ	3.03	0.42
2:D:120:ASP:OD1	2:D:124:LYS:NZ	2.50	0.42
2:J:313:MET:HE1	2:J:435:VAL:HG21	2.02	0.42
2:B:120:ASP:OD1	2:B:124:LYS:HE3	2.19	0.42
2:B:319:TYR:CZ	2:B:328:VAL:HG13	2.55	0.42
2:D:353:VAL:HG22	1:E:177:ASP:HA	2.02	0.42
1:G:137:HIS:CE1	1:G:168:SER:HB3	2.55	0.42
2:H:306:ASP:HA	2:H:307:PRO:HD3	1.88	0.42
1:K:101:TRP:CE3	1:K:187:LEU:HD13	2.54	0.42
1:K:158:GLU:HB3	1:K:159:TYR:CD2	2.55	0.42
2:L:201:ALA:HB3	2:L:267:PHE:CD1	2.55	0.41
2:D:91:GLN:HE22	2:D:125:LEU:HD21	1.84	0.41
2:D:174:ALA:HB1	2:D:207:GLU:HB2	2.02	0.41
2:D:261:PRO:C	2:D:262:TYR:CD1	2.98	0.41
2:J:395:PHE:CD2	2:J:395:PHE:C	2.98	0.41
2:N:11:GLN:CG	2:N:15:GLN:HE21	2.33	0.41
1:I:239:CYS:HB2	1:I:248:ALA:H	1.84	0.41
1:K:267:MET:SD	1:K:301:ALA:HB3	2.60	0.41
3:O:295:ASP:O	3:O:298:LYS:HE2	2.21	0.41
1:I:2:ARG:HH22	2:J:71:GLU:CD	2.28	0.41
2:L:352:LYS:HD3	2:L:353:VAL:H	1.86	0.41
2:F:273:ALA:HB1	2:F:274:PRO:HA	2.03	0.41
2:D:53:PHE:HA	2:D:63:PRO:HA	2.02	0.41
1:E:357:PRO:HB2	1:E:358:PRO:HD2	2.02	0.41
2:H:20:CYS:SG	2:H:235:VAL:HG21	2.61	0.41
2:H:174:ALA:HB3	2:H:177:VAL:O	2.21	0.41
1:C:257:MET:HE3	1:C:257:MET:HB3	1.98	0.41
2:H:392:ASP:CG	2:H:422:ARG:HH22	2.29	0.41
1:I:89:ASN:HA	1:I:119:VAL:HG11	2.03	0.41
1:K:290:THR:HG21	1:K:329:GLN:HB3	2.02	0.41
2:L:137:VAL:HG21	2:L:154:MET:HE1	2.01	0.41
1:I:258:VAL:HA	1:I:259:PRO:HD2	1.92	0.40
2:B:7:ILE:HD13	2:B:7:ILE:HG21	1.90	0.40
1:C:317:PHE:CD1	1:C:317:PHE:N	2.89	0.40
2:J:313:MET:HE3	2:J:380:ASN:OD1	2.22	0.40
1:A:385:PHE:C	1:A:385:PHE:CD2	2.99	0.40
1:C:1:MET:HA	1:C:128:ASP:OD2	2.21	0.40
2:D:154:MET:HE1	2:D:166:LYS:HB3	2.04	0.40
1:G:372:THR:HG21	1:G:426:GLN:HA	2.03	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	443/445 (100%)	413 (93%)	26 (6%)	4 (1%)	14	49
1	C	443/445 (100%)	405 (91%)	35 (8%)	3 (1%)	18	55
1	E	443/445 (100%)	414 (94%)	21 (5%)	8 (2%)	6	35
1	G	443/445 (100%)	416 (94%)	24 (5%)	3 (1%)	18	55
1	I	443/445 (100%)	405 (91%)	32 (7%)	6 (1%)	9	39
1	K	443/445 (100%)	411 (93%)	28 (6%)	4 (1%)	14	49
1	M	443/445 (100%)	404 (91%)	37 (8%)	2 (0%)	24	61
2	B	449/451 (100%)	413 (92%)	36 (8%)	0	100	100
2	D	449/451 (100%)	414 (92%)	28 (6%)	7 (2%)	7	37
2	F	449/451 (100%)	413 (92%)	33 (7%)	3 (1%)	18	55
2	H	449/451 (100%)	420 (94%)	26 (6%)	3 (1%)	18	55
2	J	449/451 (100%)	420 (94%)	27 (6%)	2 (0%)	30	65
2	L	449/451 (100%)	404 (90%)	43 (10%)	2 (0%)	30	65
2	N	449/451 (100%)	418 (93%)	26 (6%)	5 (1%)	11	44
3	O	192/194 (99%)	166 (86%)	21 (11%)	5 (3%)	4	28
All	All	6436/6466 (100%)	5936 (92%)	443 (7%)	57 (1%)	16	49

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	394	PHE
2	D	281	ALA
2	D	439	SER
1	E	394	PHE
1	G	81	PHE
2	L	404	PHE
1	M	347	ASN
1	A	96	GLY

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Mol	Chain	Res	Type
2	D	402	ARG
1	E	48	ASN
1	E	427	ASP
1	G	348	ASN
2	H	68	VAL
1	I	55	ALA
1	K	81	PHE
1	M	427	ASP
3	O	208	SER
3	O	350	VAL
2	D	141	PHE
1	E	95	SER
1	E	430	ALA
2	F	404	PHE
2	F	416	GLY
1	G	71	GLY
1	I	48	ASN
1	I	81	PHE
1	I	348	ASN
1	K	82	GLY
2	L	286	LEU
2	N	218	ASP
1	A	347	ASN
1	A	443	ASP
1	E	347	ASN
2	H	439	SER
1	I	347	ASN
1	K	95	SER
2	N	43	GLY
3	O	254	LYS
3	O	292	GLY
1	I	394	PHE
2	J	267	PHE
2	J	365	GLY
2	N	220	GLU
1	A	402	GLY
1	C	130	LEU
1	E	296	ALA
1	K	104	GLY
1	C	96	GLY
2	D	348	PRO
1	E	173	PRO

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Mol	Chain	Res	Type
2	F	267	PHE
2	H	275	VAL
2	N	32	PRO
2	D	265	ILE
2	D	350	GLY
2	N	175	PRO
3	O	226	VAL

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	381/381 (100%)	370 (97%)	11 (3%)	37	58
1	C	381/381 (100%)	374 (98%)	7 (2%)	51	67
1	E	381/381 (100%)	372 (98%)	9 (2%)	43	63
1	G	381/381 (100%)	367 (96%)	14 (4%)	30	52
1	I	381/381 (100%)	376 (99%)	5 (1%)	61	72
1	K	381/381 (100%)	374 (98%)	7 (2%)	51	67
1	M	381/381 (100%)	369 (97%)	12 (3%)	35	56
2	B	379/379 (100%)	367 (97%)	12 (3%)	34	56
2	D	379/379 (100%)	356 (94%)	23 (6%)	17	41
2	F	379/379 (100%)	369 (97%)	10 (3%)	40	61
2	H	379/379 (100%)	359 (95%)	20 (5%)	20	44
2	J	379/379 (100%)	367 (97%)	12 (3%)	34	56
2	L	379/379 (100%)	360 (95%)	19 (5%)	22	45
2	N	379/379 (100%)	368 (97%)	11 (3%)	37	58
3	O	168/168 (100%)	155 (92%)	13 (8%)	12	34
All	All	5488/5488 (100%)	5303 (97%)	185 (3%)	33	55

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	44	LEU
1	A	50	TYR
1	A	60	VAL
1	A	133	PHE
1	A	147	MET
1	A	168	SER
1	A	253	LEU
1	A	329	GLN
1	A	366	THR
1	A	412	GLU
2	B	2	ARG
2	B	194	THR
2	B	206	ASN
2	B	253	THR
2	B	265	ILE
2	B	304	LYS
2	B	329	ASN
2	B	361	THR
2	B	371	VAL
2	B	379	SER
2	B	386	GLU
2	B	439	SER
1	C	22	GLU
1	C	47	ILE
1	C	222	TYR
1	C	225	LEU
1	C	252	LYS
1	C	260	PHE
1	C	391	ARG
2	D	9	VAL
2	D	48	SER
2	D	53	PHE
2	D	66	VAL
2	D	89	PRO
2	D	103	TYR
2	D	110	ILE
2	D	121	ARG
2	D	141	PHE
2	D	150	THR
2	D	160	ASP
2	D	173	PRO
2	D	192	HIS

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Mol	Chain	Res	Type
2	D	224	TYR
2	D	236	SER
2	D	244	PHE
2	D	266	HIS
2	D	275	VAL
2	D	326	LYS
2	D	376	CYS
2	D	378	LEU
2	D	392	ASP
2	D	432	TYR
1	E	70	PRO
1	E	91	VAL
1	E	168	SER
1	E	175	VAL
1	E	178	THR
1	E	188	SER
1	E	324	LYS
1	E	382	SER
1	E	442	GLU
2	F	52	PHE
2	F	68	VAL
2	F	110	ILE
2	F	112	LYS
2	F	194	THR
2	F	200	CYS
2	F	276	ILE
2	F	295	CYS
2	F	298	PRO
2	F	326	LYS
1	G	4	ILE
1	G	11	GLN
1	G	47	ILE
1	G	50	TYR
1	G	64	ILE
1	G	84	ILE
1	G	174	LYS
1	G	188	SER
1	G	199	THR
1	G	329	GLN
1	G	342	VAL
1	G	368	ILE
1	G	395	LEU

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Mol	Chain	Res	Type
1	G	438	GLU
2	H	9	VAL
2	H	42	ILE
2	H	49	PHE
2	H	51	THR
2	H	74	VAL
2	H	98	ASP
2	H	140	SER
2	H	160	ASP
2	H	194	THR
2	H	216	ASN
2	H	244	PHE
2	H	245	ASP
2	H	253	THR
2	H	266	HIS
2	H	271	THR
2	H	340	SER
2	H	353	VAL
2	H	386	GLU
2	H	388	TRP
2	H	450	GLU
1	I	47	ILE
1	I	68	LEU
1	I	217	LEU
1	I	299	MET
1	I	415	MET
2	J	27	GLU
2	J	37	PRO
2	J	166	LYS
2	J	179	THR
2	J	200	CYS
2	J	217	LEU
2	J	227	LEU
2	J	276	ILE
2	J	346	TRP
2	J	352	LYS
2	J	379	SER
2	J	446	GLU
1	K	4	ILE
1	K	163	ILE
1	K	178	THR
1	K	291	GLN

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Mol	Chain	Res	Type
1	K	355	ASP
1	K	366	THR
1	K	368	ILE
2	L	9	VAL
2	L	36	MET
2	L	46	ASP
2	L	50	ASN
2	L	71	GLU
2	L	179	THR
2	L	194	THR
2	L	209	ILE
2	L	253	THR
2	L	257	THR
2	L	266	HIS
2	L	303	VAL
2	L	307	PRO
2	L	325	PRO
2	L	326	LYS
2	L	346	TRP
2	L	352	LYS
2	L	353	VAL
2	L	381	THR
1	M	8	GLN
1	M	15	GLN
1	M	84	ILE
1	M	117	LEU
1	M	168	SER
1	M	178	THR
1	M	240	LEU
1	M	284	LEU
1	M	329	GLN
1	M	366	THR
1	M	368	ILE
1	M	423	GLN
2	N	110	ILE
2	N	207	GLU
2	N	252	LEU
2	N	266	HIS
2	N	276	ILE
2	N	357	TYR
2	N	362	VAL
2	N	378	LEU

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Mol	Chain	Res	Type
2	N	381	THR
2	N	391	LEU
2	N	422	ARG
3	O	220	THR
3	O	226	VAL
3	O	237	SER
3	O	250	MET
3	O	265	ASN
3	O	289	SER
3	O	313	VAL
3	O	328	ILE
3	O	338	GLU
3	O	342	GLU
3	O	378	PHE
3	O	388	HIS
3	O	393	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	184	ASN
1	A	334	GLN
1	A	335	ASN
1	A	347	ASN
1	A	375	GLN
1	A	433	GLN
2	B	8	HIS
2	B	206	ASN
2	B	216	ASN
2	B	249	ASN
2	B	283	HIS
2	B	309	HIS
2	B	406	HIS
1	C	6	HIS
1	C	8	GLN
1	C	134	GLN
1	C	247	ASN
2	D	31	GLN
2	D	133	GLN
2	D	216	ASN
2	D	256	GLN

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Mol	Chain	Res	Type
2	D	266	HIS
2	D	329	ASN
2	D	406	HIS
1	E	8	GLN
1	E	14	ASN
1	E	291	GLN
1	E	329	GLN
1	E	347	ASN
1	E	348	ASN
1	E	375	GLN
1	E	424	GLN
2	F	249	ASN
2	F	300	ASN
2	F	356	ASN
2	F	393	HIS
1	G	8	GLN
1	G	14	ASN
1	G	37	HIS
1	G	105	HIS
1	G	165	ASN
1	G	190	HIS
1	G	245	GLN
1	G	247	ASN
1	G	298	ASN
1	G	332	ASN
1	G	334	GLN
1	G	375	GLN
1	G	384	GLN
1	G	414	ASN
2	H	15	GLN
2	H	61	HIS
2	H	91	GLN
2	H	128	GLN
2	H	186	ASN
2	H	309	HIS
1	I	191	GLN
1	I	307	HIS
1	I	329	GLN
1	I	384	GLN
2	J	18	ASN
2	J	61	HIS
2	J	85	GLN

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Mol	Chain	Res	Type
2	J	128	GLN
2	J	192	HIS
2	J	216	ASN
1	K	165	ASN
1	K	280	GLN
1	K	291	GLN
1	K	329	GLN
2	L	8	HIS
2	L	133	GLN
2	L	258	ASN
2	L	266	HIS
2	L	342	GLN
1	M	6	HIS
1	M	227	HIS
1	M	347	ASN
1	M	384	GLN
2	N	15	GLN
2	N	226	ASN
2	N	258	ASN
2	N	300	ASN
2	N	309	HIS
3	O	244	GLN
3	O	265	ASN
3	O	299	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](#)

Of 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	B	501	6	33,34,34	0.90	1 (3%)	50,54,54	1.53	8 (16%)
5	GTP	D	501	6	33,34,34	0.92	1 (3%)	50,54,54	1.22	5 (10%)
5	GTP	H	501	6	33,34,34	0.86	0	50,54,54	1.38	9 (18%)
4	GDP	A	501	-	29,30,30	0.81	0	45,47,47	1.43	8 (17%)
5	GTP	J	501	6	33,34,34	0.97	1 (3%)	50,54,54	1.29	5 (10%)
4	GDP	E	501	-	29,30,30	0.84	1 (3%)	45,47,47	1.43	7 (15%)
4	GDP	M	501	-	29,30,30	0.82	0	45,47,47	1.34	3 (6%)
4	GDP	C	501	-	29,30,30	0.83	1 (3%)	45,47,47	1.37	5 (11%)
5	GTP	L	501	6	33,34,34	0.94	1 (3%)	50,54,54	1.16	4 (8%)
5	GTP	N	501	6	33,34,34	0.99	2 (6%)	50,54,54	1.64	10 (20%)
5	GTP	F	501	6	33,34,34	1.03	2 (6%)	50,54,54	1.49	7 (14%)
4	GDP	I	501	-	29,30,30	0.79	0	45,47,47	1.39	6 (13%)
4	GDP	G	501	-	29,30,30	0.81	0	45,47,47	1.37	6 (13%)
4	GDP	K	501	-	29,30,30	0.74	0	45,47,47	1.37	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	B	501	6	-	5/22/38/38	0/3/3/3
5	GTP	D	501	6	-	4/22/38/38	0/3/3/3
5	GTP	H	501	6	-	6/22/38/38	0/3/3/3
4	GDP	A	501	-	-	5/16/32/32	0/3/3/3
5	GTP	J	501	6	-	9/22/38/38	0/3/3/3
4	GDP	E	501	-	-	5/16/32/32	0/3/3/3
4	GDP	M	501	-	-	2/16/32/32	0/3/3/3
4	GDP	C	501	-	-	2/16/32/32	0/3/3/3
5	GTP	L	501	6	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	N	501	6	-	4/22/38/38	0/3/3/3
5	GTP	F	501	6	-	2/22/38/38	0/3/3/3
4	GDP	I	501	-	-	4/16/32/32	0/3/3/3
4	GDP	G	501	-	-	2/16/32/32	0/3/3/3
4	GDP	K	501	-	-	2/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	GTP	PB-O3A	2.66	1.62	1.59
5	F	501	GTP	PB-O3B	2.52	1.62	1.59
5	J	501	GTP	PB-O3A	2.47	1.62	1.59
5	N	501	GTP	PB-O3A	2.39	1.62	1.59
5	F	501	GTP	PA-O3A	2.20	1.61	1.59
4	C	501	GDP	PA-O3A	2.14	1.61	1.59
5	L	501	GTP	PB-O3A	2.13	1.61	1.59
5	B	501	GTP	PA-O3A	2.10	1.61	1.59
5	N	501	GTP	PB-O3B	2.04	1.61	1.59
4	E	501	GDP	PA-O3A	2.02	1.61	1.59

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	501	GDP	N2-C2-N3	-4.82	110.26	119.67
5	B	501	GTP	O4'-C1'-N9	4.57	118.72	108.36
5	N	501	GTP	N2-C2-N1	4.23	125.69	116.76
5	B	501	GTP	O6-C6-N1	-4.15	112.30	120.11
4	K	501	GDP	C2'-C3'-C4'	-4.05	94.77	102.61
5	N	501	GTP	N2-C2-N3	-4.05	111.76	119.67
4	I	501	GDP	O2A-PA-O3A	3.83	117.61	107.27
4	A	501	GDP	N9-C8-N7	3.74	120.34	113.40
5	F	501	GTP	C3'-C2'-C1'	3.74	108.54	101.46
4	C	501	GDP	O2A-PA-O3A	3.63	117.10	107.27
5	F	501	GTP	O5'-C5'-C4'	3.56	121.12	108.99
5	B	501	GTP	O2G-PG-O1G	3.51	124.52	110.83
5	J	501	GTP	O6-C6-N1	-3.44	113.65	120.11
4	A	501	GDP	C8-N9-C4	-3.27	99.90	106.03
5	N	501	GTP	O3A-PB-O1B	-3.25	100.93	110.70
4	E	501	GDP	O2A-PA-O3A	3.25	116.05	107.27
4	E	501	GDP	N2-C2-N1	3.23	123.58	116.76
4	M	501	GDP	C1'-N9-C8	3.21	135.86	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	501	GTP	C2'-C3'-C4'	3.12	108.63	102.61
5	J	501	GTP	C2-N1-C6	-3.09	119.50	125.11
5	F	501	GTP	O4'-C1'-N9	3.01	115.17	108.36
5	F	501	GTP	O2G-PG-O1G	2.98	122.46	110.83
4	I	501	GDP	O4'-C4'-C3'	2.94	111.00	105.15
5	N	501	GTP	O3G-PG-O1G	2.94	122.28	110.83
4	I	501	GDP	C2-N3-C4	-2.90	107.30	112.30
4	G	501	GDP	O6-C6-N1	-2.86	114.73	120.11
4	A	501	GDP	C8-N7-C5	-2.82	99.24	104.26
4	G	501	GDP	C6-C5-N7	2.81	135.41	130.29
4	G	501	GDP	C2-N1-C6	-2.79	120.05	125.11
5	D	501	GTP	O4'-C4'-C3'	2.74	110.59	105.15
4	I	501	GDP	O3A-PA-O1A	-2.73	102.49	110.70
4	G	501	GDP	O2'-C2'-C3'	2.73	120.55	111.82
4	C	501	GDP	O4'-C1'-N9	2.70	114.47	108.36
5	B	501	GTP	O5'-C5'-C4'	2.68	118.12	108.99
5	N	501	GTP	C3'-C2'-C1'	2.67	106.52	101.46
4	C	501	GDP	O3B-PB-O2B	2.66	117.78	107.80
5	B	501	GTP	C2-N1-C6	-2.66	120.29	125.11
5	N	501	GTP	N9-C8-N7	-2.65	108.49	113.40
5	L	501	GTP	O3'-C3'-C4'	2.64	118.67	111.08
5	D	501	GTP	O5'-C5'-C4'	2.61	117.87	108.99
5	B	501	GTP	C2'-C3'-C4'	-2.59	97.61	102.61
5	H	501	GTP	O3A-PA-O1A	-2.57	102.96	110.70
4	M	501	GDP	O2A-PA-O3A	2.53	114.12	107.27
5	H	501	GTP	O4'-C1'-N9	2.51	114.05	108.36
4	E	501	GDP	O3B-PB-O2B	2.43	116.92	107.80
5	F	501	GTP	C2'-C3'-C4'	-2.41	97.96	102.61
4	K	501	GDP	O4'-C4'-C3'	2.40	109.93	105.15
5	D	501	GTP	C2'-C1'-N9	2.40	119.94	113.25
4	G	501	GDP	C4-C5-N7	-2.39	106.88	110.67
5	N	501	GTP	O4'-C4'-C3'	2.39	109.90	105.15
4	K	501	GDP	C4-C5-N7	-2.37	106.91	110.67
5	L	501	GTP	O4'-C1'-N9	2.35	113.68	108.36
5	D	501	GTP	O2G-PG-O1G	2.33	119.90	110.83
5	N	501	GTP	C6-C5-N7	2.32	134.51	130.29
5	J	501	GTP	O3B-PG-O1G	-2.31	98.88	111.04
4	A	501	GDP	O6-C6-C5	2.30	132.61	126.53
4	I	501	GDP	N1-C2-N3	2.30	127.53	123.32
5	D	501	GTP	C1'-N9-C8	2.29	133.25	126.73
4	G	501	GDP	O3B-PB-O3A	2.28	112.28	104.64
4	C	501	GDP	O5'-PA-O1A	-2.28	99.91	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	501	GTP	O2B-PB-O3A	2.28	113.42	107.27
4	A	501	GDP	O6-C6-N1	-2.27	115.84	120.11
4	A	501	GDP	O5'-PA-O1A	-2.23	100.09	108.94
4	E	501	GDP	C2-N1-C6	-2.23	121.06	125.11
5	F	501	GTP	O3A-PA-O1A	2.23	117.40	110.70
5	B	501	GTP	O3G-PG-O3B	-2.22	97.18	104.64
5	H	501	GTP	O3A-PB-O1B	2.22	117.39	110.70
5	H	501	GTP	O3G-PG-O1G	2.22	119.49	110.83
4	K	501	GDP	O2B-PB-O3A	2.22	112.08	104.64
5	H	501	GTP	O3B-PB-O1B	-2.22	104.03	110.70
4	K	501	GDP	O5'-PA-O1A	-2.20	100.22	108.94
4	K	501	GDP	O2A-PA-O1A	2.18	122.57	112.44
4	E	501	GDP	O2A-PA-O1A	2.17	122.55	112.44
5	L	501	GTP	O2A-PA-O1A	2.15	122.44	112.44
4	M	501	GDP	O3B-PB-O2B	2.12	115.77	107.80
5	B	501	GTP	O3B-PG-O1G	-2.12	99.90	111.04
5	F	501	GTP	O3G-PG-O1G	2.12	119.08	110.83
4	E	501	GDP	O6-C6-N1	-2.11	116.14	120.11
4	C	501	GDP	O3A-PB-O1B	-2.11	99.95	111.04
5	H	501	GTP	C8-N7-C5	-2.09	100.54	104.26
5	N	501	GTP	C5'-C4'-C3'	-2.08	107.74	115.21
5	H	501	GTP	O2A-PA-O3A	2.07	112.87	107.27
5	J	501	GTP	O3B-PB-O1B	-2.07	104.48	110.70
5	J	501	GTP	O2'-C2'-C1'	2.07	117.22	110.10
4	A	501	GDP	O3A-PB-O1B	-2.04	100.30	111.04
4	I	501	GDP	C2'-C3'-C4'	-2.02	98.71	102.61
5	L	501	GTP	O2G-PG-O3B	-2.01	97.89	104.64
5	N	501	GTP	C8-N9-C4	2.01	109.78	106.03
4	A	501	GDP	O2A-PA-O1A	2.00	121.75	112.44

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GDP	PA-O3A-PB-O2B
4	E	501	GDP	C5'-O5'-PA-O3A
4	E	501	GDP	C5'-O5'-PA-O2A
4	I	501	GDP	PA-O3A-PB-O2B
4	M	501	GDP	C5'-O5'-PA-O1A
5	B	501	GTP	PB-O3A-PA-O5'
5	H	501	GTP	C5'-O5'-PA-O1A
5	J	501	GTP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
5	J	501	GTP	C5'-O5'-PA-O3A
5	J	501	GTP	C5'-O5'-PA-O1A
5	J	501	GTP	C5'-O5'-PA-O2A
5	L	501	GTP	PB-O3B-PG-O3G
4	G	501	GDP	C3'-C4'-C5'-O5'
5	B	501	GTP	O4'-C4'-C5'-O5'
4	G	501	GDP	O4'-C4'-C5'-O5'
4	I	501	GDP	O4'-C4'-C5'-O5'
4	I	501	GDP	C3'-C4'-C5'-O5'
5	D	501	GTP	O4'-C4'-C5'-O5'
5	D	501	GTP	C3'-C4'-C5'-O5'
4	A	501	GDP	O4'-C4'-C5'-O5'
4	K	501	GDP	PA-O3A-PB-O1B
5	J	501	GTP	C4'-C5'-O5'-PA
5	B	501	GTP	C3'-C4'-C5'-O5'
4	K	501	GDP	PA-O3A-PB-O2B
4	E	501	GDP	C3'-C4'-C5'-O5'
5	H	501	GTP	PB-O3A-PA-O1A
5	N	501	GTP	PG-O3B-PB-O1B
5	J	501	GTP	PA-O3A-PB-O3B
4	M	501	GDP	C5'-O5'-PA-O3A
5	H	501	GTP	C5'-O5'-PA-O3A
5	H	501	GTP	C5'-O5'-PA-O2A
5	N	501	GTP	C5'-O5'-PA-O1A
4	E	501	GDP	PA-O3A-PB-O1B
5	H	501	GTP	PB-O3A-PA-O2A
5	B	501	GTP	PG-O3B-PB-O1B
5	F	501	GTP	PB-O3A-PA-O1A
4	A	501	GDP	C3'-C4'-C5'-O5'
4	A	501	GDP	PA-O3A-PB-O1B
5	J	501	GTP	PB-O3B-PG-O1G
4	A	501	GDP	PA-O3A-PB-O3B
4	I	501	GDP	PA-O3A-PB-O3B
5	J	501	GTP	PB-O3B-PG-O3G
5	L	501	GTP	PB-O3B-PG-O2G
4	C	501	GDP	PB-O3A-PA-O1A
5	D	501	GTP	PA-O3A-PB-O2B
5	F	501	GTP	PB-O3A-PA-O2A
5	H	501	GTP	PG-O3B-PB-O2B
5	N	501	GTP	PA-O3A-PB-O1B
4	E	501	GDP	O4'-C4'-C5'-O5'
5	N	501	GTP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
5	L	501	GTP	PB-O3B-PG-O1G
5	B	501	GTP	PG-O3B-PB-O2B
5	D	501	GTP	PG-O3B-PB-O2B
5	J	501	GTP	PA-O3A-PB-O2B
4	C	501	GDP	C3'-C4'-C5'-O5'

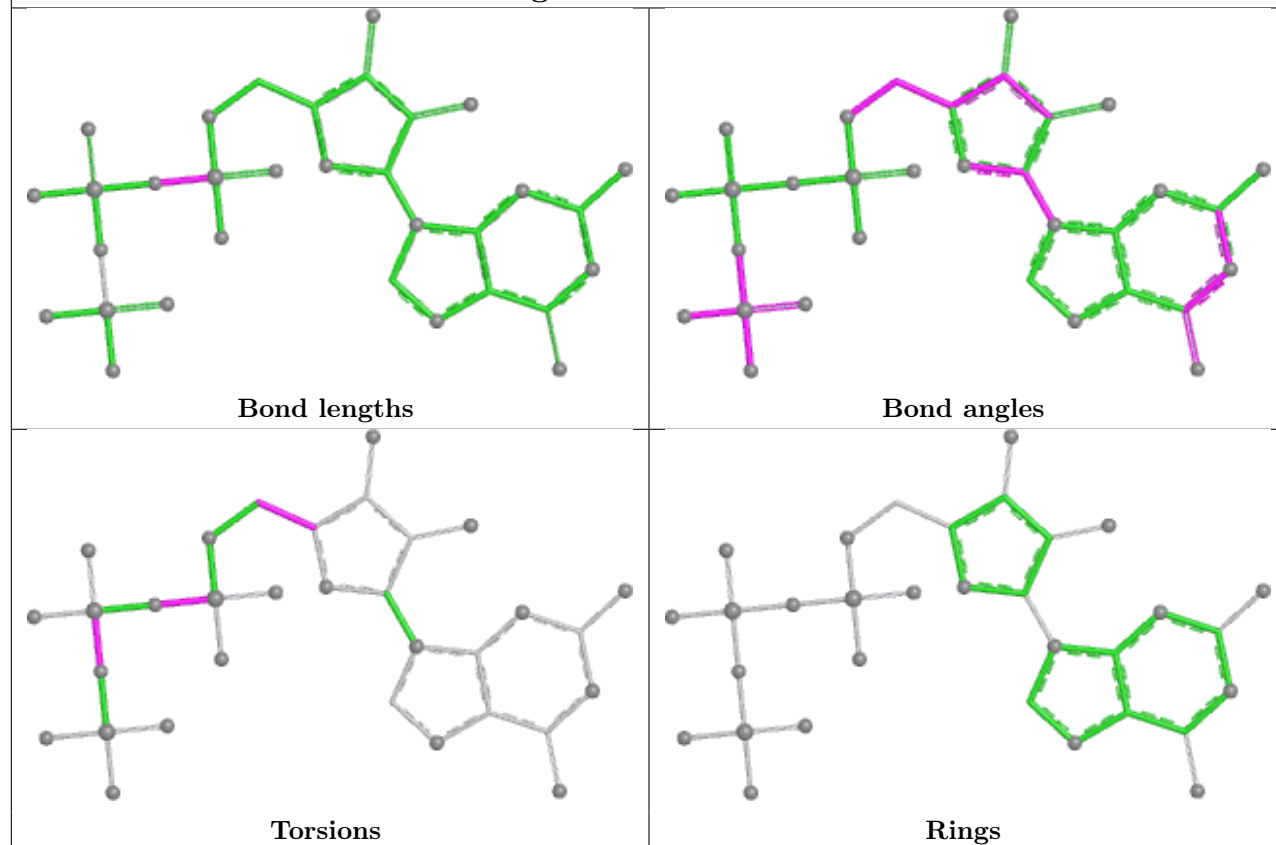
There are no ring outliers.

3 monomers are involved in 3 short contacts:

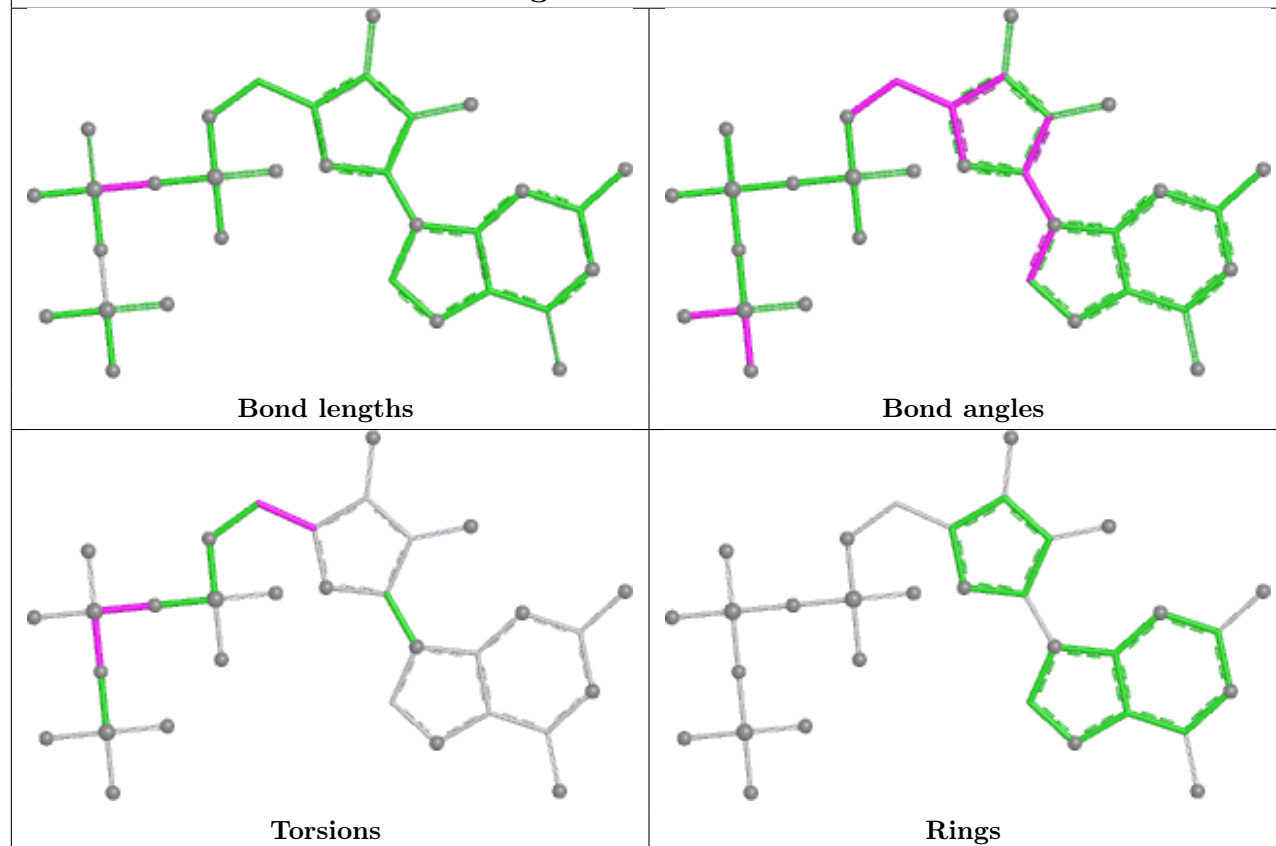
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	GTP	1	0
5	H	501	GTP	1	0
5	L	501	GTP	1	0

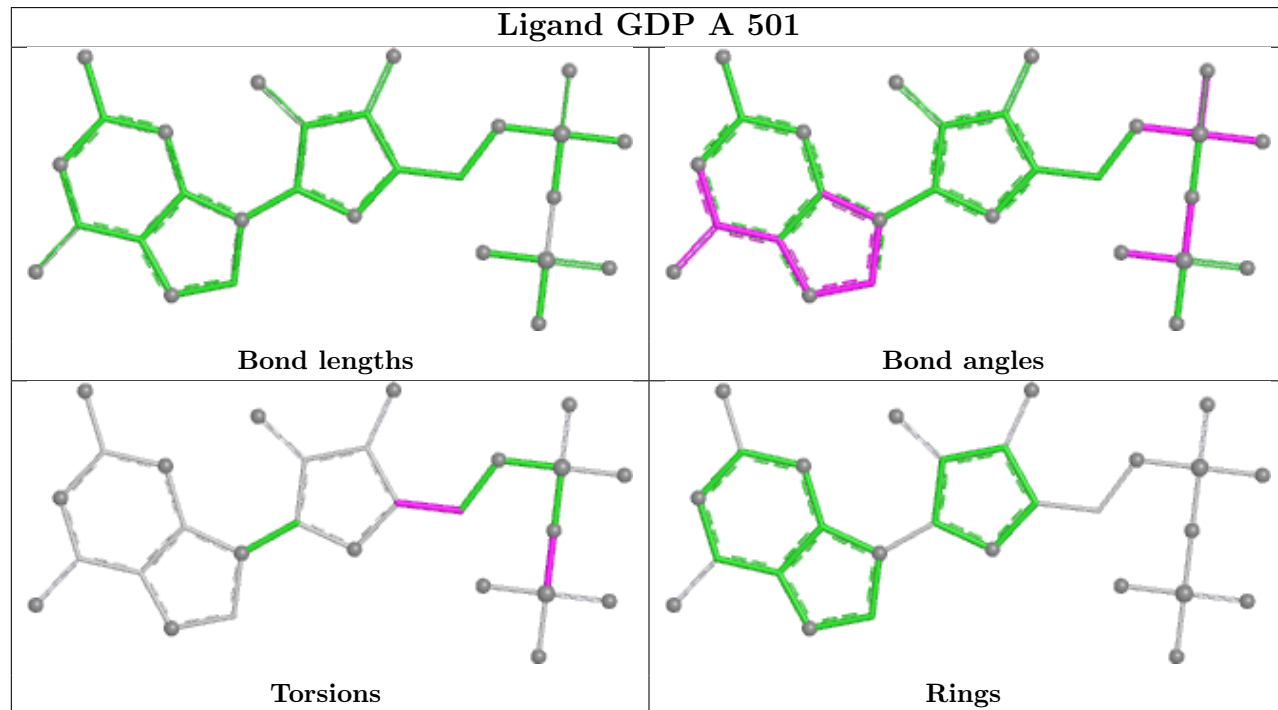
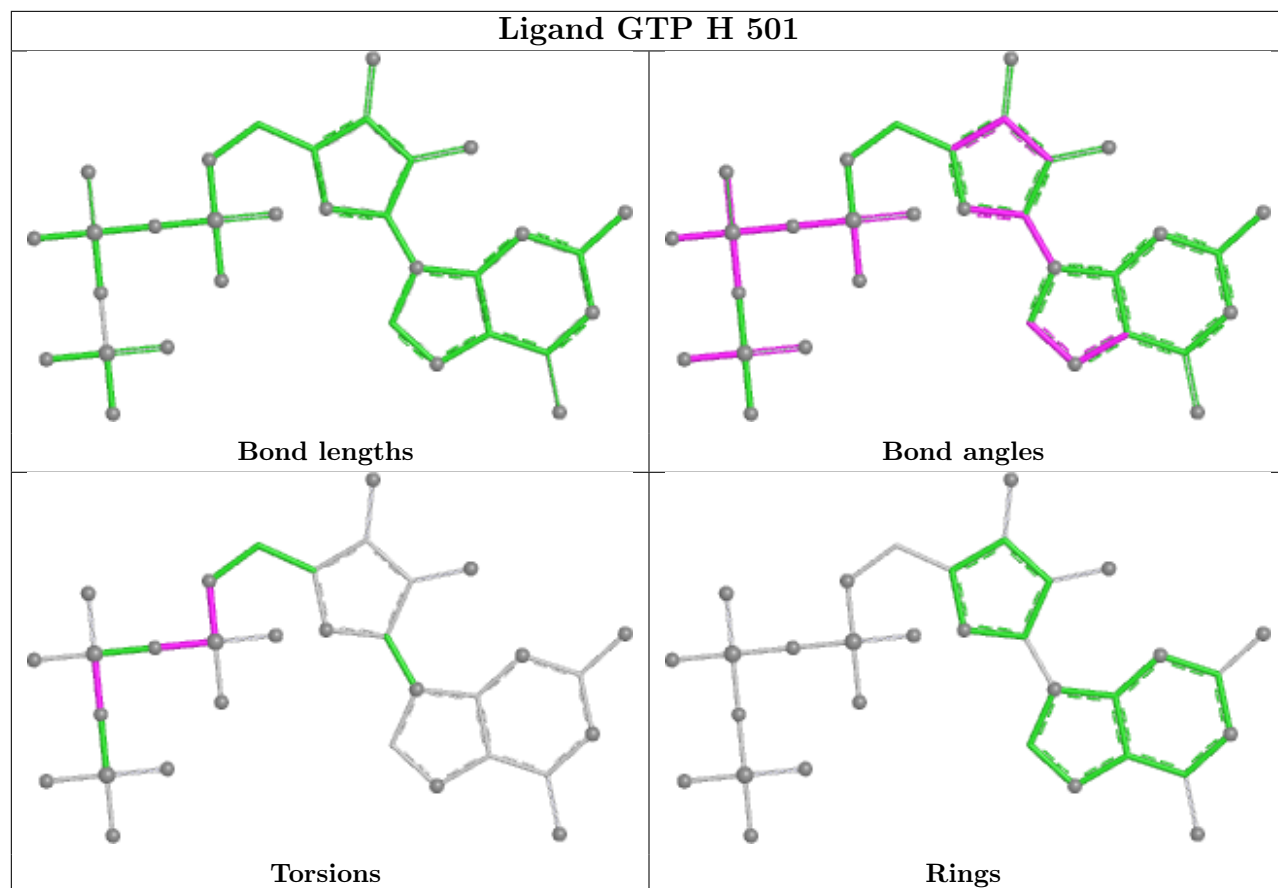
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP B 501

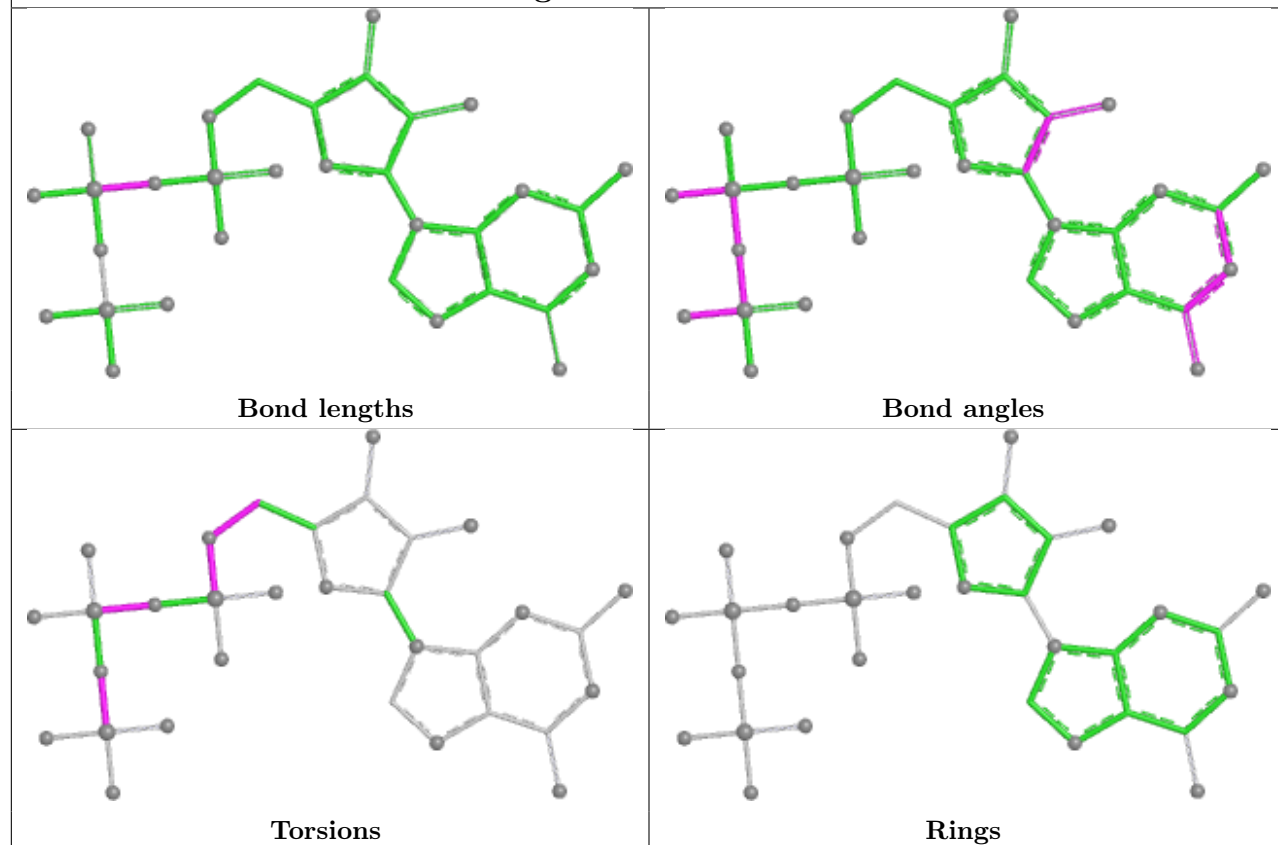


Ligand GTP D 501

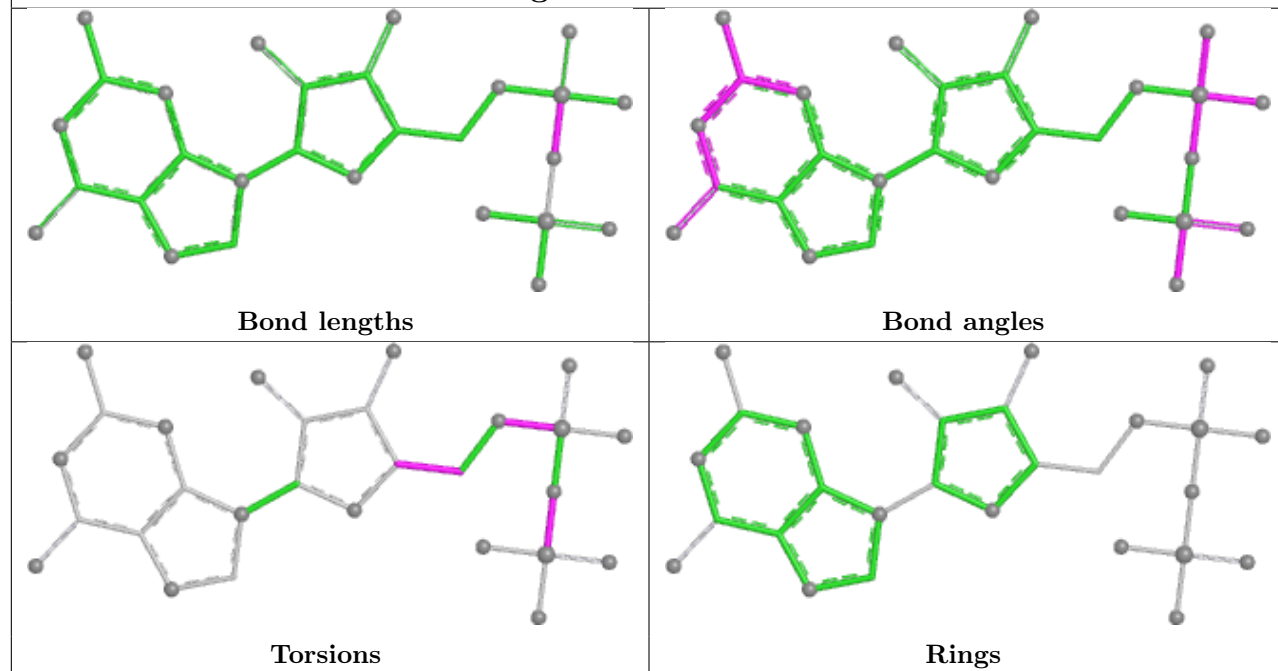


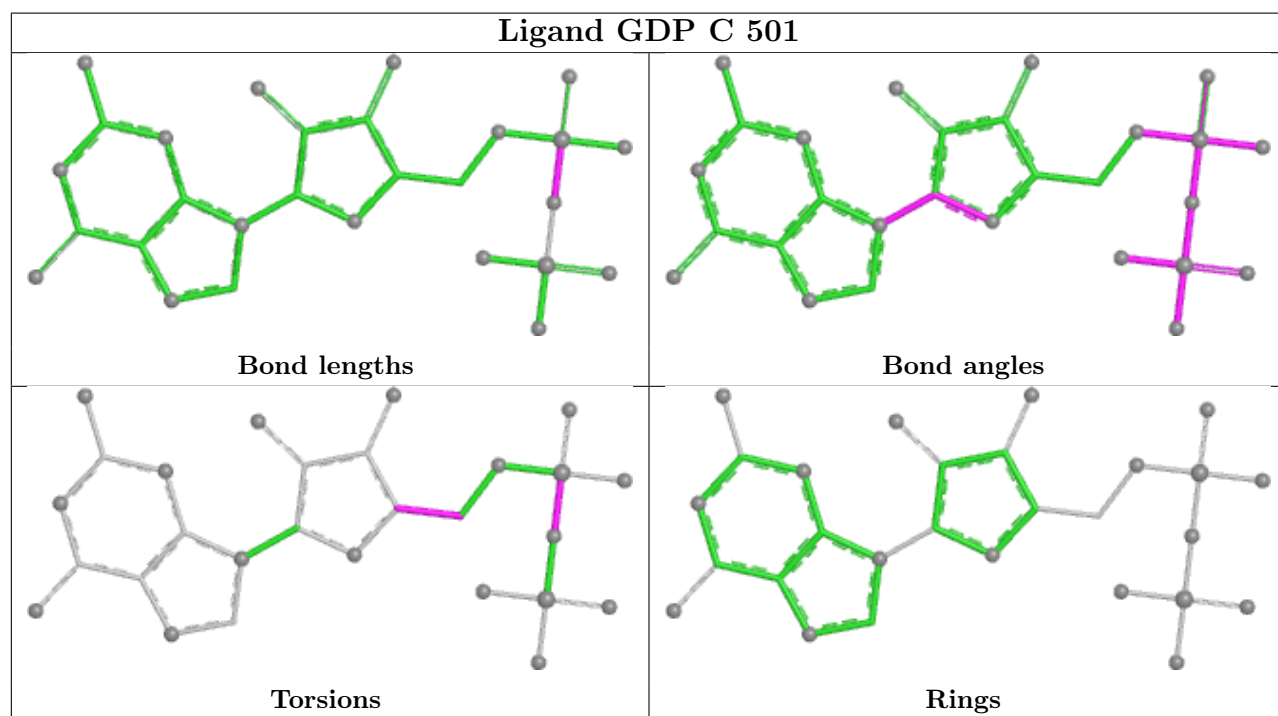
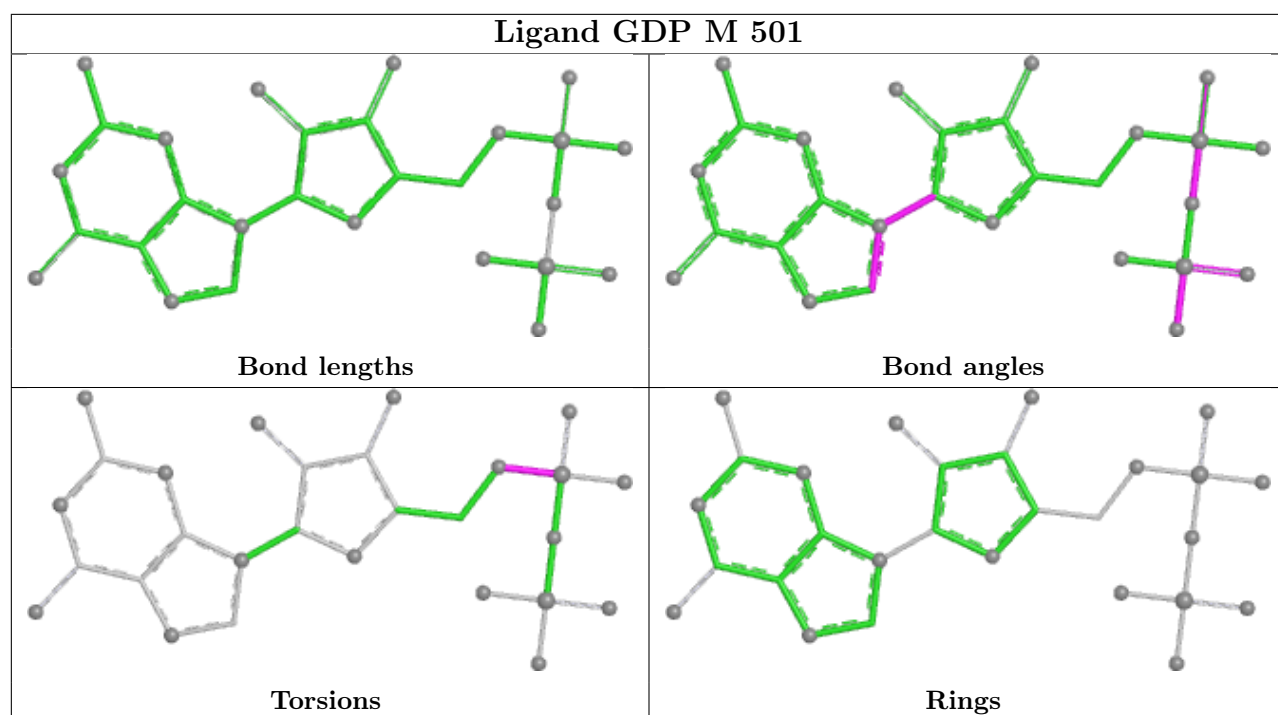


Ligand GTP J 501

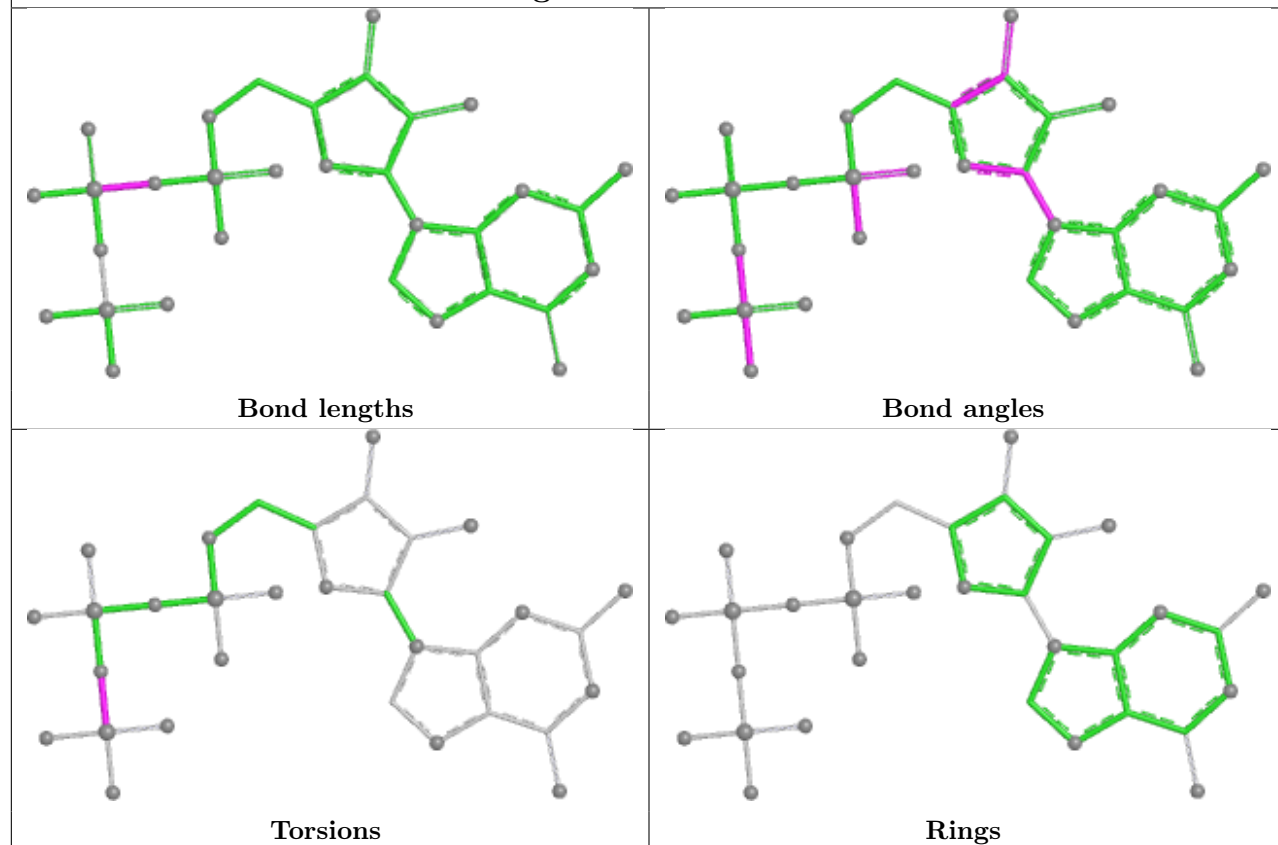


Ligand GDP E 501

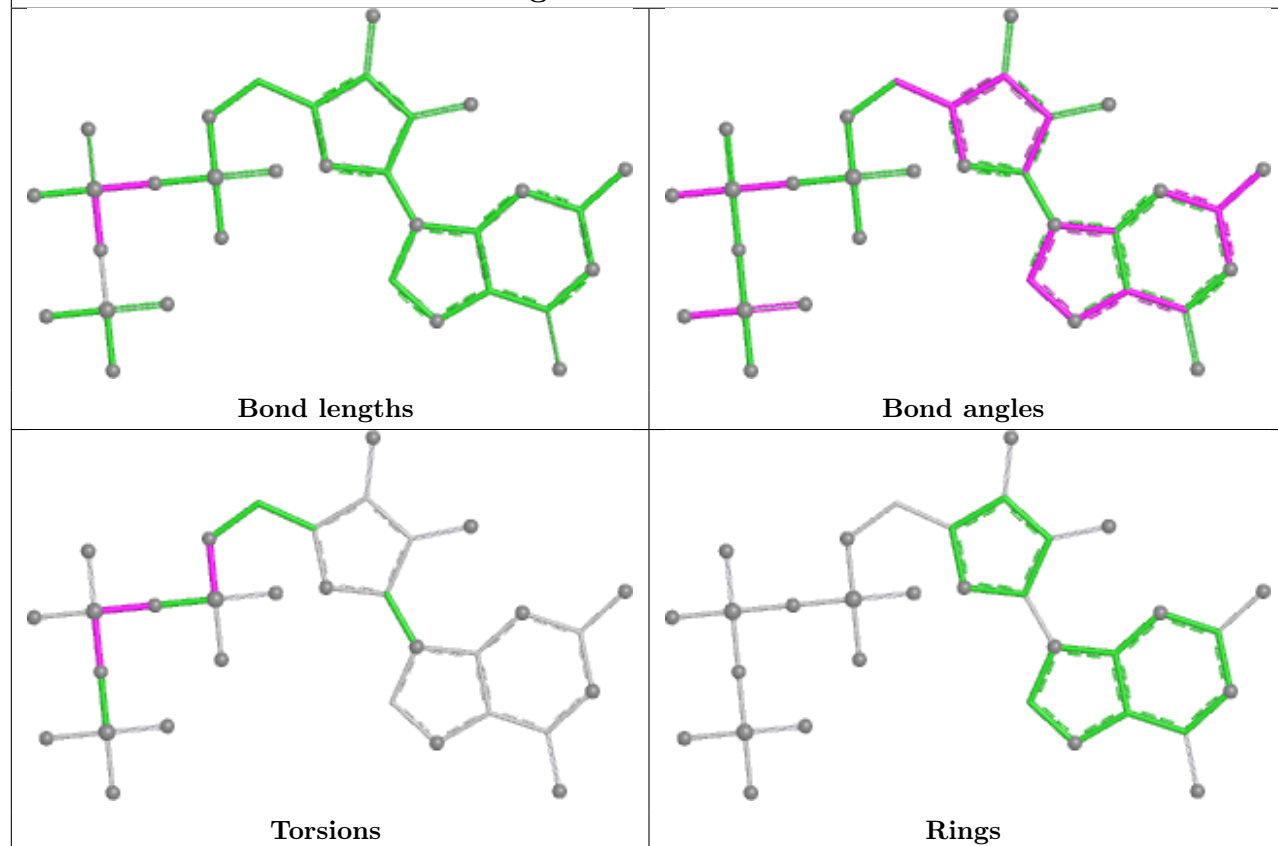




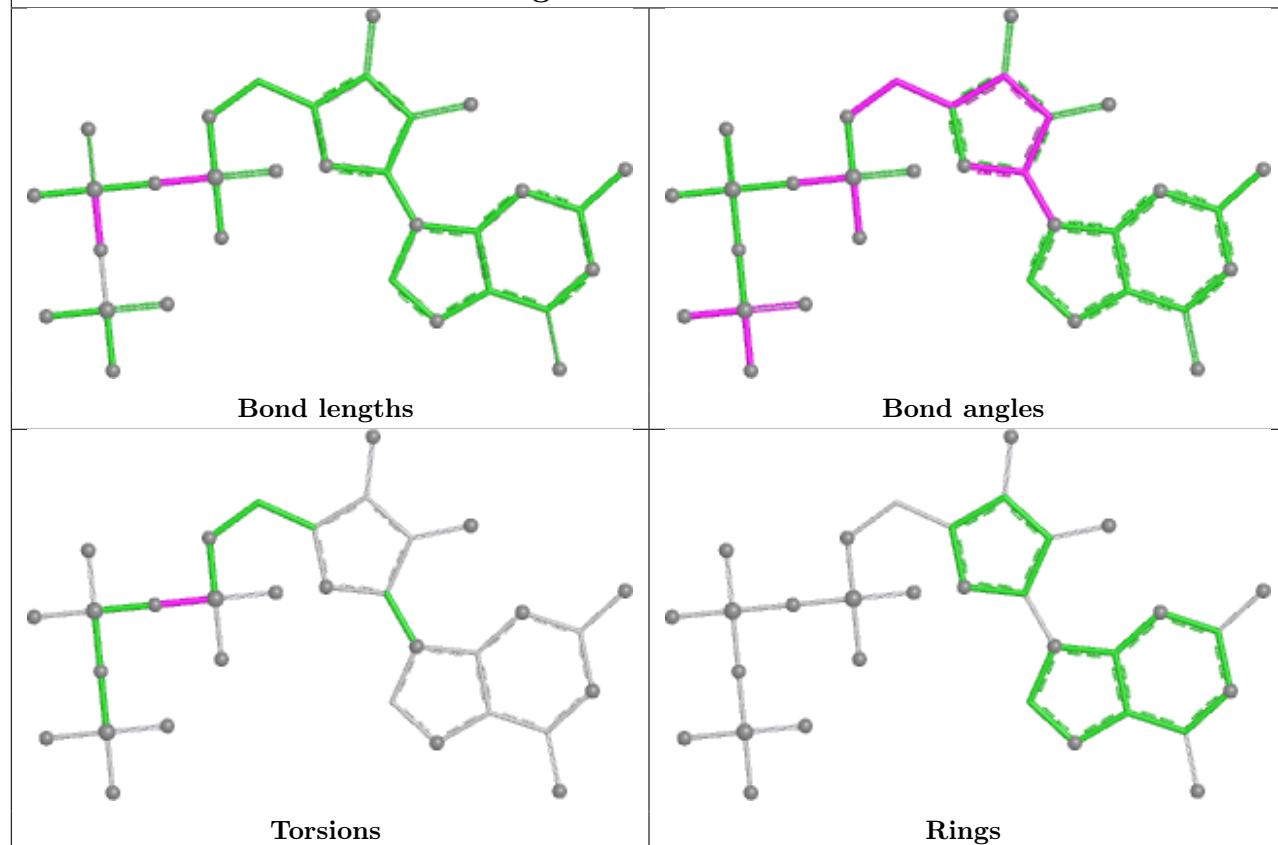
Ligand GTP L 501



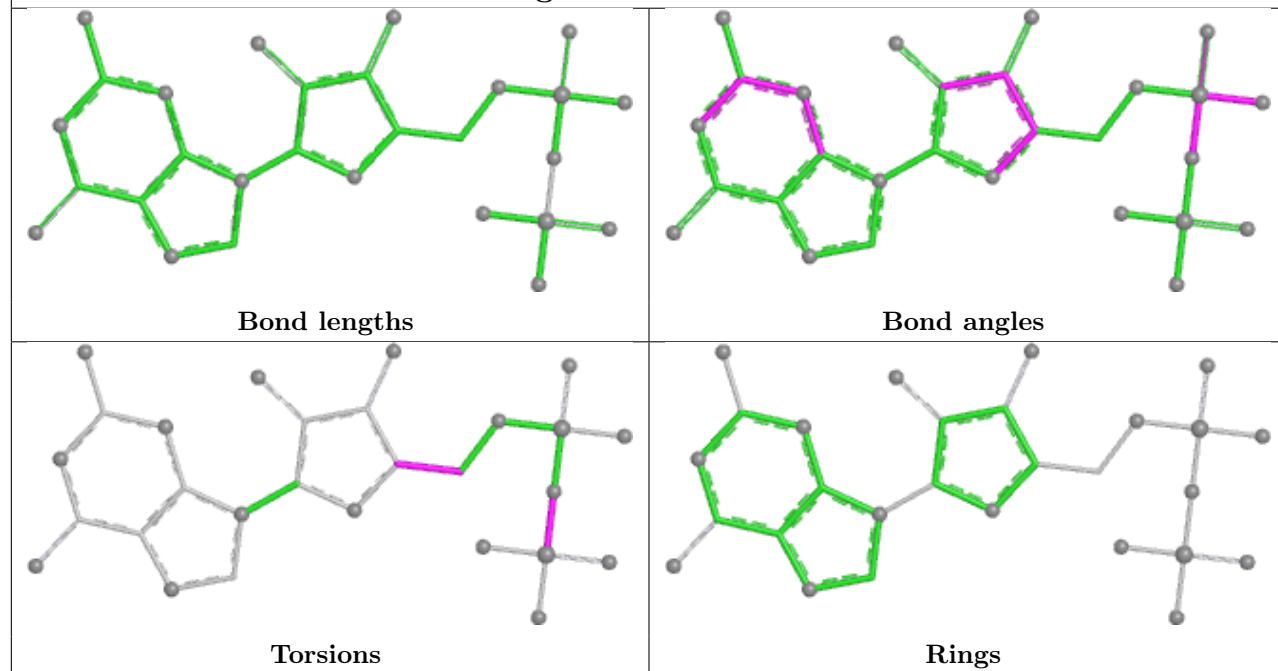
Ligand GTP N 501

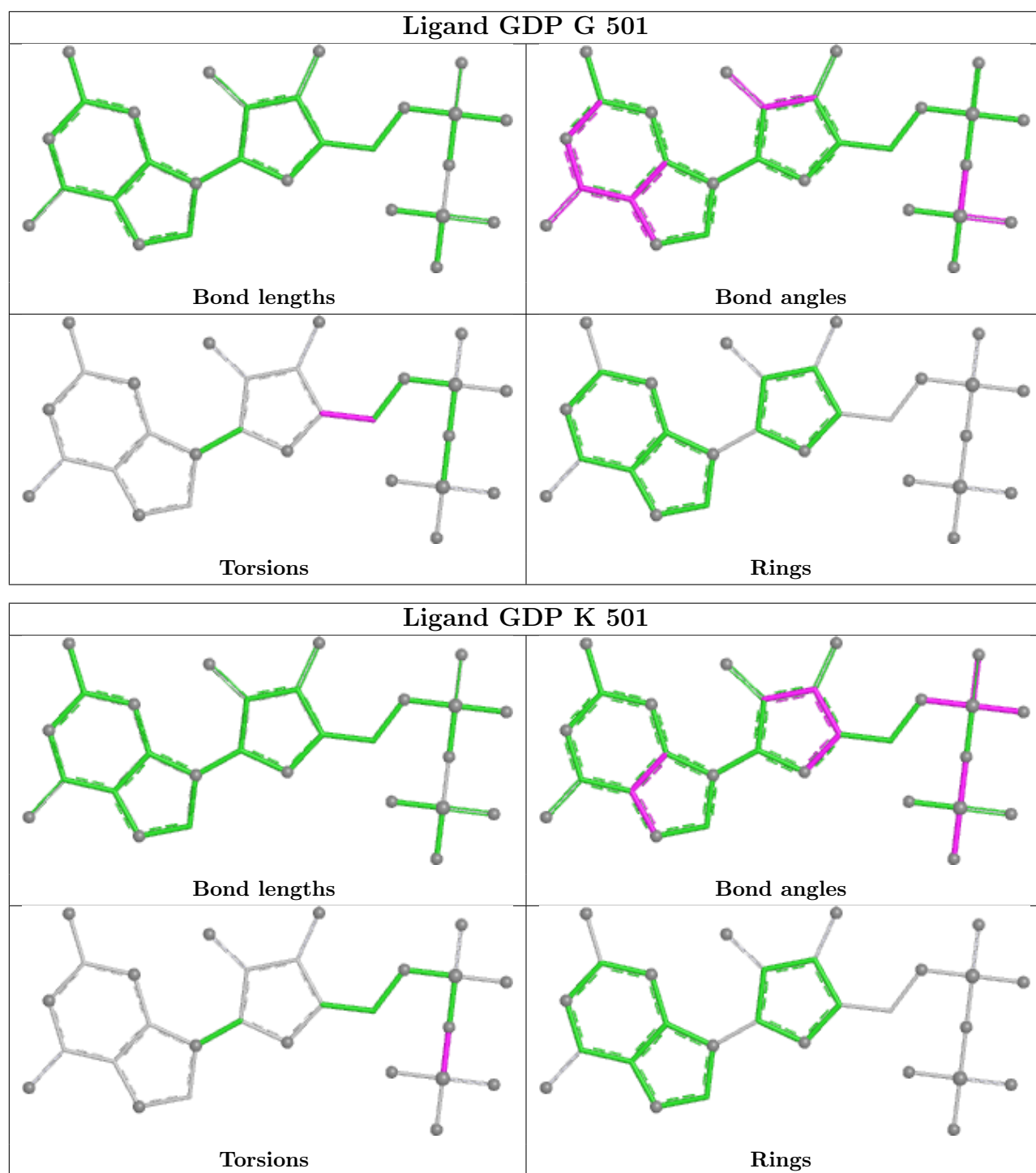


Ligand GTP F 501



Ligand GDP I 501





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.

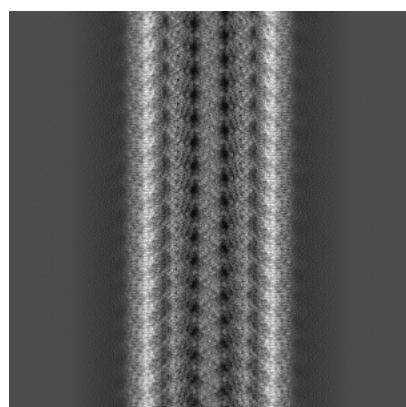
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7522. These allow visual inspection of the internal detail of the map and identification of artifacts.

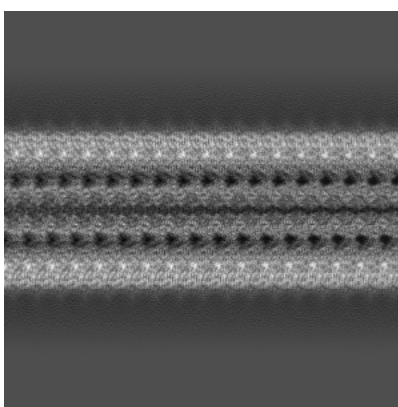
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

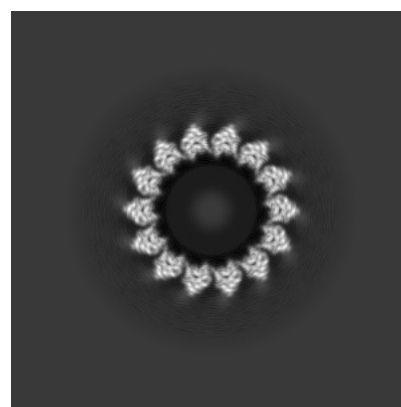
6.1.1 Primary map



X



Y

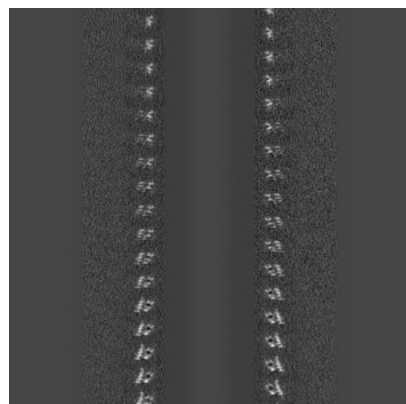


Z

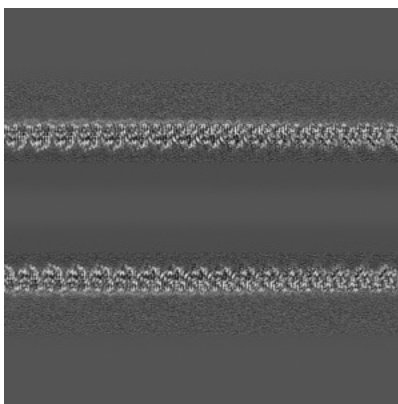
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

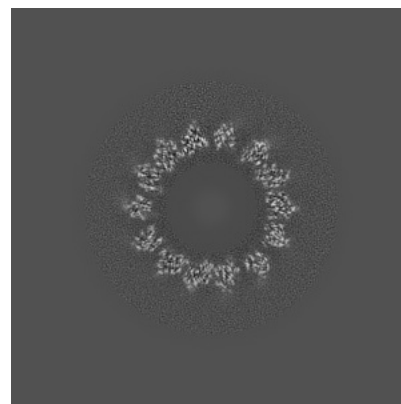
6.2.1 Primary map



X Index: 256



Y Index: 256

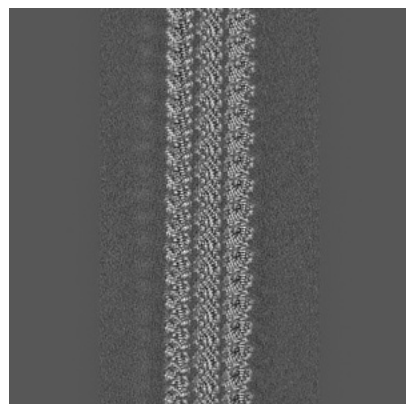


Z Index: 256

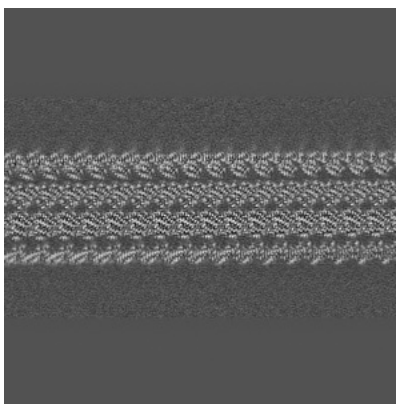
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

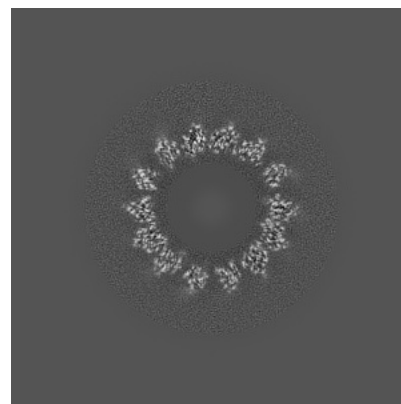
6.3.1 Primary map



X Index: 174



Y Index: 337

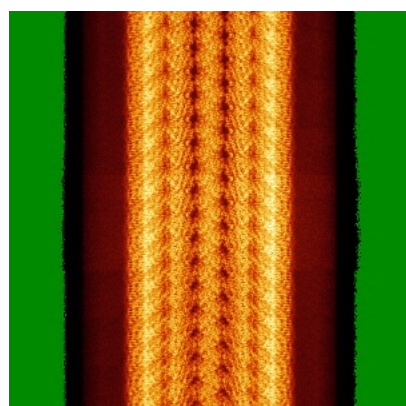


Z Index: 237

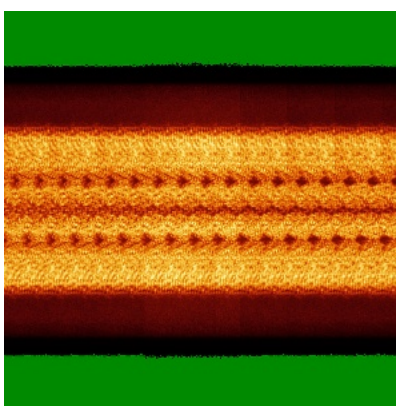
The images above show the largest variance slices of the map in three orthogonal directions.

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

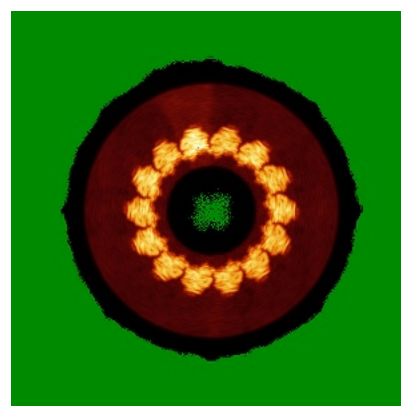
6.4.1 Primary map



X



Y

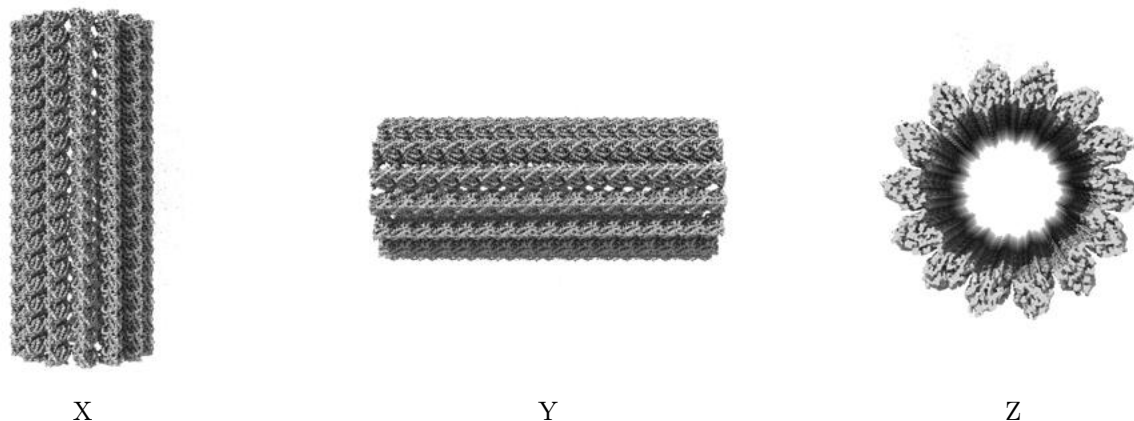


Z

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 1.26. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

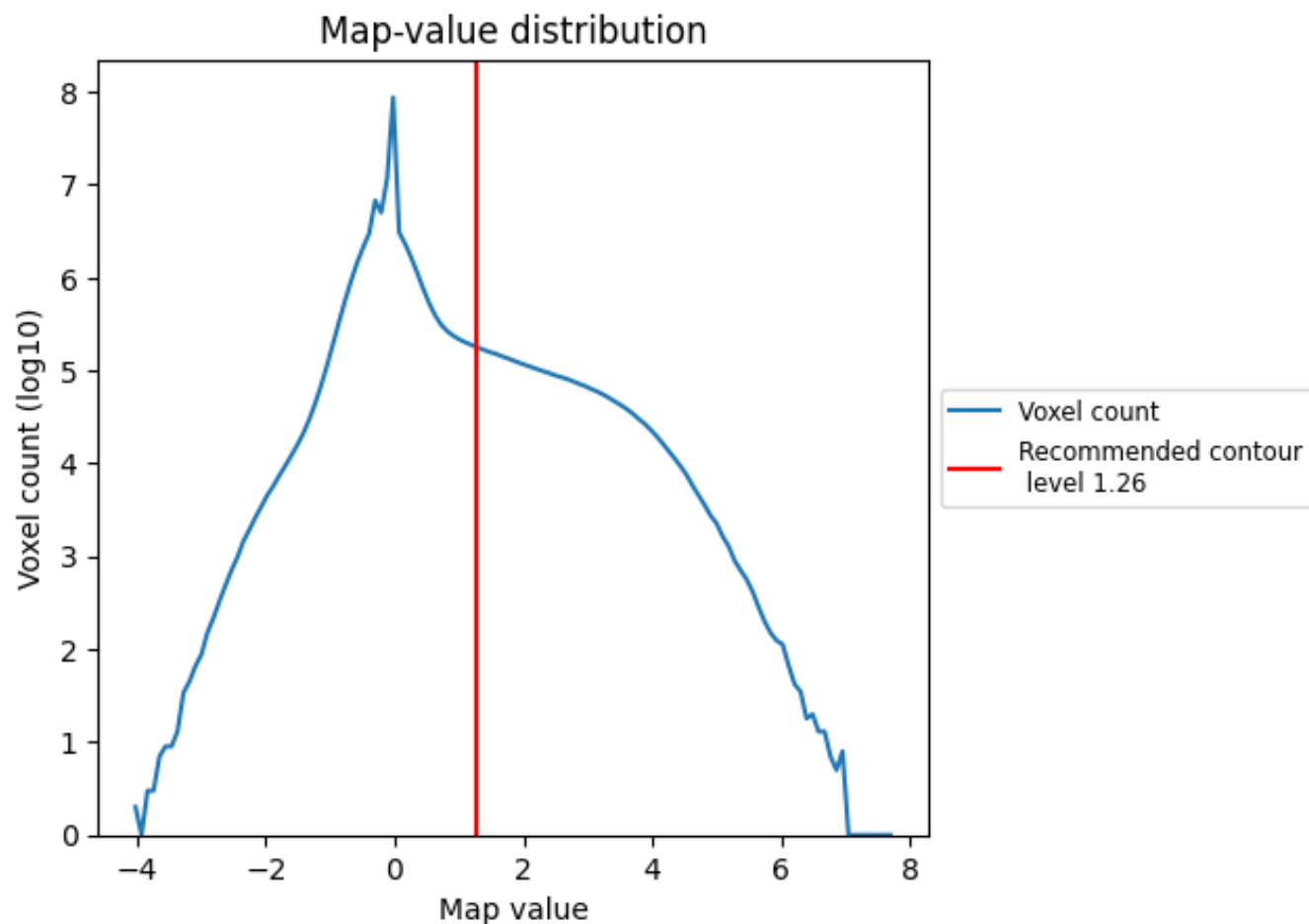
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

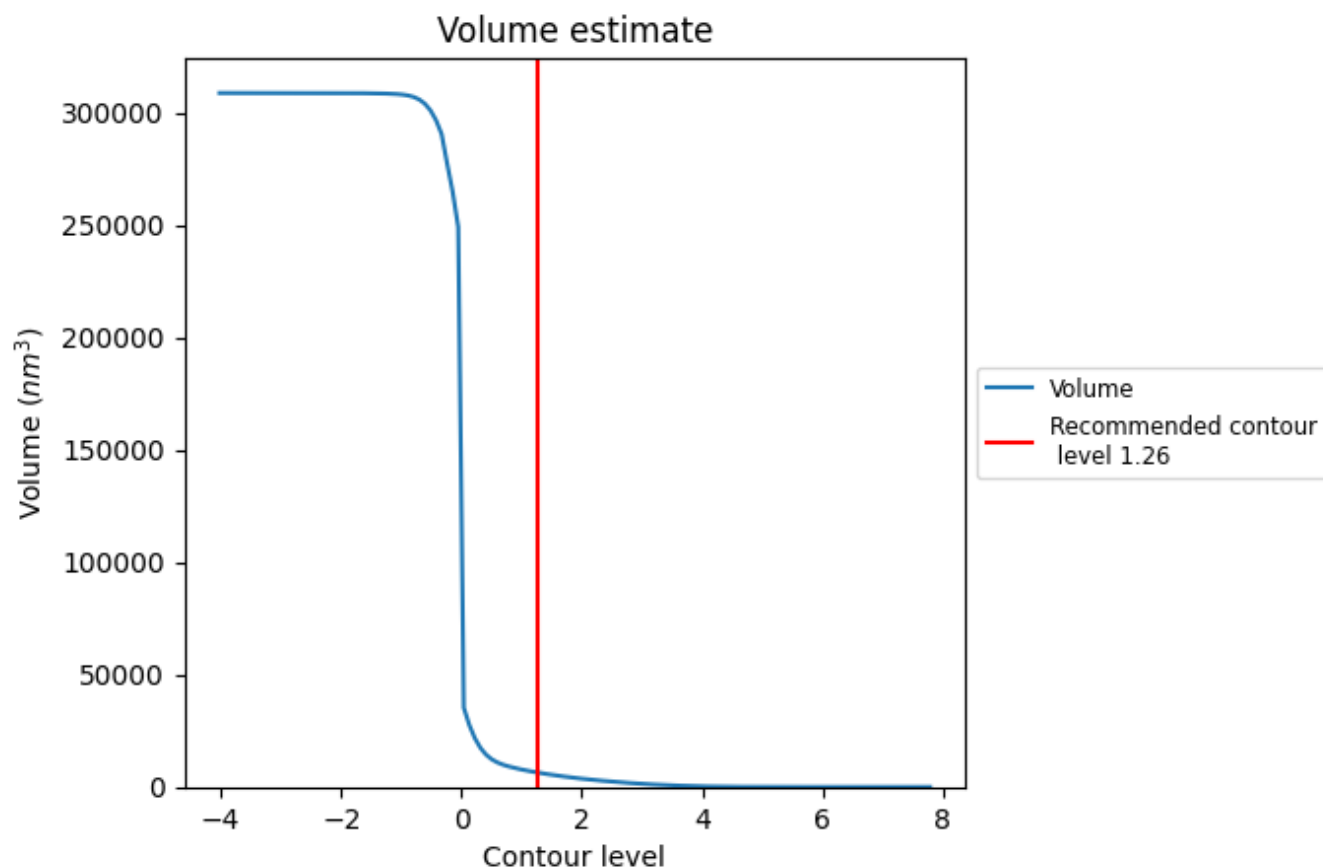
This section contains the results of statistical analysis of the map.

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.

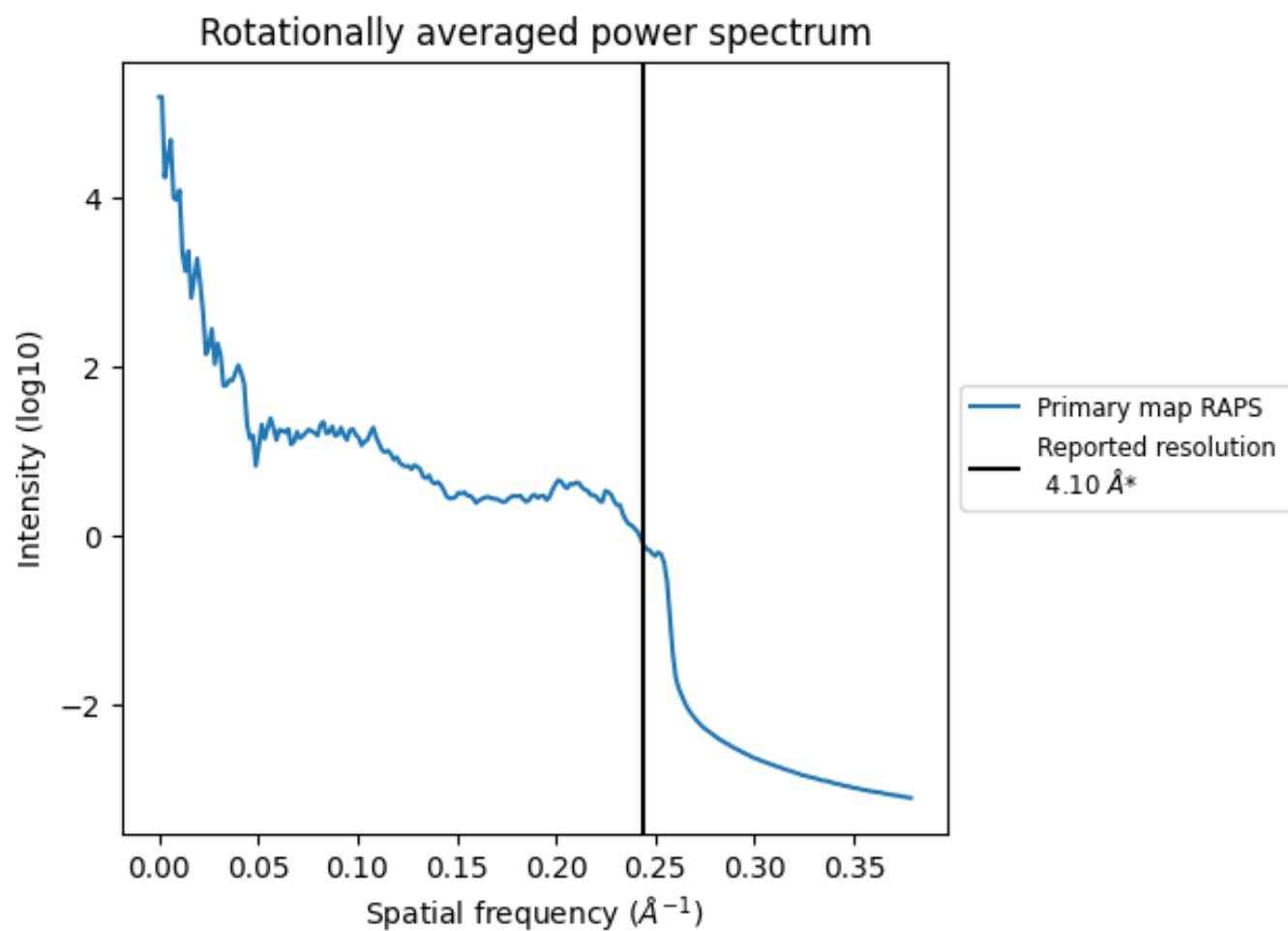
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6436 nm³; this corresponds to an approximate mass of 5814 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

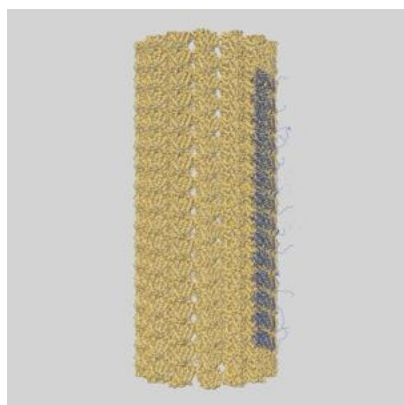
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

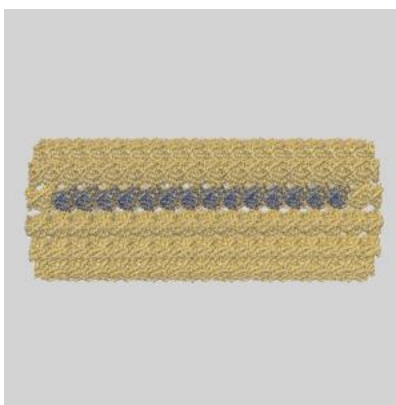
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7522 and PDB model 7PQC. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



X



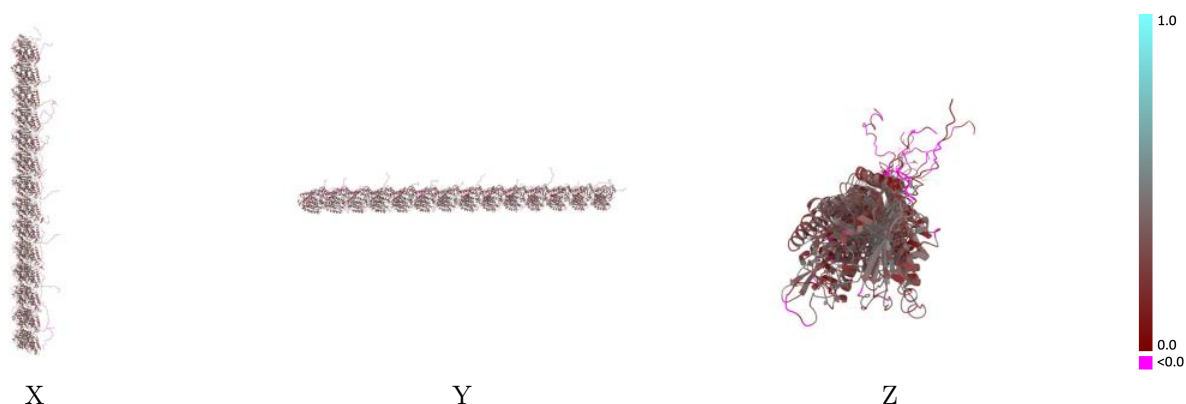
Y



Z

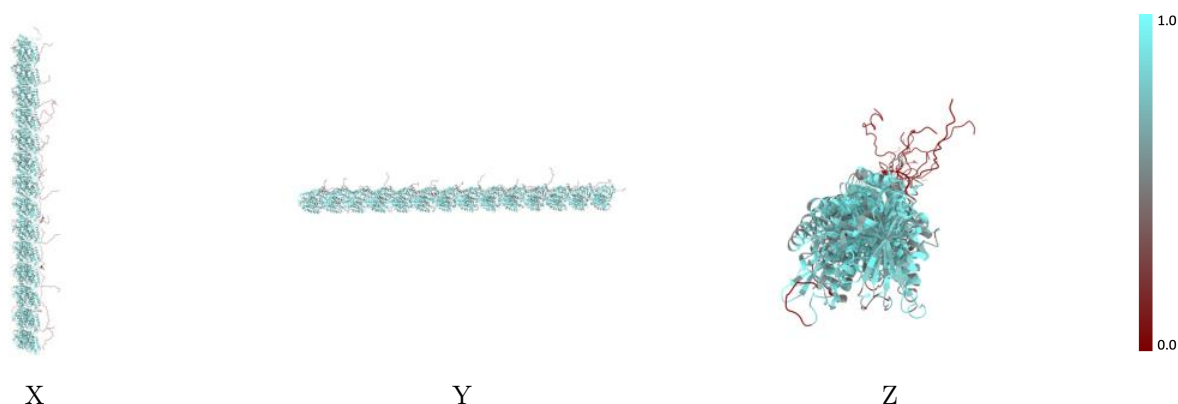
The images above show the 3D surface view of the map at the recommended contour level 1.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



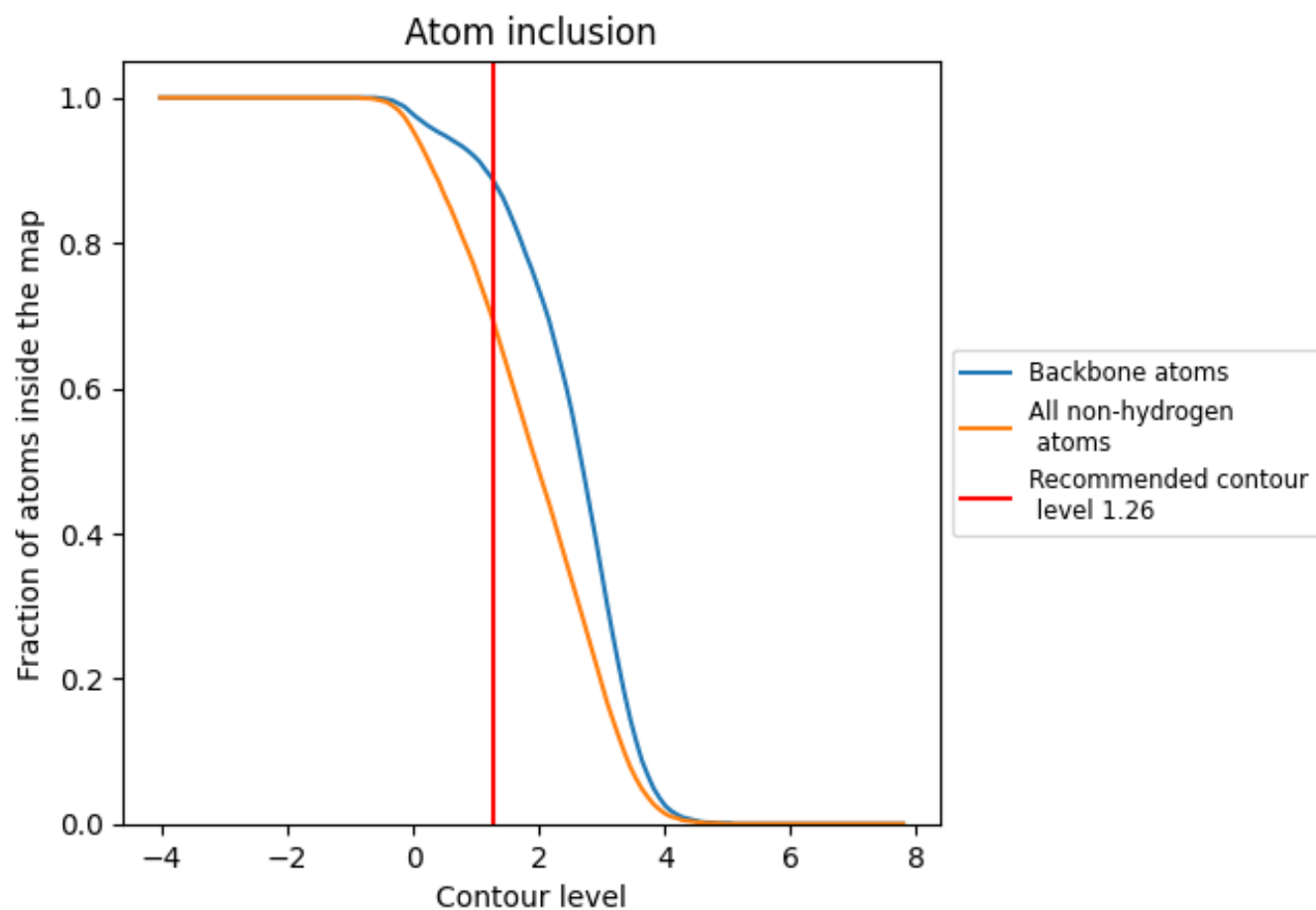
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.26).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 70% 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 (1.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6960	0.3170
A	0.7150	0.3260
B	0.7030	0.3130
C	0.7150	0.3300
D	0.7130	0.3240
E	0.7160	0.3270
F	0.7110	0.3230
G	0.7270	0.3370
H	0.7160	0.3280
I	0.7160	0.3220
J	0.7040	0.3240
K	0.7150	0.3290
L	0.6990	0.3150
M	0.7030	0.3250
N	0.7160	0.3170
O	0.1630	0.0610

1.0

0.0

<0.0