



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:49 PM UTC

PDB ID : 7PQP / pdb_00007pqp
EMDB ID : EMD-7522
Title : tau-microtubule structural ensemble based on CryoEM data
Authors : Brotzakis, Z.F.; Vendruscolo, M.
Deposited on : 2021-09-18
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:

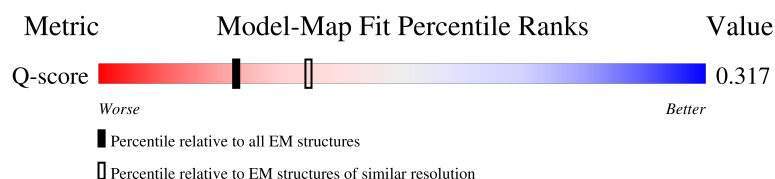
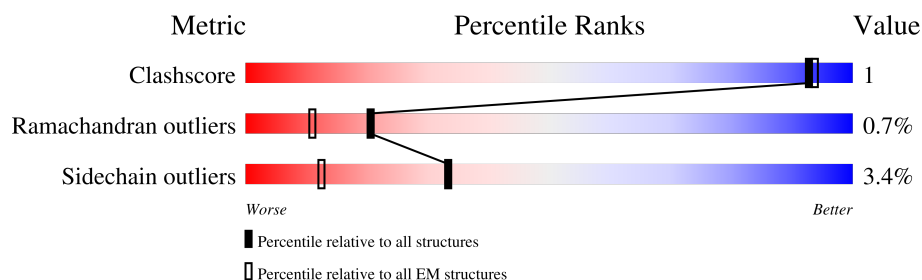
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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.



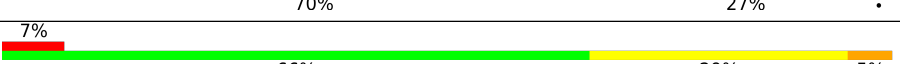
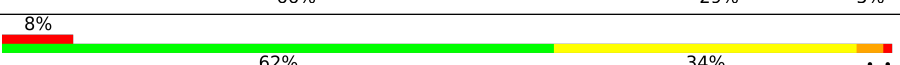
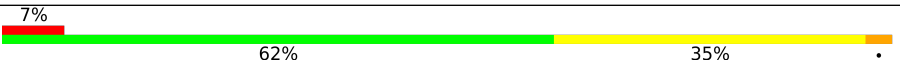
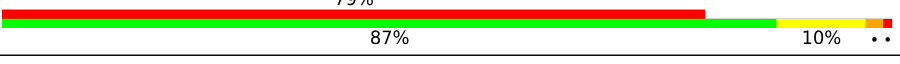
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	6% 69% 28% .
1	C	445	5% 68% 28% .
1	E	445	5% 73% 26% .
1	G	445	6% 70% 28% .

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Mol	Chain	Length	Quality of chain
1	I	445	
1	K	445	
1	M	445	
2	B	451	
2	D	451	
2	F	451	
2	H	451	
2	J	451	
2	L	451	
2	N	451	
3	O	194	

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		

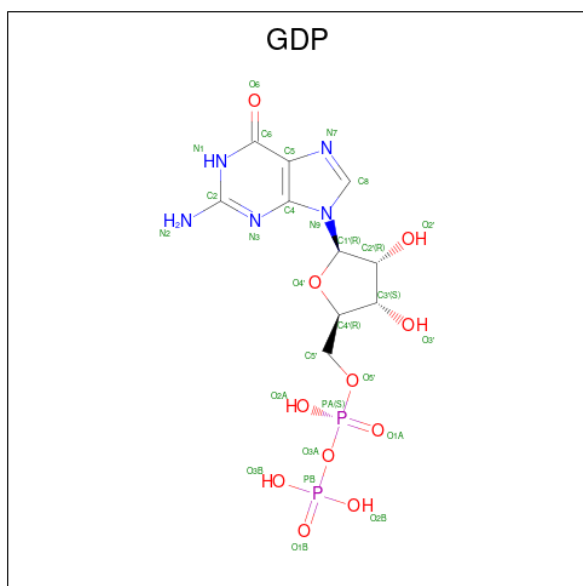
- Molecule 2 is a protein called Tubulin alpha-1B chain.

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.

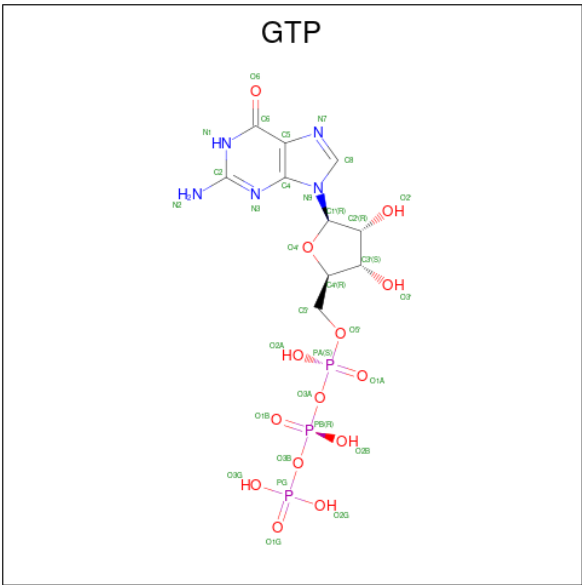
Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	194	Total	C	N	O	S	0	0
			1455	904	273	275	3		

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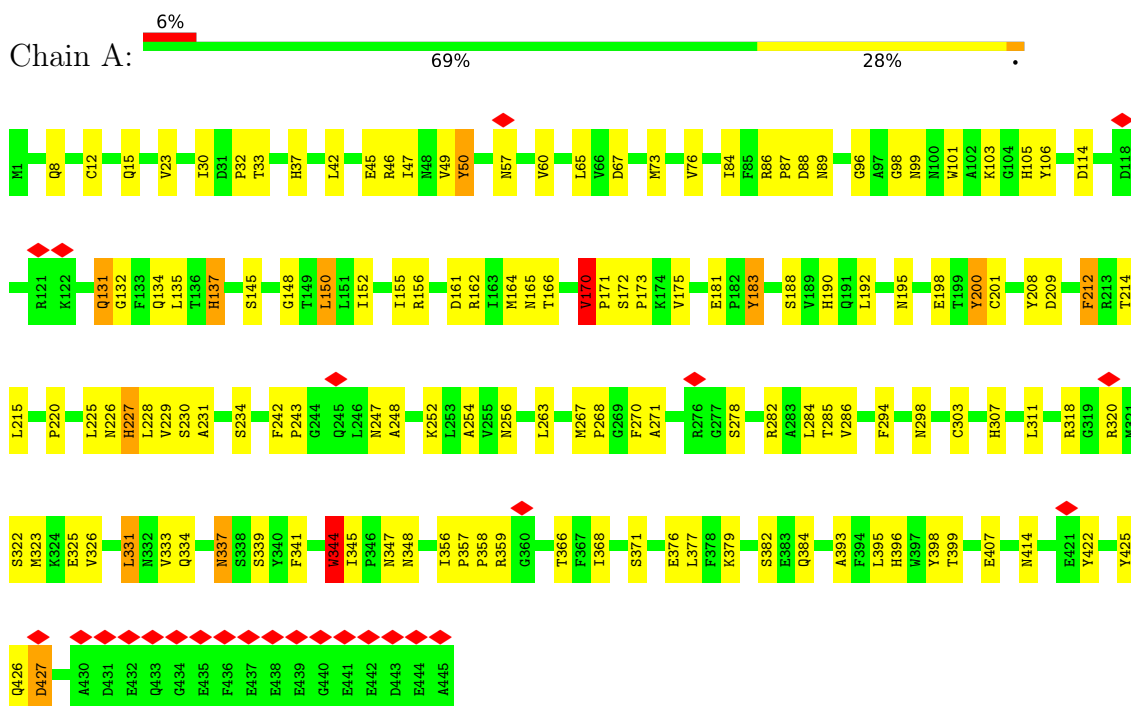
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Mol	Chain	Residues	Atoms		AltConf
6	J	1	Total 1	Mg 1	0
6	L	1	Total 1	Mg 1	0
6	N	1	Total 1	Mg 1	0

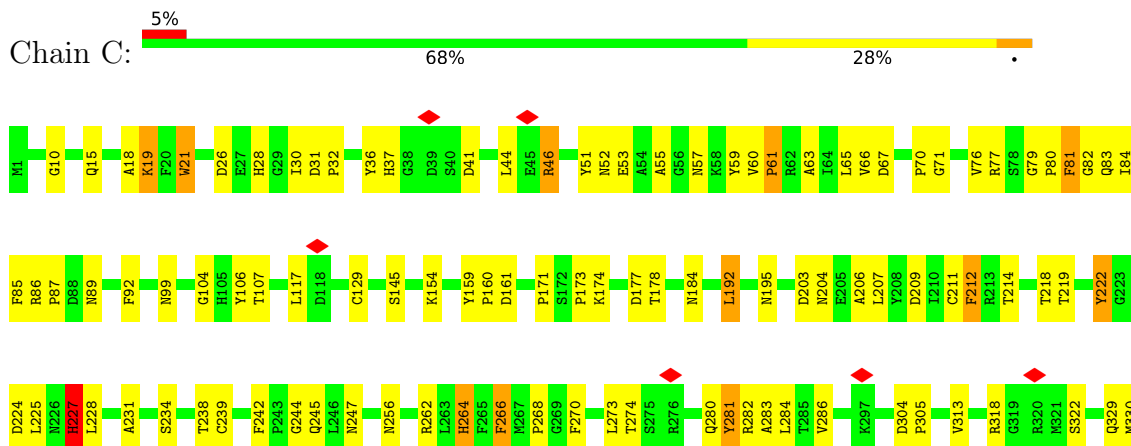
3 Residue-property plots

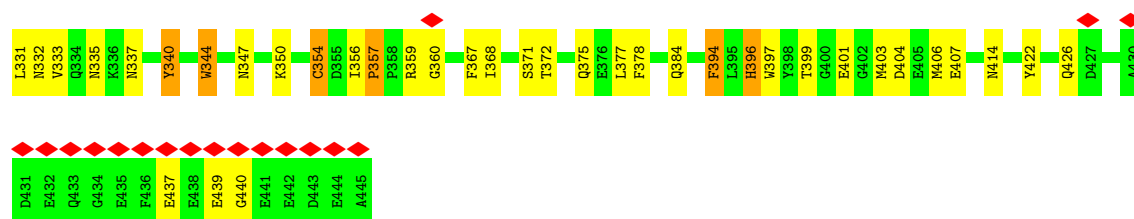
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

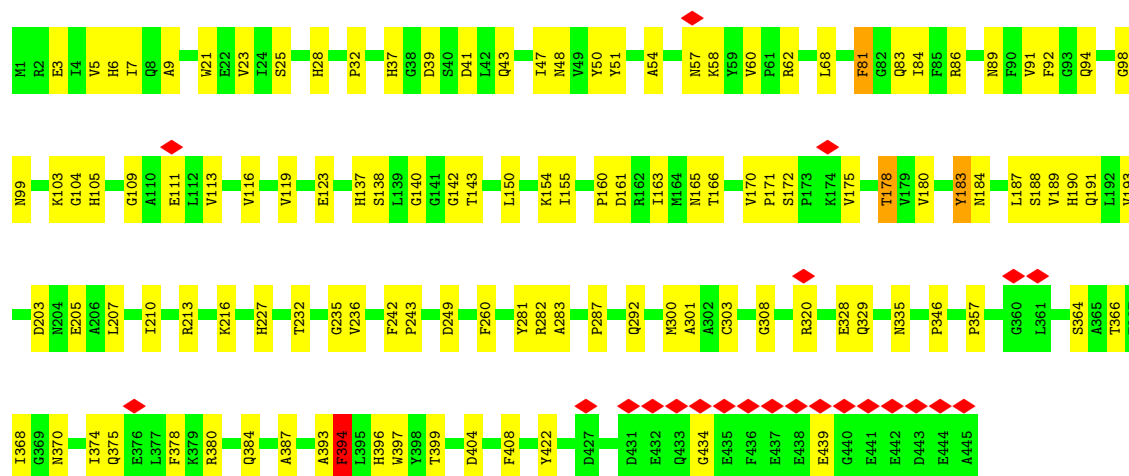
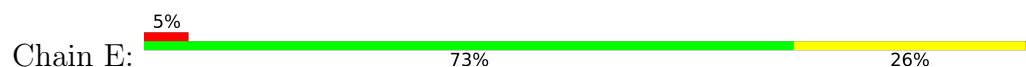


- Molecule 1: Tubulin beta chain

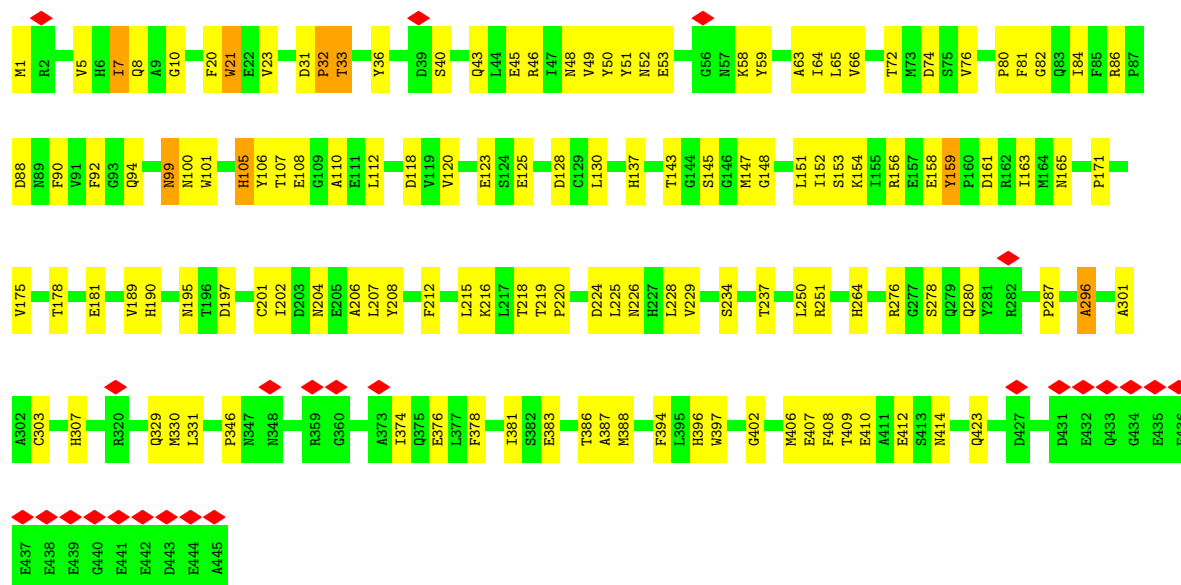




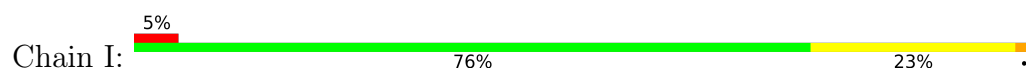
• Molecule 1: Tubulin beta chain

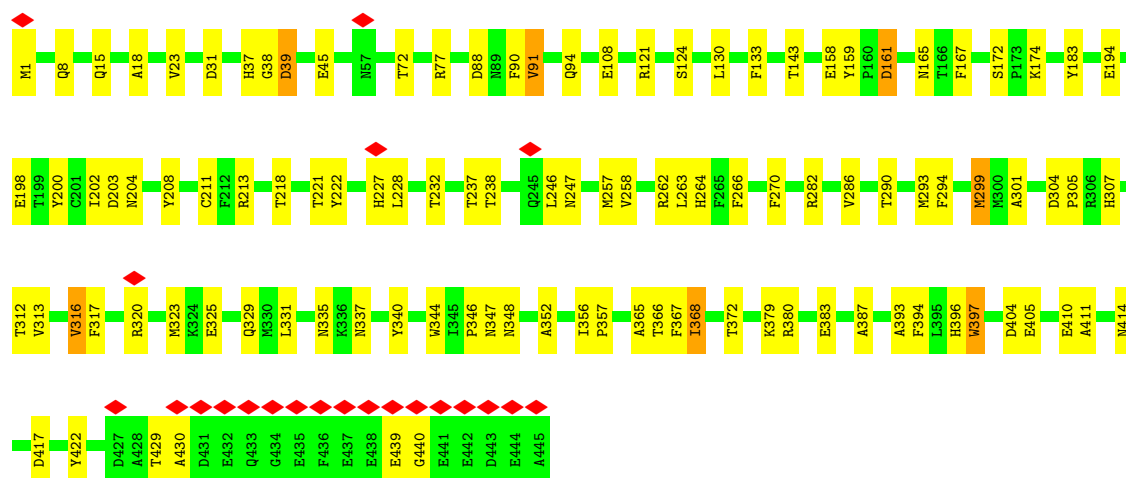


• Molecule 1: Tubulin beta chain

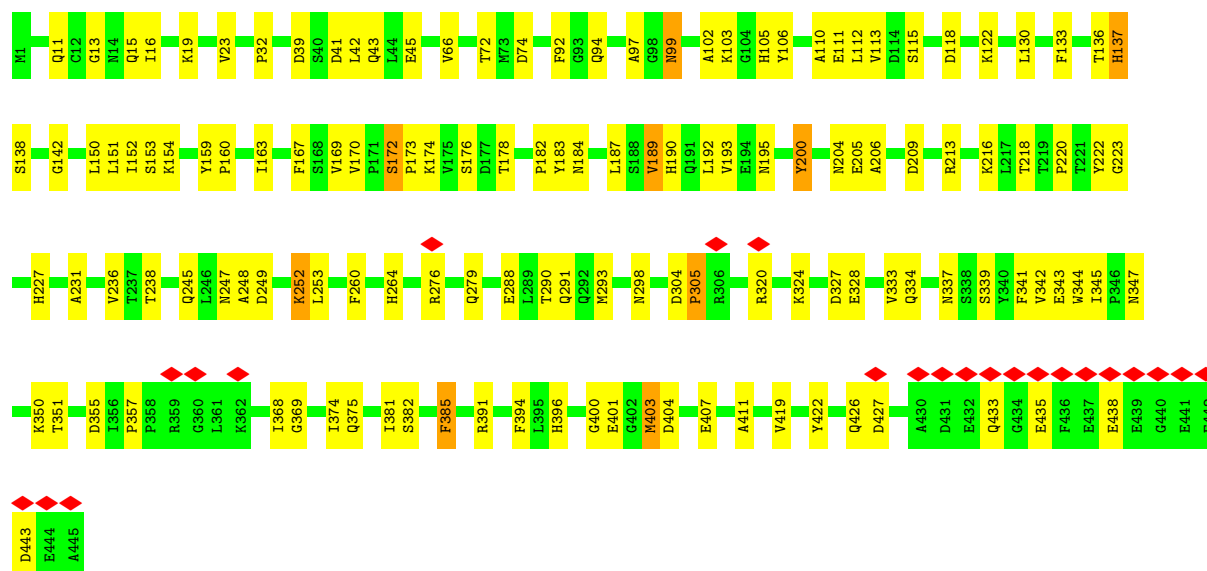


• Molecule 1: Tubulin beta chain

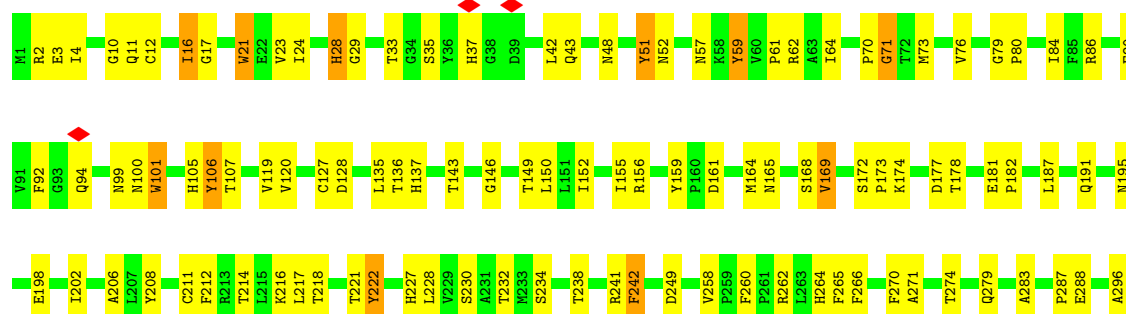


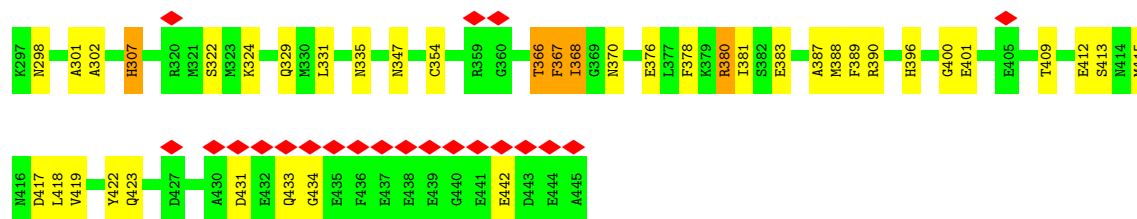


• Molecule 1: Tubulin beta chain

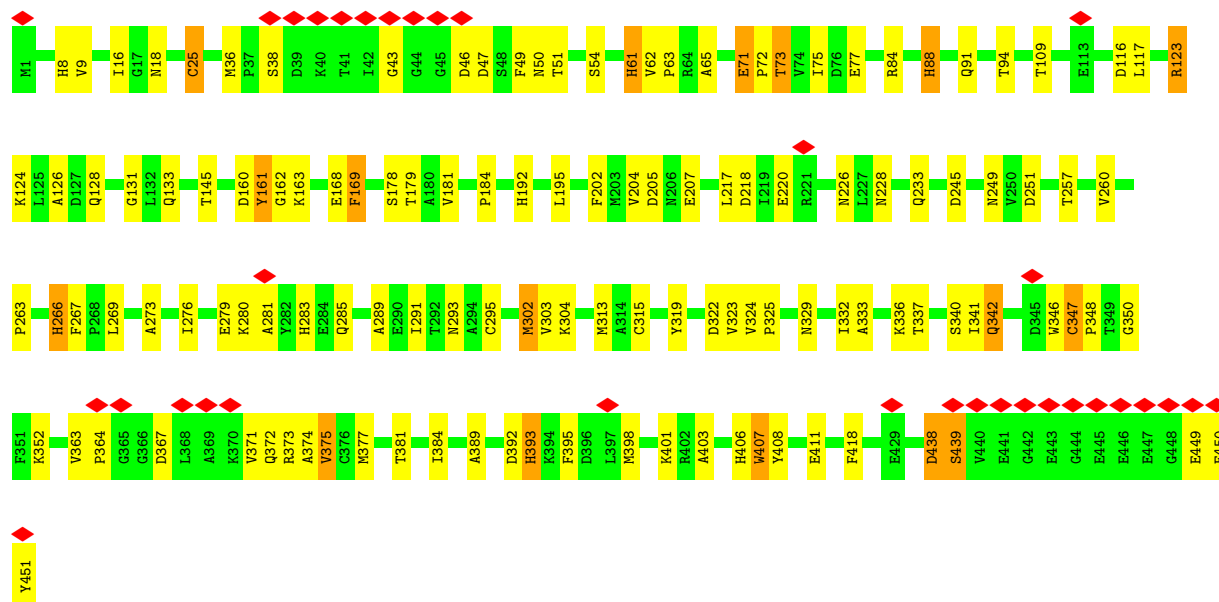


• Molecule 1: Tubulin beta chain

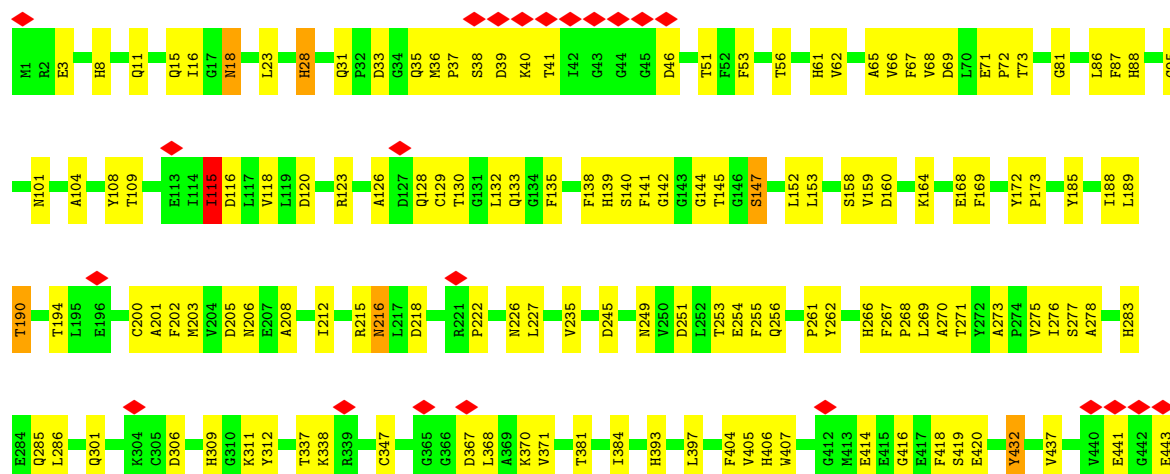




• Molecule 2: Tubulin alpha-1B chain

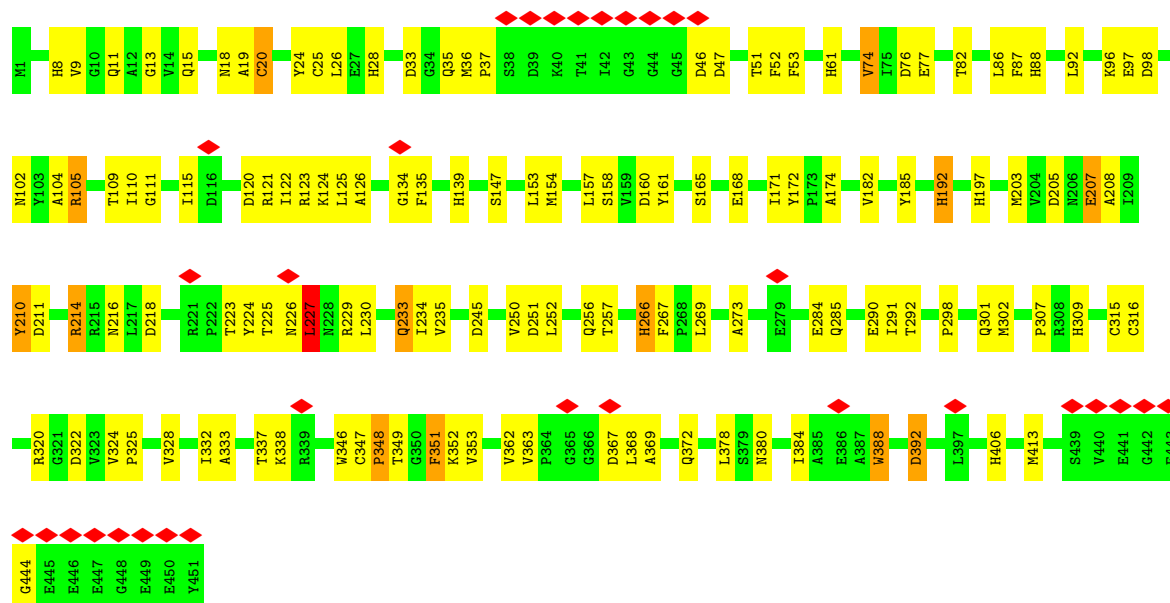


• Molecule 2: Tubulin alpha-1B chain

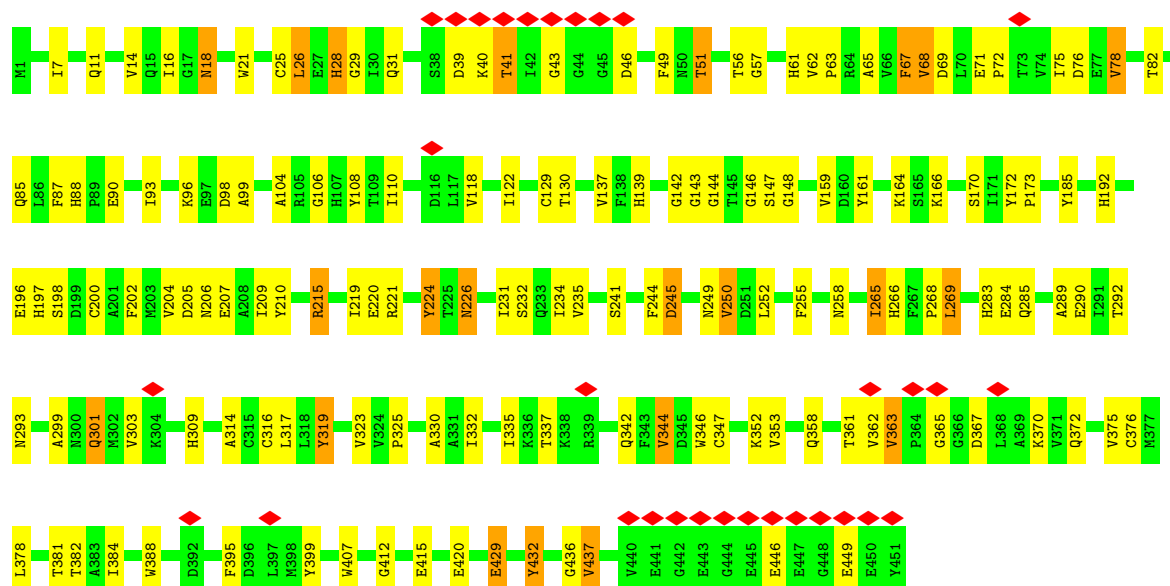




• Molecule 2: Tubulin alpha-1B chain

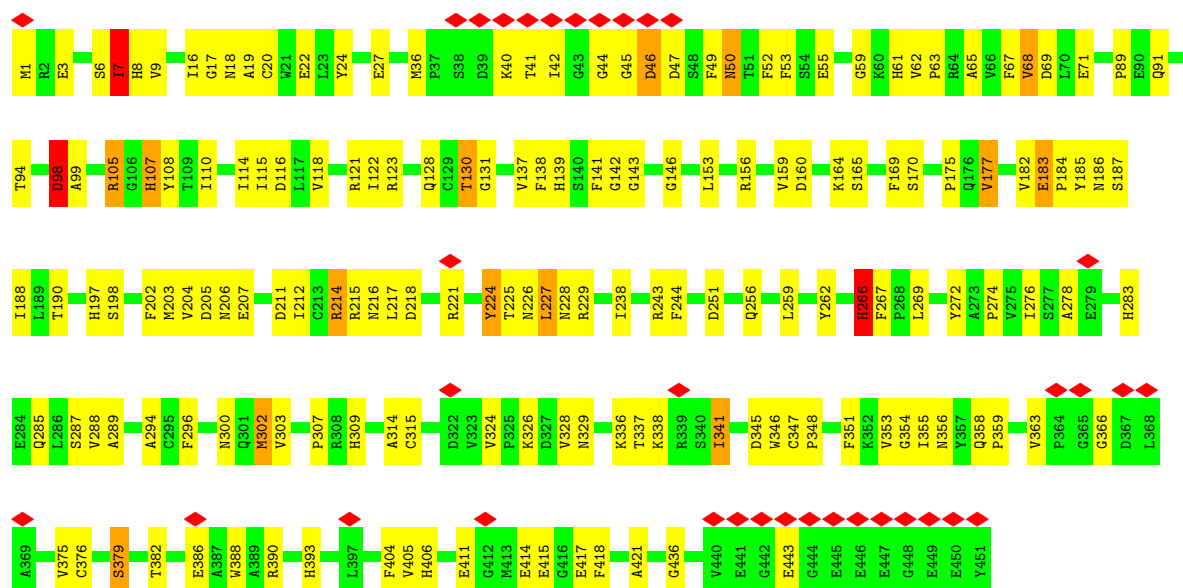


• Molecule 2: Tubulin alpha-1B chain

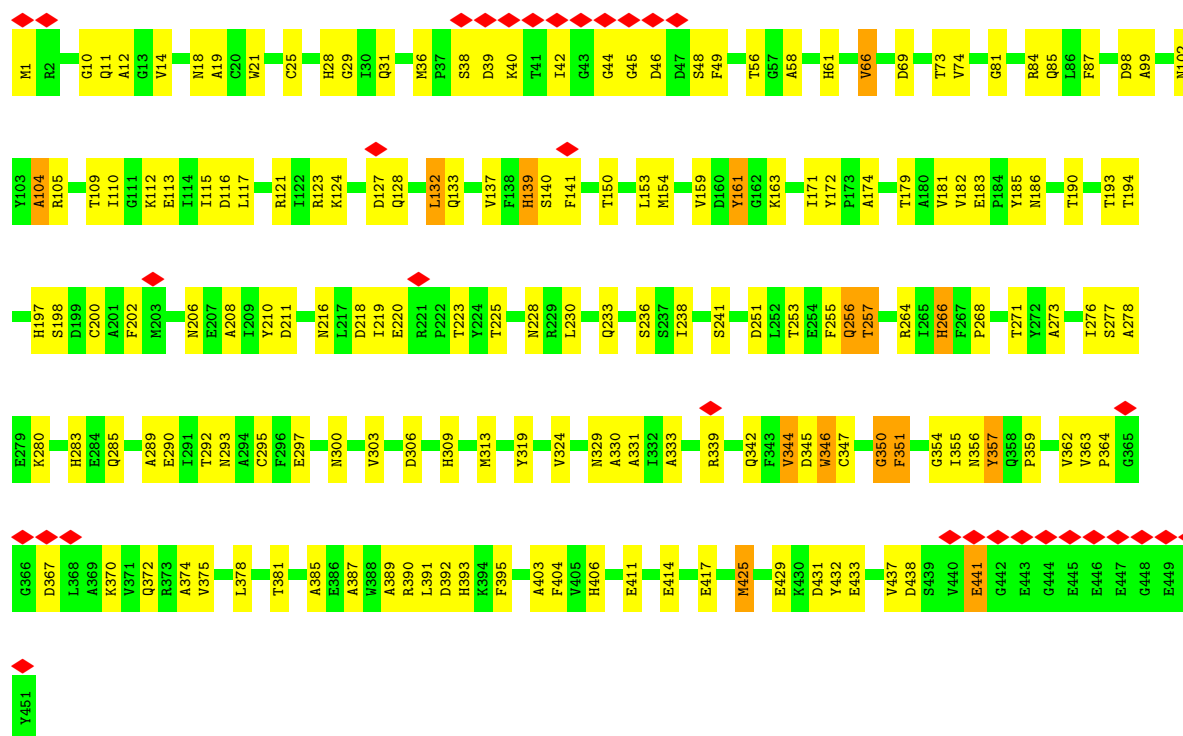


• Molecule 2: Tubulin alpha-1B chain

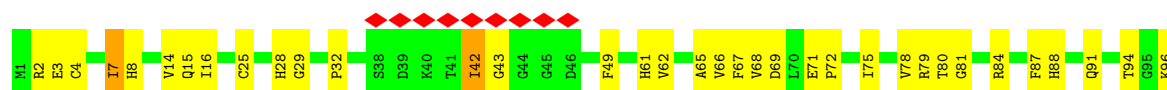


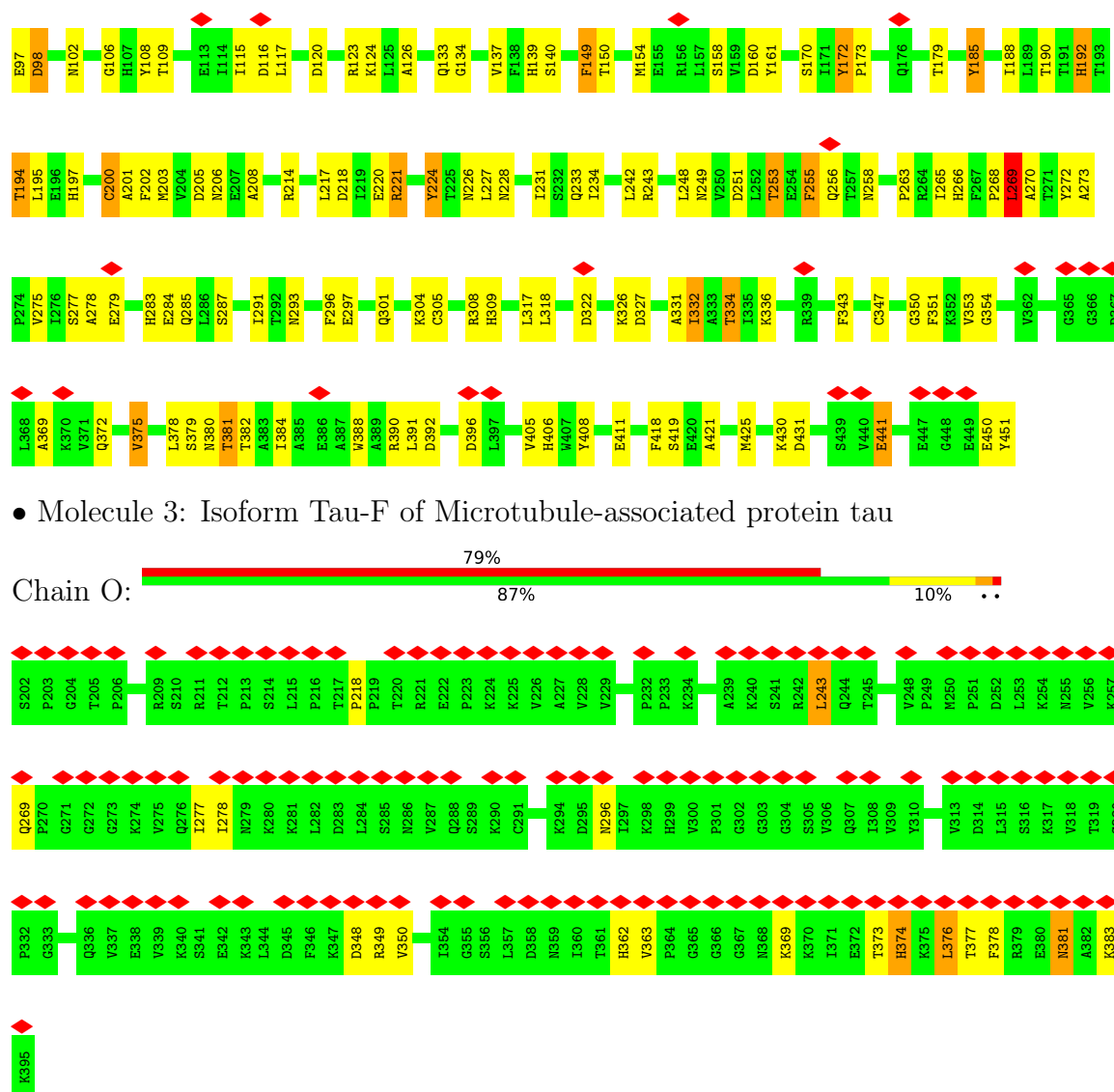


• Molecule 2: Tubulin alpha-1B chain



• Molecule 2: Tubulin alpha-1B chain





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

Chain O: 79% 87% 10% ..

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: GTP, MG, GDP

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	0.64	1/3574 (0.0%)	2.27	163/4839 (3.4%)
1	C	0.71	1/3574 (0.0%)	2.27	192/4839 (4.0%)
1	E	0.70	1/3574 (0.0%)	2.17	151/4839 (3.1%)
1	G	0.71	1/3574 (0.0%)	2.16	157/4839 (3.2%)
1	I	0.69	0/3574	2.03	116/4839 (2.4%)
1	K	0.69	0/3574	2.21	164/4839 (3.4%)
1	M	0.67	1/3574 (0.0%)	2.29	183/4839 (3.8%)
2	B	0.69	1/3603 (0.0%)	2.19	163/4889 (3.3%)
2	D	0.68	0/3603	2.22	175/4889 (3.6%)
2	F	0.65	0/3603	2.28	168/4889 (3.4%)
2	H	0.65	0/3603	2.33	188/4889 (3.8%)
2	J	0.64	0/3603	2.37	202/4889 (4.1%)
2	L	0.63	0/3603	2.31	207/4889 (4.2%)
2	N	0.64	0/3603	2.36	195/4889 (4.0%)
3	O	0.95	0/1483	1.69	29/1996 (1.5%)
All	All	0.68	6/51722 (0.0%)	2.23	2453/70092 (3.5%)

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	12
1	C	0	10
1	E	0	7
1	G	0	5
1	I	0	6
1	K	0	4
1	M	0	9
2	B	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	8
2	F	0	11
2	H	0	8
2	J	0	11
2	L	0	12
2	N	0	12
All	All	0	122

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	129	CYS	C-O	-10.29	1.11	1.23
2	B	145	THR	C-O	-7.18	1.15	1.23
1	M	347	ASN	C-O	-6.62	1.16	1.24
1	E	346	PRO	C-O	-6.53	1.16	1.24
1	A	101	TRP	CZ3-CH2	5.86	1.55	1.40
1	G	346	PRO	C-O	-5.37	1.17	1.24

All (2453) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	249	ASN	OD1-CG-ND2	-13.81	108.79	122.60
1	M	11	GLN	OE1-CD-NE2	-12.36	110.25	122.60
2	J	216	ASN	OD1-CG-ND2	-12.28	110.32	122.60
2	J	44	GLY	CA-C-N	11.84	131.92	121.86
2	J	44	GLY	C-N-CA	11.84	131.92	121.86
2	B	245	ASP	CA-CB-CG	11.49	124.09	112.60
1	I	8	GLN	OE1-CD-NE2	-11.31	111.28	122.60
2	D	206	ASN	OD1-CG-ND2	-11.19	111.41	122.60
2	F	348	PRO	N-CA-CB	11.14	114.94	103.25
2	H	146	GLY	CA-C-N	11.06	135.67	120.63
2	H	146	GLY	C-N-CA	11.06	135.67	120.63
2	H	226	ASN	CA-CB-CG	10.73	123.33	112.60
2	L	98	ASP	CA-CB-CG	10.58	123.18	112.60
1	C	31	ASP	CA-CB-CG	10.57	123.17	112.60
1	E	103	LYS	CA-C-N	10.53	131.58	120.00
1	E	103	LYS	C-N-CA	10.53	131.58	120.00
1	K	247	ASN	OD1-CG-ND2	-10.52	112.08	122.60
2	L	197	HIS	CB-CG-CD2	-10.46	117.59	131.20
2	J	358	GLN	OE1-CD-NE2	-10.46	112.14	122.60
2	B	91	GLN	OE1-CD-NE2	-10.36	112.24	122.60
2	N	29	GLY	CA-C-N	10.35	136.02	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	29	GLY	C-N-CA	10.35	136.02	123.19
2	L	81	GLY	O-C-N	-10.31	113.94	122.81
2	N	256	GLN	OE1-CD-NE2	-10.30	112.30	122.60
2	D	306	ASP	CA-C-O	-10.17	112.68	119.29
1	K	276	ARG	N-CA-C	-10.12	100.08	111.82
1	M	230	SER	CA-C-O	-10.08	108.38	119.97
1	K	99	ASN	CA-CB-CG	10.06	122.66	112.60
1	E	43	GLN	OE1-CD-NE2	-10.03	112.57	122.60
2	J	266	HIS	CA-CB-CG	10.00	123.80	113.80
1	M	265	PHE	CA-CB-CG	9.96	123.76	113.80
1	M	181	GLU	CA-C-N	9.82	129.60	119.19
1	M	181	GLU	C-N-CA	9.82	129.60	119.19
1	A	234	SER	CA-C-N	9.81	130.83	119.94
1	A	234	SER	C-N-CA	9.81	130.83	119.94
2	B	418	PHE	CA-CB-CG	9.79	123.59	113.80
2	J	61	HIS	CA-C-N	9.75	129.23	122.60
2	J	61	HIS	C-N-CA	9.75	129.23	122.60
2	L	128	GLN	OE1-CD-NE2	-9.64	112.96	122.60
2	F	353	VAL	CA-C-N	9.57	128.16	121.65
2	F	353	VAL	C-N-CA	9.57	128.16	121.65
2	L	354	GLY	O-C-N	-9.48	115.55	123.23
1	G	408	PHE	CA-CB-CG	9.47	123.27	113.80
3	O	376	LEU	N-CA-C	9.30	124.54	112.26
1	E	227	HIS	ND1-CE1-NE2	9.29	117.69	108.40
1	E	378	PHE	CA-CB-CG	-9.28	104.52	113.80
2	B	226	ASN	OD1-CG-ND2	-9.27	113.33	122.60
1	E	94	GLN	OE1-CD-NE2	-9.25	113.35	122.60
1	G	195	ASN	OD1-CG-ND2	-9.23	113.37	122.60
1	K	320	ARG	CD-NE-CZ	9.23	137.32	124.40
2	N	115	ILE	N-CA-C	9.23	119.28	110.42
1	C	264	HIS	CA-C-O	-9.22	109.07	119.95
1	A	150	LEU	N-CA-C	9.22	120.93	111.07
2	B	363	VAL	N-CA-C	9.21	116.55	108.63
2	H	16	ILE	CA-C-O	9.18	130.49	120.95
1	M	105	HIS	CB-CG-CD2	-9.16	119.29	131.20
1	G	59	TYR	CA-C-N	9.15	131.29	123.33
1	G	59	TYR	C-N-CA	9.15	131.29	123.33
2	H	342	GLN	OE1-CD-NE2	-9.11	113.49	122.60
2	H	46	ASP	CA-C-N	9.07	138.03	121.70
2	H	46	ASP	C-N-CA	9.07	138.03	121.70
1	C	414	ASN	OD1-CG-ND2	-9.04	113.56	122.60
2	N	372	GLN	OE1-CD-NE2	-9.01	113.59	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	GLY	CA-C-O	-9.01	112.49	121.86
1	E	408	PHE	CA-CB-CG	9.00	122.80	113.80
2	D	36	MET	CA-C-O	-8.96	112.56	119.46
1	C	219	THR	CA-C-N	8.96	129.39	120.52
1	C	219	THR	C-N-CA	8.96	129.39	120.52
1	C	30	ILE	CA-C-N	8.96	134.30	120.68
1	C	30	ILE	C-N-CA	8.96	134.30	120.68
1	C	266	PHE	CA-CB-CG	8.95	122.75	113.80
1	G	296	ALA	CA-C-N	8.94	136.14	122.37
1	G	296	ALA	C-N-CA	8.94	136.14	122.37
1	G	329	GLN	OE1-CD-NE2	-8.95	113.66	122.60
1	I	365	ALA	O-C-N	-8.94	112.95	123.41
1	A	137	HIS	CA-CB-CG	8.94	122.74	113.80
1	K	411	ALA	N-CA-C	8.93	121.01	111.28
1	I	194	GLU	N-CA-C	8.92	122.17	111.82
3	O	378	PHE	N-CA-C	8.86	123.45	112.47
1	C	283	ALA	N-CA-C	8.85	121.95	110.53
1	G	394	PHE	CA-CB-CG	8.84	122.64	113.80
1	E	357	PRO	CA-C-N	8.84	128.78	119.85
1	E	357	PRO	C-N-CA	8.84	128.78	119.85
1	E	37	HIS	CB-CG-CD2	-8.84	119.71	131.20
2	H	309	HIS	CA-CB-CG	8.82	122.62	113.80
2	H	93	ILE	O-C-N	-8.82	112.18	122.94
2	F	284	GLU	CA-C-N	8.79	132.77	120.29
2	F	284	GLU	C-N-CA	8.79	132.77	120.29
2	J	36	MET	CA-C-O	-8.79	111.20	120.87
2	B	217	LEU	CA-C-N	8.78	134.54	122.34
2	B	217	LEU	C-N-CA	8.78	134.54	122.34
1	E	171	PRO	CA-C-N	8.77	132.58	120.39
1	E	171	PRO	C-N-CA	8.77	132.58	120.39
1	G	158	GLU	CA-C-N	8.77	129.99	122.28
1	G	158	GLU	C-N-CA	8.77	129.99	122.28
1	A	15	GLN	OE1-CD-NE2	-8.75	113.85	122.60
2	L	113	GLU	CA-C-N	8.74	131.85	122.14
2	L	113	GLU	C-N-CA	8.74	131.85	122.14
1	M	28	HIS	CA-CB-CG	-8.73	105.07	113.80
2	D	35	GLN	OE1-CD-NE2	-8.72	113.88	122.60
1	K	182	PRO	CA-C-N	8.68	132.44	120.63
1	K	182	PRO	C-N-CA	8.68	132.44	120.63
2	D	205	ASP	CA-CB-CG	8.67	121.27	112.60
1	K	94	GLN	OE1-CD-NE2	-8.67	113.93	122.60
2	B	249	ASN	CA-C-N	8.67	135.85	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	249	ASN	C-N-CA	8.67	135.85	122.25
2	J	45	GLY	O-C-N	-8.56	117.52	123.08
1	E	213	ARG	CD-NE-CZ	8.52	136.33	124.40
2	J	46	ASP	O-C-N	-8.49	112.53	122.89
2	N	2	ARG	CD-NE-CZ	8.46	136.25	124.40
1	C	15	GLN	OE1-CD-NE2	-8.46	114.14	122.60
2	B	49	PHE	CA-CB-CG	-8.46	105.34	113.80
1	C	37	HIS	CA-CB-CG	8.45	122.25	113.80
1	C	31	ASP	CA-C-N	8.45	130.40	119.84
1	C	31	ASP	C-N-CA	8.45	130.40	119.84
1	K	19	LYS	CA-C-O	-8.45	109.69	120.00
2	D	33	ASP	CA-CB-CG	8.45	121.05	112.60
2	D	138	PHE	CA-CB-CG	8.44	122.24	113.80
1	G	99	ASN	OD1-CG-ND2	-8.44	114.16	122.60
2	L	277	SER	CA-C-N	8.44	131.59	120.28
2	L	277	SER	C-N-CA	8.44	131.59	120.28
1	A	242	PHE	O-C-N	-8.44	115.89	121.88
1	C	426	GLN	OE1-CD-NE2	-8.43	114.17	122.60
1	M	258	VAL	N-CA-C	8.40	116.47	108.15
1	G	229	VAL	CA-C-O	-8.33	111.80	121.05
2	F	172	TYR	CB-CA-C	8.32	120.16	108.76
2	J	142	GLY	CA-C-N	8.32	128.25	120.34
2	J	142	GLY	C-N-CA	8.32	128.25	120.34
2	H	303	VAL	O-C-N	-8.31	114.23	123.20
2	J	67	PHE	CA-CB-CG	8.30	122.11	113.80
1	E	397	TRP	CA-C-N	8.29	131.71	120.44
1	E	397	TRP	C-N-CA	8.29	131.71	120.44
2	H	16	ILE	O-C-N	-8.28	113.83	121.87
1	C	160	PRO	N-CA-C	8.28	124.14	114.20
1	C	357	PRO	O-C-N	-8.27	111.70	121.46
2	H	68	VAL	O-C-N	-8.27	114.51	123.03
2	N	91	GLN	OE1-CD-NE2	-8.27	114.33	122.60
2	F	192	HIS	CB-CG-CD2	-8.26	120.46	131.20
1	E	155	ILE	N-CA-C	-8.25	102.83	111.58
2	H	173	PRO	O-C-N	-8.24	113.87	123.10
2	N	102	ASN	N-CA-CB	-8.23	96.78	110.37
2	H	367	ASP	CB-CA-C	8.22	122.88	109.07
2	F	104	ALA	N-CA-C	8.21	122.56	112.54
2	D	62	VAL	CA-C-O	-8.20	113.21	119.20
1	E	249	ASP	CA-CB-CG	8.20	120.80	112.60
2	F	15	GLN	OE1-CD-NE2	-8.20	114.40	122.60
1	K	23	VAL	N-CA-CB	8.20	119.23	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	366	THR	CA-CB-CG2	8.20	124.43	110.50
2	D	133	GLN	OE1-CD-NE2	-8.19	114.41	122.60
1	G	74	ASP	CA-C-N	8.19	131.58	120.44
1	G	74	ASP	C-N-CA	8.19	131.58	120.44
1	E	161	ASP	CA-CB-CG	8.19	120.78	112.60
2	L	31	GLN	OE1-CD-NE2	-8.19	114.41	122.60
1	K	400	GLY	CA-C-N	8.17	134.95	122.37
1	K	400	GLY	C-N-CA	8.17	134.95	122.37
2	B	293	ASN	OD1-CG-ND2	-8.16	114.44	122.60
1	K	122	LYS	N-CA-C	-8.16	101.97	111.03
1	C	171	PRO	O-C-N	-8.14	113.98	123.10
2	J	221	ARG	O-C-N	-8.13	114.03	121.42
1	A	60	VAL	CA-C-N	8.12	128.07	120.03
1	A	60	VAL	C-N-CA	8.12	128.07	120.03
1	A	377	LEU	CA-C-N	8.12	131.16	120.28
1	A	377	LEU	C-N-CA	8.12	131.16	120.28
2	D	116	ASP	CA-CB-CG	8.11	120.71	112.60
2	B	228	ASN	CA-CB-CG	8.10	120.70	112.60
1	K	97	ALA	CA-C-O	8.10	127.81	118.90
1	K	375	GLN	CA-C-N	8.08	131.45	120.54
1	K	375	GLN	C-N-CA	8.08	131.45	120.54
2	H	365	GLY	CA-C-N	8.05	129.63	120.53
2	H	365	GLY	C-N-CA	8.05	129.63	120.53
2	J	7	ILE	N-CA-C	8.05	119.69	107.77
3	O	369	LYS	CA-C-N	8.05	136.20	121.70
3	O	369	LYS	C-N-CA	8.05	136.20	121.70
1	A	422	TYR	O-C-N	-8.04	111.77	122.23
1	C	61	PRO	N-CA-CB	8.02	110.78	103.33
2	D	419	SER	CA-C-O	-8.01	112.45	120.70
1	C	195	ASN	CA-CB-CG	8.01	120.61	112.60
2	N	283	HIS	CA-CB-CG	-7.99	105.81	113.80
2	D	368	LEU	CB-CA-C	7.99	122.67	109.89
1	I	365	ALA	CA-C-O	7.98	130.36	120.54
2	H	285	GLN	OE1-CD-NE2	-7.97	114.63	122.60
1	M	264	HIS	CB-CG-CD2	-7.97	120.84	131.20
1	M	415	MET	O-C-N	-7.97	113.67	122.12
1	A	134	GLN	OE1-CD-NE2	-7.96	114.64	122.60
2	J	285	GLN	OE1-CD-NE2	-7.96	114.64	122.60
1	C	384	GLN	OE1-CD-NE2	-7.93	114.67	122.60
2	H	283	HIS	CB-CG-CD2	-7.92	120.90	131.20
2	H	61	HIS	CA-CB-CG	-7.92	105.88	113.80
2	B	348	PRO	N-CA-CB	7.91	111.56	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	359	PRO	CA-C-N	7.91	129.15	119.98
2	L	359	PRO	C-N-CA	7.91	129.15	119.98
1	E	370	ASN	CA-CB-CG	7.90	120.50	112.60
1	C	304	ASP	CA-C-N	7.90	128.08	119.87
1	C	304	ASP	C-N-CA	7.90	128.08	119.87
2	J	186	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	K	293	MET	CA-C-O	-7.87	112.56	120.82
2	N	297	GLU	CA-C-N	7.86	128.28	119.32
2	N	297	GLU	C-N-CA	7.86	128.28	119.32
2	D	208	ALA	O-C-N	-7.85	113.20	122.15
2	H	372	GLN	OE1-CD-NE2	-7.85	114.75	122.60
2	F	115	ILE	N-CA-C	7.85	118.63	110.62
3	O	392	ILE	CA-C-N	7.85	136.09	121.97
3	O	392	ILE	C-N-CA	7.85	136.09	121.97
1	C	262	ARG	CB-CA-C	7.84	119.70	109.28
2	L	197	HIS	CB-CG-ND1	7.84	134.46	122.70
1	E	7	ILE	CA-C-N	7.84	133.03	122.84
1	E	7	ILE	C-N-CA	7.84	133.03	122.84
1	C	92	PHE	N-CA-C	7.83	121.29	108.99
1	E	6	HIS	CB-CG-CD2	-7.81	121.05	131.20
2	J	379	SER	CA-C-N	7.81	133.20	122.19
2	J	379	SER	C-N-CA	7.81	133.20	122.19
2	B	304	LYS	N-CA-C	7.80	121.89	112.38
2	F	233	GLN	OE1-CD-NE2	-7.80	114.80	122.60
1	K	163	ILE	CB-CA-C	7.78	124.05	111.29
2	N	32	PRO	N-CA-C	7.78	124.01	113.98
1	E	99	ASN	OD1-CG-ND2	-7.78	114.82	122.60
2	J	203	MET	CA-C-N	7.77	132.37	121.96
2	J	203	MET	C-N-CA	7.77	132.37	121.96
2	J	302	MET	CA-C-N	7.77	132.82	123.19
2	J	302	MET	C-N-CA	7.77	132.82	123.19
3	O	388	HIS	CB-CG-CD2	-7.76	121.11	131.20
1	C	313	VAL	CA-C-N	7.76	135.00	122.81
1	C	313	VAL	C-N-CA	7.76	135.00	122.81
1	M	100	ASN	CA-CB-CG	7.75	120.35	112.60
1	I	320	ARG	CA-C-O	-7.74	112.62	120.98
2	F	87	PHE	CA-CB-CG	7.74	121.54	113.80
2	J	18	ASN	OD1-CG-ND2	-7.73	114.87	122.60
1	K	276	ARG	O-C-N	-7.73	112.76	122.27
2	F	291	ILE	O-C-N	-7.71	113.89	121.83
2	N	408	TYR	CA-C-O	7.71	128.59	120.42
2	B	249	ASN	OD1-CG-ND2	-7.71	114.89	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	94	THR	CA-C-N	7.71	129.90	122.27
2	J	94	THR	C-N-CA	7.71	129.90	122.27
2	B	392	ASP	CA-CB-CG	7.71	120.31	112.60
1	E	178	THR	CA-CB-CG2	7.70	123.59	110.50
1	G	383	GLU	N-CA-C	7.70	121.94	112.23
2	J	69	ASP	OD1-CG-OD2	-7.70	104.41	122.90
2	H	266	HIS	CA-CB-CG	7.70	121.50	113.80
1	E	116	VAL	O-C-N	-7.70	113.89	121.90
2	F	25	CYS	N-CA-C	-7.70	102.58	110.97
2	J	156	ARG	CA-C-O	-7.68	112.78	120.70
1	C	245	GLN	N-CA-C	-7.68	102.85	111.14
2	H	110	ILE	CA-C-N	7.68	128.63	120.03
2	H	110	ILE	C-N-CA	7.68	128.63	120.03
1	C	242	PHE	O-C-N	7.67	126.62	121.71
3	O	383	LYS	N-CA-C	7.67	119.70	110.19
1	G	287	PRO	N-CA-CB	7.66	112.00	103.26
1	K	209	ASP	CA-CB-CG	-7.65	104.95	112.60
1	M	230	SER	O-C-N	7.64	131.67	122.27
1	G	88	ASP	CA-CB-CG	7.62	120.22	112.60
2	L	392	ASP	CA-CB-CG	7.62	120.22	112.60
1	A	89	ASN	CA-CB-CG	7.61	120.21	112.60
2	F	205	ASP	CA-CB-CG	7.61	120.21	112.60
2	F	267	PHE	CA-CB-CG	7.60	121.40	113.80
2	J	406	HIS	CB-CG-CD2	-7.59	121.33	131.20
2	B	395	PHE	CA-C-O	-7.59	113.03	121.00
2	N	228	ASN	OD1-CG-ND2	-7.58	115.02	122.60
2	F	290	GLU	CB-CG-CD	-7.57	99.73	112.60
1	M	64	ILE	CB-CA-C	7.57	121.83	110.63
1	C	368	ILE	O-C-N	-7.56	115.01	123.10
2	D	15	GLN	OE1-CD-NE2	-7.56	115.04	122.60
2	J	214	ARG	CA-C-N	7.55	130.26	120.44
2	J	214	ARG	C-N-CA	7.55	130.26	120.44
2	N	137	VAL	O-C-N	-7.54	115.27	123.03
2	D	367	ASP	CA-CB-CG	7.54	120.14	112.60
1	G	21	TRP	N-CA-C	7.54	122.23	112.89
1	G	88	ASP	CA-C-O	-7.53	109.97	119.31
1	K	66	VAL	N-CA-C	7.53	119.45	108.53
3	O	377	THR	CA-C-N	7.53	134.35	122.61
3	O	377	THR	C-N-CA	7.53	134.35	122.61
1	I	335	ASN	OD1-CG-ND2	-7.52	115.08	122.60
2	N	283	HIS	CB-CG-CD2	-7.51	121.43	131.20
1	A	398	TYR	CB-CA-C	-7.51	99.03	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	247	ASN	OD1-CG-ND2	-7.51	115.09	122.60
2	L	139	HIS	CB-CG-CD2	-7.51	121.44	131.20
1	I	307	HIS	CA-CB-CG	-7.51	106.29	113.80
1	G	43	GLN	OE1-CD-NE2	-7.50	115.10	122.60
2	H	388	TRP	CA-CB-CG	7.50	127.85	113.60
1	I	37	HIS	O-C-N	-7.49	114.58	122.30
1	K	137	HIS	CA-CB-CG	7.49	121.29	113.80
1	K	419	VAL	N-CA-C	-7.47	103.17	110.72
1	M	172	SER	CA-C-O	-7.47	113.88	120.60
2	B	38	SER	CA-C-N	7.47	131.35	120.82
2	B	38	SER	C-N-CA	7.47	131.35	120.82
2	H	285	GLN	CA-C-O	7.46	129.20	120.69
1	M	29	GLY	CA-C-N	7.46	130.50	120.50
1	M	29	GLY	C-N-CA	7.46	130.50	120.50
1	C	206	ALA	CA-C-N	7.46	130.60	120.38
1	C	206	ALA	C-N-CA	7.46	130.60	120.38
2	B	61	HIS	CB-CG-CD2	-7.46	121.50	131.20
1	M	57	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	K	72	THR	CA-CB-CG2	7.45	123.16	110.50
1	M	418	LEU	CA-C-O	-7.45	113.00	120.82
1	C	270	PHE	N-CA-C	7.44	120.68	108.99
2	J	206	ASN	OD1-CG-ND2	-7.44	115.16	122.60
1	K	304	ASP	CA-CB-CG	7.44	120.04	112.60
1	I	208	TYR	O-C-N	-7.43	114.36	122.09
2	D	66	VAL	CA-C-N	7.42	133.46	123.00
2	D	66	VAL	C-N-CA	7.42	133.46	123.00
1	C	44	LEU	N-CA-C	7.41	121.17	112.72
2	L	14	VAL	CA-CB-CG1	7.41	122.99	110.40
2	D	159	VAL	N-CA-CB	7.41	118.69	110.62
2	D	283	HIS	CA-CB-CG	-7.40	106.40	113.80
2	L	403	ALA	CA-C-N	7.39	135.66	121.54
2	L	403	ALA	C-N-CA	7.39	135.66	121.54
1	C	63	ALA	CA-C-N	7.39	132.93	123.10
1	C	63	ALA	C-N-CA	7.39	132.93	123.10
1	C	203	ASP	CA-CB-CG	7.38	119.98	112.60
1	I	211	CYS	N-CA-C	7.38	120.02	111.02
1	E	227	HIS	CE1-NE2-CD2	-7.36	101.64	109.00
2	L	438	ASP	CA-CB-CG	-7.35	105.25	112.60
1	M	279	GLN	OE1-CD-NE2	-7.35	115.25	122.60
2	H	197	HIS	CB-CG-CD2	-7.34	121.66	131.20
2	J	354	GLY	CA-C-O	-7.34	113.59	120.57
1	E	83	GLN	OE1-CD-NE2	-7.34	115.26	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	178	THR	CA-C-N	7.33	129.94	120.56
1	C	178	THR	C-N-CA	7.33	129.94	120.56
1	I	368	ILE	O-C-N	-7.33	115.48	123.03
2	N	67	PHE	CA-CB-CG	7.33	121.12	113.80
2	L	102	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	A	379	LYS	O-C-N	7.32	129.60	122.07
2	D	37	PRO	N-CA-CB	7.30	111.62	103.44
2	F	147	SER	CA-C-N	7.30	129.49	120.22
2	F	147	SER	C-N-CA	7.30	129.49	120.22
2	J	91	GLN	OE1-CD-NE2	-7.29	115.31	122.60
2	L	36	MET	CA-C-O	-7.29	114.06	120.19
1	E	9	ALA	N-CA-C	7.29	120.77	108.02
2	N	109	THR	N-CA-C	7.28	120.26	111.82
2	D	141	PHE	CA-CB-CG	7.27	121.07	113.80
1	A	183	TYR	CB-CA-C	-7.26	99.49	110.88
1	E	191	GLN	OE1-CD-NE2	-7.25	115.35	122.60
2	B	18	ASN	OD1-CG-ND2	-7.25	115.35	122.60
2	J	337	THR	N-CA-C	-7.25	103.31	111.07
2	L	441	GLU	CA-C-O	7.24	129.32	120.55
2	H	206	ASN	OD1-CG-ND2	-7.24	115.36	122.60
2	L	342	GLN	OE1-CD-NE2	-7.24	115.36	122.60
1	A	229	VAL	CA-C-N	7.22	129.82	120.44
1	A	229	VAL	C-N-CA	7.22	129.82	120.44
2	B	260	VAL	CA-C-N	7.22	127.83	120.04
2	B	260	VAL	C-N-CA	7.22	127.83	120.04
1	E	387	ALA	CA-C-N	7.21	129.81	120.44
1	E	387	ALA	C-N-CA	7.21	129.81	120.44
2	N	277	SER	N-CA-C	7.20	119.87	110.43
1	C	256	ASN	OD1-CG-ND2	-7.20	115.40	122.60
1	K	288	GLU	N-CA-C	7.20	119.13	111.28
2	F	46	ASP	O-C-N	-7.20	114.93	123.28
2	N	139	HIS	N-CA-C	7.19	120.27	108.99
1	A	422	TYR	CA-C-O	7.18	128.21	120.24
2	N	88	HIS	CA-CB-CG	7.17	120.97	113.80
2	L	292	THR	CA-CB-OG1	-7.17	98.84	109.60
1	I	23	VAL	CA-C-O	-7.17	113.10	121.05
2	B	47	ASP	CA-CB-CG	7.16	119.76	112.60
1	C	37	HIS	CB-CG-CD2	-7.15	121.91	131.20
2	J	355	ILE	CA-C-O	-7.14	111.85	120.78
1	K	279	GLN	OE1-CD-NE2	-7.14	115.46	122.60
2	L	223	THR	CA-C-O	-7.14	113.29	121.72
2	D	173	PRO	N-CA-CB	7.14	109.97	103.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	285	GLN	OE1-CD-NE2	-7.14	115.46	122.60
1	A	278	SER	CA-C-N	7.14	132.02	120.60
1	A	278	SER	C-N-CA	7.14	132.02	120.60
2	H	72	PRO	CA-C-N	7.14	130.56	120.28
2	H	72	PRO	C-N-CA	7.14	130.56	120.28
1	M	23	VAL	CA-CB-CG1	7.14	122.53	110.40
2	J	347	CYS	CA-C-O	-7.12	113.97	119.46
1	K	245	GLN	CA-C-O	7.12	127.61	119.27
2	J	143	GLY	CA-C-N	7.12	129.26	120.22
2	J	143	GLY	C-N-CA	7.12	129.26	120.22
1	E	380	ARG	CA-C-O	-7.12	113.37	120.70
2	H	325	PRO	N-CA-CB	7.11	111.07	103.39
1	A	37	HIS	CA-C-O	7.11	126.65	119.97
2	H	332	ILE	CA-CB-CG1	7.11	122.48	110.40
1	I	77	ARG	CB-CA-C	7.10	122.02	110.88
2	F	76	ASP	CA-CB-CG	7.08	119.68	112.60
2	H	255	PHE	CA-C-O	-7.08	113.28	121.07
2	B	204	VAL	CA-C-O	-7.08	113.07	121.28
2	L	11	GLN	OE1-CD-NE2	-7.08	115.52	122.60
2	N	62	VAL	CA-C-N	7.07	127.11	119.90
2	N	62	VAL	C-N-CA	7.07	127.11	119.90
2	H	301	GLN	OE1-CD-NE2	-7.07	115.53	122.60
1	G	216	LYS	CA-C-N	7.06	131.40	121.24
1	G	216	LYS	C-N-CA	7.06	131.40	121.24
2	J	267	PHE	CA-CB-CG	7.05	120.85	113.80
2	D	61	HIS	CA-C-N	7.05	130.35	123.02
2	D	61	HIS	C-N-CA	7.05	130.35	123.02
2	H	361	THR	O-C-N	-7.05	114.00	123.10
1	K	206	ALA	CA-C-N	7.04	129.71	120.28
1	K	206	ALA	C-N-CA	7.04	129.71	120.28
2	B	363	VAL	CA-C-N	7.04	126.80	119.76
2	B	363	VAL	C-N-CA	7.04	126.80	119.76
2	J	436	GLY	CA-C-N	7.04	129.93	120.50
2	J	436	GLY	C-N-CA	7.04	129.93	120.50
1	K	184	ASN	OD1-CG-ND2	-7.03	115.57	122.60
2	F	51	THR	CA-CB-OG1	7.03	120.15	109.60
1	A	396	HIS	CB-CG-CD2	-7.03	122.06	131.20
2	N	206	ASN	CA-C-O	-7.02	113.44	120.82
2	N	379	SER	N-CA-C	7.02	121.00	109.06
2	J	296	PHE	CA-C-O	7.01	126.76	119.05
2	L	433	GLU	CA-C-N	7.00	129.66	120.28
2	L	433	GLU	C-N-CA	7.00	129.66	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	203	ASP	CA-CB-CG	7.00	119.60	112.60
2	N	2	ARG	CA-C-O	-7.00	113.75	121.23
1	E	41	ASP	CA-CB-CG	6.99	119.59	112.60
2	J	228	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	M	270	PHE	CA-C-O	6.99	129.29	121.11
1	E	242	PHE	CA-C-N	6.99	126.98	119.78
1	E	242	PHE	C-N-CA	6.99	126.98	119.78
2	L	115	ILE	O-C-N	-6.99	114.41	121.96
1	M	37	HIS	ND1-CG-CD2	6.99	113.09	106.10
1	G	206	ALA	CA-C-N	6.98	129.94	120.44
1	G	206	ALA	C-N-CA	6.98	129.94	120.44
1	G	107	THR	N-CA-C	6.98	119.22	108.12
1	G	423	GLN	OE1-CD-NE2	-6.98	115.62	122.60
2	B	341	ILE	CB-CA-C	6.97	118.95	111.35
1	I	121	ARG	CA-C-O	-6.97	113.16	120.55
2	D	393	HIS	ND1-CG-CD2	6.96	113.06	106.10
2	J	382	THR	O-C-N	-6.96	114.07	122.22
1	K	205	GLU	CA-C-O	6.96	127.94	119.38
2	D	172	TYR	CA-C-N	6.96	127.51	119.99
2	D	172	TYR	C-N-CA	6.96	127.51	119.99
2	F	74	VAL	CA-C-N	6.96	134.50	121.97
2	F	74	VAL	C-N-CA	6.96	134.50	121.97
1	G	145	SER	O-C-N	6.96	129.61	122.09
2	L	276	ILE	CB-CA-C	6.96	120.75	111.21
3	O	393	VAL	N-CA-C	6.96	123.82	109.34
1	E	396	HIS	ND1-CE1-NE2	6.96	115.36	108.40
1	E	92	PHE	CA-CB-CG	6.95	120.75	113.80
1	A	384	GLN	OE1-CD-NE2	-6.95	115.65	122.60
1	M	400	GLY	O-C-N	-6.95	114.78	122.84
1	A	376	GLU	CA-C-N	6.94	129.81	120.65
1	A	376	GLU	C-N-CA	6.94	129.81	120.65
1	E	99	ASN	CB-CG-ND2	6.94	126.82	116.40
2	F	197	HIS	CB-CG-CD2	-6.94	122.17	131.20
1	K	16	ILE	CA-C-O	-6.94	113.14	120.57
1	E	180	VAL	CA-C-N	6.94	129.74	120.58
1	E	180	VAL	C-N-CA	6.94	129.74	120.58
1	E	81	PHE	CA-C-N	6.94	129.03	120.22
1	E	81	PHE	C-N-CA	6.94	129.03	120.22
3	O	381	ASN	CA-CB-CG	6.94	119.54	112.60
1	A	379	LYS	CA-C-O	-6.93	113.54	120.82
2	D	130	THR	CA-CB-CG2	6.93	122.29	110.50
2	D	73	THR	O-C-N	-6.93	112.09	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	65	ALA	CA-C-O	-6.92	112.88	120.36
2	F	233	GLN	CA-C-N	6.92	129.42	120.56
2	F	233	GLN	C-N-CA	6.92	129.42	120.56
2	N	15	GLN	OE1-CD-NE2	-6.92	115.68	122.60
1	E	104	GLY	CA-C-O	-6.92	113.33	120.66
2	N	218	ASP	CA-C-N	6.92	133.32	121.63
2	N	218	ASP	C-N-CA	6.92	133.32	121.63
2	F	20	CYS	CA-C-N	6.91	130.11	120.29
2	F	20	CYS	C-N-CA	6.91	130.11	120.29
2	N	268	PRO	N-CA-C	6.91	122.08	111.57
2	D	449	GLU	CA-C-N	6.91	134.42	122.81
2	D	449	GLU	C-N-CA	6.91	134.42	122.81
2	F	291	ILE	CA-C-N	6.91	129.42	120.44
2	F	291	ILE	C-N-CA	6.91	129.42	120.44
1	E	39	ASP	CA-CB-CG	6.90	119.50	112.60
1	G	376	GLU	CA-C-N	6.90	130.38	120.79
1	G	376	GLU	C-N-CA	6.90	130.38	120.79
2	N	87	PHE	CA-CB-CG	-6.90	106.90	113.80
1	C	305	PRO	CA-C-N	6.90	133.22	121.14
1	C	305	PRO	C-N-CA	6.90	133.22	121.14
1	K	396	HIS	CB-CG-CD2	-6.90	122.23	131.20
2	H	358	GLN	CA-C-N	6.89	127.47	120.38
2	H	358	GLN	C-N-CA	6.89	127.47	120.38
2	B	336	LYS	CA-C-N	6.89	132.36	120.58
2	B	336	LYS	C-N-CA	6.89	132.36	120.58
2	F	111	GLY	CA-C-O	6.88	127.87	120.30
2	J	393	HIS	CA-CB-CG	6.88	120.69	113.80
2	H	361	THR	CA-CB-CG2	6.88	122.19	110.50
1	K	368	ILE	CA-C-N	6.88	126.92	122.18
1	K	368	ILE	C-N-CA	6.88	126.92	122.18
2	H	362	VAL	N-CA-C	6.87	119.03	109.55
2	H	219	ILE	CB-CA-C	6.87	119.92	110.99
1	C	81	PHE	CA-CB-CG	-6.86	106.94	113.80
1	I	194	GLU	N-CA-CB	-6.86	99.65	110.28
2	J	278	ALA	O-C-N	-6.86	115.00	122.07
2	D	132	LEU	N-CA-C	-6.86	99.67	109.96
2	L	1	MET	CB-CA-C	6.86	123.13	110.10
1	M	419	VAL	CA-C-N	6.86	130.03	120.29
1	M	419	VAL	C-N-CA	6.86	130.03	120.29
1	A	227	HIS	CB-CG-CD2	-6.86	122.29	131.20
2	D	28	HIS	CB-CG-CD2	-6.85	122.30	131.20
1	E	109	GLY	O-C-N	-6.85	114.94	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	128	ASP	CB-CA-C	6.85	121.56	110.95
2	H	235	VAL	N-CA-C	6.85	119.61	111.05
2	B	192	HIS	CA-CB-CG	6.84	120.64	113.80
1	I	317	PHE	CA-CB-CG	6.84	120.64	113.80
1	E	260	PHE	CA-C-N	6.83	126.52	119.82
1	E	260	PHE	C-N-CA	6.83	126.52	119.82
2	D	267	PHE	CA-CB-CG	6.83	120.62	113.80
2	N	256	GLN	CG-CD-NE2	6.82	126.63	116.40
1	G	301	ALA	CA-C-N	6.81	133.06	121.14
1	G	301	ALA	C-N-CA	6.81	133.06	121.14
1	C	357	PRO	CA-C-N	6.81	127.20	119.92
1	C	357	PRO	C-N-CA	6.81	127.20	119.92
1	A	30	ILE	CA-C-N	6.81	129.85	120.39
1	A	30	ILE	C-N-CA	6.81	129.85	120.39
1	K	170	VAL	CA-C-N	6.81	126.77	119.76
1	K	170	VAL	C-N-CA	6.81	126.77	119.76
2	H	85	GLN	OE1-CD-NE2	-6.80	115.80	122.60
2	L	10	GLY	CA-C-O	-6.80	116.31	122.57
1	M	119	VAL	N-CA-C	6.80	117.58	110.72
1	M	51	TYR	CA-C-N	6.79	133.13	122.94
1	M	51	TYR	C-N-CA	6.79	133.13	122.94
2	N	381	THR	CA-CB-CG2	6.79	122.04	110.50
1	A	414	ASN	CA-C-N	6.79	129.67	120.44
1	A	414	ASN	C-N-CA	6.79	129.67	120.44
1	K	385	PHE	CA-CB-CG	-6.79	107.01	113.80
2	F	154	MET	N-CA-CB	6.79	120.24	110.06
2	H	209	ILE	CA-C-O	-6.78	113.32	120.57
2	N	301	GLN	OE1-CD-NE2	-6.77	115.83	122.60
2	B	179	THR	CA-C-O	-6.77	111.59	119.78
1	A	145	SER	CA-C-O	6.76	127.92	120.82
1	A	357	PRO	N-CA-CB	6.76	109.64	103.08
2	L	141	PHE	CA-CB-CG	6.76	120.56	113.80
1	A	395	LEU	CA-C-N	6.76	130.01	120.28
1	A	395	LEU	C-N-CA	6.76	130.01	120.28
1	K	200	TYR	CA-C-N	6.76	131.43	122.30
1	K	200	TYR	C-N-CA	6.76	131.43	122.30
2	L	123	ARG	O-C-N	-6.76	113.96	122.27
1	K	298	ASN	OD1-CG-ND2	-6.76	115.84	122.60
2	L	347	CYS	O-C-N	-6.76	115.27	121.42
2	L	39	ASP	CA-CB-CG	6.75	119.35	112.60
1	M	149	THR	N-CA-CB	6.75	119.79	110.01
2	B	160	ASP	CA-CB-CG	6.74	119.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	238	THR	O-C-N	-6.74	114.81	122.09
1	I	286	VAL	CA-CB-CG1	6.74	121.86	110.40
2	D	168	GLU	O-C-N	-6.74	115.17	123.33
1	K	190	HIS	CB-CG-CD2	-6.74	122.44	131.20
2	N	343	PHE	CA-CB-CG	6.74	120.53	113.80
2	F	18	ASN	CA-CB-CG	6.73	119.33	112.60
1	A	131	GLN	CG-CD-NE2	6.73	126.49	116.40
2	J	121	ARG	CA-C-N	6.73	130.36	120.74
2	J	121	ARG	C-N-CA	6.73	130.36	120.74
1	A	228	LEU	CA-C-N	6.73	129.67	120.46
1	A	228	LEU	C-N-CA	6.73	129.67	120.46
2	L	198	SER	CA-C-O	-6.72	113.87	121.81
2	N	61	HIS	O-C-N	-6.72	115.53	123.06
1	M	43	GLN	OE1-CD-NE2	-6.72	115.88	122.60
2	D	8	HIS	ND1-CG-CD2	6.72	112.82	106.10
2	J	19	ALA	CB-CA-C	6.71	120.93	109.65
1	M	3	GLU	CA-C-O	6.71	127.36	120.24
1	G	190	HIS	CB-CG-CD2	-6.71	122.47	131.20
2	N	283	HIS	CB-CG-ND1	6.71	132.77	122.70
2	J	50	ASN	OD1-CG-ND2	-6.71	115.89	122.60
2	B	374	ALA	N-CA-C	6.70	119.26	109.07
2	H	148	GLY	CA-C-O	-6.70	112.92	120.09
1	E	243	PRO	N-CA-CB	6.70	109.18	103.35
2	J	128	GLN	OE1-CD-NE2	-6.70	115.90	122.60
2	J	443	GLU	N-CA-C	6.70	121.06	113.02
1	M	143	THR	N-CA-C	6.70	118.46	111.03
1	C	83	GLN	OE1-CD-NE2	-6.69	115.91	122.60
2	H	49	PHE	CA-C-N	6.69	129.24	120.28
2	H	49	PHE	C-N-CA	6.69	129.24	120.28
2	H	130	THR	N-CA-CB	6.68	120.05	110.16
1	C	304	ASP	O-C-N	-6.68	114.42	121.30
2	F	182	VAL	CA-C-N	6.68	128.44	120.09
2	F	182	VAL	C-N-CA	6.68	128.44	120.09
1	G	197	ASP	N-CA-C	6.67	121.55	113.41
2	B	398	MET	N-CA-C	6.67	118.63	111.36
1	A	248	ALA	N-CA-C	6.67	118.53	107.20
1	M	105	HIS	CB-CG-ND1	6.66	132.69	122.70
1	K	115	SER	CA-C-N	6.66	131.51	121.65
1	K	115	SER	C-N-CA	6.66	131.51	121.65
1	I	313	VAL	O-C-N	-6.66	115.67	123.00
1	G	387	ALA	N-CA-C	6.65	119.54	111.82
1	K	264	HIS	CA-C-N	6.65	131.26	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	264	HIS	C-N-CA	6.65	131.26	122.42
2	N	220	GLU	N-CA-C	6.65	118.53	111.28
2	B	407	TRP	CA-C-O	6.64	127.61	119.97
2	N	117	LEU	N-CA-C	6.64	119.08	111.11
1	G	80	PRO	O-C-N	-6.63	114.78	123.01
2	B	63	PRO	N-CA-CB	6.63	109.09	103.25
2	D	120	ASP	CA-C-O	6.63	127.59	120.10
2	N	251	ASP	CA-C-N	6.63	129.47	120.38
2	N	251	ASP	C-N-CA	6.63	129.47	120.38
1	A	307	HIS	CB-CG-CD2	-6.63	122.58	131.20
1	E	303	CYS	O-C-N	-6.63	114.81	123.16
1	K	260	PHE	CA-C-N	6.63	128.12	119.84
1	K	260	PHE	C-N-CA	6.63	128.12	119.84
2	B	18	ASN	CA-CB-CG	6.62	119.22	112.60
1	M	169	VAL	CB-CA-C	6.62	120.32	110.98
1	G	147	MET	CA-C-N	6.62	127.16	119.94
1	G	147	MET	C-N-CA	6.62	127.16	119.94
2	L	104	ALA	CB-CA-C	6.62	121.37	110.90
1	M	208	TYR	N-CA-C	-6.61	104.15	111.36
1	M	177	ASP	CA-C-N	6.61	133.19	122.29
1	M	177	ASP	C-N-CA	6.61	133.19	122.29
2	N	309	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	A	326	VAL	N-CA-C	6.61	116.74	110.53
2	D	139	HIS	N-CA-C	6.61	117.86	108.74
1	K	374	ILE	CA-CB-CG1	6.61	121.63	110.40
2	D	266	HIS	ND1-CG-CD2	6.60	112.70	106.10
2	F	245	ASP	CA-CB-CG	6.60	119.20	112.60
2	J	159	VAL	N-CA-CB	6.60	117.81	110.62
2	H	144	GLY	O-C-N	6.59	128.59	122.19
1	M	76	VAL	N-CA-C	-6.59	104.06	110.72
1	A	170	VAL	CA-CB-CG2	6.59	121.60	110.40
2	D	393	HIS	ND1-CE1-NE2	6.59	114.99	108.40
2	L	387	ALA	CA-C-N	6.59	129.64	120.29
2	L	387	ALA	C-N-CA	6.59	129.64	120.29
1	C	60	VAL	CA-C-N	6.58	126.50	119.85
1	C	60	VAL	C-N-CA	6.58	126.50	119.85
2	H	25	CYS	CB-CA-C	6.58	121.22	110.88
2	H	78	VAL	N-CA-CB	6.58	119.00	110.57
2	H	388	TRP	O-C-N	6.58	128.94	122.09
2	N	205	ASP	CA-CB-CG	6.58	119.18	112.60
2	N	266	HIS	CA-CB-CG	6.58	120.38	113.80
1	G	23	VAL	CA-C-O	-6.58	113.67	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	181	VAL	CA-CB-CG2	6.58	121.59	110.40
2	N	375	VAL	CB-CA-C	-6.58	100.37	110.50
1	G	110	ALA	CA-C-O	-6.58	111.53	119.49
2	L	206	ASN	OD1-CG-ND2	-6.57	116.03	122.60
2	J	251	ASP	CA-C-N	6.56	129.73	120.28
2	J	251	ASP	C-N-CA	6.56	129.73	120.28
2	N	4	CYS	CA-C-N	6.56	132.52	122.68
2	N	4	CYS	C-N-CA	6.56	132.52	122.68
2	L	374	ALA	N-CA-C	6.56	118.91	109.14
2	F	384	ILE	CA-CB-CG1	6.55	121.54	110.40
1	I	365	ALA	N-CA-C	6.55	119.96	108.75
1	I	94	GLN	OE1-CD-NE2	-6.55	116.05	122.60
2	L	256	GLN	N-CA-CB	6.55	119.51	110.01
2	N	405	VAL	CA-C-O	6.55	127.58	120.57
1	M	17	GLY	CA-C-N	6.54	129.71	120.28
1	M	17	GLY	C-N-CA	6.54	129.71	120.28
1	G	280	GLN	OE1-CD-NE2	-6.54	116.06	122.60
2	B	375	VAL	O-C-N	-6.54	115.79	123.05
2	H	429	GLU	N-CA-CB	-6.54	100.14	110.28
2	J	205	ASP	CA-C-N	6.54	131.59	121.19
2	J	205	ASP	C-N-CA	6.54	131.59	121.19
1	I	15	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	M	165	ASN	CA-CB-CG	6.54	119.14	112.60
2	L	81	GLY	CA-C-N	6.53	130.24	120.31
2	L	81	GLY	C-N-CA	6.53	130.24	120.31
1	C	360	GLY	N-CA-C	6.53	124.02	115.40
1	E	86	ARG	CA-C-N	6.53	126.22	119.82
1	E	86	ARG	C-N-CA	6.53	126.22	119.82
1	K	218	THR	N-CA-C	-6.53	104.00	112.68
1	E	189	VAL	CA-C-N	6.52	129.02	120.28
1	E	189	VAL	C-N-CA	6.52	129.02	120.28
2	L	133	GLN	OE1-CD-NE2	-6.52	116.08	122.60
2	J	8	HIS	CA-C-O	-6.52	113.76	120.54
1	K	276	ARG	CD-NE-CZ	6.52	133.53	124.40
1	I	88	ASP	CA-CB-CG	6.51	119.11	112.60
2	F	25	CYS	O-C-N	-6.51	115.26	122.03
2	H	11	GLN	CG-CD-NE2	6.51	126.17	116.40
1	M	52	ASN	OD1-CG-ND2	-6.51	116.09	122.60
2	J	259	LEU	CA-C-N	6.51	134.17	122.13
2	J	259	LEU	C-N-CA	6.51	134.17	122.13
1	A	225	LEU	CA-C-N	6.51	129.65	120.28
1	A	225	LEU	C-N-CA	6.51	129.65	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	152	ILE	CA-C-N	6.51	129.65	120.28
1	G	152	ILE	C-N-CA	6.51	129.65	120.28
2	J	224	TYR	CA-C-N	6.51	130.20	120.31
2	J	224	TYR	C-N-CA	6.51	130.20	120.31
1	K	204	ASN	CA-CB-CG	6.50	119.11	112.60
2	H	129	CYS	CA-C-N	6.50	129.53	120.29
2	H	129	CYS	C-N-CA	6.50	129.53	120.29
1	I	31	ASP	CA-C-O	-6.50	114.75	120.60
1	A	198	GLU	O-C-N	-6.50	116.46	123.42
3	O	277	ILE	CA-C-N	6.50	133.40	121.70
3	O	277	ILE	C-N-CA	6.50	133.40	121.70
2	F	333	ALA	O-C-N	6.50	129.01	122.12
2	D	142	GLY	CA-C-N	6.50	128.37	122.20
2	D	142	GLY	C-N-CA	6.50	128.37	122.20
2	F	96	LYS	N-CA-CB	-6.50	99.51	110.49
2	J	16	ILE	CB-CA-C	6.50	120.94	112.24
2	H	96	LYS	CA-C-N	6.49	133.94	121.54
2	H	96	LYS	C-N-CA	6.49	133.94	121.54
2	N	226	ASN	OD1-CG-ND2	-6.49	116.11	122.60
2	H	335	ILE	CA-C-O	-6.49	114.20	120.95
2	N	354	GLY	CA-C-N	6.49	133.65	121.97
2	N	354	GLY	C-N-CA	6.49	133.65	121.97
2	H	40	LYS	CA-C-N	6.49	130.03	120.95
2	H	40	LYS	C-N-CA	6.49	130.03	120.95
1	I	348	ASN	CA-CB-CG	6.49	119.09	112.60
1	E	142	GLY	O-C-N	-6.48	114.27	122.70
1	K	178	THR	CA-CB-CG2	6.48	121.52	110.50
1	E	138	SER	CA-C-O	-6.48	112.82	120.60
1	I	325	GLU	CA-C-N	6.48	128.85	120.56
1	I	325	GLU	C-N-CA	6.48	128.85	120.56
1	M	10	GLY	O-C-N	-6.47	116.38	123.05
2	D	8	HIS	CB-CG-CD2	-6.47	122.79	131.20
2	H	62	VAL	CA-CB-CG2	6.47	121.40	110.40
1	E	84	ILE	N-CA-CB	6.47	120.28	110.58
1	I	203	ASP	O-C-N	-6.46	115.78	123.27
1	I	372	THR	N-CA-CB	6.46	120.17	110.22
1	A	286	VAL	O-C-N	6.46	124.55	120.42
1	E	232	THR	CA-C-N	6.46	128.93	120.28
1	E	232	THR	C-N-CA	6.46	128.93	120.28
2	N	353	VAL	CA-C-N	6.46	127.59	121.46
2	N	353	VAL	C-N-CA	6.46	127.59	121.46
1	A	252	LYS	CA-C-N	6.45	128.93	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	LYS	C-N-CA	6.45	128.93	120.28
1	C	357	PRO	CB-CA-C	-6.45	103.05	110.92
2	N	78	VAL	CA-CB-CG2	6.45	121.37	110.40
1	C	372	THR	CA-C-O	6.45	127.30	119.49
1	M	159	TYR	CA-C-N	6.45	127.01	120.04
1	M	159	TYR	C-N-CA	6.45	127.01	120.04
2	D	245	ASP	CA-CB-CG	6.45	119.05	112.60
2	B	406	HIS	CA-C-O	-6.44	112.19	119.79
2	J	3	GLU	N-CA-C	6.44	119.22	109.23
1	M	283	ALA	CA-C-N	6.44	131.42	122.79
1	M	283	ALA	C-N-CA	6.44	131.42	122.79
2	J	229	ARG	CD-NE-CZ	6.44	133.42	124.40
2	J	415	GLU	CA-C-N	6.44	127.27	119.99
2	J	415	GLU	C-N-CA	6.44	127.27	119.99
2	L	395	PHE	CA-CB-CG	6.44	120.24	113.80
2	B	406	HIS	CB-CG-CD2	-6.44	122.83	131.20
1	C	396	HIS	CB-CG-CD2	-6.43	122.84	131.20
2	N	381	THR	OG1-CB-CG2	-6.43	96.44	109.30
1	A	86	ARG	CD-NE-CZ	6.43	133.40	124.40
2	B	257	THR	O-C-N	6.43	130.18	122.27
2	N	214	ARG	CA-CB-CG	6.43	126.95	114.10
2	N	106	GLY	CA-C-O	-6.42	113.23	120.30
2	J	91	GLN	CG-CD-NE2	6.42	126.03	116.40
2	B	279	GLU	CA-C-N	6.42	128.88	120.28
2	B	279	GLU	C-N-CA	6.42	128.88	120.28
1	M	383	GLU	O-C-N	6.42	129.47	122.15
2	L	359	PRO	O-C-N	-6.41	113.89	121.46
2	F	234	ILE	CA-C-N	6.41	129.24	120.46
2	F	234	ILE	C-N-CA	6.41	129.24	120.46
2	D	420	GLU	N-CA-C	6.40	118.80	111.11
1	C	76	VAL	CA-CB-CG1	6.40	121.28	110.40
1	K	42	LEU	CA-C-O	-6.40	111.75	119.49
1	C	79	GLY	CA-C-N	6.40	126.76	119.92
1	C	79	GLY	C-N-CA	6.40	126.76	119.92
1	M	367	PHE	O-C-N	-6.39	115.83	123.31
2	N	72	PRO	CA-C-N	6.39	129.13	120.38
2	N	72	PRO	C-N-CA	6.39	129.13	120.38
2	J	356	ASN	CA-CB-CG	-6.39	106.21	112.60
1	A	278	SER	O-C-N	-6.38	113.87	122.43
2	J	107	HIS	CE1-NE2-CD2	-6.38	102.61	109.00
2	D	273	ALA	CA-C-O	-6.38	113.40	119.91
2	H	347	CYS	N-CA-CB	-6.38	100.91	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	333	VAL	CA-C-O	-6.38	114.78	121.41
2	J	358	GLN	CA-C-O	-6.38	114.55	119.46
1	A	320	ARG	N-CA-CB	-6.37	102.42	110.45
1	C	41	ASP	CA-CB-CG	6.37	118.97	112.60
2	D	56	THR	CA-CB-CG2	6.37	121.33	110.50
2	L	216	ASN	N-CA-C	6.37	120.66	112.12
2	B	75	ILE	CB-CA-C	6.37	121.01	112.22
1	M	302	ALA	N-CA-C	6.37	120.62	112.34
2	D	101	ASN	CA-CB-CG	6.36	118.96	112.60
1	K	41	ASP	CA-CB-CG	-6.36	106.24	112.60
2	D	309	HIS	CB-CG-CD2	-6.36	122.93	131.20
2	N	268	PRO	CA-C-N	6.36	132.95	122.07
2	N	268	PRO	C-N-CA	6.36	132.95	122.07
2	J	118	VAL	CA-C-N	6.36	129.98	120.31
2	J	118	VAL	C-N-CA	6.36	129.98	120.31
2	B	251	ASP	CA-CB-CG	6.35	118.95	112.60
2	H	361	THR	CA-C-O	6.35	129.24	121.56
2	J	99	ALA	CA-C-N	6.35	131.62	122.35
2	J	99	ALA	C-N-CA	6.35	131.62	122.35
2	L	29	GLY	CA-C-N	6.35	129.01	120.50
2	L	29	GLY	C-N-CA	6.35	129.01	120.50
1	M	264	HIS	CA-CB-CG	6.35	120.15	113.80
2	D	441	GLU	CA-C-N	6.34	128.55	122.27
2	D	441	GLU	C-N-CA	6.34	128.55	122.27
1	G	161	ASP	CA-CB-CG	6.34	118.94	112.60
2	H	337	THR	CA-C-N	6.34	130.38	121.24
2	H	337	THR	C-N-CA	6.34	130.38	121.24
1	C	333	VAL	CA-C-O	-6.34	114.50	121.29
2	J	65	ALA	O-C-N	-6.34	116.19	123.42
2	H	292	THR	CA-CB-CG2	6.34	121.28	110.50
1	M	307	HIS	CB-CG-CD2	-6.34	122.96	131.20
1	A	60	VAL	CA-C-O	-6.33	111.46	119.95
1	I	72	THR	N-CA-C	-6.33	106.14	114.31
2	B	145	THR	O-C-N	-6.33	115.03	122.81
2	H	235	VAL	CA-C-N	6.33	129.62	120.38
2	H	235	VAL	C-N-CA	6.33	129.62	120.38
2	H	381	THR	CA-CB-CG2	6.33	121.25	110.50
1	M	174	LYS	CG-CD-CE	6.33	125.85	111.30
1	I	316	VAL	CB-CA-C	6.32	118.50	111.80
1	A	226	ASN	OD1-CG-ND2	-6.32	116.28	122.60
2	D	449	GLU	O-C-N	-6.32	114.02	122.74
1	M	271	ALA	O-C-N	-6.32	115.31	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	228	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	I	228	LEU	CA-C-O	6.31	127.23	120.10
2	N	231	ILE	N-CA-C	-6.31	104.18	110.62
2	H	43	GLY	CA-C-N	6.31	127.12	120.43
2	H	43	GLY	C-N-CA	6.31	127.12	120.43
2	J	138	PHE	N-CA-C	6.31	118.81	108.52
2	N	287	SER	N-CA-C	6.30	119.41	110.14
1	I	414	ASN	CA-CB-CG	6.30	118.90	112.60
1	A	201	CYS	N-CA-C	6.30	117.42	108.54
2	B	293	ASN	CA-C-N	6.30	129.89	120.31
2	B	293	ASN	C-N-CA	6.30	129.89	120.31
1	A	285	THR	CA-C-N	6.30	126.47	120.43
1	A	285	THR	C-N-CA	6.30	126.47	120.43
2	F	210	TYR	N-CA-C	6.30	118.95	111.33
1	A	137	HIS	CB-CG-CD2	-6.29	123.02	131.20
2	J	303	VAL	CA-CB-CG1	-6.29	99.70	110.40
2	N	7	ILE	CA-C-O	-6.29	113.85	120.39
1	K	231	ALA	O-C-N	-6.29	115.46	122.12
2	L	228	ASN	N-CA-C	6.29	118.65	111.11
2	J	165	SER	N-CA-C	6.28	118.41	110.24
1	G	175	VAL	CA-C-N	6.28	132.41	122.36
1	G	175	VAL	C-N-CA	6.28	132.41	122.36
1	G	402	GLY	CA-C-O	-6.28	111.71	119.69
2	J	6	SER	O-C-N	-6.28	115.88	123.10
1	K	369	GLY	CA-C-N	6.27	132.60	123.13
1	K	369	GLY	C-N-CA	6.27	132.60	123.13
2	D	277	SER	N-CA-C	6.27	117.97	110.19
2	B	117	LEU	CA-C-O	-6.27	114.24	120.70
2	B	289	ALA	N-CA-C	6.27	118.11	111.28
1	G	225	LEU	O-C-N	-6.26	115.33	122.09
2	B	347	CYS	CA-C-N	6.26	127.67	119.84
2	B	347	CYS	C-N-CA	6.26	127.67	119.84
2	H	76	ASP	CA-CB-CG	6.26	118.86	112.60
1	G	148	GLY	N-CA-C	-6.26	104.92	112.49
2	D	115	ILE	CA-C-N	6.26	128.95	120.38
2	D	115	ILE	C-N-CA	6.26	128.95	120.38
1	E	23	VAL	O-C-N	6.26	128.19	121.87
1	G	31	ASP	CB-CA-C	6.26	117.87	108.86
2	F	13	GLY	CA-C-N	6.25	128.44	120.56
2	F	13	GLY	C-N-CA	6.25	128.44	120.56
2	D	201	ALA	CA-C-N	6.25	129.70	120.95
2	D	201	ALA	C-N-CA	6.25	129.70	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	130	THR	CA-CB-CG2	6.25	121.13	110.50
2	J	296	PHE	O-C-N	-6.25	114.66	122.35
2	L	319	TYR	CA-C-N	6.25	132.94	121.94
2	L	319	TYR	C-N-CA	6.25	132.94	121.94
2	D	139	HIS	CB-CG-CD2	-6.24	123.08	131.20
2	J	283	HIS	CB-CG-CD2	-6.24	123.08	131.20
1	M	70	PRO	N-CA-CB	6.24	109.68	102.88
1	A	294	PHE	N-CA-CB	-6.24	100.67	110.46
2	B	375	VAL	CA-C-O	6.23	127.62	120.76
1	G	218	THR	CA-C-N	6.23	137.00	121.80
1	G	218	THR	C-N-CA	6.23	137.00	121.80
2	L	185	TYR	O-C-N	6.23	128.76	122.03
2	F	225	THR	CA-C-O	-6.22	113.82	120.42
2	J	114	ILE	O-C-N	-6.22	115.90	122.06
1	I	347	ASN	OD1-CG-ND2	-6.22	116.38	122.60
2	N	123	ARG	CA-C-N	6.22	129.24	120.28
2	N	123	ARG	C-N-CA	6.22	129.24	120.28
2	B	352	LYS	CA-C-N	6.22	131.13	123.10
2	B	352	LYS	C-N-CA	6.22	131.13	123.10
2	J	62	VAL	N-CA-C	6.22	113.22	107.56
2	B	324	VAL	CA-C-N	6.22	127.61	119.84
2	B	324	VAL	C-N-CA	6.22	127.61	119.84
2	N	265	ILE	CB-CA-C	6.22	121.49	111.29
2	N	331	ALA	CA-C-N	6.22	130.50	120.55
2	N	331	ALA	C-N-CA	6.22	130.50	120.55
1	C	37	HIS	CA-C-N	6.21	127.21	120.44
1	C	37	HIS	C-N-CA	6.21	127.21	120.44
2	J	227	LEU	CB-CA-C	6.21	120.80	110.92
1	G	123	GLU	CA-C-N	6.21	128.60	120.28
1	G	123	GLU	C-N-CA	6.21	128.60	120.28
2	J	307	PRO	N-CA-CB	6.21	109.65	102.88
1	M	33	THR	CA-C-N	6.21	130.95	121.51
1	M	33	THR	C-N-CA	6.21	130.95	121.51
1	E	175	VAL	N-CA-C	6.21	116.10	108.53
1	C	107	THR	N-CA-C	6.21	118.72	108.48
1	C	192	LEU	CB-CA-C	6.21	121.40	110.85
2	H	139	HIS	ND1-CE1-NE2	6.20	114.60	108.40
2	J	287	SER	N-CA-C	6.20	118.55	110.43
1	K	113	VAL	CA-CB-CG1	6.20	120.94	110.40
1	C	347	ASN	CA-CB-CG	6.20	118.80	112.60
2	L	216	ASN	OD1-CG-ND2	-6.20	116.41	122.60
3	O	393	VAL	CA-C-N	6.20	132.85	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	393	VAL	C-N-CA	6.20	132.85	121.70
2	B	8	HIS	CB-CG-CD2	-6.19	123.15	131.20
1	C	347	ASN	CB-CA-C	6.19	123.11	112.27
1	K	174	LYS	N-CA-C	6.19	123.37	114.39
1	M	423	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	E	207	LEU	N-CA-C	6.19	119.00	111.82
2	D	108	TYR	CA-C-O	-6.18	115.29	119.68
2	F	174	ALA	N-CA-C	6.18	117.60	109.93
1	G	84	ILE	CA-C-O	-6.18	112.18	119.85
2	H	51	THR	CA-C-N	6.18	133.44	121.63
2	H	51	THR	C-N-CA	6.18	133.44	121.63
1	M	274	THR	CA-CB-CG2	6.18	121.02	110.50
1	A	101	TRP	CZ3-CH2-CZ2	-6.18	113.46	121.50
1	A	181	GLU	N-CA-C	6.18	122.04	113.45
2	F	61	HIS	CB-CG-CD2	-6.18	123.17	131.20
1	A	67	ASP	O-C-N	-6.18	116.56	123.48
1	E	329	GLN	CG-CD-NE2	6.18	125.67	116.40
2	F	328	VAL	CA-CB-CG2	6.18	120.90	110.40
2	H	144	GLY	CA-C-O	-6.18	114.11	120.66
2	L	238	ILE	CA-CB-CG2	6.17	121.00	110.50
1	M	107	THR	OG1-CB-CG2	-6.17	96.95	109.30
1	K	401	GLU	CB-CG-CD	6.17	123.09	112.60
1	E	384	GLN	CG-CD-NE2	6.17	125.66	116.40
1	C	224	ASP	CB-CA-C	-6.17	100.56	110.79
2	B	109	THR	CA-C-N	6.16	128.55	120.60
2	B	109	THR	C-N-CA	6.16	128.55	120.60
2	L	251	ASP	N-CA-C	6.16	119.60	110.48
2	N	71	GLU	CA-C-N	6.16	125.65	119.24
2	N	71	GLU	C-N-CA	6.16	125.65	119.24
2	H	220	GLU	N-CA-C	6.16	118.07	111.36
1	K	422	TYR	CB-CG-CD2	-6.16	111.57	120.80
3	O	393	VAL	O-C-N	-6.16	114.88	122.57
1	K	152	ILE	CA-C-N	6.15	130.45	120.60
1	K	152	ILE	C-N-CA	6.15	130.45	120.60
2	N	347	CYS	CA-C-N	6.15	126.27	119.87
2	N	347	CYS	C-N-CA	6.15	126.27	119.87
1	A	399	THR	CA-CB-CG2	6.15	120.96	110.50
1	I	312	THR	N-CA-C	6.15	118.12	108.96
1	G	10	GLY	O-C-N	-6.15	116.29	123.17
2	D	405	VAL	CA-C-O	-6.14	114.00	120.57
1	M	367	PHE	CA-C-O	6.14	127.14	120.32
1	M	222	TYR	CA-C-N	6.14	126.91	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	222	TYR	C-N-CA	6.14	126.91	120.03
2	N	284	GLU	CB-CA-C	6.14	121.84	109.68
2	L	117	LEU	CA-C-O	6.14	127.06	120.55
1	C	10	GLY	O-C-N	-6.14	116.19	122.70
2	L	45	GLY	O-C-N	-6.13	116.46	122.77
2	H	358	GLN	OE1-CD-NE2	-6.13	116.47	122.60
1	M	298	ASN	N-CA-C	-6.13	105.77	113.18
2	L	351	PHE	CA-CB-CG	6.13	119.93	113.80
2	H	234	ILE	CA-CB-CG1	6.12	120.81	110.40
1	M	211	CYS	CA-C-O	-6.12	113.93	120.42
2	B	169	PHE	N-CA-C	6.12	119.25	107.44
2	D	120	ASP	O-C-N	-6.12	115.06	122.22
2	F	325	PRO	N-CA-CB	6.12	110.00	103.52
2	B	205	ASP	O-C-N	-6.11	114.92	123.11
1	C	57	ASN	OD1-CG-ND2	-6.11	116.49	122.60
2	F	226	ASN	CA-C-N	6.11	130.91	120.71
2	F	226	ASN	C-N-CA	6.11	130.91	120.71
2	B	257	THR	N-CA-C	6.11	118.91	111.82
1	C	330	MET	CA-C-O	6.11	127.00	120.10
2	J	300	ASN	N-CA-C	6.11	121.48	113.30
2	L	330	ALA	N-CA-CB	-6.11	100.81	110.28
1	C	177	ASP	CA-C-N	6.10	132.68	121.94
1	C	177	ASP	C-N-CA	6.10	132.68	121.94
2	H	265	ILE	CA-CB-CG1	6.10	120.76	110.40
2	L	285	GLN	N-CA-C	6.10	120.89	112.90
2	L	85	GLN	O-C-N	-6.09	114.72	122.34
1	M	242	PHE	CA-CB-CG	6.09	119.89	113.80
1	G	107	THR	CA-C-O	-6.09	115.83	119.55
2	L	171	ILE	O-C-N	-6.09	114.96	122.57
2	L	425	MET	O-C-N	-6.09	114.78	122.27
2	H	108	TYR	CA-C-O	-6.09	111.61	120.13
1	I	39	ASP	N-CA-C	6.09	120.88	112.90
1	I	165	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	I	368	ILE	CA-C-O	6.09	126.28	120.25
2	H	63	PRO	N-CA-CB	6.09	109.11	103.39
2	H	429	GLU	CB-CA-C	6.09	122.36	110.67
1	G	153	SER	N-CA-C	6.08	118.71	111.71
2	F	353	VAL	CA-CB-CG2	6.08	120.74	110.40
1	M	29	GLY	O-C-N	6.08	129.24	122.31
2	B	8	HIS	ND1-CE1-NE2	6.08	114.48	108.40
2	J	359	PRO	CB-CA-C	-6.07	103.51	110.92
2	N	425	MET	N-CA-C	6.07	118.69	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	280	LYS	CA-C-O	-6.07	112.99	119.97
2	L	346	TRP	CG-CD1-NE1	-6.07	102.31	110.20
1	M	418	LEU	N-CA-C	6.07	117.56	111.07
1	C	145	SER	O-C-N	6.07	128.64	122.09
1	A	150	LEU	N-CA-CB	-6.07	101.21	110.01
2	D	72	PRO	CA-N-CD	-6.07	103.51	112.00
1	E	150	LEU	CA-C-N	6.07	128.41	120.28
1	E	150	LEU	C-N-CA	6.07	128.41	120.28
2	J	202	PHE	CA-CB-CG	6.07	119.86	113.80
1	K	159	TYR	O-C-N	-6.07	115.91	121.37
1	M	101	TRP	CE3-CZ3-CH2	-6.07	113.22	121.10
1	E	183	TYR	CA-CB-CG	6.06	124.82	113.90
1	M	80	PRO	N-CA-CB	6.06	108.98	103.34
1	M	37	HIS	CB-CG-CD2	-6.06	123.32	131.20
2	B	220	GLU	CA-C-O	-6.06	114.44	120.80
2	D	384	ILE	CA-C-O	-6.06	113.93	120.47
2	N	120	ASP	CA-CB-CG	-6.06	106.54	112.60
2	B	381	THR	CA-C-O	6.06	128.09	121.06
2	D	11	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	M	16	ILE	N-CA-C	-6.05	104.95	110.82
1	E	384	GLN	N-CA-C	6.04	117.87	111.28
2	N	14	VAL	CA-C-N	6.04	128.66	120.38
2	N	14	VAL	C-N-CA	6.04	128.66	120.38
2	L	12	ALA	CA-C-N	6.04	126.53	119.94
2	L	12	ALA	C-N-CA	6.04	126.53	119.94
2	B	179	THR	CA-CB-OG1	6.04	118.66	109.60
2	J	198	SER	N-CA-C	6.04	118.50	110.53
2	J	405	VAL	N-CA-C	6.04	117.51	110.62
1	A	99	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	C	372	THR	CA-CB-CG2	6.04	120.76	110.50
1	G	410	GLU	CA-C-O	-6.04	113.54	120.24
1	E	396	HIS	CE1-NE2-CD2	-6.04	102.96	109.00
2	H	147	SER	CB-CA-C	6.04	120.30	110.95
2	J	123	ARG	CD-NE-CZ	6.04	132.85	124.40
1	C	222	TYR	N-CA-C	6.03	117.86	111.28
2	J	22	GLU	CA-C-N	6.03	128.37	120.28
2	J	22	GLU	C-N-CA	6.03	128.37	120.28
2	J	351	PHE	CA-C-N	6.03	132.58	122.87
2	J	351	PHE	C-N-CA	6.03	132.58	122.87
2	D	397	LEU	CA-C-N	6.03	128.85	120.29
2	D	397	LEU	C-N-CA	6.03	128.85	120.29
1	C	242	PHE	CA-CB-CG	6.03	119.83	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	362	VAL	CA-CB-CG2	6.03	120.64	110.40
1	G	181	GLU	CA-C-O	-6.03	111.90	120.16
2	H	82	THR	O-C-N	-6.03	114.15	122.46
1	M	288	GLU	CA-C-O	6.02	126.94	120.55
2	N	392	ASP	CA-CB-CG	6.02	118.62	112.60
2	D	203	MET	N-CA-C	6.02	119.30	109.24
2	F	380	ASN	CA-C-N	6.02	132.73	122.37
2	F	380	ASN	C-N-CA	6.02	132.73	122.37
1	K	105	HIS	CB-CG-CD2	-6.02	123.37	131.20
1	A	263	LEU	CA-C-N	6.02	131.64	122.37
1	A	263	LEU	C-N-CA	6.02	131.64	122.37
1	C	268	PRO	CA-C-N	6.02	129.88	121.09
1	C	268	PRO	C-N-CA	6.02	129.88	121.09
1	E	320	ARG	N-CA-C	6.02	118.00	108.67
2	F	224	TYR	CA-CB-CG	6.02	124.73	113.90
2	B	184	PRO	N-CA-CB	6.02	109.95	103.33
2	B	340	SER	CB-CA-C	6.02	120.44	110.81
1	G	171	PRO	N-CA-C	6.02	120.30	111.03
1	I	430	ALA	CA-C-O	-6.02	112.23	119.27
1	I	439	GLU	O-C-N	-6.02	115.84	123.24
1	K	15	GLN	OE1-CD-NE2	-6.01	116.58	122.60
2	N	79	ARG	N-CA-C	6.01	120.09	112.87
1	E	434	GLY	O-C-N	-6.01	118.48	121.85
2	L	174	ALA	CA-C-N	6.01	125.72	119.05
2	L	174	ALA	C-N-CA	6.01	125.72	119.05
1	M	92	PHE	N-CA-C	6.01	118.54	109.23
2	J	63	PRO	N-CA-CB	6.00	108.65	103.31
1	I	198	GLU	O-C-N	-6.00	116.64	123.48
1	C	340	TYR	CD1-CG-CD2	6.00	127.10	118.10
2	N	28	HIS	CA-CB-CG	6.00	119.80	113.80
2	N	172	TYR	CB-CG-CD2	-6.00	111.80	120.80
2	F	349	THR	OG1-CB-CG2	-5.99	97.31	109.30
1	E	384	GLN	OE1-CD-NE2	-5.99	116.61	122.60
2	F	24	TYR	N-CA-C	5.99	118.58	111.33
2	H	71	GLU	CA-C-N	5.99	125.87	119.28
2	H	71	GLU	C-N-CA	5.99	125.87	119.28
2	N	15	GLN	CG-CD-NE2	5.99	125.39	116.40
1	K	426	GLN	OE1-CD-NE2	-5.99	116.61	122.60
2	B	161	TYR	CG-CD1-CE1	-5.99	112.22	121.20
2	B	367	ASP	CA-C-N	5.99	129.34	120.90
2	B	367	ASP	C-N-CA	5.99	129.34	120.90
1	E	21	TRP	CZ3-CH2-CZ2	-5.98	113.72	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	SER	N-CA-C	5.98	120.12	112.34
1	I	165	ASN	O-C-N	-5.98	116.37	123.06
1	I	379	LYS	CA-C-O	-5.98	114.22	120.55
2	J	59	GLY	CA-C-N	5.97	130.72	122.77
2	J	59	GLY	C-N-CA	5.97	130.72	122.77
1	M	35	SER	N-CA-CB	-5.97	100.89	110.39
1	A	356	ILE	CA-C-N	5.97	126.53	120.38
1	A	356	ILE	C-N-CA	5.97	126.53	120.38
1	C	244	GLY	CA-C-O	5.97	127.99	121.48
1	K	11	GLN	CA-C-N	5.97	128.56	120.38
1	K	11	GLN	C-N-CA	5.97	128.56	120.38
2	N	253	THR	CA-CB-CG2	5.97	120.65	110.50
2	B	342	GLN	CB-CA-C	5.97	120.05	109.72
2	D	337	THR	OG1-CB-CG2	-5.97	97.36	109.30
1	K	339	SER	N-CA-C	5.97	120.29	113.19
2	B	51	THR	CA-CB-CG2	5.97	120.64	110.50
2	D	53	PHE	CA-CB-CG	5.97	119.77	113.80
2	N	25	CYS	CA-C-O	-5.97	111.91	119.31
2	F	233	GLN	CB-CG-CD	5.96	122.74	112.60
2	B	315	CYS	N-CA-C	5.96	118.24	109.24
2	B	332	ILE	N-CA-CB	5.96	117.12	110.62
1	A	137	HIS	CA-C-O	-5.96	114.54	120.80
1	G	287	PRO	CA-N-CD	-5.96	103.66	112.00
2	D	212	ILE	N-CA-C	5.96	116.69	110.62
2	B	126	ALA	CA-C-O	-5.95	114.11	120.42
2	F	216	ASN	CA-C-O	-5.95	114.77	120.90
1	I	366	THR	CA-CB-CG2	5.95	120.62	110.50
1	G	189	VAL	CA-C-N	5.95	128.25	120.28
1	G	189	VAL	C-N-CA	5.95	128.25	120.28
2	H	432	TYR	O-C-N	-5.95	115.81	122.12
1	I	344	TRP	CA-C-O	-5.95	111.32	119.12
2	J	411	GLU	CA-C-O	5.95	126.91	119.59
1	M	11	GLN	CG-CD-NE2	5.95	125.32	116.40
1	M	202	ILE	N-CA-C	5.95	116.09	108.12
2	J	116	ASP	CA-C-O	-5.95	114.58	120.82
2	L	370	LYS	O-C-N	-5.95	113.95	122.99
1	C	440	GLY	O-C-N	-5.95	117.70	122.81
2	J	288	VAL	N-CA-CB	5.95	117.11	110.51
1	E	283	ALA	N-CA-C	5.94	117.72	110.41
1	A	345	ILE	CA-C-N	5.94	125.88	119.76
1	A	345	ILE	C-N-CA	5.94	125.88	119.76
2	F	322	ASP	CA-CB-CG	-5.94	106.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	100	ASN	CA-C-N	5.94	128.52	120.38
1	G	100	ASN	C-N-CA	5.94	128.52	120.38
1	I	344	TRP	CD2-CE2-CZ2	-5.94	116.46	122.40
2	F	324	VAL	CA-C-N	5.94	125.48	119.19
2	F	324	VAL	C-N-CA	5.94	125.48	119.19
1	G	40	SER	CA-C-N	5.94	129.05	120.38
1	G	40	SER	C-N-CA	5.94	129.05	120.38
2	H	172	TYR	CA-C-N	5.94	126.14	119.90
2	H	172	TYR	C-N-CA	5.94	126.14	119.90
1	I	266	PHE	CA-CB-CG	5.94	119.74	113.80
1	M	422	TYR	CA-C-N	5.94	128.83	120.28
1	M	422	TYR	C-N-CA	5.94	128.83	120.28
2	D	147	SER	N-CA-CB	-5.93	101.16	110.06
2	D	443	GLU	N-CA-C	5.93	120.91	113.43
2	F	53	PHE	N-CA-C	5.93	118.43	109.41
2	H	185	TYR	CB-CG-CD2	-5.93	111.90	120.80
1	A	341	PHE	CA-C-N	5.93	132.65	121.97
1	A	341	PHE	C-N-CA	5.93	132.65	121.97
1	K	290	THR	CB-CA-C	5.93	121.60	110.63
1	C	15	GLN	N-CA-C	5.93	118.98	111.69
1	C	281	TYR	N-CA-C	5.93	119.66	111.71
2	F	223	THR	N-CA-C	5.93	118.36	110.53
2	L	193	THR	CA-CB-OG1	-5.93	100.71	109.60
2	N	382	THR	CA-C-O	5.93	126.75	119.05
1	C	356	ILE	O-C-N	-5.92	117.64	121.37
2	F	33	ASP	CB-CA-C	5.92	119.97	110.09
3	O	218	PRO	N-CA-CB	5.92	106.30	103.22
2	B	72	PRO	N-CA-CB	5.91	109.92	103.30
2	F	380	ASN	O-C-N	-5.91	116.48	123.22
2	H	437	VAL	CA-CB-CG1	5.91	120.45	110.40
1	A	247	ASN	CA-C-N	5.91	129.61	121.33
1	A	247	ASN	C-N-CA	5.91	129.61	121.33
2	J	141	PHE	CA-C-N	5.91	126.50	120.00
2	J	141	PHE	C-N-CA	5.91	126.50	120.00
2	D	262	TYR	CA-C-N	5.91	127.23	119.84
2	D	262	TYR	C-N-CA	5.91	127.23	119.84
2	D	51	THR	N-CA-C	5.91	119.75	112.54
2	F	153	LEU	CA-C-N	5.91	128.47	120.38
2	F	153	LEU	C-N-CA	5.91	128.47	120.38
2	L	116	ASP	CA-C-N	5.91	128.19	120.28
2	L	116	ASP	C-N-CA	5.91	128.19	120.28
1	M	187	LEU	CA-C-O	-5.91	113.18	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	371	VAL	CA-CB-CG2	5.90	120.44	110.40
1	G	154	LYS	CA-CB-CG	-5.90	102.30	114.10
2	H	232	SER	CB-CA-C	5.90	120.25	110.81
2	H	285	GLN	CB-CG-CD	5.90	122.63	112.60
1	E	105	HIS	N-CA-C	5.90	120.54	112.04
2	J	379	SER	O-C-N	-5.90	116.16	123.36
2	F	348	PRO	CA-N-CD	-5.90	103.74	112.00
1	A	156	ARG	N-CA-CB	-5.90	101.21	110.06
1	K	253	LEU	CA-C-O	-5.90	114.62	120.70
2	B	179	THR	N-CA-C	-5.89	105.75	113.12
2	L	295	CYS	O-C-N	-5.89	114.33	122.46
2	L	345	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	145	SER	O-C-N	-5.89	116.00	122.07
2	L	292	THR	CA-CB-CG2	5.89	120.52	110.50
1	E	375	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	K	173	PRO	CA-C-N	5.89	130.99	121.98
1	K	173	PRO	C-N-CA	5.89	130.99	121.98
2	D	268	PRO	O-C-N	-5.88	115.82	123.06
1	G	381	ILE	O-C-N	-5.88	116.16	121.87
2	L	303	VAL	CB-CA-C	5.88	119.88	110.82
1	A	303	CYS	N-CA-C	5.88	119.23	110.52
2	D	226	ASN	OD1-CG-ND2	-5.88	116.72	122.60
2	B	8	HIS	ND1-CG-CD2	5.88	111.98	106.10
1	C	256	ASN	CB-CG-ND2	5.88	125.22	116.40
1	K	74	ASP	CA-CB-CG	-5.88	106.72	112.60
2	L	362	VAL	CA-C-O	5.88	126.93	120.64
1	A	347	ASN	O-C-N	5.88	130.09	122.86
2	D	222	PRO	CB-CA-C	5.88	118.57	111.46
1	G	58	LYS	CA-C-O	-5.88	114.48	120.71
2	B	439	SER	N-CA-CB	5.88	120.42	110.49
1	C	273	LEU	CA-C-N	5.88	132.48	122.37
1	C	273	LEU	C-N-CA	5.88	132.48	122.37
1	E	98	GLY	CA-C-N	5.88	132.76	121.54
1	E	98	GLY	C-N-CA	5.88	132.76	121.54
1	K	404	ASP	CA-C-O	5.87	127.39	120.69
1	G	165	ASN	CB-CG-ND2	5.87	125.21	116.40
1	M	368	ILE	CA-C-N	5.87	126.61	122.33
1	M	368	ILE	C-N-CA	5.87	126.61	122.33
2	B	71	GLU	CA-C-N	5.87	126.28	119.47
2	B	71	GLU	C-N-CA	5.87	126.28	119.47
1	G	5	VAL	CB-CA-C	5.86	118.33	110.42
1	G	46	ARG	CD-NE-CZ	5.86	132.61	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	356	ILE	CA-C-O	5.86	124.87	120.88
2	L	154	MET	N-CA-C	5.86	118.14	111.11
2	L	225	THR	CA-C-N	5.86	128.60	120.63
2	L	225	THR	C-N-CA	5.86	128.60	120.63
2	F	160	ASP	CA-C-O	-5.86	112.62	119.24
2	N	188	ILE	CA-C-O	-5.86	113.98	120.96
1	A	333	VAL	CA-C-N	5.86	128.61	120.29
1	A	333	VAL	C-N-CA	5.86	128.61	120.29
1	I	246	LEU	CA-C-O	-5.86	113.07	120.28
1	A	256	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	C	32	PRO	N-CA-CB	5.86	109.40	103.25
2	H	16	ILE	CA-C-N	5.86	126.44	120.00
2	H	16	ILE	C-N-CA	5.86	126.44	120.00
2	H	65	ALA	N-CA-C	5.86	117.75	108.79
2	L	74	VAL	CA-C-N	5.86	129.92	120.55
2	L	74	VAL	C-N-CA	5.86	129.92	120.55
2	N	173	PRO	N-CA-CB	5.86	109.53	103.38
1	E	329	GLN	OE1-CD-NE2	-5.85	116.75	122.60
1	M	335	ASN	OD1-CG-ND2	-5.85	116.75	122.60
2	D	406	HIS	O-C-N	-5.85	115.38	122.22
1	A	243	PRO	CA-C-N	5.85	129.86	121.03
1	A	243	PRO	C-N-CA	5.85	129.86	121.03
1	E	287	PRO	N-CA-C	5.85	121.55	113.65
2	J	289	ALA	CA-C-N	5.85	128.44	120.54
2	J	289	ALA	C-N-CA	5.85	128.44	120.54
2	L	44	GLY	CA-C-N	5.85	129.32	122.19
2	L	44	GLY	C-N-CA	5.85	129.32	122.19
2	H	99	ALA	N-CA-C	-5.85	106.11	113.18
2	L	290	GLU	CA-C-O	-5.85	113.49	120.10
2	B	291	ILE	CA-C-O	-5.84	114.00	120.96
1	I	282	ARG	CA-C-N	5.84	129.17	120.87
1	I	282	ARG	C-N-CA	5.84	129.17	120.87
2	F	28	HIS	CB-CG-CD2	-5.84	123.61	131.20
1	G	84	ILE	CA-C-N	5.84	133.58	121.32
1	G	84	ILE	C-N-CA	5.84	133.58	121.32
1	M	99	ASN	CA-C-N	5.84	131.60	123.07
1	M	99	ASN	C-N-CA	5.84	131.60	123.07
1	G	215	LEU	CA-C-N	5.84	130.42	122.07
1	G	215	LEU	C-N-CA	5.84	130.42	122.07
2	H	284	GLU	CB-CG-CD	5.84	122.52	112.60
1	K	160	PRO	N-CD-CG	5.83	111.95	103.20
2	L	375	VAL	CA-CB-CG1	5.83	120.32	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	231	ALA	CA-C-N	5.83	130.55	120.58
1	C	231	ALA	C-N-CA	5.83	130.55	120.58
1	G	201	CYS	O-C-N	-5.83	114.83	122.59
2	J	226	ASN	CA-C-N	5.83	128.90	120.79
2	J	226	ASN	C-N-CA	5.83	128.90	120.79
2	L	357	TYR	CA-C-N	5.83	129.36	121.20
2	L	357	TYR	C-N-CA	5.83	129.36	121.20
1	E	188	SER	CA-C-N	5.83	130.32	120.64
1	E	188	SER	C-N-CA	5.83	130.32	120.64
2	L	73	THR	CA-CB-OG1	-5.83	100.86	109.60
2	F	105	ARG	N-CA-CB	5.83	118.69	110.12
2	L	289	ALA	N-CA-C	5.83	117.32	110.97
1	M	84	ILE	CA-C-O	-5.83	114.33	120.57
1	M	137	HIS	CA-CB-CG	-5.83	107.97	113.80
1	M	149	THR	CA-C-N	5.83	128.09	120.28
1	M	149	THR	C-N-CA	5.83	128.09	120.28
2	J	69	ASP	CB-CG-OD2	5.83	131.80	118.40
2	L	429	GLU	N-CA-C	5.82	117.30	111.07
1	C	371	SER	CA-C-O	-5.82	114.41	120.70
2	L	127	ASP	N-CA-CB	-5.82	100.73	110.39
2	D	46	ASP	CA-CB-CG	5.82	118.42	112.60
1	G	251	ARG	CB-CG-CD	5.81	124.67	111.30
1	K	112	LEU	N-CA-CB	-5.81	103.27	111.00
1	I	222	TYR	CA-C-N	5.81	126.39	119.94
1	I	222	TYR	C-N-CA	5.81	126.39	119.94
1	M	413	SER	CA-C-N	5.81	128.07	120.28
1	M	413	SER	C-N-CA	5.81	128.07	120.28
2	H	245	ASP	CB-CA-C	5.81	119.39	109.80
2	J	417	GLU	CA-C-N	5.81	127.99	120.44
2	J	417	GLU	C-N-CA	5.81	127.99	120.44
1	G	112	LEU	N-CA-CB	-5.81	102.01	111.18
1	I	158	GLU	CA-C-N	5.81	129.24	122.85
1	I	158	GLU	C-N-CA	5.81	129.24	122.85
1	I	202	ILE	CA-C-O	5.81	126.49	120.39
1	E	183	TYR	CA-C-N	5.80	128.06	120.28
1	E	183	TYR	C-N-CA	5.80	128.06	120.28
1	M	29	GLY	CA-C-O	-5.80	112.32	119.69
1	E	301	ALA	CA-C-N	5.80	129.88	120.60
1	E	301	ALA	C-N-CA	5.80	129.88	120.60
2	L	264	ARG	CA-CB-CG	-5.80	102.50	114.10
2	N	251	ASP	O-C-N	-5.80	115.34	123.11
1	C	332	ASN	CA-C-N	5.80	127.95	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	332	ASN	C-N-CA	5.80	127.95	120.70
2	D	46	ASP	CA-C-N	5.80	132.14	121.70
2	D	46	ASP	C-N-CA	5.80	132.14	121.70
1	M	301	ALA	CA-C-N	5.80	129.97	120.63
1	M	301	ALA	C-N-CA	5.80	129.97	120.63
2	J	98	ASP	CA-C-O	5.80	127.70	121.55
1	K	43	GLN	OE1-CD-NE2	-5.80	116.80	122.60
2	B	88	HIS	CB-CG-CD2	-5.80	123.66	131.20
2	L	66	VAL	CA-CB-CG2	5.80	120.25	110.40
2	N	396	ASP	CA-CB-CG	5.80	118.40	112.60
3	O	388	HIS	N-CA-C	5.80	123.15	110.80
1	C	439	GLU	O-C-N	-5.79	116.45	123.29
1	E	68	LEU	CB-CA-C	5.79	120.44	110.01
2	H	198	SER	CA-C-O	-5.79	115.15	121.87
2	L	290	GLU	CA-C-N	5.79	129.82	120.55
2	L	290	GLU	C-N-CA	5.79	129.82	120.55
2	L	329	ASN	CA-CB-CG	-5.79	106.81	112.60
2	H	14	VAL	N-CA-C	5.79	115.97	110.42
1	A	215	LEU	N-CA-CB	5.79	119.03	110.53
2	D	15	GLN	CA-C-N	5.78	128.63	120.42
2	D	15	GLN	C-N-CA	5.78	128.63	120.42
1	I	37	HIS	CA-C-N	5.78	127.07	120.53
1	I	37	HIS	C-N-CA	5.78	127.07	120.53
2	L	268	PRO	N-CA-CB	5.78	108.45	103.36
2	H	376	CYS	CA-C-O	-5.78	114.27	120.92
2	J	156	ARG	CA-C-N	5.78	128.34	120.54
2	J	156	ARG	C-N-CA	5.78	128.34	120.54
1	K	382	SER	CB-CA-C	-5.78	101.80	110.88
1	M	335	ASN	N-CA-CB	-5.78	102.90	110.59
2	B	163	LYS	CB-CA-C	5.78	120.66	110.37
1	I	404	ASP	N-CA-CB	-5.78	102.24	111.43
2	J	207	GLU	CA-C-N	5.78	127.95	120.44
2	J	207	GLU	C-N-CA	5.78	127.95	120.44
2	L	233	GLN	OE1-CD-NE2	-5.78	116.82	122.60
2	L	363	VAL	CB-CA-C	5.78	116.54	110.88
1	G	49	VAL	CA-C-N	5.77	131.31	122.24
1	G	49	VAL	C-N-CA	5.77	131.31	122.24
1	E	60	VAL	O-C-N	5.77	127.68	121.10
2	N	293	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	I	294	PHE	CA-CB-CG	-5.77	108.03	113.80
2	D	188	ILE	CB-CG1-CD1	-5.77	101.68	113.80
2	J	49	PHE	CA-CB-CG	5.77	119.57	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	MET	CA-C-O	-5.77	113.42	120.05
2	F	266	HIS	CB-CG-CD2	-5.77	123.70	131.20
2	F	9	VAL	CA-CB-CG2	5.77	120.20	110.40
1	A	101	TRP	CA-C-N	5.76	128.00	120.28
1	A	101	TRP	C-N-CA	5.76	128.00	120.28
1	G	204	ASN	CA-CB-CG	5.76	118.36	112.60
1	M	195	ASN	CA-CB-CG	5.76	118.36	112.60
1	A	192	LEU	N-CA-C	5.76	117.64	111.36
2	D	337	THR	CA-CB-CG2	5.76	120.29	110.50
1	M	279	GLN	N-CA-CB	5.76	118.52	109.94
1	C	322	SER	O-C-N	5.76	130.25	122.59
1	K	192	LEU	CA-C-O	-5.76	113.85	120.24
1	M	380	ARG	CB-CA-C	5.76	121.88	110.42
2	D	61	HIS	O-C-N	-5.76	116.66	123.22
2	H	7	ILE	N-CA-CB	-5.76	103.99	111.82
1	K	345	ILE	CA-C-N	5.75	127.03	119.84
1	K	345	ILE	C-N-CA	5.75	127.03	119.84
1	A	382	SER	CA-C-N	5.75	127.99	120.28
1	A	382	SER	C-N-CA	5.75	127.99	120.28
2	D	309	HIS	ND1-CE1-NE2	5.75	114.15	108.40
2	H	67	PHE	CA-CB-CG	5.75	119.55	113.80
2	N	192	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	A	183	TYR	CB-CG-CD2	-5.75	112.17	120.80
1	A	393	ALA	CA-C-O	-5.75	114.37	120.92
2	D	432	TYR	CA-C-O	-5.75	113.60	120.10
2	F	208	ALA	CA-C-O	-5.75	114.78	120.70
1	I	357	PRO	CA-C-N	5.75	127.02	119.84
1	I	357	PRO	C-N-CA	5.75	127.02	119.84
2	B	77	GLU	CA-C-O	5.75	126.64	120.55
2	D	69	ASP	CA-C-N	5.75	131.19	121.14
2	D	69	ASP	C-N-CA	5.75	131.19	121.14
2	D	309	HIS	ND1-CG-CD2	5.74	111.84	106.10
2	L	61	HIS	ND1-CG-CD2	5.74	111.84	106.10
2	B	406	HIS	ND1-CG-CD2	5.74	111.84	106.10
2	D	255	PHE	CA-C-N	5.74	127.97	120.28
2	D	255	PHE	C-N-CA	5.74	127.97	120.28
2	B	303	VAL	CA-CB-CG1	5.74	120.16	110.40
1	M	127	CYS	CA-C-O	-5.74	115.31	121.56
2	B	348	PRO	CA-N-CD	-5.74	103.97	112.00
1	C	209	ASP	O-C-N	-5.73	115.22	122.27
2	H	122	ILE	CA-C-N	5.73	128.24	120.44
2	H	122	ILE	C-N-CA	5.73	128.24	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	161	ASP	N-CA-C	5.73	119.53	112.54
1	I	299	MET	N-CA-CB	-5.73	101.41	110.06
1	A	57	ASN	OD1-CG-ND2	-5.73	116.87	122.60
2	B	178	SER	CB-CA-C	5.73	119.10	109.48
1	I	227	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	K	154	LYS	N-CA-C	5.72	120.76	113.55
2	B	94	THR	N-CA-C	5.72	118.88	109.72
1	G	278	SER	CA-C-O	-5.72	111.61	119.05
1	M	206	ALA	CA-C-O	-5.72	114.35	120.42
2	F	86	LEU	N-CA-C	5.72	117.19	111.07
2	H	205	ASP	CA-CB-CG	5.72	118.32	112.60
2	B	280	LYS	CB-CA-C	5.72	120.28	110.79
2	B	389	ALA	CA-C-O	-5.72	114.46	120.63
1	E	37	HIS	ND1-CG-CD2	5.72	111.82	106.10
2	J	358	GLN	O-C-N	5.72	126.17	121.31
2	L	150	THR	CA-CB-CG2	5.72	120.22	110.50
2	L	364	PRO	N-CA-CB	5.72	108.69	103.15
2	L	414	GLU	CA-C-O	-5.72	114.70	121.16
2	D	104	ALA	CA-C-O	-5.71	114.49	120.55
1	C	173	PRO	N-CA-CB	5.71	109.77	103.26
2	F	8	HIS	ND1-CE1-NE2	5.71	114.11	108.40
1	K	39	ASP	CA-C-N	5.71	131.53	122.62
1	K	39	ASP	C-N-CA	5.71	131.53	122.62
2	L	137	VAL	N-CA-C	5.71	116.09	107.75
1	K	138	SER	O-C-N	5.71	129.36	122.68
2	H	221	ARG	O-C-N	-5.71	114.76	121.32
1	M	150	LEU	CB-CA-C	5.71	120.26	110.79
1	M	173	PRO	N-CA-C	5.71	121.26	113.84
1	C	209	ASP	CA-C-N	5.70	128.52	120.42
1	C	209	ASP	C-N-CA	5.70	128.52	120.42
2	J	156	ARG	O-C-N	5.70	128.25	122.09
1	C	227	HIS	CB-CG-CD2	-5.70	123.79	131.20
2	B	267	PHE	CA-CB-CG	5.70	119.50	113.80
1	K	245	GLN	CA-CB-CG	5.70	125.50	114.10
2	N	224	TYR	CA-C-N	5.70	130.22	120.71
2	N	224	TYR	C-N-CA	5.70	130.22	120.71
3	O	388	HIS	CB-CA-C	5.70	121.75	110.42
1	E	48	ASN	CA-C-O	-5.69	113.82	120.20
1	A	76	VAL	CA-CB-CG2	5.69	120.08	110.40
2	H	420	GLU	CA-C-N	5.69	128.18	120.38
2	H	420	GLU	C-N-CA	5.69	128.18	120.38
2	J	212	ILE	N-CA-C	5.69	116.43	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	248	LEU	O-C-N	5.69	130.44	123.44
1	A	114	ASP	CA-C-N	5.69	131.68	121.66
1	A	114	ASP	C-N-CA	5.69	131.68	121.66
2	J	393	HIS	CB-CG-CD2	-5.69	123.80	131.20
2	L	69	ASP	CA-CB-CG	5.69	118.29	112.60
1	I	410	GLU	CA-C-O	-5.69	114.39	120.42
1	M	43	GLN	CG-CD-NE2	5.69	124.93	116.40
1	K	110	ALA	N-CA-C	5.68	119.32	112.38
1	K	178	THR	CA-C-N	5.68	127.84	120.56
1	K	178	THR	C-N-CA	5.68	127.84	120.56
2	L	110	ILE	CA-C-N	5.68	126.41	119.99
2	L	110	ILE	C-N-CA	5.68	126.41	119.99
1	G	31	ASP	CA-CB-CG	-5.68	106.92	112.60
2	J	388	TRP	CG-CD2-CE3	5.68	139.58	133.90
2	N	296	PHE	CB-CA-C	5.68	119.10	109.55
2	B	283	HIS	N-CA-C	5.68	119.31	112.38
1	C	354	CYS	CB-CA-C	5.68	119.11	109.80
2	D	40	LYS	CA-CB-CG	-5.68	102.74	114.10
2	F	160	ASP	N-CA-CB	-5.68	103.04	110.59
2	F	203	MET	CA-C-N	5.68	130.99	122.58
2	F	203	MET	C-N-CA	5.68	130.99	122.58
2	H	87	PHE	O-C-N	-5.68	116.61	123.03
1	I	357	PRO	N-CA-CB	5.68	108.59	103.08
2	J	42	ILE	CA-CB-CG2	5.68	120.15	110.50
2	H	226	ASN	CB-CG-ND2	5.67	124.91	116.40
1	I	37	HIS	ND1-CE1-NE2	5.67	114.07	108.40
2	D	368	LEU	CA-C-O	-5.67	114.29	120.81
1	I	313	VAL	CB-CA-C	5.67	121.38	111.18
1	A	270	PHE	CA-CB-CG	5.66	119.46	113.80
2	B	329	ASN	CA-CB-CG	-5.66	106.94	112.60
2	F	207	GLU	CA-C-N	5.66	128.14	120.44
2	F	207	GLU	C-N-CA	5.66	128.14	120.44
2	B	283	HIS	N-CA-CB	-5.66	100.69	110.32
1	M	120	VAL	CA-C-N	5.66	128.66	120.79
1	M	120	VAL	C-N-CA	5.66	128.66	120.79
2	B	43	GLY	CA-C-N	5.66	128.87	121.85
2	B	43	GLY	C-N-CA	5.66	128.87	121.85
2	F	346	TRP	N-CA-CB	-5.66	102.30	110.56
1	K	385	PHE	N-CA-C	5.66	117.31	111.03
1	E	364	SER	N-CA-CB	-5.66	102.74	111.46
2	F	211	ASP	CA-CB-CG	5.66	118.26	112.60
2	N	390	ARG	N-CA-C	5.66	117.53	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	346	PRO	N-CA-CB	5.66	108.27	103.35
1	G	190	HIS	N-CA-C	5.66	117.44	111.28
1	M	137	HIS	CB-CG-CD2	-5.66	123.85	131.20
2	B	54	SER	O-C-N	-5.65	116.63	123.13
1	I	397	TRP	CD2-CE3-CZ3	5.65	125.95	118.60
1	M	287	PRO	N-CA-C	5.65	122.94	113.78
1	C	238	THR	CA-C-O	-5.65	113.12	119.79
2	D	311	LYS	CA-C-O	-5.65	113.33	120.28
1	C	26	ASP	CA-CB-CG	5.65	118.25	112.60
2	F	134	GLY	N-CA-C	5.65	117.79	110.45
1	G	159	TYR	CA-C-O	-5.65	115.67	121.32
1	C	404	ASP	CA-C-N	5.64	129.71	120.63
1	C	404	ASP	C-N-CA	5.64	129.71	120.63
1	E	89	ASN	CA-CB-CG	-5.64	106.96	112.60
2	N	431	ASP	CA-C-O	-5.64	113.73	120.10
2	J	118	VAL	N-CA-C	5.64	116.28	110.36
1	G	225	LEU	CA-C-N	5.64	130.22	120.58
1	G	225	LEU	C-N-CA	5.64	130.22	120.58
2	H	88	HIS	ND1-CG-CD2	5.64	111.74	106.10
2	J	146	GLY	CA-C-N	5.64	129.54	121.71
2	J	146	GLY	C-N-CA	5.64	129.54	121.71
2	J	294	ALA	CA-C-O	-5.64	113.73	120.10
2	B	25	CYS	O-C-N	5.63	128.12	122.03
1	E	6	HIS	CB-CG-ND1	5.63	131.15	122.70
1	E	399	THR	CA-CB-OG1	-5.63	101.16	109.60
1	M	198	GLU	CB-CG-CD	-5.63	103.03	112.60
1	E	6	HIS	CA-CB-CG	5.62	119.42	113.80
2	N	172	TYR	CD1-CG-CD2	5.62	126.53	118.10
2	N	430	LYS	CA-C-O	-5.62	114.46	120.42
1	G	92	PHE	CA-CB-CG	5.62	119.42	113.80
2	N	272	TYR	CA-C-N	5.62	133.86	122.45
2	N	272	TYR	C-N-CA	5.62	133.86	122.45
1	G	8	GLN	CA-CB-CG	5.62	125.34	114.10
1	C	247	ASN	CA-C-N	5.62	131.19	121.64
1	C	247	ASN	C-N-CA	5.62	131.19	121.64
1	E	25	SER	CA-C-N	5.62	127.74	120.44
1	E	25	SER	C-N-CA	5.62	127.74	120.44
1	E	190	HIS	CA-C-O	5.62	126.51	120.55
2	L	110	ILE	CA-CB-CG1	5.62	119.95	110.40
1	A	337	ASN	CA-CB-CG	5.62	118.22	112.60
1	A	359	ARG	CA-C-O	-5.62	114.87	121.16
2	L	28	HIS	CB-CG-CD2	-5.62	123.90	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	TRP	CE3-CZ3-CH2	-5.61	113.80	121.10
1	M	400	GLY	CA-C-O	5.61	126.31	119.01
1	C	283	ALA	CA-C-O	-5.61	115.49	121.94
1	C	77	ARG	CD-NE-CZ	5.61	132.25	124.40
2	H	266	HIS	CA-C-N	5.61	130.67	122.98
2	H	266	HIS	C-N-CA	5.61	130.67	122.98
2	J	186	ASN	CA-C-N	5.61	128.06	120.38
2	J	186	ASN	C-N-CA	5.61	128.06	120.38
2	N	249	ASN	N-CA-CB	-5.61	102.21	110.85
1	A	247	ASN	CA-CB-CG	5.61	118.21	112.60
1	G	178	THR	CA-CB-OG1	5.61	118.01	109.60
2	H	118	VAL	N-CA-CB	5.61	117.75	110.57
1	M	442	GLU	O-C-N	-5.61	116.11	122.84
1	A	152	ILE	CA-C-N	5.60	127.72	120.44
1	A	152	ILE	C-N-CA	5.60	127.72	120.44
2	J	190	THR	CA-C-O	-5.60	114.93	120.70
1	M	181	GLU	O-C-N	-5.60	114.88	121.32
1	K	32	PRO	N-CA-C	5.60	120.86	113.86
2	L	56	THR	CA-CB-OG1	5.60	118.00	109.60
1	I	213	ARG	CA-C-N	5.60	128.05	120.44
1	I	213	ARG	C-N-CA	5.60	128.05	120.44
2	N	419	SER	CA-C-O	-5.60	114.49	120.42
1	A	334	GLN	O-C-N	-5.59	115.77	122.15
2	L	25	CYS	CA-CB-SG	-5.59	101.54	114.40
2	L	161	TYR	N-CA-C	5.59	120.26	113.38
2	N	106	GLY	O-C-N	5.59	128.38	122.28
2	B	251	ASP	CB-CA-C	5.59	120.31	110.36
1	C	18	ALA	N-CA-C	5.59	118.14	111.71
1	C	234	SER	N-CA-C	-5.59	105.10	111.14
1	C	437	GLU	O-C-N	-5.59	116.87	123.41
2	D	256	GLN	CB-CA-C	5.59	120.07	110.79
2	D	338	LYS	CA-CB-CG	-5.59	102.92	114.10
1	K	111	GLU	CA-C-O	5.59	126.04	119.28
1	K	249	ASP	CA-CB-CG	5.59	118.19	112.60
2	N	126	ALA	CA-C-N	5.59	129.54	120.60
2	N	126	ALA	C-N-CA	5.59	129.54	120.60
2	B	25	CYS	CA-C-O	-5.59	115.14	120.90
1	M	234	SER	CA-C-N	5.58	126.14	120.00
1	M	234	SER	C-N-CA	5.58	126.14	120.00
2	J	50	ASN	CA-C-N	5.58	130.04	120.72
2	J	50	ASN	C-N-CA	5.58	130.04	120.72
1	K	369	GLY	O-C-N	5.58	128.27	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	273	ALA	O-C-N	-5.58	117.95	121.85
2	H	330	ALA	N-CA-CB	-5.58	101.92	110.12
1	G	303	CYS	N-CA-C	5.58	118.82	109.95
2	J	303	VAL	O-C-N	-5.58	117.32	123.18
2	N	309	HIS	CB-CG-ND1	5.58	131.06	122.70
1	I	174	LYS	N-CA-C	5.58	120.20	112.45
1	M	161	ASP	CB-CA-C	5.58	119.35	109.65
1	C	305	PRO	N-CD-CG	5.57	111.56	103.20
2	D	39	ASP	CA-C-O	5.57	127.22	120.81
2	F	82	THR	OG1-CB-CG2	-5.57	98.16	109.30
1	I	31	ASP	CA-C-N	5.57	126.81	119.84
1	I	31	ASP	C-N-CA	5.57	126.81	119.84
2	J	115	ILE	O-C-N	-5.57	116.45	121.91
2	L	105	ARG	CD-NE-CZ	5.57	132.20	124.40
3	O	374	HIS	N-CA-C	5.57	122.67	110.80
2	F	351	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	344	TRP	NE1-CE2-CZ2	5.57	138.46	130.10
2	B	162	GLY	N-CA-C	5.57	120.53	113.24
1	I	232	THR	CA-CB-CG2	5.57	119.97	110.50
2	L	46	ASP	CA-C-N	5.57	131.72	121.70
2	L	46	ASP	C-N-CA	5.57	131.72	121.70
2	N	326	LYS	CA-C-O	-5.57	114.65	120.55
2	B	46	ASP	O-C-N	-5.56	115.78	123.12
2	N	334	THR	CA-CB-OG1	5.56	117.94	109.60
1	C	37	HIS	ND1-CG-CD2	5.56	111.66	106.10
1	C	84	ILE	CA-C-N	5.56	128.77	120.87
1	C	84	ILE	C-N-CA	5.56	128.77	120.87
1	I	367	PHE	N-CA-C	5.56	118.99	110.20
1	A	242	PHE	CA-C-O	5.56	126.01	120.28
1	K	403	MET	CA-C-O	-5.56	114.90	120.96
1	M	101	TRP	CD2-CE3-CZ3	5.56	125.83	118.60
2	H	65	ALA	N-CA-CB	-5.56	102.94	111.56
1	I	380	ARG	CD-NE-CZ	5.56	132.18	124.40
2	B	295	CYS	CA-C-O	5.55	126.27	119.05
2	J	98	ASP	OD1-CG-OD2	-5.55	109.57	122.90
2	D	285	GLN	CB-CA-C	5.55	118.89	109.84
2	F	20	CYS	O-C-N	-5.55	115.82	122.15
2	L	179	THR	CB-CA-C	5.55	119.30	109.75
2	L	344	VAL	N-CA-CB	5.55	116.58	110.53
2	B	403	ALA	CA-C-N	5.55	132.14	121.54
2	B	403	ALA	C-N-CA	5.55	132.14	121.54
2	F	35	GLN	OE1-CD-NE2	-5.55	117.05	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	227	HIS	CA-CB-CG	-5.55	108.25	113.80
2	L	425	MET	N-CA-C	5.55	118.26	111.82
1	A	325	GLU	CB-CA-C	5.55	119.59	110.88
1	C	344	TRP	CD2-CE3-CZ3	5.55	125.81	118.60
1	G	86	ARG	CA-C-O	-5.54	114.25	119.80
1	C	67	ASP	CA-CB-CG	5.54	118.14	112.60
1	M	73	MET	CA-C-O	-5.54	114.64	120.63
1	A	271	ALA	O-C-N	5.54	126.16	121.84
2	D	71	GLU	CA-CB-CG	5.54	125.19	114.10
2	F	37	PRO	CA-C-N	5.54	134.28	121.87
2	F	37	PRO	C-N-CA	5.54	134.28	121.87
1	G	130	LEU	N-CA-CB	-5.54	100.76	109.51
2	H	231	ILE	CA-C-N	5.54	128.02	120.54
2	H	231	ILE	C-N-CA	5.54	128.02	120.54
2	N	185	TYR	CA-CB-CG	5.54	123.88	113.90
1	I	172	SER	CA-C-N	5.54	125.20	119.05
1	I	172	SER	C-N-CA	5.54	125.20	119.05
2	J	107	HIS	ND1-CE1-NE2	5.54	113.94	108.40
2	B	73	THR	O-C-N	-5.54	115.46	122.27
1	E	243	PRO	N-CD-CG	5.54	111.51	103.20
2	L	391	LEU	N-CA-CB	-5.54	101.97	110.16
1	E	48	ASN	N-CA-C	5.54	118.83	111.75
1	I	313	VAL	CA-CB-CG2	5.54	119.81	110.40
1	K	169	VAL	CA-C-N	5.54	130.38	122.24
1	K	169	VAL	C-N-CA	5.54	130.38	122.24
2	H	290	GLU	CA-C-O	-5.53	115.20	120.90
1	M	94	GLN	OE1-CD-NE2	-5.53	117.07	122.60
2	B	333	ALA	N-CA-C	5.53	118.83	111.75
1	G	118	ASP	CA-C-N	5.53	128.04	120.46
1	G	118	ASP	C-N-CA	5.53	128.04	120.46
1	A	190	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	E	23	VAL	CA-C-O	-5.53	114.65	120.57
2	L	19	ALA	N-CA-C	-5.53	106.58	113.55
1	A	318	ARG	CD-NE-CZ	5.53	132.14	124.40
1	C	262	ARG	O-C-N	5.53	128.85	121.67
1	I	124	SER	O-C-N	-5.53	115.85	122.15
1	A	322	SER	N-CA-C	5.52	117.71	109.59
2	D	226	ASN	O-C-N	5.52	128.06	122.09
2	F	367	ASP	CA-C-N	5.52	128.61	120.82
2	F	367	ASP	C-N-CA	5.52	128.61	120.82
2	B	407	TRP	CE2-CD2-CG	5.52	113.83	107.20
2	L	18	ASN	OD1-CG-ND2	-5.52	117.08	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	417	ASP	N-CA-C	5.52	117.30	111.28
1	K	396	HIS	O-C-N	-5.52	115.76	122.22
2	D	301	GLN	CB-CA-C	5.52	118.86	109.53
1	E	335	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	C	84	ILE	CA-C-O	5.52	126.69	119.85
2	H	41	THR	CA-CB-OG1	5.52	117.88	109.60
1	M	76	VAL	CA-C-O	-5.52	115.00	120.85
2	B	77	GLU	O-C-N	-5.51	116.28	122.12
2	F	227	LEU	CA-C-N	5.51	128.69	120.31
2	F	227	LEU	C-N-CA	5.51	128.69	120.31
2	J	55	GLU	CA-C-N	5.51	131.25	122.59
2	J	55	GLU	C-N-CA	5.51	131.25	122.59
1	K	174	LYS	O-C-N	5.51	127.87	122.19
1	A	37	HIS	ND1-CE1-NE2	5.51	113.91	108.40
2	D	407	TRP	CG-CD2-CE3	5.51	139.41	133.90
2	L	306	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	89	ASN	CA-C-N	-5.51	115.09	122.42
1	C	89	ASN	C-N-CA	-5.51	115.09	122.42
2	N	269	LEU	CB-CA-C	5.51	118.93	109.51
1	G	206	ALA	O-C-N	-5.51	114.54	122.36
2	N	190	THR	CA-CB-OG1	-5.51	101.34	109.60
2	N	201	ALA	N-CA-CB	-5.51	102.31	110.90
2	N	278	ALA	O-C-N	5.51	127.82	122.09
1	G	45	GLU	O-C-N	5.50	127.95	122.12
2	N	81	GLY	CA-C-N	5.50	127.66	120.28
2	N	81	GLY	C-N-CA	5.50	127.66	120.28
1	C	154	LYS	N-CA-C	5.50	118.11	111.40
2	D	3	GLU	N-CA-C	5.50	117.63	108.99
2	D	164	LYS	CA-C-N	5.50	128.66	120.95
2	D	164	LYS	C-N-CA	5.50	128.66	120.95
1	E	62	ARG	N-CA-CB	-5.50	101.19	110.49
2	H	252	LEU	O-C-N	-5.50	115.78	122.22
1	C	337	ASN	CA-C-N	5.50	128.41	120.38
1	C	337	ASN	C-N-CA	5.50	128.41	120.38
1	K	227	HIS	ND1-CE1-NE2	5.50	113.90	108.40
1	M	12	CYS	CA-C-N	5.50	126.05	119.94
1	M	12	CYS	C-N-CA	5.50	126.05	119.94
1	C	70	PRO	N-CD-CG	5.50	111.45	103.20
1	G	151	LEU	O-C-N	-5.50	115.50	122.27
1	A	88	ASP	N-CA-CB	-5.50	100.32	110.32
2	H	323	VAL	CA-C-N	5.50	128.74	123.02
2	H	323	VAL	C-N-CA	5.50	128.74	123.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	309	HIS	CB-CG-CD2	-5.50	124.06	131.20
2	F	285	GLN	OE1-CD-NE2	-5.50	117.11	122.60
3	O	387	ASP	CA-C-N	5.49	132.03	121.54
3	O	387	ASP	C-N-CA	5.49	132.03	121.54
1	A	311	LEU	N-CA-C	-5.49	104.94	111.03
2	B	367	ASP	CA-CB-CG	-5.49	107.11	112.60
2	F	444	GLY	O-C-N	-5.49	119.10	123.27
2	B	168	GLU	CA-C-N	5.49	130.70	122.47
2	B	168	GLU	C-N-CA	5.49	130.70	122.47
2	F	369	ALA	CA-C-O	-5.49	115.50	121.87
2	J	238	ILE	CA-CB-CG2	5.49	119.83	110.50
2	F	182	VAL	CA-CB-CG2	5.49	119.73	110.40
1	M	431	ASP	CA-C-N	5.49	130.40	122.44
1	M	431	ASP	C-N-CA	5.49	130.40	122.44
1	E	54	ALA	CA-C-N	5.48	131.63	122.20
1	E	54	ALA	C-N-CA	5.48	131.63	122.20
1	C	340	TYR	CB-CG-CD2	-5.48	112.58	120.80
1	E	123	GLU	CA-C-O	-5.48	114.71	120.63
2	J	141	PHE	CA-CB-CG	5.48	119.28	113.80
2	N	49	PHE	CA-C-O	-5.48	114.72	120.63
2	N	327	ASP	N-CA-C	5.48	117.33	111.36
1	A	209	ASP	CA-C-N	5.48	128.20	120.42
1	A	209	ASP	C-N-CA	5.48	128.20	120.42
1	C	394	PHE	CA-CB-CG	-5.47	108.33	113.80
1	I	45	GLU	N-CA-CB	-5.47	101.78	109.94
2	J	98	ASP	O-C-N	-5.47	116.08	122.81
1	K	103	LYS	O-C-N	-5.47	115.27	122.39
2	H	139	HIS	N-CA-CB	-5.47	102.59	111.24
1	K	170	VAL	CA-C-O	-5.47	113.95	120.90
2	L	276	ILE	N-CA-CB	-5.47	103.01	110.56
2	B	323	VAL	CA-C-N	5.47	129.27	123.25
2	B	323	VAL	C-N-CA	5.47	129.27	123.25
1	G	90	PHE	CA-C-N	5.47	129.55	122.93
1	G	90	PHE	C-N-CA	5.47	129.55	122.93
2	H	268	PRO	N-CA-CB	5.47	108.52	102.72
1	M	218	THR	CA-C-N	5.47	128.66	122.59
1	M	218	THR	C-N-CA	5.47	128.66	122.59
2	D	158	SER	CA-C-N	5.47	127.53	120.70
2	D	158	SER	C-N-CA	5.47	127.53	120.70
2	F	309	HIS	CE1-NE2-CD2	5.47	114.47	109.00
2	H	106	GLY	O-C-N	-5.47	116.44	122.24
1	A	242	PHE	CA-C-N	5.47	125.93	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	PHE	C-N-CA	5.47	125.93	120.52
2	H	429	GLU	CA-C-O	-5.47	113.69	119.97
2	N	195	LEU	N-CA-C	5.47	119.45	112.34
2	B	124	LYS	CA-C-N	5.46	127.86	120.38
2	B	124	LYS	C-N-CA	5.46	127.86	120.38
1	K	152	ILE	CA-C-O	-5.46	115.27	120.95
1	K	396	HIS	ND1-CE1-NE2	5.46	113.86	108.40
1	M	92	PHE	CA-C-N	5.46	129.48	121.67
1	M	92	PHE	C-N-CA	5.46	129.48	121.67
1	A	23	VAL	CA-C-O	-5.46	113.95	120.78
1	C	367	PHE	N-CA-CB	-5.46	101.51	110.41
2	H	26	LEU	N-CA-CB	-5.46	101.82	110.28
1	C	19	LYS	CA-C-O	-5.46	113.35	119.79
2	D	86	LEU	CA-C-O	5.46	126.32	120.70
2	L	324	VAL	N-CA-CB	-5.46	106.58	112.37
2	B	406	HIS	CG-CD2-NE2	-5.46	101.74	107.20
2	D	38	SER	CA-C-N	5.46	128.59	120.95
2	D	38	SER	C-N-CA	5.46	128.59	120.95
2	L	183	GLU	CA-C-N	5.46	124.91	119.24
2	L	183	GLU	C-N-CA	5.46	124.91	119.24
2	L	356	ASN	CA-CB-CG	5.46	118.06	112.60
1	M	324	LYS	N-CA-C	5.46	117.31	111.36
1	C	242	PHE	N-CA-CB	-5.45	101.36	111.18
2	F	82	THR	CA-C-N	5.45	131.25	122.14
2	F	82	THR	C-N-CA	5.45	131.25	122.14
2	L	219	ILE	CA-CB-CG1	5.45	119.67	110.40
1	M	16	ILE	CB-CA-C	5.45	119.18	112.04
2	N	304	LYS	N-CA-C	5.45	119.56	113.01
2	N	388	TRP	NE1-CE2-CD2	-5.45	100.31	107.40
2	D	123	ARG	N-CA-C	5.45	117.93	111.33
2	B	283	HIS	CA-C-O	5.45	126.08	119.49
2	F	298	PRO	N-CA-C	5.45	123.69	112.47
2	J	41	THR	OG1-CB-CG2	-5.45	98.40	109.30
1	M	155	ILE	CA-C-N	5.45	128.59	120.31
1	M	155	ILE	C-N-CA	5.45	128.59	120.31
2	B	218	ASP	N-CA-CB	-5.45	103.63	111.91
2	F	214	ARG	N-CA-C	5.45	118.39	111.69
1	A	161	ASP	CA-CB-CG	5.44	118.04	112.60
2	D	31	GLN	N-CA-CB	-5.44	102.21	110.05
2	J	105	ARG	CA-C-O	-5.44	115.09	120.70
1	A	358	PRO	O-C-N	-5.44	116.33	122.91
2	L	390	ARG	CA-C-O	5.44	126.28	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	408	TYR	CA-C-N	5.44	127.91	120.46
2	N	408	TYR	C-N-CA	5.44	127.91	120.46
2	B	181	VAL	CB-CA-C	-5.44	103.45	112.26
2	H	56	THR	CA-CB-CG2	5.44	119.75	110.50
2	J	328	VAL	CA-CB-CG2	-5.44	101.16	110.40
2	L	433	GLU	CA-CB-CG	-5.44	103.22	114.10
2	L	218	ASP	O-C-N	-5.44	116.06	122.58
1	C	280	GLN	N-CA-C	5.43	119.17	112.54
1	C	404	ASP	CA-CB-CG	5.43	118.03	112.60
2	D	414	GLU	O-C-N	-5.43	116.97	123.06
2	H	224	TYR	CA-CB-CG	5.43	123.68	113.90
1	C	66	VAL	N-CA-C	5.43	116.49	108.45
2	D	16	ILE	CA-C-N	5.43	125.97	119.94
2	D	16	ILE	C-N-CA	5.43	125.97	119.94
1	G	94	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	K	45	GLU	N-CA-C	5.43	116.88	111.07
1	K	426	GLN	CG-CD-NE2	5.43	124.54	116.40
2	D	128	GLN	O-C-N	-5.43	114.88	122.37
2	H	159	VAL	O-C-N	-5.43	115.67	121.80
2	N	220	GLU	CA-C-N	5.43	128.49	122.74
2	N	220	GLU	C-N-CA	5.43	128.49	122.74
1	C	104	GLY	CA-C-N	5.42	127.99	120.29
1	C	104	GLY	C-N-CA	5.42	127.99	120.29
1	K	189	VAL	CA-CB-CG1	5.42	119.62	110.40
1	A	200	TYR	N-CA-CB	-5.42	101.96	110.69
1	G	307	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	K	102	ALA	N-CA-C	5.42	117.19	111.28
2	D	11	GLN	N-CA-C	5.42	119.61	112.89
2	D	216	ASN	N-CA-C	-5.42	104.86	112.12
2	D	235	VAL	N-CA-C	5.42	116.15	110.62
1	M	182	PRO	N-CA-C	5.42	120.67	113.57
2	D	118	VAL	CA-CB-CG1	5.42	119.61	110.40
1	G	208	TYR	O-C-N	-5.42	116.38	122.12
1	M	396	HIS	CB-CG-CD2	-5.42	124.16	131.20
2	H	207	GLU	O-C-N	-5.41	115.08	122.33
1	K	176	SER	CB-CA-C	5.41	120.06	109.35
2	L	346	TRP	NE1-CE2-CD2	-5.41	100.37	107.40
1	E	282	ARG	CB-CA-C	5.41	119.30	109.83
2	H	215	ARG	CA-C-N	5.41	127.80	120.44
2	H	215	ARG	C-N-CA	5.41	127.80	120.44
1	C	403	MET	CA-C-O	-5.41	115.83	121.99
1	C	228	LEU	CA-C-O	-5.41	114.82	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	341	PHE	N-CA-C	5.41	118.39	109.85
1	M	100	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	A	231	ALA	CA-C-O	-5.40	115.15	120.82
2	D	88	HIS	CA-CB-CG	5.40	119.20	113.80
1	K	183	TYR	CA-C-N	5.40	127.78	120.38
1	K	183	TYR	C-N-CA	5.40	127.78	120.38
2	B	116	ASP	CA-C-O	-5.40	113.76	119.97
1	G	234	SER	CA-C-N	5.40	126.09	119.99
1	G	234	SER	C-N-CA	5.40	126.09	119.99
1	G	237	THR	N-CA-CB	5.40	118.77	110.61
2	H	269	LEU	CB-CA-C	5.40	118.44	109.53
2	L	182	VAL	CA-CB-CG2	5.40	119.58	110.40
1	M	409	THR	OG1-CB-CG2	-5.40	98.49	109.30
1	G	137	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	K	381	ILE	CA-C-N	5.40	127.46	120.44
1	K	381	ILE	C-N-CA	5.40	127.46	120.44
2	F	315	CYS	CA-C-O	5.40	127.32	121.06
2	F	406	HIS	CA-C-O	-5.40	114.00	120.10
2	L	85	GLN	CA-C-N	5.40	128.52	120.31
2	L	85	GLN	C-N-CA	5.40	128.52	120.31
2	J	346	TRP	N-CA-CB	-5.40	102.02	110.44
1	C	335	ASN	OD1-CG-ND2	-5.39	117.20	122.60
1	C	212	PHE	N-CA-C	5.39	118.08	111.82
2	L	208	ALA	O-C-N	-5.39	115.22	122.23
1	M	433	GLN	OE1-CD-NE2	-5.39	117.21	122.60
2	N	158	SER	CA-C-N	5.39	129.99	121.09
2	N	158	SER	C-N-CA	5.39	129.99	121.09
2	F	291	ILE	N-CA-C	-5.39	105.28	110.72
1	K	305	PRO	N-CA-C	5.39	123.57	112.47
1	E	393	ALA	CA-C-N	5.39	131.83	121.54
1	E	393	ALA	C-N-CA	5.39	131.83	121.54
1	I	211	CYS	CB-CA-C	5.39	119.49	110.92
2	F	123	ARG	N-CA-C	5.39	117.15	111.28
2	L	319	TYR	CB-CA-C	5.39	119.26	109.62
2	F	372	GLN	OE1-CD-NE2	-5.38	117.22	122.60
2	J	278	ALA	CA-C-O	5.38	126.47	120.82
2	J	366	GLY	N-CA-C	5.38	121.09	112.58
1	G	105	HIS	CB-CG-CD2	-5.38	124.20	131.20
1	G	156	ARG	CA-C-O	-5.38	114.02	120.10
1	M	376	GLU	CA-CB-CG	5.38	124.86	114.10
2	H	301	GLN	CG-CD-NE2	5.38	124.47	116.40
2	L	363	VAL	CA-CB-CG1	5.38	119.55	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	192	HIS	CB-CG-CD2	-5.38	124.21	131.20
2	F	211	ASP	CA-C-N	5.38	127.83	120.46
2	F	211	ASP	C-N-CA	5.38	127.83	120.46
2	B	63	PRO	CB-CA-C	-5.37	104.74	111.56
2	B	62	VAL	CA-C-N	5.37	125.38	119.90
2	B	62	VAL	C-N-CA	5.37	125.38	119.90
2	B	257	THR	CA-CB-CG2	5.37	119.63	110.50
2	F	160	ASP	CA-CB-CG	5.37	117.97	112.60
1	M	152	ILE	O-C-N	5.37	127.15	121.89
1	A	426	GLN	CA-CB-CG	5.37	124.83	114.10
1	C	264	HIS	CA-C-N	5.37	129.18	121.50
1	C	264	HIS	C-N-CA	5.37	129.18	121.50
2	L	202	PHE	CA-CB-CG	5.37	119.17	113.80
1	C	192	LEU	N-CA-CB	-5.37	102.22	110.16
1	G	52	ASN	CA-CB-CG	-5.37	107.23	112.60
3	O	388	HIS	CA-C-N	5.37	131.36	121.70
3	O	388	HIS	C-N-CA	5.37	131.36	121.70
2	D	218	ASP	CA-C-N	5.36	128.27	120.98
2	D	218	ASP	C-N-CA	5.36	128.27	120.98
1	G	120	VAL	N-CA-CB	5.36	116.47	110.62
2	J	353	VAL	CA-C-N	5.36	126.25	122.33
2	J	353	VAL	C-N-CA	5.36	126.25	122.33
2	F	309	HIS	CG-CD2-NE2	-5.36	101.84	107.20
2	H	210	TYR	CA-C-N	5.36	127.90	120.29
2	H	210	TYR	C-N-CA	5.36	127.90	120.29
1	C	266	PHE	CA-C-N	5.36	130.19	121.83
1	C	266	PHE	C-N-CA	5.36	130.19	121.83
2	F	413	MET	O-C-N	-5.36	117.06	123.06
2	H	75	ILE	O-C-N	5.36	129.26	122.57
2	H	268	PRO	CA-C-N	5.36	130.01	122.09
2	H	268	PRO	C-N-CA	5.36	130.01	122.09
2	H	317	LEU	CA-C-N	5.36	131.75	122.32
2	H	317	LEU	C-N-CA	5.36	131.75	122.32
2	L	61	HIS	CG-CD2-NE2	-5.36	101.84	107.20
2	F	88	HIS	CA-C-N	5.35	125.17	119.28
2	F	88	HIS	C-N-CA	5.35	125.17	119.28
1	M	165	ASN	O-C-N	-5.35	116.65	123.24
2	N	270	ALA	N-CA-CB	-5.35	102.38	111.69
1	K	291	GLN	O-C-N	-5.35	116.45	122.12
2	H	314	ALA	N-CA-C	5.35	117.20	109.07
2	H	363	VAL	CG1-CB-CG2	-5.35	99.03	110.80
2	H	381	THR	O-C-N	-5.35	117.49	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	197	HIS	N-CA-C	5.35	119.57	112.72
2	B	325	PRO	CA-C-N	5.35	128.44	120.31
2	B	325	PRO	C-N-CA	5.35	128.44	120.31
1	C	184	ASN	CA-CB-CG	5.35	117.95	112.60
2	D	18	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	K	105	HIS	ND1-CG-CD2	5.35	111.45	106.10
1	K	223	GLY	O-C-N	-5.35	116.98	122.17
2	L	355	ILE	O-C-N	-5.35	117.52	123.03
2	N	120	ASP	CB-CA-C	5.35	119.67	110.79
1	C	214	THR	CB-CA-C	5.35	117.63	109.34
2	D	41	THR	CA-C-O	5.35	126.20	120.32
1	G	378	PHE	CA-CB-CG	5.35	119.15	113.80
1	I	204	ASN	CA-C-O	-5.35	113.82	119.97
2	L	372	GLN	OE1-CD-NE2	-5.35	117.25	122.60
2	D	144	GLY	O-C-N	-5.35	116.45	122.28
1	G	212	PHE	CA-CB-CG	5.35	119.15	113.80
1	E	328	GLU	CA-CB-CG	5.34	124.79	114.10
2	H	88	HIS	CA-C-N	5.34	124.86	119.19
2	H	88	HIS	C-N-CA	5.34	124.86	119.19
2	J	300	ASN	CA-CB-CG	5.34	117.94	112.60
2	D	23	LEU	CA-C-N	5.34	127.97	120.28
2	D	23	LEU	C-N-CA	5.34	127.97	120.28
1	K	337	ASN	CA-C-N	5.34	127.97	120.28
1	K	337	ASN	C-N-CA	5.34	127.97	120.28
1	K	438	GLU	CB-CG-CD	5.34	121.68	112.60
1	K	172	SER	N-CA-CB	-5.34	102.83	110.04
2	L	141	PHE	CA-C-N	5.34	131.88	121.41
2	L	141	PHE	C-N-CA	5.34	131.88	121.41
2	N	369	ALA	O-C-N	-5.34	116.33	122.95
1	G	48	ASN	CA-C-N	5.34	129.38	120.62
1	G	48	ASN	C-N-CA	5.34	129.38	120.62
1	M	266	PHE	CA-C-N	5.34	129.03	121.61
1	M	266	PHE	C-N-CA	5.34	129.03	121.61
1	C	86	ARG	CB-CA-C	5.34	118.48	109.67
2	H	142	GLY	CA-C-N	5.34	125.75	120.31
2	H	142	GLY	C-N-CA	5.34	125.75	120.31
2	L	109	THR	N-CA-CB	5.34	118.03	110.13
2	B	337	THR	CA-C-O	-5.33	114.32	120.24
2	B	38	SER	CA-C-O	-5.33	115.48	121.40
3	O	363	VAL	CA-C-N	5.33	125.09	119.76
3	O	363	VAL	C-N-CA	5.33	125.09	119.76
2	F	19	ALA	O-C-N	-5.33	116.07	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	208	ALA	N-CA-CB	-5.33	102.13	109.91
2	N	334	THR	N-CA-CB	5.33	118.78	109.72
1	A	87	PRO	N-CA-C	5.33	121.69	113.75
2	F	320	ARG	CD-NE-CZ	5.33	131.86	124.40
1	K	334	GLN	OE1-CD-NE2	-5.33	117.27	122.60
2	L	390	ARG	CB-CG-CD	5.33	123.56	111.30
1	A	137	HIS	N-CA-C	5.33	115.06	108.19
1	K	407	GLU	CA-C-N	5.33	127.73	120.54
1	K	407	GLU	C-N-CA	5.33	127.73	120.54
2	L	278	ALA	O-C-N	5.33	127.77	122.12
2	H	28	HIS	CB-CG-CD2	-5.33	124.28	131.20
1	M	172	SER	N-CA-C	5.32	117.63	110.29
1	C	340	TYR	CA-CB-CG	5.32	123.48	113.90
1	E	166	THR	CA-CB-CG2	5.32	119.55	110.50
2	F	203	MET	CG-SD-CE	-5.32	89.19	100.90
2	J	221	ARG	CA-C-N	5.32	125.08	119.76
2	J	221	ARG	C-N-CA	5.32	125.08	119.76
2	B	133	GLN	OE1-CD-NE2	-5.32	117.28	122.60
2	N	2	ARG	N-CA-C	5.32	116.93	108.79
1	C	397	TRP	CD2-CE3-CZ3	5.32	125.51	118.60
1	M	24	ILE	CA-C-N	5.32	127.35	120.44
1	M	24	ILE	C-N-CA	5.32	127.35	120.44
2	D	418	PHE	CA-CB-CG	-5.31	108.49	113.80
2	D	67	PHE	CA-CB-CG	5.31	119.11	113.80
2	H	69	ASP	OD1-CG-OD2	-5.31	110.15	122.90
1	E	119	VAL	CA-C-N	5.31	127.73	120.46
1	E	119	VAL	C-N-CA	5.31	127.73	120.46
1	G	32	PRO	CB-CA-C	-5.31	103.87	111.62
1	G	82	GLY	N-CA-C	5.31	120.51	114.67
2	L	153	LEU	O-C-N	-5.31	115.78	122.20
2	L	385	ALA	N-CA-C	5.31	118.86	112.38
2	J	89	PRO	N-CA-C	5.31	120.74	113.84
2	D	368	LEU	N-CA-CB	-5.31	101.94	109.85
1	M	389	PHE	CA-CB-CG	5.31	119.11	113.80
1	G	49	VAL	CB-CA-C	-5.30	104.31	112.05
2	H	258	ASN	CA-C-O	-5.30	112.88	118.77
1	A	214	THR	CA-CB-OG1	5.30	117.56	109.60
2	H	98	ASP	CA-CB-CG	5.30	117.90	112.60
2	L	39	ASP	CB-CA-C	5.30	120.30	112.03
2	N	65	ALA	N-CA-C	5.30	117.25	109.24
1	E	140	GLY	N-CA-C	5.30	120.50	114.67
2	F	290	GLU	O-C-N	5.30	127.53	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	293	ASN	CB-CA-C	5.30	119.20	110.88
2	H	407	TRP	CE2-CD2-CE3	-5.30	113.50	118.80
1	I	108	GLU	N-CA-C	5.30	117.14	111.36
1	E	137	HIS	CB-CG-CD2	-5.30	124.31	131.20
2	H	207	GLU	N-CA-CB	5.30	118.46	110.30
1	E	170	VAL	CA-CB-CG2	5.30	119.40	110.40
1	I	221	THR	N-CA-CB	5.30	118.94	110.46
1	E	28	HIS	CE1-NE2-CD2	-5.29	103.71	109.00
1	E	161	ASP	N-CA-CB	-5.29	102.34	110.44
1	K	39	ASP	N-CA-C	5.29	119.49	113.19
2	F	122	ILE	CB-CG1-CD1	5.29	124.91	113.80
1	C	256	ASN	N-CA-CB	-5.29	102.75	110.47
1	G	33	THR	N-CA-C	5.29	119.22	112.34
1	G	215	LEU	CD1-CG-CD2	-5.29	99.16	110.80
1	I	387	ALA	CA-C-O	-5.29	114.81	120.42
2	H	147	SER	N-CA-C	-5.29	105.16	111.03
2	B	65	ALA	CA-C-N	5.29	130.47	122.91
2	B	65	ALA	C-N-CA	5.29	130.47	122.91
2	J	345	ASP	N-CA-CB	-5.28	101.14	110.39
2	F	115	ILE	CA-C-O	-5.28	115.46	120.95
1	A	282	ARG	N-CA-C	5.28	116.87	108.79
1	M	161	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	337	ASN	CA-C-N	5.28	128.33	120.31
1	A	337	ASN	C-N-CA	5.28	128.33	120.31
1	E	329	GLN	N-CA-C	-5.28	105.11	112.45
2	B	207	GLU	CB-CG-CD	-5.28	103.63	112.60
1	G	7	ILE	CA-CB-CG1	5.28	119.37	110.40
1	C	46	ARG	CB-CG-CD	5.28	123.44	111.30
2	N	249	ASN	OD1-CG-ND2	5.28	127.88	122.60
2	H	415	GLU	CA-C-N	5.27	125.83	119.98
2	H	415	GLU	C-N-CA	5.27	125.83	119.98
2	H	88	HIS	CB-CG-CD2	-5.27	124.34	131.20
1	M	4	ILE	CA-C-N	5.27	129.65	122.90
1	M	4	ILE	C-N-CA	5.27	129.65	122.90
2	B	276	ILE	CA-C-O	-5.27	115.76	121.19
1	G	374	ILE	CB-CG1-CD1	5.27	124.86	113.80
2	L	346	TRP	CD1-NE1-CE2	5.27	118.39	108.90
1	E	47	ILE	CA-C-N	5.27	128.07	120.38
1	E	47	ILE	C-N-CA	5.27	128.07	120.38
1	E	137	HIS	CB-CG-ND1	5.27	130.60	122.70
2	F	392	ASP	CB-CA-C	5.27	120.38	110.63
2	J	336	LYS	CA-C-N	5.27	127.29	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	336	LYS	C-N-CA	5.27	127.29	120.44
2	L	393	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	M	232	THR	N-CA-CB	5.27	118.05	110.20
2	D	190	THR	O-C-N	5.27	127.70	122.12
2	H	446	GLU	CA-C-N	5.26	129.77	120.87
2	H	446	GLU	C-N-CA	5.26	129.77	120.87
1	C	51	TYR	N-CA-C	5.26	117.19	109.24
2	D	135	PHE	CA-CB-CG	5.26	119.06	113.80
2	F	229	ARG	N-CA-C	-5.26	106.36	112.89
1	I	38	GLY	CA-C-N	5.26	131.20	121.52
1	I	38	GLY	C-N-CA	5.26	131.20	121.52
1	I	167	PHE	CA-CB-CG	5.26	119.06	113.80
2	N	134	GLY	N-CA-C	5.26	117.69	110.69
2	F	158	SER	N-CA-CB	5.26	117.64	110.01
2	L	128	GLN	CG-CD-NE2	5.26	124.29	116.40
1	K	11	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	G	202	ILE	CB-CG1-CD1	5.25	124.83	113.80
2	L	46	ASP	CA-CB-CG	-5.25	107.34	112.60
2	B	323	VAL	N-CA-C	5.25	117.42	108.86
2	H	104	ALA	O-C-N	-5.25	116.55	122.12
2	L	431	ASP	CA-C-O	-5.25	114.41	120.24
1	C	399	THR	CA-C-N	5.25	130.14	120.79
1	C	399	THR	C-N-CA	5.25	130.14	120.79
1	C	145	SER	N-CA-CB	-5.25	102.46	110.07
1	E	308	GLY	CA-C-N	5.25	130.83	121.75
1	E	308	GLY	C-N-CA	5.25	130.83	121.75
2	L	280	LYS	O-C-N	5.25	128.72	122.27
2	L	375	VAL	N-CA-C	5.25	115.83	108.17
1	I	263	LEU	CB-CA-C	5.25	118.93	111.74
2	F	135	PHE	N-CA-C	5.25	117.95	109.40
1	M	221	THR	O-C-N	-5.25	116.82	123.17
2	B	50	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	C	41	ASP	CA-C-N	5.24	127.56	120.38
1	C	41	ASP	C-N-CA	5.24	127.56	120.38
2	J	177	VAL	CA-CB-CG1	5.24	119.31	110.40
1	M	99	ASN	N-CA-C	5.24	119.51	113.38
2	N	75	ILE	CA-C-N	5.24	127.56	120.38
2	N	75	ILE	C-N-CA	5.24	127.56	120.38
2	N	255	PHE	CA-CB-CG	5.24	119.04	113.80
2	D	172	TYR	N-CA-C	5.24	117.03	109.48
1	G	76	VAL	CA-C-O	-5.24	115.50	120.95
2	J	141	PHE	N-CA-C	5.24	119.39	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	132	LEU	CA-C-N	5.24	127.83	120.28
2	L	132	LEU	C-N-CA	5.24	127.83	120.28
2	L	153	LEU	CB-CA-C	5.24	119.54	110.84
2	F	368	LEU	CB-CA-C	5.24	118.07	109.90
1	K	334	GLN	N-CA-C	5.24	116.99	111.28
2	L	69	ASP	OD1-CG-OD2	-5.24	110.33	122.90
2	L	339	ARG	CA-C-N	5.24	127.56	120.38
2	L	339	ARG	C-N-CA	5.24	127.56	120.38
1	A	215	LEU	CA-C-N	5.24	132.60	123.91
1	A	215	LEU	C-N-CA	5.24	132.60	123.91
2	H	90	GLU	CA-CB-CG	-5.24	103.63	114.10
2	L	293	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	A	331	LEU	CB-CA-C	5.24	119.10	110.88
1	C	87	PRO	N-CD-CG	5.24	111.05	103.20
1	C	378	PHE	CA-C-N	5.24	127.72	120.29
1	C	378	PHE	C-N-CA	5.24	127.72	120.29
2	J	309	HIS	CA-C-N	5.23	126.90	120.51
2	J	309	HIS	C-N-CA	5.23	126.90	120.51
2	N	16	ILE	CA-C-N	5.23	125.76	120.00
2	N	16	ILE	C-N-CA	5.23	125.76	120.00
1	C	174	LYS	CA-C-O	-5.23	113.65	119.67
2	B	123	ARG	N-CA-C	5.23	117.66	111.33
2	J	363	VAL	CA-CB-CG1	5.23	119.29	110.40
2	D	51	THR	O-C-N	5.23	129.44	122.43
1	M	135	LEU	CA-C-O	-5.23	114.70	120.24
2	D	384	ILE	CB-CA-C	5.22	120.72	112.26
1	K	400	GLY	O-C-N	-5.22	116.88	122.73
2	L	266	HIS	N-CA-C	5.22	119.16	112.26
2	N	411	GLU	CB-CG-CD	5.22	121.48	112.60
2	D	3	GLU	O-C-N	-5.22	117.43	123.33
2	F	92	LEU	CA-C-O	-5.22	115.11	120.54
2	J	53	PHE	CA-CB-CG	5.22	119.02	113.80
2	J	116	ASP	CA-CB-CG	-5.22	107.38	112.60
2	L	406	HIS	CB-CG-CD2	-5.22	124.41	131.20
2	D	447	GLU	N-CA-C	5.22	118.23	110.14
2	J	363	VAL	O-C-N	-5.22	115.50	121.14
2	L	324	VAL	CA-CB-CG1	5.22	119.28	110.40
2	N	351	PHE	N-CA-C	5.22	117.26	108.96
2	B	285	GLN	CB-CA-C	5.22	118.24	109.89
2	F	174	ALA	N-CA-CB	-5.22	102.79	110.14
2	B	128	GLN	CB-CG-CD	5.21	121.47	112.60
2	D	128	GLN	N-CA-C	-5.21	106.69	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	201	CYS	CA-C-N	5.21	129.10	121.80
1	G	201	CYS	C-N-CA	5.21	129.10	121.80
2	J	137	VAL	CA-C-N	5.21	130.35	123.05
2	J	137	VAL	C-N-CA	5.21	130.35	123.05
2	J	164	LYS	CA-C-O	-5.21	114.97	120.92
2	D	160	ASP	CA-CB-CG	5.21	117.81	112.60
2	D	185	TYR	CA-CB-CG	5.21	123.28	113.90
2	L	98	ASP	CA-C-O	5.21	127.07	121.55
2	N	308	ARG	N-CA-C	5.21	117.70	111.71
2	H	31	GLN	N-CA-CB	-5.21	103.70	109.74
1	G	376	GLU	CA-C-O	-5.21	115.00	120.63
1	A	45	GLU	N-CA-C	5.21	118.89	112.54
1	A	195	ASN	N-CA-CB	-5.21	103.04	110.80
1	A	298	ASN	N-CA-CB	-5.21	101.66	110.41
2	H	166	LYS	CA-CB-CG	-5.21	103.69	114.10
2	L	28	HIS	CA-C-N	5.21	132.58	121.18
2	L	28	HIS	C-N-CA	5.21	132.58	121.18
2	N	291	ILE	CA-CB-CG1	5.21	119.25	110.40
1	I	429	THR	CA-C-N	5.21	130.82	121.66
1	I	429	THR	C-N-CA	5.21	130.82	121.66
1	A	230	SER	N-CA-C	5.20	116.64	111.07
1	I	258	VAL	N-CA-C	5.20	113.30	108.15
1	M	106	TYR	CA-C-O	-5.20	113.15	119.03
1	C	331	LEU	CB-CA-C	5.20	120.77	110.42
2	D	53	PHE	CA-C-N	5.20	130.10	122.77
2	D	53	PHE	C-N-CA	5.20	130.10	122.77
2	H	11	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	E	57	ASN	CA-CB-CG	5.20	117.80	112.60
2	F	125	LEU	CA-C-O	5.20	127.94	120.51
2	F	363	VAL	O-C-N	5.20	127.02	121.10
1	G	226	ASN	CA-C-N	5.19	127.76	120.28
1	G	226	ASN	C-N-CA	5.19	127.76	120.28
2	D	367	ASP	CA-C-N	5.19	128.22	120.95
2	D	367	ASP	C-N-CA	5.19	128.22	120.95
2	D	441	GLU	CB-CA-C	5.19	120.40	109.65
1	M	79	GLY	CA-C-N	5.19	124.95	119.76
1	M	79	GLY	C-N-CA	5.19	124.95	119.76
1	A	87	PRO	N-CD-CG	5.19	110.99	103.20
1	E	292	GLN	CA-C-N	-5.19	112.42	120.31
1	E	292	GLN	C-N-CA	-5.19	112.42	120.31
1	E	404	ASP	CB-CA-C	5.19	118.30	109.53
2	F	98	ASP	CB-CA-C	5.19	118.91	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	438	ASP	CA-C-N	5.19	131.45	121.54
2	B	438	ASP	C-N-CA	5.19	131.45	121.54
1	C	99	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	C	159	TYR	CA-C-N	5.19	125.88	120.12
1	C	159	TYR	C-N-CA	5.19	125.88	120.12
2	D	270	ALA	CA-C-N	5.19	130.72	121.75
2	D	270	ALA	C-N-CA	5.19	130.72	121.75
1	E	119	VAL	CA-CB-CG1	5.19	119.22	110.40
2	F	245	ASP	N-CA-C	5.19	117.38	110.53
2	F	337	THR	N-CA-C	-5.19	105.69	112.23
1	I	203	ASP	CA-C-O	5.19	125.85	120.30
1	I	264	HIS	CB-CG-CD2	-5.19	124.46	131.20
2	N	96	LYS	CB-CA-C	5.19	120.10	109.67
1	A	67	ASP	CA-CB-CG	-5.19	107.41	112.60
1	A	234	SER	O-C-N	-5.19	115.49	122.23
2	D	15	GLN	O-C-N	-5.19	116.24	122.15
2	H	370	LYS	CB-CA-C	5.19	118.29	109.84
1	I	329	GLN	N-CA-CB	5.19	117.74	110.12
2	D	301	GLN	OE1-CD-NE2	-5.18	117.42	122.60
2	F	218	ASP	N-CA-CB	-5.18	102.33	111.40
2	N	194	THR	CA-C-O	-5.18	113.20	119.27
1	A	33	THR	N-CA-C	5.18	118.38	111.75
1	K	357	PRO	CA-C-N	5.18	125.47	119.92
1	K	357	PRO	C-N-CA	5.18	125.47	119.92
1	A	323	MET	N-CA-C	5.18	116.93	111.28
2	L	273	ALA	O-C-N	-5.18	116.78	122.06
1	A	341	PHE	O-C-N	-5.18	117.04	123.36
2	L	441	GLU	O-C-N	-5.18	115.57	122.20
1	A	101	TRP	CD2-CE2-CZ2	5.18	127.58	122.40
2	F	234	ILE	O-C-N	-5.18	116.52	121.90
2	F	309	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	K	252	LYS	N-CA-C	5.18	116.92	111.28
1	M	370	ASN	CA-CB-CG	5.18	117.78	112.60
1	C	359	ARG	CA-C-O	-5.18	114.75	120.70
1	M	28	HIS	ND1-CE1-NE2	5.18	113.58	108.40
2	N	120	ASP	CA-C-N	5.18	127.22	120.28
2	N	120	ASP	C-N-CA	5.18	127.22	120.28
2	J	382	THR	N-CA-C	5.17	117.66	111.71
1	K	227	HIS	CA-C-N	5.17	129.43	120.58
1	K	227	HIS	C-N-CA	5.17	129.43	120.58
2	J	314	ALA	CB-CA-C	5.17	119.92	109.68
1	G	190	HIS	CB-CG-ND1	5.17	130.46	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	257	THR	CA-CB-CG2	5.17	119.29	110.50
1	C	329	GLN	N-CA-CB	5.17	118.20	110.19
2	J	274	PRO	N-CD-CG	5.17	110.00	103.80
2	D	251	ASP	O-C-N	-5.17	116.96	122.85
1	K	443	ASP	CB-CA-C	5.17	118.84	110.37
1	C	397	TRP	CE3-CZ3-CH2	-5.17	114.39	121.10
2	J	68	VAL	O-C-N	-5.17	117.71	123.03
1	K	195	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	M	191	GLN	CB-CA-C	-5.17	100.34	110.11
1	A	73	MET	CG-SD-CE	-5.17	89.54	100.90
2	J	187	SER	O-C-N	-5.17	116.65	122.12
1	M	388	MET	CA-C-O	-5.17	115.02	120.55
2	N	172	TYR	CA-C-O	-5.17	115.31	120.63
2	B	393	HIS	CB-CG-ND1	-5.16	114.95	122.70
1	C	245	GLN	CA-C-O	-5.16	115.38	120.70
2	F	347	CYS	CA-C-N	5.16	126.29	119.84
2	F	347	CYS	C-N-CA	5.16	126.29	119.84
1	G	264	HIS	CA-C-N	5.16	130.27	122.99
1	G	264	HIS	C-N-CA	5.16	130.27	122.99
1	I	393	ALA	N-CA-C	5.16	117.52	110.24
1	K	103	LYS	CA-CB-CG	-5.16	103.77	114.10
1	K	248	ALA	N-CA-C	5.16	116.37	108.52
2	D	189	LEU	N-CA-CB	-5.16	102.27	110.22
1	E	5	VAL	N-CA-CB	-5.16	99.63	111.81
2	J	153	LEU	N-CA-CB	-5.16	102.52	110.16
1	E	384	GLN	CA-C-N	5.16	127.96	120.79
1	E	384	GLN	C-N-CA	5.16	127.96	120.79
2	F	126	ALA	O-C-N	-5.16	116.72	122.09
1	G	88	ASP	N-CA-C	5.16	119.29	112.89
2	H	39	ASP	CA-C-O	-5.16	115.76	121.28
1	K	433	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	C	41	ASP	CA-C-O	5.16	125.70	119.31
1	A	156	ARG	N-CA-C	5.16	117.57	111.33
2	J	256	GLN	CA-C-N	5.16	128.15	120.31
2	J	256	GLN	C-N-CA	5.16	128.15	120.31
2	L	271	THR	N-CA-CB	-5.16	101.94	111.53
2	B	407	TRP	O-C-N	-5.15	115.93	122.27
1	C	256	ASN	CA-C-O	5.15	125.23	119.41
2	F	309	HIS	CA-CB-CG	5.15	118.95	113.80
2	J	71	GLU	CA-C-O	-5.15	115.43	119.66
2	H	18	ASN	N-CA-C	5.15	117.80	111.82
2	H	143	GLY	CA-C-O	-5.15	116.94	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	CYS	CA-CB-SG	-5.15	102.56	114.40
1	I	18	ALA	O-C-N	-5.15	116.73	122.09
2	L	283	HIS	CA-CB-CG	5.15	118.95	113.80
1	M	59	TYR	CA-C-O	5.15	125.70	120.24
1	M	387	ALA	N-CA-C	5.15	117.56	111.33
2	N	380	ASN	O-C-N	-5.15	117.21	123.13
2	F	338	LYS	CB-CA-C	5.14	120.28	112.00
1	E	439	GLU	CA-C-N	5.14	125.22	120.34
1	E	439	GLU	C-N-CA	5.14	125.22	120.34
2	J	218	ASP	N-CA-C	5.14	119.13	112.86
2	N	234	ILE	CB-CA-C	5.14	119.72	111.29
1	C	397	TRP	NE1-CE2-CZ2	5.14	137.81	130.10
2	J	414	GLU	N-CA-C	5.14	118.44	110.17
2	L	331	ALA	O-C-N	5.14	128.01	122.15
2	N	28	HIS	N-CA-CB	-5.14	103.15	110.80
2	N	285	GLN	CA-C-O	5.14	126.50	120.80
2	F	121	ARG	N-CA-CB	5.13	117.73	110.13
1	M	434	GLY	O-C-N	-5.13	118.39	122.81
2	N	293	ASN	CA-C-N	5.13	127.67	120.28
2	N	293	ASN	C-N-CA	5.13	127.67	120.28
2	D	173	PRO	CA-N-CD	-5.13	104.81	112.00
2	L	38	SER	O-C-N	-5.13	117.53	123.33
1	E	283	ALA	CA-C-O	-5.13	116.14	121.99
1	I	411	ALA	CA-C-O	-5.13	114.98	120.42
1	K	344	TRP	NE1-CE2-CD2	-5.13	100.73	107.40
1	E	184	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	G	20	PHE	CA-CB-CG	-5.13	108.67	113.80
1	G	414	ASN	CA-CB-CG	5.13	117.73	112.60
2	F	257	THR	N-CA-C	5.13	118.64	112.38
1	G	276	ARG	CA-C-N	5.13	125.63	119.94
1	G	276	ARG	C-N-CA	5.13	125.63	119.94
2	H	249	ASN	CA-C-O	-5.13	114.75	120.54
1	I	405	GLU	CA-C-O	5.13	125.89	120.10
2	J	198	SER	CA-CB-OG	5.13	121.36	111.10
2	L	283	HIS	CB-CG-CD2	-5.13	124.53	131.20
2	N	305	CYS	CB-CA-C	5.13	118.20	109.53
1	C	437	GLU	CA-C-N	5.13	128.83	121.50
1	C	437	GLU	C-N-CA	5.13	128.83	121.50
2	D	81	GLY	CA-C-N	5.13	127.87	120.38
2	D	81	GLY	C-N-CA	5.13	127.87	120.38
2	D	278	ALA	CA-C-N	5.13	127.42	120.65
2	D	278	ALA	C-N-CA	5.13	127.42	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	237	THR	CA-C-N	5.13	127.42	120.65
1	I	237	THR	C-N-CA	5.13	127.42	120.65
1	E	28	HIS	CB-CG-ND1	5.12	130.39	122.70
2	H	323	VAL	N-CA-CB	-5.12	104.34	111.41
1	I	383	GLU	CA-C-N	5.12	127.66	120.28
1	I	383	GLU	C-N-CA	5.12	127.66	120.28
1	C	184	ASN	N-CA-C	5.12	116.56	110.97
1	G	407	GLU	CB-CA-C	5.12	120.51	110.67
1	K	411	ALA	N-CA-CB	-5.12	102.59	110.12
2	N	75	ILE	CA-C-O	-5.12	114.54	119.92
3	O	362	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	M	84	ILE	N-CA-C	5.12	117.45	111.05
2	N	266	HIS	ND1-CE1-NE2	5.12	113.52	108.40
1	A	173	PRO	N-CA-CB	5.12	108.06	103.20
1	K	160	PRO	CB-CA-C	5.12	120.01	111.56
2	N	200	CYS	O-C-N	5.12	128.90	123.42
2	N	322	ASP	CA-C-N	5.12	129.60	122.23
2	N	322	ASP	C-N-CA	5.12	129.60	122.23
1	E	394	PHE	CA-CB-CG	-5.12	108.68	113.80
1	G	125	GLU	N-CA-C	-5.12	106.62	112.92
1	G	220	PRO	CB-CA-C	-5.12	104.40	111.21
2	H	289	ALA	CA-C-N	5.12	127.59	120.63
2	H	289	ALA	C-N-CA	5.12	127.59	120.63
1	C	401	GLU	O-C-N	-5.12	116.16	122.25
1	M	329	GLN	N-CA-CB	5.12	117.73	110.16
2	N	202	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	98	GLY	CA-C-N	5.12	134.02	125.02
1	A	98	GLY	C-N-CA	5.12	134.02	125.02
1	I	380	ARG	N-CA-C	5.12	116.94	111.36
2	L	367	ASP	O-C-N	-5.12	117.25	123.13
1	M	80	PRO	N-CA-C	-5.12	103.16	111.19
2	F	77	GLU	O-C-N	-5.11	115.98	122.27
2	H	344	VAL	CA-C-O	5.11	126.69	121.58
2	L	159	VAL	CA-C-O	5.11	124.97	119.35
2	H	412	GLY	N-CA-C	5.11	122.17	115.47
2	L	346	TRP	NE1-CE2-CZ2	5.11	137.77	130.10
1	M	71	GLY	CA-C-N	5.11	127.13	120.28
1	M	71	GLY	C-N-CA	5.11	127.13	120.28
2	N	326	LYS	N-CA-C	5.11	116.85	111.28
2	L	350	GLY	CA-C-O	-5.11	111.68	120.57
2	H	21	TRP	O-C-N	-5.11	115.99	122.27
2	H	137	VAL	N-CA-C	5.11	115.40	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	45	GLU	CA-C-O	-5.11	115.12	120.63
1	G	128	ASP	O-C-N	5.11	127.54	122.03
1	G	330	MET	CA-C-N	5.11	127.54	120.29
1	G	330	MET	C-N-CA	5.11	127.54	120.29
2	J	315	CYS	CA-C-N	5.10	129.97	122.77
2	J	315	CYS	C-N-CA	5.10	129.97	122.77
2	L	223	THR	N-CA-C	5.10	118.07	110.52
2	J	40	LYS	CA-C-N	5.10	128.01	120.82
2	J	40	LYS	C-N-CA	5.10	128.01	120.82
1	K	328	GLU	N-CA-C	5.10	118.61	112.38
2	L	58	ALA	O-C-N	-5.10	115.81	122.59
2	L	236	SER	N-CA-C	5.10	116.84	111.28
2	N	69	ASP	OD1-CG-OD2	-5.10	110.66	122.90
1	A	212	PHE	N-CA-C	5.10	116.53	110.97
1	E	163	ILE	CA-CB-CG1	5.10	119.07	110.40
1	G	165	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	I	337	ASN	CA-CB-CG	-5.10	107.50	112.60
2	J	376	CYS	N-CA-CB	-5.10	102.30	110.46
2	N	382	THR	CA-C-N	5.10	129.23	120.72
2	N	382	THR	C-N-CA	5.10	129.23	120.72
2	D	61	HIS	CB-CG-CD2	-5.10	124.58	131.20
1	K	178	THR	O-C-N	-5.10	117.16	123.33
2	D	88	HIS	CB-CG-CD2	-5.09	124.58	131.20
2	L	432	TYR	CA-C-O	5.09	125.65	119.49
1	M	177	ASP	CA-CB-CG	-5.09	107.51	112.60
1	A	12	CYS	O-C-N	-5.09	116.73	122.12
2	B	408	TYR	CA-C-N	5.09	127.07	120.56
2	B	408	TYR	C-N-CA	5.09	127.07	120.56
1	C	313	VAL	O-C-N	-5.09	117.39	123.04
1	C	377	LEU	CB-CA-C	5.09	118.87	110.88
2	J	160	ASP	CA-CB-CG	5.08	117.69	112.60
1	K	13	GLY	CA-C-N	5.08	131.52	122.06
1	K	13	GLY	C-N-CA	5.08	131.52	122.06
1	K	419	VAL	N-CA-CB	5.08	118.21	110.58
2	N	258	ASN	CA-CB-CG	5.08	117.69	112.60
1	M	90	PHE	CA-CB-CG	5.08	118.88	113.80
1	C	28	HIS	N-CA-CB	-5.08	102.97	110.49
2	F	301	GLN	OE1-CD-NE2	-5.08	117.52	122.60
2	H	197	HIS	ND1-CG-CD2	5.08	111.18	106.10
2	J	24	TYR	CA-C-N	5.08	127.05	120.44
2	J	24	TYR	C-N-CA	5.08	127.05	120.44
2	L	220	GLU	CA-C-N	5.08	128.44	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	220	GLU	C-N-CA	5.08	128.44	122.85
1	C	207	LEU	CA-C-O	-5.08	115.14	120.63
2	H	344	VAL	CA-CB-CG1	5.08	119.04	110.40
1	K	236	VAL	CA-C-O	5.08	125.96	120.47
2	L	84	ARG	CA-C-O	-5.08	114.36	120.10
1	A	148	GLY	CA-C-O	-5.08	115.52	120.75
2	B	313	MET	CA-CB-CG	-5.08	103.94	114.10
2	D	36	MET	O-C-N	5.08	125.63	121.31
2	H	129	CYS	CA-C-O	-5.08	115.47	121.16
2	J	197	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	M	21	TRP	N-CA-C	5.08	119.47	113.28
1	E	58	LYS	N-CA-C	5.08	117.00	108.73
2	N	224	TYR	O-C-N	-5.08	115.79	122.39
2	D	227	LEU	N-CA-C	-5.07	105.64	111.07
2	F	88	HIS	O-C-N	-5.07	116.89	121.31
1	G	207	LEU	CA-C-N	5.07	127.33	120.38
1	G	207	LEU	C-N-CA	5.07	127.33	120.38
1	K	291	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	C	55	ALA	CA-C-O	5.07	127.76	120.51
2	H	28	HIS	ND1-CE1-NE2	5.07	113.47	108.40
2	N	200	CYS	N-CA-CB	-5.07	103.70	111.56
1	A	42	LEU	N-CA-CB	-5.07	101.52	110.39
2	B	364	PRO	N-CA-CB	5.07	108.06	103.34
2	F	120	ASP	CA-CB-CG	5.07	117.67	112.60
2	F	139	HIS	CA-C-O	5.07	126.73	121.36
1	I	159	TYR	N-CA-CB	-5.07	104.20	110.79
2	J	269	LEU	CA-C-O	-5.07	115.33	120.71
2	J	276	ILE	CA-C-O	-5.07	116.61	121.63
1	M	62	ARG	CD-NE-CZ	5.07	131.50	124.40
2	N	285	GLN	O-C-N	-5.07	117.26	123.19
1	E	99	ASN	N-CA-CB	5.07	119.06	110.49
2	F	273	ALA	N-CA-CB	-5.07	103.73	110.77
1	I	91	VAL	CB-CA-C	5.07	116.35	111.23
2	N	350	GLY	CA-C-N	5.07	129.14	122.30
2	N	350	GLY	C-N-CA	5.07	129.14	122.30
2	N	406	HIS	CB-CG-CD2	-5.07	124.61	131.20
2	N	273	ALA	N-CA-C	5.06	116.43	108.23
1	E	62	ARG	CB-CA-C	5.06	120.49	110.42
1	K	151	LEU	N-CA-C	5.06	117.19	111.11
2	L	333	ALA	CA-C-O	-5.06	114.38	120.10
2	J	18	ASN	CB-CA-C	5.06	119.72	110.36
2	L	241	SER	CA-C-N	5.06	127.06	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	241	SER	C-N-CA	5.06	127.06	120.28
2	J	390	ARG	O-C-N	5.06	127.91	122.15
2	N	353	VAL	O-C-N	-5.06	117.74	123.20
2	B	373	ARG	CB-CA-C	5.05	120.70	109.94
2	D	123	ARG	O-C-N	5.05	127.48	122.12
1	E	301	ALA	N-CA-C	5.05	116.87	109.24
1	E	370	ASN	CB-CA-C	5.05	119.70	112.12
1	G	108	GLU	N-CA-CB	5.05	117.55	110.12
1	G	163	ILE	CA-C-O	-5.05	116.38	121.59
1	M	59	TYR	N-CA-C	5.05	116.63	108.34
2	N	124	LYS	CA-C-N	5.05	129.27	120.68
2	N	124	LYS	C-N-CA	5.05	129.27	120.68
2	D	72	PRO	N-CA-CB	5.05	108.16	103.41
2	F	251	ASP	CA-CB-CG	5.05	117.65	112.60
2	F	388	TRP	N-CA-C	-5.05	105.66	111.07
2	L	392	ASP	CA-C-O	-5.05	113.05	119.31
2	B	350	GLY	N-CA-C	5.05	120.23	114.67
2	N	332	ILE	CB-CG1-CD1	5.05	124.41	113.80
3	O	243	LEU	CB-CG-CD1	5.05	125.85	110.70
2	B	84	ARG	CD-NE-CZ	5.05	131.47	124.40
2	F	307	PRO	N-CA-C	5.05	122.87	112.47
1	K	118	ASP	CA-C-O	-5.05	115.50	120.90
1	M	90	PHE	CA-C-O	-5.05	115.75	121.66
1	E	249	ASP	N-CA-CB	-5.05	101.96	110.49
1	G	331	LEU	CA-C-O	-5.05	115.07	120.42
2	F	292	THR	CA-C-N	5.05	127.29	120.38
2	F	292	THR	C-N-CA	5.05	127.29	120.38
2	J	27	GLU	N-CA-C	-5.05	105.97	111.82
2	N	405	VAL	N-CA-C	5.04	117.36	111.05
1	C	173	PRO	N-CA-C	5.04	121.27	113.75
1	K	427	ASP	CA-CB-CG	5.04	117.64	112.60
2	N	149	PHE	CA-C-O	-5.04	113.84	119.79
1	C	53	GLU	O-C-N	-5.04	117.26	122.96
2	F	102	ASN	OD1-CG-ND2	-5.04	117.56	122.60
2	J	185	TYR	CA-CB-CG	5.04	122.97	113.90
2	N	233	GLN	N-CA-C	5.04	119.28	113.18
1	E	203	ASP	CA-C-N	5.04	127.74	120.38
1	E	203	ASP	C-N-CA	5.04	127.74	120.38
1	M	262	ARG	CB-CA-C	5.04	118.76	109.99
1	C	71	GLY	CA-C-N	5.04	126.99	120.44
1	C	71	GLY	C-N-CA	5.04	126.99	120.44
1	C	245	GLN	CB-CA-C	5.04	118.86	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	340	TYR	N-CA-CB	-5.04	102.91	111.27
1	M	42	LEU	N-CA-C	5.04	117.42	111.33
2	L	38	SER	N-CA-C	5.04	116.90	108.99
2	F	47	ASP	CA-CB-CG	5.04	117.64	112.60
2	B	377	MET	O-C-N	-5.03	117.38	123.27
2	J	122	ILE	CA-C-N	5.03	128.37	120.82
2	J	122	ILE	C-N-CA	5.03	128.37	120.82
2	L	306	ASP	N-CA-C	-5.03	101.97	109.42
2	N	98	ASP	CA-C-O	5.03	127.71	120.51
1	A	284	LEU	CA-C-N	5.03	130.12	121.87
1	A	284	LEU	C-N-CA	5.03	130.12	121.87
1	A	333	VAL	CA-C-O	-5.03	115.72	120.95
1	K	92	PHE	CA-C-N	5.03	127.77	121.83
1	K	92	PHE	C-N-CA	5.03	127.77	121.83
2	N	8	HIS	CB-CG-CD2	-5.03	124.66	131.20
2	N	188	ILE	CB-CA-C	5.03	118.63	112.04
2	J	175	PRO	N-CD-CG	5.03	110.74	103.20
2	B	302	MET	N-CA-C	5.03	119.14	112.30
1	E	160	PRO	O-C-N	-5.03	116.20	122.23
2	F	88	HIS	CB-CG-CD2	-5.03	124.67	131.20
2	L	87	PHE	CA-CB-CG	5.03	118.83	113.80
1	M	378	PHE	CA-C-N	5.03	126.97	120.44
1	M	378	PHE	C-N-CA	5.03	126.97	120.44
1	A	220	PRO	N-CA-CB	5.02	108.02	103.15
1	C	204	ASN	OD1-CG-ND2	-5.02	117.58	122.60
2	H	250	VAL	N-CA-CB	-5.02	104.48	111.41
2	L	441	GLU	CB-CA-C	5.02	119.22	111.13
2	B	133	GLN	CA-C-O	5.02	126.13	120.00
2	D	109	THR	N-CA-CB	-5.02	102.22	110.40
2	L	48	SER	N-CA-C	5.02	118.90	112.87
2	N	16	ILE	CA-C-O	5.02	125.94	120.57
2	N	221	ARG	O-C-N	-5.02	116.90	121.17
2	F	171	ILE	N-CA-CB	-5.02	105.25	110.82
2	J	9	VAL	N-CA-C	5.02	115.08	107.75
1	K	227	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	A	396	HIS	ND1-CG-CD2	5.02	111.12	106.10
2	F	165	SER	N-CA-CB	5.02	117.33	109.85
2	L	295	CYS	CA-CB-SG	-5.02	102.86	114.40
2	N	88	HIS	CB-CA-C	5.02	117.54	109.51
2	N	160	ASP	CA-C-N	5.02	130.54	122.86
2	N	160	ASP	C-N-CA	5.02	130.54	122.86
2	N	258	ASN	CB-CG-ND2	5.02	123.93	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	52	ASN	CA-CB-CG	5.02	117.62	112.60
1	M	216	LYS	CA-C-N	5.02	128.67	121.50
1	M	216	LYS	C-N-CA	5.02	128.67	121.50
1	C	57	ASN	CB-CA-C	5.01	120.40	110.42
1	C	107	THR	CA-CB-CG2	5.01	119.02	110.50
1	E	154	LYS	CA-C-O	-5.01	113.21	119.38
2	F	36	MET	CB-CA-C	5.01	116.64	108.87
1	M	149	THR	CA-CB-OG1	5.01	117.12	109.60
2	N	384	ILE	CB-CA-C	5.01	121.37	111.79
1	K	279	GLN	CA-C-O	5.01	126.04	120.63
2	D	153	LEU	CA-C-O	-5.01	115.24	120.55
1	G	396	HIS	N-CA-C	5.01	117.47	111.71
1	G	406	MET	CA-C-N	5.01	127.92	120.31
1	G	406	MET	C-N-CA	5.01	127.92	120.31
1	I	305	PRO	CA-C-N	5.01	129.09	120.72
1	I	305	PRO	C-N-CA	5.01	129.09	120.72
1	M	217	LEU	N-CA-CB	-5.01	102.19	109.95
2	B	91	GLN	CB-CA-C	5.01	119.25	110.64
2	D	87	PHE	CA-C-N	5.01	127.35	120.39
2	D	87	PHE	C-N-CA	5.01	127.35	120.39
2	D	254	GLU	N-CA-C	5.01	117.63	111.82
1	E	380	ARG	O-C-N	5.01	127.50	122.09
2	F	26	LEU	CA-C-N	5.01	128.99	120.88
2	F	26	LEU	C-N-CA	5.01	128.99	120.88
2	F	168	GLU	CA-C-N	5.01	130.06	123.05
2	F	168	GLU	C-N-CA	5.01	130.06	123.05
1	G	224	ASP	CA-C-O	-5.01	113.41	119.27
1	K	137	HIS	ND1-CG-CD2	5.01	111.11	106.10
1	K	355	ASP	CA-CB-CG	-5.01	107.59	112.60
2	N	331	ALA	CA-C-O	-5.00	114.22	119.97
1	A	165	ASN	OD1-CG-ND2	-5.00	117.60	122.60
2	B	36	MET	O-C-N	-5.00	116.28	121.28
2	B	233	GLN	OE1-CD-NE2	-5.00	117.60	122.60
1	C	305	PRO	CA-N-CD	-5.00	105.00	112.00
1	E	170	VAL	CA-C-N	5.00	124.91	119.76
1	E	170	VAL	C-N-CA	5.00	124.91	119.76
1	M	241	ARG	N-CA-C	5.00	116.73	111.28
1	A	47	ILE	O-C-N	-5.00	116.99	121.89

There are no chirality outliers.

All (122) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	TYR	Sidechain
1	A	131	GLN	Peptide
1	A	175	VAL	Peptide
1	A	183	TYR	Sidechain
1	A	200	TYR	Sidechain
1	A	208	TYR	Sidechain
1	A	212	PHE	Sidechain
1	A	32	PRO	Peptide
1	A	344	TRP	Peptide
1	A	371	SER	Mainchain
1	A	425	TYR	Sidechain
1	A	50	TYR	Sidechain
2	B	161	TYR	Sidechain
2	B	302	MET	Peptide
2	B	347	CYS	Peptide
2	B	393	HIS	Sidechain
2	B	411	GLU	Peptide
2	B	61	HIS	Sidechain
2	B	88	HIS	Sidechain
1	C	106	TYR	Sidechain
1	C	222	TYR	Sidechain
1	C	227	HIS	Sidechain
1	C	264	HIS	Sidechain
1	C	281	TYR	Sidechain
1	C	36	TYR	Sidechain
1	C	375	GLN	Mainchain
1	C	422	TYR	Sidechain
1	C	59	TYR	Sidechain
1	C	85	PHE	Sidechain
2	D	202	PHE	Sidechain
2	D	215	ARG	Peptide
2	D	28	HIS	Sidechain
2	D	312	TYR	Sidechain
2	D	370	LYS	Mainchain
2	D	404	PHE	Sidechain
2	D	432	TYR	Sidechain
2	D	449	GLU	Mainchain
1	E	111	GLU	Mainchain
1	E	165	ASN	Sidechain
1	E	183	TYR	Sidechain
1	E	281	TYR	Sidechain
1	E	422	TYR	Sidechain
1	E	50	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	E	51	TYR	Sidechain
2	F	11	GLN	Mainchain
2	F	161	TYR	Sidechain
2	F	185	TYR	Sidechain
2	F	192	HIS	Sidechain
2	F	210	TYR	Sidechain
2	F	227	LEU	Mainchain
2	F	233	GLN	Mainchain
2	F	302	MET	Peptide
2	F	316	CYS	Mainchain
2	F	74	VAL	Mainchain
2	F	97	GLU	Mainchain
1	G	106	TYR	Sidechain
1	G	159	TYR	Sidechain
1	G	36	TYR	Sidechain
1	G	50	TYR	Sidechain
1	G	51	TYR	Sidechain
2	H	161	TYR	Sidechain
2	H	244	PHE	Sidechain
2	H	28	HIS	Sidechain
2	H	319	TYR	Sidechain
2	H	353	VAL	Peptide
2	H	429	GLU	Sidechain
2	H	67	PHE	Sidechain
2	H	68	VAL	Peptide
1	I	183	TYR	Sidechain
1	I	200	TYR	Sidechain
1	I	218	THR	Mainchain
1	I	270	PHE	Sidechain
1	I	422	TYR	Sidechain
1	I	90	PHE	Sidechain
2	J	169	PHE	Peptide
2	J	177	VAL	Peptide
2	J	183	GLU	Sidechain
2	J	244	PHE	Mainchain
2	J	262	TYR	Sidechain
2	J	266	HIS	Sidechain
2	J	272	TYR	Sidechain
2	J	302	MET	Peptide
2	J	341	ILE	Peptide
2	J	68	VAL	Peptide
2	J	98	ASP	Sidechain

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Mol	Chain	Res	Type	Group
1	K	106	TYR	Sidechain
1	K	222	TYR	Sidechain
1	K	385	PHE	Sidechain
1	K	391	ARG	Sidechain
2	L	139	HIS	Sidechain,Peptide
2	L	140	SER	Peptide
2	L	161	TYR	Sidechain
2	L	172	TYR	Sidechain
2	L	21	TRP	Mainchain
2	L	255	PHE	Sidechain
2	L	351	PHE	Sidechain
2	L	357	TYR	Sidechain
2	L	389	ALA	Mainchain
2	L	417	GLU	Peptide
2	L	99	ALA	Peptide
1	M	106	TYR	Sidechain
1	M	21	TRP	Peptide
1	M	222	TYR	Sidechain
1	M	227	HIS	Sidechain
1	M	260	PHE	Peptide
1	M	307	HIS	Sidechain
1	M	367	PHE	Sidechain
1	M	51	TYR	Sidechain
1	M	59	TYR	Sidechain
2	N	108	TYR	Sidechain
2	N	116	ASP	Peptide
2	N	149	PHE	Sidechain
2	N	161	TYR	Sidechain
2	N	170	SER	Peptide
2	N	185	TYR	Sidechain
2	N	194	THR	Mainchain
2	N	243	ARG	Mainchain
2	N	255	PHE	Sidechain
2	N	3	GLU	Peptide
2	N	451	TYR	Sidechain
2	N	68	VAL	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3498	0	3342	10	0
1	C	3498	0	3342	12	0
1	E	3498	0	3342	6	0
1	G	3498	0	3342	6	0
1	I	3498	0	3342	7	0
1	K	3498	0	3342	14	0
1	M	3498	0	3342	13	0
2	B	3524	0	3409	12	0
2	D	3524	0	3409	6	0
2	F	3524	0	3409	9	0
2	H	3524	0	3409	13	0
2	J	3524	0	3409	14	0
2	L	3524	0	3409	8	0
2	N	3524	0	3409	16	0
3	O	1455	0	1526	3	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	0	0
5	D	32	0	12	0	0
5	F	32	0	12	0	0
5	H	32	0	12	0	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	137	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 1.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2:ARG:NH2	1:M:249:ASP:HB3	2.03	0.74
1:A:155:ILE:HG22	1:A:164:MET:HE1	1.70	0.72
2:H:382:THR:HG21	2:H:436:GLY:HA3	1.77	0.67
2:B:269:LEU:HD23	2:B:269:LEU:H	1.62	0.65
1:G:101:TRP:CH2	1:G:105:HIS:CG	2.86	0.64
2:B:123:ARG:HH11	2:B:123:ARG:HG3	1.61	0.64
2:H:202:PHE:CE1	2:H:378:LEU:HD13	2.38	0.59
2:F:256:GLN:HB3	1:G:397:TRP:CZ2	2.38	0.59
1:A:105:HIS:CE1	1:A:150:LEU:HD13	2.38	0.58
2:N:150:THR:HG22	2:N:154:MET:HE2	1.86	0.58
1:K:189:VAL:O	1:K:193:VAL:HG12	2.05	0.57
1:M:238:THR:HG22	1:M:354:CYS:SG	2.46	0.56
2:H:319:TYR:CD2	2:H:375:VAL:HG22	2.41	0.56
1:A:155:ILE:CG2	1:A:164:MET:HE1	2.36	0.56
2:J:326:LYS:HD3	1:K:220:PRO:HG3	1.88	0.55
2:D:147:SER:HB2	2:D:190:THR:HG21	1.88	0.55
2:J:211:ASP:CG	2:J:215:ARG:HH22	2.15	0.55
1:I:257:MET:HE2	1:I:368:ILE:HG22	1.88	0.55
3:O:388:HIS:CG	3:O:389:GLY:HA2	2.42	0.54
1:K:324:LYS:HE2	2:L:210:TYR:HB3	1.89	0.53
1:M:2:ARG:HH11	2:N:97:GLU:HA	1.75	0.52
1:K:167:PHE:CE2	1:K:200:TYR:CE1	2.98	0.52
1:M:16:ILE:HG22	1:M:136:THR:HG21	1.91	0.52
2:J:105:ARG:NH2	2:J:110:ILE:HD11	2.25	0.51
1:A:170:VAL:HB	1:A:171:PRO:HD2	1.92	0.51
1:K:187:LEU:HD22	1:K:403:MET:HE1	1.92	0.51
1:M:28:HIS:CE1	1:M:242:PHE:CZ	2.98	0.51
1:K:252:LYS:HE2	5:L:501:GTP:O1G	2.10	0.51
1:M:2:ARG:NH1	2:N:98:ASP:H	2.08	0.50
2:H:164:LYS:HE2	2:H:164:LYS:HA	1.94	0.50
1:K:213:ARG:O	1:K:216:LYS:HE2	2.12	0.49
2:N:7:ILE:HG23	2:N:66:VAL:HG23	1.94	0.49
2:L:297:GLU:HB3	2:L:300:ASN:HD22	1.78	0.49
2:B:438:ASP:CG	2:B:439:SER:H	2.21	0.49
2:N:133:GLN:HE22	2:N:242:LEU:HD22	1.77	0.48
2:F:252:LEU:HD12	2:F:252:LEU:N	2.28	0.48
3:O:393:VAL:HB	3:O:394:TYR:HA	1.93	0.48
1:E:235:GLY:HA3	1:E:366:THR:HG21	1.96	0.48
2:J:52:PHE:CZ	2:J:243:ARG:HD3	2.49	0.48
1:C:212:PHE:CD1	1:C:218:THR:HA	2.48	0.48
1:G:101:TRP:CH2	1:G:105:HIS:CD2	3.02	0.48
1:M:156:ARG:HH11	1:M:164:MET:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:104:ALA:HB1	2:L:411:GLU:HB2	1.95	0.47
2:L:121:ARG:NH2	2:L:124:LYS:CB	2.78	0.47
2:N:269:LEU:C	2:N:269:LEU:HD12	2.38	0.47
1:I:396:HIS:CE1	1:I:397:TRP:CE2	3.03	0.47
2:J:17:GLY:HA2	2:J:20:CYS:SG	2.55	0.46
1:M:101:TRP:CD1	1:M:146:GLY:HA2	2.51	0.46
2:B:195:LEU:HD13	2:B:266:HIS:CE1	2.50	0.46
2:L:344:VAL:HG21	2:L:346:TRP:CZ2	2.51	0.46
1:E:210:ILE:CD1	1:E:300:MET:HG2	2.45	0.46
2:L:121:ARG:NH2	2:L:124:LYS:HB2	2.30	0.46
2:J:182:VAL:C	2:J:184:PRO:HD2	2.41	0.46
1:A:368:ILE:HD12	1:A:368:ILE:N	2.31	0.45
2:B:71:GLU:HG3	2:B:73:THR:H	1.81	0.45
2:J:1:MET:HA	2:J:130:THR:OG1	2.17	0.45
1:K:342:VAL:HG22	1:K:343:GLU:N	2.31	0.45
1:G:32:PRO:HB3	1:G:81:PHE:H	1.81	0.45
2:H:241:SER:CB	2:H:250:VAL:H	2.30	0.45
2:J:46:ASP:HA	2:J:47:ASP:HB2	1.97	0.45
1:M:2:ARG:NH2	1:M:249:ASP:CB	2.78	0.45
2:N:133:GLN:HE22	2:N:242:LEU:CD2	2.29	0.45
1:C:282:ARG:NH2	1:C:284:LEU:HD12	2.32	0.45
2:F:250:VAL:HG22	2:F:352:LYS:HE3	1.99	0.45
2:F:227:LEU:HD23	2:F:227:LEU:C	2.42	0.44
1:C:406:MET:HE3	1:C:407:GLU:OE2	2.17	0.44
2:H:26:LEU:HD13	2:H:363:VAL:HG22	1.97	0.44
1:M:322:SER:CB	2:N:221:ARG:HB2	2.47	0.44
2:N:317:LEU:C	2:N:318:LEU:HD22	2.43	0.44
2:B:263:PRO:HD3	1:C:396:HIS:CG	2.52	0.44
2:F:20:CYS:SG	2:F:235:VAL:HG21	2.58	0.44
2:D:286:LEU:HD13	2:D:371:VAL:HG12	2.00	0.44
1:G:21:TRP:CZ2	1:G:63:ALA:HB2	2.53	0.44
2:J:107:HIS:HD2	2:J:108:TYR:CE2	2.35	0.44
2:B:319:TYR:CD2	2:B:375:VAL:HG22	2.53	0.43
2:F:332:ILE:CG2	2:F:351:PHE:CE1	3.02	0.43
2:N:269:LEU:HD12	2:N:269:LEU:O	2.18	0.43
2:B:169:PHE:CE2	2:B:202:PHE:CD2	3.07	0.43
2:B:342:GLN:HG2	2:B:451:TYR:CE2	2.53	0.43
1:E:32:PRO:HA	1:E:81:PHE:CE1	2.53	0.43
2:J:188:ILE:HG22	2:J:421:ALA:HB1	1.99	0.43
1:M:2:ARG:HH22	1:M:249:ASP:CG	2.26	0.43
2:D:126:ALA:HA	2:D:129:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HB3	1:A:166:THR:HG23	2.01	0.43
1:M:380:ARG:NH1	1:M:381:ILE:HD11	2.34	0.43
1:C:21:TRP:CZ3	1:C:61:PRO:HB3	2.54	0.43
2:D:261:PRO:HA	1:E:394:PHE:CD1	2.54	0.42
2:H:215:ARG:NH2	2:H:299:ALA:HB1	2.34	0.42
2:H:344:VAL:HG21	2:H:346:TRP:CE2	2.54	0.42
1:I:290:THR:HA	1:I:293:MET:HG2	2.02	0.42
1:G:64:ILE:C	1:G:65:LEU:HD12	2.43	0.42
2:J:183:GLU:N	2:J:184:PRO:HD2	2.34	0.42
2:N:80:THR:HA	2:N:84:ARG:CZ	2.49	0.42
3:O:393:VAL:HB	3:O:394:TYR:CA	2.49	0.42
1:A:46:ARG:O	1:A:49:VAL:HG23	2.19	0.42
2:F:105:ARG:NH2	2:F:110:ILE:HG13	2.34	0.42
2:F:157:LEU:HD23	2:F:157:LEU:HA	1.93	0.42
1:K:167:PHE:CD2	1:K:200:TYR:CD1	3.08	0.42
1:A:344:TRP:CE3	2:B:401:LYS:HG3	2.55	0.42
2:H:265:ILE:HG23	2:H:432:TYR:CZ	2.55	0.42
1:I:316:VAL:HG22	1:I:352:ALA:HB3	2.01	0.42
2:D:216:ASN:HB3	2:D:275:VAL:O	2.20	0.42
1:C:318:ARG:NH2	1:C:357:PRO:O	2.53	0.42
1:K:167:PHE:CE2	1:K:200:TYR:CD1	3.08	0.42
2:N:192:HIS:CD2	2:N:421:ALA:HA	2.54	0.42
2:H:18:ASN:HD21	2:H:78:VAL:HG22	1.86	0.41
2:H:319:TYR:CD2	2:H:375:VAL:CG2	3.03	0.41
2:N:172:TYR:CD1	2:N:203:MET:HE3	2.56	0.41
2:H:316:CYS:HA	2:H:352:LYS:O	2.21	0.41
2:L:163:LYS:HZ1	1:M:401:GLU:CD	2.28	0.41
2:N:332:ILE:HG22	2:N:336:LYS:HE3	2.02	0.41
1:K:130:LEU:HD21	1:K:133:PHE:CZ	2.55	0.41
1:K:150:LEU:O	1:K:153:SER:HB2	2.21	0.41
1:I:299:MET:C	1:I:301:ALA:H	2.28	0.41
2:N:42:ILE:HD12	2:N:43:GLY:N	2.36	0.41
2:B:449:GLU:HG2	2:B:451:TYR:O	2.21	0.41
1:C:19:LYS:HE3	1:C:227:HIS:CG	2.55	0.41
1:I:323:MET:HE2	2:J:224:TYR:CZ	2.55	0.41
2:L:313:MET:HA	2:L:344:VAL:HG22	2.03	0.41
1:C:80:PRO:C	1:C:82:GLY:H	2.29	0.41
2:H:395:PHE:CZ	2:H:399:TYR:CD2	3.08	0.41
1:I:262:ARG:HH22	1:I:417:ASP:CG	2.28	0.41
1:E:187:LEU:HD23	1:E:187:LEU:HA	1.87	0.41
1:C:192:LEU:C	1:C:192:LEU:HD23	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:378:LEU:HA	2:F:378:LEU:HD23	1.91	0.40
2:J:7:ILE:HD13	2:J:7:ILE:HG21	1.94	0.40
2:J:139:HIS:CE1	2:J:170:SER:HB3	2.56	0.40
1:K:99:ASN:HA	1:K:142:GLY:HA3	2.03	0.40
1:K:167:PHE:CZ	1:K:200:TYR:CE1	3.10	0.40
1:A:254:ALA:HB1	2:B:407:TRP:CH2	2.57	0.40
1:C:19:LYS:CE	1:C:227:HIS:CG	3.05	0.40
1:C:239:CYS:SG	1:C:354:CYS:HB2	2.61	0.40
1:C:344:TRP:CD1	1:C:344:TRP:H	2.37	0.40
2:N:332:ILE:CG2	2:N:336:LYS:HE3	2.51	0.40
1:E:374:ILE:HD12	1:E:374:ILE:HA	2.01	0.40
1:A:96:GLY:O	1:A:103:LYS:HE2	2.21	0.40
2:D:115:ILE:HG12	2:D:152:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/445 (100%)	407 (92%)	33 (7%)	3 (1%)	18	55
1	C	443/445 (100%)	415 (94%)	26 (6%)	2 (0%)	24	61
1	E	443/445 (100%)	409 (92%)	32 (7%)	2 (0%)	24	61
1	G	443/445 (100%)	413 (93%)	29 (6%)	1 (0%)	43	76
1	I	443/445 (100%)	413 (93%)	27 (6%)	3 (1%)	18	55
1	K	443/445 (100%)	409 (92%)	32 (7%)	2 (0%)	24	61
1	M	443/445 (100%)	413 (93%)	26 (6%)	4 (1%)	14	49
2	B	449/451 (100%)	417 (93%)	29 (6%)	3 (1%)	18	55
2	D	449/451 (100%)	415 (92%)	31 (7%)	3 (1%)	18	55
2	F	449/451 (100%)	414 (92%)	34 (8%)	1 (0%)	43	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	449/451 (100%)	415 (92%)	32 (7%)	2 (0%)	30	65
2	J	449/451 (100%)	416 (93%)	28 (6%)	5 (1%)	11	44
2	L	449/451 (100%)	419 (93%)	25 (6%)	5 (1%)	11	44
2	N	449/451 (100%)	412 (92%)	36 (8%)	1 (0%)	43	76
3	O	192/194 (99%)	162 (84%)	23 (12%)	7 (4%)	2	22
All	All	6436/6466 (100%)	5949 (92%)	443 (7%)	44 (1%)	20	55

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	404	PHE
3	O	390	ALA
2	B	322	ASP
1	C	81	PHE
1	C	394	PHE
2	H	29	GLY
2	J	348	PRO
1	K	394	PHE
2	L	132	LEU
2	L	350	GLY
2	L	404	PHE
3	O	350	VAL
3	O	388	HIS
2	B	281	ALA
1	E	394	PHE
2	H	57	GLY
1	I	394	PHE
1	M	48	ASN
3	O	278	ILE
3	O	393	VAL
1	A	348	ASN
2	D	416	GLY
1	G	296	ALA
2	J	338	LYS
2	L	186	ASN
1	M	296	ALA
1	A	268	PRO
1	E	216	LYS
2	L	112	LYS
1	M	128	ASP

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Mol	Chain	Res	Type
2	N	441	GLU
3	O	269	GLN
1	A	427	ASP
2	D	437	VAL
1	I	304	ASP
2	J	341	ILE
1	K	305	PRO
3	O	349	ARG
1	M	71	GLY
2	D	95	GLY
2	B	131	GLY
2	F	348	PRO
2	J	131	GLY
1	I	440	GLY

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%)	366 (96%)	15 (4%)	28	51
1	C	381/381 (100%)	371 (97%)	10 (3%)	40	61
1	E	381/381 (100%)	371 (97%)	10 (3%)	40	61
1	G	381/381 (100%)	366 (96%)	15 (4%)	28	51
1	I	381/381 (100%)	372 (98%)	9 (2%)	43	63
1	K	381/381 (100%)	373 (98%)	8 (2%)	47	65
1	M	381/381 (100%)	368 (97%)	13 (3%)	32	55
2	B	379/379 (100%)	371 (98%)	8 (2%)	47	65
2	D	379/379 (100%)	365 (96%)	14 (4%)	30	52
2	F	379/379 (100%)	369 (97%)	10 (3%)	40	61
2	H	379/379 (100%)	365 (96%)	14 (4%)	30	52
2	J	379/379 (100%)	364 (96%)	15 (4%)	28	50
2	L	379/379 (100%)	361 (95%)	18 (5%)	23	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	379/379 (100%)	358 (94%)	21 (6%)	19	44
3	O	168/168 (100%)	161 (96%)	7 (4%)	26	49
All	All	5488/5488 (100%)	5301 (97%)	187 (3%)	33	55

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	50	TYR
1	A	65	LEU
1	A	84	ILE
1	A	137	HIS
1	A	162	ARG
1	A	170	VAL
1	A	172	SER
1	A	188	SER
1	A	227	HIS
1	A	331	LEU
1	A	337	ASN
1	A	366	THR
1	A	407	GLU
1	A	427	ASP
2	B	9	VAL
2	B	16	ILE
2	B	25	CYS
2	B	266	HIS
2	B	346	TRP
2	B	372	GLN
2	B	384	ILE
2	B	450	GLU
1	C	46	ARG
1	C	65	LEU
1	C	117	LEU
1	C	161	ASP
1	C	225	LEU
1	C	266	PHE
1	C	274	THR
1	C	286	VAL
1	C	340	TYR
1	C	350	LYS
2	D	18	ASN

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Mol	Chain	Res	Type
2	D	68	VAL
2	D	115	ILE
2	D	140	SER
2	D	145	THR
2	D	169	PHE
2	D	194	THR
2	D	200	CYS
2	D	253	THR
2	D	269	LEU
2	D	271	THR
2	D	276	ILE
2	D	347	CYS
2	D	381	THR
1	E	3	GLU
1	E	91	VAL
1	E	113	VAL
1	E	143	THR
1	E	172	SER
1	E	178	THR
1	E	193	VAL
1	E	205	GLU
1	E	236	VAL
1	E	368	ILE
2	F	52	PHE
2	F	109	THR
2	F	124	LYS
2	F	207	GLU
2	F	214	ARG
2	F	230	LEU
2	F	266	HIS
2	F	269	LEU
2	F	388	TRP
2	F	392	ASP
1	G	1	MET
1	G	7	ILE
1	G	33	THR
1	G	53	GLU
1	G	66	VAL
1	G	72	THR
1	G	99	ASN
1	G	143	THR
1	G	219	THR

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Mol	Chain	Res	Type
1	G	228	LEU
1	G	250	LEU
1	G	386	THR
1	G	388	MET
1	G	409	THR
1	G	412	GLU
2	H	41	THR
2	H	51	THR
2	H	170	SER
2	H	196	GLU
2	H	200	CYS
2	H	204	VAL
2	H	224	TYR
2	H	226	ASN
2	H	245	ASP
2	H	269	LEU
2	H	301	GLN
2	H	384	ILE
2	H	437	VAL
2	H	449	GLU
1	I	1	MET
1	I	39	ASP
1	I	91	VAL
1	I	130	LEU
1	I	133	PHE
1	I	143	THR
1	I	161	ASP
1	I	238	THR
1	I	331	LEU
2	J	7	ILE
2	J	50	ASN
2	J	98	ASP
2	J	204	VAL
2	J	214	ARG
2	J	217	LEU
2	J	225	THR
2	J	227	LEU
2	J	266	HIS
2	J	324	VAL
2	J	329	ASN
2	J	375	VAL
2	J	379	SER

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Mol	Chain	Res	Type
2	J	386	GLU
2	J	418	PHE
1	K	136	THR
1	K	137	HIS
1	K	172	SER
1	K	327	ASP
1	K	347	ASN
1	K	350	LYS
1	K	351	THR
1	K	435	GLU
2	L	40	LYS
2	L	42	ILE
2	L	49	PHE
2	L	66	VAL
2	L	190	THR
2	L	194	THR
2	L	200	CYS
2	L	211	ASP
2	L	230	LEU
2	L	253	THR
2	L	256	GLN
2	L	257	THR
2	L	266	HIS
2	L	378	LEU
2	L	381	THR
2	L	425	MET
2	L	437	VAL
2	L	441	GLU
1	M	61	PRO
1	M	86	ARG
1	M	168	SER
1	M	169	VAL
1	M	178	THR
1	M	212	PHE
1	M	214	THR
1	M	228	LEU
1	M	331	LEU
1	M	366	THR
1	M	368	ILE
1	M	390	ARG
1	M	412	GLU
2	N	42	ILE

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Mol	Chain	Res	Type
2	N	94	THR
2	N	140	SER
2	N	179	THR
2	N	200	CYS
2	N	217	LEU
2	N	224	TYR
2	N	227	LEU
2	N	253	THR
2	N	263	PRO
2	N	269	LEU
2	N	275	VAL
2	N	279	GLU
2	N	334	THR
2	N	375	VAL
2	N	378	LEU
2	N	381	THR
2	N	391	LEU
2	N	418	PHE
2	N	441	GLU
2	N	450	GLU
3	O	243	LEU
3	O	296	ASN
3	O	348	ASP
3	O	373	THR
3	O	374	HIS
3	O	376	LEU
3	O	381	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	48	ASN
1	A	83	GLN
1	A	89	ASN
1	A	134	GLN
1	A	307	HIS
2	B	31	GLN
2	B	50	ASN
2	B	216	ASN
2	B	249	ASN
2	B	266	HIS

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Mol	Chain	Res	Type
1	C	43	GLN
1	C	48	ASN
1	C	134	GLN
1	C	247	ASN
1	C	292	GLN
1	C	335	ASN
1	C	348	ASN
1	C	370	ASN
2	D	91	GLN
2	D	139	HIS
2	D	216	ASN
2	D	249	ASN
2	D	329	ASN
2	D	393	HIS
1	E	11	GLN
1	E	43	GLN
1	E	137	HIS
1	E	247	ASN
1	E	291	GLN
1	E	329	GLN
1	E	332	ASN
1	E	334	GLN
1	E	416	ASN
2	F	18	ASN
2	F	233	GLN
2	F	372	GLN
1	G	89	ASN
1	G	100	ASN
1	G	105	HIS
1	G	279	GLN
1	G	298	ASN
1	G	329	GLN
1	G	334	GLN
1	G	347	ASN
1	G	384	GLN
2	H	18	ASN
2	H	28	HIS
2	H	85	GLN
2	H	197	HIS
2	H	226	ASN
2	H	283	HIS
1	I	14	ASN

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Mol	Chain	Res	Type
1	I	165	ASN
1	I	384	GLN
2	J	107	HIS
2	J	249	ASN
2	J	266	HIS
2	J	309	HIS
2	J	358	GLN
1	K	57	ASN
1	K	184	ASN
1	K	348	ASN
1	K	423	GLN
2	L	31	GLN
2	L	91	GLN
2	L	186	ASN
2	L	216	ASN
2	L	300	ASN
1	M	52	ASN
1	M	131	GLN
1	M	134	GLN
1	M	195	ASN
1	M	337	ASN
2	N	85	GLN
2	N	133	GLN
2	N	249	ASN
2	N	300	ASN
2	N	301	GLN
2	N	393	HIS
3	O	374	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

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	L	501	6	33,34,34	0.98	1 (3%)	50,54,54	1.48	9 (18%)
4	GDP	I	501	-	29,30,30	0.74	0	45,47,47	1.13	2 (4%)
5	GTP	B	501	6	33,34,34	0.98	2 (6%)	50,54,54	1.01	3 (6%)
5	GTP	J	501	6	33,34,34	0.93	1 (3%)	50,54,54	1.27	5 (10%)
5	GTP	N	501	6	33,34,34	0.90	2 (6%)	50,54,54	0.97	2 (4%)
5	GTP	F	501	6	33,34,34	0.79	0	50,54,54	0.90	0
4	GDP	G	501	-	29,30,30	0.77	0	45,47,47	1.36	4 (8%)
5	GTP	H	501	6	33,34,34	0.79	0	50,54,54	0.90	1 (2%)
4	GDP	E	501	-	29,30,30	0.83	0	45,47,47	1.05	5 (11%)
4	GDP	M	501	-	29,30,30	0.80	0	45,47,47	1.20	5 (11%)
4	GDP	A	501	-	29,30,30	0.84	0	45,47,47	1.69	10 (22%)
5	GTP	D	501	6	33,34,34	0.96	1 (3%)	50,54,54	1.32	8 (16%)
4	GDP	C	501	-	29,30,30	0.82	0	45,47,47	1.97	14 (31%)
4	GDP	K	501	-	29,30,30	0.82	0	45,47,47	1.46	7 (15%)

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	L	501	6	-	7/22/38/38	0/3/3/3
4	GDP	I	501	-	-	4/16/32/32	0/3/3/3
5	GTP	B	501	6	-	5/22/38/38	0/3/3/3
5	GTP	J	501	6	-	3/22/38/38	0/3/3/3
5	GTP	N	501	6	-	1/22/38/38	0/3/3/3
5	GTP	F	501	6	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GDP	G	501	-	-	3/16/32/32	0/3/3/3
5	GTP	H	501	6	-	1/22/38/38	0/3/3/3
4	GDP	E	501	-	-	2/16/32/32	0/3/3/3
4	GDP	M	501	-	-	1/16/32/32	0/3/3/3
4	GDP	A	501	-	-	2/16/32/32	0/3/3/3
5	GTP	D	501	6	-	2/22/38/38	0/3/3/3
4	GDP	C	501	-	-	2/16/32/32	0/3/3/3
4	GDP	K	501	-	-	2/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	501	GTP	PB-O3B	2.60	1.62	1.59
5	N	501	GTP	PG-O3G	-2.25	1.46	1.54
5	B	501	GTP	PG-O2G	-2.25	1.46	1.54
5	D	501	GTP	PA-O3A	2.24	1.61	1.59
5	N	501	GTP	PG-O2G	-2.20	1.46	1.54
5	B	501	GTP	PG-O3G	-2.19	1.46	1.54
5	J	501	GTP	PB-O3B	2.06	1.61	1.59

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	GDP	C2'-C3'-C4'	-5.31	92.34	102.61
4	C	501	GDP	O4'-C4'-C3'	4.77	114.62	105.15
4	A	501	GDP	O6-C6-N1	-4.41	111.81	120.11
4	I	501	GDP	O2A-PA-O3A	4.35	119.03	107.27
4	A	501	GDP	O2'-C2'-C1'	4.35	125.07	110.10
5	L	501	GTP	O6-C6-N1	-3.96	112.66	120.11
4	A	501	GDP	C3'-C2'-C1'	-3.96	93.97	101.46
4	C	501	GDP	C2-N3-C4	3.94	119.09	112.30
4	C	501	GDP	N1-C2-N3	-3.58	116.77	123.32
4	G	501	GDP	O2A-PA-O3A	3.53	116.81	107.27
5	D	501	GTP	O6-C6-N1	-3.43	113.67	120.11
5	J	501	GTP	N2-C2-N1	-3.42	109.54	116.76
4	C	501	GDP	O4'-C1'-C2'	-3.25	99.65	106.62
4	K	501	GDP	O2A-PA-O3A	3.20	115.93	107.27
4	K	501	GDP	C2-N1-C6	-3.18	119.34	125.11
4	G	501	GDP	O4'-C1'-N9	3.16	115.52	108.36
4	M	501	GDP	O4'-C1'-N9	3.16	115.52	108.36
4	K	501	GDP	O6-C6-N1	-3.14	114.21	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	GTP	C6-C5-N7	3.04	135.82	130.29
4	C	501	GDP	C6-C5-N7	3.02	135.78	130.29
4	A	501	GDP	C2-N1-C6	-2.95	119.75	125.11
5	L	501	GTP	N2-C2-N3	2.84	125.22	119.67
4	E	501	GDP	O4'-C4'-C5'	2.80	118.30	109.33
4	K	501	GDP	C6-C5-C4	-2.77	114.67	118.83
5	D	501	GTP	O5'-C5'-C4'	2.66	118.05	108.99
5	L	501	GTP	O2G-PG-O3B	-2.65	95.74	104.64
5	L	501	GTP	O3A-PA-O1A	-2.62	102.81	110.70
5	D	501	GTP	N2-C2-N3	-2.62	114.56	119.67
4	E	501	GDP	O6-C6-N1	-2.61	115.20	120.11
4	I	501	GDP	O3B-PB-O2B	2.60	117.57	107.80
4	C	501	GDP	O2'-C2'-C1'	-2.57	101.24	110.10
4	C	501	GDP	O3B-PB-O2B	2.57	117.43	107.80
5	D	501	GTP	O2G-PG-O1G	2.48	120.50	110.83
4	A	501	GDP	O3'-C3'-C4'	2.47	118.18	111.08
4	M	501	GDP	O4'-C4'-C5'	2.45	117.18	109.33
4	A	501	GDP	C8-N7-C5	-2.45	99.90	104.26
4	A	501	GDP	O3B-PB-O2B	2.44	116.95	107.80
4	G	501	GDP	O4'-C4'-C3'	2.42	109.95	105.15
5	B	501	GTP	O2A-PA-O3A	2.41	113.79	107.27
4	M	501	GDP	O3B-PB-O2B	2.41	116.85	107.80
5	N	501	GTP	O2B-PB-O3A	-2.41	100.76	107.27
5	H	501	GTP	O2B-PB-O3A	-2.39	100.80	107.27
5	L	501	GTP	O2B-PB-O1B	2.38	123.54	112.44
5	B	501	GTP	O6-C6-N1	-2.38	115.64	120.11
5	L	501	GTP	O2A-PA-O3A	2.37	113.69	107.27
5	L	501	GTP	O4'-C4'-C5'	-2.37	101.75	109.33
4	K	501	GDP	C3'-C2'-C1'	-2.36	97.00	101.46
4	M	501	GDP	O6-C6-N1	-2.34	115.72	120.11
5	B	501	GTP	O2B-PB-O3A	-2.31	101.02	107.27
5	D	501	GTP	N2-C2-N1	2.28	121.57	116.76
5	N	501	GTP	O2A-PA-O3A	2.27	113.41	107.27
5	J	501	GTP	O3G-PG-O2G	2.26	116.29	107.80
4	C	501	GDP	C3'-C2'-C1'	2.26	105.74	101.46
4	G	501	GDP	O2'-C2'-C1'	-2.26	102.32	110.10
4	E	501	GDP	C5'-C4'-C3'	-2.23	107.20	115.21
5	L	501	GTP	O4'-C1'-C2'	-2.22	101.87	106.62
4	C	501	GDP	O3A-PB-O1B	-2.21	99.39	111.04
5	J	501	GTP	O4'-C1'-N9	2.20	113.34	108.36
4	C	501	GDP	C5'-C4'-C3'	-2.19	107.32	115.21
4	C	501	GDP	O2A-PA-O1A	2.18	122.60	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	501	GDP	C1'-N9-C8	2.18	132.91	126.73
5	L	501	GTP	N2-C2-N1	-2.13	112.27	116.76
4	K	501	GDP	C5-C6-N1	2.12	118.65	113.25
4	C	501	GDP	N2-C2-N1	2.10	121.19	116.76
4	E	501	GDP	O2A-PA-O1A	2.09	122.18	112.44
5	J	501	GTP	N1-C2-N3	2.08	127.14	123.32
5	D	501	GTP	C6-C5-C4	-2.07	115.71	118.83
4	C	501	GDP	O3'-C3'-C2'	2.06	118.44	111.82
5	D	501	GTP	C2-N1-C6	-2.05	121.39	125.11
4	A	501	GDP	C2'-C3'-C4'	2.05	106.57	102.61
4	E	501	GDP	C6-C5-C4	-2.05	115.75	118.83
4	A	501	GDP	C4-C5-N7	2.04	113.90	110.67
4	M	501	GDP	O2'-C2'-C3'	2.03	118.33	111.82
5	J	501	GTP	C2-N1-C6	-2.02	121.44	125.11
4	A	501	GDP	N1-C2-N3	2.00	126.98	123.32

There are no chirality outliers.

All (38) torsion outliers are listed below:

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

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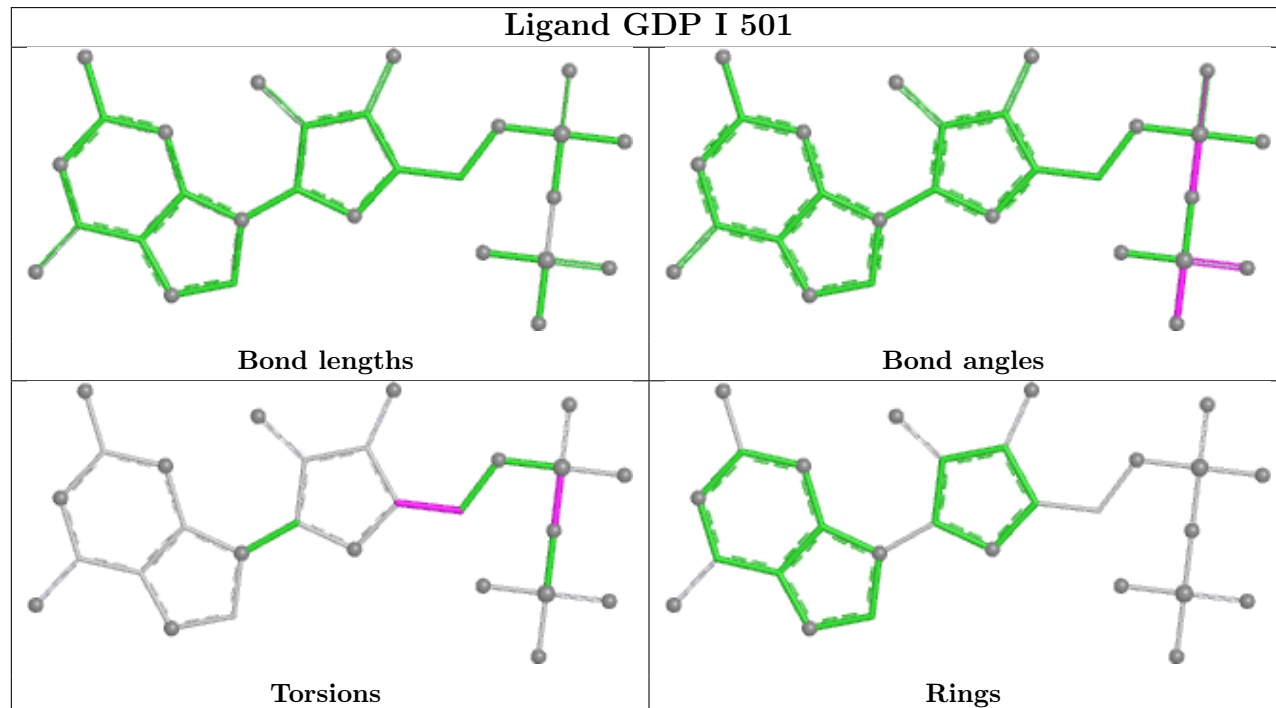
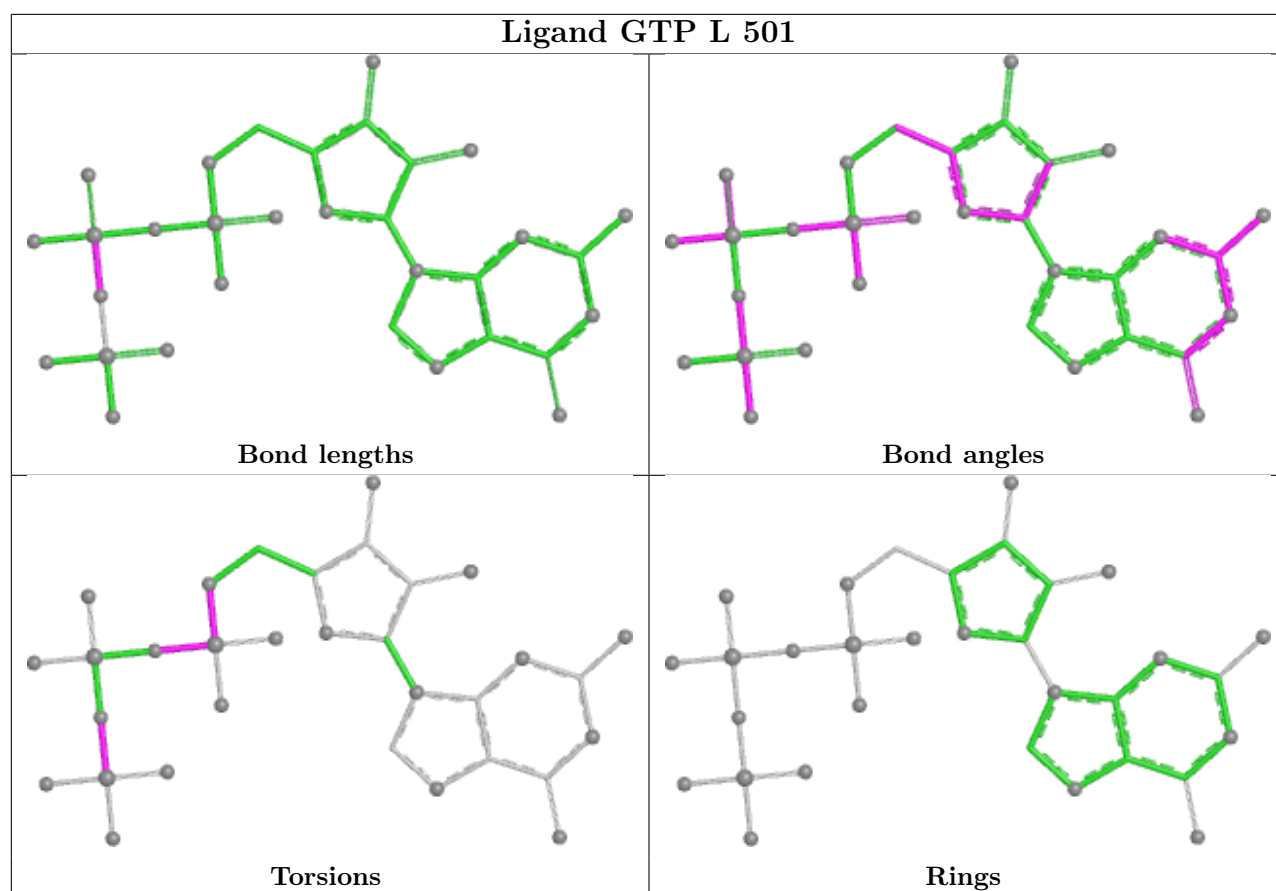
Mol	Chain	Res	Type	Atoms
4	I	501	GDP	PB-O3A-PA-O2A
4	K	501	GDP	PA-O3A-PB-O1B
5	F	501	GTP	C4'-C5'-O5'-PA
4	E	501	GDP	C3'-C4'-C5'-O5'
4	C	501	GDP	PA-O3A-PB-O1B
4	A	501	GDP	PA-O3A-PB-O3B
5	J	501	GTP	PB-O3B-PG-O3G
5	L	501	GTP	PB-O3B-PG-O2G
4	I	501	GDP	PB-O3A-PA-O1A
5	L	501	GTP	PB-O3A-PA-O1A
5	B	501	GTP	PG-O3B-PB-O2B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

There are no ring outliers.

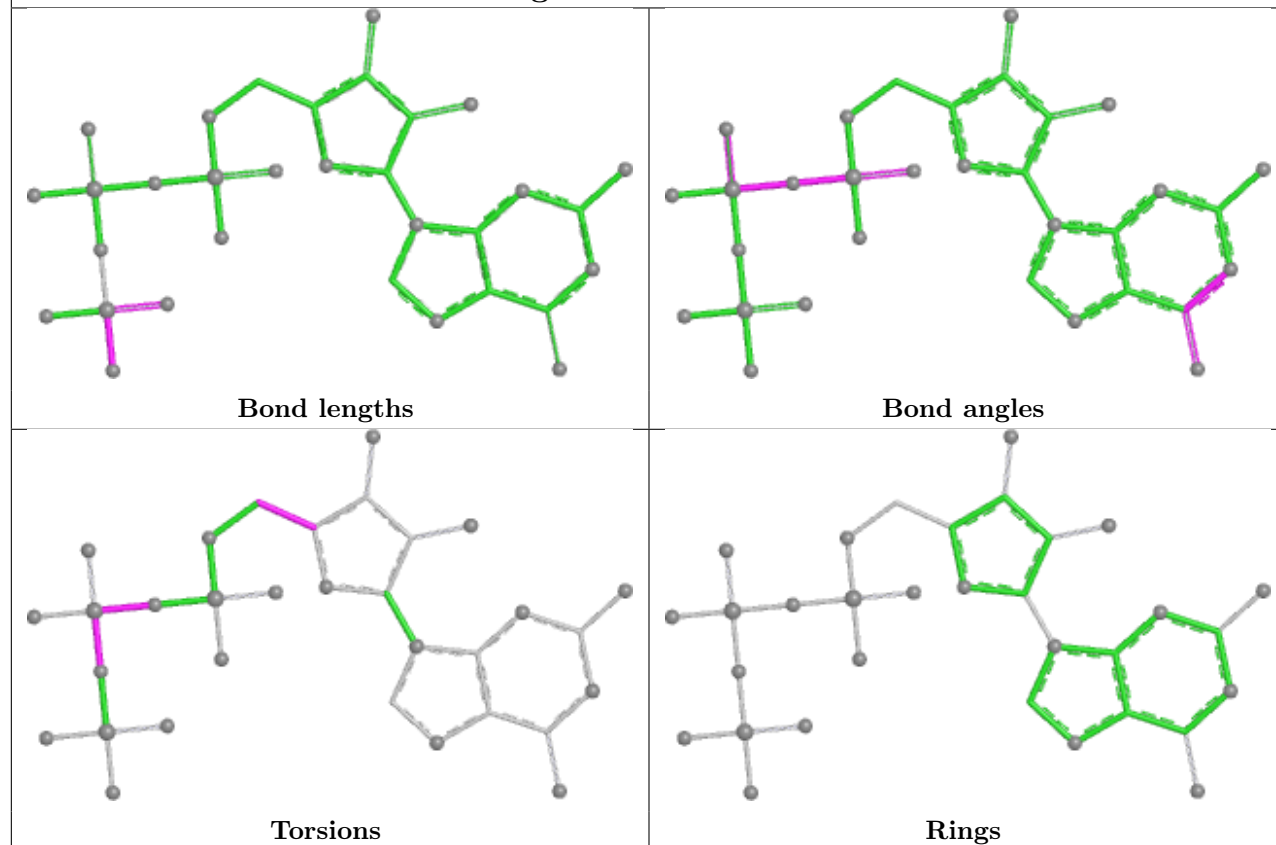
1 monomer is involved in 1 short contact:

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

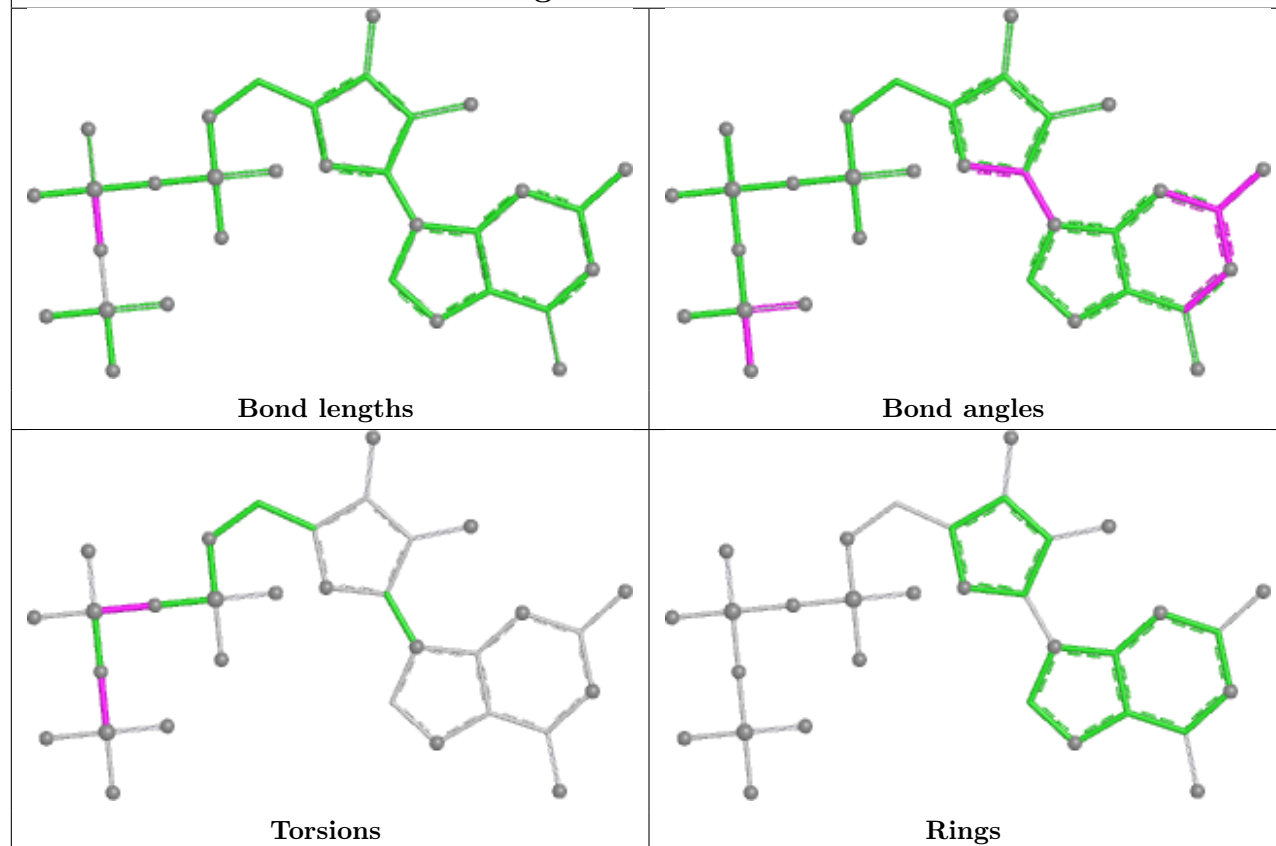
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



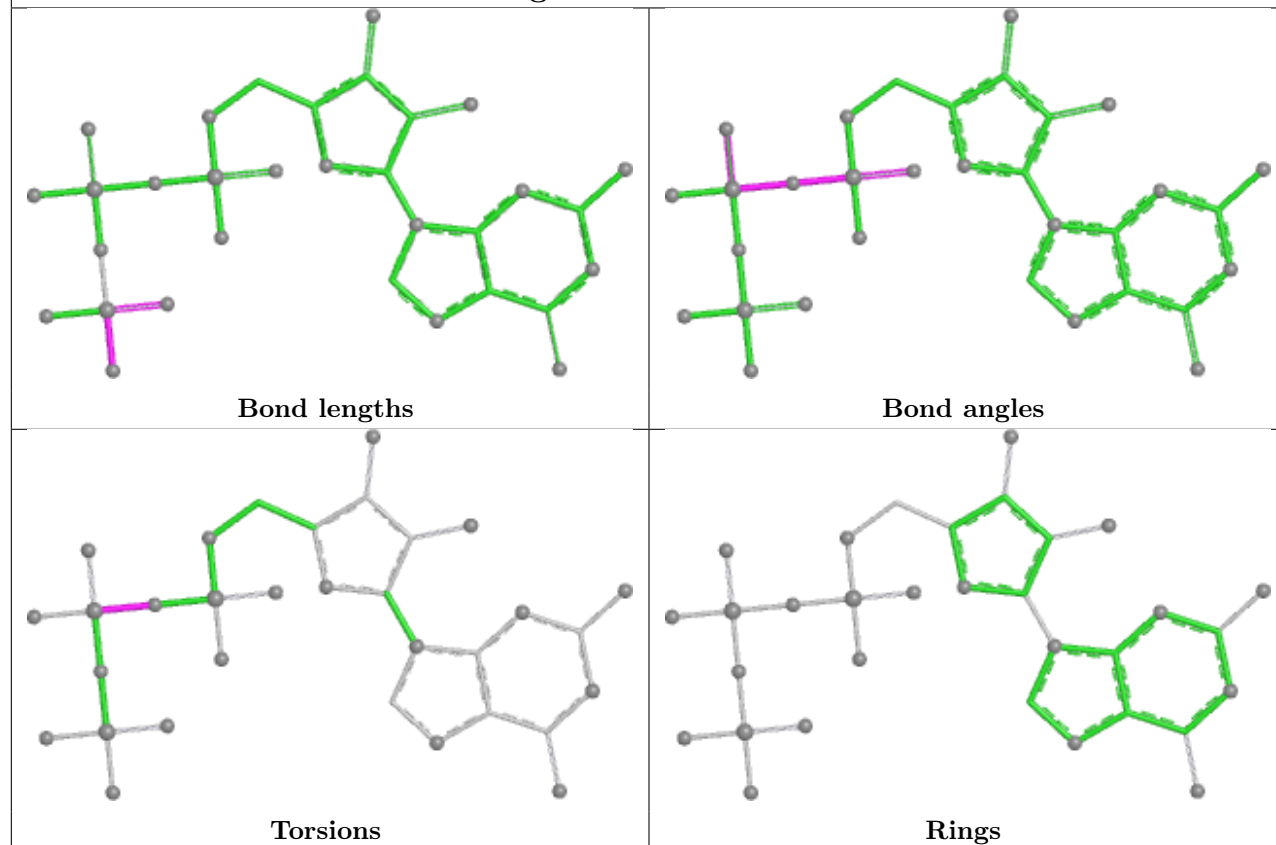
Ligand GTP B 501



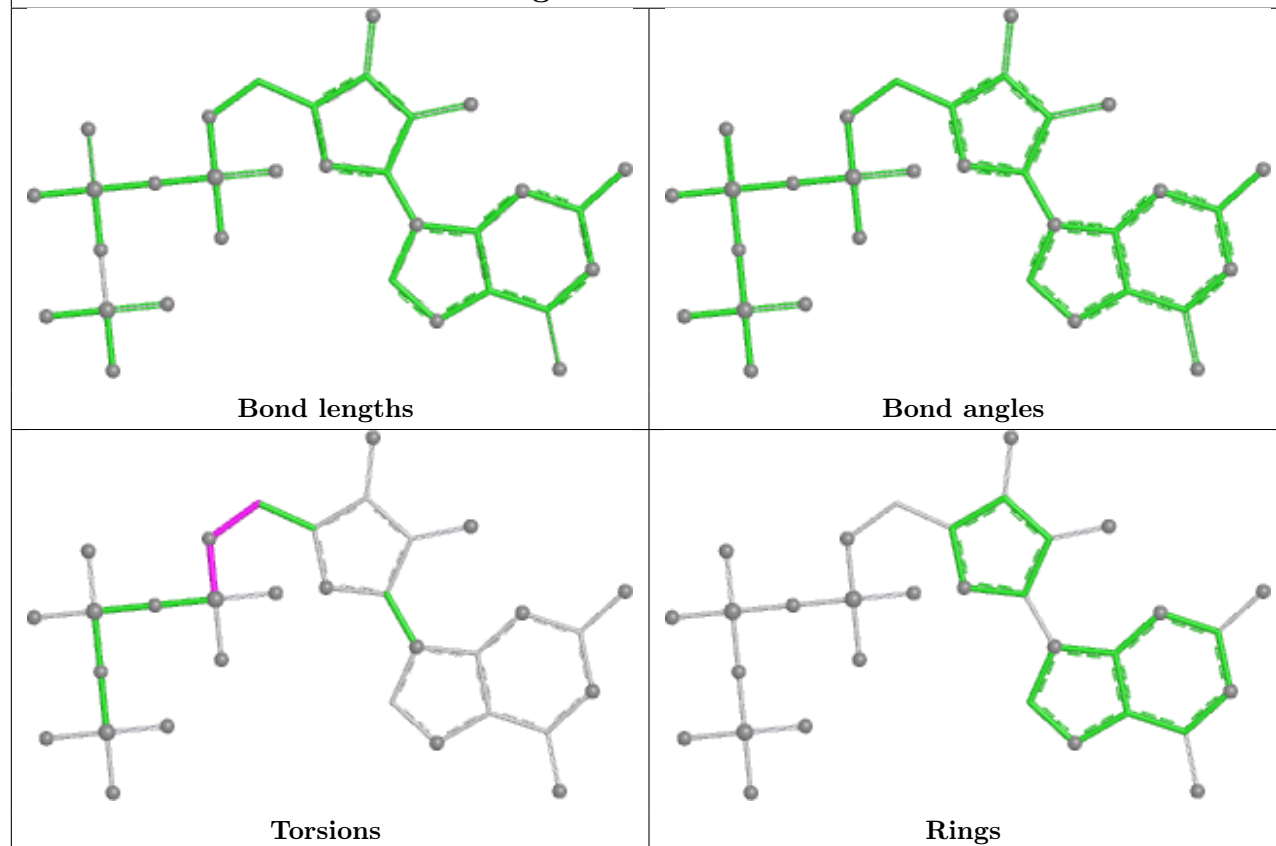
Ligand GTP J 501

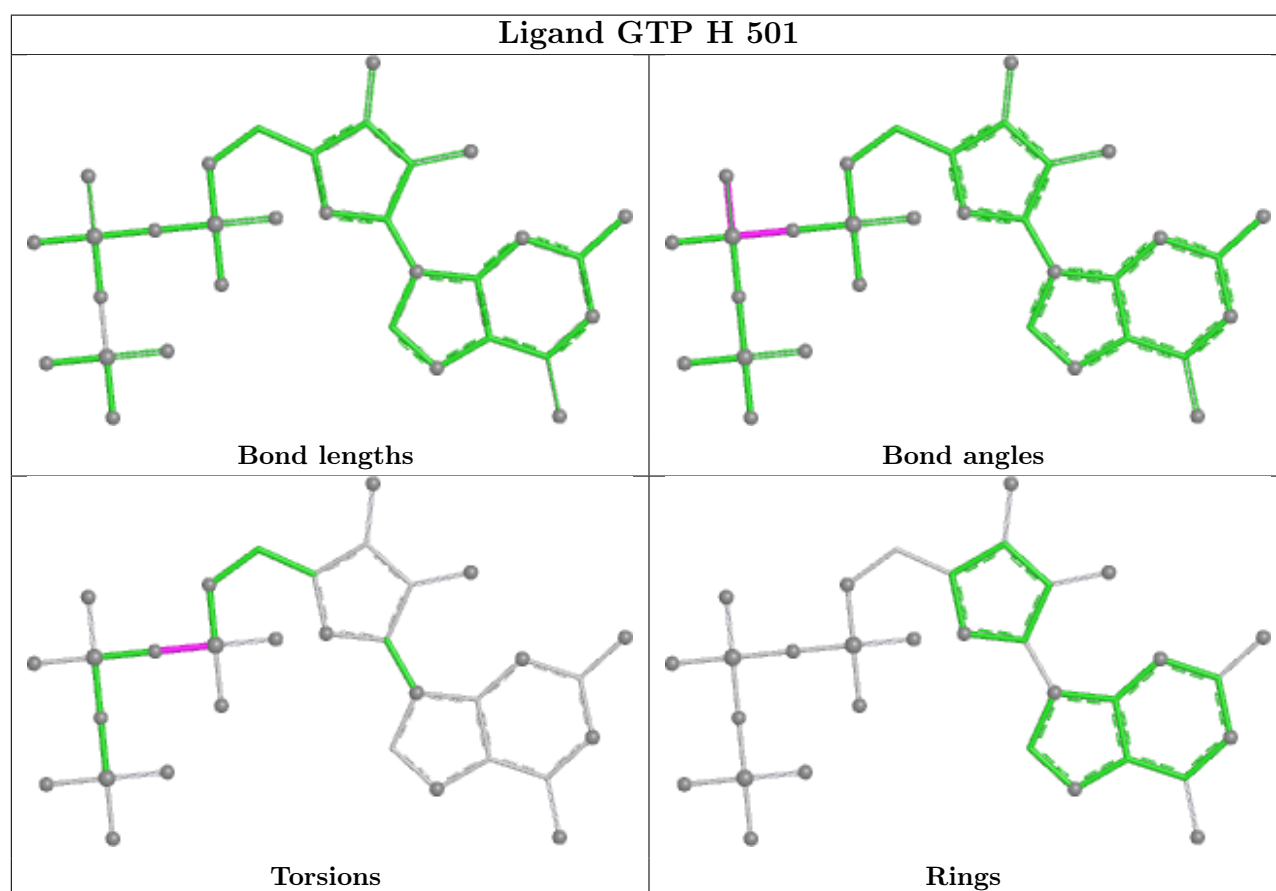
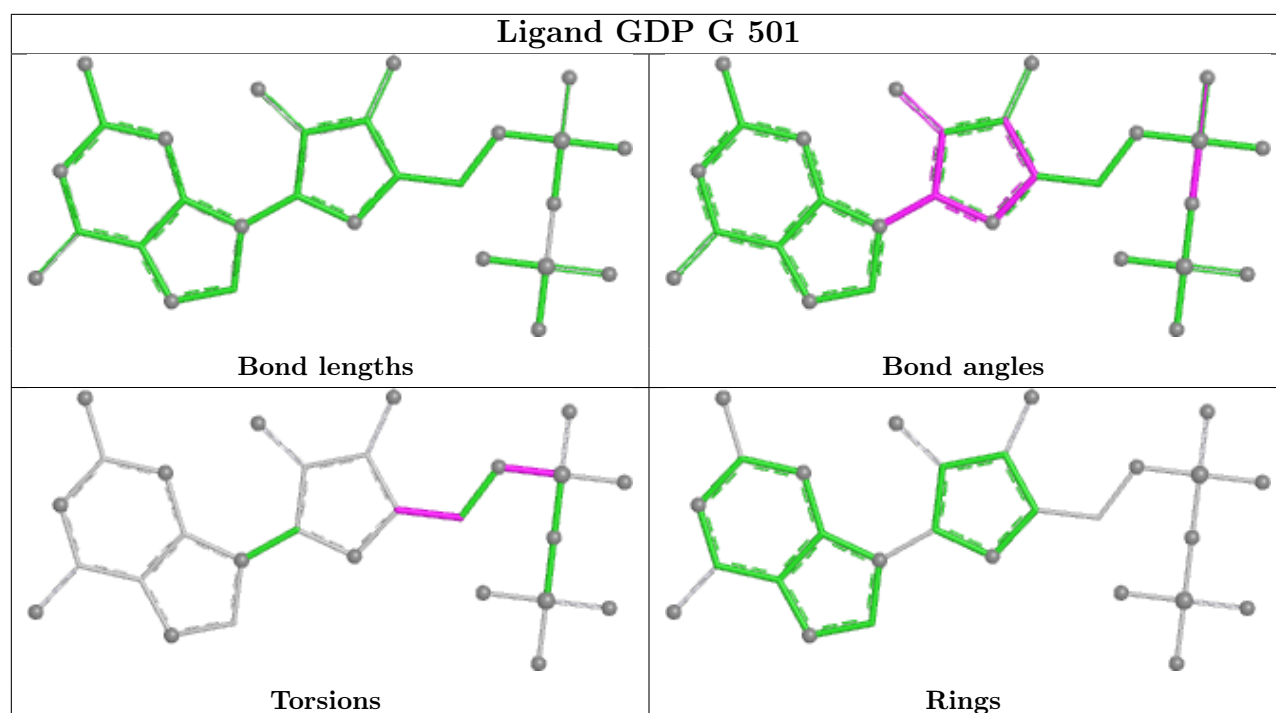


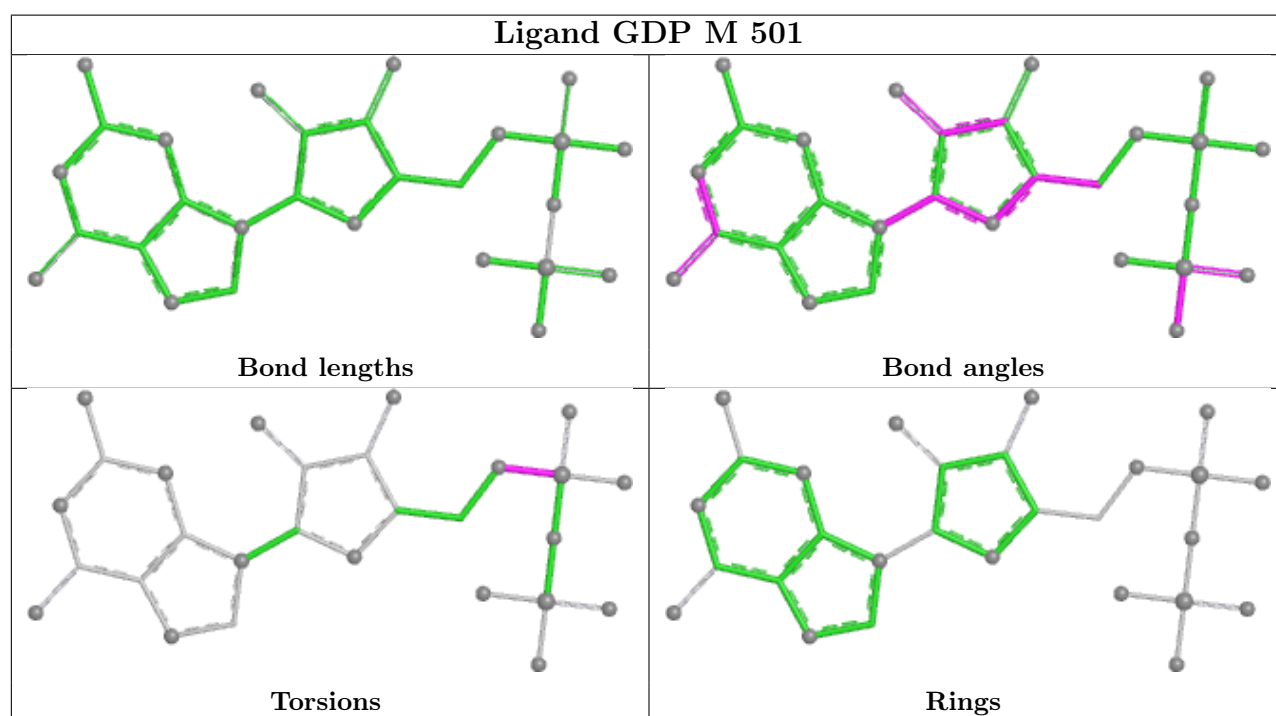
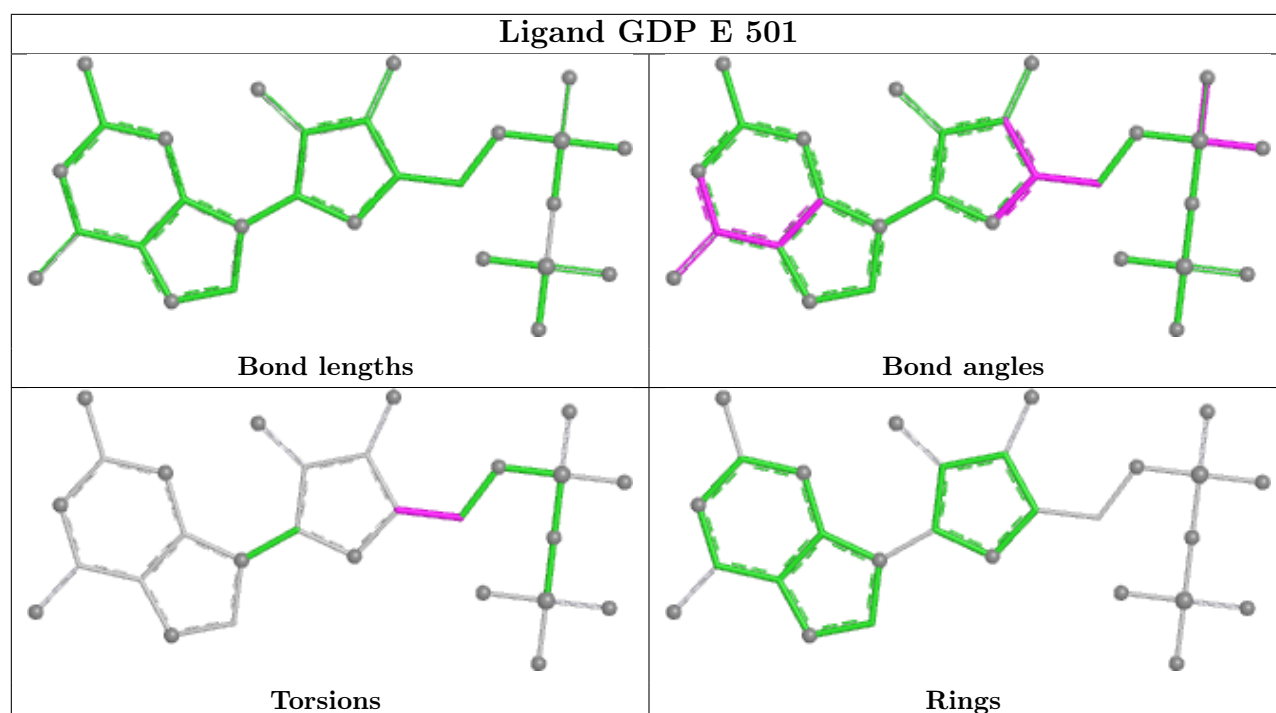
Ligand GTP N 501

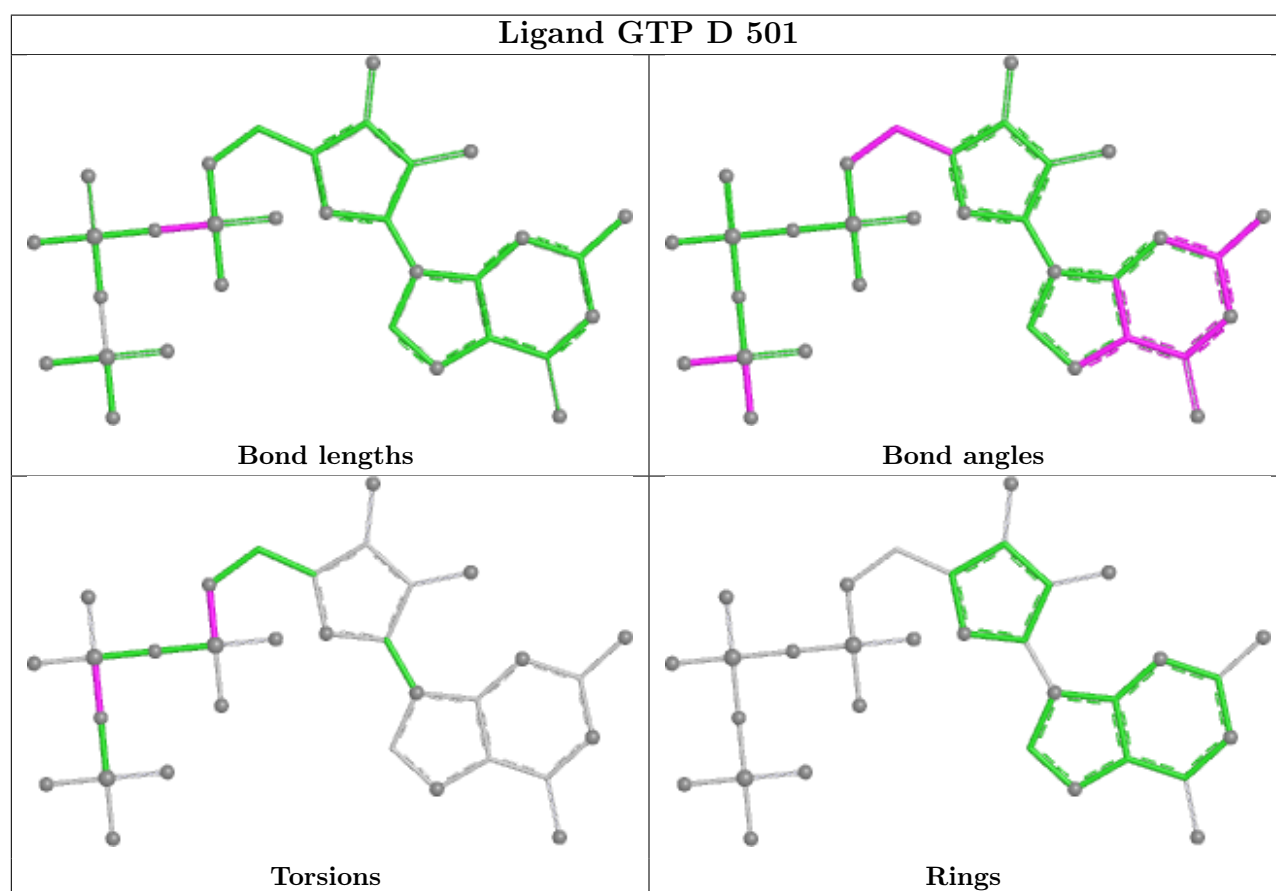
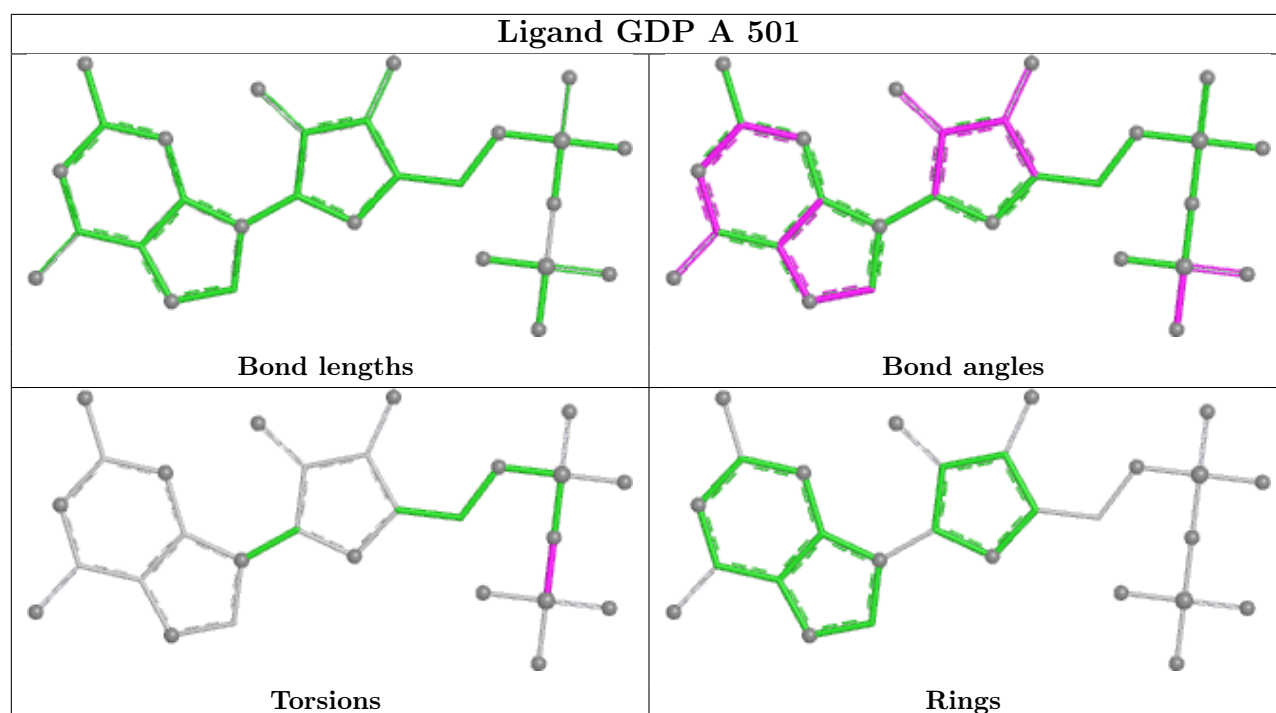


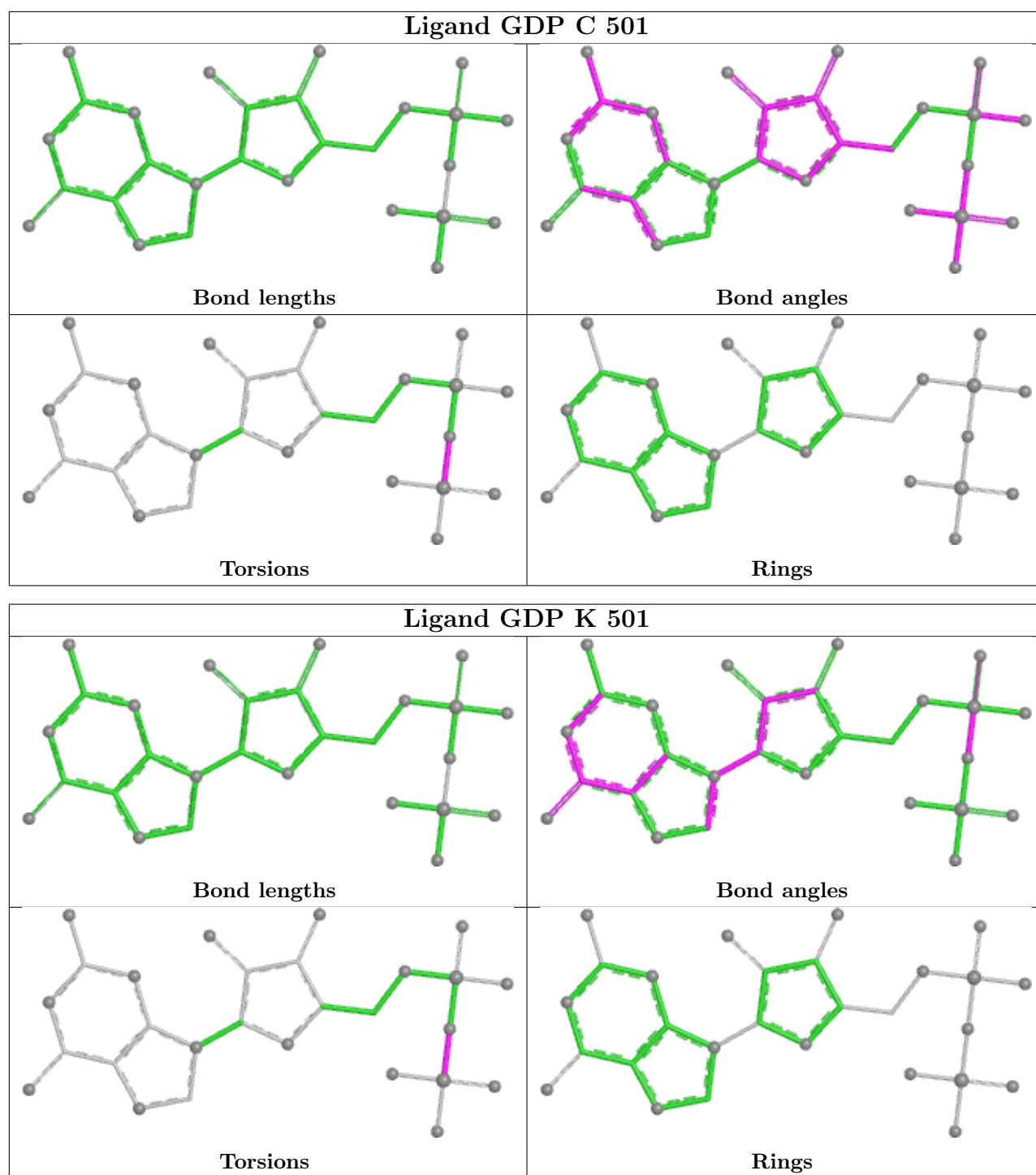
Ligand GTP F 501











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.

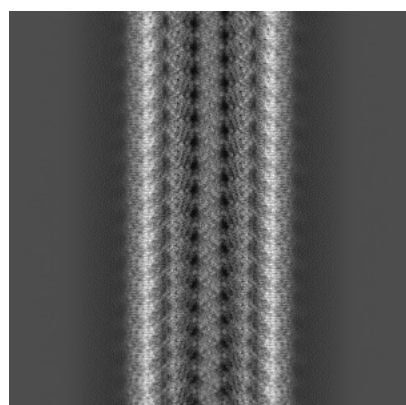
6 Map visualisation [i](#)

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.

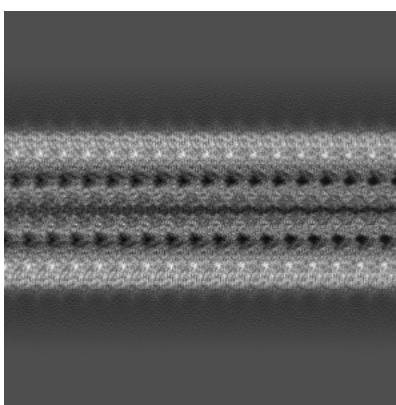
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

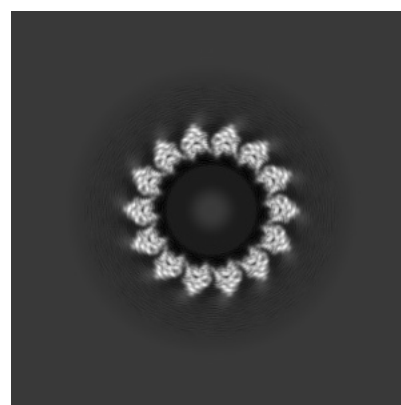
6.1.1 Primary map



X



Y

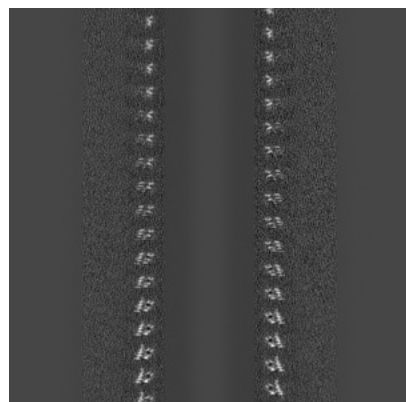


Z

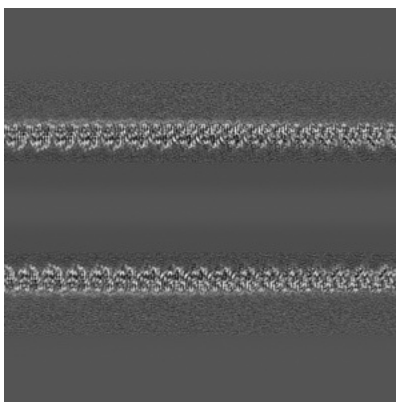
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

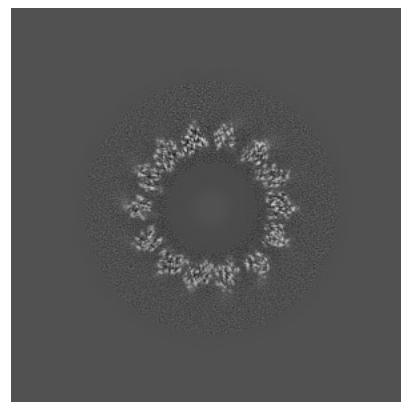
6.2.1 Primary map



X Index: 256



Y Index: 256

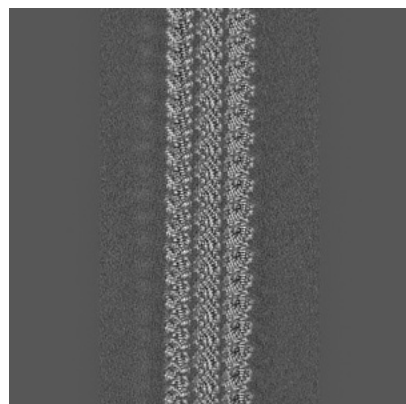


Z Index: 256

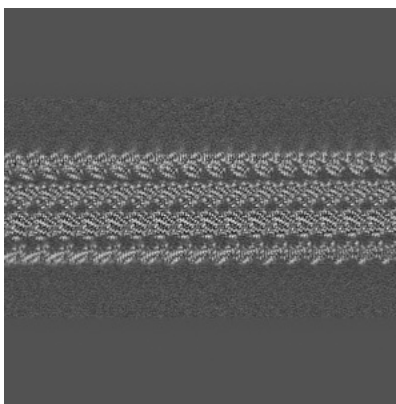
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

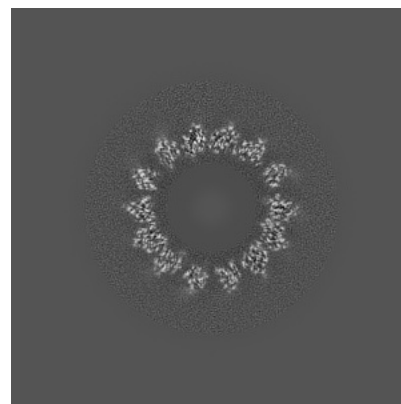
6.3.1 Primary map



X Index: 174



Y Index: 337

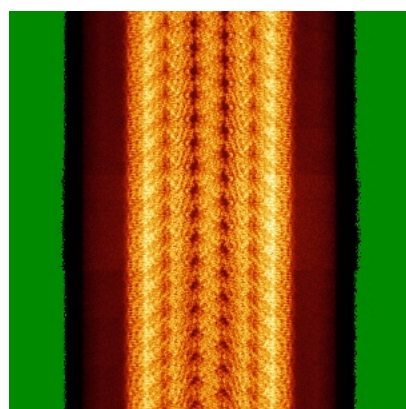


Z Index: 237

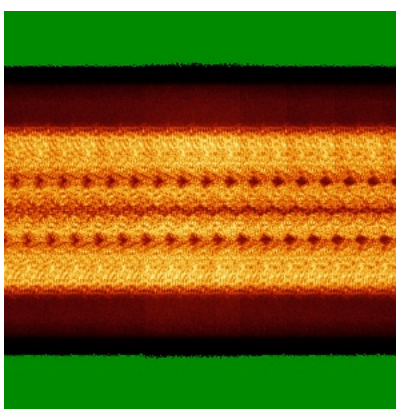
The images above show the largest variance slices of the map in three orthogonal directions.

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

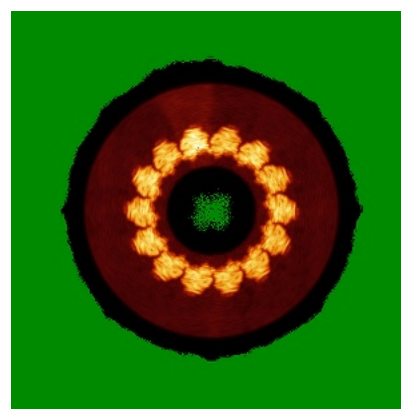
6.4.1 Primary map



X



Y

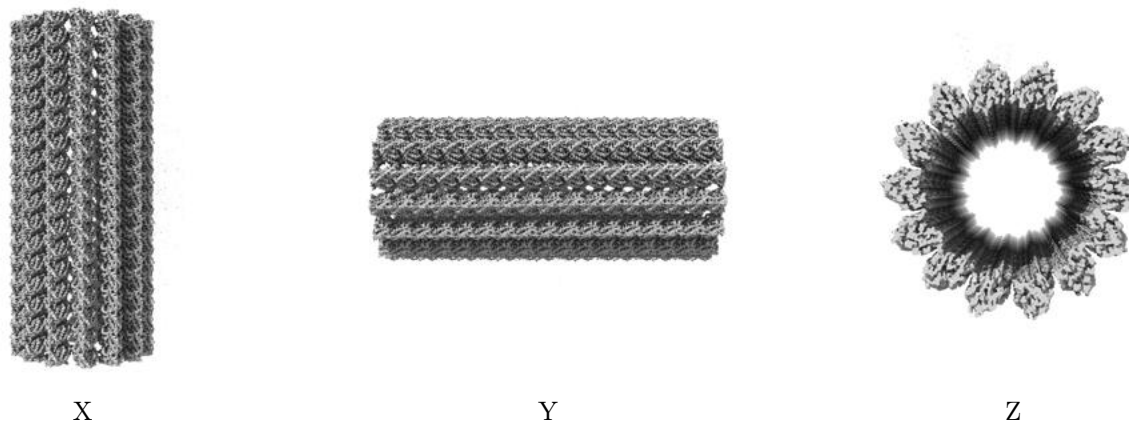


Z

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.

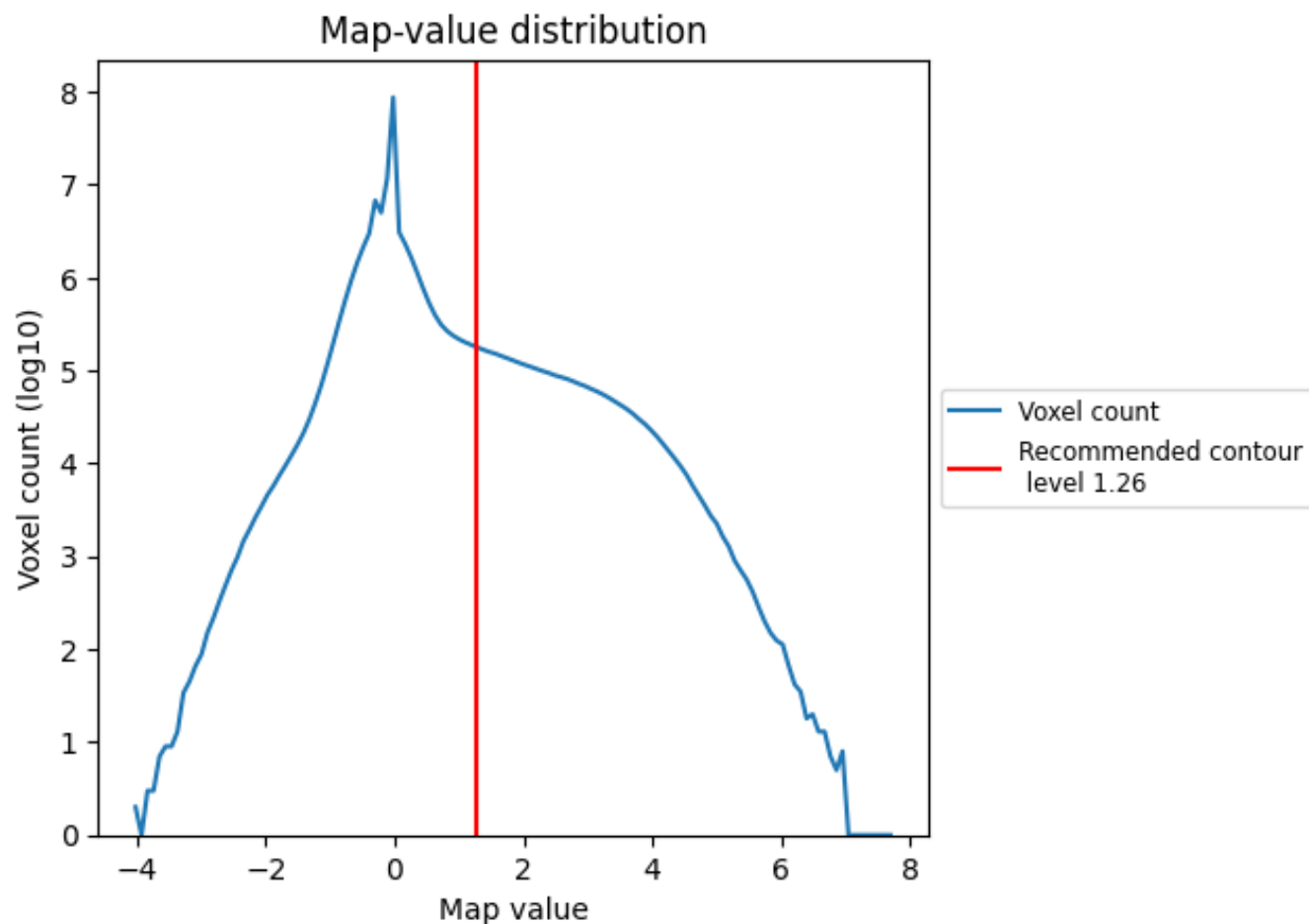
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

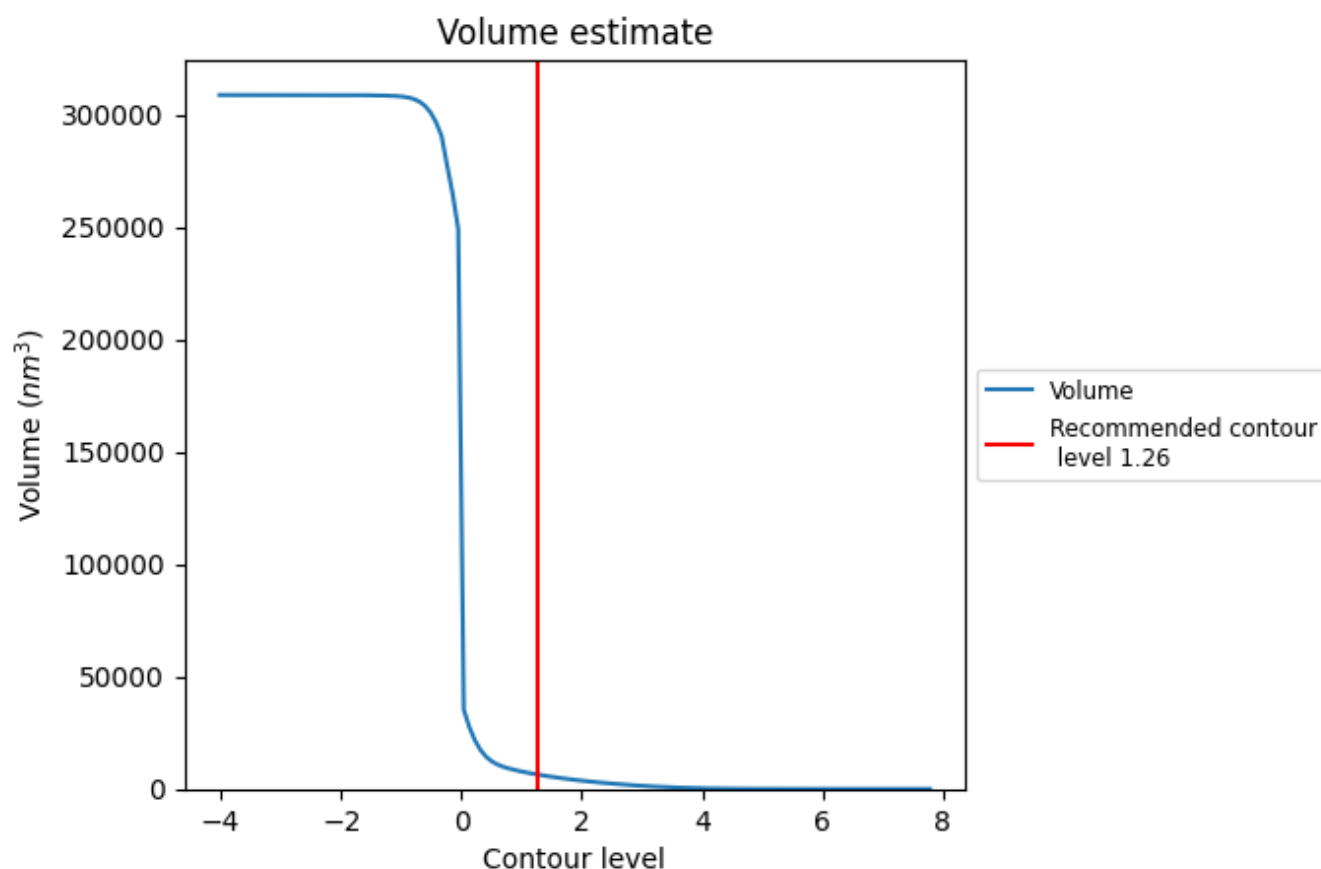
This section contains the results of statistical analysis of the map.

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.

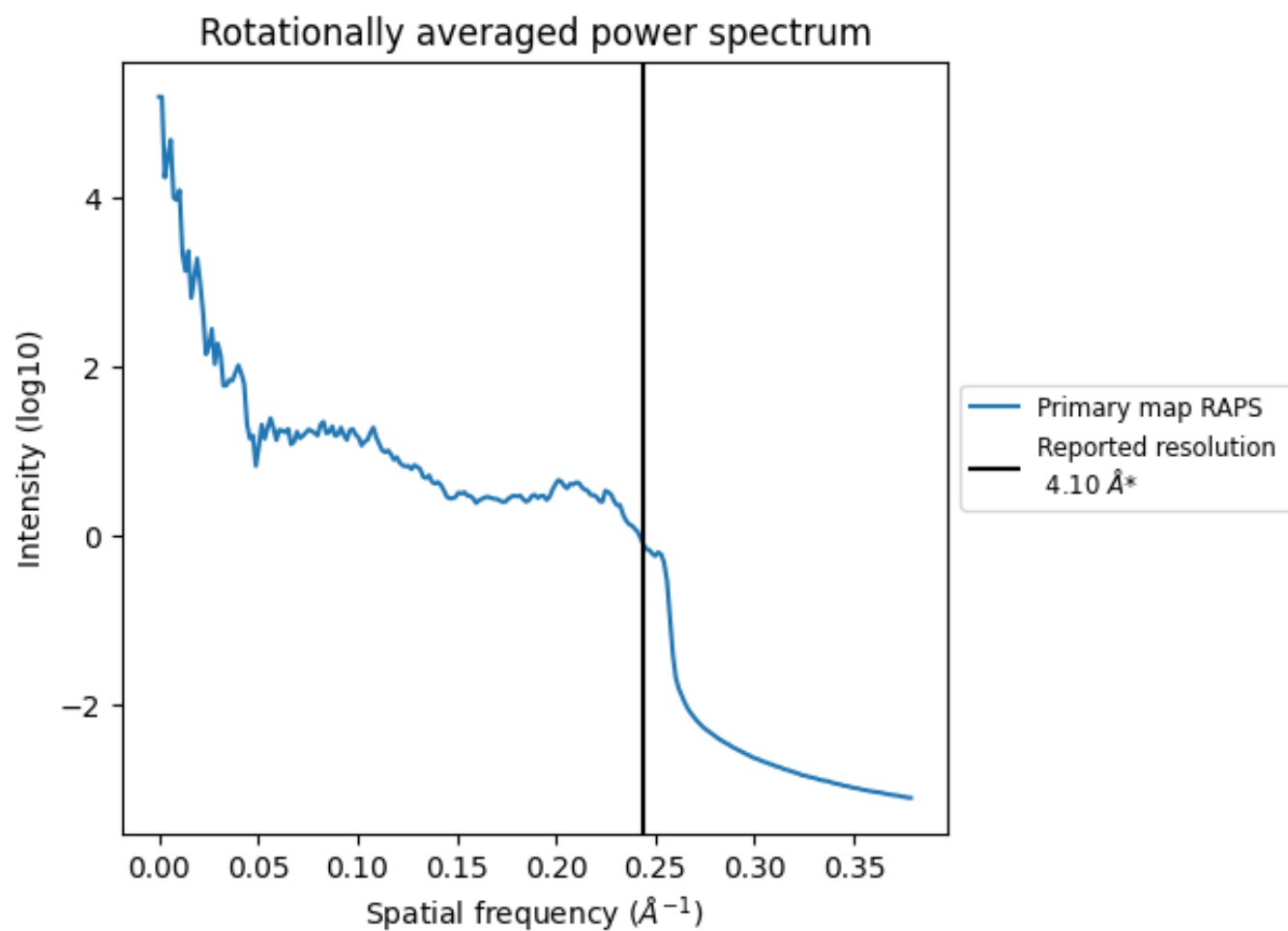
7.2 Volume estimate [i](#)



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 ⓘ



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

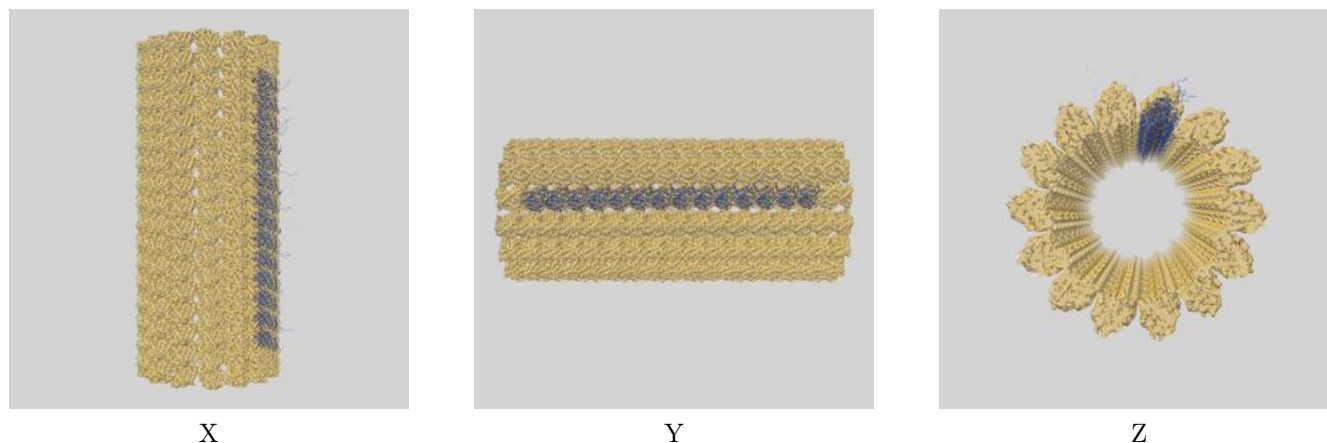
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

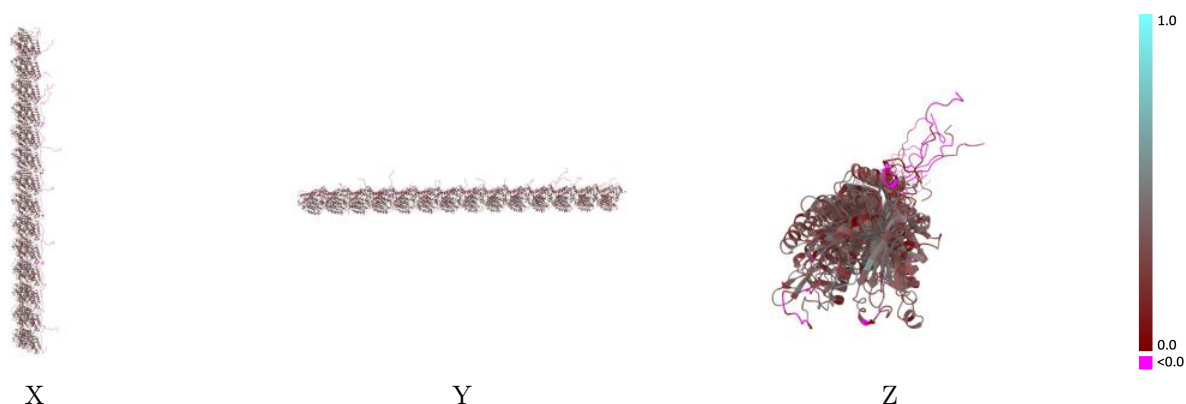
This section contains information regarding the fit between EMDB map EMD-7522 and PDB model 7PQP. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



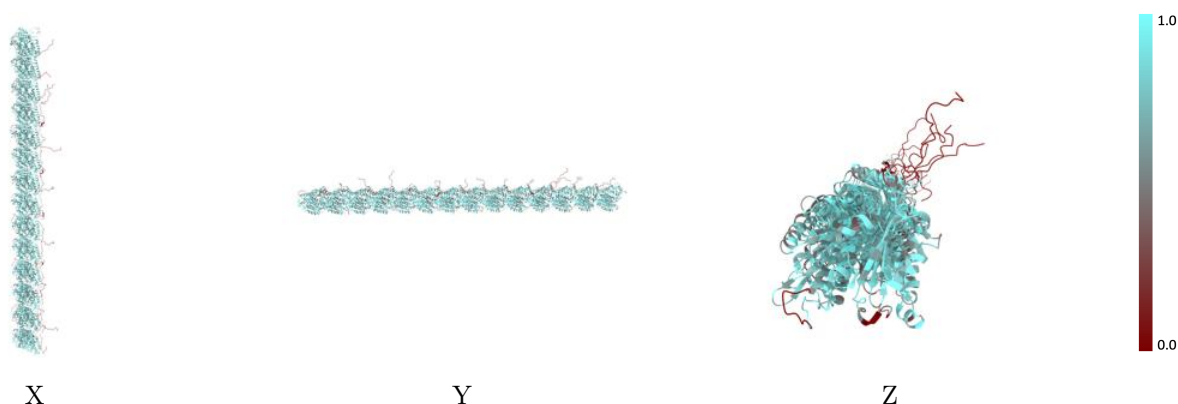
The images above show the 3D surface view of the map at the recommended contour level 1.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



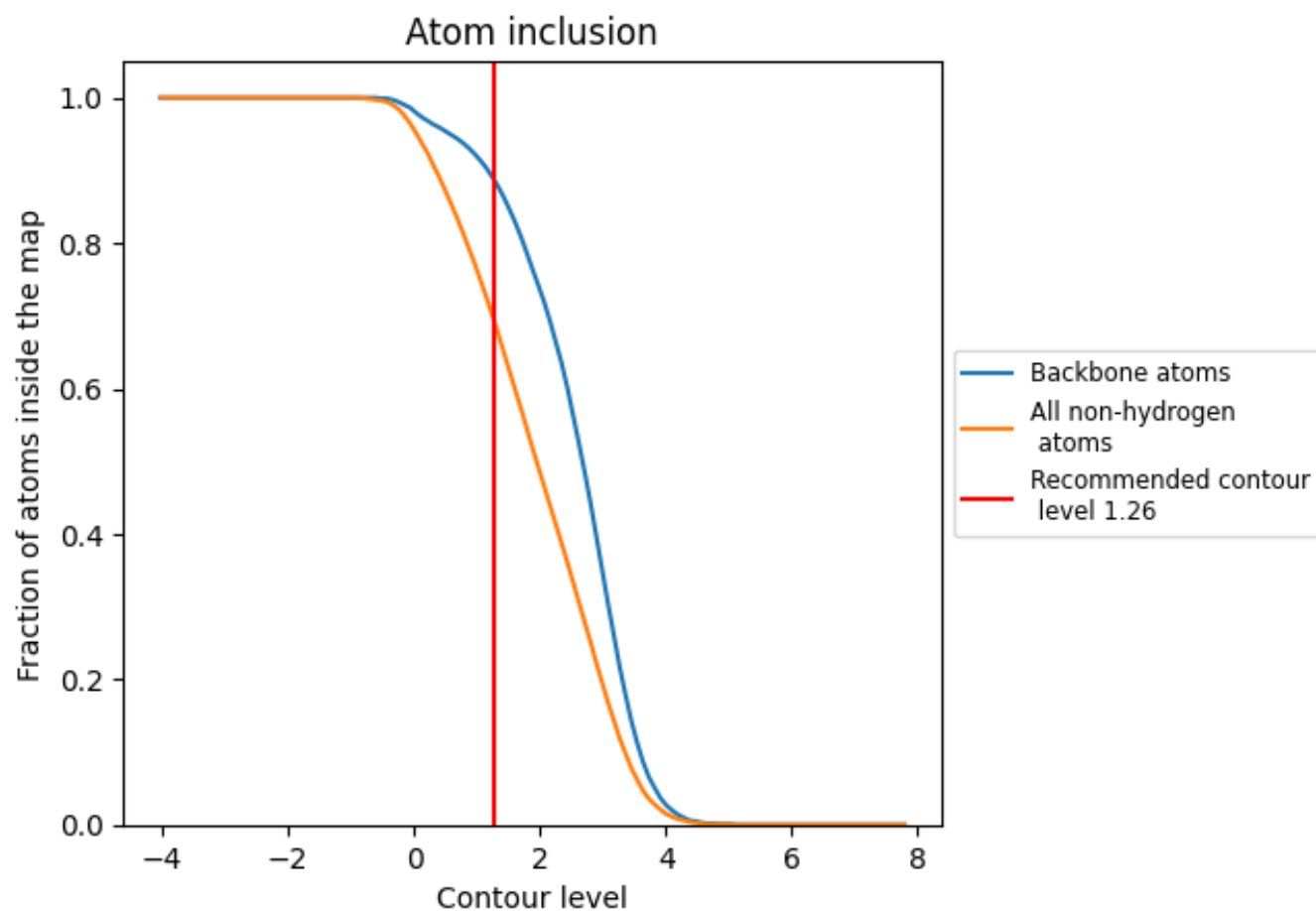
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.6970	0.3170
A	0.7170	0.3200
B	0.7010	0.3140
C	0.7140	0.3280
D	0.7120	0.3190
E	0.7170	0.3280
F	0.7140	0.3270
G	0.7310	0.3340
H	0.7190	0.3300
I	0.7120	0.3360
J	0.7070	0.3240
K	0.7120	0.3260
L	0.7000	0.3190
M	0.7040	0.3220
N	0.7100	0.3120
O	0.1890	0.0700

