



Full wwPDB EM Validation Report ⓘ

Oct 6, 2025 – 01:07 PM EDT

PDB ID : 9NRJ / pdb_00009nrj
EMDB ID : EMD-49735
Title : abTCR bound to SAR444200, a novel anti-GPC3 T-cell engager, for the treatment of GPC3+ solid tumors
Authors : Svidritskiy, E.; Qiu, Y.; Yanfeng, Z.
Deposited on : 2025-03-14
Resolution : 3.40 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:

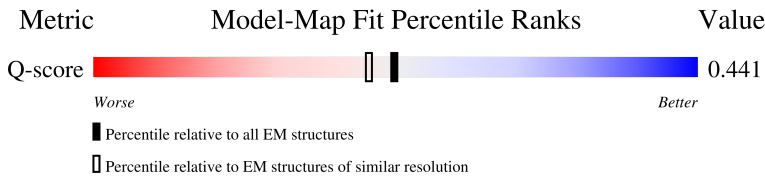
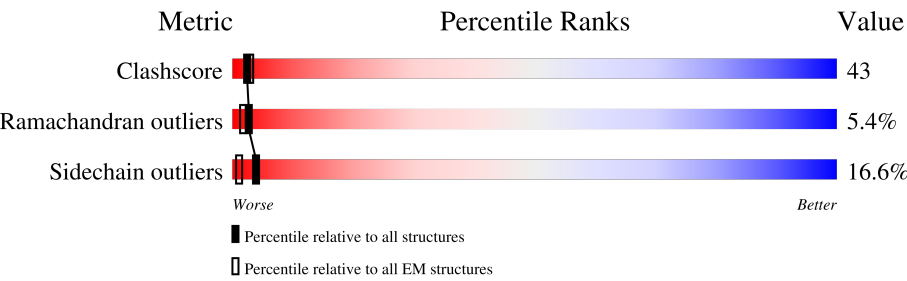
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	199	 27% 32% 48% 18%
2	B	242	 19% 6% 28% 38% 28%
3	C	114	 55% 14% 41% 28% 17%
4	T	117	 29% 29% 36% 31%

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Mol	Chain	Length	Quality of chain
5	D	3	<div>67%</div> <div>  100% </div>
6	E	3	<div>100%</div> <div>  100% </div>
7	F	2	<div>100%</div> <div>  100% </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	D	1	X	-	-	-
7	NAG	F	1	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5386 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 M1-specific T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	199	Total	C	N	O	S	0	0
			1530	958	255	310	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	ALA	GLY	conflict	UNP P0DSE1
A	111	ASN	-	insertion	UNP P0DSE1
A	158	CYS	THR	conflict	UNP P0DSE1

- Molecule 2 is a protein called M1-specific T cell receptor beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	242	Total	C	N	O	S	0	0
			1945	1224	336	379	6		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	97	SER	ILE	conflict	UNP P0DSE2
B	124	GLU	LYS	conflict	UNP P0DSE2
B	171	CYS	SER	conflict	UNP P0DSE2
B	189	SER	CYS	conflict	UNP P0DSE2

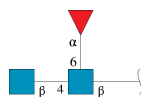
- Molecule 3 is a protein called 2C04.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	114	Total	C	N	O	S	0	0
			885	558	159	165	3		

- Molecule 4 is a protein called TCE01.

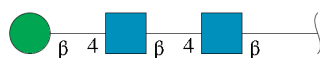
Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	117	Total	C	N	O	S	0	0
			921	578	162	178	3		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

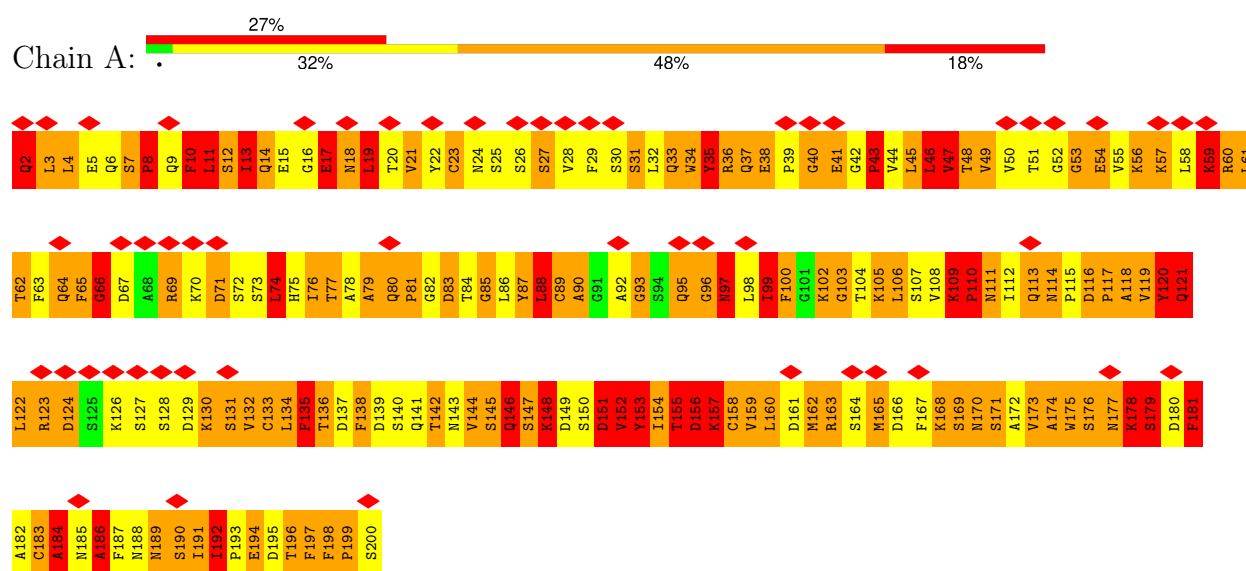


Mol	Chain	Residues	Atoms				AltConf	Trace
7	F	2	Total	C	N	O	0	0
			28	16	2	10		

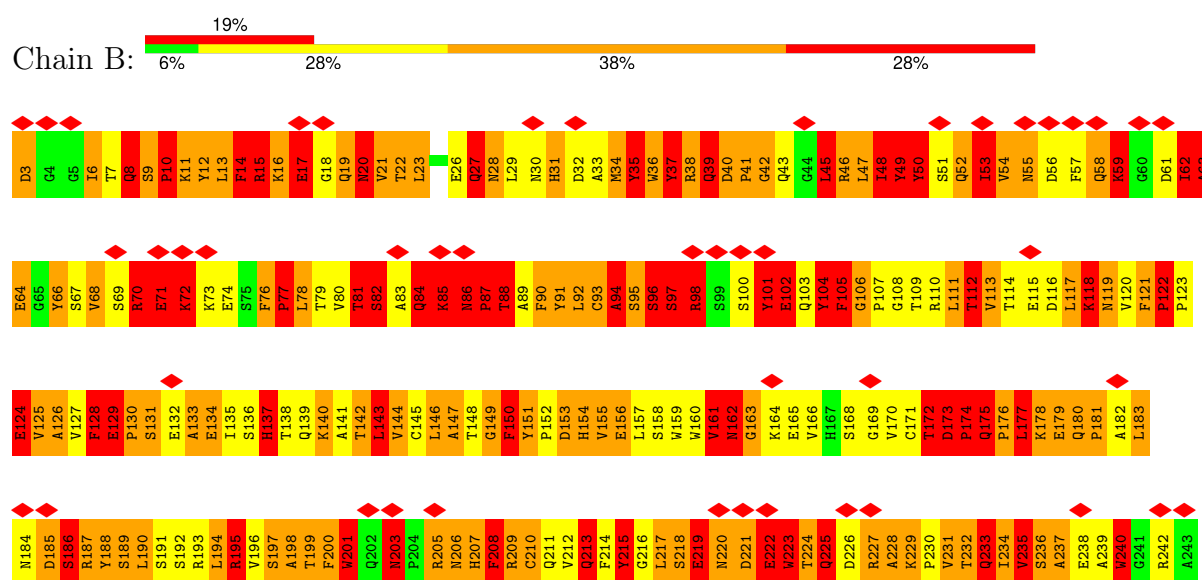
3 Residue-property plots

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: M1-specific T cell receptor alpha chain

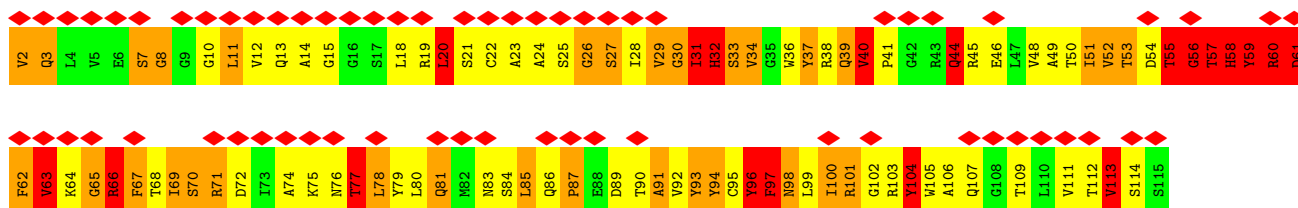


• Molecule 2: M1-specific T cell receptor beta chain

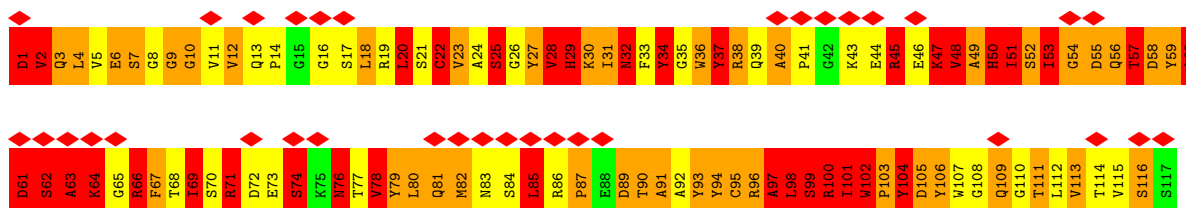




• Molecule 3: 2C04



• Molecule 4: TCE01



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95366	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.175	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	166.0, 166.0, 166.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, FUC

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	3.80	218/1560 (14.0%)	4.89	518/2111 (24.5%)
2	B	3.44	232/1998 (11.6%)	4.87	674/2716 (24.8%)
3	C	2.45	60/902 (6.7%)	4.28	245/1222 (20.0%)
4	T	3.37	130/943 (13.8%)	5.22	360/1277 (28.2%)
All	All	3.40	640/5403 (11.8%)	4.85	1797/7326 (24.5%)

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	2	69
2	B	0	98
3	C	0	28
4	T	2	69
All	All	4	264

All (640) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	VAL	C-O	33.65	1.64	1.24
1	A	153	TYR	C-O	26.79	1.57	1.24
2	B	50	TYR	C-O	26.27	1.58	1.23
1	A	151	ASP	C-O	25.10	1.55	1.24
2	B	207	HIS	CA-CB	24.39	1.87	1.53
2	B	58	GLN	C-O	22.53	1.51	1.23
1	A	132	VAL	C-O	19.08	1.43	1.24
2	B	211	GLN	C-N	-18.74	1.10	1.33
1	A	123	ARG	C-O	18.66	1.46	1.23
1	A	21	VAL	CA-C	-18.34	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	ASP	C-N	17.22	1.57	1.33
2	B	92	LEU	C-O	16.98	1.44	1.23
2	B	209	ARG	C-N	-16.66	1.10	1.33
1	A	158	CYS	C-O	16.20	1.43	1.23
1	A	82	GLY	C-O	15.58	1.40	1.24
2	B	121	PHE	CA-C	-15.45	1.35	1.52
1	A	178	LYS	C-O	-14.99	1.05	1.24
2	B	31	HIS	CG-ND1	14.93	1.54	1.38
4	T	96	ARG	CA-C	-14.57	1.33	1.52
1	A	109	LYS	CA-C	-14.56	1.34	1.52
4	T	50	HIS	CE1-NE2	14.54	1.47	1.32
1	A	90	ALA	CA-CB	14.53	1.74	1.54
1	A	30	SER	C-O	14.28	1.41	1.24
1	A	176	SER	C-O	14.24	1.42	1.23
2	B	175	GLN	CA-C	14.08	1.68	1.52
2	B	85	LYS	C-O	14.06	1.41	1.24
1	A	154	ILE	C-O	13.99	1.38	1.24
2	B	235	VAL	C-N	-13.94	1.14	1.33
2	B	42	GLY	C-N	-13.86	1.14	1.33
2	B	50	TYR	C-N	13.83	1.52	1.33
2	B	232	THR	C-N	-13.83	1.15	1.33
4	T	34	TYR	C-N	-13.75	1.14	1.33
1	A	2	GLN	N-CA	13.16	1.71	1.46
1	A	173	VAL	C-O	13.04	1.37	1.24
4	T	34	TYR	CA-C	-12.95	1.36	1.52
2	B	34	MET	C-O	12.64	1.40	1.23
2	B	31	HIS	ND1-CE1	12.64	1.45	1.32
4	T	96	ARG	C-N	-12.62	1.17	1.34
2	B	232	THR	C-O	-12.58	1.08	1.24
2	B	208	PHE	C-N	-12.21	1.18	1.33
2	B	62	ILE	C-N	12.16	1.50	1.33
2	B	50	TYR	CA-C	12.14	1.67	1.52
2	B	97	SER	CA-CB	-12.06	1.37	1.53
1	A	153	TYR	CA-C	12.03	1.68	1.52
2	B	125	VAL	CA-C	-12.01	1.40	1.52
1	A	73	SER	CA-C	-11.89	1.37	1.52
1	A	62	THR	C-N	-11.88	1.18	1.33
2	B	82	SER	C-O	-11.87	1.09	1.24
2	B	121	PHE	C-N	-11.84	1.19	1.33
1	A	76	ILE	C-N	-11.75	1.17	1.33
2	B	207	HIS	N-CA	11.66	1.61	1.46
1	A	165	MET	SD-CE	11.38	2.08	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	34	VAL	CA-CB	-11.31	1.38	1.54
2	B	122	PRO	N-CD	-11.30	1.31	1.47
4	T	98	LEU	CA-C	-11.26	1.39	1.52
2	B	49	TYR	C-O	11.24	1.38	1.23
1	A	11	LEU	CA-C	11.09	1.66	1.52
4	T	106	TYR	C-N	-10.84	1.19	1.33
1	A	185	ASN	C-O	10.81	1.38	1.24
1	A	174	ALA	C-O	10.79	1.37	1.23
1	A	44	VAL	CA-C	-10.73	1.40	1.52
2	B	232	THR	CA-C	-10.66	1.37	1.52
1	A	110	PRO	CA-CB	-10.61	1.39	1.54
1	A	61	LEU	C-N	-10.59	1.19	1.33
1	A	133	CYS	C-O	10.58	1.36	1.24
1	A	75	HIS	CD2-NE2	-10.49	1.26	1.37
2	B	87	PRO	N-CA	-10.46	1.35	1.47
1	A	107	SER	N-CA	-10.45	1.34	1.46
1	A	32	LEU	C-N	-10.41	1.20	1.33
1	A	132	VAL	CA-C	10.40	1.65	1.52
4	T	4	LEU	C-O	10.40	1.36	1.24
1	A	152	VAL	C-N	10.39	1.48	1.33
1	A	168	LYS	N-CA	-10.34	1.33	1.45
1	A	185	ASN	C-N	10.33	1.49	1.33
1	A	190	SER	CA-CB	10.28	1.69	1.53
1	A	17	GLU	C-N	-10.23	1.18	1.33
1	A	124	ASP	CG-OD2	10.21	1.44	1.25
2	B	189	SER	CA-CB	-10.21	1.34	1.53
2	B	37	TYR	CA-C	-10.12	1.40	1.52
2	B	192	SER	CA-CB	-10.12	1.32	1.54
2	B	180	GLN	CA-CB	10.10	1.69	1.53
2	B	89	ALA	C-O	9.99	1.36	1.24
1	A	200	SER	C-OXT	9.97	1.43	1.23
2	B	35	TYR	C-O	9.96	1.35	1.23
1	A	116	ASP	CG-OD2	9.94	1.44	1.25
1	A	118	ALA	CA-C	9.92	1.64	1.52
4	T	113	VAL	C-N	-9.90	1.20	1.33
1	A	178	LYS	CA-C	9.86	1.66	1.52
2	B	37	TYR	C-O	-9.81	1.12	1.24
4	T	111	THR	CA-C	-9.74	1.40	1.52
4	T	98	LEU	C-N	-9.71	1.20	1.33
1	A	13	ILE	CA-C	-9.70	1.40	1.52
1	A	110	PRO	N-CD	-9.69	1.34	1.47
1	A	119	VAL	CA-CB	-9.69	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	69	ILE	CA-C	-9.68	1.42	1.52
4	T	33	PHE	N-CA	-9.63	1.33	1.46
4	T	60	ALA	CA-CB	9.59	1.69	1.53
1	A	17	GLU	C-O	-9.58	1.10	1.23
4	T	32	ASN	C-N	-9.54	1.20	1.33
1	A	123	ARG	C-N	9.42	1.46	1.33
2	B	146	LEU	CA-CB	9.41	1.67	1.53
4	T	48	VAL	C-O	9.41	1.35	1.24
3	C	39	GLN	C-N	9.35	1.41	1.33
1	A	56	LYS	C-N	-9.32	1.20	1.33
2	B	78	LEU	CA-C	-9.32	1.40	1.52
2	B	162	ASN	CA-CB	-9.31	1.37	1.53
2	B	201	TRP	CA-C	-9.30	1.40	1.52
2	B	71	GLU	C-O	9.26	1.34	1.23
4	T	1	ASP	N-CA	9.21	1.63	1.46
1	A	152	VAL	CA-C	9.19	1.64	1.52
2	B	95	SER	CA-CB	-9.15	1.40	1.53
1	A	174	ALA	N-CA	9.13	1.57	1.45
4	T	116	SER	C-O	-9.12	1.12	1.24
2	B	9	SER	C-O	9.12	1.35	1.24
3	C	68	THR	C-O	9.12	1.35	1.24
1	A	8	PRO	CA-CB	9.11	1.70	1.53
2	B	92	LEU	CA-C	-9.11	1.41	1.52
1	A	176	SER	C-N	9.10	1.45	1.33
3	C	91	ALA	N-CA	9.10	1.57	1.46
4	T	100	ARG	CG-CD	9.09	1.79	1.52
1	A	174	ALA	CA-C	9.09	1.63	1.52
1	A	159	VAL	N-CA	9.08	1.57	1.46
4	T	21	SER	C-N	9.07	1.45	1.33
2	B	13	LEU	CA-CB	-9.07	1.36	1.54
4	T	101	ILE	N-CA	9.06	1.57	1.46
3	C	103	ARG	CD-NE	8.92	1.58	1.46
1	A	192	ILE	N-CA	-8.91	1.35	1.46
1	A	152	VAL	N-CA	-8.88	1.35	1.46
2	B	53	ILE	CA-CB	-8.84	1.42	1.54
2	B	31	HIS	CE1-NE2	8.83	1.41	1.32
1	A	112	ILE	C-N	-8.83	1.21	1.33
4	T	70	SER	N-CA	8.81	1.57	1.45
1	A	87	TYR	C-N	-8.81	1.21	1.33
1	A	139	ASP	CA-C	-8.80	1.40	1.53
2	B	213	GLN	CA-CB	8.79	1.68	1.53
2	B	72	LYS	CA-C	8.77	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	103	PRO	N-CA	-8.76	1.32	1.47
1	A	140	SER	CA-CB	-8.75	1.38	1.53
1	A	147	SER	CB-OG	8.74	1.59	1.42
3	C	98	ASN	CA-CB	-8.72	1.40	1.53
2	B	62	ILE	C-O	8.71	1.34	1.23
1	A	109	LYS	C-N	-8.71	1.22	1.33
1	A	199	PRO	C-N	8.71	1.45	1.33
2	B	210	CYS	C-N	-8.70	1.20	1.33
3	C	102	GLY	C-O	8.66	1.31	1.23
1	A	32	LEU	CA-C	-8.66	1.41	1.52
4	T	104	TYR	CA-C	8.64	1.64	1.52
2	B	189	SER	CB-OG	8.63	1.59	1.42
2	B	58	GLN	C-N	8.63	1.44	1.33
4	T	100	ARG	C-N	8.62	1.45	1.33
1	A	21	VAL	C-N	-8.62	1.23	1.33
2	B	120	VAL	C-O	8.62	1.33	1.24
4	T	32	ASN	CA-C	-8.62	1.40	1.52
2	B	48	ILE	CA-CB	8.60	1.66	1.54
2	B	181	PRO	N-CD	-8.60	1.35	1.47
2	B	120	VAL	CA-C	-8.58	1.42	1.52
4	T	52	SER	CA-CB	-8.55	1.40	1.53
2	B	34	MET	N-CA	-8.54	1.35	1.45
4	T	22	CYS	CA-C	-8.52	1.42	1.52
4	T	108	GLY	CA-C	-8.46	1.44	1.52
3	C	64	LYS	CA-C	8.45	1.64	1.52
4	T	23	VAL	N-CA	8.45	1.56	1.46
2	B	20	ASN	C-N	8.43	1.44	1.33
2	B	125	VAL	CA-CB	-8.43	1.43	1.55
1	A	169	SER	CA-C	-8.34	1.42	1.52
2	B	213	GLN	CA-C	-8.31	1.42	1.52
4	T	50	HIS	CG-ND1	8.31	1.47	1.38
1	A	132	VAL	CA-CB	-8.30	1.43	1.54
2	B	51	SER	C-O	-8.30	1.14	1.24
2	B	134	GLU	CA-CB	-8.30	1.40	1.53
2	B	131	SER	CA-C	-8.24	1.42	1.52
2	B	46	ARG	CA-C	8.23	1.63	1.52
1	A	184	ALA	C-N	-8.22	1.22	1.33
1	A	179	SER	CA-CB	-8.22	1.39	1.53
1	A	197	PHE	C-O	8.21	1.34	1.24
2	B	176	PRO	CA-C	8.21	1.64	1.52
2	B	18	GLY	C-N	-8.20	1.23	1.33
2	B	198	ALA	C-O	8.18	1.34	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	58	HIS	CE1-NE2	-8.17	1.24	1.32
2	B	191	SER	C-O	8.16	1.34	1.23
2	B	208	PHE	C-O	8.16	1.34	1.23
2	B	195	ARG	C-N	-8.15	1.22	1.33
2	B	155	VAL	CA-C	-8.13	1.44	1.52
2	B	37	TYR	CB-CG	8.11	1.69	1.51
2	B	196	VAL	C-N	-8.11	1.23	1.33
2	B	212	VAL	N-CA	-8.08	1.36	1.46
4	T	19	ARG	NE-CZ	-8.08	1.24	1.33
1	A	71	ASP	C-N	-8.07	1.23	1.33
2	B	52	GLN	CA-CB	8.07	1.66	1.53
1	A	21	VAL	C-O	-8.05	1.14	1.23
1	A	47	VAL	CA-C	-8.05	1.42	1.52
2	B	148	THR	C-N	-8.05	1.21	1.33
1	A	153	TYR	N-CA	8.04	1.56	1.46
2	B	92	LEU	C-N	8.03	1.44	1.33
2	B	47	LEU	CA-C	8.02	1.62	1.52
4	T	47	LYS	C-O	8.01	1.33	1.23
4	T	78	VAL	C-O	8.00	1.33	1.24
1	A	119	VAL	C-N	-7.99	1.21	1.33
4	T	62	SER	CA-CB	7.98	1.67	1.53
1	A	171	SER	C-N	-7.97	1.23	1.33
2	B	46	ARG	NE-CZ	7.97	1.41	1.33
2	B	116	ASP	CA-C	-7.96	1.42	1.52
4	T	4	LEU	CA-C	-7.95	1.43	1.52
1	A	12	SER	CA-CB	7.95	1.66	1.53
2	B	87	PRO	CA-C	-7.90	1.45	1.52
2	B	174	PRO	N-CD	-7.90	1.36	1.47
1	A	35	TYR	N-CA	7.89	1.55	1.46
2	B	193	ARG	CD-NE	-7.89	1.35	1.46
4	T	30	LYS	C-O	7.89	1.34	1.24
1	A	83	ASP	C-O	7.87	1.34	1.24
1	A	159	VAL	CA-CB	-7.87	1.44	1.54
1	A	197	PHE	CA-CB	-7.86	1.43	1.53
1	A	74	LEU	CA-C	-7.86	1.44	1.53
1	A	131	SER	N-CA	7.85	1.55	1.46
1	A	167	PHE	C-N	-7.82	1.22	1.33
4	T	36	TRP	NE1-CE2	-7.82	1.28	1.37
4	T	53	ILE	CA-C	-7.81	1.42	1.52
1	A	120	TYR	N-CA	-7.81	1.36	1.45
3	C	83	ASN	C-N	-7.81	1.24	1.33
2	B	126	ALA	N-CA	7.80	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	7	SER	C-O	-7.78	1.15	1.24
1	A	89	CYS	CA-CB	7.77	1.66	1.53
2	B	151	TYR	CG-CD1	-7.76	1.23	1.39
4	T	7	SER	CA-C	-7.75	1.43	1.52
1	A	34	TRP	N-CA	-7.73	1.36	1.46
1	A	89	CYS	C-O	7.71	1.33	1.23
2	B	155	VAL	N-CA	-7.71	1.36	1.46
2	B	224	THR	N-CA	-7.71	1.35	1.46
1	A	110	PRO	N-CA	-7.69	1.39	1.46
2	B	36	TRP	CD2-CE2	-7.66	1.28	1.41
2	B	176	PRO	C-N	7.66	1.44	1.33
4	T	53	ILE	C-O	7.63	1.32	1.24
2	B	91	TYR	C-N	7.62	1.45	1.33
2	B	215	TYR	N-CA	-7.62	1.36	1.46
1	A	119	VAL	CA-C	7.60	1.62	1.52
4	T	78	VAL	CA-C	-7.59	1.43	1.52
2	B	160	TRP	C-O	7.59	1.33	1.23
2	B	186	SER	CA-C	-7.59	1.43	1.52
3	C	39	GLN	C-O	7.58	1.32	1.24
4	T	106	TYR	C-O	-7.58	1.14	1.23
4	T	107	TRP	N-CA	-7.58	1.37	1.46
1	A	105	LYS	C-N	-7.54	1.23	1.33
2	B	84	GLN	CD-NE2	-7.48	1.17	1.33
2	B	173	ASP	CA-C	-7.47	1.45	1.53
1	A	175	TRP	CB-CG	7.47	1.73	1.50
4	T	98	LEU	C-O	-7.43	1.15	1.24
4	T	36	TRP	CA-CB	7.38	1.66	1.53
3	C	90	THR	N-CA	7.36	1.55	1.46
1	A	100	PHE	N-CA	-7.36	1.36	1.46
2	B	39	GLN	CA-C	-7.36	1.43	1.52
4	T	103	PRO	C-O	7.33	1.38	1.23
2	B	169	GLY	C-O	7.32	1.33	1.24
2	B	186	SER	C-N	-7.32	1.22	1.33
2	B	93	CYS	C-N	7.31	1.44	1.33
1	A	6	GLN	CA-C	-7.30	1.43	1.52
1	A	107	SER	CA-CB	-7.29	1.40	1.53
4	T	99	SER	C-N	-7.29	1.24	1.33
1	A	64	GLN	CA-C	-7.28	1.43	1.52
2	B	198	ALA	CA-C	-7.28	1.42	1.52
4	T	5	VAL	N-CA	7.26	1.55	1.46
3	C	2	VAL	C-N	7.25	1.43	1.33
4	T	51	ILE	C-N	-7.25	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	61	ASP	C-O	7.24	1.32	1.24
4	T	60	ALA	C-N	7.22	1.43	1.33
1	A	198	PHE	CA-CB	-7.19	1.42	1.53
2	B	94	ALA	C-O	-7.18	1.15	1.23
2	B	107	PRO	N-CA	-7.17	1.38	1.47
4	T	53	ILE	CB-CG2	7.15	1.76	1.52
4	T	71	ARG	N-CA	7.15	1.55	1.45
1	A	121	GLN	CA-CB	7.15	1.64	1.53
2	B	195	ARG	CA-C	-7.15	1.43	1.52
3	C	2	VAL	N-CA	7.14	1.59	1.46
1	A	73	SER	C-N	-7.14	1.23	1.33
3	C	68	THR	CA-C	-7.13	1.43	1.52
4	T	115	VAL	CA-CB	7.13	1.62	1.53
2	B	238	GLU	N-CA	-7.12	1.37	1.46
1	A	7	SER	CA-C	-7.11	1.45	1.52
1	A	90	ALA	N-CA	7.10	1.57	1.46
2	B	49	TYR	CA-C	7.08	1.61	1.52
4	T	48	VAL	C-N	-7.05	1.24	1.33
2	B	154	HIS	C-N	-7.05	1.24	1.33
2	B	199	THR	N-CA	7.04	1.55	1.46
1	A	43	PRO	CA-C	7.03	1.62	1.52
1	A	143	ASN	CA-CB	-7.03	1.43	1.53
1	A	198	PHE	C-O	7.01	1.33	1.23
3	C	40	VAL	CA-C	-7.01	1.47	1.53
4	T	115	VAL	CA-C	-7.00	1.44	1.52
3	C	98	ASN	N-CA	7.00	1.54	1.46
1	A	173	VAL	CA-CB	-7.00	1.45	1.54
2	B	123	PRO	N-CD	-6.99	1.38	1.47
1	A	31	SER	CA-C	-6.98	1.44	1.52
1	A	113	GLN	N-CA	-6.98	1.37	1.45
4	T	100	ARG	NE-CZ	-6.98	1.25	1.33
4	T	58	ASP	CA-C	-6.98	1.43	1.53
1	A	18	ASN	C-N	6.97	1.42	1.33
2	B	34	MET	CG-SD	-6.97	1.63	1.80
2	B	137	HIS	CG-ND1	-6.94	1.30	1.38
1	A	46	LEU	C-N	-6.93	1.24	1.33
1	A	36	ARG	CA-C	-6.92	1.44	1.52
2	B	38	ARG	N-CA	6.92	1.55	1.46
4	T	102	TRP	C-O	6.88	1.31	1.23
2	B	240	TRP	CA-CB	6.86	1.64	1.53
1	A	54	GLU	C-N	-6.85	1.24	1.33
1	A	162	MET	C-O	6.84	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	ASP	C-O	-6.84	1.14	1.23
2	B	14	PHE	C-N	-6.84	1.24	1.33
1	A	7	SER	C-O	6.83	1.30	1.24
1	A	170	ASN	CA-CB	-6.83	1.42	1.53
3	C	60	ARG	C-O	6.83	1.32	1.24
1	A	63	PHE	C-N	-6.82	1.24	1.33
2	B	215	TYR	CA-C	-6.81	1.44	1.52
1	A	37	GLN	C-O	6.80	1.32	1.23
2	B	223	TRP	NE1-CE2	-6.80	1.29	1.37
2	B	238	GLU	CA-C	-6.80	1.43	1.52
1	A	17	GLU	CA-C	-6.79	1.44	1.53
2	B	137	HIS	CD2-NE2	-6.79	1.30	1.37
3	C	19	ARG	N-CA	-6.79	1.38	1.46
2	B	105	PHE	CA-C	-6.78	1.43	1.53
1	A	34	TRP	CA-C	-6.76	1.44	1.52
1	A	179	SER	CB-OG	6.75	1.55	1.42
2	B	174	PRO	N-CA	-6.74	1.38	1.47
1	A	66	GLY	C-O	-6.74	1.14	1.23
3	C	36	TRP	C-N	-6.74	1.24	1.33
1	A	49	VAL	C-O	6.73	1.32	1.24
1	A	174	ALA	CA-CB	6.72	1.66	1.54
4	T	18	LEU	CA-C	-6.72	1.44	1.52
4	T	113	VAL	N-CA	6.72	1.54	1.46
2	B	156	GLU	CA-C	-6.71	1.45	1.52
4	T	2	VAL	CA-C	6.71	1.60	1.52
1	A	19	LEU	CA-C	-6.70	1.44	1.52
4	T	114	THR	N-CA	-6.70	1.38	1.46
4	T	10	GLY	C-O	6.69	1.32	1.23
4	T	65	GLY	CA-C	6.68	1.61	1.51
4	T	80	LEU	CA-C	-6.67	1.44	1.52
4	T	52	SER	N-CA	-6.67	1.38	1.45
1	A	191	ILE	CA-CB	-6.67	1.44	1.53
2	B	13	LEU	CB-CG	-6.66	1.40	1.53
3	C	81	GLN	CA-C	-6.66	1.44	1.52
1	A	133	CYS	N-CA	-6.64	1.38	1.46
3	C	79	TYR	N-CA	6.64	1.54	1.45
2	B	36	TRP	CG-CD2	-6.64	1.31	1.43
2	B	151	TYR	CA-C	-6.62	1.44	1.52
1	A	2	GLN	C-N	6.61	1.42	1.33
2	B	192	SER	CA-C	-6.61	1.44	1.52
4	T	102	TRP	CA-CB	6.60	1.64	1.53
1	A	183	CYS	C-O	6.59	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	50	HIS	CA-CB	6.59	1.65	1.53
1	A	116	ASP	CG-OD1	6.58	1.37	1.25
4	T	37	TYR	CG-CD1	-6.57	1.25	1.39
2	B	62	ILE	N-CA	6.56	1.54	1.45
4	T	48	VAL	CA-C	-6.55	1.44	1.52
1	A	159	VAL	C-N	-6.54	1.24	1.33
3	C	98	ASN	CG-OD1	-6.51	1.11	1.23
1	A	183	CYS	CA-C	6.50	1.61	1.52
1	A	156	ASP	N-CA	6.50	1.53	1.45
2	B	36	TRP	C-N	6.50	1.43	1.33
1	A	175	TRP	CG-CD1	6.49	1.53	1.36
1	A	30	SER	CA-CB	-6.49	1.43	1.53
2	B	89	ALA	N-CA	6.48	1.53	1.46
1	A	191	ILE	C-O	6.47	1.34	1.23
2	B	236	SER	N-CA	-6.47	1.36	1.46
1	A	74	LEU	C-N	-6.46	1.24	1.33
1	A	74	LEU	C-O	6.46	1.31	1.23
3	C	97	PHE	CA-CB	-6.45	1.41	1.53
2	B	125	VAL	C-N	-6.44	1.25	1.33
1	A	11	LEU	C-N	-6.44	1.24	1.33
1	A	28	VAL	C-N	-6.44	1.24	1.33
1	A	34	TRP	C-O	-6.44	1.16	1.23
4	T	101	ILE	CA-CB	-6.43	1.45	1.54
1	A	192	ILE	CA-CB	-6.43	1.45	1.54
2	B	12	TYR	C-N	-6.42	1.25	1.33
1	A	90	ALA	C-N	-6.42	1.24	1.33
4	T	68	THR	C-O	6.40	1.31	1.24
3	C	11	LEU	CA-C	-6.39	1.45	1.52
1	A	185	ASN	CA-C	6.36	1.63	1.52
3	C	60	ARG	N-CA	-6.35	1.38	1.46
2	B	201	TRP	CD2-CE3	-6.34	1.30	1.40
2	B	198	ALA	C-N	6.33	1.42	1.33
1	A	58	LEU	CA-C	-6.33	1.46	1.53
3	C	64	LYS	N-CA	6.33	1.53	1.45
4	T	92	ALA	CA-C	-6.32	1.44	1.52
2	B	113	VAL	N-CA	-6.32	1.38	1.46
2	B	63	ALA	CA-CB	6.31	1.64	1.53
4	T	25	SER	C-N	-6.28	1.22	1.33
2	B	31	HIS	N-CA	-6.26	1.38	1.45
1	A	35	TYR	C-N	-6.26	1.24	1.33
4	T	89	ASP	CG-OD2	6.26	1.37	1.25
2	B	93	CYS	CA-C	-6.25	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	90	THR	N-CA	6.25	1.53	1.46
2	B	228	ALA	N-CA	6.25	1.54	1.46
4	T	109	GLN	C-N	6.25	1.41	1.33
3	C	102	GLY	C-N	6.24	1.42	1.33
2	B	79	THR	CA-CB	-6.23	1.38	1.54
1	A	75	HIS	ND1-CE1	-6.22	1.26	1.32
1	A	76	ILE	CA-C	-6.22	1.45	1.52
2	B	233	GLN	C-N	-6.22	1.23	1.33
4	T	74	SER	CA-C	-6.20	1.44	1.52
1	A	99	ILE	C-N	-6.19	1.24	1.33
1	A	120	TYR	C-O	-6.18	1.15	1.23
2	B	213	GLN	N-CA	6.18	1.53	1.46
1	A	194	GLU	CA-C	-6.16	1.44	1.52
1	A	153	TYR	C-N	6.15	1.42	1.33
4	T	105	ASP	N-CA	-6.14	1.38	1.45
3	C	97	PHE	N-CA	-6.14	1.38	1.46
1	A	175	TRP	C-N	-6.13	1.25	1.33
2	B	70	ARG	CD-NE	6.13	1.54	1.46
2	B	77	PRO	CA-CB	6.13	1.62	1.53
4	T	81	GLN	N-CA	6.12	1.55	1.46
1	A	57	LYS	N-CA	-6.12	1.38	1.46
1	A	132	VAL	C-N	6.12	1.42	1.33
2	B	189	SER	N-CA	-6.12	1.38	1.45
2	B	153	ASP	CG-OD1	6.11	1.36	1.25
3	C	71	ARG	CA-C	-6.10	1.44	1.52
4	T	28	VAL	CB-CG1	-6.10	1.32	1.52
1	A	130	LYS	C-O	6.09	1.31	1.23
2	B	89	ALA	C-N	6.08	1.42	1.33
1	A	88	LEU	N-CA	-6.08	1.38	1.45
2	B	123	PRO	CA-CB	-6.08	1.46	1.53
2	B	145	CYS	CA-C	-6.07	1.45	1.52
1	A	31	SER	C-O	6.06	1.31	1.23
2	B	48	ILE	C-N	6.06	1.42	1.33
3	C	44	GLN	CD-NE2	6.06	1.46	1.33
4	T	103	PRO	N-CD	-6.05	1.39	1.47
1	A	155	THR	C-O	6.05	1.32	1.23
2	B	36	TRP	NE1-CE2	-6.00	1.30	1.37
4	T	33	PHE	C-N	5.98	1.41	1.33
4	T	2	VAL	CA-CB	-5.98	1.46	1.54
2	B	31	HIS	C-O	-5.97	1.16	1.23
4	T	39	GLN	C-O	5.96	1.31	1.24
4	T	3	GLN	C-N	-5.96	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	187	ARG	C-N	5.95	1.42	1.33
2	B	15	ARG	CD-NE	-5.94	1.38	1.46
2	B	76	PHE	C-O	-5.94	1.19	1.24
2	B	112	THR	C-O	-5.94	1.17	1.24
2	B	21	VAL	CA-C	5.93	1.60	1.52
1	A	143	ASN	N-CA	-5.92	1.38	1.46
4	T	2	VAL	C-N	-5.92	1.25	1.33
2	B	89	ALA	CA-CB	-5.92	1.49	1.54
2	B	230	PRO	N-CD	-5.91	1.39	1.47
3	C	27	SER	C-O	-5.91	1.16	1.24
4	T	7	SER	C-N	5.90	1.39	1.32
1	A	199	PRO	N-CA	-5.90	1.39	1.47
4	T	104	TYR	N-CA	-5.89	1.39	1.46
4	T	67	PHE	C-N	-5.88	1.25	1.33
3	C	104	TYR	CA-CB	-5.88	1.44	1.53
1	A	99	ILE	CA-CB	-5.87	1.46	1.53
1	A	19	LEU	C-N	-5.87	1.26	1.33
2	B	26	GLU	CA-C	5.86	1.59	1.52
3	C	112	THR	C-O	-5.86	1.17	1.23
2	B	37	TYR	C-N	5.85	1.42	1.33
2	B	76	PHE	N-CA	-5.85	1.40	1.46
1	A	145	SER	C-O	5.83	1.30	1.23
4	T	51	ILE	C-O	5.83	1.30	1.23
1	A	150	SER	CA-C	5.82	1.60	1.53
2	B	229	LYS	N-CA	5.81	1.54	1.46
2	B	173	ASP	CA-CB	5.81	1.61	1.53
2	B	81	THR	C-O	5.81	1.32	1.23
2	B	181	PRO	C-O	5.81	1.31	1.24
4	T	76	ASN	C-O	-5.81	1.16	1.24
4	T	4	LEU	N-CA	-5.80	1.39	1.46
1	A	184	ALA	C-O	5.80	1.30	1.24
3	C	39	GLN	CA-CB	5.79	1.62	1.53
2	B	91	TYR	CE1-CZ	-5.79	1.24	1.38
4	T	114	THR	CA-C	5.79	1.59	1.52
1	A	189	ASN	C-N	-5.77	1.25	1.33
2	B	84	GLN	CA-C	5.76	1.59	1.52
1	A	97	ASN	C-N	5.76	1.41	1.33
4	T	50	HIS	CA-C	-5.75	1.45	1.52
3	C	36	TRP	C-O	-5.75	1.16	1.23
2	B	95	SER	C-N	-5.74	1.26	1.33
1	A	114	ASN	C-N	5.74	1.40	1.33
2	B	117	LEU	N-CA	5.73	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	ASN	C-N	5.73	1.38	1.33
4	T	20	LEU	C-N	5.73	1.41	1.33
1	A	75	HIS	C-N	-5.72	1.25	1.33
1	A	86	LEU	C-O	5.72	1.30	1.24
2	B	216	GLY	C-N	5.71	1.41	1.33
2	B	190	LEU	CB-CG	-5.70	1.42	1.53
4	T	87	PRO	CA-CB	-5.69	1.45	1.53
1	A	72	SER	CB-OG	5.68	1.53	1.42
1	A	130	LYS	CG-CD	5.68	1.69	1.52
2	B	214	PHE	C-N	5.66	1.41	1.33
4	T	38	ARG	C-N	-5.65	1.26	1.33
4	T	70	SER	C-O	5.64	1.31	1.23
1	A	130	LYS	CA-C	-5.64	1.45	1.52
3	C	58	HIS	CG-CD2	-5.63	1.29	1.35
1	A	92	ALA	C-O	-5.62	1.17	1.23
2	B	201	TRP	NE1-CE2	5.62	1.43	1.37
4	T	57	THR	CA-CB	5.62	1.62	1.53
4	T	50	HIS	C-N	-5.62	1.27	1.33
1	A	135	PHE	N-CA	5.61	1.53	1.46
1	A	132	VAL	CB-CG2	5.61	1.71	1.52
2	B	37	TYR	CA-CB	-5.61	1.44	1.53
4	T	56	GLN	CA-C	-5.60	1.45	1.52
4	T	53	ILE	CA-CB	5.60	1.60	1.54
1	A	144	VAL	C-N	5.59	1.41	1.33
2	B	209	ARG	C-O	5.59	1.30	1.23
1	A	135	PHE	CA-CB	-5.58	1.45	1.53
2	B	91	TYR	CG-CD2	-5.57	1.27	1.39
3	C	8	GLY	C-O	5.57	1.31	1.23
2	B	177	LEU	C-O	-5.56	1.17	1.24
1	A	43	PRO	N-CD	-5.56	1.40	1.47
3	C	111	VAL	C-N	5.56	1.41	1.33
3	C	66	ARG	C-N	-5.55	1.24	1.33
3	C	53	THR	N-CA	5.55	1.53	1.46
4	T	61	ASP	C-N	5.54	1.41	1.33
1	A	10	PHE	CA-CB	-5.52	1.44	1.53
2	B	181	PRO	N-CA	-5.52	1.40	1.47
4	T	71	ARG	CZ-NH2	5.52	1.40	1.33
1	A	109	LYS	CB-CG	5.52	1.69	1.52
2	B	40	ASP	C-O	5.51	1.31	1.23
2	B	235	VAL	CA-C	-5.51	1.45	1.52
1	A	88	LEU	C-N	-5.51	1.25	1.33
4	T	59	TYR	C-O	5.50	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	LEU	CA-CB	5.49	1.60	1.53
1	A	55	VAL	C-N	-5.49	1.25	1.33
1	A	89	CYS	CA-C	-5.49	1.45	1.53
1	A	131	SER	C-N	5.48	1.41	1.33
2	B	26	GLU	C-O	5.48	1.30	1.23
2	B	77	PRO	C-O	5.47	1.31	1.24
3	C	94	TYR	CD2-CE2	5.46	1.55	1.38
4	T	93	TYR	CA-C	-5.46	1.46	1.52
2	B	43	GLN	N-CA	-5.46	1.39	1.46
4	T	60	ALA	CA-C	-5.46	1.45	1.52
1	A	129	ASP	N-CA	5.44	1.52	1.46
2	B	94	ALA	CA-C	-5.44	1.45	1.52
2	B	152	PRO	N-CD	-5.44	1.40	1.47
1	A	87	TYR	CG-CD1	-5.44	1.27	1.39
1	A	144	VAL	CA-CB	-5.43	1.46	1.53
1	A	69	ARG	CD-NE	5.43	1.53	1.46
2	B	96	SER	CA-CB	5.43	1.63	1.53
2	B	105	PHE	C-N	5.43	1.41	1.33
3	C	10	GLY	C-O	-5.43	1.18	1.24
3	C	84	SER	N-CA	-5.43	1.39	1.46
3	C	56	GLY	C-O	-5.42	1.16	1.23
2	B	242	ARG	C-O	5.42	1.30	1.23
2	B	16	LYS	C-O	5.42	1.31	1.23
3	C	103	ARG	C-N	5.41	1.41	1.33
4	T	11	VAL	N-CA	5.40	1.52	1.46
2	B	162	ASN	C-O	-5.40	1.17	1.24
1	A	4	LEU	C-O	5.39	1.30	1.23
2	B	157	LEU	C-N	-5.39	1.25	1.33
2	B	82	SER	C-N	5.39	1.40	1.33
1	A	199	PRO	CA-CB	-5.39	1.46	1.53
2	B	154	HIS	ND1-CE1	5.38	1.38	1.32
1	A	50	VAL	C-N	5.38	1.41	1.33
3	C	103	ARG	CZ-NH2	5.37	1.40	1.33
4	T	6	GLU	C-N	5.37	1.40	1.33
4	T	99	SER	CB-OG	5.36	1.52	1.42
2	B	90	PHE	C-N	5.36	1.40	1.33
4	T	28	VAL	N-CA	-5.36	1.39	1.46
2	B	124	GLU	C-N	-5.35	1.26	1.33
2	B	85	LYS	CG-CD	5.33	1.68	1.52
3	C	85	LEU	C-N	-5.33	1.25	1.33
1	A	195	ASP	CG-OD1	-5.33	1.15	1.25
3	C	60	ARG	CA-C	-5.33	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	84	SER	C-N	-5.32	1.26	1.33
1	A	191	ILE	C-N	5.32	1.39	1.33
2	B	170	VAL	CA-CB	-5.32	1.47	1.54
2	B	160	TRP	N-CA	5.31	1.54	1.47
4	T	87	PRO	C-N	5.31	1.41	1.33
2	B	22	THR	C-N	5.30	1.40	1.33
1	A	39	PRO	C-N	5.30	1.41	1.33
1	A	56	LYS	CA-C	-5.29	1.46	1.52
2	B	108	GLY	C-N	5.29	1.40	1.33
2	B	130	PRO	C-O	5.29	1.30	1.23
3	C	90	THR	C-O	5.29	1.30	1.23
1	A	196	THR	C-N	5.29	1.41	1.33
2	B	111	LEU	N-CA	5.29	1.52	1.46
1	A	48	THR	CA-C	-5.29	1.46	1.52
1	A	168	LYS	CG-CD	5.29	1.68	1.52
2	B	188	TYR	CG-CD2	-5.28	1.28	1.39
4	T	37	TYR	CE1-CZ	-5.28	1.25	1.38
1	A	200	SER	N-CA	5.28	1.56	1.46
2	B	236	SER	CA-CB	5.28	1.62	1.53
3	C	62	PHE	C-N	5.28	1.39	1.33
1	A	64	GLN	N-CA	-5.27	1.39	1.46
1	A	151	ASP	N-CA	-5.27	1.39	1.46
2	B	6	ILE	CA-CB	5.27	1.61	1.54
1	A	161	ASP	C-N	-5.25	1.26	1.33
2	B	107	PRO	C-N	5.25	1.41	1.33
2	B	130	PRO	N-CD	-5.25	1.40	1.47
4	T	66	ARG	CA-C	5.25	1.59	1.52
3	C	37	TYR	N-CA	-5.25	1.38	1.46
4	T	61	ASP	N-CA	5.25	1.52	1.46
1	A	172	ALA	C-O	5.23	1.30	1.23
1	A	61	LEU	CA-CB	5.23	1.61	1.53
2	B	206	ASN	N-CA	-5.23	1.39	1.46
4	T	62	SER	CB-OG	5.22	1.52	1.42
1	A	16	GLY	C-N	-5.22	1.26	1.33
2	B	188	TYR	CG-CD1	-5.22	1.28	1.39
1	A	69	ARG	NE-CZ	5.21	1.38	1.33
2	B	150	PHE	CA-C	-5.21	1.46	1.52
4	T	37	TYR	CG-CD2	-5.21	1.28	1.39
2	B	136	SER	CA-CB	-5.21	1.45	1.53
1	A	89	CYS	N-CA	5.20	1.52	1.45
4	T	53	ILE	N-CA	5.20	1.52	1.46
3	C	96	TYR	C-O	-5.20	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	71	ARG	CZ-NH1	5.18	1.40	1.32
2	B	105	PHE	CG-CD1	-5.18	1.27	1.38
4	T	102	TRP	C-N	-5.17	1.24	1.34
2	B	73	LYS	CA-C	5.17	1.59	1.52
4	T	80	LEU	N-CA	5.17	1.52	1.46
2	B	93	CYS	N-CA	5.17	1.51	1.45
2	B	237	ALA	N-CA	-5.17	1.39	1.46
4	T	63	ALA	C-O	5.16	1.30	1.23
1	A	8	PRO	N-CA	-5.16	1.38	1.47
2	B	117	LEU	C-O	-5.16	1.17	1.24
1	A	57	LYS	C-N	-5.15	1.25	1.34
2	B	77	PRO	C-N	5.14	1.40	1.33
3	C	113	VAL	CA-C	-5.13	1.46	1.52
1	A	108	VAL	C-N	-5.12	1.23	1.33
4	T	3	GLN	N-CA	-5.11	1.39	1.46
1	A	190	SER	CB-OG	5.11	1.52	1.42
4	T	104	TYR	CG-CD1	-5.11	1.28	1.39
2	B	36	TRP	C-O	5.10	1.30	1.23
4	T	97	ALA	C-O	5.10	1.29	1.23
2	B	189	SER	CA-C	5.10	1.58	1.52
2	B	195	ARG	NE-CZ	-5.10	1.27	1.33
4	T	90	THR	C-O	5.10	1.30	1.24
3	C	96	TYR	CG-CD2	5.09	1.50	1.39
1	A	129	ASP	C-N	5.09	1.41	1.33
2	B	50	TYR	CB-CG	5.09	1.62	1.51
2	B	96	SER	C-O	5.08	1.30	1.23
3	C	57	THR	N-CA	-5.07	1.39	1.45
1	A	13	ILE	C-N	-5.07	1.25	1.33
2	B	38	ARG	C-O	5.06	1.30	1.23
2	B	46	ARG	CD-NE	5.06	1.53	1.46
2	B	168	SER	C-N	5.05	1.39	1.33
2	B	214	PHE	N-CA	-5.05	1.39	1.46
3	C	23	ALA	C-O	5.04	1.30	1.23
2	B	197	SER	CA-CB	5.04	1.60	1.53
1	A	7	SER	N-CA	-5.04	1.41	1.45
2	B	173	ASP	CG-OD2	5.03	1.34	1.25
2	B	186	SER	CA-CB	-5.03	1.45	1.53
4	T	105	ASP	CG-OD2	5.02	1.34	1.25
3	C	106	ALA	C-N	5.02	1.41	1.33
2	B	205	ARG	CA-C	-5.01	1.45	1.52
3	C	7	SER	CA-CB	-5.01	1.45	1.53
2	B	106	GLY	CA-C	5.00	1.59	1.51

All (1797) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	8	GLY	CA-C-O	-23.40	105.61	122.45
2	B	92	LEU	O-C-N	21.75	149.81	123.27
2	B	37	TYR	CA-C-O	-21.45	97.87	120.40
2	B	92	LEU	CA-C-O	-21.44	96.01	120.66
4	T	97	ALA	CB-CA-C	-21.37	84.94	111.43
3	C	97	PHE	CB-CA-C	21.28	148.22	109.70
2	B	19	GLN	OE1-CD-NE2	20.86	143.46	122.60
1	A	168	LYS	N-CA-CB	-20.54	79.22	110.85
1	A	185	ASN	N-CA-C	-20.15	90.36	112.93
2	B	195	ARG	CB-CA-C	-19.97	78.24	110.79
2	B	35	TYR	CA-C-O	-19.64	96.38	120.54
2	B	84	GLN	OE1-CD-NE2	-19.57	103.03	122.60
4	T	96	ARG	CA-C-O	-19.29	99.67	120.89
2	B	77	PRO	CB-CA-C	-19.23	79.82	111.56
1	A	174	ALA	CA-C-O	19.14	143.03	121.40
4	T	18	LEU	CA-C-N	-19.10	94.74	122.44
4	T	18	LEU	C-N-CA	-19.10	94.74	122.44
2	B	77	PRO	N-CA-CB	-19.05	83.24	103.25
2	B	213	GLN	N-CA-CB	19.02	137.99	110.04
3	C	62	PHE	N-CA-C	-18.78	88.66	112.88
1	A	138	PHE	N-CA-CB	-18.71	78.88	110.49
1	A	152	VAL	CA-C-N	-18.64	85.95	121.54
1	A	152	VAL	C-N-CA	-18.64	85.95	121.54
1	A	183	CYS	N-CA-C	18.56	130.93	111.07
2	B	96	SER	CA-C-O	-18.51	101.34	121.33
1	A	130	LYS	CA-C-N	-18.35	95.41	122.94
1	A	130	LYS	C-N-CA	-18.35	95.41	122.94
4	T	33	PHE	CA-CB-CG	18.30	132.10	113.80
2	B	47	LEU	CA-C-O	18.28	141.19	120.54
2	B	148	THR	CA-C-N	-18.11	98.63	123.08
2	B	148	THR	C-N-CA	-18.11	98.63	123.08
2	B	105	PHE	CA-C-O	-18.04	100.03	121.32
4	T	7	SER	CA-C-O	-17.98	100.91	120.33
2	B	72	LYS	O-C-N	-17.97	98.69	122.59
4	T	61	ASP	CA-C-O	-17.76	95.12	120.51
1	A	71	ASP	CA-CB-CG	17.64	130.24	112.60
1	A	123	ARG	O-C-N	17.46	140.75	123.46
1	A	175	TRP	NE1-CE2-CD2	17.44	130.07	107.40
4	T	71	ARG	CB-CA-C	-17.36	73.11	110.45
2	B	175	GLN	N-CA-CB	-17.25	78.12	109.68
1	A	174	ALA	N-CA-C	-17.21	83.26	109.24
2	B	207	HIS	N-CA-CB	17.19	139.01	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	21	SER	CA-C-N	-17.06	99.46	123.00
4	T	21	SER	C-N-CA	-17.06	99.46	123.00
4	T	49	ALA	N-CA-CB	-17.03	84.40	110.97
1	A	139	ASP	CB-CA-C	-16.92	80.22	109.83
2	B	62	ILE	CA-C-O	-16.82	105.58	121.72
1	A	154	ILE	CA-C-N	16.50	150.01	121.29
1	A	154	ILE	C-N-CA	16.50	150.01	121.29
2	B	160	TRP	CA-C-N	-16.45	99.48	122.34
2	B	160	TRP	C-N-CA	-16.45	99.48	122.34
1	A	118	ALA	O-C-N	-16.41	103.26	123.44
2	B	189	SER	N-CA-CB	-16.34	84.73	111.20
4	T	22	CYS	CA-C-O	-16.33	102.58	120.38
2	B	27	GLN	CB-CA-C	-16.31	80.17	109.70
2	B	88	THR	N-CA-CB	-16.28	81.25	111.52
3	C	44	GLN	CA-C-N	-16.17	94.02	122.64
3	C	44	GLN	C-N-CA	-16.17	94.02	122.64
1	A	13	ILE	CB-CA-C	-16.17	84.78	111.29
2	B	41	PRO	N-CA-CB	16.13	120.19	103.25
2	B	207	HIS	CA-CB-CG	-16.12	97.68	113.80
1	A	158	CYS	CA-C-N	-16.10	96.73	122.50
1	A	158	CYS	C-N-CA	-16.10	96.73	122.50
1	A	192	ILE	N-CA-CB	-16.10	88.67	111.21
2	B	48	ILE	CA-C-N	-16.05	97.39	122.59
2	B	48	ILE	C-N-CA	-16.05	97.39	122.59
2	B	122	PRO	CB-CA-C	-16.04	91.35	110.92
2	B	147	ALA	CB-CA-C	-16.00	85.17	110.78
1	A	137	ASP	CA-C-N	-15.97	91.04	121.54
1	A	137	ASP	C-N-CA	-15.97	91.04	121.54
4	T	71	ARG	NE-CZ-NH1	-15.91	105.59	121.50
3	C	94	TYR	CA-C-N	-15.90	94.56	123.03
3	C	94	TYR	C-N-CA	-15.90	94.56	123.03
4	T	66	ARG	CB-CA-C	-15.84	78.89	110.42
2	B	49	TYR	N-CA-CB	-15.84	83.99	111.55
4	T	48	VAL	CA-C-N	-15.82	94.48	122.32
4	T	48	VAL	C-N-CA	-15.82	94.48	122.32
1	A	175	TRP	CB-CG-CD1	15.79	150.58	126.90
4	T	70	SER	CA-C-N	-15.73	94.54	121.75
4	T	70	SER	C-N-CA	-15.73	94.54	121.75
3	C	34	VAL	CA-CB-CG2	-15.69	83.74	110.40
2	B	35	TYR	O-C-N	15.67	141.74	123.41
2	B	229	LYS	CB-CA-C	-15.63	86.83	108.87
1	A	138	PHE	CA-CB-CG	15.62	129.43	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	VAL	CA-C-O	-15.50	109.15	122.63
2	B	104	TYR	CA-C-N	-15.46	97.03	122.39
2	B	104	TYR	C-N-CA	-15.46	97.03	122.39
2	B	210	CYS	CB-CA-C	-15.45	89.29	111.23
4	T	78	VAL	O-C-N	15.44	138.89	123.14
2	B	91	TYR	CA-C-O	-15.39	104.36	120.98
1	A	175	TRP	CE2-CD2-CE3	15.33	134.13	118.80
4	T	34	TYR	N-CA-C	-15.25	85.05	108.99
4	T	78	VAL	CA-C-O	-15.17	103.43	120.72
4	T	60	ALA	N-CA-CB	15.10	136.01	110.49
1	A	178	LYS	O-C-N	-15.09	102.52	122.59
3	C	34	VAL	N-CA-CB	-15.07	92.75	112.34
1	A	175	TRP	CG-CD2-CE3	-15.06	118.84	133.90
2	B	50	TYR	CD1-CG-CD2	-15.05	95.52	118.10
1	A	175	TRP	CD1-NE1-CE2	-15.01	81.88	108.90
2	B	124	GLU	CA-C-N	-14.99	102.63	123.17
2	B	124	GLU	C-N-CA	-14.99	102.63	123.17
2	B	209	ARG	CB-CA-C	-14.86	85.46	110.43
3	C	64	LYS	CA-C-O	14.85	137.75	121.56
2	B	82	SER	CA-C-N	14.83	145.32	122.93
2	B	82	SER	C-N-CA	14.83	145.32	122.93
2	B	17	GLU	N-CA-C	-14.69	88.79	110.52
1	A	155	THR	CA-CB-OG1	-14.68	87.57	109.60
4	T	4	LEU	N-CA-CB	-14.53	88.23	110.90
1	A	151	ASP	O-C-N	14.51	141.89	122.59
1	A	36	ARG	N-CA-C	-14.48	86.56	109.72
2	B	214	PHE	CA-C-O	-14.48	104.25	120.32
1	A	105	LYS	CB-CA-C	-14.39	87.66	111.41
1	A	188	ASN	CA-C-N	-14.35	97.44	122.26
1	A	188	ASN	C-N-CA	-14.35	97.44	122.26
4	T	57	THR	N-CA-CB	14.34	134.72	110.49
1	A	197	PHE	CB-CA-C	-14.24	87.31	110.81
4	T	18	LEU	O-C-N	14.21	139.39	123.33
3	C	63	VAL	CA-C-O	-14.10	104.75	120.26
2	B	158	SER	CA-C-N	-14.00	100.83	122.81
2	B	158	SER	C-N-CA	-14.00	100.83	122.81
2	B	78	LEU	CA-C-O	-13.95	104.31	120.49
3	C	102	GLY	CA-C-O	-13.90	112.22	122.37
2	B	198	ALA	N-CA-C	-13.87	94.75	112.23
3	C	40	VAL	CA-C-O	-13.87	109.08	119.20
3	C	71	ARG	CB-CA-C	-13.86	82.85	110.42
2	B	175	GLN	CB-CG-CD	-13.85	89.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	113	VAL	N-CA-CB	13.78	128.75	112.35
2	B	68	VAL	N-CA-C	-13.76	88.74	108.42
1	A	152	VAL	CA-C-O	13.76	137.97	120.78
4	T	87	PRO	N-CA-CB	13.68	116.64	103.51
1	A	169	SER	CB-CA-C	-13.66	91.22	110.34
4	T	2	VAL	N-CA-CB	-13.62	92.05	112.35
4	T	99	SER	O-C-N	-13.59	107.41	123.31
2	B	38	ARG	CA-C-N	-13.57	103.63	122.77
2	B	38	ARG	C-N-CA	-13.57	103.63	122.77
2	B	201	TRP	CA-C-O	-13.52	103.73	119.15
2	B	125	VAL	N-CA-CB	-13.50	90.46	112.06
3	C	31	ILE	CA-C-N	-13.50	95.76	121.54
3	C	31	ILE	C-N-CA	-13.50	95.76	121.54
2	B	97	SER	CA-C-O	-13.49	106.27	120.84
1	A	11	LEU	CB-CA-C	13.47	136.73	109.38
4	T	65	GLY	O-C-N	-13.42	105.26	122.70
2	B	211	GLN	CB-CA-C	-13.37	86.90	109.50
1	A	175	TRP	CG-CD1-NE1	13.37	127.58	110.20
2	B	139	GLN	CB-CG-CD	-13.32	89.95	112.60
3	C	113	VAL	CA-C-O	-13.27	106.58	120.51
1	A	185	ASN	CA-C-N	-13.21	98.02	121.14
1	A	185	ASN	C-N-CA	-13.21	98.02	121.14
1	A	120	TYR	N-CA-CB	-13.20	88.52	111.08
4	T	48	VAL	N-CA-CB	13.16	132.95	111.23
2	B	52	GLN	CB-CG-CD	-13.10	90.33	112.60
2	B	150	PHE	CB-CA-C	-13.07	83.58	109.33
4	T	93	TYR	CA-C-O	-13.06	105.96	120.32
4	T	100	ARG	CB-CG-CD	13.05	141.31	111.30
1	A	130	LYS	O-C-N	13.00	139.13	123.27
2	B	62	ILE	O-C-N	12.93	134.71	122.69
1	A	76	ILE	CB-CA-C	-12.87	91.45	110.62
2	B	120	VAL	N-CA-C	-12.85	89.89	108.53
1	A	176	SER	O-C-N	12.79	137.12	123.56
2	B	176	PRO	CB-CA-C	-12.79	90.46	111.56
2	B	151	TYR	CB-CA-C	-12.77	93.04	109.65
4	T	50	HIS	CA-C-O	-12.77	107.21	121.51
4	T	100	ARG	NE-CZ-NH1	-12.77	108.73	121.50
3	C	24	ALA	CA-C-N	12.76	142.62	122.59
3	C	24	ALA	C-N-CA	12.76	142.62	122.59
2	B	47	LEU	O-C-N	-12.75	108.69	123.22
2	B	121	PHE	O-C-N	12.74	130.95	121.65
1	A	191	ILE	CA-C-N	-12.73	98.57	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ILE	C-N-CA	-12.73	98.57	122.13
2	B	97	SER	CB-CA-C	-12.72	89.94	111.31
2	B	206	ASN	N-CA-CB	-12.71	90.86	110.06
2	B	94	ALA	CA-C-O	-12.70	105.36	120.60
4	T	57	THR	CB-CA-C	-12.68	85.19	110.42
2	B	72	LYS	N-CA-CB	-12.68	89.07	110.49
4	T	79	TYR	CA-C-N	-12.65	104.89	122.86
4	T	79	TYR	C-N-CA	-12.65	104.89	122.86
1	A	174	ALA	CB-CA-C	-12.64	82.27	110.07
2	B	50	TYR	CB-CG-CD1	12.62	139.74	120.80
2	B	89	ALA	N-CA-CB	-12.61	96.65	109.51
1	A	198	PHE	CA-CB-CG	-12.58	101.22	113.80
1	A	173	VAL	CB-CA-C	-12.57	91.89	110.62
4	T	104	TYR	CA-C-N	-12.57	100.93	122.67
4	T	104	TYR	C-N-CA	-12.57	100.93	122.67
4	T	25	SER	CA-C-N	-12.54	100.09	123.03
4	T	25	SER	C-N-CA	-12.54	100.09	123.03
2	B	175	GLN	CB-CA-C	12.52	130.32	109.67
2	B	180	GLN	N-CA-CB	12.48	132.59	110.37
2	B	23	LEU	CA-C-O	12.46	133.96	120.38
4	T	26	GLY	N-CA-C	-12.43	95.23	111.52
1	A	109	LYS	CB-CA-C	-12.43	85.68	110.17
4	T	104	TYR	N-CA-CB	-12.41	90.95	109.82
1	A	132	VAL	N-CA-C	-12.37	90.03	108.46
4	T	70	SER	CA-C-O	-12.35	107.25	121.58
1	A	80	GLN	CB-CG-CD	12.33	133.56	112.60
1	A	31	SER	O-C-N	12.25	137.22	123.25
1	A	159	VAL	N-CA-C	12.17	127.36	108.87
1	A	195	ASP	CA-CB-CG	12.15	124.75	112.60
1	A	87	TYR	CA-C-O	-12.14	106.24	122.51
2	B	21	VAL	CA-CB-CG1	-12.11	89.82	110.40
1	A	177	ASN	CA-C-N	-12.09	98.45	121.54
1	A	177	ASN	C-N-CA	-12.09	98.45	121.54
2	B	186	SER	CA-C-N	-12.08	97.75	122.03
2	B	186	SER	C-N-CA	-12.08	97.75	122.03
1	A	89	CYS	N-CA-C	-12.06	92.67	110.52
2	B	39	GLN	N-CA-C	-11.99	88.67	108.34
1	A	88	LEU	CB-CA-C	-11.96	87.46	109.46
4	T	71	ARG	CG-CD-NE	-11.95	85.70	112.00
4	T	30	LYS	O-C-N	11.95	134.76	122.10
1	A	23	CYS	CA-C-N	-11.93	103.27	122.36
1	A	23	CYS	C-N-CA	-11.93	103.27	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	VAL	CB-CA-C	-11.93	91.72	111.29
2	B	93	CYS	CA-C-O	-11.92	107.21	121.28
4	T	52	SER	CA-C-N	11.92	136.48	120.50
4	T	52	SER	C-N-CA	11.92	136.48	120.50
3	C	97	PHE	CB-CG-CD1	-11.91	100.46	120.70
1	A	139	ASP	O-C-N	11.90	136.27	122.94
3	C	95	CYS	N-CA-CB	-11.89	93.21	111.05
2	B	61	ASP	CA-C-N	-11.86	109.08	122.48
2	B	61	ASP	C-N-CA	-11.86	109.08	122.48
3	C	63	VAL	O-C-N	-11.85	106.71	122.11
2	B	173	ASP	N-CA-C	-11.82	96.01	109.60
4	T	99	SER	CA-C-N	-11.81	101.71	120.60
4	T	99	SER	C-N-CA	-11.81	101.71	120.60
2	B	15	ARG	CB-CG-CD	11.80	138.44	111.30
2	B	85	LYS	CB-CA-C	-11.78	86.97	110.42
2	B	213	GLN	CA-CB-CG	-11.78	90.53	114.10
2	B	50	TYR	N-CA-C	-11.78	91.79	109.81
4	T	30	LYS	N-CA-C	-11.76	99.62	114.56
2	B	71	GLU	N-CA-C	-11.75	90.81	108.79
2	B	225	GLN	CB-CA-C	-11.71	87.12	110.42
3	C	68	THR	O-C-N	11.71	138.16	122.59
2	B	213	GLN	CA-C-O	-11.70	109.15	121.55
2	B	110	ARG	CA-C-N	-11.69	105.41	122.94
2	B	110	ARG	C-N-CA	-11.69	105.41	122.94
1	A	17	GLU	CB-CG-CD	11.67	132.44	112.60
1	A	156	ASP	CB-CA-C	-11.67	87.02	109.66
4	T	56	GLN	CA-C-N	-11.66	99.27	121.54
4	T	56	GLN	C-N-CA	-11.66	99.27	121.54
2	B	172	THR	O-C-N	-11.65	110.10	123.27
1	A	131	SER	CA-C-N	-11.64	106.76	122.94
1	A	131	SER	C-N-CA	-11.64	106.76	122.94
2	B	90	PHE	CB-CA-C	-11.62	91.14	110.19
3	C	61	ASP	CA-C-N	-11.59	104.52	122.60
3	C	61	ASP	C-N-CA	-11.59	104.52	122.60
1	A	97	ASN	CA-C-O	-11.58	104.24	120.11
4	T	5	VAL	N-CA-CB	-11.55	98.13	110.72
2	B	12	TYR	CA-C-N	-11.50	103.59	122.21
2	B	12	TYR	C-N-CA	-11.50	103.59	122.21
2	B	191	SER	CB-CA-C	-11.48	87.38	109.66
4	T	98	LEU	CA-C-O	-11.43	108.12	120.24
1	A	159	VAL	N-CA-CB	-11.41	94.81	110.56
2	B	156	GLU	CA-C-O	-11.38	105.91	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	230	PRO	N-CA-CB	11.38	110.43	102.35
4	T	71	ARG	CA-C-O	-11.38	109.04	121.33
1	A	183	CYS	CB-CA-C	11.37	128.73	110.88
4	T	108	GLY	O-C-N	11.33	134.07	123.65
2	B	207	HIS	N-CA-C	-11.32	87.95	107.99
2	B	131	SER	CB-CA-C	-11.31	91.41	109.84
2	B	142	THR	CA-CB-OG1	11.29	126.54	109.60
2	B	41	PRO	CA-N-CD	-11.29	96.19	112.00
1	A	160	LEU	CB-CA-C	-11.28	90.22	109.51
2	B	129	GLU	CB-CA-C	-11.28	92.62	108.86
4	T	34	TYR	O-C-N	-11.26	110.61	123.33
2	B	104	TYR	N-CA-CB	-11.25	93.02	110.46
1	A	153	TYR	CA-C-O	11.23	136.57	120.51
1	A	30	SER	CA-C-N	-11.21	102.36	121.75
1	A	30	SER	C-N-CA	-11.21	102.36	121.75
4	T	30	LYS	CA-C-N	-11.20	106.90	122.91
4	T	30	LYS	C-N-CA	-11.20	106.90	122.91
1	A	139	ASP	CA-C-O	-11.19	108.51	121.72
1	A	172	ALA	N-CA-CB	-11.19	90.70	111.52
2	B	31	HIS	N-CA-CB	-11.16	93.02	111.66
2	B	21	VAL	N-CA-CB	-11.16	93.15	111.45
4	T	59	TYR	CA-C-N	-11.11	100.32	121.54
4	T	59	TYR	C-N-CA	-11.11	100.32	121.54
4	T	47	LYS	CB-CA-C	-11.11	90.52	109.51
1	A	174	ALA	N-CA-CB	-11.10	92.38	111.69
4	T	69	ILE	CA-C-O	-11.10	108.15	121.80
1	A	178	LYS	CA-C-N	-11.06	100.41	121.54
1	A	178	LYS	C-N-CA	-11.06	100.41	121.54
2	B	103	GLN	CA-C-N	-11.06	103.54	122.67
2	B	103	GLN	C-N-CA	-11.06	103.54	122.67
3	C	20	LEU	N-CA-CB	-11.05	93.39	109.85
2	B	81	THR	CB-CA-C	-11.04	93.83	111.28
4	T	2	VAL	CG1-CB-CG2	11.04	135.08	110.80
1	A	137	ASP	N-CA-CB	-11.03	95.90	112.78
4	T	21	SER	CA-C-O	-11.01	108.71	121.16
2	B	49	TYR	CA-C-O	11.00	134.31	121.44
3	C	2	VAL	N-CA-CB	10.99	130.19	111.50
2	B	58	GLN	O-C-N	10.97	135.72	123.33
2	B	59	LYS	N-CA-CB	10.94	125.93	110.17
1	A	165	MET	CB-CG-SD	-10.88	80.06	112.70
1	A	199	PRO	N-CA-C	-10.87	90.07	112.47
4	T	68	THR	CA-C-N	-10.86	105.67	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	68	THR	C-N-CA	-10.86	105.67	121.85
1	A	82	GLY	CA-C-N	-10.86	102.73	122.38
1	A	82	GLY	C-N-CA	-10.86	102.73	122.38
2	B	156	GLU	CA-C-N	-10.84	107.75	122.72
2	B	156	GLU	C-N-CA	-10.84	107.75	122.72
1	A	174	ALA	O-C-N	-10.83	110.06	123.17
2	B	10	PRO	CA-C-N	-10.82	103.86	120.31
2	B	10	PRO	C-N-CA	-10.82	103.86	120.31
3	C	68	THR	CA-C-N	-10.82	102.85	122.43
3	C	68	THR	C-N-CA	-10.82	102.85	122.43
1	A	93	GLY	CA-C-O	-10.80	110.41	121.64
3	C	8	GLY	O-C-N	10.78	136.71	122.70
1	A	119	VAL	CB-CA-C	-10.77	96.45	111.21
3	C	30	GLY	CA-C-N	-10.76	102.60	121.97
3	C	30	GLY	C-N-CA	-10.76	102.60	121.97
4	T	95	CYS	CA-C-O	-10.76	108.54	121.56
1	A	97	ASN	CB-CA-C	-10.75	94.54	110.24
2	B	36	TRP	O-C-N	10.75	136.39	123.27
2	B	76	PHE	CA-CB-CG	-10.73	103.07	113.80
1	A	114	ASN	CB-CA-C	10.69	131.23	110.17
3	C	61	ASP	O-C-N	10.69	136.81	122.59
1	A	192	ILE	CA-CB-CG1	10.69	128.57	110.40
1	A	5	GLU	CA-C-N	-10.68	106.92	122.94
1	A	5	GLU	C-N-CA	-10.68	106.92	122.94
3	C	41	PRO	CB-CA-C	10.68	124.90	111.23
2	B	19	GLN	CG-CD-OE1	-10.66	99.47	120.80
1	A	46	LEU	CA-C-N	-10.63	102.84	121.97
1	A	46	LEU	C-N-CA	-10.63	102.84	121.97
2	B	46	ARG	CD-NE-CZ	10.63	139.28	124.40
2	B	71	GLU	CB-CG-CD	10.63	130.67	112.60
3	C	103	ARG	CD-NE-CZ	-10.62	109.53	124.40
4	T	73	GLU	N-CA-C	-10.61	99.59	112.54
4	T	69	ILE	N-CA-C	-10.59	94.73	109.45
3	C	98	ASN	CA-CB-CG	10.54	123.14	112.60
2	B	61	ASP	N-CA-C	-10.52	99.78	111.14
2	B	105	PHE	CA-C-N	-10.51	105.36	121.87
2	B	105	PHE	C-N-CA	-10.51	105.36	121.87
4	T	19	ARG	N-CA-CB	10.49	127.26	110.90
2	B	201	TRP	N-CA-C	-10.48	100.48	113.38
2	B	128	PHE	CA-CB-CG	-10.48	103.32	113.80
1	A	99	ILE	CA-CB-CG2	-10.47	92.70	110.50
1	A	119	VAL	N-CA-CB	-10.47	96.11	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ASN	CB-CG-ND2	-10.46	100.72	116.40
1	A	130	LYS	CA-C-O	-10.45	108.64	120.66
1	A	174	ALA	CA-C-N	10.45	146.22	122.19
1	A	174	ALA	C-N-CA	10.45	146.22	122.19
2	B	88	THR	O-C-N	-10.44	111.53	123.33
1	A	190	SER	N-CA-CB	-10.40	94.48	110.29
4	T	33	PHE	CB-CA-C	-10.38	89.76	110.42
2	B	43	GLN	CA-C-N	10.35	136.47	121.67
2	B	43	GLN	C-N-CA	10.35	136.47	121.67
2	B	131	SER	CA-C-O	-10.35	108.89	120.69
1	A	154	ILE	N-CA-C	-10.35	93.04	108.46
1	A	2	GLN	CA-C-O	-10.34	103.22	120.80
2	B	76	PHE	CA-C-O	-10.33	108.30	120.08
1	A	120	TYR	CA-C-O	-10.33	109.44	121.11
4	T	92	ALA	N-CA-C	-10.33	93.34	109.76
1	A	132	VAL	N-CA-CB	-10.30	94.54	111.44
1	A	165	MET	N-CA-C	-10.30	101.48	114.56
1	A	31	SER	CA-C-O	-10.27	110.24	121.33
2	B	173	ASP	CA-C-O	10.26	129.97	120.02
2	B	88	THR	N-CA-C	-10.25	92.89	108.99
3	C	97	PHE	N-CA-C	-10.25	91.44	108.76
2	B	201	TRP	CG-CD2-CE3	-10.24	123.66	133.90
2	B	27	GLN	CG-CD-NE2	10.24	131.76	116.40
1	A	114	ASN	N-CA-CB	-10.23	92.16	110.37
3	C	67	PHE	CB-CA-C	-10.20	91.33	112.44
3	C	62	PHE	O-C-N	10.19	134.37	122.25
1	A	99	ILE	CA-C-O	-10.17	109.30	120.48
2	B	89	ALA	CB-CA-C	-10.16	99.52	114.87
2	B	228	ALA	CA-C-O	-10.16	105.97	120.51
2	B	74	GLU	N-CA-CB	-10.16	94.98	110.73
1	A	109	LYS	CA-C-O	-10.15	106.25	120.16
1	A	121	GLN	CB-CA-C	10.15	126.27	109.53
1	A	188	ASN	CA-C-O	-10.15	106.90	119.38
4	T	96	ARG	O-C-N	10.13	134.82	123.48
1	A	34	TRP	CA-C-O	-10.12	110.40	121.23
3	C	46	GLU	CB-CA-C	-10.12	88.39	109.94
1	A	116	ASP	CB-CA-C	-10.09	96.44	111.27
1	A	118	ALA	N-CA-CB	-10.09	93.96	110.71
2	B	121	PHE	N-CA-CB	-10.08	97.03	111.25
4	T	84	SER	O-C-N	10.07	135.83	123.44
1	A	117	PRO	CB-CA-C	10.07	124.60	111.21
3	C	111	VAL	CA-C-N	-10.07	107.65	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	111	VAL	C-N-CA	-10.07	107.65	122.65
3	C	112	THR	CA-C-O	-10.07	109.62	120.80
1	A	82	GLY	O-C-N	10.05	134.50	122.84
4	T	2	VAL	CB-CA-C	-10.05	94.73	110.52
1	A	144	VAL	CA-C-N	10.03	135.04	120.90
1	A	144	VAL	C-N-CA	10.03	135.04	120.90
2	B	77	PRO	CB-CG-CD	-10.02	74.04	106.10
1	A	69	ARG	CB-CG-CD	10.01	134.32	111.30
1	A	196	THR	CA-C-O	-10.01	109.65	120.36
3	C	67	PHE	CA-CB-CG	10.01	123.81	113.80
2	B	123	PRO	CB-CA-C	-9.99	96.76	110.85
3	C	100	ILE	O-C-N	9.98	132.33	122.25
2	B	149	GLY	CA-C-N	-9.97	107.16	122.81
2	B	149	GLY	C-N-CA	-9.97	107.16	122.81
4	T	96	ARG	CA-C-N	-9.97	107.38	121.33
4	T	96	ARG	C-N-CA	-9.97	107.38	121.33
2	B	46	ARG	NE-CZ-NH1	9.96	131.46	121.50
3	C	60	ARG	CA-CB-CG	9.95	134.01	114.10
2	B	35	TYR	CG-CD1-CE1	-9.95	106.28	121.20
2	B	213	GLN	CA-C-N	-9.94	107.43	122.74
2	B	213	GLN	C-N-CA	-9.94	107.43	122.74
1	A	165	MET	N-CA-CB	-9.92	97.80	111.00
1	A	10	PHE	O-C-N	-9.91	112.14	123.33
4	T	62	SER	CA-CB-OG	9.91	130.91	111.10
2	B	209	ARG	CA-C-N	-9.90	107.61	122.47
2	B	209	ARG	C-N-CA	-9.90	107.61	122.47
2	B	40	ASP	N-CA-CB	9.89	121.21	109.74
4	T	116	SER	O-C-N	-9.89	112.10	123.27
4	T	52	SER	N-CA-CB	-9.88	95.14	110.56
2	B	157	LEU	CB-CA-C	-9.87	93.46	109.75
3	C	81	GLN	CA-C-O	-9.87	110.80	121.56
4	T	82	MET	N-CA-C	-9.87	89.39	107.75
4	T	48	VAL	CG1-CB-CG2	-9.86	89.10	110.80
4	T	48	VAL	O-C-N	9.84	134.87	122.57
2	B	177	LEU	CB-CA-C	-9.84	94.15	110.29
1	A	7	SER	N-CA-C	-9.83	93.21	108.55
2	B	156	GLU	CB-CA-C	-9.80	96.31	110.62
3	C	67	PHE	N-CA-C	-9.79	94.38	109.65
3	C	32	HIS	N-CA-CB	9.79	127.04	110.49
2	B	10	PRO	CB-CA-C	-9.79	87.54	112.00
2	B	224	THR	CA-CB-OG1	9.77	124.25	109.60
1	A	166	ASP	CA-C-O	-9.76	109.66	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	97	PHE	CA-CB-CG	-9.76	104.04	113.80
3	C	49	ALA	CA-C-O	-9.76	110.37	121.40
1	A	88	LEU	O-C-N	-9.75	111.94	122.96
4	T	30	LYS	N-CA-CB	9.75	123.97	111.00
1	A	144	VAL	CB-CA-C	-9.75	102.31	113.22
2	B	140	LYS	CB-CA-C	-9.74	93.83	112.43
2	B	143	LEU	CA-C-O	9.72	132.10	120.92
2	B	222	GLU	CB-CA-C	-9.71	91.09	110.42
1	A	186	ALA	N-CA-CB	-9.71	94.58	110.40
3	C	39	GLN	O-C-N	9.68	135.72	123.14
4	T	89	ASP	N-CA-CB	9.68	125.73	110.73
2	B	50	TYR	CE1-CZ-CE2	-9.66	100.98	120.30
2	B	121	PHE	CA-C-O	-9.66	111.45	120.34
3	C	94	TYR	O-C-N	9.64	135.04	123.27
1	A	22	TYR	N-CA-CB	9.64	126.50	111.56
1	A	73	SER	CA-C-O	-9.63	110.20	120.99
1	A	152	VAL	CB-CA-C	9.63	127.09	111.29
1	A	175	TRP	NE1-CE2-CZ2	-9.60	115.69	130.10
4	T	31	ILE	CA-C-N	9.59	139.17	121.52
4	T	31	ILE	C-N-CA	9.59	139.17	121.52
4	T	59	TYR	N-CA-CB	9.58	126.01	111.35
2	B	192	SER	CA-C-O	-9.58	109.95	121.06
3	C	25	SER	N-CA-CB	-9.57	94.89	111.55
2	B	12	TYR	CA-C-O	-9.56	110.38	120.70
1	A	155	THR	N-CA-CB	-9.55	97.26	110.25
2	B	21	VAL	N-CA-C	9.54	122.57	108.45
4	T	31	ILE	CA-CB-CG1	9.52	126.58	110.40
1	A	175	TRP	CA-C-O	9.52	131.62	121.06
1	A	151	ASP	CA-C-O	-9.51	106.91	120.51
4	T	64	LYS	CB-CG-CD	9.49	133.13	111.30
4	T	60	ALA	N-CA-C	-9.49	90.60	110.80
4	T	101	ILE	CA-C-O	-9.49	108.92	120.78
4	T	96	ARG	N-CA-CB	9.47	127.97	111.39
3	C	60	ARG	N-CA-CB	-9.47	94.49	110.49
4	T	59	TYR	CB-CA-C	-9.47	92.27	112.82
1	A	10	PHE	CB-CA-C	-9.47	89.78	109.94
1	A	31	SER	CA-C-N	-9.45	105.12	121.85
1	A	31	SER	C-N-CA	-9.45	105.12	121.85
2	B	175	GLN	CA-C-N	9.43	131.62	119.84
2	B	175	GLN	C-N-CA	9.43	131.62	119.84
1	A	77	THR	N-CA-C	-9.39	93.21	108.52
4	T	9	GLY	CA-C-N	9.39	139.81	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	9	GLY	C-N-CA	9.39	139.81	121.41
1	A	41	GLU	CA-C-N	-9.37	107.16	121.87
1	A	41	GLU	C-N-CA	-9.37	107.16	121.87
1	A	183	CYS	N-CA-CB	-9.36	96.43	110.01
4	T	29	HIS	CB-CA-C	-9.36	98.13	111.14
2	B	91	TYR	CA-C-N	-9.35	107.59	122.73
2	B	91	TYR	C-N-CA	-9.35	107.59	122.73
2	B	27	GLN	N-CA-CB	9.34	126.95	110.80
1	A	48	THR	N-CA-C	-9.33	91.68	108.48
2	B	105	PHE	CB-CA-C	-9.33	91.08	113.19
4	T	113	VAL	N-CA-C	9.31	122.48	108.23
2	B	83	ALA	N-CA-CB	-9.29	96.12	111.53
2	B	106	GLY	O-C-N	-9.28	112.49	121.77
3	C	45	ARG	NE-CZ-NH1	-9.28	112.22	121.50
4	T	71	ARG	NH1-CZ-NH2	9.26	131.33	119.30
1	A	18	ASN	O-C-N	-9.25	111.86	122.68
1	A	129	ASP	N-CA-C	-9.25	98.79	111.56
1	A	158	CYS	O-C-N	9.25	134.01	123.19
1	A	85	GLY	CA-C-O	-9.24	110.85	121.47
4	T	4	LEU	CB-CA-C	-9.23	97.14	110.62
1	A	191	ILE	N-CA-C	9.23	119.93	106.55
1	A	44	VAL	N-CA-C	-9.18	95.22	108.53
4	T	6	GLU	CA-CB-CG	-9.17	95.76	114.10
2	B	37	TYR	CD1-CG-CD2	-9.16	104.36	118.10
4	T	28	VAL	N-CA-C	-9.16	90.28	109.34
2	B	181	PRO	CA-C-N	-9.15	106.40	120.31
2	B	181	PRO	C-N-CA	-9.15	106.40	120.31
1	A	87	TYR	CA-C-N	-9.14	106.21	121.39
1	A	87	TYR	C-N-CA	-9.14	106.21	121.39
2	B	52	GLN	CA-CB-CG	9.14	132.39	114.10
3	C	97	PHE	O-C-N	-9.14	112.61	123.31
4	T	64	LYS	CB-CA-C	-9.14	95.38	110.19
1	A	132	VAL	CA-CB-CG1	-9.14	94.86	110.40
1	A	19	LEU	N-CA-C	9.14	120.77	107.88
1	A	73	SER	O-C-N	9.14	133.66	123.33
2	B	102	GLU	O-C-N	-9.13	112.68	123.27
3	C	51	ILE	N-CA-C	-9.12	94.85	108.17
4	T	114	THR	N-CA-CB	-9.12	96.25	110.57
3	C	7	SER	CA-C-N	-9.11	103.55	121.41
3	C	7	SER	C-N-CA	-9.11	103.55	121.41
2	B	195	ARG	NE-CZ-NH2	-9.10	111.01	119.20
2	B	154	HIS	CA-CB-CG	9.09	122.89	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	49	TYR	N-CA-C	-9.08	95.45	109.52
4	T	51	ILE	N-CA-C	-9.08	96.44	108.06
2	B	64	GLU	CA-C-N	-9.08	107.36	122.25
2	B	64	GLU	C-N-CA	-9.08	107.36	122.25
1	A	191	ILE	O-C-N	9.07	132.43	122.36
1	A	137	ASP	CB-CA-C	9.05	125.99	111.23
4	T	31	ILE	N-CA-C	-9.05	95.22	108.71
1	A	191	ILE	CA-C-O	-9.03	112.12	121.70
2	B	155	VAL	CA-CB-CG2	9.03	125.74	110.40
3	C	91	ALA	CB-CA-C	-9.03	92.46	110.42
1	A	30	SER	O-C-N	9.02	132.44	122.15
2	B	158	SER	N-CA-CB	-9.02	95.85	111.55
1	A	173	VAL	N-CA-CB	-8.99	95.74	111.39
4	T	7	SER	N-CA-CB	8.99	124.51	110.84
2	B	35	TYR	CB-CG-CD2	-8.99	107.32	120.80
3	C	104	TYR	N-CA-CB	-8.98	95.77	110.41
3	C	94	TYR	CA-C-O	-8.98	110.33	120.66
2	B	233	GLN	N-CA-CB	-8.97	97.38	111.56
4	T	53	ILE	CB-CG1-CD1	8.96	132.63	113.80
1	A	132	VAL	CB-CA-C	-8.96	96.70	110.50
3	C	87	PRO	CB-CA-C	-8.96	98.61	111.68
4	T	67	PHE	CB-CA-C	-8.95	95.57	109.89
2	B	39	GLN	CB-CA-C	-8.95	95.82	110.14
2	B	124	GLU	CB-CG-CD	8.95	127.81	112.60
4	T	94	TYR	CB-CA-C	-8.95	91.71	109.33
3	C	101	ARG	CG-CD-NE	8.94	131.66	112.00
3	C	40	VAL	N-CA-C	-8.93	97.77	107.77
2	B	117	LEU	CB-CA-C	-8.93	92.66	110.42
2	B	215	TYR	CA-C-O	-8.93	111.06	120.70
1	A	122	LEU	CA-C-N	-8.92	103.80	121.91
1	A	122	LEU	C-N-CA	-8.92	103.80	121.91
4	T	48	VAL	CA-CB-CG1	-8.92	95.24	110.40
2	B	20	ASN	CA-C-O	-8.91	111.45	121.07
2	B	191	SER	N-CA-C	-8.90	95.79	109.85
1	A	185	ASN	N-CA-CB	-8.89	98.29	110.56
2	B	198	ALA	O-C-N	8.89	134.24	122.33
1	A	129	ASP	CA-C-N	-8.88	108.34	122.73
1	A	129	ASP	C-N-CA	-8.88	108.34	122.73
3	C	79	TYR	CB-CA-C	-8.88	90.82	109.38
1	A	143	ASN	N-CA-CB	-8.88	95.73	110.47
1	A	73	SER	CA-C-N	-8.88	109.16	122.47
1	A	73	SER	C-N-CA	-8.88	109.16	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	52	SER	CA-C-O	-8.87	110.83	121.66
2	B	239	ALA	N-CA-CB	-8.87	96.25	111.69
1	A	20	THR	CA-CB-OG1	8.87	122.90	109.60
2	B	199	THR	N-CA-CB	8.87	125.11	110.39
4	T	23	VAL	CB-CA-C	-8.86	99.67	111.81
1	A	28	VAL	CA-CB-CG2	8.86	125.46	110.40
2	B	225	GLN	N-CA-CB	-8.86	95.52	110.49
1	A	144	VAL	CA-CB-CG1	-8.86	95.35	110.40
4	T	60	ALA	CA-C-N	8.86	138.45	121.54
4	T	60	ALA	C-N-CA	8.86	138.45	121.54
1	A	182	ALA	N-CA-C	-8.85	96.94	109.69
2	B	154	HIS	CB-CA-C	-8.85	98.32	111.77
2	B	203	ASN	CA-C-O	-8.84	111.46	119.59
1	A	177	ASN	CB-CA-C	-8.83	93.29	109.54
1	A	198	PHE	CB-CA-C	-8.83	95.10	108.61
1	A	155	THR	CA-CB-CG2	-8.83	95.49	110.50
1	A	177	ASN	N-CA-C	-8.83	98.05	110.50
1	A	199	PRO	CB-CA-C	8.83	126.12	111.56
1	A	153	TYR	CB-CA-C	-8.81	92.89	110.42
1	A	160	LEU	CA-C-O	-8.81	110.79	121.36
1	A	63	PHE	CB-CA-C	-8.80	92.25	109.68
3	C	113	VAL	O-C-N	8.80	131.25	122.71
4	T	97	ALA	CA-C-O	-8.79	111.21	120.09
4	T	32	ASN	N-CA-CB	8.78	123.49	110.33
3	C	72	ASP	N-CA-C	-8.77	95.99	109.85
1	A	175	TRP	CD1-CG-CD2	-8.77	92.28	106.30
4	T	83	ASN	N-CA-C	-8.77	102.29	113.16
1	A	57	LYS	CB-CA-C	8.76	126.11	109.37
1	A	162	MET	CA-C-O	8.76	132.03	122.13
1	A	195	ASP	N-CA-CB	-8.75	92.00	111.69
4	T	32	ASN	CB-CA-C	8.75	127.25	109.67
1	A	87	TYR	N-CA-C	8.73	122.01	109.71
2	B	188	TYR	N-CA-CB	8.72	125.99	111.08
1	A	180	ASP	N-CA-CB	8.70	126.91	110.90
2	B	197	SER	CA-C-N	-8.70	105.89	120.68
2	B	197	SER	C-N-CA	-8.70	105.89	120.68
3	C	58	HIS	CB-CG-CD2	-8.68	119.92	131.20
4	T	81	GLN	CB-CA-C	-8.67	97.20	111.68
4	T	53	ILE	CA-CB-CG2	8.66	125.22	110.50
3	C	39	GLN	CA-C-N	-8.65	114.02	123.02
3	C	39	GLN	C-N-CA	-8.65	114.02	123.02
2	B	190	LEU	CA-C-N	-8.65	108.29	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	190	LEU	C-N-CA	-8.65	108.29	122.81
2	B	175	GLN	CA-CB-CG	8.64	131.38	114.10
4	T	81	GLN	CA-C-O	-8.64	111.71	121.39
1	A	123	ARG	CB-CA-C	-8.64	95.92	110.43
3	C	46	GLU	CA-C-O	-8.64	111.32	120.99
4	T	63	ALA	N-CA-CB	-8.64	99.99	110.53
2	B	205	ARG	CA-C-N	-8.63	109.08	121.42
2	B	205	ARG	C-N-CA	-8.63	109.08	121.42
4	T	60	ALA	CA-C-O	-8.62	108.18	120.51
3	C	37	TYR	CB-CG-CD2	-8.62	107.87	120.80
3	C	98	ASN	O-C-N	-8.62	113.12	123.29
1	A	33	GLN	CB-CA-C	-8.61	91.55	111.09
4	T	114	THR	O-C-N	-8.59	113.15	123.29
1	A	153	TYR	N-CA-CB	8.59	125.00	110.49
2	B	121	PHE	CB-CA-C	-8.59	96.66	109.97
4	T	45	ARG	N-CA-CB	-8.58	95.98	110.49
4	T	101	ILE	CB-CA-C	-8.58	97.22	111.29
1	A	187	PHE	N-CA-CB	-8.58	98.82	111.51
3	C	76	ASN	O-C-N	8.57	132.31	122.20
4	T	2	VAL	O-C-N	-8.57	113.44	122.95
1	A	78	ALA	N-CA-CB	8.56	124.96	110.49
2	B	187	ARG	N-CA-C	-8.56	98.17	110.59
3	C	67	PHE	O-C-N	-8.55	111.35	122.72
2	B	70	ARG	NE-CZ-NH2	8.54	126.89	119.20
1	A	119	VAL	CG1-CB-CG2	8.53	129.57	110.80
2	B	40	ASP	N-CA-C	-8.52	98.94	110.36
1	A	198	PHE	CA-C-N	-8.51	109.20	119.84
1	A	198	PHE	C-N-CA	-8.51	109.20	119.84
2	B	68	VAL	CB-CA-C	-8.50	95.88	111.18
4	T	80	LEU	CA-C-O	-8.49	111.16	120.33
4	T	95	CYS	CB-CA-C	-8.48	94.44	109.71
2	B	62	ILE	N-CA-CB	8.48	122.00	112.34
1	A	181	PHE	CB-CA-C	8.47	123.81	109.50
2	B	187	ARG	NE-CZ-NH2	8.47	126.82	119.20
2	B	175	GLN	O-C-N	-8.46	112.82	121.28
1	A	89	CYS	O-C-N	-8.45	113.48	122.94
3	C	44	GLN	CG-CD-NE2	8.45	129.07	116.40
4	T	59	TYR	O-C-N	8.44	132.54	122.75
2	B	125	VAL	CB-CA-C	-8.44	95.78	110.38
4	T	76	ASN	O-C-N	-8.44	111.36	122.59
2	B	217	LEU	O-C-N	8.43	133.05	123.19
2	B	232	THR	CA-C-N	-8.43	108.05	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	232	THR	C-N-CA	-8.43	108.05	121.87
2	B	7	THR	CA-CB-OG1	-8.43	96.96	109.60
2	B	70	ARG	N-CA-CB	-8.40	96.20	110.83
2	B	168	SER	CA-C-N	8.40	135.40	120.77
2	B	168	SER	C-N-CA	8.40	135.40	120.77
2	B	242	ARG	O-C-N	8.38	132.87	123.48
1	A	193	PRO	CA-C-O	-8.38	111.84	121.56
1	A	184	ALA	N-CA-C	8.37	121.46	111.33
2	B	71	GLU	CB-CA-C	-8.36	95.07	110.62
4	T	38	ARG	CB-CG-CD	8.36	130.52	111.30
2	B	239	ALA	O-C-N	8.35	133.28	123.17
1	A	73	SER	N-CA-C	-8.35	95.88	108.99
1	A	106	LEU	N-CA-C	8.35	122.01	110.24
2	B	101	TYR	N-CA-CB	-8.35	96.38	110.49
2	B	56	ASP	CA-C-O	8.35	130.21	120.69
1	A	88	LEU	CA-C-O	8.34	131.06	121.47
3	C	10	GLY	CA-C-O	-8.34	114.50	121.76
2	B	119	ASN	CA-C-N	-8.34	112.34	123.10
2	B	119	ASN	C-N-CA	-8.34	112.34	123.10
1	A	175	TRP	CD2-CE2-CZ2	-8.34	114.06	122.40
2	B	201	TRP	CB-CA-C	-8.33	95.15	109.65
2	B	90	PHE	CA-C-O	-8.31	111.17	120.32
4	T	71	ARG	N-CA-CB	8.30	125.53	111.66
2	B	154	HIS	CA-C-N	-8.30	111.80	123.17
2	B	154	HIS	C-N-CA	-8.30	111.80	123.17
4	T	37	TYR	CD1-CE1-CZ	8.30	134.54	119.60
2	B	23	LEU	N-CA-CB	8.30	123.60	110.57
3	C	44	GLN	CA-C-O	-8.29	111.98	120.77
2	B	187	ARG	CB-CA-C	8.29	126.18	110.51
1	A	97	ASN	O-C-N	8.28	134.69	123.34
4	T	104	TYR	CB-CG-CD1	-8.28	108.38	120.80
3	C	97	PHE	CA-C-O	8.28	129.50	120.32
2	B	225	GLN	OE1-CD-NE2	-8.27	114.33	122.60
4	T	23	VAL	N-CA-C	8.27	119.45	106.88
4	T	56	GLN	CA-C-O	-8.27	108.68	120.51
3	C	86	GLN	N-CA-C	-8.26	95.95	109.82
1	A	169	SER	O-C-N	8.24	133.48	123.26
2	B	82	SER	O-C-N	8.24	133.55	122.59
3	C	66	ARG	N-CA-CB	8.24	124.41	110.49
3	C	37	TYR	CB-CA-C	-8.23	91.89	111.65
4	T	51	ILE	CA-C-N	-8.23	107.76	122.74
4	T	51	ILE	C-N-CA	-8.23	107.76	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	71	ARG	CB-CG-CD	8.23	130.23	111.30
1	A	121	GLN	CA-C-N	8.22	133.40	122.30
1	A	121	GLN	C-N-CA	8.22	133.40	122.30
1	A	179	SER	O-C-N	-8.21	111.67	122.59
1	A	138	PHE	O-C-N	-8.21	111.67	122.59
2	B	229	LYS	N-CA-C	-8.21	99.73	110.07
4	T	22	CYS	CA-C-N	-8.20	112.78	122.95
4	T	22	CYS	C-N-CA	-8.20	112.78	122.95
4	T	44	GLU	N-CA-CB	-8.19	97.35	110.46
1	A	153	TYR	N-CA-C	8.19	128.25	110.80
2	B	120	VAL	CG1-CB-CG2	-8.18	92.80	110.80
4	T	8	GLY	N-CA-C	-8.17	103.71	112.04
4	T	113	VAL	CB-CA-C	-8.17	101.07	110.96
2	B	13	LEU	CB-CA-C	-8.17	92.11	110.07
2	B	159	TRP	CB-CA-C	-8.15	93.28	109.33
1	A	21	VAL	CG1-CB-CG2	-8.14	92.89	110.80
1	A	142	THR	CA-CB-OG1	-8.14	97.39	109.60
2	B	173	ASP	CA-CB-CG	8.13	120.73	112.60
2	B	49	TYR	CB-CA-C	-8.13	93.12	109.79
1	A	140	SER	N-CA-C	-8.13	103.37	113.20
1	A	178	LYS	N-CA-CB	-8.12	96.77	110.49
2	B	146	LEU	CA-C-O	-8.12	111.45	120.70
1	A	152	VAL	CA-CB-CG2	8.11	124.19	110.40
3	C	104	TYR	CA-CB-CG	-8.11	99.31	113.90
4	T	111	THR	CA-C-O	-8.10	110.88	120.60
2	B	62	ILE	CA-C-N	-8.09	106.09	121.54
2	B	62	ILE	C-N-CA	-8.09	106.09	121.54
2	B	120	VAL	CA-C-N	-8.09	108.38	122.38
2	B	120	VAL	C-N-CA	-8.09	108.38	122.38
3	C	50	THR	CB-CA-C	-8.09	96.97	109.99
4	T	57	THR	OG1-CB-CG2	-8.08	93.14	109.30
2	B	83	ALA	CB-CA-C	8.07	126.40	112.27
2	B	165	GLU	CB-CA-C	-8.07	96.68	109.84
1	A	64	GLN	CB-CA-C	-8.07	96.08	109.80
3	C	39	GLN	N-CA-CB	8.06	123.48	110.90
3	C	45	ARG	NE-CZ-NH2	8.05	126.45	119.20
4	T	87	PRO	O-C-N	8.05	133.25	122.30
2	B	73	LYS	CA-C-N	-8.03	110.07	122.60
2	B	73	LYS	C-N-CA	-8.03	110.07	122.60
3	C	101	ARG	CB-CA-C	8.03	123.97	111.28
2	B	217	LEU	CA-C-O	-8.02	111.90	120.80
2	B	19	GLN	N-CA-C	-8.02	95.19	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	VAL	N-CA-C	-8.00	97.05	108.65
2	B	199	THR	CB-CA-C	-8.00	93.59	110.31
2	B	155	VAL	CA-C-O	-8.00	113.41	121.49
4	T	20	LEU	CB-CA-C	7.99	122.25	110.26
4	T	58	ASP	CA-C-N	-7.99	108.38	122.84
4	T	58	ASP	C-N-CA	-7.99	108.38	122.84
1	A	177	ASN	OD1-CG-ND2	7.98	130.58	122.60
4	T	78	VAL	N-CA-C	-7.98	96.96	108.53
2	B	232	THR	N-CA-C	-7.97	98.08	109.96
3	C	97	PHE	N-CA-CB	-7.97	97.01	110.80
2	B	213	GLN	N-CA-C	-7.97	99.52	110.35
2	B	151	TYR	CG-CD1-CE1	-7.96	109.26	121.20
4	T	108	GLY	CA-C-O	-7.96	112.34	121.49
1	A	151	ASP	CA-C-N	-7.94	107.67	121.97
1	A	151	ASP	C-N-CA	-7.94	107.67	121.97
2	B	208	PHE	CA-C-N	-7.94	105.78	121.91
2	B	208	PHE	C-N-CA	-7.94	105.78	121.91
3	C	67	PHE	N-CA-CB	-7.94	97.31	110.65
1	A	132	VAL	O-C-N	7.94	131.59	123.10
2	B	105	PHE	N-CA-CB	-7.93	96.60	110.87
1	A	113	GLN	N-CA-C	-7.92	97.33	109.85
4	T	37	TYR	CG-CD2-CE2	7.91	133.07	121.20
2	B	156	GLU	O-C-N	7.91	133.42	123.14
1	A	198	PHE	CA-C-O	-7.90	112.50	120.63
3	C	90	THR	CB-CA-C	-7.90	96.50	109.53
4	T	79	TYR	O-C-N	7.89	133.41	123.15
2	B	160	TRP	O-C-N	7.89	133.78	123.06
2	B	135	ILE	N-CA-CB	7.88	119.77	110.55
3	C	101	ARG	NE-CZ-NH2	7.88	126.29	119.20
2	B	240	TRP	CZ3-CH2-CZ2	-7.87	111.27	121.50
4	T	40	ALA	N-CA-CB	7.87	124.38	110.37
4	T	51	ILE	O-C-N	7.87	130.75	123.19
4	T	18	LEU	CA-C-O	-7.86	112.18	120.99
2	B	205	ARG	O-C-N	7.86	133.52	122.36
1	A	87	TYR	CB-CG-CD2	7.85	132.57	120.80
1	A	157	LYS	N-CA-CB	7.83	121.88	109.51
2	B	171	CYS	CA-C-O	-7.83	112.18	120.40
1	A	166	ASP	O-C-N	7.83	132.90	122.41
2	B	150	PHE	CA-CB-CG	-7.82	105.98	113.80
3	C	91	ALA	N-CA-CB	7.81	123.69	110.49
3	C	64	LYS	N-CA-C	7.81	121.51	110.50
1	A	87	TYR	CD1-CG-CD2	-7.81	106.39	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	26	GLU	CA-C-O	-7.81	111.97	121.11
2	B	184	ASN	CA-CB-CG	-7.81	104.79	112.60
2	B	235	VAL	N-CA-C	-7.80	93.11	109.34
2	B	163	GLY	N-CA-C	-7.79	103.79	115.32
1	A	169	SER	CA-C-O	-7.78	110.48	119.98
3	C	11	LEU	CB-CG-CD1	-7.78	87.35	110.70
1	A	44	VAL	CB-CA-C	-7.78	98.99	110.81
2	B	192	SER	O-C-N	7.77	132.29	123.27
1	A	67	ASP	CA-C-N	-7.77	110.22	122.73
1	A	67	ASP	C-N-CA	-7.77	110.22	122.73
2	B	173	ASP	N-CA-CB	-7.75	98.35	109.75
1	A	120	TYR	CB-CA-C	-7.75	94.06	109.33
3	C	63	VAL	N-CA-C	-7.75	103.71	111.77
3	C	65	GLY	CA-C-N	-7.75	106.75	121.54
3	C	65	GLY	C-N-CA	-7.75	106.75	121.54
4	T	91	ALA	N-CA-CB	7.74	123.55	111.24
4	T	82	MET	N-CA-CB	7.74	123.16	110.39
4	T	90	THR	CB-CA-C	-7.73	97.61	110.29
1	A	177	ASN	O-C-N	7.73	131.98	122.86
2	B	111	LEU	CB-CG-CD1	-7.72	87.54	110.70
2	B	76	PHE	N-CA-CB	-7.71	97.45	111.03
2	B	39	GLN	OE1-CD-NE2	-7.71	114.89	122.60
3	C	22	CYS	N-CA-CB	7.71	121.62	110.37
3	C	39	GLN	CA-CB-CG	-7.71	98.69	114.10
2	B	70	ARG	NE-CZ-NH1	-7.70	113.80	121.50
1	A	34	TRP	O-C-N	-7.69	115.19	123.42
1	A	29	PHE	CA-C-N	7.67	131.18	120.29
1	A	29	PHE	C-N-CA	7.67	131.18	120.29
2	B	171	CYS	CA-C-N	-7.67	112.14	122.72
2	B	171	CYS	C-N-CA	-7.67	112.14	122.72
4	T	104	TYR	CB-CA-C	7.66	123.11	110.92
2	B	131	SER	O-C-N	7.66	132.00	123.04
2	B	213	GLN	O-C-N	7.66	132.23	122.81
3	C	102	GLY	CA-C-N	-7.65	110.56	121.50
3	C	102	GLY	C-N-CA	-7.65	110.56	121.50
2	B	177	LEU	N-CA-CB	7.65	122.34	109.87
3	C	2	VAL	CA-C-O	-7.65	107.80	120.80
2	B	164	LYS	N-CA-C	-7.64	96.47	109.24
2	B	80	VAL	N-CA-CB	-7.64	97.08	111.21
3	C	89	ASP	CA-C-N	-7.64	110.78	122.09
3	C	89	ASP	C-N-CA	-7.64	110.78	122.09
1	A	148	LYS	CA-CB-CG	7.64	129.38	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	56	GLN	CB-CA-C	-7.64	95.22	110.42
3	C	72	ASP	N-CA-CB	7.63	123.56	111.20
2	B	102	GLU	CB-CA-C	-7.61	97.52	110.16
2	B	86	ASN	CB-CA-C	7.61	125.16	110.17
1	A	154	ILE	O-C-N	7.61	131.24	123.10
1	A	24	ASN	CA-CB-CG	7.60	120.20	112.60
1	A	93	GLY	O-C-N	7.60	131.97	122.85
2	B	72	LYS	N-CA-C	7.60	126.99	110.80
2	B	115	GLU	CA-C-N	7.60	136.06	121.54
2	B	115	GLU	C-N-CA	7.60	136.06	121.54
4	T	85	LEU	CA-C-N	7.60	134.42	122.26
4	T	85	LEU	C-N-CA	7.60	134.42	122.26
4	T	114	THR	CA-C-O	7.60	128.66	120.38
1	A	3	LEU	N-CA-CB	7.59	121.25	109.48
1	A	119	VAL	N-CA-C	7.59	120.41	108.87
3	C	20	LEU	O-C-N	-7.58	113.60	122.93
3	C	3	GLN	CA-C-O	-7.57	112.06	120.69
2	B	162	ASN	CB-CG-OD1	-7.57	105.66	120.80
3	C	29	VAL	N-CA-C	-7.56	103.87	111.88
2	B	205	ARG	N-CA-CB	7.55	121.49	110.47
1	A	88	LEU	N-CA-C	7.55	121.65	110.48
1	A	6	GLN	CA-C-N	-7.54	109.60	123.11
1	A	6	GLN	C-N-CA	-7.54	109.60	123.11
2	B	16	LYS	N-CA-CB	7.54	121.22	110.44
1	A	137	ASP	O-C-N	7.54	132.59	122.04
4	T	27	TYR	CB-CA-C	-7.54	98.14	109.90
4	T	113	VAL	CA-C-N	-7.54	112.60	123.00
4	T	113	VAL	C-N-CA	-7.54	112.60	123.00
2	B	35	TYR	N-CA-CB	-7.53	97.50	111.13
1	A	175	TRP	CD2-CE3-CZ3	-7.53	108.82	118.60
2	B	209	ARG	N-CA-CB	-7.53	100.12	111.56
4	T	105	ASP	O-C-N	-7.52	114.12	122.84
4	T	1	ASP	O-C-N	-7.52	110.97	123.00
1	A	21	VAL	CA-CB-CG2	7.52	123.18	110.40
3	C	32	HIS	CB-CA-C	-7.52	95.46	110.42
2	B	145	CYS	CB-CA-C	-7.51	96.72	109.72
2	B	130	PRO	O-C-N	7.51	132.05	123.04
1	A	177	ASN	N-CA-CB	7.50	120.97	110.17
1	A	111	ASN	CB-CA-C	-7.50	99.08	111.68
2	B	122	PRO	O-C-N	-7.50	112.61	121.46
4	T	91	ALA	CB-CA-C	-7.49	97.93	109.99
2	B	214	PHE	CA-C-N	-7.48	111.72	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	214	PHE	C-N-CA	-7.48	111.72	122.94
2	B	81	THR	CA-CB-OG1	-7.48	98.38	109.60
3	C	71	ARG	NE-CZ-NH2	-7.48	112.47	119.20
4	T	24	ALA	N-CA-C	-7.48	97.05	109.24
2	B	69	SER	N-CA-C	-7.48	96.75	109.24
2	B	128	PHE	CZ-CE2-CD2	-7.48	106.54	120.00
2	B	181	PRO	N-CA-CB	7.47	111.10	103.25
2	B	105	PHE	CD1-CG-CD2	-7.46	107.40	118.60
4	T	67	PHE	N-CA-CB	-7.46	98.73	109.85
1	A	112	ILE	CB-CA-C	-7.44	102.38	111.08
3	C	111	VAL	O-C-N	7.44	131.29	123.26
3	C	44	GLN	CA-CB-CG	7.43	128.97	114.10
4	T	84	SER	N-CA-CB	7.43	123.04	110.71
1	A	182	ALA	O-C-N	7.43	133.35	122.81
2	B	158	SER	O-C-N	7.43	132.80	123.15
4	T	100	ARG	O-C-N	-7.43	112.74	122.39
2	B	37	TYR	CB-CG-CD1	7.42	131.94	120.80
2	B	41	PRO	O-C-N	7.42	132.66	122.64
1	A	22	TYR	CB-CA-C	-7.42	96.82	110.62
1	A	102	LYS	CA-C-O	7.42	128.47	119.49
4	T	63	ALA	CA-C-O	-7.42	113.06	122.63
4	T	53	ILE	CG1-CB-CG2	7.41	132.93	110.70
2	B	233	GLN	CA-C-O	-7.41	113.52	121.45
2	B	120	VAL	CA-C-O	-7.41	112.28	120.72
2	B	50	TYR	CG-CD1-CE1	7.40	132.31	121.20
3	C	91	ALA	O-C-N	7.39	132.42	122.59
4	T	32	ASN	CA-C-N	-7.39	107.43	121.54
4	T	32	ASN	C-N-CA	-7.39	107.43	121.54
3	C	97	PHE	CB-CG-CD2	7.38	133.24	120.70
4	T	74	SER	CA-C-N	-7.38	110.85	122.65
4	T	74	SER	C-N-CA	-7.38	110.85	122.65
1	A	182	ALA	CA-C-O	-7.37	112.69	121.60
2	B	196	VAL	N-CA-CB	-7.36	99.08	111.23
2	B	50	TYR	O-C-N	7.35	133.45	122.94
2	B	155	VAL	CB-CA-C	-7.35	97.66	110.38
4	T	104	TYR	CA-C-O	-7.35	112.99	121.07
1	A	181	PHE	CA-CB-CG	7.34	121.14	113.80
2	B	194	LEU	CA-C-N	-7.33	112.70	123.11
2	B	194	LEU	C-N-CA	-7.33	112.70	123.11
2	B	90	PHE	O-C-N	7.33	131.92	123.27
2	B	105	PHE	N-CA-C	7.33	117.94	108.34
2	B	29	LEU	N-CA-C	-7.33	99.06	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ASP	N-CA-CB	7.32	123.19	112.13
2	B	190	LEU	CA-C-O	7.32	129.68	121.11
2	B	37	TYR	CA-C-N	-7.32	111.26	122.09
2	B	37	TYR	C-N-CA	-7.32	111.26	122.09
1	A	136	THR	CA-C-N	7.31	136.05	123.91
1	A	136	THR	C-N-CA	7.31	136.05	123.91
2	B	212	VAL	CB-CA-C	-7.31	100.18	110.12
1	A	92	ALA	N-CA-C	7.30	120.57	110.35
2	B	205	ARG	N-CA-C	-7.30	104.50	113.41
2	B	190	LEU	CB-CG-CD2	-7.30	88.81	110.70
1	A	43	PRO	N-CA-C	7.29	127.49	112.47
1	A	99	ILE	N-CA-CB	-7.29	102.72	111.90
2	B	215	TYR	CA-C-N	-7.28	107.13	121.41
2	B	215	TYR	C-N-CA	-7.28	107.13	121.41
3	C	77	THR	CA-C-O	-7.28	113.46	121.33
3	C	91	ALA	CA-C-O	-7.28	110.10	120.51
1	A	155	THR	CA-C-N	-7.28	110.58	122.81
1	A	155	THR	C-N-CA	-7.28	110.58	122.81
1	A	21	VAL	CA-C-O	-7.27	114.51	121.64
1	A	187	PHE	CB-CA-C	-7.27	98.95	111.45
2	B	137	HIS	CB-CA-C	-7.26	96.93	110.01
1	A	41	GLU	CA-C-O	-7.26	112.91	121.11
2	B	124	GLU	N-CA-CB	7.26	120.74	110.36
2	B	184	ASN	N-CA-CB	7.26	122.46	110.85
1	A	29	PHE	CA-CB-CG	-7.25	106.55	113.80
1	A	20	THR	CB-CA-C	-7.23	96.92	110.16
4	T	62	SER	CA-C-O	-7.23	110.17	120.51
2	B	72	LYS	CA-C-O	7.22	130.83	120.51
2	B	91	TYR	CG-CD1-CE1	7.22	132.03	121.20
3	C	107	GLN	CA-C-O	7.21	128.29	119.79
4	T	58	ASP	N-CA-C	-7.20	99.32	109.69
1	A	106	LEU	CA-C-N	-7.20	112.58	122.95
1	A	106	LEU	C-N-CA	-7.20	112.58	122.95
3	C	96	TYR	O-C-N	-7.20	114.92	123.27
2	B	238	GLU	CB-CA-C	-7.18	98.43	109.99
4	T	77	THR	CA-CB-CG2	-7.18	98.30	110.50
4	T	106	TYR	CA-C-O	7.18	130.15	121.68
1	A	108	VAL	CB-CA-C	-7.17	101.38	111.21
2	B	119	ASN	CA-CB-CG	7.17	119.77	112.60
2	B	227	ARG	CB-CG-CD	7.16	127.78	111.30
4	T	13	GLN	N-CA-CB	-7.16	100.62	110.29
1	A	32	LEU	N-CA-CB	7.16	124.84	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122	PRO	N-CA-CB	7.16	110.02	103.08
2	B	205	ARG	CB-CG-CD	7.16	127.76	111.30
2	B	27	GLN	OE1-CD-NE2	-7.16	115.44	122.60
2	B	222	GLU	N-CA-CB	7.15	122.57	110.49
1	A	79	ALA	N-CA-CB	-7.15	99.56	110.42
1	A	49	VAL	CB-CA-C	7.14	122.45	110.95
2	B	66	TYR	CB-CA-C	-7.14	96.11	111.11
1	A	89	CYS	CA-C-O	-7.14	113.29	121.72
2	B	104	TYR	CA-C-O	-7.14	112.82	121.89
2	B	227	ARG	CB-CA-C	-7.14	96.79	111.22
2	B	110	ARG	CB-CG-CD	7.14	127.72	111.30
1	A	39	PRO	CA-N-CD	7.14	121.99	112.00
2	B	212	VAL	N-CA-CB	-7.13	101.43	111.99
4	T	114	THR	CB-CA-C	-7.13	97.38	109.72
2	B	225	GLN	CB-CG-CD	-7.12	100.50	112.60
1	A	193	PRO	CA-C-N	-7.11	111.88	122.83
1	A	193	PRO	C-N-CA	-7.11	111.88	122.83
4	T	109	GLN	CA-C-O	-7.11	112.96	120.92
1	A	33	GLN	CA-C-N	-7.11	108.62	121.62
1	A	33	GLN	C-N-CA	-7.11	108.62	121.62
1	A	186	ALA	O-C-N	-7.10	112.67	122.46
2	B	64	GLU	N-CA-CB	-7.09	98.31	109.87
1	A	173	VAL	CA-C-O	7.09	128.96	120.67
2	B	91	TYR	O-C-N	7.09	132.07	122.57
1	A	108	VAL	CA-C-O	7.08	130.01	121.02
2	B	49	TYR	CA-CB-CG	-7.08	101.16	113.90
2	B	201	TRP	N-CA-CB	-7.07	99.99	110.53
1	A	41	GLU	N-CA-CB	7.07	123.17	111.08
2	B	43	GLN	O-C-N	7.07	132.00	122.59
4	T	98	LEU	CB-CG-CD1	7.07	131.91	110.70
1	A	158	CYS	N-CA-CB	-7.07	98.86	110.52
2	B	147	ALA	N-CA-CB	7.07	122.03	110.37
2	B	50	TYR	CE1-CZ-OH	7.07	141.10	119.90
1	A	102	LYS	CG-CD-CE	7.06	127.55	111.30
4	T	79	TYR	CA-C-O	-7.06	113.18	121.44
1	A	173	VAL	CA-CB-CG1	-7.06	98.41	110.40
1	A	84	THR	CA-CB-OG1	-7.05	99.03	109.60
1	A	134	LEU	CA-C-O	-7.05	112.82	120.36
1	A	170	ASN	CA-CB-CG	-7.04	105.56	112.60
4	T	53	ILE	N-CA-C	-7.04	99.49	109.63
2	B	19	GLN	O-C-N	-7.03	115.04	123.27
1	A	162	MET	N-CA-C	-7.03	95.52	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	LEU	CA-C-O	-7.03	111.59	119.67
2	B	112	THR	CB-CA-C	-7.02	98.50	110.16
1	A	56	LYS	O-C-N	7.02	132.01	123.16
1	A	171	SER	CA-C-O	-7.01	113.48	121.40
2	B	58	GLN	CB-CA-C	-7.01	95.00	109.94
2	B	215	TYR	N-CA-CB	-7.01	98.63	110.83
2	B	186	SER	N-CA-CB	-7.01	99.62	110.56
2	B	174	PRO	CA-N-CD	7.01	121.81	112.00
1	A	167	PHE	CA-CB-CG	7.00	120.80	113.80
1	A	146	GLN	N-CA-CB	-6.99	98.73	109.92
2	B	85	LYS	CA-CB-CG	6.99	128.09	114.10
1	A	5	GLU	O-C-N	6.99	131.62	123.30
1	A	51	THR	CA-C-N	6.99	126.74	120.10
1	A	51	THR	C-N-CA	6.99	126.74	120.10
1	A	150	SER	O-C-N	-6.99	114.14	122.46
2	B	11	LYS	O-C-N	-6.99	113.67	122.27
2	B	89	ALA	CA-C-N	-6.98	113.27	123.05
2	B	89	ALA	C-N-CA	-6.98	113.27	123.05
1	A	144	VAL	N-CA-C	6.98	113.68	106.21
1	A	175	TRP	CB-CG-CD2	-6.98	117.03	126.80
1	A	40	GLY	CA-C-N	-6.98	111.86	122.81
1	A	40	GLY	C-N-CA	-6.98	111.86	122.81
2	B	78	LEU	CA-C-N	-6.97	111.74	122.62
2	B	78	LEU	C-N-CA	-6.97	111.74	122.62
1	A	29	PHE	CB-CA-C	-6.97	94.08	109.56
2	B	217	LEU	N-CA-CB	6.96	122.00	110.52
1	A	108	VAL	CG1-CB-CG2	6.96	126.10	110.80
1	A	137	ASP	N-CA-C	-6.95	105.24	113.38
2	B	91	TYR	N-CA-C	6.95	120.18	108.23
4	T	79	TYR	N-CA-CB	6.94	123.63	111.55
2	B	209	ARG	CG-CD-NE	6.94	127.28	112.00
3	C	39	GLN	CA-C-O	-6.94	111.51	120.25
1	A	28	VAL	N-CA-CB	-6.93	98.60	111.91
3	C	26	GLY	CA-C-O	-6.93	113.09	121.83
4	T	39	GLN	CB-CA-C	-6.93	100.64	110.34
2	B	161	VAL	N-CA-CB	-6.92	98.81	112.24
4	T	94	TYR	CA-C-O	-6.92	113.29	121.11
4	T	23	VAL	CA-C-O	-6.91	112.74	120.97
4	T	96	ARG	CB-CA-C	-6.91	97.51	110.16
4	T	6	GLU	CB-CA-C	-6.91	97.73	109.83
2	B	55	ASN	CA-CB-CG	6.91	119.51	112.60
1	A	176	SER	N-CA-C	-6.90	98.03	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	37	TYR	CG-CD2-CE2	-6.90	110.85	121.20
4	T	101	ILE	CA-CB-CG1	-6.89	98.68	110.40
1	A	142	THR	CB-CA-C	-6.88	98.62	109.84
1	A	167	PHE	O-C-N	6.87	131.38	123.27
2	B	143	LEU	CB-CA-C	-6.87	98.19	109.53
2	B	151	TYR	CG-CD2-CE2	6.87	131.50	121.20
1	A	131	SER	N-CA-C	-6.87	98.21	109.40
3	C	91	ALA	CA-C-N	-6.87	113.77	123.11
3	C	91	ALA	C-N-CA	-6.87	113.77	123.11
4	T	76	ASN	CB-CG-ND2	6.87	126.70	116.40
2	B	17	GLU	N-CA-CB	-6.86	99.48	110.46
1	A	52	GLY	CA-C-O	-6.86	113.89	121.71
1	A	19	LEU	CB-CA-C	-6.86	98.20	111.78
4	T	19	ARG	N-CA-C	-6.85	95.95	107.80
4	T	98	LEU	CB-CA-C	-6.85	99.18	110.14
4	T	106	TYR	O-C-N	-6.84	113.16	122.94
2	B	40	ASP	CA-C-O	-6.84	113.50	120.96
2	B	41	PRO	CA-CB-CG	-6.84	91.50	104.50
1	A	46	LEU	N-CA-CB	6.83	120.31	110.40
1	A	169	SER	CA-C-N	-6.83	110.05	121.39
1	A	169	SER	C-N-CA	-6.83	110.05	121.39
3	C	45	ARG	CG-CD-NE	-6.83	96.98	112.00
3	C	36	TRP	CB-CG-CD1	6.83	137.14	126.90
2	B	30	ASN	N-CA-C	-6.82	98.14	109.46
2	B	235	VAL	N-CA-CB	6.79	122.44	111.23
3	C	37	TYR	CD1-CE1-CZ	-6.79	107.38	119.60
2	B	56	ASP	CA-CB-CG	6.79	119.39	112.60
2	B	61	ASP	O-C-N	6.79	129.42	122.09
2	B	13	LEU	O-C-N	-6.78	114.97	123.17
2	B	36	TRP	CB-CA-C	-6.78	95.92	109.35
2	B	70	ARG	CG-CD-NE	-6.77	97.10	112.00
3	C	96	TYR	CB-CG-CD1	-6.77	110.65	120.80
1	A	65	PHE	CB-CA-C	6.76	120.69	109.53
4	T	20	LEU	CA-C-N	-6.76	111.99	122.87
4	T	20	LEU	C-N-CA	-6.76	111.99	122.87
4	T	61	ASP	CA-C-N	6.75	134.43	121.54
4	T	61	ASP	C-N-CA	6.75	134.43	121.54
1	A	158	CYS	CA-C-O	-6.75	113.31	120.80
2	B	112	THR	CA-CB-CG2	-6.74	99.04	110.50
2	B	173	ASP	O-C-N	-6.74	114.73	121.27
2	B	158	SER	CA-CB-OG	6.74	124.57	111.10
3	C	48	VAL	CA-C-N	-6.74	111.30	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	48	VAL	C-N-CA	-6.74	111.30	122.21
2	B	91	TYR	CD1-CG-CD2	-6.73	108.00	118.10
1	A	13	ILE	CA-CB-CG2	6.73	121.94	110.50
2	B	20	ASN	N-CA-CB	-6.73	98.46	109.56
4	T	38	ARG	CA-CB-CG	6.73	127.55	114.10
2	B	176	PRO	N-CA-C	6.72	126.31	112.47
1	A	117	PRO	CA-CB-CG	-6.72	91.74	104.50
2	B	234	ILE	CB-CA-C	-6.71	101.98	111.38
3	C	34	VAL	CA-C-O	6.71	126.19	120.22
2	B	50	TYR	CZ-CE2-CD2	6.71	131.68	119.60
1	A	19	LEU	CA-C-O	-6.71	113.94	121.25
2	B	87	PRO	CA-N-CD	6.71	121.39	112.00
4	T	80	LEU	N-CA-C	-6.71	96.08	108.02
2	B	122	PRO	CA-N-CD	-6.70	102.62	112.00
2	B	140	LYS	N-CA-CB	-6.70	98.62	110.14
1	A	169	SER	N-CA-CB	6.69	121.37	110.32
2	B	119	ASN	O-C-N	6.69	130.58	122.35
2	B	104	TYR	CB-CA-C	-6.68	98.89	110.45
2	B	200	PHE	CA-CB-CG	-6.68	107.11	113.80
1	A	147	SER	CA-C-N	-6.67	112.01	122.49
1	A	147	SER	C-N-CA	-6.67	112.01	122.49
4	T	8	GLY	CA-C-N	-6.67	108.33	121.41
4	T	8	GLY	C-N-CA	-6.67	108.33	121.41
2	B	118	LYS	CA-C-O	-6.67	111.47	119.27
4	T	34	TYR	CG-CD2-CE2	6.67	131.20	121.20
1	A	46	LEU	N-CA-C	-6.66	105.15	113.55
1	A	67	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	159	VAL	CG1-CB-CG2	6.66	125.45	110.80
2	B	86	ASN	CA-C-N	-6.66	110.67	120.46
2	B	86	ASN	C-N-CA	-6.66	110.67	120.46
1	A	69	ARG	CB-CA-C	6.66	120.34	111.82
4	T	101	ILE	CA-CB-CG2	-6.64	99.21	110.50
3	C	38	ARG	CB-CA-C	-6.64	96.18	110.45
1	A	71	ASP	CB-CA-C	-6.63	99.02	110.95
3	C	15	GLY	O-C-N	6.63	129.98	122.42
1	A	29	PHE	O-C-N	6.63	130.96	123.27
1	A	155	THR	CB-CA-C	-6.63	96.52	111.30
2	B	31	HIS	CG-ND1-CE1	-6.63	98.03	109.30
4	T	19	ARG	CB-CA-C	-6.62	100.95	110.62
1	A	28	VAL	CA-C-N	6.62	133.22	122.29
1	A	28	VAL	C-N-CA	6.62	133.22	122.29
1	A	108	VAL	N-CA-C	6.62	118.93	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	58	GLN	CB-CG-CD	6.62	123.85	112.60
2	B	130	PRO	N-CA-C	-6.60	101.30	111.13
4	T	106	TYR	CA-CB-CG	-6.60	102.02	113.90
3	C	18	LEU	CA-C-N	-6.60	111.80	121.76
3	C	18	LEU	C-N-CA	-6.60	111.80	121.76
3	C	44	GLN	CG-CD-OE1	-6.60	107.60	120.80
1	A	117	PRO	N-CD-CG	-6.60	93.31	103.20
4	T	72	ASP	N-CA-CB	6.60	121.07	110.65
3	C	49	ALA	CA-C-N	-6.59	107.10	121.87
3	C	49	ALA	C-N-CA	-6.59	107.10	121.87
2	B	35	TYR	CB-CA-C	-6.59	96.64	109.68
3	C	98	ASN	CB-CA-C	-6.59	98.33	109.72
1	A	93	GLY	N-CA-C	-6.58	101.32	112.77
2	B	39	GLN	CB-CG-CD	-6.58	101.41	112.60
4	T	5	VAL	N-CA-C	-6.58	99.10	108.58
2	B	224	THR	CA-C-O	-6.58	111.81	119.64
1	A	48	THR	O-C-N	6.58	131.53	123.44
2	B	105	PHE	CE1-CZ-CE2	-6.58	108.16	120.00
1	A	199	PRO	CA-C-O	-6.58	108.63	120.60
2	B	67	SER	O-C-N	-6.58	115.75	123.25
2	B	103	GLN	OE1-CD-NE2	-6.57	116.03	122.60
1	A	115	PRO	CA-N-CD	-6.57	102.81	112.00
2	B	190	LEU	O-C-N	-6.57	115.17	123.24
3	C	33	SER	CA-C-O	-6.57	114.20	121.23
2	B	94	ALA	N-CA-CB	6.56	122.88	111.13
4	T	52	SER	CB-CA-C	-6.56	98.98	109.80
1	A	78	ALA	O-C-N	6.56	131.31	122.59
2	B	53	ILE	CA-C-N	-6.54	113.55	122.91
2	B	53	ILE	C-N-CA	-6.54	113.55	122.91
3	C	80	LEU	N-CA-CB	6.54	121.53	110.87
2	B	31	HIS	CB-CA-C	-6.54	96.39	110.45
4	T	16	GLY	O-C-N	-6.53	115.86	122.59
1	A	112	ILE	N-CA-CB	-6.53	103.64	110.95
2	B	142	THR	CA-CB-CG2	-6.52	99.42	110.50
3	C	87	PRO	N-CA-C	-6.51	105.72	113.86
1	A	4	LEU	N-CA-C	-6.51	99.60	109.95
1	A	186	ALA	CB-CA-C	6.51	123.59	109.99
2	B	105	PHE	O-C-N	6.51	132.83	122.61
4	T	11	VAL	CA-CB-CG1	6.51	121.46	110.40
2	B	124	GLU	CA-C-O	-6.50	114.33	121.87
2	B	187	ARG	CA-C-O	-6.50	114.29	121.89
2	B	23	LEU	CA-C-N	-6.50	111.60	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	23	LEU	C-N-CA	-6.50	111.60	122.64
2	B	91	TYR	CE1-CZ-CE2	-6.49	107.31	120.30
4	T	66	ARG	NE-CZ-NH1	-6.49	115.01	121.50
4	T	73	GLU	N-CA-CB	6.49	121.17	110.39
1	A	7	SER	CA-C-O	-6.49	114.53	120.50
1	A	104	THR	CA-C-O	-6.49	113.27	120.60
2	B	177	LEU	CD1-CG-CD2	-6.49	96.53	110.80
1	A	124	ASP	N-CA-CB	6.49	119.72	110.44
1	A	198	PHE	N-CA-C	-6.49	101.96	110.39
2	B	29	LEU	CA-C-N	-6.48	113.05	122.19
2	B	29	LEU	C-N-CA	-6.48	113.05	122.19
1	A	43	PRO	CB-CA-C	-6.48	100.87	111.56
2	B	42	GLY	O-C-N	6.48	131.12	122.70
2	B	179	GLU	CB-CA-C	-6.47	99.19	109.80
1	A	6	GLN	O-C-N	6.46	131.63	123.23
1	A	154	ILE	CA-C-O	-6.46	113.43	120.67
2	B	101	TYR	O-C-N	-6.46	114.00	122.59
2	B	57	PHE	N-CA-CB	-6.46	99.44	111.13
4	T	6	GLU	O-C-N	6.46	130.17	122.94
1	A	48	THR	N-CA-CB	6.46	121.43	110.71
1	A	159	VAL	CA-C-O	-6.45	112.82	121.02
2	B	98	ARG	N-CA-CB	6.45	121.39	110.49
2	B	235	VAL	CB-CA-C	-6.45	100.71	111.29
2	B	227	ARG	CA-C-N	-6.45	109.22	121.54
2	B	227	ARG	C-N-CA	-6.45	109.22	121.54
1	A	149	ASP	CA-C-N	-6.43	112.51	122.16
1	A	149	ASP	C-N-CA	-6.43	112.51	122.16
2	B	64	GLU	CB-CA-C	-6.43	99.74	110.29
4	T	21	SER	N-CA-C	-6.42	99.75	109.95
3	C	65	GLY	CA-C-O	-6.41	111.67	119.68
4	T	14	PRO	CA-C-N	6.40	134.35	121.93
4	T	14	PRO	C-N-CA	6.40	134.35	121.93
2	B	231	VAL	O-C-N	-6.40	114.57	122.57
1	A	148	LYS	N-CA-C	-6.40	104.09	112.41
2	B	191	SER	N-CA-CB	-6.40	100.83	111.20
2	B	154	HIS	N-CA-C	-6.39	92.84	107.48
3	C	101	ARG	CA-C-N	6.39	131.19	122.63
3	C	101	ARG	C-N-CA	6.39	131.19	122.63
2	B	141	ALA	N-CA-CB	6.38	121.27	110.49
1	A	44	VAL	O-C-N	6.37	129.64	123.14
2	B	195	ARG	CA-CB-CG	6.37	126.85	114.10
1	A	34	TRP	N-CA-C	-6.37	99.05	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	13	GLN	CB-CG-CD	6.36	123.42	112.60
4	T	26	GLY	O-C-N	-6.36	116.70	123.00
4	T	7	SER	CB-CA-C	6.36	120.22	110.62
2	B	105	PHE	CD1-CE1-CZ	6.35	131.43	120.00
4	T	19	ARG	CB-CG-CD	-6.35	96.69	111.30
3	C	11	LEU	N-CA-CB	6.35	121.01	110.85
3	C	49	ALA	O-C-N	6.35	130.85	123.17
4	T	46	GLU	CA-C-O	-6.35	113.62	120.92
2	B	79	THR	CB-CA-C	-6.35	96.11	109.38
2	B	115	GLU	CA-C-O	-6.34	113.70	120.42
2	B	9	SER	N-CA-C	-6.34	102.52	108.22
3	C	111	VAL	CA-C-O	-6.33	113.74	120.39
2	B	58	GLN	N-CA-C	-6.33	99.05	108.99
4	T	108	GLY	N-CA-C	-6.33	101.85	111.10
2	B	122	PRO	N-CA-C	6.33	118.42	110.70
3	C	51	ILE	CA-CB-CG2	6.33	121.25	110.50
4	T	76	ASN	OD1-CG-ND2	-6.32	116.28	122.60
4	T	13	GLN	CA-C-N	6.32	127.74	119.84
4	T	13	GLN	C-N-CA	6.32	127.74	119.84
3	C	38	ARG	N-CA-CB	6.31	122.20	111.66
1	A	127	SER	CA-C-N	6.31	136.71	122.19
1	A	127	SER	C-N-CA	6.31	136.71	122.19
2	B	88	THR	CB-CA-C	-6.29	96.53	109.94
1	A	110	PRO	O-C-N	-6.29	115.59	123.21
1	A	121	GLN	CA-C-O	-6.29	113.68	120.92
2	B	47	LEU	CB-CA-C	-6.29	99.48	109.80
3	C	104	TYR	CB-CA-C	-6.29	98.75	109.51
1	A	33	GLN	N-CA-C	-6.29	99.60	108.96
1	A	160	LEU	CB-CG-CD2	-6.28	91.85	110.70
4	T	67	PHE	O-C-N	-6.28	115.21	122.93
1	A	189	ASN	CB-CA-C	-6.28	98.73	109.65
3	C	76	ASN	N-CA-C	-6.28	104.20	113.61
1	A	69	ARG	CG-CD-NE	-6.27	98.20	112.00
2	B	85	LYS	CA-C-O	6.26	129.46	120.51
1	A	47	VAL	CA-C-O	-6.25	112.96	120.78
3	C	2	VAL	N-CA-C	-6.25	93.49	111.00
2	B	29	LEU	O-C-N	-6.24	115.98	123.03
1	A	35	TYR	N-CA-C	6.23	118.61	108.76
3	C	112	THR	N-CA-C	6.23	119.97	109.76
2	B	74	GLU	CB-CA-C	-6.22	100.20	110.72
1	A	159	VAL	CB-CA-C	-6.22	102.69	111.21
2	B	138	THR	N-CA-C	-6.22	106.66	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	69	ILE	CA-C-O	-6.22	112.87	121.51
4	T	34	TYR	N-CA-CB	6.22	123.08	111.52
2	B	11	LYS	CA-C-N	6.22	132.26	122.94
2	B	11	LYS	C-N-CA	6.22	132.26	122.94
2	B	20	ASN	N-CA-C	6.22	119.05	110.35
2	B	164	LYS	CA-C-O	-6.21	113.52	120.66
3	C	3	GLN	CA-C-N	-6.21	112.08	122.64
3	C	3	GLN	C-N-CA	-6.21	112.08	122.64
4	T	92	ALA	CA-C-N	-6.21	114.36	123.05
4	T	92	ALA	C-N-CA	-6.21	114.36	123.05
2	B	131	SER	CA-C-N	-6.21	108.89	121.18
2	B	131	SER	C-N-CA	-6.21	108.89	121.18
1	A	153	TYR	CA-C-N	-6.20	114.32	122.94
1	A	153	TYR	C-N-CA	-6.20	114.32	122.94
2	B	17	GLU	CA-C-O	-6.20	114.40	121.72
2	B	144	VAL	N-CA-CB	-6.20	100.94	110.86
2	B	174	PRO	N-CA-CB	-6.20	96.75	103.25
3	C	53	THR	CA-C-N	6.19	133.18	122.09
3	C	53	THR	C-N-CA	6.19	133.18	122.09
1	A	72	SER	CA-C-O	-6.19	114.81	121.38
1	A	102	LYS	N-CA-CB	-6.19	99.80	110.32
2	B	138	THR	CA-CB-CG2	-6.19	99.98	110.50
1	A	163	ARG	CG-CD-NE	-6.18	98.39	112.00
4	T	32	ASN	CA-CB-CG	6.18	118.78	112.60
2	B	146	LEU	CA-CB-CG	-6.18	94.66	116.30
4	T	28	VAL	CA-C-N	-6.18	112.70	122.95
4	T	28	VAL	C-N-CA	-6.18	112.70	122.95
1	A	2	GLN	CA-C-N	6.17	129.88	121.05
1	A	2	GLN	C-N-CA	6.17	129.88	121.05
1	A	177	ASN	CA-C-O	-6.17	114.83	121.56
1	A	179	SER	N-CA-CB	6.16	120.90	110.49
2	B	50	TYR	CG-CD2-CE2	6.16	130.44	121.20
4	T	59	TYR	N-CA-C	-6.16	99.48	107.73
1	A	17	GLU	O-C-N	-6.16	115.08	122.65
1	A	33	GLN	O-C-N	-6.16	116.02	123.10
4	T	24	ALA	N-CA-CB	6.16	120.46	110.43
2	B	183	LEU	N-CA-CB	6.15	119.16	110.36
3	C	52	VAL	CA-C-N	-6.15	111.62	122.26
3	C	52	VAL	C-N-CA	-6.15	111.62	122.26
1	A	188	ASN	O-C-N	6.15	130.67	122.43
3	C	100	ILE	N-CA-CB	6.15	118.97	112.21
4	T	93	TYR	CA-C-N	-6.14	113.17	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	93	TYR	C-N-CA	-6.14	113.17	122.81
3	C	105	TRP	CB-CG-CD2	-6.13	118.21	126.80
1	A	122	LEU	CA-C-O	-6.13	113.56	120.43
4	T	66	ARG	N-CA-CB	6.13	120.85	110.49
3	C	38	ARG	CA-C-O	-6.13	114.71	121.33
3	C	64	LYS	CB-CA-C	6.12	120.81	109.54
3	C	90	THR	CA-C-N	-6.12	109.85	121.54
3	C	90	THR	C-N-CA	-6.12	109.85	121.54
4	T	53	ILE	CA-CB-CG1	-6.12	100.00	110.40
4	T	85	LEU	CB-CA-C	6.12	121.53	109.66
1	A	165	MET	CA-C-N	6.12	130.82	122.19
1	A	165	MET	C-N-CA	6.12	130.82	122.19
4	T	11	VAL	CA-CB-CG2	6.12	120.80	110.40
4	T	50	HIS	CA-CB-CG	-6.12	107.68	113.80
1	A	19	LEU	CA-C-N	-6.11	109.90	121.63
1	A	19	LEU	C-N-CA	-6.11	109.90	121.63
1	A	106	LEU	O-C-N	6.11	130.42	122.97
4	T	113	VAL	CG1-CB-CG2	6.11	124.23	110.80
3	C	69	ILE	CA-CB-CG2	-6.10	100.13	110.50
2	B	196	VAL	CB-CA-C	-6.10	101.29	111.29
1	A	197	PHE	CD1-CG-CD2	-6.09	109.46	118.60
1	A	14	GLN	N-CA-C	-6.09	101.50	110.52
2	B	224	THR	N-CA-C	-6.09	105.75	113.43
1	A	71	ASP	O-C-N	-6.09	117.20	123.29
1	A	172	ALA	CA-C-O	6.09	127.81	120.99
2	B	177	LEU	O-C-N	-6.09	115.53	123.02
2	B	57	PHE	O-C-N	-6.09	116.29	123.41
1	A	172	ALA	O-C-N	-6.08	116.45	123.33
1	A	51	THR	CA-C-O	-6.08	114.54	121.72
2	B	22	THR	CB-CA-C	-6.08	99.93	109.84
3	C	102	GLY	O-C-N	6.08	129.56	123.48
1	A	118	ALA	CB-CA-C	6.08	120.13	109.80
4	T	89	ASP	CA-C-N	-6.08	112.91	121.72
4	T	89	ASP	C-N-CA	-6.08	112.91	121.72
2	B	62	ILE	CA-CB-CG2	-6.07	100.19	110.50
2	B	227	ARG	CA-C-O	-6.06	114.27	121.60
2	B	105	PHE	CB-CG-CD2	6.06	131.00	120.70
3	C	58	HIS	CA-CB-CG	-6.06	107.74	113.80
4	T	100	ARG	CD-NE-CZ	-6.06	115.92	124.40
2	B	161	VAL	N-CA-C	6.06	118.50	109.17
2	B	8	GLN	N-CA-CB	6.05	121.97	111.13
2	B	116	ASP	CA-C-N	-6.05	109.97	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	116	ASP	C-N-CA	-6.05	109.97	121.54
1	A	145	SER	N-CA-C	-6.05	101.71	110.24
3	C	2	VAL	O-C-N	6.04	132.67	123.00
2	B	195	ARG	NE-CZ-NH1	6.04	127.54	121.50
3	C	101	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	A	44	VAL	CA-C-O	-6.04	113.84	120.72
1	A	197	PHE	CA-C-O	6.04	127.04	120.58
2	B	193	ARG	CG-CD-NE	-6.04	98.72	112.00
4	T	100	ARG	CA-CB-CG	6.04	126.17	114.10
2	B	14	PHE	CB-CG-CD1	-6.03	110.44	120.70
2	B	30	ASN	CB-CA-C	6.03	119.69	109.80
3	C	36	TRP	CD2-CE2-CZ2	-6.03	116.37	122.40
2	B	237	ALA	CA-C-O	-6.03	114.78	121.23
3	C	63	VAL	CA-C-N	6.03	130.40	120.94
3	C	63	VAL	C-N-CA	6.03	130.40	120.94
1	A	35	TYR	CA-C-O	-6.02	114.27	120.89
1	A	36	ARG	CB-CA-C	-6.02	97.47	109.33
2	B	133	ALA	O-C-N	6.02	128.59	122.09
2	B	110	ARG	CG-CD-NE	-6.02	98.76	112.00
3	C	59	TYR	N-CA-CB	6.02	120.72	111.22
1	A	154	ILE	N-CA-CB	-6.01	101.58	111.44
2	B	147	ALA	CA-C-O	-6.01	114.29	120.54
2	B	240	TRP	CE2-CD2-CE3	-6.00	112.80	118.80
2	B	52	GLN	OE1-CD-NE2	-6.00	116.60	122.60
3	C	74	ALA	CA-C-N	6.00	130.64	122.07
3	C	74	ALA	C-N-CA	6.00	130.64	122.07
2	B	190	LEU	CB-CA-C	5.99	121.91	109.38
1	A	7	SER	O-C-N	-5.99	117.88	121.71
1	A	200	SER	CB-CA-C	5.99	121.48	110.10
2	B	102	GLU	CB-CG-CD	5.99	122.78	112.60
2	B	69	SER	O-C-N	-5.99	115.97	123.27
4	T	85	LEU	CA-C-O	-5.99	114.45	121.46
2	B	29	LEU	CA-C-O	5.99	128.96	121.66
4	T	95	CYS	CA-CB-SG	5.98	128.16	114.40
2	B	116	ASP	CB-CA-C	-5.98	98.52	110.42
4	T	79	TYR	N-CA-C	-5.98	100.25	109.52
2	B	15	ARG	NE-CZ-NH2	5.98	124.58	119.20
4	T	94	TYR	CE1-CZ-OH	5.98	137.83	119.90
1	A	71	ASP	N-CA-C	-5.97	99.06	108.14
1	A	89	CYS	CB-CA-C	5.97	120.28	109.83
2	B	214	PHE	CB-CA-C	-5.97	98.90	109.70
2	B	143	LEU	O-C-N	-5.96	116.24	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	11	LEU	O-C-N	5.96	130.67	123.16
4	T	100	ARG	CG-CD-NE	-5.96	98.89	112.00
1	A	14	GLN	N-CA-CB	5.96	119.99	110.46
3	C	61	ASP	CA-C-O	-5.95	112.00	120.51
2	B	16	LYS	CA-C-N	-5.95	110.11	122.07
2	B	16	LYS	C-N-CA	-5.95	110.11	122.07
2	B	215	TYR	O-C-N	5.95	130.96	123.23
2	B	110	ARG	CA-C-O	-5.94	113.83	120.54
1	A	35	TYR	CA-C-N	-5.94	113.48	122.81
1	A	35	TYR	C-N-CA	-5.94	113.48	122.81
2	B	76	PHE	CA-C-N	5.93	127.26	119.84
2	B	76	PHE	C-N-CA	5.93	127.26	119.84
3	C	59	TYR	CA-C-N	-5.93	110.20	121.54
3	C	59	TYR	C-N-CA	-5.93	110.20	121.54
4	T	21	SER	N-CA-CB	-5.93	101.36	110.85
2	B	45	LEU	O-C-N	-5.92	116.58	123.27
2	B	119	ASN	OD1-CG-ND2	5.92	128.52	122.60
1	A	154	ILE	CA-CB-CG2	-5.92	100.44	110.50
2	B	118	LYS	CG-CD-CE	5.92	124.91	111.30
3	C	90	THR	CA-CB-OG1	5.92	118.47	109.60
2	B	96	SER	N-CA-C	-5.91	100.09	109.07
3	C	92	VAL	CA-C-O	-5.91	113.75	120.66
1	A	173	VAL	O-C-N	-5.91	116.80	123.18
4	T	92	ALA	O-C-N	5.91	129.95	123.04
1	A	42	GLY	CA-C-N	5.90	127.22	119.84
1	A	42	GLY	C-N-CA	5.90	127.22	119.84
2	B	118	LYS	N-CA-C	-5.90	105.91	113.23
1	A	128	SER	CB-CA-C	-5.90	99.88	110.03
1	A	156	ASP	N-CA-CB	5.90	120.76	111.20
1	A	83	ASP	O-C-N	5.90	130.51	122.37
1	A	110	PRO	CA-N-CD	5.89	120.25	112.00
2	B	61	ASP	CA-CB-CG	5.89	118.49	112.60
4	T	102	TRP	CG-CD1-NE1	5.89	117.86	110.20
2	B	50	TYR	N-CA-CB	-5.89	102.22	111.05
3	C	76	ASN	CA-C-N	-5.89	111.57	121.75
3	C	76	ASN	C-N-CA	-5.89	111.57	121.75
2	B	208	PHE	CA-C-O	-5.88	114.79	121.72
2	B	31	HIS	N-CA-C	-5.87	100.14	109.07
4	T	93	TYR	O-C-N	5.87	130.20	123.27
1	A	61	LEU	N-CA-CB	5.87	118.92	110.06
3	C	34	VAL	CG1-CB-CG2	5.87	123.71	110.80
2	B	132	GLU	N-CA-C	-5.87	105.97	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLN	O-C-N	5.85	129.95	123.16
2	B	221	ASP	CB-CA-C	5.85	118.41	109.34
1	A	159	VAL	O-C-N	-5.85	116.04	122.83
2	B	223	TRP	CA-C-N	-5.85	110.47	122.58
2	B	223	TRP	C-N-CA	-5.85	110.47	122.58
3	C	44	GLN	CB-CA-C	-5.84	103.97	113.37
2	B	237	ALA	N-CA-CB	-5.84	102.51	111.56
2	B	39	GLN	CA-C-O	-5.84	114.05	120.24
2	B	200	PHE	CD1-CE1-CZ	-5.84	109.49	120.00
2	B	128	PHE	N-CA-CB	-5.83	100.37	110.17
2	B	180	GLN	N-CA-C	-5.83	96.92	109.81
3	C	81	GLN	CB-CA-C	-5.83	98.81	109.54
1	A	123	ARG	CA-CB-CG	5.82	125.75	114.10
2	B	107	PRO	CA-C-O	-5.82	110.00	120.60
2	B	216	GLY	CA-C-N	-5.82	113.98	122.65
2	B	216	GLY	C-N-CA	-5.82	113.98	122.65
3	C	99	LEU	N-CA-C	-5.81	98.42	110.80
1	A	84	THR	CA-C-O	-5.81	114.80	121.19
1	A	15	GLU	CB-CG-CD	-5.81	102.72	112.60
4	T	47	LYS	O-C-N	5.81	129.56	123.06
1	A	183	CYS	CA-C-O	5.80	126.91	120.82
1	A	132	VAL	CG1-CB-CG2	5.79	123.54	110.80
1	A	136	THR	OG1-CB-CG2	5.79	120.88	109.30
4	T	7	SER	CA-C-N	-5.79	113.54	122.69
4	T	7	SER	C-N-CA	-5.79	113.54	122.69
1	A	119	VAL	O-C-N	-5.79	116.12	122.83
3	C	105	TRP	N-CA-CB	5.79	120.63	111.43
4	T	99	SER	N-CA-CB	-5.78	100.80	110.80
3	C	81	GLN	N-CA-C	-5.78	102.35	110.50
1	A	176	SER	CB-CA-C	-5.78	100.69	109.99
4	T	83	ASN	CA-C-N	-5.78	111.84	121.89
4	T	83	ASN	C-N-CA	-5.78	111.84	121.89
4	T	6	GLU	CB-CG-CD	5.77	122.41	112.60
1	A	70	LYS	O-C-N	-5.77	114.76	122.49
2	B	212	VAL	O-C-N	5.76	128.97	123.03
2	B	214	PHE	N-CA-CB	5.76	120.76	110.80
3	C	103	ARG	N-CA-C	5.76	118.92	109.76
4	T	107	TRP	CB-CA-C	-5.76	100.05	111.91
2	B	14	PHE	CA-C-N	-5.75	111.96	121.80
2	B	14	PHE	C-N-CA	-5.75	111.96	121.80
3	C	112	THR	CB-CA-C	5.75	119.15	109.48
1	A	189	ASN	CA-CB-CG	-5.75	106.85	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	99	SER	CB-CA-C	-5.74	99.30	109.70
1	A	170	ASN	N-CA-CB	-5.74	101.57	110.29
2	B	35	TYR	CA-C-N	5.74	132.03	122.73
2	B	35	TYR	C-N-CA	5.74	132.03	122.73
3	C	46	GLU	O-C-N	5.74	129.81	123.33
1	A	18	ASN	N-CA-CB	-5.74	101.70	110.42
4	T	1	ASP	CA-C-O	-5.73	111.06	120.80
2	B	35	TYR	CB-CG-CD1	5.73	129.40	120.80
3	C	61	ASP	N-CA-C	-5.73	98.60	110.80
2	B	148	THR	OG1-CB-CG2	-5.73	97.84	109.30
1	A	32	LEU	CA-C-O	-5.73	114.58	120.99
2	B	45	LEU	CB-CA-C	5.72	119.19	109.75
2	B	118	LYS	N-CA-CB	-5.72	101.52	110.44
4	T	62	SER	CA-C-N	5.71	130.51	122.05
4	T	62	SER	C-N-CA	5.71	130.51	122.05
2	B	185	ASP	CA-CB-CG	5.71	118.31	112.60
4	T	110	GLY	N-CA-C	5.71	119.87	112.68
3	C	77	THR	OG1-CB-CG2	-5.71	97.89	109.30
2	B	37	TYR	CA-CB-CG	-5.70	103.64	113.90
3	C	19	ARG	CA-C-N	5.70	128.93	120.95
3	C	19	ARG	C-N-CA	5.70	128.93	120.95
1	A	38	GLU	CB-CA-C	-5.69	100.96	108.76
3	C	52	VAL	CA-CB-CG1	-5.69	100.72	110.40
4	T	53	ILE	CA-C-O	-5.69	115.10	121.36
4	T	68	THR	CA-C-O	-5.69	114.17	120.38
2	B	134	GLU	CA-C-N	5.69	127.73	120.56
2	B	134	GLU	C-N-CA	5.69	127.73	120.56
2	B	207	HIS	CB-CA-C	5.69	120.06	110.79
1	A	70	LYS	CB-CG-CD	5.69	124.38	111.30
3	C	64	LYS	N-CA-CB	-5.69	101.98	110.17
1	A	45	LEU	N-CA-C	-5.69	100.41	109.96
1	A	60	ARG	CA-C-N	5.69	129.55	121.42
1	A	60	ARG	C-N-CA	5.69	129.55	121.42
2	B	191	SER	CA-C-N	-5.69	112.91	122.29
2	B	191	SER	C-N-CA	-5.69	112.91	122.29
2	B	90	PHE	CA-C-N	5.68	131.38	122.17
2	B	90	PHE	C-N-CA	5.68	131.38	122.17
4	T	113	VAL	CA-CB-CG1	5.68	120.06	110.40
1	A	144	VAL	N-CA-CB	-5.68	106.60	112.28
2	B	40	ASP	CA-CB-CG	5.68	118.28	112.60
2	B	161	VAL	CB-CA-C	-5.68	103.43	111.38
1	A	11	LEU	O-C-N	-5.67	116.46	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ARG	CB-CA-C	5.67	120.21	110.79
3	C	64	LYS	CA-C-N	5.67	130.10	120.91
3	C	64	LYS	C-N-CA	5.67	130.10	120.91
2	B	42	GLY	N-CA-C	-5.67	99.74	113.18
2	B	139	GLN	OE1-CD-NE2	5.66	128.26	122.60
4	T	115	VAL	CB-CA-C	-5.66	103.39	111.31
2	B	114	THR	CB-CA-C	-5.65	99.95	109.50
2	B	141	ALA	CA-C-N	5.65	130.19	122.84
2	B	141	ALA	C-N-CA	5.65	130.19	122.84
1	A	37	GLN	CB-CA-C	-5.65	102.94	110.79
2	B	104	TYR	N-CA-C	5.65	118.82	110.46
1	A	107	SER	O-C-N	-5.65	114.41	122.99
3	C	3	GLN	N-CA-CB	5.64	118.69	109.95
1	A	12	SER	N-CA-C	-5.64	101.18	109.81
1	A	109	LYS	N-CA-C	-5.64	97.35	109.81
2	B	68	VAL	CG1-CB-CG2	-5.64	98.39	110.80
4	T	102	TRP	CG-CD2-CE3	-5.64	128.26	133.90
2	B	206	ASN	CA-C-N	5.64	131.12	123.11
2	B	206	ASN	C-N-CA	5.64	131.12	123.11
2	B	163	GLY	CA-C-N	-5.64	113.60	122.73
2	B	163	GLY	C-N-CA	-5.64	113.60	122.73
1	A	108	VAL	O-C-N	-5.63	116.30	122.83
1	A	65	PHE	CA-CB-CG	5.63	119.43	113.80
3	C	68	THR	CA-C-O	-5.63	112.46	120.51
4	T	6	GLU	CA-C-N	-5.63	114.87	122.86
4	T	6	GLU	C-N-CA	-5.63	114.87	122.86
4	T	25	SER	CA-C-O	5.63	128.02	121.44
2	B	194	LEU	N-CA-C	-5.62	98.07	107.80
2	B	69	SER	CA-C-N	-5.62	114.51	122.94
2	B	69	SER	C-N-CA	-5.62	114.51	122.94
2	B	113	VAL	CG1-CB-CG2	-5.62	98.44	110.80
1	A	100	PHE	CB-CG-CD1	-5.61	111.16	120.70
2	B	133	ALA	CA-C-O	-5.61	114.92	120.70
3	C	34	VAL	O-C-N	-5.61	117.93	122.97
1	A	59	LYS	CB-CA-C	5.60	121.56	110.42
4	T	35	GLY	CA-C-N	-5.60	114.81	122.93
4	T	35	GLY	C-N-CA	-5.60	114.81	122.93
3	C	30	GLY	O-C-N	-5.59	115.43	122.70
1	A	20	THR	CA-C-O	-5.59	114.74	120.89
2	B	178	LYS	CB-CA-C	-5.59	101.13	110.29
2	B	19	GLN	CA-CB-CG	5.59	125.27	114.10
2	B	33	ALA	N-CA-CB	5.58	119.53	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	VAL	CA-CB-CG2	-5.58	100.91	110.40
4	T	18	LEU	N-CA-C	-5.58	100.23	108.99
1	A	176	SER	N-CA-CB	5.58	120.11	111.24
1	A	179	SER	CB-CA-C	5.58	121.52	110.42
4	T	5	VAL	CA-CB-CG2	5.57	119.88	110.40
4	T	111	THR	CA-C-N	-5.57	113.53	121.50
4	T	111	THR	C-N-CA	-5.57	113.53	121.50
4	T	3	GLN	CB-CA-C	-5.57	99.34	110.42
1	A	155	THR	CA-C-O	-5.57	116.17	122.01
4	T	28	VAL	CA-CB-CG1	5.56	119.85	110.40
2	B	145	CYS	CA-C-O	-5.56	114.32	120.38
2	B	166	VAL	CG1-CB-CG2	-5.56	98.58	110.80
3	C	50	THR	CA-C-O	-5.56	114.53	120.75
1	A	37	GLN	OE1-CD-NE2	-5.55	117.05	122.60
2	B	126	ALA	CB-CA-C	-5.55	98.11	109.94
4	T	33	PHE	N-CA-C	-5.55	98.98	110.80
4	T	47	LYS	CD-CE-NZ	-5.55	94.14	111.90
2	B	208	PHE	N-CA-C	-5.54	102.32	110.52
2	B	39	GLN	CG-CD-OE1	5.54	131.88	120.80
2	B	137	HIS	N-CA-C	5.54	120.03	113.16
3	C	71	ARG	CA-C-N	-5.54	113.51	122.81
3	C	71	ARG	C-N-CA	-5.54	113.51	122.81
4	T	30	LYS	CB-CA-C	-5.54	100.49	109.13
4	T	80	LEU	CB-CG-CD1	5.54	127.31	110.70
2	B	21	VAL	CA-C-N	5.53	129.41	121.50
2	B	21	VAL	C-N-CA	5.53	129.41	121.50
1	A	61	LEU	O-C-N	5.53	129.54	123.01
1	A	158	CYS	CB-CA-C	-5.53	100.19	109.48
1	A	82	GLY	N-CA-C	-5.53	108.59	114.67
1	A	192	ILE	CB-CA-C	5.52	121.41	111.36
2	B	31	HIS	ND1-CE1-NE2	5.52	113.92	108.40
4	T	27	TYR	CA-C-N	-5.52	112.04	121.97
4	T	27	TYR	C-N-CA	-5.52	112.04	121.97
4	T	86	ARG	CA-C-O	-5.52	115.02	120.26
4	T	33	PHE	O-C-N	-5.51	115.26	122.59
2	B	46	ARG	CB-CG-CD	5.51	123.98	111.30
2	B	48	ILE	N-CA-CB	-5.51	102.14	111.23
2	B	200	PHE	CZ-CE2-CD2	-5.51	110.08	120.00
1	A	86	LEU	CA-C-N	-5.51	114.40	122.06
1	A	86	LEU	C-N-CA	-5.51	114.40	122.06
2	B	168	SER	O-C-N	5.51	129.61	123.05
2	B	115	GLU	O-C-N	5.51	128.43	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ASN	CA-C-O	5.51	125.43	119.15
2	B	72	LYS	CB-CA-C	5.50	121.37	110.42
2	B	136	SER	CB-CA-C	-5.50	102.20	110.90
1	A	167	PHE	CA-C-N	-5.50	113.24	122.92
1	A	167	PHE	C-N-CA	-5.50	113.24	122.92
2	B	84	GLN	N-CA-CB	-5.50	103.28	110.59
2	B	196	VAL	CA-C-N	-5.50	111.17	120.95
2	B	196	VAL	C-N-CA	-5.50	111.17	120.95
3	C	101	ARG	CD-NE-CZ	5.49	132.09	124.40
2	B	151	TYR	CB-CG-CD2	-5.49	112.56	120.80
4	T	77	THR	N-CA-CB	-5.49	100.95	110.17
1	A	8	PRO	N-CA-CB	-5.48	96.57	102.60
2	B	211	GLN	CA-C-N	-5.48	114.31	122.70
2	B	211	GLN	C-N-CA	-5.48	114.31	122.70
4	T	38	ARG	CG-CD-NE	-5.48	99.95	112.00
4	T	38	ARG	N-CA-CB	-5.48	103.07	111.56
3	C	60	ARG	N-CA-C	-5.47	99.14	110.80
1	A	145	SER	CB-CA-C	-5.47	100.89	109.70
2	B	158	SER	N-CA-C	5.46	117.99	109.52
1	A	103	GLY	O-C-N	5.46	129.80	122.70
1	A	166	ASP	CA-C-N	5.46	130.69	123.05
1	A	166	ASP	C-N-CA	5.46	130.69	123.05
2	B	110	ARG	CD-NE-CZ	5.46	132.04	124.40
2	B	214	PHE	O-C-N	5.46	129.69	123.31
2	B	134	GLU	N-CA-C	-5.45	105.42	111.36
3	C	104	TYR	CB-CG-CD2	-5.45	112.63	120.80
2	B	97	SER	N-CA-C	5.45	117.88	107.75
2	B	158	SER	CB-CA-C	-5.44	98.63	109.79
4	T	31	ILE	CB-CA-C	5.44	118.65	110.98
2	B	187	ARG	CG-CD-NE	-5.44	100.03	112.00
3	C	72	ASP	CA-C-O	-5.44	115.10	121.46
2	B	116	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	12	SER	CA-C-O	-5.44	115.26	121.68
2	B	12	TYR	O-C-N	5.43	130.29	123.23
2	B	109	THR	OG1-CB-CG2	5.43	120.15	109.30
2	B	189	SER	CA-CB-OG	5.42	121.94	111.10
2	B	170	VAL	CB-CA-C	-5.42	104.19	110.91
2	B	137	HIS	O-C-N	-5.42	114.89	122.37
1	A	35	TYR	CB-CA-C	-5.41	100.26	110.16
2	B	144	VAL	O-C-N	-5.41	117.20	122.93
4	T	90	THR	OG1-CB-CG2	5.41	120.11	109.30
3	C	36	TRP	CG-CD2-CE3	-5.40	128.50	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	18	LEU	N-CA-CB	5.39	121.55	111.52
2	B	161	VAL	O-C-N	-5.39	115.89	122.36
1	A	143	ASN	CB-CA-C	-5.39	102.00	110.79
2	B	22	THR	CA-C-O	-5.39	114.54	120.69
2	B	196	VAL	CA-C-O	5.39	127.52	120.78
4	T	80	LEU	CA-C-N	-5.39	114.79	122.77
4	T	80	LEU	C-N-CA	-5.39	114.79	122.77
2	B	146	LEU	CB-CA-C	5.39	120.49	111.22
4	T	37	TYR	N-CA-CB	-5.38	100.88	110.14
2	B	38	ARG	CA-CB-CG	-5.38	103.34	114.10
3	C	70	SER	CA-C-O	-5.38	112.81	120.51
4	T	8	GLY	O-C-N	5.38	129.61	123.21
1	A	19	LEU	N-CA-CB	-5.38	102.02	111.49
2	B	77	PRO	CA-C-N	5.37	129.51	121.72
2	B	77	PRO	C-N-CA	5.37	129.51	121.72
2	B	110	ARG	NH1-CZ-NH2	5.37	126.28	119.30
2	B	73	LYS	N-CA-C	5.37	122.23	110.80
2	B	87	PRO	CA-C-N	-5.37	112.35	121.85
2	B	87	PRO	C-N-CA	-5.37	112.35	121.85
4	T	84	SER	CA-C-O	-5.36	112.97	120.21
3	C	32	HIS	N-CA-C	-5.36	99.38	110.80
4	T	29	HIS	N-CA-CB	-5.36	102.86	110.79
4	T	58	ASP	CA-C-O	5.36	128.08	121.60
2	B	56	ASP	O-C-N	-5.36	116.77	123.04
4	T	103	PRO	N-CA-C	-5.36	98.18	112.10
4	T	69	ILE	N-CA-CB	-5.35	101.63	111.91
2	B	150	PHE	CA-C-O	-5.35	115.06	121.11
1	A	35	TYR	CG-CD1-CE1	5.35	129.23	121.20
2	B	157	LEU	CD1-CG-CD2	-5.35	99.03	110.80
2	B	9	SER	O-C-N	5.35	126.58	121.71
2	B	121	PHE	CA-CB-CG	5.35	119.15	113.80
1	A	111	ASN	N-CA-CB	5.34	118.40	110.49
2	B	111	LEU	CD1-CG-CD2	-5.34	99.04	110.80
1	A	11	LEU	CA-C-N	-5.34	113.47	123.03
1	A	11	LEU	C-N-CA	-5.34	113.47	123.03
2	B	18	GLY	CA-C-O	5.34	125.91	119.82
3	C	44	GLN	N-CA-C	-5.34	100.72	109.80
1	A	13	ILE	CA-C-N	-5.34	111.34	122.07
1	A	13	ILE	C-N-CA	-5.34	111.34	122.07
1	A	175	TRP	N-CA-CB	5.34	120.71	111.69
2	B	45	LEU	CA-C-N	-5.34	114.19	122.09
2	B	45	LEU	C-N-CA	-5.34	114.19	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	THR	CA-CB-CG2	5.33	119.57	110.50
3	C	15	GLY	N-CA-C	-5.33	107.17	114.64
4	T	29	HIS	CB-CG-CD2	-5.33	124.27	131.20
3	C	90	THR	CA-CB-CG2	5.33	119.56	110.50
2	B	37	TYR	N-CA-C	5.32	117.34	108.02
4	T	72	ASP	CB-CA-C	-5.32	102.17	110.74
2	B	37	TYR	CG-CD1-CE1	5.32	129.18	121.20
1	A	181	PHE	O-C-N	-5.32	116.98	123.10
2	B	209	ARG	CA-CB-CG	5.32	124.74	114.10
1	A	32	LEU	N-CA-C	-5.31	100.65	108.99
2	B	18	GLY	O-C-N	-5.31	117.12	122.54
3	C	60	ARG	CB-CA-C	5.31	120.99	110.42
1	A	117	PRO	O-C-N	-5.31	116.73	123.10
2	B	114	THR	CA-CB-OG1	5.31	117.56	109.60
4	T	5	VAL	O-C-N	-5.30	116.90	122.95
3	C	20	LEU	CD1-CG-CD2	-5.30	99.14	110.80
3	C	93	TYR	N-CA-CB	-5.30	101.77	110.41
2	B	160	TRP	CB-CA-C	-5.30	104.51	111.82
1	A	62	THR	CB-CA-C	-5.29	100.39	109.65
4	T	100	ARG	NE-CZ-NH2	-5.29	114.44	119.20
4	T	103	PRO	CA-C-O	5.29	132.88	120.20
4	T	77	THR	N-CA-C	5.28	117.36	108.96
2	B	225	GLN	CA-C-N	-5.27	114.06	122.29
2	B	225	GLN	C-N-CA	-5.27	114.06	122.29
2	B	91	TYR	CB-CA-C	5.27	119.95	111.05
1	A	63	PHE	N-CA-CB	5.26	120.66	111.13
2	B	128	PHE	O-C-N	-5.26	117.08	123.13
2	B	200	PHE	N-CA-C	5.26	119.75	113.23
4	T	96	ARG	N-CA-C	-5.26	100.45	108.76
2	B	6	ILE	CA-CB-CG2	5.26	119.44	110.50
1	A	50	VAL	O-C-N	5.25	129.14	122.57
3	C	97	PHE	CA-C-N	5.25	130.25	123.00
3	C	97	PHE	C-N-CA	5.25	130.25	123.00
1	A	58	LEU	N-CA-C	-5.25	97.99	107.60
2	B	128	PHE	CA-C-O	5.25	126.31	120.43
4	T	60	ALA	O-C-N	5.25	129.57	122.59
1	A	64	GLN	O-C-N	5.24	129.89	123.44
3	C	40	VAL	CB-CA-C	5.24	116.81	110.78
3	C	34	VAL	CB-CA-C	-5.24	104.44	110.41
1	A	93	GLY	CA-C-N	5.23	132.02	122.50
1	A	93	GLY	C-N-CA	5.23	132.02	122.50
2	B	130	PRO	N-CD-CG	5.23	111.04	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	81	THR	N-CA-C	5.22	119.24	111.87
3	C	48	VAL	CA-CB-CG2	5.22	119.28	110.40
1	A	73	SER	CA-CB-OG	5.22	121.54	111.10
4	T	106	TYR	N-CA-C	-5.22	101.82	109.81
1	A	133	CYS	N-CA-CB	-5.22	101.93	110.43
2	B	219	GLU	O-C-N	-5.22	115.65	122.59
2	B	210	CYS	O-C-N	-5.21	116.47	123.14
2	B	128	PHE	CG-CD2-CE2	5.21	129.56	120.70
1	A	194	GLU	CA-C-O	-5.21	113.43	120.15
3	C	81	GLN	CB-CG-CD	5.20	121.44	112.60
1	A	198	PHE	CE1-CZ-CE2	-5.20	110.64	120.00
4	T	19	ARG	CA-CB-CG	5.20	124.50	114.10
2	B	31	HIS	CG-CD2-NE2	5.20	112.40	107.20
4	T	29	HIS	N-CA-C	5.20	119.32	112.25
3	C	40	VAL	N-CA-CB	5.19	117.62	111.23
4	T	37	TYR	CB-CG-CD1	5.19	128.59	120.80
4	T	60	ALA	CB-CA-C	5.19	120.75	110.42
1	A	146	GLN	N-CA-C	5.19	116.98	110.24
3	C	11	LEU	CA-CB-CG	5.19	134.46	116.30
4	T	107	TRP	N-CA-C	-5.19	101.38	108.38
2	B	178	LYS	N-CA-C	-5.19	101.31	109.25
2	B	222	GLU	N-CA-C	-5.19	99.75	110.80
1	A	188	ASN	N-CA-C	-5.18	106.22	112.54
2	B	146	LEU	CA-C-N	5.18	129.57	122.84
2	B	146	LEU	C-N-CA	5.18	129.57	122.84
2	B	141	ALA	CB-CA-C	-5.18	100.12	110.42
2	B	237	ALA	O-C-N	5.17	128.96	123.42
2	B	237	ALA	CA-C-N	-5.17	110.28	121.87
2	B	237	ALA	C-N-CA	-5.17	110.28	121.87
3	C	19	ARG	N-CA-C	-5.17	98.61	107.61
4	T	37	TYR	CG-CD1-CE1	-5.17	113.45	121.20
2	B	144	VAL	CA-CB-CG1	5.17	119.18	110.40
1	A	200	SER	N-CA-CB	5.17	119.28	110.50
2	B	103	GLN	CA-C-O	-5.16	114.64	120.32
3	C	66	ARG	N-CA-C	5.16	121.79	110.80
4	T	36	TRP	CA-C-O	-5.16	115.24	120.71
1	A	137	ASP	CA-C-O	-5.16	114.26	119.78
3	C	77	THR	CA-CB-OG1	5.16	117.33	109.60
1	A	159	VAL	CA-CB-CG1	5.15	119.16	110.40
1	A	133	CYS	CB-CA-C	-5.15	101.25	109.75
4	T	80	LEU	CB-CA-C	-5.15	102.84	110.62
4	T	37	TYR	CE1-CZ-CE2	-5.15	110.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	THR	OG1-CB-CG2	-5.14	99.01	109.30
2	B	135	ILE	CA-C-O	-5.14	115.72	121.17
4	T	33	PHE	CA-C-N	-5.14	112.75	121.85
4	T	33	PHE	C-N-CA	-5.14	112.75	121.85
4	T	55	ASP	N-CA-CB	5.14	119.18	110.49
1	A	18	ASN	N-CA-C	-5.14	103.14	110.59
2	B	46	ARG	NE-CZ-NH2	-5.13	114.58	119.20
2	B	176	PRO	CA-C-N	5.13	129.16	121.72
2	B	176	PRO	C-N-CA	5.13	129.16	121.72
2	B	178	LYS	N-CA-CB	-5.12	101.52	109.87
1	A	163	ARG	CA-C-N	-5.12	111.76	121.54
1	A	163	ARG	C-N-CA	-5.12	111.76	121.54
3	C	69	ILE	CA-C-N	-5.12	111.76	121.54
3	C	69	ILE	C-N-CA	-5.12	111.76	121.54
3	C	21	SER	N-CA-C	-5.11	101.52	109.14
2	B	195	ARG	O-C-N	-5.11	116.69	123.13
3	C	45	ARG	O-C-N	-5.10	116.00	122.43
2	B	193	ARG	CB-CG-CD	5.10	123.03	111.30
3	C	36	TRP	CB-CG-CD2	-5.10	119.66	126.80
1	A	25	SER	N-CA-CB	5.10	119.31	111.46
2	B	110	ARG	NE-CZ-NH1	-5.10	116.40	121.50
2	B	26	GLU	CB-CG-CD	5.10	121.27	112.60
2	B	123	PRO	N-CA-C	-5.09	102.61	111.32
4	T	94	TYR	OH-CZ-CE2	-5.09	104.62	119.90
2	B	3	ASP	CA-CB-CG	5.09	117.69	112.60
3	C	8	GLY	CA-C-N	-5.09	113.72	123.29
3	C	8	GLY	C-N-CA	-5.09	113.72	123.29
2	B	199	THR	CA-CB-OG1	-5.09	101.96	109.60
4	T	30	LYS	CG-CD-CE	5.09	123.01	111.30
4	T	103	PRO	CB-CA-C	-5.09	99.28	112.00
4	T	81	GLN	N-CA-CB	5.09	118.97	110.53
4	T	102	TRP	N-CA-C	-5.09	103.74	110.40
4	T	106	TYR	CG-CD2-CE2	5.08	128.83	121.20
2	B	219	GLU	CA-C-N	-5.08	111.83	121.54
2	B	219	GLU	C-N-CA	-5.08	111.83	121.54
2	B	48	ILE	CA-C-O	-5.08	114.43	120.78
2	B	236	SER	N-CA-CB	-5.08	102.83	111.31
4	T	91	ALA	CA-C-O	-5.08	115.07	120.75
3	C	54	ASP	CB-CA-C	-5.07	100.36	109.24
2	B	228	ALA	N-CA-C	5.07	121.60	110.80
1	A	6	GLN	CB-CA-C	-5.07	99.69	109.37
3	C	111	VAL	N-CA-CB	-5.07	104.42	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	46	ARG	N-CA-CB	-5.07	102.03	110.23
2	B	189	SER	O-C-N	-5.06	116.33	123.11
4	T	102	TRP	CD1-CG-CD2	-5.06	98.21	106.30
1	A	8	PRO	CA-C-N	5.06	130.83	121.52
1	A	8	PRO	C-N-CA	5.06	130.83	121.52
4	T	99	SER	CA-CB-OG	5.06	121.22	111.10
4	T	100	ARG	CA-C-O	-5.05	113.38	119.49
2	B	201	TRP	CZ3-CH2-CZ2	-5.05	114.94	121.50
4	T	22	CYS	N-CA-C	-5.04	100.95	109.07
1	A	143	ASN	CB-CG-ND2	-5.04	108.84	116.40
2	B	17	GLU	CB-CG-CD	-5.04	104.03	112.60
4	T	106	TYR	N-CA-CB	-5.04	103.49	111.05
4	T	34	TYR	CD1-CG-CD2	-5.04	110.54	118.10
2	B	183	LEU	CA-C-N	-5.04	114.76	122.87
2	B	183	LEU	C-N-CA	-5.04	114.76	122.87
4	T	46	GLU	CB-CA-C	-5.04	101.22	109.53
1	A	44	VAL	N-CA-CB	5.03	120.52	111.21
2	B	35	TYR	CZ-CE2-CD2	-5.03	110.54	119.60
4	T	32	ASN	O-C-N	5.03	129.50	122.36
2	B	125	VAL	O-C-N	-5.03	116.55	122.58
2	B	230	PRO	CA-C-O	-5.02	114.53	122.82
4	T	89	ASP	N-CA-C	-5.02	106.41	112.88
1	A	193	PRO	CB-CA-C	5.02	117.65	111.23
4	T	45	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	A	189	ASN	O-C-N	-5.01	115.86	122.42
1	A	39	PRO	CA-C-N	5.01	130.66	121.85
1	A	39	PRO	C-N-CA	5.01	130.66	121.85
1	A	187	PHE	CA-C-N	5.01	129.08	120.72
1	A	187	PHE	C-N-CA	5.01	129.08	120.72
2	B	226	ASP	N-CA-C	-5.01	106.10	113.61
2	B	118	LYS	O-C-N	5.01	129.32	122.46
2	B	82	SER	CA-C-O	-5.00	113.36	120.51
4	T	10	GLY	CA-C-O	-5.00	111.86	120.57

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	152	VAL	CA
1	A	192	ILE	CB
4	T	31	ILE	CB
4	T	53	ILE	CB

All (264) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	PHE	Mainchain
1	A	105	LYS	Peptide,Mainchain
1	A	109	LYS	Mainchain
1	A	11	LEU	Mainchain
1	A	110	PRO	Mainchain
1	A	111	ASN	Mainchain
1	A	118	ALA	Peptide
1	A	12	SER	Mainchain
1	A	120	TYR	Sidechain
1	A	121	GLN	Mainchain
1	A	13	ILE	Mainchain
1	A	135	PHE	Mainchain
1	A	141	GLN	Mainchain
1	A	144	VAL	Mainchain
1	A	152	VAL	Peptide
1	A	155	THR	Mainchain
1	A	160	LEU	Mainchain
1	A	17	GLU	Mainchain
1	A	171	SER	Peptide,Mainchain
1	A	179	SER	Peptide
1	A	18	ASN	Mainchain
1	A	181	PHE	Sidechain,Mainchain
1	A	184	ALA	Mainchain
1	A	186	ALA	Mainchain
1	A	19	LEU	Mainchain
1	A	191	ILE	Mainchain
1	A	192	ILE	Mainchain
1	A	194	GLU	Mainchain
1	A	196	THR	Mainchain
1	A	197	PHE	Sidechain,Mainchain
1	A	198	PHE	Peptide,Sidechain,Mainchain
1	A	2	GLN	Peptide
1	A	21	VAL	Mainchain
1	A	33	GLN	Mainchain
1	A	34	TRP	Mainchain
1	A	35	TYR	Sidechain
1	A	37	GLN	Mainchain
1	A	38	GLU	Peptide
1	A	41	GLU	Mainchain
1	A	43	PRO	Peptide,Mainchain
1	A	46	LEU	Mainchain
1	A	54	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	56	LYS	Mainchain
1	A	57	LYS	Mainchain
1	A	60	ARG	Sidechain,Mainchain
1	A	62	THR	Mainchain
1	A	66	GLY	Mainchain
1	A	7	SER	Peptide,Mainchain
1	A	74	LEU	Mainchain
1	A	81	PRO	Mainchain
1	A	85	GLY	Mainchain
1	A	87	TYR	Sidechain,Mainchain
1	A	88	LEU	Mainchain
1	A	89	CYS	Peptide,Mainchain
1	A	9	GLN	Mainchain
1	A	90	ALA	Mainchain
1	A	96	GLY	Peptide
1	A	99	ILE	Mainchain
2	B	101	TYR	Mainchain
2	B	102	GLU	Peptide,Mainchain
2	B	104	TYR	Mainchain
2	B	105	PHE	Sidechain,Mainchain
2	B	11	LYS	Mainchain
2	B	112	THR	Mainchain
2	B	118	LYS	Peptide,Mainchain
2	B	12	TYR	Sidechain
2	B	122	PRO	Mainchain
2	B	124	GLU	Mainchain
2	B	128	PHE	Sidechain
2	B	129	GLU	Peptide
2	B	13	LEU	Mainchain
2	B	137	HIS	Sidechain
2	B	14	PHE	Sidechain
2	B	142	THR	Peptide
2	B	144	VAL	Mainchain
2	B	147	ALA	Mainchain
2	B	150	PHE	Mainchain
2	B	151	TYR	Mainchain
2	B	155	VAL	Mainchain
2	B	156	GLU	Mainchain
2	B	16	LYS	Peptide
2	B	161	VAL	Peptide
2	B	162	ASN	Peptide,Sidechain,Mainchain
2	B	17	GLU	Mainchain

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Mol	Chain	Res	Type	Group
2	B	172	THR	Mainchain
2	B	173	ASP	Mainchain
2	B	175	GLN	Peptide
2	B	177	LEU	Mainchain
2	B	180	GLN	Mainchain
2	B	181	PRO	Mainchain
2	B	182	ALA	Mainchain
2	B	183	LEU	Peptide
2	B	186	SER	Mainchain
2	B	188	TYR	Sidechain
2	B	19	GLN	Peptide,Sidechain
2	B	195	ARG	Mainchain
2	B	20	ASN	Peptide,Mainchain
2	B	200	PHE	Sidechain
2	B	201	TRP	Mainchain
2	B	203	ASN	Mainchain
2	B	206	ASN	Sidechain
2	B	208	PHE	Mainchain
2	B	209	ARG	Sidechain
2	B	210	CYS	Mainchain
2	B	213	GLN	Mainchain
2	B	215	TYR	Peptide,Sidechain
2	B	22	THR	Mainchain
2	B	220	ASN	Peptide
2	B	224	THR	Mainchain
2	B	225	GLN	Peptide,Sidechain
2	B	228	ALA	Mainchain
2	B	232	THR	Mainchain
2	B	233	GLN	Mainchain
2	B	235	VAL	Mainchain
2	B	236	SER	Mainchain
2	B	237	ALA	Mainchain
2	B	240	TRP	Mainchain
2	B	28	ASN	Sidechain
2	B	35	TYR	Sidechain
2	B	37	TYR	Sidechain,Mainchain
2	B	38	ARG	Mainchain
2	B	39	GLN	Mainchain
2	B	42	GLY	Mainchain
2	B	45	LEU	Peptide,Mainchain
2	B	48	ILE	Mainchain
2	B	50	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	53	ILE	Peptide
2	B	66	TYR	Sidechain
2	B	70	ARG	Sidechain
2	B	71	GLU	Mainchain
2	B	72	LYS	Peptide
2	B	76	PHE	Mainchain
2	B	81	THR	Mainchain
2	B	82	SER	Mainchain
2	B	84	GLN	Peptide,Sidechain
2	B	86	ASN	Mainchain
2	B	87	PRO	Peptide,Mainchain
2	B	88	THR	Mainchain
2	B	91	TYR	Sidechain
2	B	94	ALA	Mainchain
2	B	96	SER	Peptide,Mainchain
2	B	97	SER	Mainchain
3	C	104	TYR	Sidechain
3	C	113	VAL	Mainchain
3	C	114	SER	Peptide
3	C	14	ALA	Mainchain
3	C	27	SER	Mainchain
3	C	29	VAL	Peptide
3	C	30	GLY	Peptide
3	C	31	ILE	Mainchain
3	C	37	TYR	Sidechain,Mainchain
3	C	40	VAL	Mainchain
3	C	55	THR	Mainchain
3	C	56	GLY	Mainchain
3	C	58	HIS	Sidechain
3	C	59	TYR	Mainchain
3	C	61	ASP	Peptide
3	C	63	VAL	Peptide,Mainchain
3	C	67	PHE	Mainchain
3	C	7	SER	Peptide,Mainchain
3	C	71	ARG	Peptide
3	C	77	THR	Mainchain
3	C	93	TYR	Sidechain
3	C	96	TYR	Mainchain
3	C	97	PHE	Sidechain
3	C	98	ASN	Sidechain,Mainchain
4	T	1	ASP	Peptide,Mainchain
4	T	10	GLY	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
4	T	100	ARG	Sidechain,Mainchain
4	T	101	ILE	Peptide,Mainchain
4	T	102	TRP	Mainchain
4	T	104	TYR	Sidechain
4	T	105	ASP	Peptide,Mainchain
4	T	106	TYR	Sidechain,Mainchain
4	T	109	GLN	Mainchain
4	T	112	LEU	Peptide
4	T	113	VAL	Mainchain
4	T	116	SER	Mainchain
4	T	12	VAL	Mainchain
4	T	2	VAL	Peptide
4	T	20	LEU	Mainchain
4	T	23	VAL	Peptide,Mainchain
4	T	25	SER	Mainchain
4	T	28	VAL	Peptide
4	T	29	HIS	Peptide,Sidechain
4	T	30	LYS	Peptide
4	T	34	TYR	Sidechain,Mainchain
4	T	36	TRP	Mainchain
4	T	37	TYR	Sidechain
4	T	43	LYS	Mainchain
4	T	45	ARG	Sidechain
4	T	50	HIS	Mainchain
4	T	51	ILE	Mainchain
4	T	52	SER	Mainchain
4	T	53	ILE	Mainchain
4	T	54	GLY	Peptide
4	T	56	GLN	Mainchain
4	T	58	ASP	Mainchain
4	T	59	TYR	Peptide
4	T	60	ALA	Peptide,Mainchain
4	T	61	ASP	Peptide,Mainchain
4	T	62	SER	Mainchain
4	T	63	ALA	Mainchain
4	T	64	LYS	Peptide
4	T	66	ARG	Peptide
4	T	7	SER	Mainchain
4	T	71	ARG	Sidechain
4	T	74	SER	Mainchain
4	T	76	ASN	Peptide,Mainchain
4	T	79	TYR	Sidechain

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Mol	Chain	Res	Type	Group
4	T	81	GLN	Peptide,Mainchain
4	T	85	LEU	Mainchain
4	T	9	GLY	Peptide
4	T	90	THR	Mainchain
4	T	91	ALA	Mainchain
4	T	93	TYR	Mainchain
4	T	94	TYR	Sidechain
4	T	95	CYS	Peptide
4	T	97	ALA	Peptide,Mainchain
4	T	98	LEU	Mainchain
4	T	99	SER	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1530	0	1474	169	0
2	B	1945	0	1833	175	0
3	C	885	0	878	48	0
4	T	921	0	883	123	0
5	D	38	0	34	0	0
6	E	39	0	34	0	0
7	F	28	0	25	0	0
All	All	5386	0	5161	452	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 43.

All (452) 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)
4:T:53:ILE:CG2	4:T:53:ILE:CB	1.76	1.60
4:T:53:ILE:CG2	4:T:53:ILE:HB	1.29	1.59
4:T:100:ARG:CG	4:T:100:ARG:CD	1.79	1.55
1:A:2:GLN:N	1:A:2:GLN:CA	1.71	1.54
2:B:207:HIS:CB	2:B:207:HIS:CA	1.87	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:51:ILE:CD1	4:T:69:ILE:HG22	1.40	1.48
1:A:120:TYR:CE1	2:B:134:GLU:CA	2.00	1.44
1:A:165:MET:SD	1:A:165:MET:CE	2.08	1.41
1:A:152:VAL:O	1:A:152:VAL:C	1.64	1.41
1:A:120:TYR:CE1	2:B:134:GLU:HA	1.57	1.39
1:A:120:TYR:HE1	2:B:134:GLU:CA	1.30	1.36
4:T:49:ALA:CB	4:T:69:ILE:HD11	1.55	1.35
4:T:51:ILE:HD11	4:T:69:ILE:CG2	1.59	1.30
3:C:31:ILE:CG2	3:C:32:HIS:H	1.42	1.30
4:T:63:ALA:HB3	4:T:67:PHE:CE2	1.72	1.22
2:B:175:GLN:HG3	4:T:102:TRP:CG	1.74	1.22
1:A:153:TYR:O	1:A:174:ALA:HA	1.36	1.21
4:T:63:ALA:HB3	4:T:67:PHE:CD2	1.75	1.20
1:A:152:VAL:CG2	1:A:176:SER:HB2	1.70	1.19
1:A:120:TYR:HE1	2:B:134:GLU:N	1.40	1.18
3:C:33:SER:C	3:C:34:VAL:HG23	1.55	1.16
1:A:132:VAL:HG23	1:A:132:VAL:O	1.40	1.16
1:A:152:VAL:O	1:A:175:TRP:O	1.64	1.15
4:T:51:ILE:CD1	4:T:69:ILE:CG2	2.21	1.14
4:T:63:ALA:CB	4:T:67:PHE:CE2	2.32	1.11
1:A:152:VAL:HG22	1:A:176:SER:HB2	1.30	1.11
1:A:126:LYS:NZ	2:B:127:VAL:O	1.84	1.10
3:C:31:ILE:HG22	3:C:32:HIS:N	1.48	1.10
2:B:175:GLN:HG3	4:T:102:TRP:CD2	1.87	1.09
1:A:153:TYR:O	1:A:174:ALA:CA	2.00	1.09
4:T:47:LYS:HE2	4:T:60:ALA:HB2	1.32	1.08
2:B:14:PHE:O	2:B:15:ARG:HG2	1.52	1.07
1:A:151:ASP:OD1	1:A:176:SER:OG	1.71	1.07
1:A:121:GLN:HB2	1:A:183:CYS:SG	1.96	1.06
4:T:49:ALA:HB3	4:T:69:ILE:CD1	1.85	1.05
2:B:207:HIS:CB	2:B:207:HIS:HA	1.79	1.05
4:T:51:ILE:HG13	4:T:69:ILE:HG21	1.36	1.05
1:A:120:TYR:CZ	2:B:134:GLU:HA	1.91	1.04
1:A:120:TYR:CE1	2:B:134:GLU:N	2.21	1.04
1:A:97:ASN:HD22	1:A:97:ASN:N	1.47	1.03
2:B:35:TYR:O	2:B:94:ALA:N	1.92	1.02
1:A:88:LEU:HD22	1:A:100:PHE:HD2	1.22	1.02
1:A:132:VAL:O	1:A:132:VAL:CG2	2.08	1.01
2:B:14:PHE:O	2:B:15:ARG:CG	2.07	1.01
1:A:120:TYR:CE1	2:B:134:GLU:CB	2.44	1.01
2:B:62:ILE:HG13	2:B:63:ALA:N	1.76	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:HIS:HB3	2:B:240:TRP:CZ2	1.97	0.99
4:T:40:ALA:HB1	4:T:41:PRO:HD2	1.42	0.99
3:C:31:ILE:HG22	3:C:32:HIS:H	0.85	0.99
3:C:39:GLN:HB2	3:C:94:TYR:HE2	1.23	0.99
4:T:47:LYS:CE	4:T:60:ALA:HB2	1.93	0.98
4:T:63:ALA:CB	4:T:67:PHE:CD2	2.46	0.98
1:A:151:ASP:O	1:A:177:ASN:N	1.94	0.98
1:A:132:VAL:HG12	1:A:175:TRP:CB	1.94	0.97
1:A:132:VAL:HG12	1:A:175:TRP:HB3	0.99	0.97
1:A:14:GLN:HB3	3:C:44:GLN:HE22	1.24	0.97
2:B:234:ILE:HG22	2:B:235:VAL:H	1.29	0.97
3:C:87:PRO:HA	3:C:113:VAL:O	1.64	0.96
2:B:84:GLN:HB3	2:B:85:LYS:HD2	1.48	0.96
1:A:163:ARG:O	1:A:164:SER:HB2	1.66	0.95
1:A:132:VAL:CG1	1:A:175:TRP:HB3	1.95	0.94
2:B:37:TYR:HE1	2:B:47:LEU:HB2	1.33	0.93
3:C:33:SER:C	3:C:34:VAL:CG2	2.41	0.93
2:B:128:PHE:HE2	2:B:146:LEU:HB3	1.32	0.93
1:A:177:ASN:O	1:A:178:LYS:C	2.08	0.93
2:B:117:LEU:O	2:B:117:LEU:HG	1.66	0.93
2:B:128:PHE:CE2	2:B:146:LEU:HB3	2.03	0.92
2:B:207:HIS:CA	2:B:207:HIS:CG	2.51	0.92
4:T:2:VAL:HG12	4:T:3:GLN:N	1.84	0.92
2:B:175:GLN:CG	4:T:102:TRP:CD2	2.52	0.92
4:T:96:ARG:HD3	4:T:98:LEU:HD11	1.50	0.91
2:B:100:SER:O	2:B:101:TYR:HB2	1.69	0.91
1:A:153:TYR:HD2	4:T:100:ARG:HD3	1.34	0.91
4:T:49:ALA:CB	4:T:69:ILE:CD1	2.43	0.91
4:T:51:ILE:CG1	4:T:69:ILE:HG21	2.01	0.91
1:A:178:LYS:O	1:A:179:SER:C	2.00	0.90
2:B:177:LEU:HD12	2:B:177:LEU:H	1.36	0.90
2:B:173:ASP:HB2	2:B:190:LEU:HD12	1.55	0.88
1:A:97:ASN:N	1:A:97:ASN:ND2	2.18	0.88
2:B:128:PHE:HE2	2:B:146:LEU:CB	1.87	0.88
1:A:96:GLY:C	1:A:97:ASN:HD22	1.81	0.87
2:B:37:TYR:HB2	2:B:92:LEU:O	1.74	0.87
3:C:2:VAL:HG23	3:C:26:GLY:HA3	1.54	0.87
4:T:49:ALA:HB3	4:T:69:ILE:HD11	0.88	0.87
4:T:51:ILE:CG1	4:T:69:ILE:CG2	2.52	0.87
1:A:153:TYR:CD2	4:T:100:ARG:HD3	2.10	0.86
2:B:85:LYS:HG2	2:B:85:LYS:O	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TYR:CE1	2:B:134:GLU:HB2	2.10	0.85
1:A:145:SER:HA	4:T:29:HIS:HB2	1.58	0.85
1:A:152:VAL:C	1:A:175:TRP:O	2.21	0.83
4:T:2:VAL:HG12	4:T:3:GLN:H	1.38	0.83
2:B:117:LEU:O	2:B:117:LEU:CG	2.26	0.82
1:A:88:LEU:HD22	1:A:100:PHE:CD2	2.12	0.82
1:A:152:VAL:HG23	1:A:176:SER:HB2	1.59	0.82
2:B:14:PHE:C	2:B:15:ARG:HG2	2.05	0.82
2:B:21:VAL:O	2:B:21:VAL:HG13	1.78	0.81
4:T:96:ARG:HD3	4:T:98:LEU:CD1	2.10	0.81
2:B:3:ASP:HB3	2:B:105:PHE:H	1.46	0.81
2:B:173:ASP:HB2	2:B:190:LEU:CD1	2.11	0.80
3:C:2:VAL:HG12	3:C:3:GLN:H	1.45	0.80
2:B:178:LYS:O	4:T:100:ARG:HB3	1.81	0.80
2:B:9:SER:HB2	2:B:10:PRO:HA	1.61	0.80
2:B:234:ILE:HG22	2:B:235:VAL:N	1.91	0.80
1:A:14:GLN:OE1	3:C:44:GLN:NE2	2.15	0.79
1:A:155:THR:HG22	1:A:156:ASP:N	1.95	0.79
1:A:152:VAL:O	1:A:153:TYR:CD1	2.34	0.79
3:C:39:GLN:HB2	3:C:94:TYR:CE2	2.14	0.79
4:T:47:LYS:CE	4:T:60:ALA:CB	2.61	0.79
1:A:148:LYS:HB3	4:T:54:GLY:HA3	1.64	0.79
2:B:177:LEU:HD12	2:B:177:LEU:N	1.97	0.79
4:T:100:ARG:CG	4:T:100:ARG:NE	2.46	0.78
1:A:14:GLN:HB3	3:C:44:GLN:NE2	1.98	0.78
1:A:153:TYR:HD2	4:T:100:ARG:CD	1.96	0.78
3:C:33:SER:O	3:C:34:VAL:HG23	1.84	0.77
4:T:34:TYR:HE1	4:T:53:ILE:HD11	1.48	0.77
2:B:131:SER:HB3	2:B:134:GLU:H	1.50	0.77
2:B:207:HIS:HB3	2:B:240:TRP:HZ2	1.47	0.77
2:B:223:TRP:NE1	2:B:229:LYS:HA	1.98	0.77
1:A:122:LEU:HB2	1:A:132:VAL:O	1.85	0.77
1:A:14:GLN:CB	3:C:44:GLN:HE22	1.97	0.77
2:B:84:GLN:HB3	2:B:85:LYS:CD	2.15	0.76
1:A:122:LEU:HB2	1:A:132:VAL:HG23	1.68	0.76
4:T:22:CYS:N	4:T:78:VAL:O	2.18	0.76
1:A:40:GLY:HA2	2:B:90:PHE:CE2	2.21	0.76
1:A:19:LEU:HD22	1:A:106:LEU:HD11	1.67	0.75
1:A:153:TYR:CD2	4:T:100:ARG:CD	2.69	0.75
1:A:154:ILE:HA	1:A:174:ALA:HA	1.68	0.75
4:T:47:LYS:HE3	4:T:60:ALA:CB	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:ILE:HD12	2:B:27:GLN:HB3	1.67	0.75
2:B:37:TYR:N	2:B:92:LEU:O	2.19	0.74
1:A:152:VAL:O	1:A:153:TYR:HD1	1.69	0.74
3:C:52:VAL:HG12	3:C:53:THR:N	2.03	0.73
3:C:85:LEU:HB3	3:C:113:VAL:HG11	1.69	0.73
1:A:146:GLN:HG3	4:T:32:ASN:ND2	2.03	0.73
2:B:62:ILE:CG1	2:B:63:ALA:N	2.51	0.72
1:A:155:THR:HG22	1:A:156:ASP:H	1.53	0.72
4:T:34:TYR:CE1	4:T:53:ILE:HD11	2.23	0.72
2:B:104:TYR:N	2:B:104:TYR:CD1	2.58	0.72
2:B:31:HIS:ND1	2:B:96:SER:C	2.49	0.71
1:A:19:LEU:HD12	1:A:19:LEU:O	1.89	0.71
4:T:49:ALA:HB1	4:T:69:ILE:HD11	1.65	0.71
1:A:189:ASN:O	1:A:189:ASN:ND2	2.24	0.71
4:T:51:ILE:HD12	4:T:69:ILE:HG22	1.68	0.71
4:T:47:LYS:HG2	4:T:48:VAL:N	2.03	0.71
1:A:109:LYS:HB3	1:A:110:PRO:HD2	1.74	0.70
2:B:37:TYR:CE1	2:B:47:LEU:HB2	2.23	0.70
4:T:51:ILE:HD11	4:T:69:ILE:HG22	0.73	0.70
2:B:124:GLU:C	2:B:125:VAL:CG2	2.62	0.69
3:C:39:GLN:O	3:C:91:ALA:HB1	1.92	0.69
1:A:153:TYR:CD2	4:T:100:ARG:CZ	2.75	0.69
2:B:124:GLU:C	2:B:125:VAL:HG23	2.16	0.69
4:T:1:ASP:C	4:T:2:VAL:HG23	2.11	0.68
3:C:31:ILE:HG23	3:C:32:HIS:H	1.53	0.68
1:A:152:VAL:CG2	1:A:176:SER:CB	2.61	0.68
3:C:96:TYR:CD1	3:C:96:TYR:C	2.71	0.68
4:T:12:VAL:HG11	4:T:18:LEU:HD11	1.74	0.68
4:T:49:ALA:HB1	4:T:69:ILE:CD1	2.23	0.68
4:T:40:ALA:HB1	4:T:41:PRO:CD	2.23	0.68
2:B:179:GLU:OE2	2:B:189:SER:HB3	1.94	0.68
4:T:96:ARG:NE	4:T:98:LEU:HD13	2.10	0.67
3:C:31:ILE:CG2	3:C:32:HIS:N	2.10	0.67
1:A:153:TYR:CD2	4:T:100:ARG:NE	2.63	0.66
2:B:112:THR:OG1	2:B:154:HIS:CE1	2.48	0.66
4:T:2:VAL:CG1	4:T:3:GLN:N	2.58	0.66
1:A:14:GLN:CB	3:C:44:GLN:NE2	2.58	0.66
4:T:47:LYS:HE3	4:T:60:ALA:HB3	1.76	0.66
4:T:53:ILE:HB	4:T:53:ILE:HG23	1.62	0.66
2:B:34:MET:HE3	2:B:70:ARG:HH22	1.61	0.65
1:A:146:GLN:HG3	4:T:32:ASN:HD22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLN:HA	1:A:2:GLN:NE2	2.11	0.65
1:A:95:GLN:CD	2:B:50:TYR:OH	2.40	0.65
4:T:61:ASP:C	4:T:62:SER:O	2.34	0.65
1:A:14:GLN:CG	3:C:44:GLN:NE2	2.60	0.64
1:A:152:VAL:HA	1:A:175:TRP:O	1.97	0.64
1:A:2:GLN:N	1:A:2:GLN:C	2.55	0.64
3:C:104:TYR:N	3:C:104:TYR:CD2	2.61	0.64
1:A:35:TYR:CE2	1:A:45:LEU:HD13	2.32	0.64
1:A:116:ASP:OD1	2:B:137:HIS:HE1	1.79	0.64
1:A:152:VAL:O	1:A:153:TYR:CA	2.45	0.64
4:T:53:ILE:CG2	4:T:53:ILE:O	2.45	0.64
1:A:117:PRO:HB3	1:A:138:PHE:CA	2.27	0.64
2:B:62:ILE:O	2:B:63:ALA:HB2	1.97	0.64
1:A:145:SER:HA	4:T:29:HIS:O	1.97	0.64
1:A:146:GLN:NE2	1:A:154:ILE:O	2.31	0.64
2:B:34:MET:O	2:B:50:TYR:HA	1.99	0.63
1:A:153:TYR:N	4:T:100:ARG:NH1	2.46	0.63
1:A:152:VAL:HG23	1:A:176:SER:CB	2.26	0.63
1:A:120:TYR:HE1	2:B:133:ALA:C	2.04	0.63
2:B:175:GLN:HG2	4:T:102:TRP:CD2	2.33	0.63
1:A:155:THR:OG1	1:A:173:VAL:O	2.06	0.63
1:A:10:PHE:O	1:A:11:LEU:CB	2.44	0.62
1:A:121:GLN:CB	1:A:183:CYS:SG	2.79	0.62
3:C:33:SER:O	3:C:34:VAL:CG2	2.43	0.62
2:B:81:THR:O	2:B:82:SER:O	2.17	0.62
1:A:98:LEU:HD21	2:B:101:TYR:HB3	1.79	0.62
1:A:163:ARG:O	1:A:164:SER:CB	2.42	0.62
1:A:47:VAL:HG22	1:A:48:THR:H	1.63	0.62
4:T:102:TRP:CD1	4:T:103:PRO:HA	2.35	0.62
1:A:152:VAL:O	1:A:153:TYR:CB	2.48	0.62
2:B:128:PHE:CE2	2:B:146:LEU:CB	2.72	0.61
2:B:37:TYR:HE1	2:B:47:LEU:CB	2.10	0.61
1:A:19:LEU:HD12	1:A:19:LEU:C	2.25	0.61
2:B:177:LEU:H	2:B:177:LEU:CD1	2.10	0.61
2:B:172:THR:O	2:B:173:ASP:C	2.36	0.61
2:B:223:TRP:CE2	2:B:229:LYS:HA	2.36	0.61
2:B:130:PRO:HD2	2:B:201:TRP:CZ2	2.36	0.60
1:A:184:ALA:C	1:A:186:ALA:N	2.59	0.60
2:B:37:TYR:CB	2:B:92:LEU:O	2.49	0.60
3:C:52:VAL:HG12	3:C:53:THR:H	1.65	0.60
4:T:99:SER:O	4:T:100:ARG:C	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:LYS:O	2:B:85:LYS:CG	2.43	0.60
2:B:14:PHE:O	2:B:15:ARG:CD	2.49	0.60
1:A:43:PRO:HD2	2:B:105:PHE:CG	2.36	0.60
3:C:2:VAL:HG12	3:C:3:GLN:N	2.14	0.59
4:T:45:ARG:HH11	4:T:45:ARG:CG	2.15	0.59
1:A:47:VAL:HG13	1:A:48:THR:N	2.16	0.59
2:B:34:MET:CE	2:B:70:ARG:HH22	2.15	0.59
2:B:143:LEU:HD12	2:B:143:LEU:H	1.67	0.59
1:A:151:ASP:OD1	1:A:151:ASP:C	2.44	0.59
2:B:8:GLN:NE2	2:B:36:TRP:CZ3	2.71	0.59
1:A:163:ARG:HH22	1:A:168:LYS:HG3	1.68	0.59
4:T:96:ARG:CD	4:T:98:LEU:CD1	2.79	0.58
1:A:154:ILE:HA	1:A:174:ALA:CA	2.33	0.58
2:B:222:GLU:O	2:B:223:TRP:HB2	2.04	0.58
4:T:2:VAL:HG22	4:T:27:TYR:O	2.04	0.58
4:T:2:VAL:HG11	4:T:31:ILE:HD11	1.85	0.58
3:C:57:THR:C	3:C:58:HIS:CG	2.82	0.58
2:B:35:TYR:CD1	2:B:50:TYR:HB2	2.39	0.58
2:B:50:TYR:O	2:B:58:GLN:O	2.22	0.57
4:T:100:ARG:CD	4:T:100:ARG:HG3	2.20	0.57
1:A:109:LYS:HB3	1:A:110:PRO:CD	2.31	0.57
2:B:81:THR:C	2:B:82:SER:O	2.47	0.57
4:T:12:VAL:CG1	4:T:18:LEU:HD11	2.34	0.57
3:C:2:VAL:CG2	3:C:26:GLY:HA3	2.31	0.57
1:A:116:ASP:CG	1:A:116:ASP:O	2.46	0.57
2:B:219:GLU:O	2:B:220:ASN:HB3	2.04	0.57
3:C:60:ARG:O	3:C:61:ASP:HB2	2.05	0.57
4:T:96:ARG:CD	4:T:98:LEU:HD13	2.34	0.57
2:B:48:ILE:HA	2:B:62:ILE:O	2.06	0.56
2:B:149:GLY:HA2	2:B:187:ARG:NH2	2.20	0.56
2:B:62:ILE:HG13	2:B:63:ALA:H	1.65	0.56
2:B:68:VAL:HA	2:B:77:PRO:O	2.05	0.56
4:T:63:ALA:HB2	4:T:67:PHE:CE2	2.37	0.56
4:T:2:VAL:CG1	4:T:3:GLN:H	2.13	0.56
2:B:234:ILE:CG2	2:B:235:VAL:H	2.11	0.56
1:A:153:TYR:CE2	4:T:100:ARG:CZ	2.89	0.56
1:A:173:VAL:HG12	1:A:174:ALA:N	2.19	0.56
1:A:177:ASN:O	1:A:179:SER:N	2.37	0.56
1:A:76:ILE:HG22	1:A:77:THR:N	2.20	0.56
4:T:51:ILE:HD11	4:T:69:ILE:CB	2.34	0.56
2:B:121:PHE:HB3	2:B:122:PRO:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:GLN:HB2	2:B:215:TYR:CZ	2.42	0.55
1:A:95:GLN:CD	2:B:50:TYR:HH	2.15	0.55
4:T:53:ILE:HB	4:T:53:ILE:HG21	1.65	0.55
2:B:85:LYS:O	2:B:86:ASN:C	2.49	0.55
1:A:148:LYS:HE2	1:A:189:ASN:OD1	2.07	0.54
1:A:153:TYR:H	4:T:100:ARG:HH12	1.56	0.54
1:A:102:LYS:N	1:A:102:LYS:HD2	2.20	0.54
1:A:74:LEU:C	1:A:74:LEU:HD12	2.33	0.54
2:B:41:PRO:CB	4:T:102:TRP:HE1	2.21	0.54
4:T:63:ALA:HB1	4:T:67:PHE:CD2	2.41	0.54
1:A:93:GLY:HA3	1:A:97:ASN:H	1.72	0.54
2:B:140:LYS:HG3	2:B:195:ARG:HH11	1.73	0.53
2:B:32:ASP:O	2:B:52:GLN:O	2.26	0.53
1:A:152:VAL:HG22	1:A:181:PHE:CE1	2.43	0.53
2:B:39:GLN:OE1	2:B:45:LEU:CD1	2.56	0.53
4:T:40:ALA:CB	4:T:41:PRO:HD2	2.28	0.53
2:B:34:MET:HG3	2:B:70:ARG:NH1	2.23	0.53
4:T:37:TYR:N	4:T:37:TYR:CD1	2.75	0.53
1:A:153:TYR:N	4:T:100:ARG:HH12	2.07	0.53
1:A:61:LEU:HD23	1:A:74:LEU:HD11	1.90	0.53
3:C:87:PRO:CA	3:C:113:VAL:O	2.49	0.52
4:T:45:ARG:HH11	4:T:45:ARG:HG2	1.73	0.52
4:T:47:LYS:CG	4:T:48:VAL:N	2.63	0.52
1:A:14:GLN:O	1:A:17:GLU:HG3	2.10	0.52
2:B:221:ASP:O	2:B:222:GLU:HG3	2.09	0.52
2:B:219:GLU:O	2:B:220:ASN:CB	2.52	0.52
4:T:6:GLU:HB2	4:T:111:THR:HG23	1.91	0.52
1:A:117:PRO:HB3	1:A:138:PHE:HA	1.92	0.52
4:T:102:TRP:CG	4:T:103:PRO:HA	2.44	0.52
3:C:104:TYR:H	3:C:104:TYR:HD2	1.56	0.52
4:T:1:ASP:C	4:T:2:VAL:CG2	2.73	0.52
2:B:173:ASP:O	2:B:174:PRO:C	2.49	0.51
1:A:81:PRO:C	1:A:83:ASP:N	2.68	0.51
1:A:145:SER:HA	4:T:29:HIS:CB	2.37	0.51
2:B:231:VAL:O	2:B:233:GLN:HG2	2.11	0.51
4:T:102:TRP:HA	4:T:103:PRO:C	2.36	0.51
1:A:47:VAL:HG22	1:A:48:THR:N	2.26	0.51
2:B:34:MET:HG3	2:B:70:ARG:HH12	1.76	0.51
2:B:41:PRO:HB3	4:T:102:TRP:HE1	1.76	0.50
3:C:52:VAL:CG1	3:C:53:THR:N	2.71	0.50
2:B:161:VAL:C	2:B:163:GLY:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:O	1:A:153:TYR:C	2.54	0.50
1:A:8:PRO:HB3	1:A:10:PHE:O	2.12	0.50
2:B:35:TYR:CD1	2:B:50:TYR:CB	2.95	0.50
2:B:62:ILE:CD1	2:B:63:ALA:H	2.25	0.50
2:B:35:TYR:HD1	2:B:50:TYR:HB3	1.75	0.49
2:B:125:VAL:HG12	2:B:126:ALA:N	2.27	0.49
2:B:54:VAL:HG22	2:B:55:ASN:N	2.26	0.49
4:T:37:TYR:HE1	4:T:50:HIS:HE1	1.60	0.49
4:T:102:TRP:HA	4:T:104:TYR:N	2.28	0.49
1:A:135:PHE:C	1:A:135:PHE:CD1	2.82	0.49
2:B:84:GLN:O	2:B:85:LYS:HB3	2.11	0.49
1:A:14:GLN:CD	3:C:44:GLN:NE2	2.70	0.49
2:B:20:ASN:N	2:B:20:ASN:OD1	2.43	0.49
1:A:120:TYR:CD1	2:B:134:GLU:N	2.79	0.49
1:A:123:ARG:HD2	1:A:124:ASP:H	1.77	0.49
2:B:62:ILE:CG1	2:B:63:ALA:H	2.20	0.49
2:B:197:SER:O	2:B:198:ALA:C	2.51	0.49
1:A:81:PRO:C	1:A:83:ASP:H	2.19	0.49
1:A:120:TYR:CE1	2:B:133:ALA:C	2.86	0.49
2:B:39:GLN:OE1	2:B:45:LEU:HD12	2.13	0.49
2:B:35:TYR:HD1	2:B:50:TYR:CB	2.26	0.49
3:C:12:VAL:HG21	3:C:85:LEU:HD13	1.94	0.49
3:C:39:GLN:CB	3:C:94:TYR:HE2	2.10	0.49
4:T:17:SER:HA	4:T:82:MET:O	2.13	0.49
1:A:153:TYR:H	4:T:100:ARG:NH1	2.09	0.48
1:A:184:ALA:C	1:A:186:ALA:H	2.20	0.48
2:B:208:PHE:CD1	2:B:208:PHE:N	2.80	0.48
3:C:59:TYR:O	3:C:60:ARG:CB	2.50	0.48
1:A:116:ASP:CG	2:B:137:HIS:HE1	2.22	0.48
1:A:23:CYS:O	1:A:71:ASP:HA	2.14	0.48
2:B:234:ILE:CG2	2:B:235:VAL:N	2.68	0.48
4:T:47:LYS:HD2	4:T:50:HIS:NE2	2.28	0.48
2:B:14:PHE:O	2:B:15:ARG:HD3	2.14	0.48
4:T:49:ALA:HB1	4:T:69:ILE:CG1	2.44	0.48
1:A:120:TYR:CD1	2:B:134:GLU:HB2	2.49	0.48
2:B:14:PHE:CG	2:B:15:ARG:N	2.82	0.48
2:B:8:GLN:NE2	2:B:36:TRP:HZ3	2.09	0.48
2:B:175:GLN:CG	4:T:102:TRP:CE3	2.96	0.48
2:B:223:TRP:CD1	2:B:229:LYS:HA	2.49	0.48
1:A:119:VAL:H	1:A:119:VAL:HG23	1.18	0.48
4:T:53:ILE:O	4:T:53:ILE:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LEU:HD13	1:A:99:ILE:HG22	1.96	0.47
1:A:97:ASN:CG	1:A:97:ASN:O	2.51	0.47
1:A:95:GLN:OE1	2:B:50:TYR:OH	2.32	0.47
2:B:27:GLN:N	2:B:27:GLN:CD	2.72	0.47
2:B:86:ASN:N	2:B:87:PRO:HD3	2.28	0.47
1:A:122:LEU:CB	1:A:132:VAL:HG23	2.40	0.47
2:B:17:GLU:HA	2:B:113:VAL:CG1	2.45	0.47
2:B:82:SER:O	2:B:84:GLN:NE2	2.45	0.47
1:A:153:TYR:CD2	4:T:100:ARG:NH1	2.82	0.47
2:B:104:TYR:HD1	2:B:104:TYR:H	1.61	0.47
4:T:101:ILE:H	4:T:101:ILE:HG23	1.46	0.47
2:B:130:PRO:HD2	2:B:201:TRP:CE2	2.49	0.47
4:T:2:VAL:HG22	4:T:27:TYR:HB2	1.96	0.47
1:A:136:THR:C	1:A:138:PHE:N	2.71	0.47
4:T:47:LYS:HD2	4:T:50:HIS:CD2	2.50	0.47
1:A:26:SER:O	1:A:27:SER:CB	2.63	0.47
1:A:152:VAL:CG2	1:A:181:PHE:CE1	2.98	0.47
2:B:37:TYR:CE1	2:B:47:LEU:HA	2.49	0.46
2:B:175:GLN:HG2	4:T:102:TRP:CE3	2.50	0.46
3:C:55:THR:HB	3:C:58:HIS:HE1	1.80	0.46
1:A:131:SER:C	1:A:132:VAL:HG13	2.40	0.46
4:T:38:ARG:HD2	4:T:48:VAL:HG21	1.97	0.46
2:B:32:ASP:C	2:B:52:GLN:O	2.58	0.46
4:T:51:ILE:HG13	4:T:69:ILE:CG2	2.15	0.46
1:A:40:GLY:HA2	2:B:90:PHE:CZ	2.51	0.46
1:A:117:PRO:HB3	1:A:138:PHE:CB	2.45	0.46
1:A:151:ASP:CG	1:A:179:SER:OG	2.59	0.46
3:C:96:TYR:O	3:C:97:PHE:CB	2.57	0.46
4:T:2:VAL:CG2	4:T:27:TYR:O	2.63	0.46
4:T:100:ARG:HH11	4:T:100:ARG:HD2	1.30	0.46
1:A:183:CYS:O	1:A:186:ALA:N	2.48	0.46
1:A:153:TYR:C	1:A:174:ALA:HA	2.39	0.46
4:T:100:ARG:CD	4:T:100:ARG:HG2	2.20	0.46
1:A:153:TYR:O	1:A:175:TRP:N	2.49	0.46
2:B:118:LYS:HD3	2:B:118:LYS:N	2.29	0.46
2:B:37:TYR:CE1	2:B:47:LEU:CA	2.98	0.46
2:B:217:LEU:O	2:B:231:VAL:HA	2.16	0.45
1:A:170:ASN:HD22	1:A:170:ASN:HA	1.57	0.45
1:A:10:PHE:O	1:A:11:LEU:HB2	2.14	0.45
1:A:47:VAL:O	1:A:47:VAL:CG1	2.60	0.45
2:B:41:PRO:HB2	4:T:102:TRP:NE1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:31:ILE:HD13	4:T:31:ILE:HG21	1.71	0.45
1:A:153:TYR:HD2	4:T:100:ARG:NE	2.09	0.45
2:B:150:PHE:N	2:B:150:PHE:CD1	2.82	0.45
2:B:213:GLN:H	2:B:213:GLN:HG2	1.78	0.45
2:B:217:LEU:HD23	2:B:217:LEU:HA	1.63	0.45
1:A:14:GLN:HG3	3:C:44:GLN:NE2	2.33	0.45
3:C:69:ILE:H	3:C:69:ILE:HG22	1.48	0.45
1:A:79:ALA:HA	1:A:83:ASP:OD2	2.17	0.44
2:B:37:TYR:CD1	2:B:47:LEU:HA	2.52	0.44
2:B:186:SER:O	2:B:187:ARG:C	2.55	0.44
4:T:47:LYS:HD2	4:T:50:HIS:HE2	1.82	0.44
1:A:109:LYS:CB	1:A:110:PRO:HD2	2.44	0.44
1:A:116:ASP:OD2	2:B:137:HIS:CE1	2.71	0.44
2:B:54:VAL:HG23	2:B:70:ARG:HG3	2.00	0.44
2:B:203:ASN:C	2:B:205:ARG:H	2.25	0.44
1:A:192:ILE:HD13	1:A:192:ILE:HG21	1.81	0.44
2:B:8:GLN:OE1	2:B:106:GLY:HA3	2.18	0.44
2:B:128:PHE:HE2	2:B:146:LEU:HB2	1.74	0.44
1:A:121:GLN:HA	1:A:133:CYS:HA	1.99	0.44
1:A:155:THR:CB	1:A:173:VAL:O	2.66	0.43
2:B:37:TYR:CD2	2:B:105:PHE:HE2	2.35	0.43
4:T:49:ALA:HB1	4:T:69:ILE:HG13	2.00	0.43
2:B:48:ILE:HB	2:B:49:TYR:H	1.65	0.43
2:B:68:VAL:O	2:B:68:VAL:HG23	2.18	0.43
2:B:149:GLY:HA2	2:B:187:ARG:HH21	1.80	0.43
3:C:61:ASP:C	3:C:63:VAL:H	1.99	0.43
2:B:71:GLU:O	2:B:72:LYS:HB2	2.17	0.43
2:B:86:ASN:N	2:B:87:PRO:CD	2.82	0.43
1:A:130:LYS:HB2	1:A:130:LYS:HE2	1.82	0.43
2:B:31:HIS:ND1	2:B:97:SER:N	2.66	0.43
1:A:138:PHE:HE2	1:A:157:LYS:HZ2	1.65	0.43
2:B:121:PHE:HB3	2:B:122:PRO:CD	2.49	0.43
1:A:100:PHE:N	1:A:100:PHE:CD1	2.87	0.43
1:A:53:GLY:HA2	1:A:65:PHE:O	2.18	0.43
1:A:152:VAL:O	1:A:153:TYR:HB2	2.17	0.43
1:A:113:GLN:O	1:A:114:ASN:HB2	2.18	0.43
2:B:130:PRO:HG2	2:B:201:TRP:CD2	2.54	0.43
4:T:4:LEU:HD11	4:T:97:ALA:HB2	2.00	0.43
1:A:178:LYS:H	1:A:178:LYS:HG3	1.36	0.43
1:A:36:ARG:HB2	1:A:46:LEU:HD11	2.00	0.42
4:T:20:LEU:O	4:T:80:LEU:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:47:LYS:CG	4:T:48:VAL:H	2.31	0.42
1:A:163:ARG:NE	1:A:163:ARG:HA	2.33	0.42
2:B:39:GLN:OE1	2:B:45:LEU:HD11	2.18	0.42
2:B:81:THR:O	2:B:82:SER:C	2.53	0.42
1:A:14:GLN:HG3	3:C:44:GLN:CD	2.45	0.42
4:T:61:ASP:O	4:T:62:SER:O	2.38	0.42
1:A:154:ILE:CA	1:A:174:ALA:HA	2.42	0.42
4:T:40:ALA:CB	4:T:41:PRO:CD	2.93	0.42
1:A:102:LYS:O	1:A:103:GLY:O	2.38	0.42
1:A:2:GLN:N	1:A:2:GLN:CB	2.69	0.42
1:A:130:LYS:HD2	1:A:175:TRP:CZ3	2.54	0.42
2:B:127:VAL:CG1	2:B:143:LEU:HD23	2.50	0.42
1:A:159:VAL:H	1:A:159:VAL:HG23	1.33	0.41
4:T:37:TYR:HE1	4:T:50:HIS:CE1	2.37	0.41
1:A:132:VAL:H	1:A:132:VAL:HG22	1.41	0.41
2:B:3:ASP:CB	2:B:105:PHE:H	2.24	0.41
2:B:37:TYR:CA	2:B:92:LEU:O	2.67	0.41
2:B:36:TRP:CE2	2:B:78:LEU:HB2	2.55	0.41
1:A:119:VAL:HA	1:A:134:LEU:O	2.20	0.41
2:B:129:GLU:HA	2:B:130:PRO:HD3	1.87	0.41
2:B:174:PRO:HB2	2:B:175:GLN:H	1.50	0.41
2:B:36:TRP:HA	2:B:93:CYS:HA	2.02	0.41
2:B:53:ILE:HB	2:B:54:VAL:H	1.79	0.41
2:B:41:PRO:HB2	4:T:102:TRP:HE1	1.86	0.41
3:C:65:GLY:O	3:C:66:ARG:HB3	2.19	0.41
2:B:118:LYS:O	2:B:227:ARG:NH2	2.54	0.41
3:C:55:THR:HB	3:C:58:HIS:CE1	2.56	0.41
2:B:37:TYR:CE1	2:B:47:LEU:CB	2.97	0.41
3:C:2:VAL:HG23	3:C:26:GLY:CA	2.38	0.41
3:C:8:GLY:O	3:C:20:LEU:HD23	2.20	0.41
4:T:38:ARG:O	4:T:45:ARG:HA	2.22	0.40
1:A:138:PHE:CD2	1:A:142:THR:HB	2.56	0.40
4:T:87:PRO:C	4:T:89:ASP:H	2.30	0.40
2:B:59:LYS:HB2	2:B:59:LYS:HE2	1.56	0.40
2:B:176:PRO:O	4:T:104:TYR:CE1	2.74	0.40
3:C:77:THR:C	3:C:78:LEU:HD23	2.46	0.40
4:T:31:ILE:O	4:T:53:ILE:HD12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/199 (99%)	165 (84%)	21 (11%)	11 (6%)	1	10
2	B	240/242 (99%)	199 (83%)	28 (12%)	13 (5%)	1	10
3	C	112/114 (98%)	95 (85%)	13 (12%)	4 (4%)	3	16
4	T	115/117 (98%)	95 (83%)	12 (10%)	8 (7%)	1	6
All	All	664/672 (99%)	554 (83%)	74 (11%)	36 (5%)	3	10

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	PRO
1	A	27	SER
1	A	53	GLY
1	A	95	GLN
1	A	151	ASP
1	A	153	TYR
2	B	63	ALA
2	B	72	LYS
2	B	82	SER
2	B	85	LYS
2	B	162	ASN
2	B	218	SER
2	B	222	GLU
2	B	225	GLN
4	T	55	ASP
1	A	47	VAL
2	B	98	ARG
2	B	174	PRO
2	B	223	TRP
4	T	62	SER
1	A	59	LYS
1	A	199	PRO

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Mol	Chain	Res	Type
2	B	185	ASP
3	C	32	HIS
4	T	57	THR
4	T	60	ALA
4	T	76	ASN
1	A	13	ILE
2	B	153	ASP
3	C	66	ARG
4	T	28	VAL
1	A	66	GLY
3	C	31	ILE
4	T	61	ASP
4	T	66	ARG
3	C	56	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	175/175 (100%)	149 (85%)	26 (15%)	2	9
2	B	213/213 (100%)	180 (84%)	33 (16%)	2	9
3	C	94/94 (100%)	76 (81%)	18 (19%)	1	4
4	T	97/97 (100%)	78 (80%)	19 (20%)	1	3
All	All	579/579 (100%)	483 (83%)	96 (17%)	4	7

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	3	LEU
1	A	11	LEU
1	A	13	ILE
1	A	31	SER
1	A	49	VAL
1	A	59	LYS

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Mol	Chain	Res	Type
1	A	64	GLN
1	A	69	ARG
1	A	74	LEU
1	A	80	GLN
1	A	97	ASN
1	A	109	LYS
1	A	146	GLN
1	A	147	SER
1	A	148	LYS
1	A	152	VAL
1	A	153	TYR
1	A	156	ASP
1	A	157	LYS
1	A	158	CYS
1	A	162	MET
1	A	169	SER
1	A	178	LYS
1	A	190	SER
1	A	192	ILE
2	B	8	GLN
2	B	10	PRO
2	B	15	ARG
2	B	23	LEU
2	B	27	GLN
2	B	28	ASN
2	B	40	ASP
2	B	46	ARG
2	B	49	TYR
2	B	59	LYS
2	B	62	ILE
2	B	64	GLU
2	B	71	GLU
2	B	77	PRO
2	B	84	GLN
2	B	85	LYS
2	B	88	THR
2	B	95	SER
2	B	97	SER
2	B	98	ARG
2	B	102	GLU
2	B	111	LEU
2	B	119	ASN

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Mol	Chain	Res	Type
2	B	124	GLU
2	B	143	LEU
2	B	150	PHE
2	B	175	GLN
2	B	177	LEU
2	B	194	LEU
2	B	199	THR
2	B	213	GLN
2	B	218	SER
2	B	219	GLU
3	C	11	LEU
3	C	20	LEU
3	C	28	ILE
3	C	40	VAL
3	C	44	GLN
3	C	51	ILE
3	C	55	THR
3	C	57	THR
3	C	60	ARG
3	C	62	PHE
3	C	70	SER
3	C	75	LYS
3	C	78	LEU
3	C	81	GLN
3	C	97	PHE
3	C	100	ILE
3	C	101	ARG
3	C	109	THR
4	T	22	CYS
4	T	25	SER
4	T	28	VAL
4	T	32	ASN
4	T	45	ARG
4	T	47	LYS
4	T	48	VAL
4	T	53	ILE
4	T	57	THR
4	T	64	LYS
4	T	66	ARG
4	T	69	ILE
4	T	71	ARG
4	T	74	SER

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Mol	Chain	Res	Type
4	T	78	VAL
4	T	85	LEU
4	T	98	LEU
4	T	100	ARG
4	T	104	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	14	GLN
1	A	64	GLN
1	A	97	ASN
1	A	170	ASN
1	A	185	ASN
2	B	103	GLN
2	B	137	HIS
2	B	154	HIS
2	B	180	GLN
2	B	202	GLN
2	B	206	ASN
3	C	3	GLN
3	C	44	GLN
3	C	58	HIS
3	C	81	GLN
4	T	3	GLN
4	T	32	ASN
4	T	50	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	NAG	D	1	1,5	14,14,15	3.48	6 (42%)	17,19,21	3.53	12 (70%)
5	NAG	D	2	5	14,14,15	1.06	1 (7%)	17,19,21	2.59	3 (17%)
5	FUC	D	3	5	10,10,11	1.09	0	14,14,16	1.53	3 (21%)
6	NAG	E	1	1,6	14,14,15	2.78	7 (50%)	17,19,21	3.86	11 (64%)
6	NAG	E	2	6	14,14,15	1.46	2 (14%)	17,19,21	2.60	4 (23%)
6	BMA	E	3	6	11,11,12	1.77	4 (36%)	15,15,17	3.17	4 (26%)
7	NAG	F	1	2,7	14,14,15	1.15	1 (7%)	17,19,21	2.57	6 (35%)
7	NAG	F	2	7	14,14,15	0.71	0	17,19,21	1.31	1 (5%)

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	NAG	D	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	D	2	5	-	0/6/23/26	0/1/1/1
5	FUC	D	3	5	-	-	0/1/1/1
6	NAG	E	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	E	2	6	-	2/6/23/26	0/1/1/1
6	BMA	E	3	6	-	1/2/19/22	0/1/1/1
7	NAG	F	1	2,7	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	F	2	7	-	0/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1	NAG	C2-N2	-8.27	1.32	1.46
5	D	1	NAG	C1-C2	-7.56	1.42	1.52
6	E	1	NAG	O5-C1	5.64	1.53	1.43
6	E	1	NAG	C1-C2	-5.40	1.45	1.52
6	E	1	NAG	C2-N2	3.91	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1	NAG	C7-N2	-3.72	1.22	1.34
5	D	1	NAG	O3-C3	3.60	1.51	1.43
6	E	3	BMA	O5-C5	3.22	1.49	1.43
7	F	1	NAG	C8-C7	3.10	1.57	1.50
6	E	1	NAG	C8-C7	2.83	1.56	1.50
5	D	1	NAG	O5-C1	-2.82	1.39	1.43
6	E	2	NAG	C2-N2	2.77	1.50	1.46
6	E	1	NAG	C3-C2	2.58	1.57	1.52
6	E	2	NAG	C1-C2	2.49	1.55	1.52
6	E	3	BMA	C2-C3	2.41	1.56	1.52
6	E	3	BMA	O4-C4	2.27	1.48	1.43
6	E	1	NAG	C6-C5	2.24	1.59	1.51
6	E	1	NAG	O5-C5	2.22	1.47	1.43
6	E	3	BMA	O5-C1	2.19	1.47	1.43
5	D	2	NAG	C3-C2	2.13	1.57	1.52
5	D	1	NAG	O5-C5	2.12	1.47	1.43

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	3	BMA	C1-O5-C5	10.53	126.30	112.19
6	E	1	NAG	O5-C5-C6	8.48	124.17	107.66
6	E	1	NAG	C4-C3-C2	8.14	122.95	111.02
5	D	2	NAG	C1-O5-C5	7.75	122.58	112.19
5	D	1	NAG	C2-N2-C7	-7.40	112.98	122.90
6	E	1	NAG	C2-N2-C7	6.44	131.54	122.90
6	E	2	NAG	C1-C2-N2	6.03	119.93	110.43
5	D	2	NAG	C1-C2-N2	5.96	119.82	110.43
6	E	2	NAG	C4-C3-C2	-5.74	102.61	111.02
7	F	1	NAG	O5-C1-C2	5.60	119.96	111.29
5	D	1	NAG	C1-O5-C5	5.33	119.32	112.19
7	F	1	NAG	C2-N2-C7	5.15	129.81	122.90
5	D	1	NAG	C8-C7-N2	-4.56	108.56	116.12
5	D	1	NAG	O5-C5-C4	-4.54	99.77	110.83
6	E	2	NAG	C1-O5-C5	4.25	117.88	112.19
6	E	1	NAG	O5-C1-C2	4.25	117.86	111.29
5	D	1	NAG	O7-C7-N2	4.08	129.18	121.98
7	F	1	NAG	C1-C2-N2	3.80	116.43	110.43
7	F	1	NAG	O7-C7-N2	-3.80	115.27	121.98
5	D	1	NAG	C1-C2-N2	3.78	116.39	110.43
6	E	1	NAG	O4-C4-C3	-3.41	102.34	110.38
6	E	3	BMA	O4-C4-C5	3.40	117.69	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	3	FUC	O3-C3-C2	3.35	116.88	110.05
5	D	1	NAG	C4-C3-C2	-3.29	106.20	111.02
5	D	1	NAG	C3-C4-C5	-3.17	104.48	110.23
6	E	3	BMA	C2-C3-C4	3.15	116.41	110.86
6	E	1	NAG	O7-C7-N2	-3.12	116.48	121.98
5	D	1	NAG	C6-C5-C4	2.98	120.32	113.02
5	D	1	NAG	O5-C1-C2	2.96	115.88	111.29
7	F	2	NAG	O5-C1-C2	2.91	115.80	111.29
6	E	1	NAG	C3-C4-C5	-2.82	105.11	110.23
6	E	3	BMA	O6-C6-C5	-2.48	102.89	111.33
6	E	1	NAG	O3-C3-C4	2.46	116.17	110.38
7	F	1	NAG	C8-C7-N2	2.38	120.06	116.12
6	E	1	NAG	O7-C7-C8	2.29	126.13	122.05
5	D	1	NAG	O5-C5-C6	2.28	112.11	107.66
6	E	1	NAG	C1-O5-C5	2.26	115.22	112.19
5	D	3	FUC	O5-C1-C2	-2.22	105.50	110.79
5	D	2	NAG	O4-C4-C3	2.17	115.50	110.38
6	E	2	NAG	O5-C5-C4	2.14	116.03	110.83
5	D	3	FUC	O5-C5-C6	2.14	112.04	107.40
7	F	1	NAG	O5-C5-C6	2.11	111.77	107.66
5	D	1	NAG	O6-C6-C5	-2.05	104.34	111.33
6	E	1	NAG	C6-C5-C4	-2.01	108.09	113.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	1	NAG	C1
7	F	1	NAG	C1

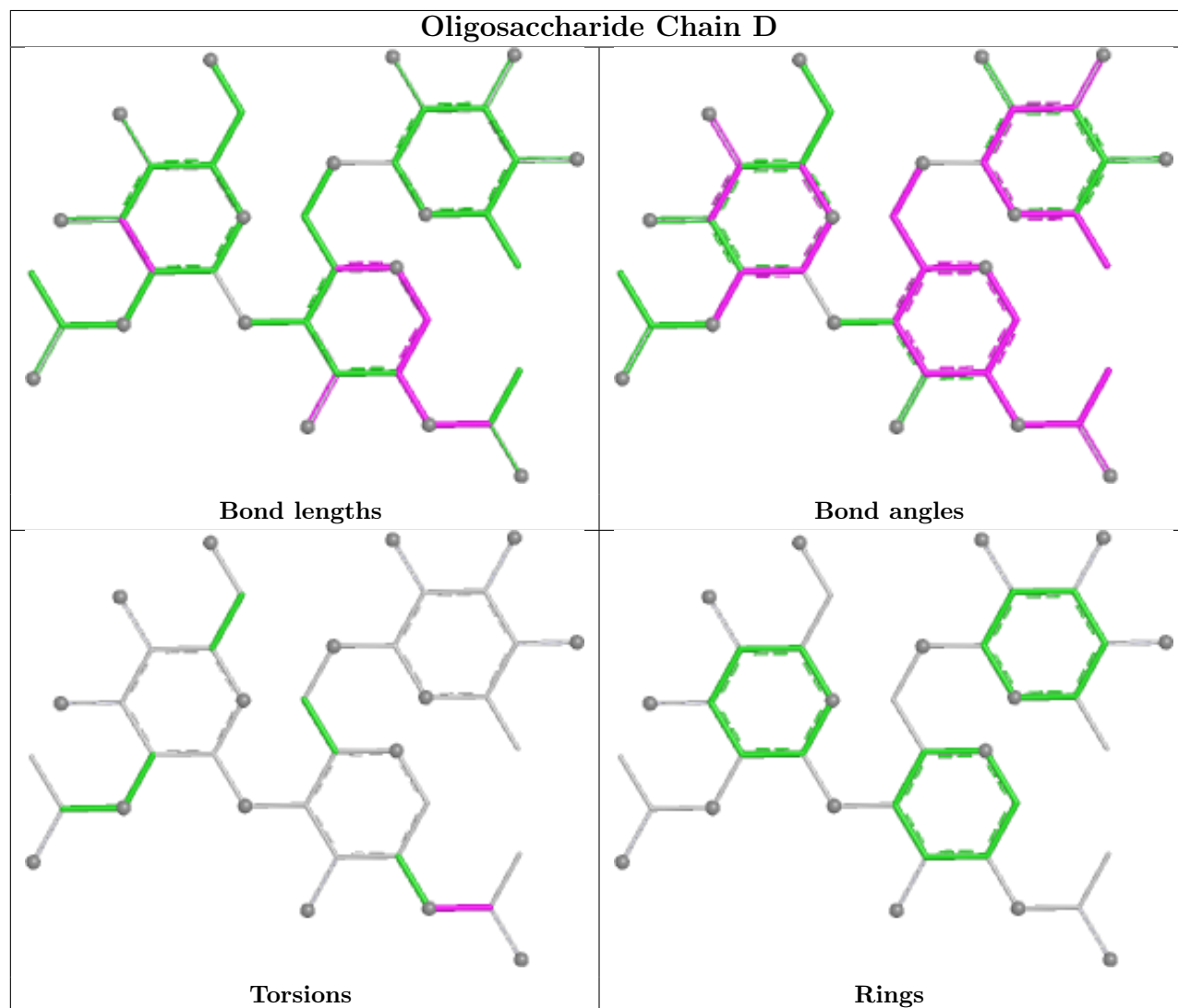
All (10) torsion outliers are listed below:

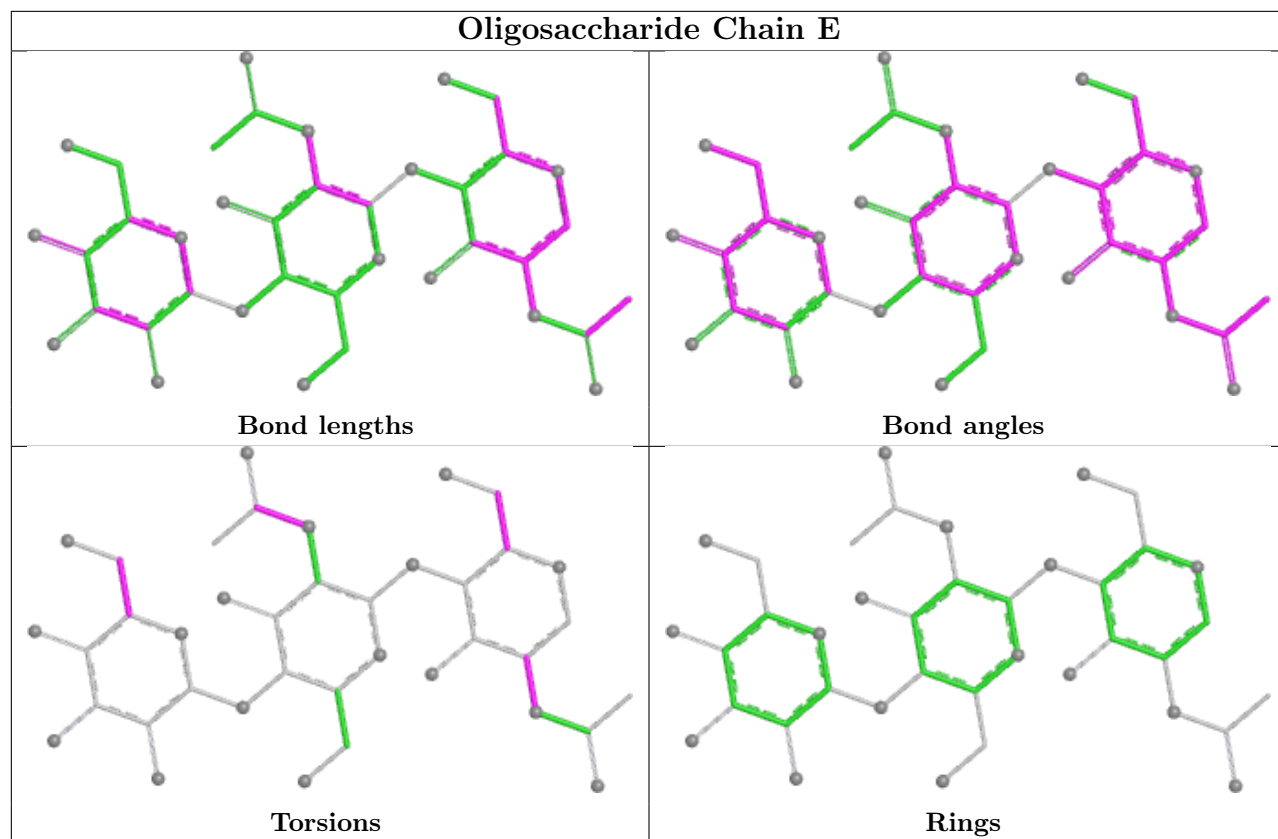
Mol	Chain	Res	Type	Atoms
6	E	2	NAG	O7-C7-N2-C2
6	E	2	NAG	C8-C7-N2-C2
6	E	1	NAG	O5-C5-C6-O6
6	E	1	NAG	C4-C5-C6-O6
5	D	1	NAG	C8-C7-N2-C2
5	D	1	NAG	O7-C7-N2-C2
6	E	3	BMA	C4-C5-C6-O6
7	F	1	NAG	C4-C5-C6-O6
7	F	1	NAG	O5-C5-C6-O6
6	E	1	NAG	C1-C2-N2-C7

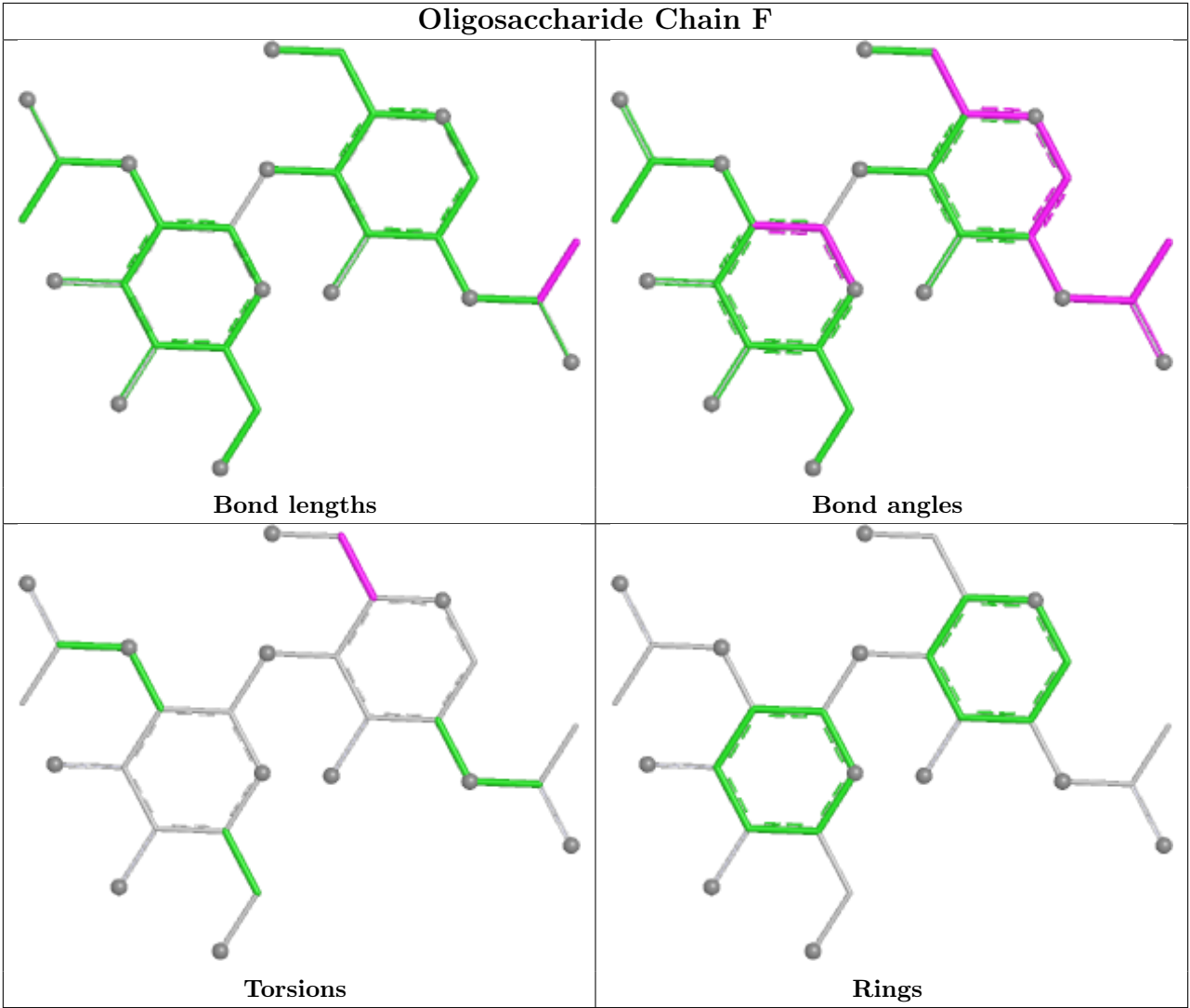
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	7

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	A	6
4	T	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	32:LEU	C	33:GLN	N	1.20
1	A	56:LYS	C	57:LYS	N	1.20
1	T	32:ASN	C	33:PHE	N	1.20
1	T	98:LEU	C	99:SER	N	1.20
1	T	113:VAL	C	114:THR	N	1.20
1	A	61:LEU	C	62:THR	N	1.19
1	B	121:PHE	C	122:PRO	N	1.19
1	T	106:TYR	C	107:TRP	N	1.19
1	A	17:GLU	C	18:ASN	N	1.18
1	A	62:THR	C	63:PHE	N	1.18
1	B	208:PHE	C	209:ARG	N	1.18
1	A	76:ILE	C	77:THR	N	1.17
1	T	96:ARG	C	97:ALA	N	1.16
1	B	232:THR	C	233:GLN	N	1.15
1	B	42:GLY	C	43:GLN	N	1.14
1	B	235:VAL	C	236:SER	N	1.14
1	T	34:TYR	C	35:GLY	N	1.14
1	B	209:ARG	C	210:CYS	N	1.10
1	B	211:GLN	C	212:VAL	N	1.10

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49735. These allow visual inspection of the internal detail of the map and identification of artifacts.

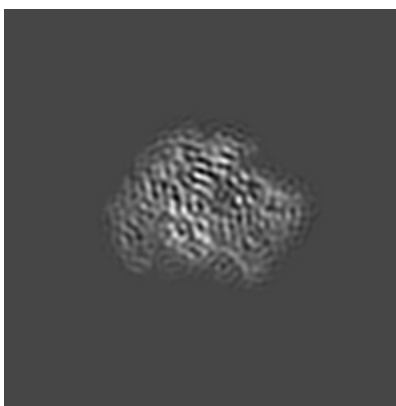
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

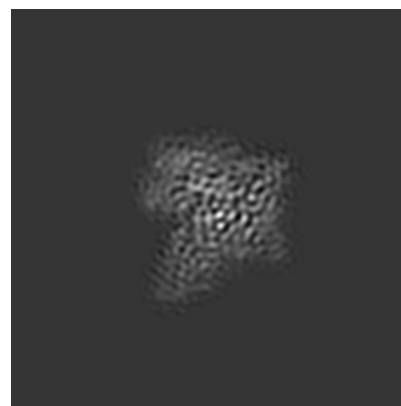
6.1.1 Primary map



X

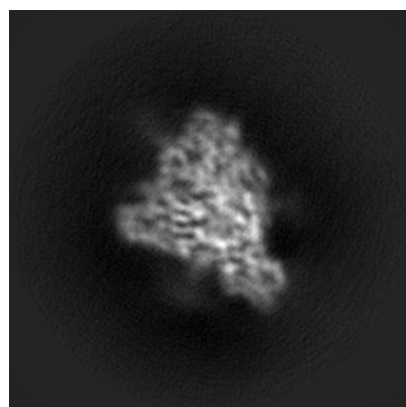


Y

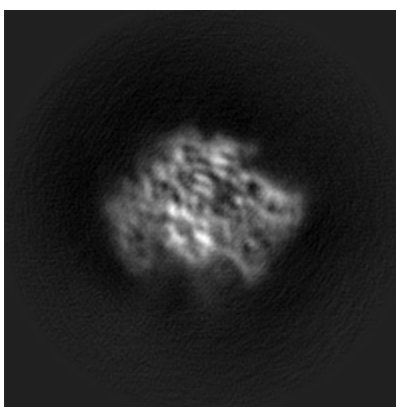


Z

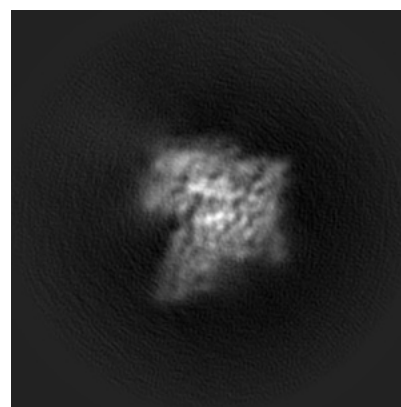
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

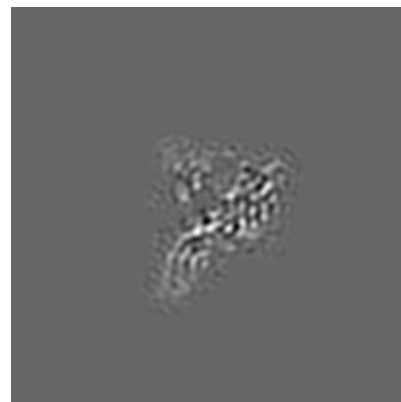
6.2.1 Primary map



X Index: 100

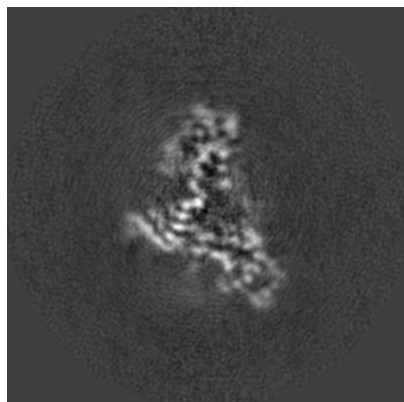


Y Index: 100

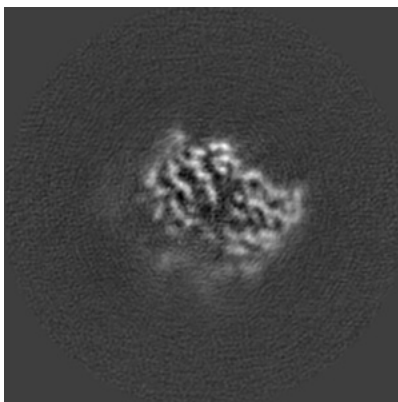


Z Index: 100

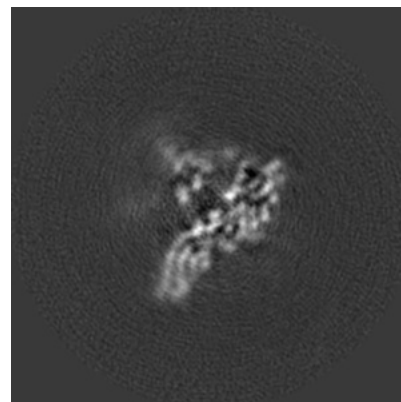
6.2.2 Raw map



X Index: 100



Y Index: 100



Z Index: 100

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: 96

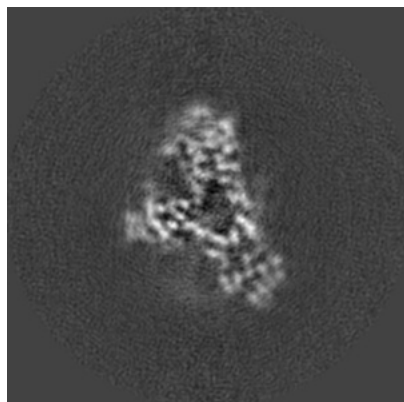


Y Index: 107

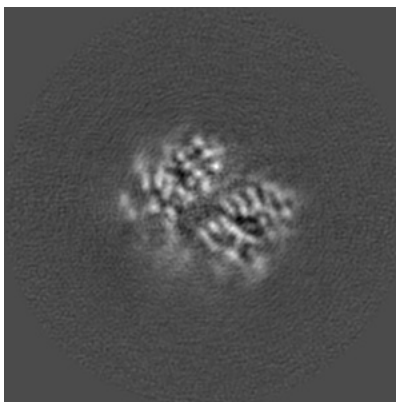


Z Index: 95

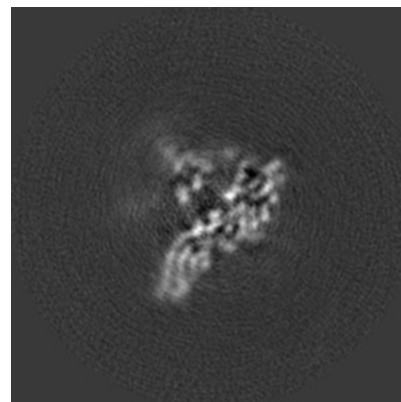
6.3.2 Raw map



X Index: 97



Y Index: 107

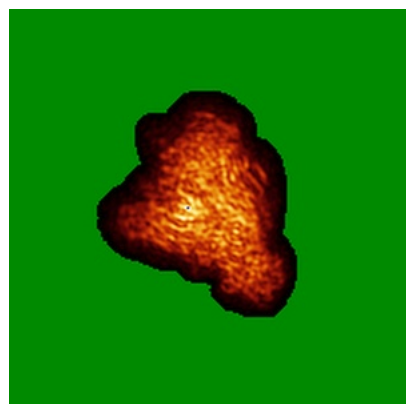


Z Index: 100

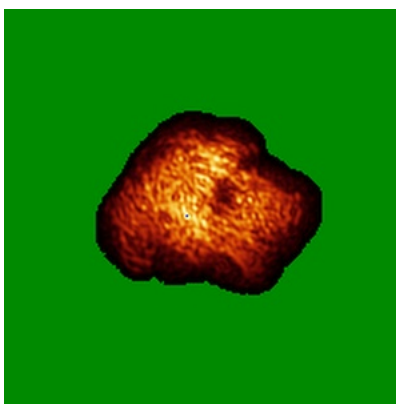
The images above show the largest variance slices of the map in three orthogonal directions.

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

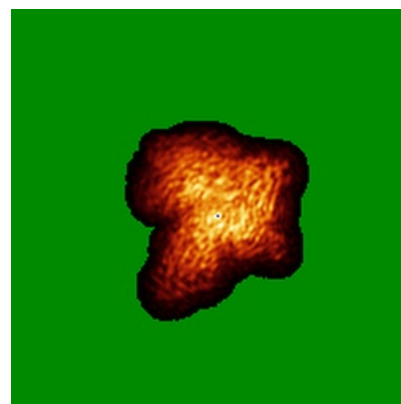
6.4.1 Primary map



X

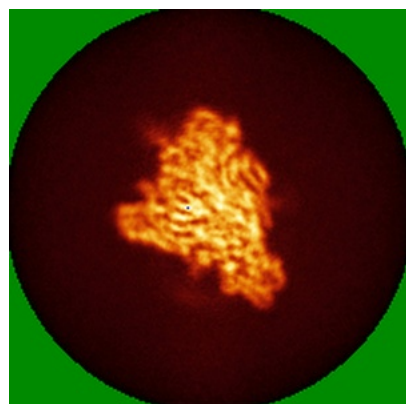


Y

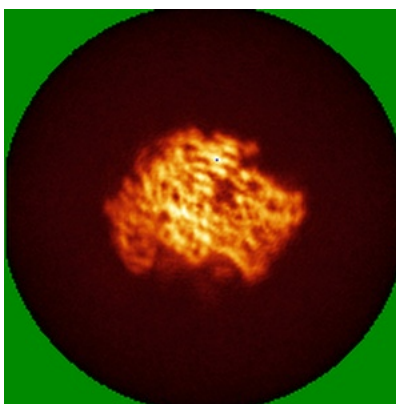


Z

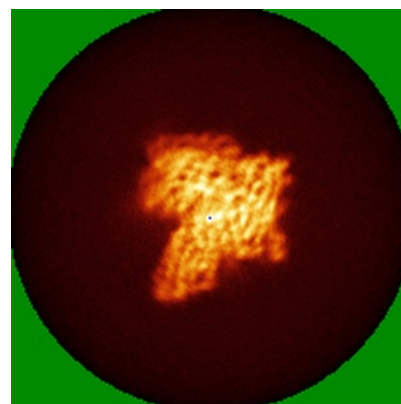
6.4.2 Raw map



X



Y

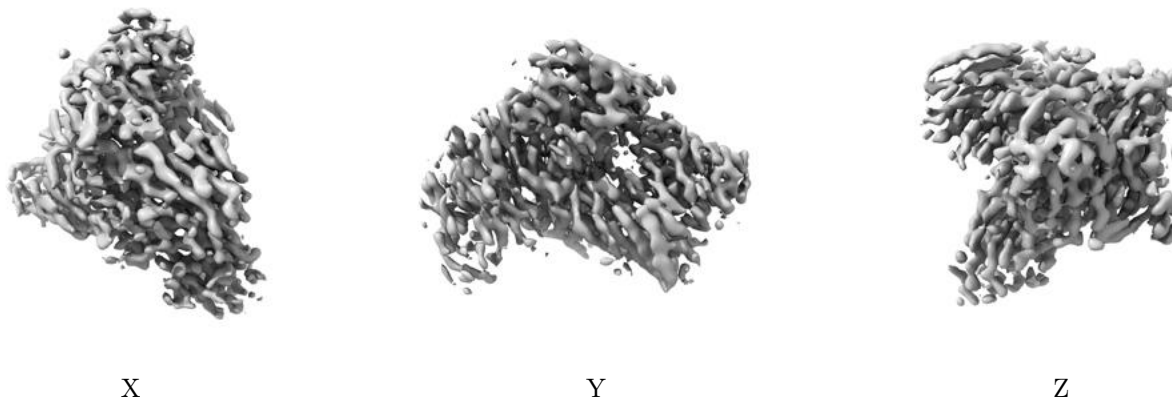


Z

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

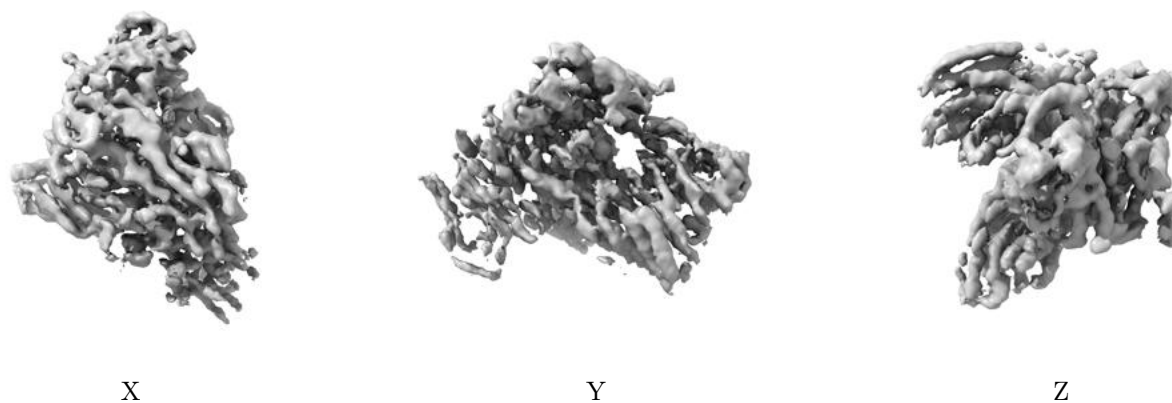
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

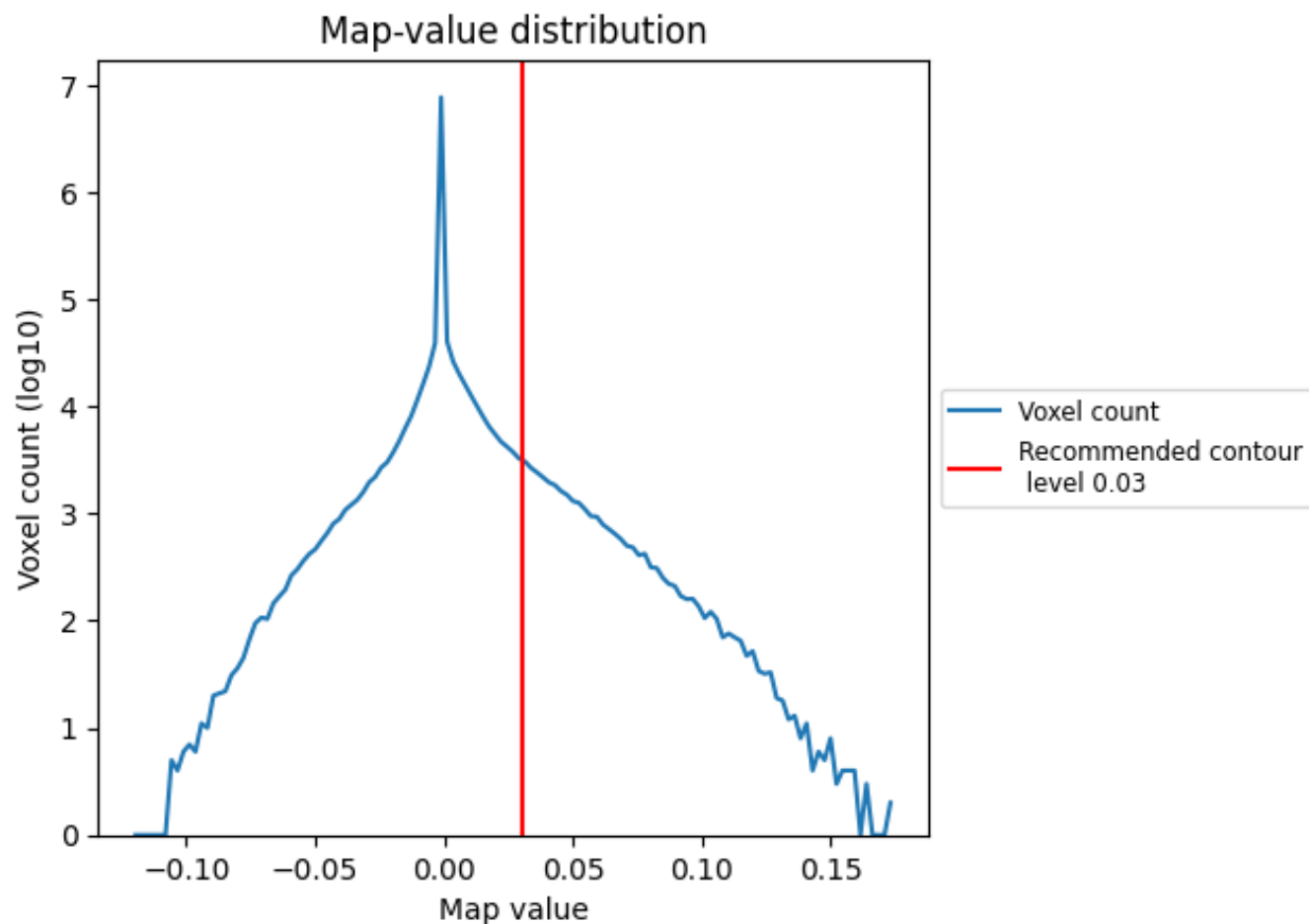
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

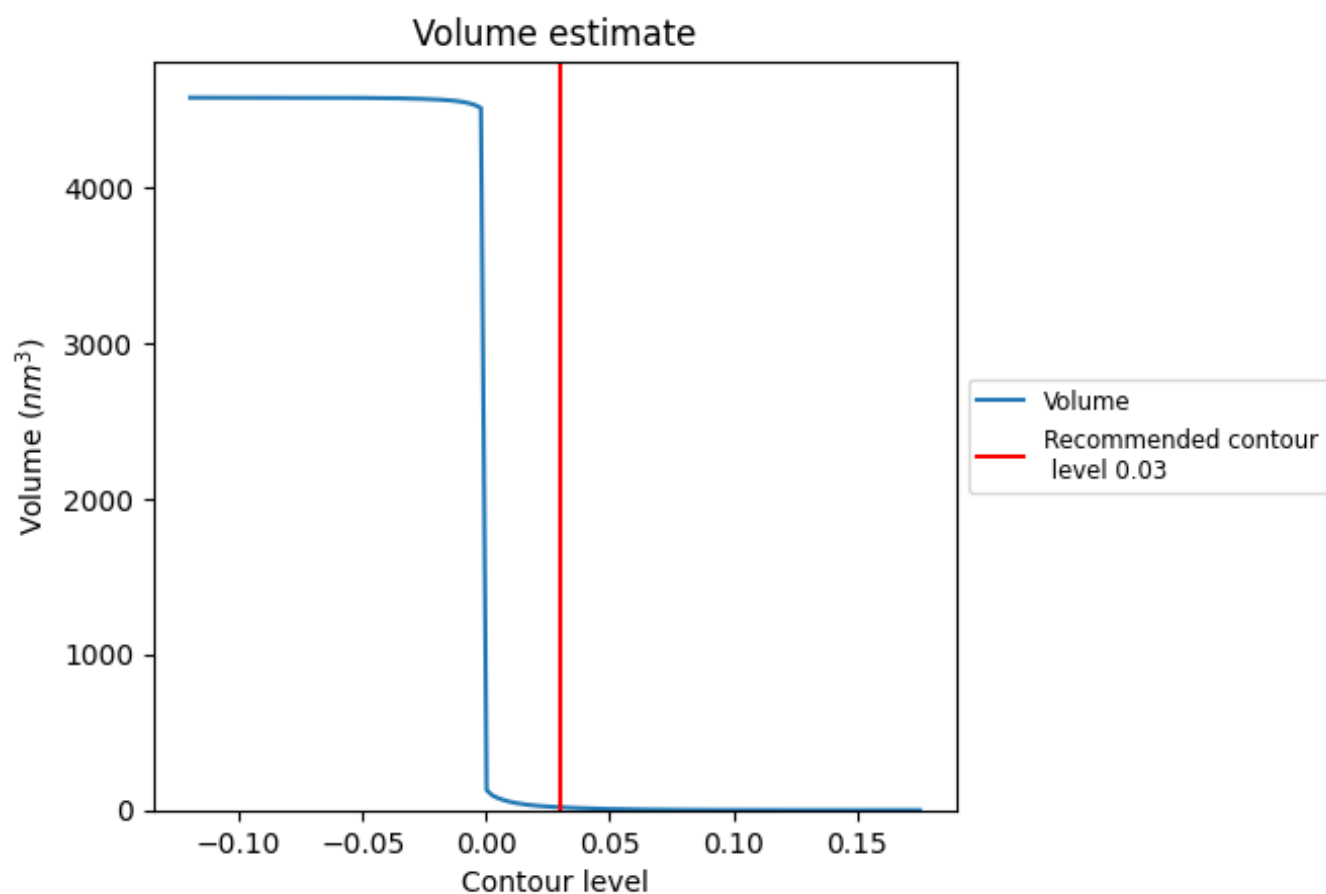
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

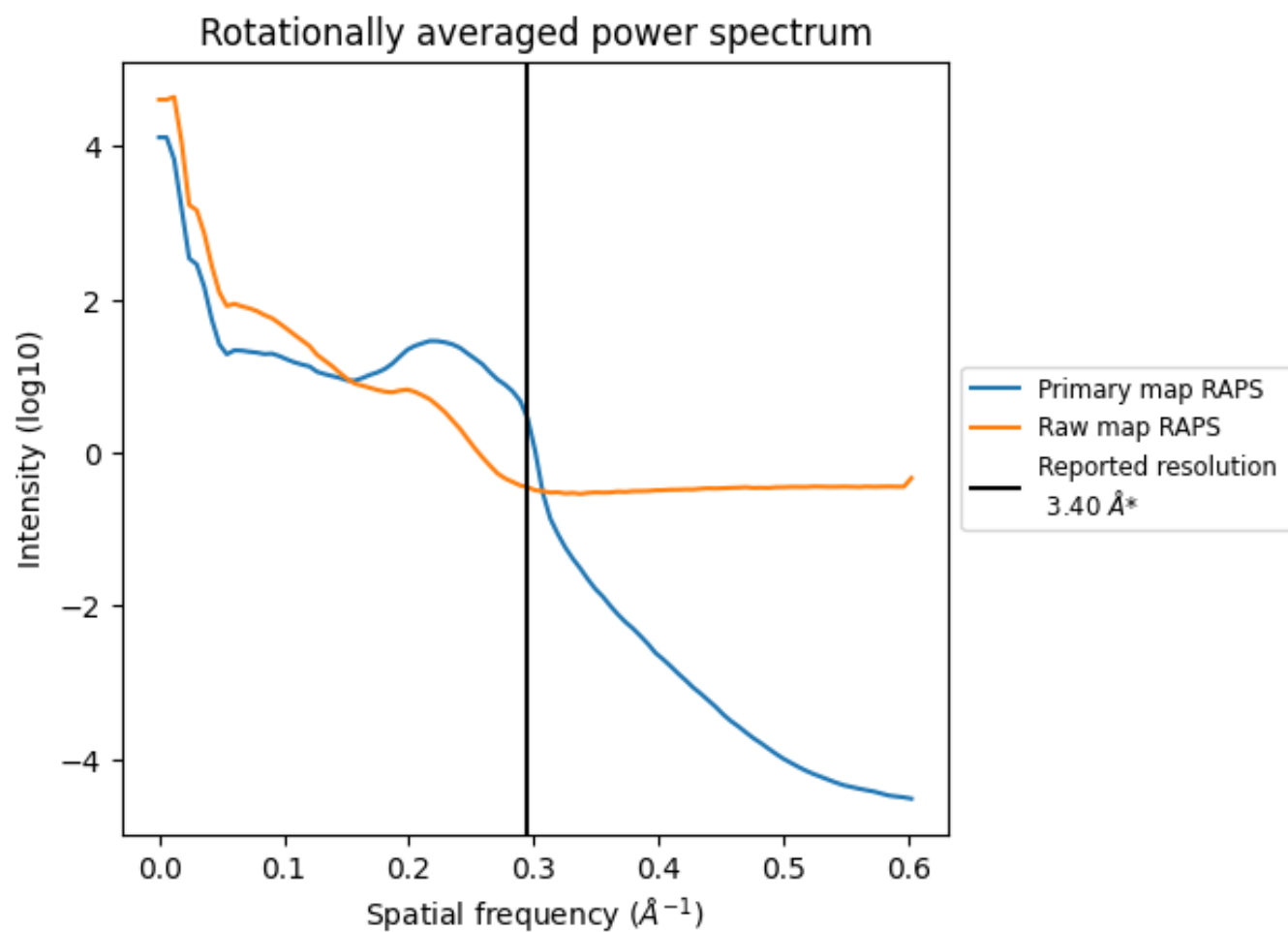
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 18 nm³; this corresponds to an approximate mass of 17 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 ⓘ

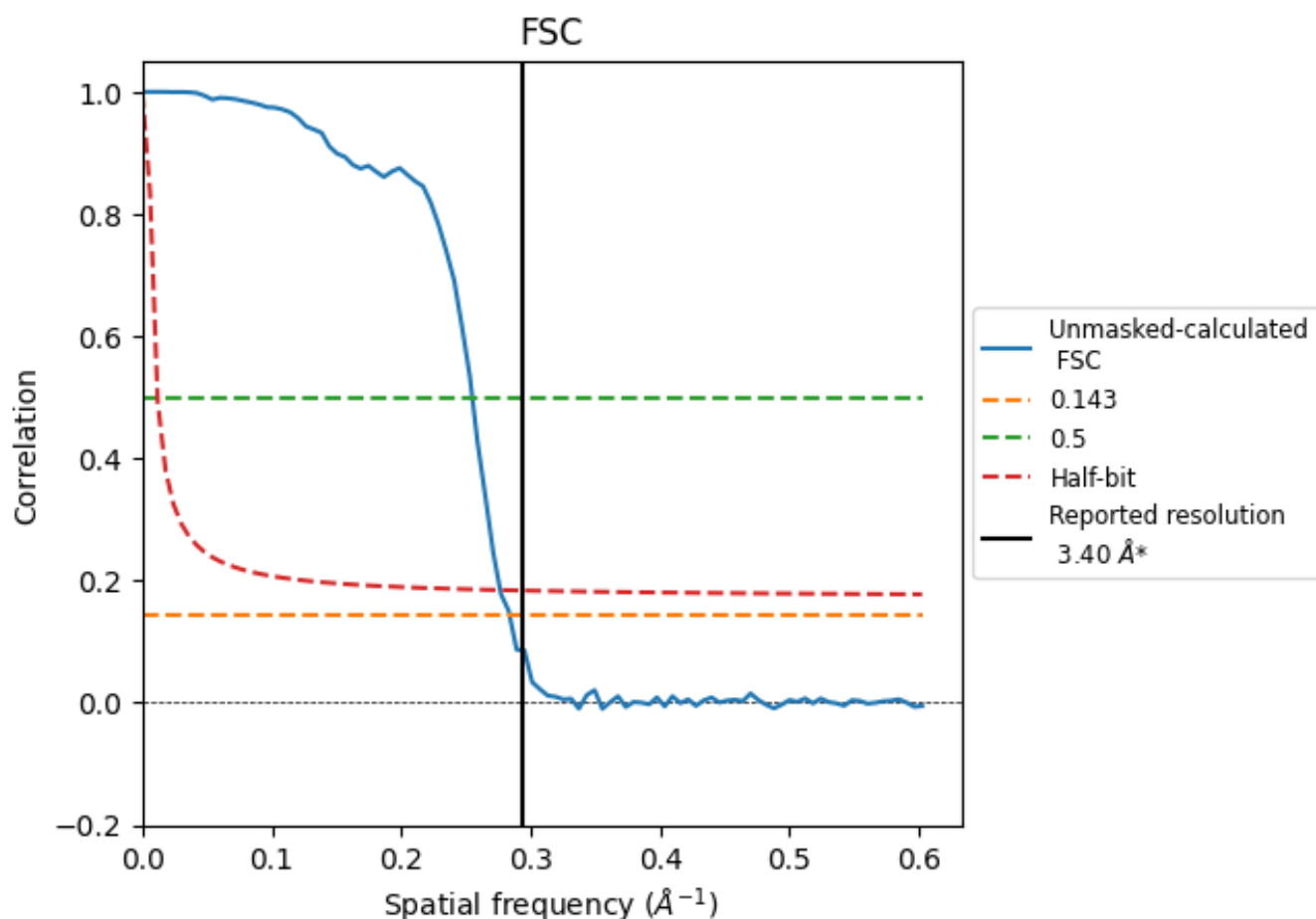


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

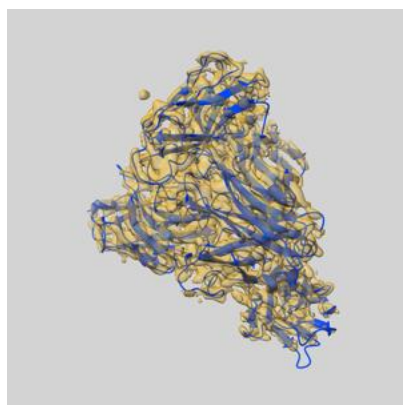
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.52	3.92	3.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

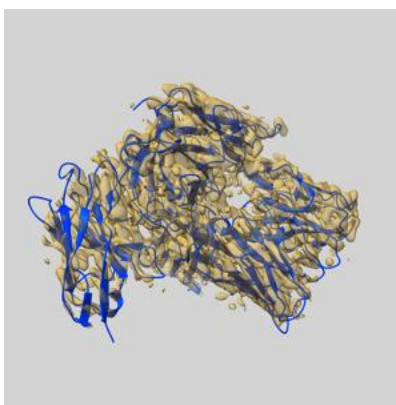
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49735 and PDB model 9NRJ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

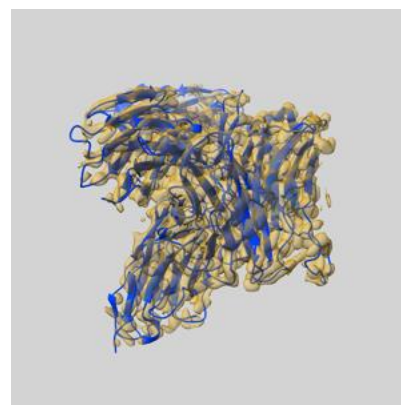
9.1 Map-model overlay [i](#)



X



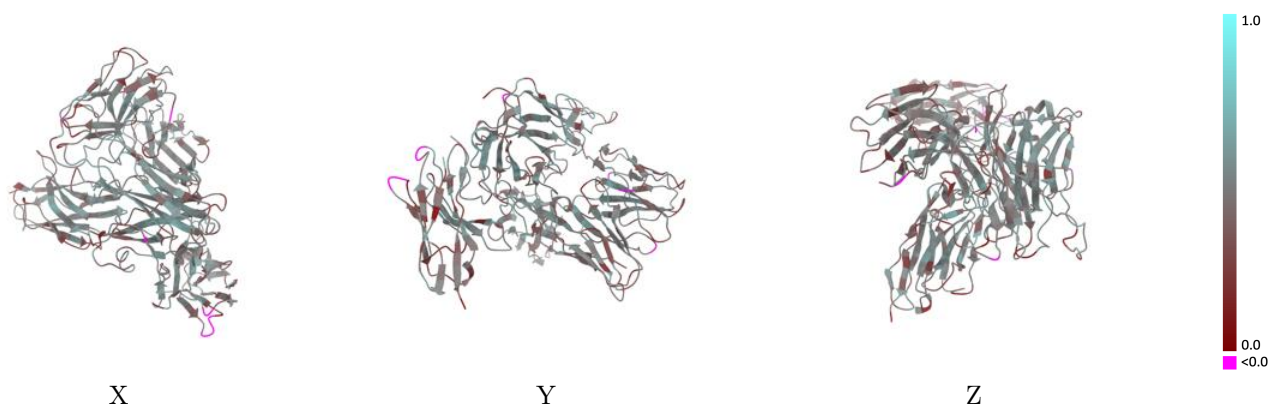
Y



Z

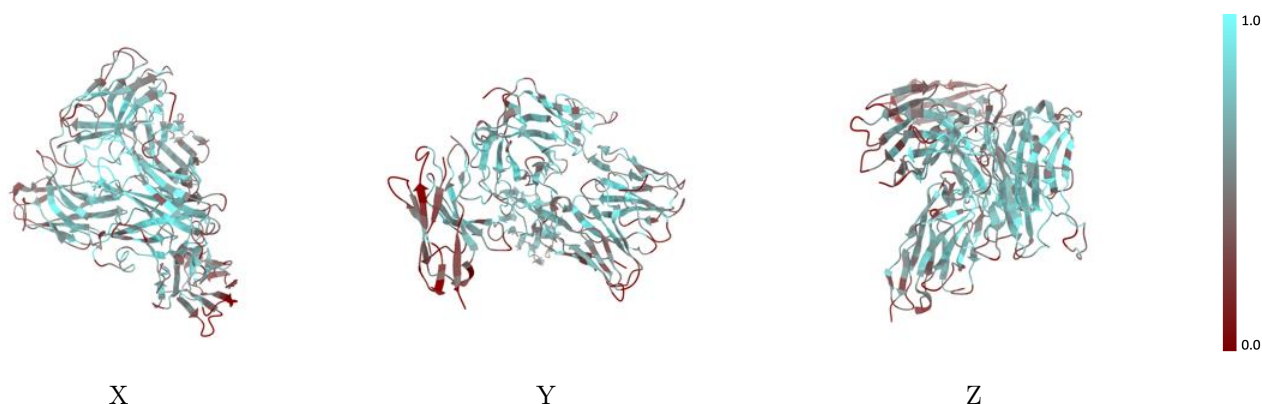
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



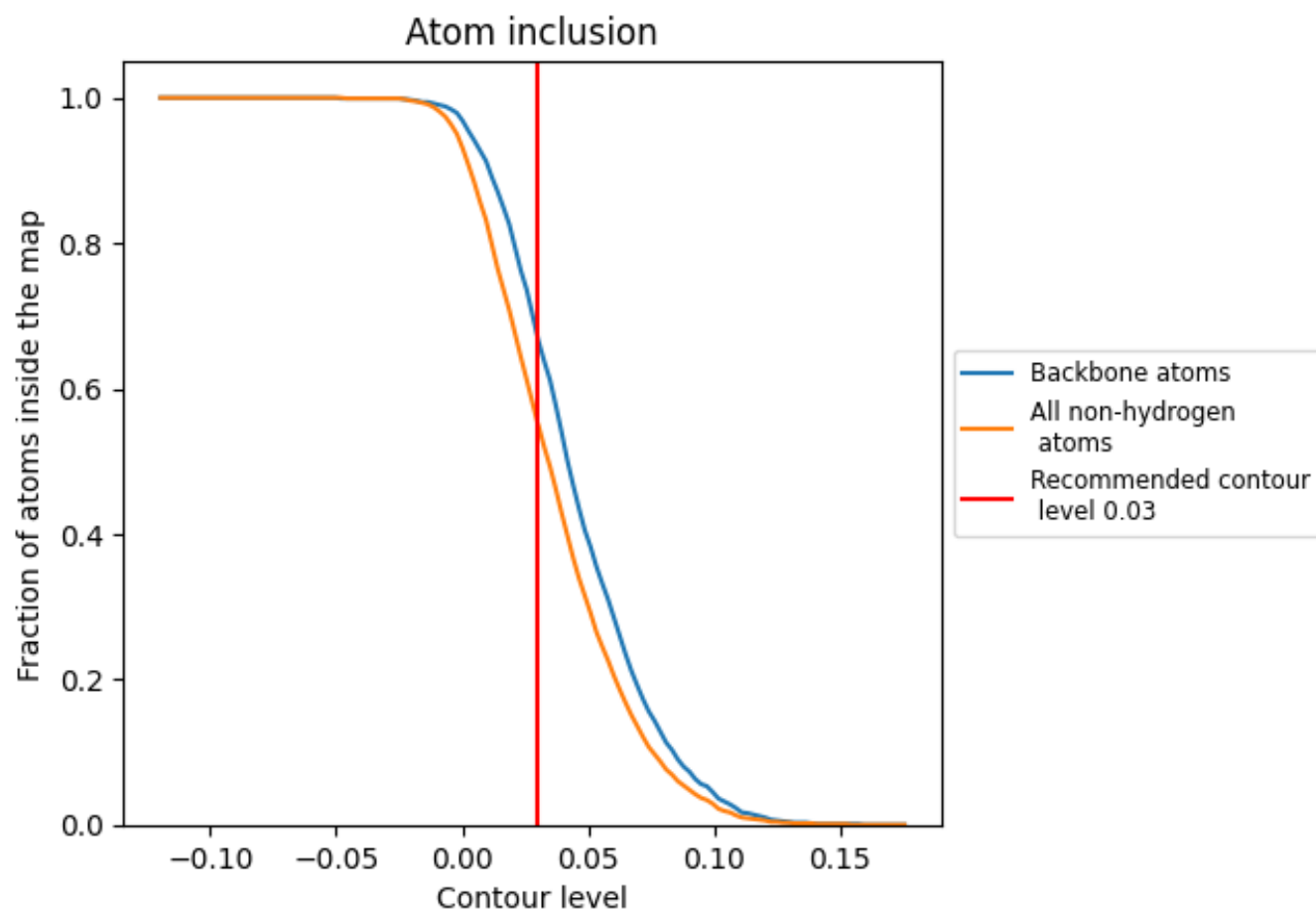
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5510	<div></div> 0.4410
A	<div></div> 0.5580	<div></div> 0.4370
B	<div></div> 0.6220	<div></div> 0.4620
C	<div></div> 0.4060	<div></div> 0.4050
D	<div></div> 0.3160	<div></div> 0.3190
E	<div></div> 0.0260	<div></div> 0.1690
F	<div></div> 0.1070	<div></div> 0.4290
T	<div></div> 0.5770	<div></div> 0.4580

1.0

0.0

<0.0