



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:49 AM UTC

PDB ID : 5G06 / pdb_00005g06
EMDB ID : EMD-3366
Title : Cryo-EM structure of yeast cytoplasmic exosome
Authors : Liu, J.J.; Niu, C.Y.; Wu, Y.; Tan, D.; Wang, Y.; Ye, M.D.; Liu, Y.; Zhao, W.W.; Zhou, K.; Liu, Q.S.; Dai, J.B.; Yang, X.R.; Dong, M.Q.; Huang, N.; Wang, H.W.
Deposited on : 2016-03-17
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

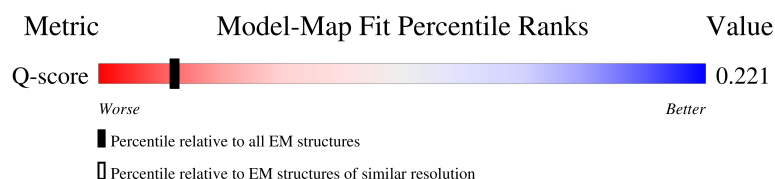
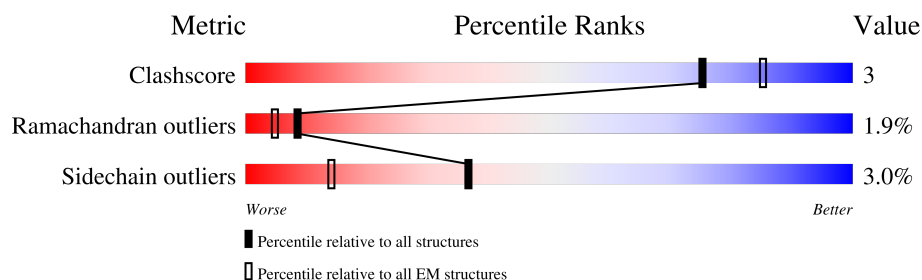
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	305	7% 42% 53% • •
2	B	246	41% 48% 7% •
3	C	394	7% 36% 43% 5% 15% •
4	D	223	47% 51% •

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Mol	Chain	Length	Quality of chain
5	E	265	43%52%
6	F	250	31%47%6%16%
7	G	240	45%47%5%
8	H	359	37%40%5%18%
9	I	292	11%35%37%5%22%
10	J	1001	6%43%51%5%
11	P	747	8%5%5%87%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 26794 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 EXOSOME COMPLEX COMPONENT RRP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	302	Total	C	N	O	S	0	0
			2350	1474	402	457	17		

- Molecule 2 is a protein called EXOSOME COMPLEX COMPONENT SKI6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	240	Total	C	N	O	S	0	0
			1890	1182	338	362	8		

- Molecule 3 is a protein called EXOSOME COMPLEX COMPONENT RRP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2622	1653	455	503	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	363	MET	VAL	conflict	UNP P25359

- Molecule 4 is a protein called EXOSOME COMPLEX COMPONENT RRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	223	Total	C	N	O	S	0	0
			1707	1073	289	335	10		

- Molecule 5 is a protein called EXOSOME COMPLEX COMPONENT RRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	265	Total	C	N	O	S	0	0
			2048	1307	336	400	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	138	ILE	VAL	conflict	UNP Q12277

- Molecule 6 is a protein called EXOSOME COMPLEX COMPONENT MTR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	211	Total	C	N	O	S	0	0
			1627	1018	276	323	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	75	SER	THR	conflict	UNP P48240

- Molecule 7 is a protein called EXOSOME COMPLEX COMPONENT RRP40.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	236	Total	C	N	O	S	0	0
			1831	1169	301	350	11		

- Molecule 8 is a protein called EXOSOME COMPLEX COMPONENT RRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	293	Total	C	N	O	S	0	0
			2277	1419	411	435	12		

- Molecule 9 is a protein called EXOSOME COMPLEX COMPONENT CSL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	227	Total	C	N	O	S	0	0
			1750	1093	310	338	9		

- Molecule 10 is a protein called EXOSOME COMPLEX EXONUCLEASE DIS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	993	Total	C	N	O	S	0	0
			7942	5002	1395	1509	36		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	171	ASN	ASP	conflict	UNP Q08162
J	551	ASN	ASP	conflict	UNP Q08162

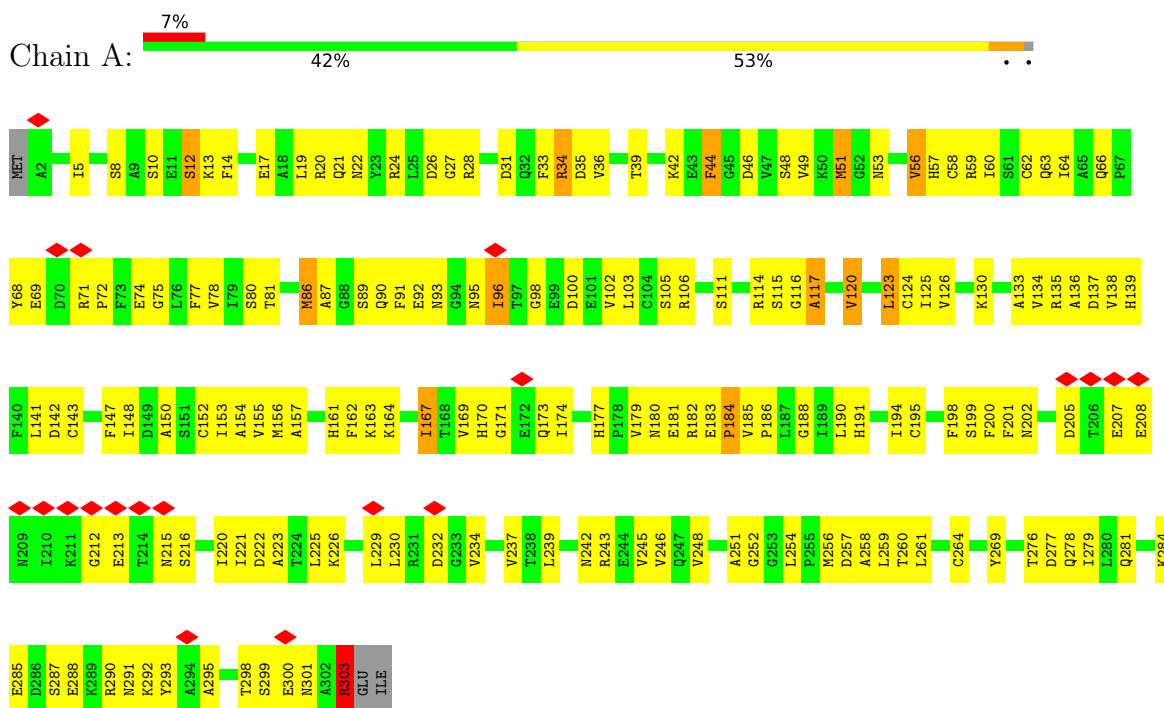
- Molecule 11 is a protein called SUPERKILLER PROTEIN 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	P	95	750	475	128	146	1	0	0

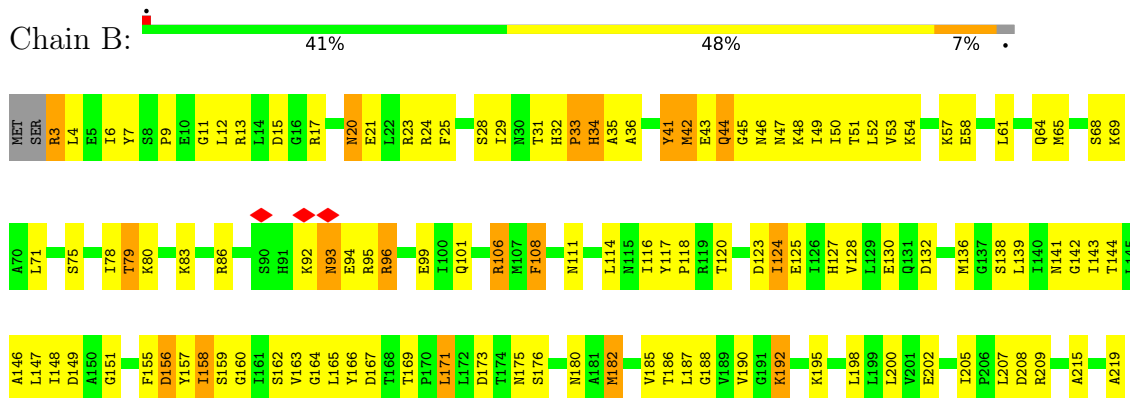
3 Residue-property plots

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

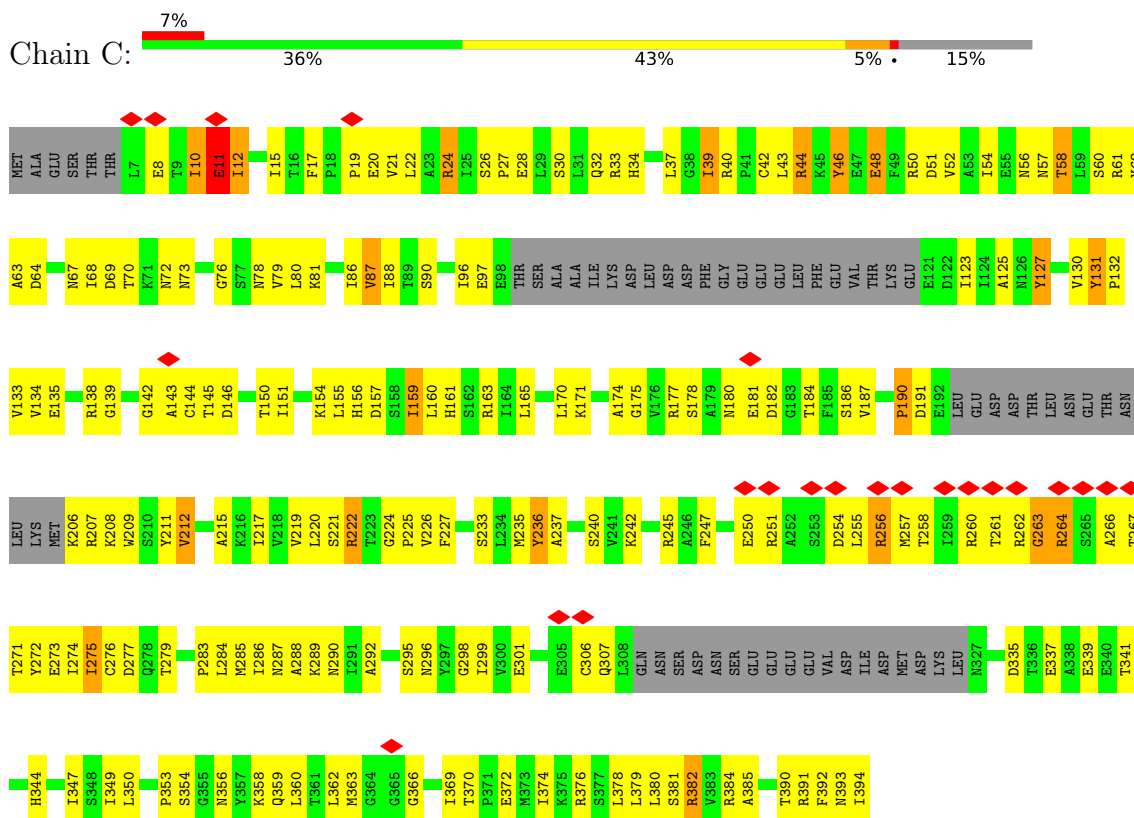
• Molecule 1: EXOSOME COMPLEX COMPONENT RRP45



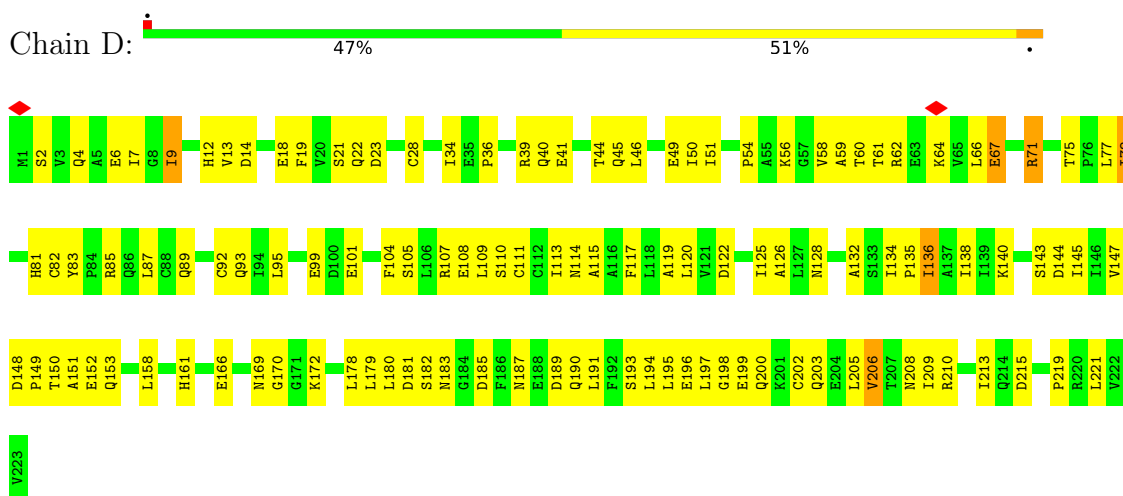
• Molecule 2: EXOSOME COMPLEX COMPONENT SKI6



- Molecule 3: EXOSOME COMPLEX COMPONENT RRP43

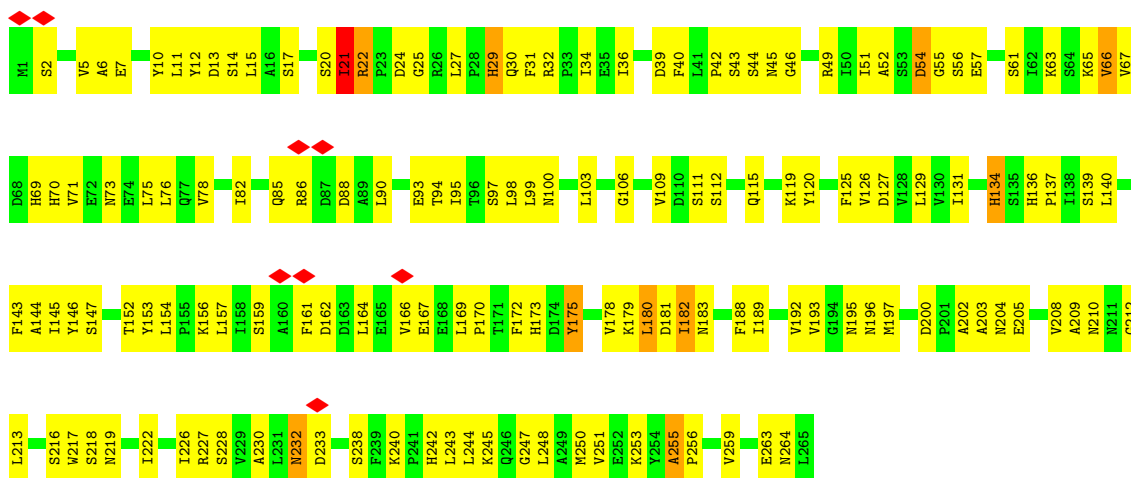


- Molecule 4: EXOSOME COMPLEX COMPONENT RRP46

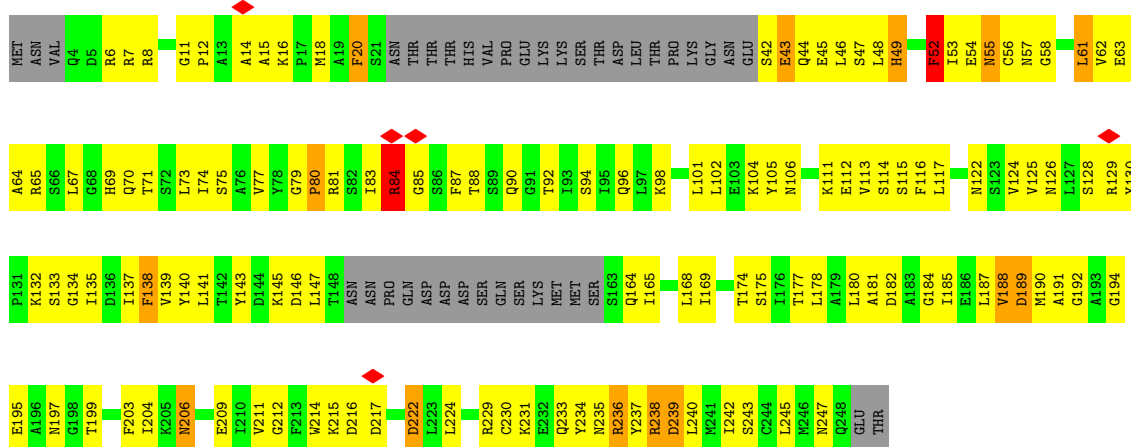


- Molecule 5: EXOSOME COMPLEX COMPONENT RRP42

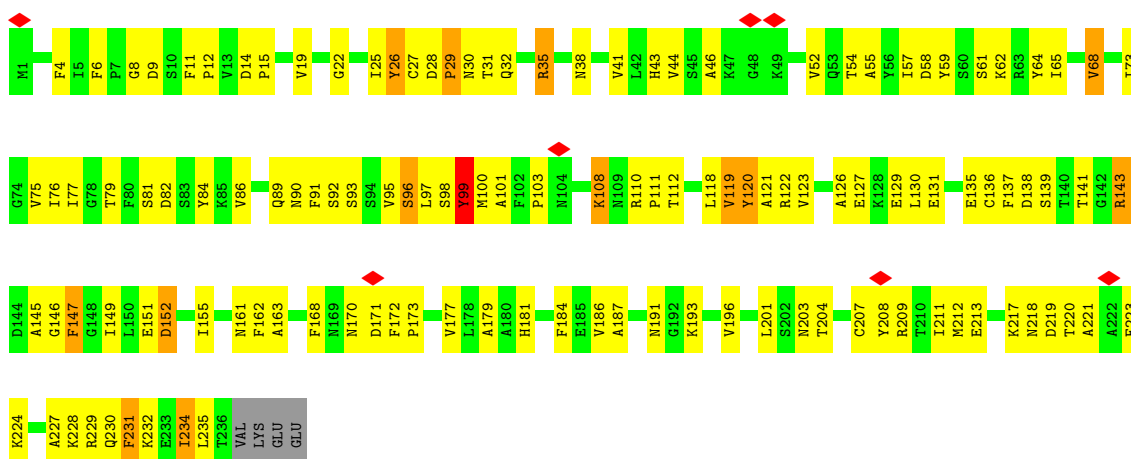




• Molecule 6: EXOSOME COMPLEX COMPONENT MTR3

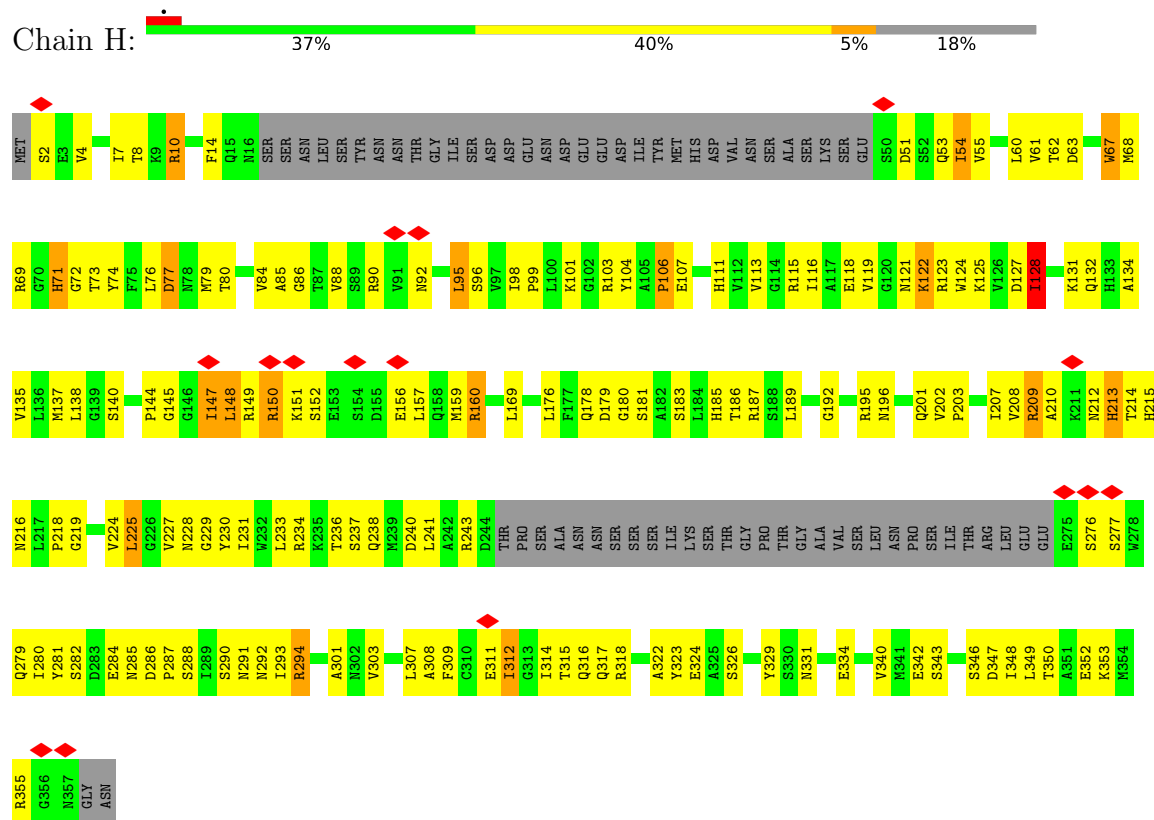


• Molecule 7: EXOSOME COMPLEX COMPONENT RRP40



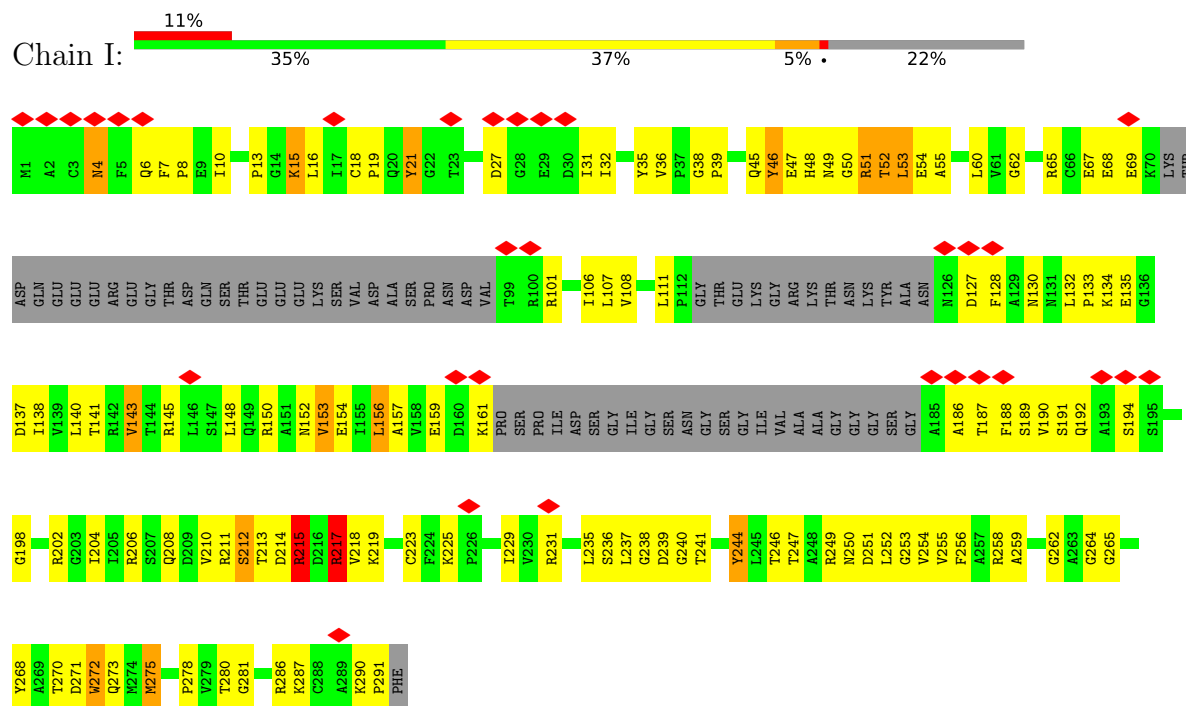
• Molecule 8: EXOSOME COMPLEX COMPONENT RRP4

Chain H:



• Molecule 9: EXOSOME COMPLEX COMPONENT CSL4

Chain I:



• Molecule 10: EXOSOME COMPLEX EXONUCLEASE DIS3

Chain J:





Chain P: 87%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25000	Depositor
Resolution determination method	Not provided	
CTF correction method	MICROGRAPHS	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	21	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.112	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	235.1772, 235.1772, 235.1772	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	2.33	97/2386 (4.1%)	2.49	168/3218 (5.2%)
2	B	2.33	79/1914 (4.1%)	2.43	118/2577 (4.6%)
3	C	2.25	91/2659 (3.4%)	2.50	185/3596 (5.1%)
4	D	2.33	64/1725 (3.7%)	2.48	124/2339 (5.3%)
5	E	2.32	85/2087 (4.1%)	2.43	133/2836 (4.7%)
6	F	2.36	80/1649 (4.9%)	2.50	120/2222 (5.4%)
7	G	2.30	83/1868 (4.4%)	2.38	123/2531 (4.9%)
8	H	2.32	92/2311 (4.0%)	2.46	153/3118 (4.9%)
9	I	2.33	76/1774 (4.3%)	2.35	95/2398 (4.0%)
10	J	2.32	347/8097 (4.3%)	2.44	534/10972 (4.9%)
11	P	2.32	30/763 (3.9%)	2.59	72/1031 (7.0%)
All	All	2.32	1124/27233 (4.1%)	2.45	1825/36838 (5.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	7
3	C	0	10
4	D	0	2
5	E	0	4
6	F	0	5
7	G	0	7
8	H	0	5
9	I	0	6
10	J	0	26
11	P	0	1
All	All	0	76

All (1124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	265	GLY	CA-C	-11.10	1.42	1.52
10	J	113	VAL	N-CA	-10.84	1.38	1.46
1	A	130	LYS	CA-C	-10.60	1.39	1.52
2	B	188	GLY	CA-C	-10.53	1.40	1.51
3	C	298	GLY	CA-C	-10.48	1.39	1.51
5	E	251	VAL	CA-C	-10.37	1.37	1.52
1	A	201	PHE	CA-C	-9.84	1.40	1.52
8	H	350	THR	N-CA	-9.82	1.34	1.46
3	C	178	SER	CA-C	-9.75	1.41	1.52
6	F	56	CYS	CA-C	-9.62	1.40	1.52
9	I	18	CYS	CA-CB	9.61	1.68	1.54
4	D	56	LYS	CA-C	-9.60	1.40	1.52
7	G	110	ARG	CZ-NH2	9.52	1.45	1.33
10	J	590	ARG	NE-CZ	9.48	1.43	1.33
10	J	105	PRO	N-CA	-9.39	1.40	1.47
10	J	486	LEU	CA-C	-9.12	1.41	1.52
10	J	886	ARG	CZ-NH2	9.10	1.45	1.33
4	D	161	HIS	CE1-NE2	8.96	1.41	1.32
1	A	24	ARG	CD-NE	8.96	1.58	1.46
10	J	186	LYS	N-CA	8.91	1.55	1.46
6	F	216	ASP	CA-C	-8.90	1.43	1.52
2	B	175	ASN	C-N	8.88	1.45	1.33
10	J	361	ASN	CA-CB	8.85	1.62	1.53
9	I	249	ARG	NE-CZ	8.79	1.42	1.33
3	C	62	TYR	CA-C	-8.75	1.40	1.52
4	D	147	VAL	CA-CB	8.71	1.64	1.54
4	D	149	PRO	CA-C	-8.68	1.43	1.52
3	C	50	ARG	NE-CZ	8.61	1.42	1.33
5	E	21	ILE	N-CA	-8.60	1.36	1.46
10	J	41	LEU	CA-C	-8.59	1.41	1.52
10	J	469	ARG	NE-CZ	8.58	1.42	1.33
11	P	91	VAL	CA-CB	8.54	1.58	1.54
10	J	937	GLY	CA-C	-8.52	1.43	1.51
6	F	44	GLN	CA-C	-8.51	1.42	1.52
1	A	133	ALA	CA-C	-8.51	1.42	1.52
1	A	220	ILE	CA-C	-8.45	1.42	1.52
6	F	129	ARG	CD-NE	8.44	1.58	1.46
4	D	45	GLN	N-CA	-8.42	1.35	1.46
10	J	899	ILE	C-N	8.41	1.44	1.33
2	B	3	ARG	CD-NE	8.35	1.57	1.46
5	E	98	LEU	CA-C	-8.34	1.42	1.52
6	F	169	ILE	CA-C	-8.33	1.44	1.52
7	G	46	ALA	CA-C	-8.32	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	11	LEU	CA-C	-8.29	1.42	1.52
9	I	157	ALA	CA-C	-8.27	1.41	1.52
9	I	258	ARG	CD-NE	8.24	1.57	1.46
1	A	114	ARG	CD-NE	8.19	1.57	1.46
5	E	164	LEU	CA-C	-8.18	1.43	1.53
10	J	113	VAL	CA-C	8.14	1.59	1.53
10	J	226	PRO	N-CA	8.12	1.53	1.47
1	A	134	VAL	CA-C	-8.09	1.42	1.52
10	J	42	ARG	NE-CZ	8.07	1.42	1.33
1	A	287	SER	C-N	8.07	1.44	1.34
1	A	35	ASP	N-CA	8.06	1.55	1.46
10	J	288	GLY	CA-C	8.05	1.63	1.51
10	J	393	VAL	C-N	8.05	1.43	1.33
8	H	101	LYS	N-CA	-8.03	1.36	1.46
10	J	721	LEU	N-CA	-8.03	1.35	1.45
3	C	150	THR	CA-CB	-8.02	1.40	1.53
10	J	214	ILE	CA-CB	8.01	1.64	1.54
2	B	235	HIS	ND1-CE1	8.00	1.40	1.32
8	H	195	ARG	CD-NE	8.00	1.57	1.46
10	J	499	VAL	CA-CB	-7.99	1.44	1.54
2	B	24	ARG	CA-C	-7.99	1.42	1.52
11	P	55	ARG	CA-C	-7.98	1.42	1.52
3	C	384	ARG	NE-CZ	7.98	1.41	1.33
10	J	309	ARG	NE-CZ	7.97	1.41	1.33
8	H	122	LYS	CA-C	-7.97	1.42	1.52
10	J	711	ASP	CA-C	-7.96	1.42	1.53
10	J	28	ARG	NE-CZ	7.96	1.41	1.33
7	G	143	ARG	CD-NE	7.93	1.57	1.46
10	J	137	ARG	CD-NE	7.92	1.57	1.46
1	A	220	ILE	C-N	7.91	1.41	1.33
10	J	515	LYS	CA-C	-7.91	1.43	1.52
8	H	329	TYR	N-CA	-7.90	1.36	1.46
10	J	144	ARG	CD-NE	7.86	1.57	1.46
10	J	281	SER	CA-C	-7.84	1.43	1.52
1	A	153	ILE	CA-CB	-7.83	1.44	1.54
10	J	600	ARG	CA-C	-7.82	1.43	1.52
10	J	41	LEU	C-N	7.79	1.43	1.33
10	J	15	ASP	CA-CB	7.76	1.65	1.53
10	J	39	HIS	C-N	7.76	1.44	1.33
3	C	157	ASP	N-CA	-7.74	1.36	1.46
1	A	135	ARG	NE-CZ	7.72	1.41	1.33
3	C	206	LYS	C-N	7.72	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	464	LEU	CA-CB	7.70	1.65	1.53
9	I	202	ARG	NE-CZ	7.70	1.41	1.33
3	C	146	ASP	N-CA	7.68	1.55	1.46
10	J	444	LEU	CA-C	-7.66	1.42	1.52
10	J	220	GLN	C-N	7.65	1.43	1.33
10	J	27	SER	CA-C	-7.65	1.43	1.52
1	A	34	ARG	CZ-NH2	7.65	1.43	1.33
9	I	6	GLN	CA-C	-7.65	1.42	1.52
10	J	831	HIS	CA-C	-7.64	1.43	1.52
4	D	128	ASN	CA-C	-7.64	1.42	1.52
6	F	64	ALA	CA-C	-7.64	1.43	1.52
3	C	215	ALA	CA-C	-7.63	1.43	1.52
10	J	790	LEU	C-N	7.63	1.43	1.33
10	J	35	ILE	CA-C	7.59	1.62	1.52
7	G	92	SER	CA-C	-7.58	1.43	1.52
10	J	393	VAL	N-CA	-7.58	1.38	1.46
6	F	230	CYS	N-CA	-7.56	1.36	1.46
8	H	77	ASP	N-CA	-7.53	1.36	1.46
1	A	152	CYS	C-N	7.53	1.43	1.33
1	A	161	HIS	CE1-NE2	-7.52	1.25	1.32
6	F	112	GLU	CA-C	-7.52	1.43	1.52
1	A	184	PRO	C-N	7.52	1.39	1.32
2	B	42	MET	C-N	7.50	1.43	1.33
7	G	64	TYR	CA-CB	7.50	1.64	1.53
3	C	226	VAL	N-CA	-7.49	1.38	1.46
6	F	11	GLY	C-N	7.49	1.42	1.33
10	J	740	ARG	CZ-NH2	7.48	1.43	1.33
10	J	960	LEU	CA-C	-7.48	1.44	1.52
10	J	242	ASP	C-N	7.47	1.43	1.33
7	G	64	TYR	C-N	7.46	1.41	1.33
10	J	604	LEU	CA-C	-7.46	1.43	1.52
1	A	56	VAL	CA-C	-7.44	1.44	1.52
10	J	535	ARG	NE-CZ	7.43	1.41	1.33
3	C	175	GLY	C-N	7.42	1.44	1.33
5	E	140	LEU	CA-C	-7.42	1.43	1.52
6	F	165	ILE	N-CA	-7.42	1.35	1.46
8	H	216	ASN	CA-C	-7.39	1.43	1.52
6	F	125	VAL	CA-C	-7.38	1.43	1.52
10	J	994	ARG	CA-C	-7.38	1.44	1.52
6	F	104	LYS	CA-CB	7.37	1.64	1.53
8	H	279	GLN	CA-CB	7.37	1.63	1.53
5	E	61	SER	C-N	7.37	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	217	ILE	CA-C	-7.37	1.43	1.52
8	H	318	ARG	NE-CZ	7.34	1.41	1.33
10	J	930	VAL	CA-C	-7.34	1.45	1.52
8	H	349	LEU	C-N	7.32	1.43	1.33
10	J	102	LEU	N-CA	-7.31	1.37	1.46
7	G	213	GLU	CA-C	-7.31	1.43	1.52
7	G	112	THR	N-CA	-7.31	1.38	1.46
10	J	439	ARG	C-N	7.30	1.43	1.33
10	J	544	PRO	CA-C	7.30	1.58	1.52
5	E	70	HIS	ND1-CE1	7.29	1.39	1.32
6	F	238	ARG	CD-NE	7.29	1.56	1.46
9	I	15	LYS	C-N	7.28	1.43	1.33
10	J	819	PHE	CA-CB	7.25	1.63	1.53
6	F	117	LEU	N-CA	-7.25	1.37	1.46
7	G	230	GLN	N-CA	-7.25	1.37	1.46
10	J	19	VAL	CA-C	-7.22	1.44	1.52
2	B	95	ARG	CA-C	-7.21	1.43	1.52
5	E	227	ARG	NE-CZ	7.21	1.41	1.33
10	J	986	VAL	N-CA	-7.20	1.38	1.46
6	F	67	LEU	CA-C	-7.19	1.43	1.52
10	J	841	HIS	ND1-CE1	7.19	1.39	1.32
1	A	138	VAL	CA-CB	-7.19	1.45	1.54
5	E	232	ASN	CA-CB	-7.18	1.45	1.54
4	D	89	GLN	CA-C	-7.18	1.43	1.52
1	A	215	ASN	CA-CB	7.17	1.63	1.53
11	P	88	ILE	N-CA	-7.13	1.38	1.46
8	H	140	SER	CA-C	-7.12	1.44	1.53
5	E	43	SER	N-CA	-7.12	1.36	1.46
10	J	295	PHE	CA-C	-7.11	1.44	1.52
5	E	45	ASN	CA-C	-7.10	1.43	1.52
10	J	830	ARG	CD-NE	7.09	1.56	1.46
1	A	78	VAL	CA-C	-7.09	1.43	1.52
5	E	244	LEU	N-CA	-7.07	1.37	1.46
5	E	109	VAL	CA-C	-7.07	1.44	1.52
8	H	60	LEU	C-N	7.07	1.42	1.33
5	E	159	SER	C-N	7.06	1.43	1.33
1	A	194	ILE	CA-CB	-7.05	1.45	1.54
8	H	294	ARG	CD-NE	7.05	1.56	1.46
8	H	209	ARG	CD-NE	7.04	1.56	1.46
10	J	759	PRO	N-CA	-7.04	1.38	1.47
6	F	57	ASN	CA-C	7.03	1.62	1.52
10	J	649	ARG	CD-NE	7.03	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	127	HIS	ND1-CE1	7.03	1.39	1.32
2	B	219	ALA	CA-C	-7.03	1.43	1.52
5	E	32	ARG	CD-NE	7.02	1.56	1.46
6	F	194	GLY	CA-C	-7.02	1.45	1.52
4	D	93	GLN	N-CA	-7.01	1.37	1.46
7	G	27	CYS	CA-C	-7.01	1.44	1.52
1	A	57	HIS	N-CA	-7.00	1.36	1.45
2	B	130	GLU	N-CA	-6.99	1.37	1.46
10	J	215	THR	CA-C	-6.99	1.44	1.52
4	D	136	ILE	CA-C	6.99	1.61	1.52
1	A	186	PRO	C-N	6.98	1.42	1.33
7	G	204	THR	C-N	6.98	1.43	1.33
10	J	600	ARG	CD-NE	6.96	1.55	1.46
3	C	21	VAL	CA-C	-6.95	1.44	1.52
10	J	503	LEU	C-N	6.95	1.42	1.33
10	J	709	THR	CA-CB	6.95	1.64	1.54
1	A	243	ARG	NE-CZ	6.95	1.40	1.33
10	J	76	PRO	CA-C	-6.95	1.46	1.53
3	C	208	LYS	C-N	6.93	1.42	1.33
10	J	398	ARG	NE-CZ	6.93	1.40	1.33
10	J	496	SER	CA-C	-6.91	1.43	1.53
10	J	754	ARG	NE-CZ	6.91	1.40	1.33
5	E	5	VAL	C-N	6.90	1.43	1.33
9	I	10	ILE	CA-CB	6.89	1.63	1.54
8	H	51	ASP	CA-C	-6.89	1.44	1.52
9	I	215	ARG	CD-NE	6.89	1.55	1.46
9	I	145	ARG	NE-CZ	6.88	1.40	1.33
4	D	196	GLU	C-N	6.88	1.43	1.33
10	J	12	ARG	NE-CZ	6.87	1.40	1.33
10	J	143	LYS	CA-C	-6.87	1.47	1.53
9	I	286	ARG	CA-CB	6.87	1.64	1.53
2	B	163	VAL	C-N	6.86	1.39	1.33
8	H	10	ARG	CA-CB	6.86	1.65	1.53
2	B	208	ASP	C-N	6.86	1.42	1.33
8	H	103	ARG	CD-NE	6.85	1.55	1.46
3	C	360	LEU	CA-C	-6.84	1.44	1.52
1	A	213	GLU	CA-C	-6.83	1.44	1.52
9	I	252	LEU	C-N	6.83	1.43	1.32
7	G	95	VAL	C-N	6.83	1.42	1.33
10	J	660	ARG	CZ-NH1	6.82	1.42	1.32
8	H	74	TYR	CZ-OH	6.81	1.52	1.38
10	J	756	ALA	CA-C	-6.80	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	67	VAL	CA-C	6.79	1.60	1.52
6	F	6	ARG	NE-CZ	6.79	1.40	1.33
7	G	130	LEU	CA-C	-6.79	1.44	1.52
4	D	199	GLU	N-CA	-6.79	1.38	1.46
10	J	37	ARG	CZ-NH1	6.79	1.42	1.32
9	I	272	TRP	N-CA	-6.78	1.36	1.46
10	J	401	ARG	CZ-NH2	6.78	1.42	1.33
5	E	75	LEU	C-N	6.78	1.42	1.33
5	E	180	LEU	CA-CB	6.78	1.62	1.53
5	E	147	SER	CA-C	-6.78	1.44	1.52
5	E	197	MET	N-CA	-6.77	1.38	1.46
10	J	122	ARG	CZ-NH2	6.77	1.42	1.33
10	J	14	ALA	N-CA	-6.77	1.38	1.46
9	I	231	ARG	C-N	6.77	1.42	1.33
1	A	31	ASP	C-N	6.77	1.43	1.33
4	D	179	LEU	C-N	6.76	1.42	1.33
11	P	9	PHE	C-N	6.76	1.42	1.33
4	D	77	LEU	N-CA	6.75	1.54	1.46
2	B	221	ALA	C-N	6.74	1.43	1.34
10	J	526	PRO	C-N	6.74	1.42	1.33
4	D	39	ARG	NE-CZ	6.74	1.40	1.33
8	H	10	ARG	CZ-NH1	6.74	1.42	1.32
8	H	234	ARG	C-N	6.74	1.42	1.33
9	I	51	ARG	NE-CZ	6.73	1.40	1.33
4	D	125	ILE	N-CA	-6.72	1.38	1.46
11	P	82	LYS	C-O	-6.72	1.16	1.24
10	J	652	PHE	CA-C	-6.72	1.44	1.52
11	P	37	HIS	ND1-CE1	6.71	1.39	1.32
7	G	96	SER	CA-C	-6.70	1.44	1.52
6	F	63	GLU	C-N	6.70	1.42	1.33
10	J	245	LEU	C-N	6.70	1.43	1.33
1	A	91	PHE	CA-C	-6.68	1.44	1.52
5	E	70	HIS	CA-CB	6.67	1.63	1.53
7	G	223	PHE	C-N	6.67	1.42	1.33
1	A	21	GLN	N-CA	-6.67	1.37	1.46
2	B	95	ARG	CD-NE	6.67	1.55	1.46
4	D	39	ARG	CD-NE	6.66	1.55	1.46
10	J	269	LYS	N-CA	-6.65	1.38	1.46
8	H	225	LEU	CA-CB	6.65	1.63	1.53
8	H	213	HIS	CA-C	-6.65	1.43	1.52
10	J	98	ALA	C-N	6.65	1.42	1.33
9	I	101	ARG	NE-CZ	6.65	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	202	ARG	NE-CZ	6.64	1.40	1.33
5	E	131	ILE	N-CA	-6.64	1.38	1.46
7	G	118	LEU	N-CA	-6.64	1.37	1.46
3	C	163	ARG	CA-CB	6.63	1.64	1.53
10	J	376	ASP	C-O	-6.63	1.16	1.24
1	A	92	GLU	C-N	6.63	1.42	1.33
2	B	158	ILE	N-CA	-6.63	1.38	1.46
5	E	212	GLY	C-N	6.63	1.42	1.33
10	J	534	LEU	N-CA	-6.62	1.39	1.46
2	B	47	ASN	CA-CB	6.62	1.61	1.53
10	J	611	ASP	CA-CB	6.62	1.61	1.53
1	A	139	HIS	CA-C	-6.62	1.44	1.52
1	A	120	VAL	CA-CB	-6.61	1.46	1.54
5	E	115	GLN	N-CA	-6.61	1.37	1.46
4	D	120	LEU	C-N	6.61	1.42	1.33
9	I	4	ASN	CA-C	-6.61	1.44	1.52
10	J	569	HIS	CA-C	-6.60	1.44	1.53
10	J	36	VAL	CA-C	-6.60	1.44	1.52
10	J	968	ASP	C-N	6.59	1.41	1.32
3	C	222	ARG	CZ-NH1	6.59	1.42	1.32
10	J	298	PRO	CA-C	-6.59	1.44	1.52
9	I	275	MET	C-N	6.59	1.42	1.33
10	J	169	ARG	CA-CB	6.58	1.63	1.53
7	G	201	LEU	C-N	6.57	1.42	1.33
3	C	163	ARG	CD-NE	6.57	1.55	1.46
8	H	101	LYS	CA-CB	6.57	1.64	1.53
8	H	307	LEU	CA-CB	6.57	1.64	1.53
3	C	207	ARG	NE-CZ	6.57	1.40	1.33
7	G	177	VAL	CA-C	6.56	1.60	1.52
3	C	262	ARG	CD-NE	6.56	1.55	1.46
2	B	75	SER	CA-C	-6.55	1.45	1.52
7	G	204	THR	CA-C	-6.55	1.44	1.52
10	J	814	MET	C-N	6.55	1.42	1.33
11	P	33	SER	N-CA	-6.55	1.38	1.46
2	B	198	LEU	CA-C	-6.55	1.45	1.52
9	I	219	LYS	CA-C	-6.55	1.44	1.52
1	A	257	ASP	CA-C	-6.54	1.44	1.53
3	C	86	ILE	N-CA	-6.54	1.38	1.46
8	H	69	ARG	N-CA	-6.54	1.37	1.46
10	J	603	MET	C-N	6.54	1.44	1.33
10	J	161	LEU	CA-C	-6.54	1.43	1.52
9	I	108	VAL	CA-C	-6.54	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	59	ILE	N-CA	-6.54	1.38	1.46
3	C	160	LEU	CA-C	-6.53	1.44	1.52
10	J	94	VAL	N-CA	-6.53	1.38	1.46
10	J	590	ARG	CD-NE	6.52	1.55	1.46
7	G	121	ALA	N-CA	-6.52	1.38	1.46
2	B	229	ASP	CA-CB	6.52	1.63	1.53
1	A	28	ARG	NE-CZ	6.52	1.40	1.33
10	J	537	LYS	CA-C	-6.51	1.44	1.52
4	D	126	ALA	CA-C	-6.51	1.44	1.52
8	H	216	ASN	C-N	6.51	1.41	1.32
5	E	78	VAL	CA-C	-6.50	1.44	1.52
7	G	229	ARG	NE-CZ	6.50	1.40	1.33
10	J	80	SER	CA-CB	6.50	1.63	1.53
2	B	225	ARG	NE-CZ	6.50	1.40	1.33
8	H	55	VAL	C-N	6.49	1.40	1.33
10	J	156	THR	C-N	6.49	1.42	1.33
10	J	216	LYS	C-N	6.49	1.42	1.33
8	H	284	GLU	CA-C	-6.48	1.44	1.52
9	I	27	ASP	N-CA	-6.48	1.37	1.46
10	J	596	LEU	C-N	6.48	1.41	1.33
10	J	69	LYS	C-N	6.47	1.42	1.33
10	J	495	PHE	CA-CB	6.47	1.64	1.53
5	E	95	ILE	C-N	6.47	1.42	1.33
5	E	56	SER	CA-C	-6.46	1.44	1.52
5	E	192	VAL	C-N	6.46	1.41	1.33
4	D	107	ARG	C-N	6.46	1.41	1.33
4	D	82	CYS	C-N	6.46	1.40	1.33
5	E	120	TYR	C-N	6.46	1.42	1.33
10	J	287	GLU	CA-C	-6.45	1.44	1.52
4	D	138	ILE	CA-CB	-6.44	1.46	1.54
3	C	245	ARG	CA-C	-6.44	1.44	1.52
7	G	184	PHE	CA-C	-6.42	1.44	1.52
5	E	27	LEU	CA-CB	6.42	1.62	1.53
5	E	162	ASP	CA-C	-6.42	1.44	1.53
6	F	61	LEU	CA-C	-6.42	1.44	1.52
9	I	236	SER	CA-C	-6.42	1.44	1.52
10	J	120	GLU	CA-C	-6.42	1.44	1.52
1	A	12	SER	CA-C	-6.41	1.44	1.52
8	H	189	LEU	N-CA	-6.41	1.37	1.46
11	P	64	ARG	NE-CZ	6.41	1.40	1.33
7	G	186	VAL	N-CA	-6.41	1.38	1.46
10	J	569	HIS	ND1-CE1	6.41	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	87	VAL	C-N	6.41	1.41	1.33
8	H	276	SER	N-CA	-6.41	1.37	1.45
7	G	146	GLY	C-N	6.41	1.42	1.33
4	D	183	ASN	CA-C	-6.40	1.44	1.52
10	J	508	HIS	CE1-NE2	6.40	1.39	1.32
1	A	258	ALA	N-CA	-6.39	1.38	1.46
5	E	243	LEU	C-N	6.39	1.42	1.33
6	F	73	LEU	N-CA	-6.39	1.38	1.46
9	I	225	LYS	N-CA	-6.39	1.40	1.46
11	P	55	ARG	CA-CB	6.39	1.63	1.53
11	P	59	ILE	CA-C	-6.39	1.44	1.52
2	B	160	GLY	CA-C	-6.38	1.47	1.52
6	F	206	ASN	CA-CB	6.38	1.62	1.53
7	G	193	LYS	CA-C	-6.38	1.44	1.52
10	J	217	SER	C-N	6.38	1.42	1.33
5	E	156	LYS	CA-C	-6.37	1.44	1.52
6	F	239	ASP	CA-C	-6.36	1.44	1.52
10	J	738	VAL	C-N	6.36	1.42	1.33
3	C	54	ILE	CA-C	-6.36	1.45	1.52
2	B	21	GLU	C-N	6.36	1.42	1.33
10	J	232	ARG	CZ-NH1	6.36	1.41	1.32
2	B	128	VAL	CA-C	6.35	1.60	1.52
10	J	344	ASN	N-CA	-6.35	1.41	1.46
2	B	117	TYR	CA-CB	6.34	1.61	1.53
5	E	25	GLY	C-N	6.34	1.41	1.33
10	J	488	HIS	N-CA	-6.34	1.38	1.46
5	E	212	GLY	N-CA	6.34	1.51	1.44
6	F	238	ARG	NE-CZ	6.34	1.40	1.33
7	G	173	PRO	CA-CB	6.34	1.62	1.53
2	B	120	THR	C-N	6.34	1.41	1.33
6	F	137	ILE	CA-C	-6.33	1.45	1.52
6	F	46	LEU	CA-C	-6.33	1.45	1.52
10	J	229	ASP	CA-CB	6.33	1.63	1.53
10	J	553	ALA	N-CA	-6.33	1.37	1.45
4	D	191	LEU	N-CA	-6.32	1.38	1.46
1	A	68	TYR	CA-C	-6.32	1.44	1.52
2	B	7	TYR	CA-CB	6.32	1.64	1.53
10	J	755	HIS	ND1-CE1	6.32	1.38	1.32
11	P	81	GLU	C-O	-6.30	1.16	1.24
5	E	88	ASP	CA-C	-6.30	1.47	1.52
9	I	154	GLU	CA-C	-6.30	1.44	1.52
10	J	291	SER	CA-C	-6.30	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	192	VAL	N-CA	-6.29	1.39	1.46
8	H	150	ARG	CZ-NH1	6.29	1.41	1.32
7	G	122	ARG	NE-CZ	6.28	1.40	1.33
8	H	131	LYS	CA-C	-6.28	1.44	1.52
2	B	79	THR	CA-C	-6.27	1.44	1.53
3	C	76	GLY	CA-C	-6.27	1.44	1.51
5	E	192	VAL	CA-CB	-6.27	1.46	1.54
6	F	77	VAL	CA-C	-6.27	1.44	1.52
10	J	643	LYS	C-N	6.27	1.41	1.33
10	J	855	HIS	C-O	-6.27	1.16	1.24
10	J	178	CYS	CA-C	-6.26	1.45	1.52
5	E	7	GLU	C-N	6.26	1.42	1.33
10	J	78	GLU	CA-C	-6.26	1.45	1.52
10	J	435	ARG	C-N	6.26	1.41	1.33
1	A	147	PHE	CA-C	6.26	1.60	1.52
5	E	146	TYR	CA-C	-6.26	1.44	1.52
2	B	61	LEU	CA-C	-6.25	1.45	1.52
5	E	217	TRP	C-N	6.25	1.42	1.33
8	H	54	ILE	CA-C	6.25	1.60	1.52
10	J	37	ARG	CA-CB	-6.25	1.44	1.53
5	E	209	ALA	CA-C	-6.25	1.44	1.52
4	D	179	LEU	CA-C	-6.24	1.44	1.52
10	J	430	CYS	C-N	6.24	1.40	1.32
8	H	169	LEU	N-CA	6.24	1.53	1.46
3	C	347	ILE	CA-CB	-6.24	1.46	1.54
5	E	208	VAL	CA-CB	6.24	1.61	1.54
11	P	74	ALA	N-CA	-6.24	1.41	1.47
10	J	772	THR	CA-C	-6.23	1.44	1.52
10	J	855	HIS	CA-C	-6.23	1.45	1.52
5	E	189	ILE	CA-C	-6.22	1.45	1.52
8	H	86	GLY	CA-C	-6.22	1.45	1.52
10	J	22	LYS	C-N	6.22	1.41	1.33
10	J	583	LEU	C-N	6.22	1.42	1.33
1	A	117	ALA	CA-CB	-6.21	1.43	1.53
3	C	33	ARG	CD-NE	6.21	1.54	1.46
9	I	259	ALA	C-N	6.21	1.42	1.33
1	A	60	ILE	C-N	6.20	1.42	1.33
10	J	42	ARG	CD-NE	6.20	1.54	1.46
10	J	50	ARG	CD-NE	6.20	1.54	1.46
7	G	235	LEU	C-N	6.19	1.42	1.33
3	C	384	ARG	C-N	6.19	1.41	1.33
10	J	137	ARG	NE-CZ	6.18	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	GLU	CA-C	-6.18	1.45	1.52
8	H	127	ASP	CA-C	-6.18	1.45	1.52
9	I	241	THR	CB-OG1	-6.18	1.33	1.43
10	J	553	ALA	C-N	6.18	1.41	1.33
4	D	62	ARG	NE-CZ	6.17	1.39	1.33
5	E	143	PHE	CB-CG	6.17	1.64	1.50
10	J	292	LEU	N-CA	-6.17	1.38	1.46
3	C	369	ILE	CA-CB	-6.17	1.46	1.54
9	I	36	VAL	CA-C	-6.17	1.45	1.52
10	J	660	ARG	NE-CZ	6.17	1.39	1.33
1	A	120	VAL	N-CA	-6.16	1.40	1.46
7	G	143	ARG	NE-CZ	6.16	1.39	1.33
1	A	180	ASN	C-N	6.16	1.41	1.33
3	C	299	ILE	N-CA	-6.16	1.39	1.46
10	J	353	ASP	CA-C	-6.16	1.44	1.53
1	A	171	GLY	CA-C	-6.15	1.43	1.51
10	J	450	VAL	N-CA	6.15	1.53	1.46
2	B	95	ARG	NE-CZ	6.15	1.39	1.33
10	J	958	TYR	CA-C	-6.14	1.44	1.52
8	H	148	LEU	CA-CB	6.14	1.63	1.53
10	J	385	LYS	C-N	6.14	1.41	1.33
6	F	147	LEU	CA-C	-6.14	1.44	1.52
10	J	263	ARG	N-CA	-6.13	1.38	1.46
4	D	81	HIS	ND1-CE1	6.13	1.38	1.32
8	H	96	SER	CA-CB	6.13	1.64	1.53
3	C	381	SER	CA-CB	6.13	1.63	1.53
10	J	315	GLN	CA-C	-6.12	1.44	1.52
2	B	223	ARG	NE-CZ	6.12	1.39	1.33
1	A	63	GLN	N-CA	-6.11	1.38	1.46
10	J	811	ARG	CZ-NH1	6.11	1.41	1.32
10	J	149	HIS	CE1-NE2	-6.11	1.26	1.32
3	C	354	SER	CA-C	-6.10	1.46	1.52
10	J	836	VAL	N-CA	-6.10	1.39	1.46
10	J	230	ASP	N-CA	-6.09	1.38	1.46
5	E	238	SER	C-N	6.09	1.41	1.33
7	G	122	ARG	CZ-NH2	6.08	1.41	1.33
4	D	181	ASP	CA-CB	6.08	1.62	1.53
10	J	900	GLU	N-CA	-6.08	1.39	1.46
10	J	984	ARG	N-CA	-6.08	1.38	1.46
10	J	649	ARG	CA-CB	6.07	1.62	1.53
10	J	773	ARG	CD-NE	6.07	1.54	1.46
5	E	67	VAL	N-CA	-6.07	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	24	PHE	CA-C	-6.06	1.45	1.52
9	I	132	LEU	CA-CB	6.06	1.61	1.54
9	I	198	GLY	CA-C	6.06	1.58	1.52
3	C	177	ARG	NE-CZ	6.05	1.39	1.33
9	I	21	TYR	CA-C	-6.05	1.45	1.52
5	E	202	ALA	C-N	-6.05	1.26	1.33
4	D	2	SER	N-CA	-6.05	1.40	1.46
10	J	149	HIS	ND1-CE1	6.05	1.38	1.32
5	E	188	PHE	CA-C	-6.05	1.45	1.52
9	I	231	ARG	CA-C	-6.04	1.45	1.52
10	J	61	PRO	CA-C	-6.04	1.45	1.52
8	H	135	VAL	CA-C	-6.04	1.45	1.52
10	J	199	ARG	CZ-NH2	6.04	1.41	1.33
10	J	548	VAL	CA-CB	-6.04	1.46	1.54
2	B	106	ARG	CD-NE	6.04	1.54	1.46
8	H	185	HIS	ND1-CE1	6.04	1.38	1.32
9	I	152	ASN	CA-CB	6.04	1.62	1.53
10	J	350	GLY	N-CA	-6.04	1.36	1.45
10	J	448	ARG	CZ-NH1	6.04	1.41	1.32
10	J	128	VAL	C-N	6.04	1.41	1.33
1	A	48	SER	CA-C	-6.03	1.45	1.52
7	G	110	ARG	CA-C	-6.03	1.46	1.53
10	J	417	SER	CA-CB	6.02	1.63	1.53
10	J	879	MET	CA-CB	6.02	1.62	1.53
6	F	18	MET	CA-C	6.01	1.60	1.52
10	J	782	SER	CA-C	-6.01	1.45	1.52
10	J	896	ARG	CZ-NH1	6.00	1.41	1.32
2	B	116	ILE	N-CA	-6.00	1.37	1.46
6	F	122	ASN	CA-C	-6.00	1.44	1.52
4	D	134	ILE	CB-CG1	5.99	1.65	1.53
10	J	325	GLU	N-CA	-5.99	1.38	1.46
10	J	754	ARG	C-N	5.99	1.41	1.33
9	I	65	ARG	NE-CZ	5.99	1.39	1.33
10	J	535	ARG	CA-C	-5.99	1.44	1.52
10	J	247	ARG	NE-CZ	5.98	1.39	1.33
9	I	153	VAL	N-CA	-5.97	1.39	1.46
9	I	231	ARG	NE-CZ	5.97	1.39	1.33
10	J	267	GLY	N-CA	5.97	1.53	1.45
8	H	185	HIS	CG-CD2	-5.97	1.29	1.35
9	I	107	LEU	C-N	5.96	1.41	1.33
3	C	264	ARG	CD-NE	5.95	1.54	1.46
7	G	68	VAL	CA-C	-5.95	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	273	GLN	CA-C	-5.95	1.47	1.52
1	A	134	VAL	N-CA	-5.95	1.39	1.46
10	J	725	SER	CA-C	-5.95	1.44	1.52
3	C	254	ASP	C-N	5.95	1.41	1.33
8	H	180	GLY	C-N	5.94	1.41	1.33
5	E	193	VAL	C-O	-5.94	1.18	1.24
1	A	138	VAL	C-N	5.93	1.41	1.33
2	B	239	ARG	NE-CZ	5.93	1.39	1.33
3	C	177	ARG	CD-NE	5.93	1.54	1.46
8	H	308	ALA	CA-C	-5.93	1.45	1.52
10	J	232	ARG	NE-CZ	5.93	1.39	1.33
10	J	649	ARG	NE-CZ	5.93	1.39	1.33
10	J	397	ARG	CA-C	-5.92	1.45	1.52
3	C	378	LEU	CA-CB	5.92	1.63	1.53
10	J	165	THR	CA-C	-5.92	1.45	1.52
2	B	125	GLU	C-N	5.92	1.40	1.33
10	J	327	LYS	N-CA	-5.91	1.38	1.45
10	J	968	ASP	CA-C	-5.91	1.45	1.52
4	D	143	SER	C-N	5.91	1.40	1.33
10	J	170	ASN	C-N	5.91	1.42	1.33
8	H	157	LEU	N-CA	-5.91	1.39	1.46
2	B	17	ARG	NE-CZ	5.89	1.39	1.33
7	G	217	LYS	N-CA	-5.89	1.39	1.46
2	B	148	ILE	CA-CB	-5.89	1.46	1.54
2	B	198	LEU	CA-CB	5.89	1.64	1.53
1	A	106	ARG	C-N	5.87	1.41	1.33
2	B	13	ARG	CZ-NH2	5.87	1.41	1.33
7	G	101	ALA	CA-CB	-5.87	1.43	1.53
1	A	207	GLU	CA-CB	5.87	1.62	1.53
7	G	92	SER	C-N	5.87	1.41	1.33
1	A	281	GLN	CA-C	-5.87	1.44	1.52
10	J	241	PHE	CA-C	-5.87	1.45	1.52
2	B	226	ASP	C-N	5.87	1.41	1.33
1	A	71	ARG	NE-CZ	5.86	1.39	1.33
7	G	58	ASP	C-N	5.86	1.42	1.33
6	F	113	VAL	N-CA	-5.86	1.39	1.46
7	G	30	ASN	CA-C	-5.86	1.45	1.52
10	J	713	ASN	CA-CB	5.86	1.62	1.53
9	I	281	GLY	C-N	5.85	1.41	1.33
10	J	572	ASP	CA-CB	5.85	1.60	1.53
10	J	172	ARG	CD-NE	5.84	1.54	1.46
6	F	81	ARG	N-CA	-5.84	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	49	SER	CA-C	-5.84	1.45	1.52
10	J	450	VAL	CA-C	-5.84	1.45	1.52
10	J	950	SER	CA-CB	5.84	1.61	1.53
1	A	126	VAL	C-O	-5.84	1.17	1.24
2	B	223	ARG	CZ-NH2	5.83	1.41	1.33
10	J	74	ASP	C-N	5.83	1.40	1.33
10	J	476	SER	CA-CB	5.83	1.61	1.53
10	J	786	LEU	CA-C	-5.83	1.45	1.52
2	B	94	GLU	CA-C	-5.83	1.45	1.52
2	B	53	VAL	C-N	5.83	1.41	1.33
4	D	221	LEU	CA-C	-5.83	1.45	1.52
8	H	346	SER	C-N	5.83	1.41	1.33
6	F	104	LYS	CA-C	-5.83	1.45	1.52
11	P	12	LYS	CA-CB	5.82	1.62	1.53
1	A	225	LEU	C-N	5.82	1.41	1.33
7	G	29	PRO	N-CA	-5.82	1.39	1.47
1	A	80	SER	CA-C	-5.81	1.45	1.52
2	B	136	MET	CA-C	-5.81	1.44	1.52
9	I	212	SER	CA-CB	5.81	1.63	1.53
10	J	488	HIS	ND1-CE1	5.81	1.38	1.32
6	F	70	GLN	CA-C	-5.81	1.45	1.52
10	J	491	GLU	CA-CB	5.81	1.62	1.53
2	B	28	SER	CA-C	-5.80	1.45	1.52
3	C	233	SER	N-CA	-5.80	1.38	1.46
6	F	236	ARG	C-N	5.80	1.42	1.33
7	G	81	SER	CA-C	-5.80	1.45	1.52
2	B	202	GLU	CA-C	-5.80	1.45	1.52
3	C	144	CYS	N-CA	-5.80	1.38	1.46
1	A	36	VAL	N-CA	-5.80	1.39	1.46
1	A	239	LEU	CA-C	-5.80	1.45	1.52
10	J	1000	LEU	CA-CB	5.80	1.62	1.53
7	G	22	GLY	CA-C	-5.79	1.43	1.51
3	C	211	TYR	CA-CB	5.79	1.62	1.53
6	F	203	PHE	C-N	5.79	1.41	1.33
8	H	96	SER	CA-C	-5.79	1.45	1.52
10	J	466	HIS	CD2-NE2	5.79	1.44	1.37
4	D	81	HIS	CD2-NE2	5.79	1.44	1.37
2	B	207	LEU	CA-C	-5.78	1.44	1.52
10	J	836	VAL	CA-C	5.78	1.60	1.52
8	H	88	VAL	C-N	5.78	1.40	1.33
10	J	665	THR	CA-C	-5.78	1.45	1.52
3	C	245	ARG	N-CA	5.78	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	137	ARG	N-CA	-5.78	1.39	1.46
10	J	105	PRO	CA-CB	-5.77	1.47	1.53
10	J	769	MET	CA-C	-5.77	1.45	1.52
9	I	190	VAL	CA-C	5.77	1.59	1.52
3	C	382	ARG	CZ-NH1	5.77	1.40	1.32
5	E	245	LYS	CA-C	5.77	1.60	1.52
7	G	11	PHE	N-CA	5.77	1.54	1.45
2	B	171	LEU	N-CA	-5.76	1.39	1.46
3	C	376	ARG	CA-C	5.76	1.60	1.52
10	J	495	PHE	N-CA	-5.76	1.39	1.46
10	J	16	GLY	CA-C	-5.76	1.45	1.51
10	J	202	ARG	N-CA	-5.75	1.39	1.46
2	B	108	PHE	CA-C	-5.75	1.44	1.52
10	J	847	ARG	CD-NE	5.75	1.54	1.46
9	I	67	GLU	C-N	5.74	1.41	1.33
2	B	44	GLN	C-N	5.74	1.42	1.33
10	J	744	ASP	CA-C	5.74	1.60	1.52
8	H	124	TRP	N-CA	-5.73	1.39	1.45
6	F	74	ILE	N-CA	-5.73	1.39	1.46
10	J	884	ILE	N-CA	-5.73	1.38	1.46
7	G	143	ARG	CA-C	-5.73	1.45	1.52
6	F	238	ARG	CZ-NH2	5.72	1.40	1.33
10	J	611	ASP	C-N	5.72	1.41	1.33
6	F	229	ARG	CZ-NH2	5.72	1.40	1.33
8	H	160	ARG	CD-NE	5.72	1.54	1.46
2	B	151	GLY	C-N	5.72	1.40	1.33
8	H	72	GLY	C-N	5.72	1.41	1.33
1	A	124	CYS	CA-C	-5.72	1.45	1.52
8	H	116	ILE	N-CA	-5.72	1.39	1.46
10	J	263	ARG	CD-NE	5.72	1.54	1.46
10	J	839	TYR	CA-C	-5.72	1.45	1.52
10	J	615	LEU	N-CA	-5.71	1.38	1.46
10	J	935	VAL	CA-C	-5.71	1.46	1.52
1	A	120	VAL	CA-C	-5.70	1.45	1.52
5	E	204	ASN	N-CA	-5.70	1.39	1.46
6	F	146	ASP	N-CA	-5.70	1.39	1.46
11	P	23	PRO	CA-CB	5.70	1.63	1.53
10	J	516	LEU	CA-C	-5.70	1.45	1.53
2	B	231	GLU	CA-CB	5.70	1.62	1.53
7	G	209	ARG	NE-CZ	5.70	1.39	1.33
10	J	568	VAL	CA-C	-5.70	1.45	1.52
11	P	11	ILE	CA-C	-5.70	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	244	TYR	C-O	-5.69	1.17	1.24
4	D	60	THR	CA-CB	-5.69	1.45	1.54
9	I	159	GLU	N-CA	-5.69	1.39	1.46
10	J	597	VAL	CA-C	-5.69	1.43	1.52
5	E	247	GLY	C-N	5.69	1.40	1.33
9	I	133	PRO	N-CA	-5.69	1.40	1.47
1	A	123	LEU	CA-C	-5.68	1.45	1.52
8	H	85	ALA	C-N	5.68	1.39	1.32
2	B	200	LEU	CA-C	-5.68	1.45	1.52
2	B	86	ARG	CZ-NH1	5.67	1.40	1.32
3	C	258	THR	N-CA	-5.67	1.41	1.46
7	G	229	ARG	CZ-NH1	5.67	1.40	1.32
2	B	32	HIS	ND1-CE1	5.66	1.38	1.32
8	H	128	ILE	CA-CB	5.66	1.60	1.54
7	G	26	TYR	CA-CB	5.66	1.63	1.53
10	J	32	ALA	C-N	5.66	1.41	1.33
6	F	138	PHE	CA-C	-5.65	1.45	1.52
4	D	200	GLN	C-N	-5.65	1.26	1.34
10	J	172	ARG	NE-CZ	5.65	1.39	1.33
10	J	740	ARG	CZ-NH1	5.64	1.40	1.32
1	A	89	SER	CA-C	-5.64	1.46	1.52
1	A	157	ALA	CA-C	-5.64	1.45	1.52
5	E	120	TYR	N-CA	-5.64	1.39	1.46
10	J	984	ARG	NE-CZ	5.64	1.39	1.33
10	J	848	ARG	CA-C	-5.64	1.45	1.52
10	J	888	HIS	C-N	5.64	1.41	1.33
11	P	35	LYS	C-N	5.63	1.41	1.34
5	E	134	HIS	CA-CB	5.63	1.62	1.53
7	G	127	GLU	CA-C	-5.63	1.45	1.52
1	A	161	HIS	CA-CB	5.62	1.62	1.53
6	F	8	ARG	NE-CZ	5.62	1.39	1.33
6	F	134	GLY	N-CA	-5.62	1.40	1.45
7	G	161	ASN	N-CA	-5.62	1.39	1.46
10	J	285	PHE	CA-CB	5.62	1.62	1.53
10	J	896	ARG	CD-NE	5.61	1.54	1.46
10	J	966	ASN	CA-C	-5.61	1.45	1.52
4	D	194	LEU	CA-CB	5.61	1.62	1.53
5	E	127	ASP	CA-CB	5.61	1.62	1.53
1	A	174	ILE	CA-C	-5.61	1.45	1.52
3	C	267	THR	C-N	5.60	1.40	1.33
3	C	362	LEU	CA-C	-5.60	1.46	1.52
10	J	827	PRO	C-N	5.60	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	82	ASP	CA-CB	5.60	1.62	1.53
10	J	621	ARG	NE-CZ	5.60	1.39	1.33
1	A	198	PHE	CA-C	-5.60	1.46	1.52
4	D	205	LEU	N-CA	-5.60	1.39	1.46
11	P	15	LYS	N-CA	-5.60	1.39	1.46
8	H	115	ARG	CD-NE	5.60	1.54	1.46
10	J	359	SER	CA-C	-5.59	1.46	1.53
10	J	452	SER	CA-C	-5.59	1.45	1.52
11	P	44	ILE	C-N	5.59	1.41	1.33
5	E	106	GLY	C-N	5.59	1.41	1.33
11	P	49	ASN	CA-C	-5.59	1.45	1.52
3	C	269	ARG	CZ-NH2	5.58	1.40	1.33
1	A	5	ILE	CA-C	-5.58	1.45	1.52
8	H	233	LEU	N-CA	-5.58	1.39	1.46
6	F	84	ARG	NE-CZ	5.58	1.39	1.33
9	I	47	GLU	C-O	-5.58	1.17	1.24
10	J	816	ALA	CA-C	-5.58	1.45	1.52
1	A	59	ARG	NE-CZ	5.57	1.39	1.33
2	B	25	PHE	C-O	-5.57	1.17	1.24
10	J	738	VAL	CA-CB	-5.57	1.47	1.54
11	P	92	PRO	C-N	5.57	1.41	1.33
4	D	99	GLU	C-N	5.57	1.41	1.33
2	B	33	PRO	N-CD	-5.56	1.40	1.47
5	E	111	SER	C-N	5.56	1.41	1.33
9	I	60	LEU	C-N	5.56	1.39	1.33
3	C	363	MET	N-CA	-5.56	1.40	1.46
4	D	210	ARG	CA-CB	5.56	1.61	1.53
4	D	95	LEU	N-CA	5.56	1.53	1.46
5	E	210	ASN	N-CA	-5.56	1.39	1.46
3	C	260	ARG	CA-CB	5.55	1.62	1.53
9	I	210	VAL	CA-C	5.55	1.59	1.52
5	E	137	PRO	C-N	5.55	1.40	1.33
10	J	230	ASP	CA-CB	5.54	1.64	1.54
10	J	443	GLU	N-CA	-5.54	1.39	1.46
6	F	124	VAL	CA-CB	-5.54	1.47	1.54
10	J	198	ASP	C-N	5.53	1.41	1.34
6	F	174	THR	CA-CB	5.53	1.61	1.53
6	F	209	GLU	CA-C	-5.53	1.46	1.52
10	J	978	LYS	C-N	5.53	1.40	1.33
10	J	31	GLY	C-N	5.52	1.41	1.33
3	C	97	GLU	N-CA	-5.52	1.39	1.46
5	E	69	HIS	ND1-CE1	5.52	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	300	LEU	C-N	5.52	1.40	1.33
7	G	68	VAL	N-CA	-5.52	1.40	1.46
10	J	992	SER	CA-C	5.52	1.59	1.52
10	J	543	ASP	CA-CB	5.51	1.62	1.53
7	G	61	SER	CA-C	-5.51	1.45	1.52
10	J	991	THR	CA-C	5.51	1.60	1.53
5	E	63	LYS	CA-C	5.51	1.60	1.53
9	I	143	VAL	N-CA	-5.51	1.40	1.46
8	H	236	THR	N-CA	-5.50	1.39	1.46
4	D	22	GLN	CA-C	-5.49	1.45	1.52
7	G	184	PHE	C-N	5.49	1.41	1.33
6	F	231	LYS	N-CA	5.49	1.52	1.46
1	A	223	ALA	C-N	5.49	1.41	1.33
2	B	185	VAL	N-CA	-5.49	1.39	1.46
8	H	290	SER	CA-CB	5.49	1.61	1.53
10	J	421	ASN	CA-CB	5.48	1.61	1.53
10	J	820	TYR	N-CA	-5.48	1.38	1.45
2	B	162	SER	N-CA	-5.48	1.39	1.45
8	H	115	ARG	C-N	5.48	1.41	1.33
10	J	960	LEU	CB-CG	5.48	1.64	1.53
8	H	195	ARG	CZ-NH2	5.48	1.40	1.33
10	J	598	ASP	CA-CB	5.48	1.62	1.53
10	J	769	MET	CA-CB	5.48	1.61	1.53
4	D	85	ARG	N-CA	5.47	1.54	1.46
3	C	207	ARG	CA-C	-5.47	1.45	1.52
5	E	17	SER	C-N	5.47	1.40	1.33
9	I	231	ARG	CD-NE	5.47	1.53	1.46
5	E	66	VAL	C-N	5.47	1.41	1.33
6	F	62	VAL	C-N	5.46	1.40	1.33
10	J	792	ARG	CZ-NH1	5.46	1.40	1.32
1	A	248	VAL	CA-C	-5.46	1.45	1.52
2	B	49	ILE	C-O	-5.46	1.18	1.24
3	C	237	ALA	CA-C	-5.46	1.46	1.52
7	G	171	ASP	C-O	-5.46	1.16	1.24
10	J	279	GLN	N-CA	-5.46	1.39	1.46
10	J	781	GLU	CA-C	-5.46	1.46	1.52
10	J	858	LEU	C-N	5.46	1.41	1.34
4	D	21	SER	CA-C	-5.46	1.46	1.53
3	C	190	PRO	CA-C	5.45	1.60	1.52
10	J	940	ARG	CZ-NH2	5.45	1.40	1.33
10	J	18	SER	N-CA	-5.45	1.39	1.45
2	B	48	LYS	CA-CB	-5.45	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	236	ARG	NE-CZ	5.45	1.39	1.33
10	J	35	ILE	N-CA	-5.45	1.40	1.46
10	J	240	SER	N-CA	-5.45	1.41	1.46
3	C	258	THR	C-N	5.45	1.40	1.33
3	C	391	ARG	CZ-NH1	5.45	1.40	1.32
7	G	58	ASP	C-O	-5.44	1.17	1.24
9	I	54	GLU	C-N	5.44	1.40	1.33
9	I	211	ARG	CZ-NH1	5.44	1.40	1.32
6	F	70	GLN	N-CA	-5.44	1.39	1.45
11	P	71	ILE	C-N	5.44	1.40	1.33
3	C	132	PRO	N-CD	-5.44	1.40	1.47
10	J	34	LYS	C-N	5.44	1.40	1.33
10	J	477	ALA	CA-CB	5.44	1.61	1.53
10	J	302	VAL	C-O	5.44	1.30	1.24
10	J	449	ILE	CA-CB	-5.43	1.46	1.54
2	B	124	ILE	CA-C	-5.43	1.46	1.52
6	F	217	ASP	C-N	5.43	1.39	1.33
9	I	206	ARG	CZ-NH1	5.43	1.40	1.32
1	A	138	VAL	N-CA	-5.43	1.39	1.46
10	J	822	GLY	CA-C	-5.43	1.42	1.51
6	F	75	SER	N-CA	-5.43	1.39	1.45
9	I	272	TRP	CA-C	-5.43	1.43	1.52
1	A	300	GLU	C-N	5.42	1.40	1.33
3	C	79	VAL	N-CA	-5.42	1.39	1.46
10	J	20	THR	N-CA	-5.42	1.39	1.45
9	I	189	SER	CA-C	5.42	1.59	1.52
9	I	264	GLY	CA-C	-5.42	1.45	1.51
1	A	26	ASP	C-N	5.42	1.41	1.33
7	G	8	GLY	CA-C	-5.42	1.44	1.51
10	J	709	THR	CA-C	5.42	1.60	1.52
8	H	213	HIS	ND1-CE1	5.42	1.38	1.32
6	F	62	VAL	CA-C	-5.41	1.45	1.52
10	J	11	LYS	CA-C	5.41	1.58	1.52
6	F	49	HIS	C-N	5.41	1.40	1.33
7	G	19	VAL	CA-CB	5.41	1.62	1.54
6	F	15	ALA	CA-CB	5.40	1.62	1.53
10	J	831	HIS	CB-CG	-5.40	1.42	1.50
10	J	129	TYR	N-CA	-5.40	1.40	1.46
2	B	224	VAL	CA-C	-5.40	1.45	1.52
1	A	245	VAL	N-CA	-5.39	1.39	1.46
7	G	41	VAL	N-CA	5.39	1.52	1.46
9	I	273	GLN	C-N	5.39	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	521	ALA	CA-C	-5.39	1.45	1.52
1	A	98	GLY	C-N	5.39	1.41	1.33
5	E	159	SER	N-CA	-5.39	1.39	1.46
4	D	83	TYR	CA-C	-5.39	1.48	1.52
10	J	171	ASN	N-CA	-5.39	1.39	1.46
10	J	50	ARG	CZ-NH1	5.38	1.40	1.32
10	J	169	ARG	NE-CZ	5.38	1.39	1.33
11	P	23	PRO	CA-C	-5.38	1.47	1.53
9	I	188	PHE	C-O	-5.38	1.17	1.23
10	J	848	ARG	NE-CZ	5.38	1.39	1.33
10	J	170	ASN	CA-C	-5.38	1.45	1.52
3	C	209	TRP	CA-C	-5.38	1.45	1.52
5	E	44	SER	C-N	5.38	1.41	1.33
10	J	65	ASN	CA-CB	5.38	1.61	1.53
10	J	112	ILE	CB-CG1	5.38	1.64	1.53
6	F	7	ARG	CA-C	-5.37	1.45	1.52
9	I	137	ASP	CA-C	-5.37	1.45	1.52
10	J	912	SER	CA-C	-5.37	1.46	1.52
3	C	138	ARG	CA-C	-5.36	1.46	1.52
5	E	167	GLU	CA-CB	5.36	1.61	1.53
10	J	959	LYS	N-CA	-5.36	1.39	1.46
10	J	909	ASN	CA-C	5.36	1.59	1.52
10	J	998	LEU	CA-CB	5.36	1.61	1.53
3	C	251	ARG	CD-NE	5.36	1.53	1.46
9	I	150	ARG	NE-CZ	5.36	1.39	1.33
1	A	182	ARG	CD-NE	5.36	1.53	1.46
3	C	224	GLY	CA-C	-5.36	1.44	1.51
3	C	225	PRO	CA-C	-5.36	1.46	1.52
8	H	318	ARG	CD-NE	5.36	1.53	1.46
3	C	245	ARG	CZ-NH2	5.36	1.40	1.33
10	J	885	ASN	C-N	5.35	1.40	1.33
10	J	931	PRO	C-N	5.35	1.41	1.33
1	A	20	ARG	NE-CZ	5.35	1.39	1.33
6	F	56	CYS	C-N	5.35	1.41	1.34
9	I	286	ARG	CZ-NH2	5.35	1.40	1.33
2	B	78	ILE	CA-C	-5.35	1.45	1.52
6	F	45	GLU	CA-C	-5.35	1.46	1.52
8	H	149	ARG	CD-NE	5.35	1.53	1.46
10	J	51	SER	C-O	-5.35	1.17	1.24
10	J	903	VAL	C-O	-5.35	1.17	1.24
10	J	940	ARG	C-N	5.35	1.41	1.33
3	C	96	ILE	N-CA	-5.34	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	35	ARG	NE-CZ	5.34	1.39	1.33
10	J	124	LYS	CA-C	-5.34	1.46	1.52
10	J	470	ASP	N-CA	-5.34	1.39	1.46
3	C	350	LEU	C-N	5.34	1.41	1.33
5	E	196	ASN	CA-C	-5.34	1.46	1.52
10	J	63	ALA	C-N	5.34	1.41	1.33
4	D	78	ILE	CA-C	-5.34	1.46	1.52
10	J	674	MET	CA-C	-5.34	1.45	1.52
1	A	142	ASP	N-CA	-5.34	1.39	1.45
5	E	159	SER	CA-C	-5.33	1.45	1.52
7	G	65	ILE	CA-CB	-5.33	1.49	1.54
4	D	105	SER	N-CA	-5.33	1.39	1.46
8	H	229	GLY	CA-C	-5.33	1.44	1.51
10	J	883	ASN	C-N	5.33	1.40	1.33
1	A	186	PRO	N-CA	-5.32	1.41	1.46
2	B	209	ARG	CD-NE	5.32	1.53	1.46
4	D	209	ILE	CA-CB	-5.32	1.47	1.54
8	H	181	SER	CA-C	-5.32	1.46	1.52
9	I	69	GLU	CA-C	5.32	1.59	1.52
6	F	192	GLY	C-N	5.32	1.40	1.33
7	G	136	CYS	CA-CB	5.32	1.60	1.53
8	H	208	VAL	C-N	5.32	1.41	1.33
7	G	93	SER	N-CA	-5.31	1.39	1.46
8	H	312	ILE	N-CA	-5.31	1.40	1.46
4	D	81	HIS	CE1-NE2	-5.31	1.27	1.32
10	J	657	ALA	CA-C	5.31	1.59	1.52
2	B	51	THR	N-CA	-5.31	1.39	1.45
5	E	82	ILE	CA-C	-5.31	1.45	1.52
10	J	868	SER	C-N	5.31	1.40	1.33
2	B	69	LYS	C-N	5.30	1.40	1.33
3	C	344	HIS	ND1-CE1	5.30	1.37	1.32
4	D	206	VAL	C-O	-5.30	1.18	1.24
6	F	224	LEU	CA-C	-5.30	1.46	1.52
3	C	33	ARG	NE-CZ	5.30	1.38	1.33
10	J	531	ARG	NE-CZ	5.30	1.38	1.33
1	A	78	VAL	N-CA	-5.29	1.40	1.46
10	J	801	PHE	N-CA	5.29	1.52	1.46
4	D	13	VAL	CA-C	-5.29	1.46	1.52
10	J	656	GLN	N-CA	-5.29	1.40	1.46
3	C	61	ARG	CD-NE	5.29	1.53	1.46
8	H	287	PRO	N-CA	-5.29	1.42	1.47
4	D	153	GLN	C-O	-5.29	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	172	LYS	CA-C	-5.29	1.46	1.52
3	C	362	LEU	C-N	5.29	1.40	1.33
7	G	96	SER	C-N	5.29	1.40	1.33
9	I	140	LEU	CB-CG	5.29	1.64	1.53
10	J	18	SER	C-N	5.29	1.40	1.33
6	F	224	LEU	C-N	5.28	1.40	1.33
10	J	382	ARG	CD-NE	5.28	1.53	1.46
6	F	77	VAL	N-CA	-5.28	1.40	1.46
10	J	48	LEU	CA-CB	5.28	1.61	1.53
10	J	908	ARG	CZ-NH2	5.28	1.40	1.33
7	G	207	CYS	CA-CB	5.28	1.61	1.53
1	A	21	GLN	C-N	5.27	1.41	1.33
4	D	85	ARG	CZ-NH1	5.27	1.40	1.32
7	G	65	ILE	CA-C	5.27	1.57	1.52
10	J	181	TYR	N-CA	-5.27	1.39	1.46
10	J	240	SER	C-N	5.27	1.40	1.33
2	B	80	LYS	CA-CB	5.27	1.62	1.53
3	C	174	ALA	CA-C	-5.27	1.46	1.52
10	J	531	ARG	CZ-NH1	5.26	1.40	1.32
3	C	212	VAL	CA-C	-5.26	1.46	1.52
6	F	116	PHE	CA-CB	5.26	1.61	1.53
7	G	43	HIS	CB-CG	-5.26	1.42	1.50
2	B	54	LYS	C-N	5.26	1.41	1.33
10	J	416	SER	CA-C	-5.26	1.46	1.52
9	I	239	ASP	C-N	5.26	1.40	1.33
10	J	932	LYS	N-CA	-5.26	1.39	1.46
8	H	4	VAL	CA-C	-5.25	1.44	1.52
10	J	119	ASP	CA-C	5.25	1.59	1.52
2	B	143	ILE	CA-CB	-5.25	1.48	1.54
5	E	119	LYS	CA-CB	5.25	1.62	1.53
10	J	667	ASN	C-N	5.25	1.40	1.33
1	A	256	MET	C-N	5.25	1.40	1.33
4	D	39	ARG	C-N	5.25	1.41	1.33
7	G	44	VAL	CA-C	-5.25	1.46	1.52
10	J	39	HIS	CE1-NE2	-5.25	1.27	1.32
6	F	235	ASN	CA-C	-5.25	1.46	1.52
9	I	106	ILE	N-CA	-5.24	1.39	1.46
3	C	44	ARG	NE-CZ	5.24	1.38	1.33
10	J	702	LYS	CA-CB	5.24	1.61	1.53
7	G	25	ILE	N-CA	-5.24	1.40	1.46
10	J	189	ASP	CA-C	5.24	1.59	1.53
11	P	79	PHE	C-N	5.24	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	ASP	C-N	5.23	1.41	1.33
8	H	90	ARG	NE-CZ	5.23	1.38	1.33
3	C	255	LEU	C-N	5.23	1.40	1.33
8	H	326	SER	CA-C	-5.23	1.45	1.52
10	J	280	ILE	CB-CG1	5.23	1.64	1.53
7	G	219	ASP	N-CA	-5.23	1.39	1.46
5	E	152	THR	C-O	-5.23	1.17	1.24
1	A	182	ARG	NE-CZ	5.22	1.38	1.33
2	B	149	ASP	CA-CB	5.22	1.61	1.53
2	B	31	THR	CA-C	-5.22	1.45	1.52
8	H	301	ALA	CA-CB	5.22	1.61	1.53
9	I	65	ARG	CD-NE	5.22	1.53	1.46
3	C	306	CYS	C-N	5.21	1.40	1.33
6	F	199	THR	N-CA	-5.21	1.39	1.46
1	A	292	LYS	C-N	5.21	1.41	1.33
8	H	113	VAL	N-CA	-5.21	1.40	1.46
6	F	243	SER	N-CA	5.21	1.52	1.46
4	D	14	ASP	C-O	5.21	1.30	1.24
8	H	317	GLN	CA-CB	5.21	1.61	1.53
10	J	938	LEU	C-N	5.21	1.40	1.33
4	D	122	ASP	C-N	5.21	1.40	1.33
5	E	264	ASN	CA-CB	5.21	1.60	1.53
2	B	144	THR	N-CA	-5.20	1.40	1.46
7	G	119	VAL	N-CA	-5.20	1.40	1.46
8	H	243	ARG	CZ-NH1	5.20	1.40	1.32
10	J	641	PHE	C-N	5.20	1.40	1.33
10	J	909	ASN	CA-CB	5.20	1.61	1.53
1	A	136	ALA	CA-CB	5.20	1.61	1.53
3	C	390	THR	C-N	5.20	1.40	1.33
5	E	222	ILE	N-CA	-5.20	1.40	1.46
5	E	97	SER	CA-C	-5.20	1.46	1.52
2	B	236	ALA	C-N	5.19	1.40	1.33
3	C	60	SER	CA-C	-5.19	1.45	1.53
6	F	212	GLY	C-O	-5.19	1.18	1.24
8	H	353	LYS	C-O	-5.19	1.18	1.24
3	C	256	ARG	C-N	5.19	1.40	1.33
10	J	848	ARG	CZ-NH2	5.19	1.40	1.33
6	F	211	VAL	CA-CB	-5.19	1.49	1.54
8	H	137	MET	CA-C	-5.19	1.46	1.52
10	J	786	LEU	N-CA	-5.19	1.40	1.46
10	J	230	ASP	CA-C	5.18	1.59	1.52
11	P	66	SER	N-CA	-5.18	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	ASP	CA-C	-5.18	1.46	1.52
6	F	12	PRO	N-CD	-5.18	1.40	1.47
6	F	69	HIS	ND1-CE1	5.18	1.37	1.32
8	H	290	SER	C-N	5.18	1.40	1.33
10	J	905	GLN	CA-C	5.18	1.59	1.52
10	J	224	LEU	CA-C	5.18	1.59	1.52
8	H	127	ASP	N-CA	-5.18	1.39	1.46
9	I	206	ARG	NE-CZ	5.18	1.38	1.33
10	J	387	GLN	CA-C	5.18	1.57	1.52
10	J	516	LEU	N-CA	-5.18	1.40	1.46
10	J	53	THR	CA-C	5.17	1.59	1.52
1	A	124	CYS	C-N	5.17	1.39	1.33
1	A	195	CYS	C-N	5.17	1.40	1.33
6	F	191	ALA	CA-C	-5.17	1.46	1.52
10	J	838	ILE	C-N	5.17	1.39	1.33
1	A	183	GLU	N-CA	-5.17	1.38	1.46
7	G	14	ASP	CA-C	-5.17	1.46	1.53
10	J	110	ASP	C-O	-5.17	1.17	1.23
10	J	930	VAL	CA-CB	-5.17	1.47	1.54
11	P	93	LYS	CA-C	5.17	1.59	1.52
3	C	264	ARG	CZ-NH1	5.16	1.40	1.32
4	D	87	LEU	C-N	5.16	1.40	1.33
7	G	99	TYR	CA-CB	5.16	1.61	1.53
7	G	100	MET	CA-CB	5.15	1.60	1.53
1	A	92	GLU	CA-C	-5.15	1.46	1.52
4	D	140	LYS	N-CA	-5.15	1.39	1.46
5	E	100	ASN	C-N	5.15	1.41	1.33
6	F	77	VAL	CA-CB	-5.15	1.48	1.54
7	G	108	LYS	N-CA	-5.15	1.39	1.46
1	A	278	GLN	CA-C	-5.15	1.46	1.52
10	J	923	ASN	C-N	5.15	1.40	1.33
7	G	93	SER	C-N	5.14	1.40	1.33
10	J	294	ARG	N-CA	5.14	1.52	1.46
1	A	51	MET	CA-CB	5.14	1.60	1.53
1	A	191	HIS	CA-C	-5.14	1.46	1.52
5	E	57	GLU	CA-C	-5.14	1.46	1.52
7	G	126	ALA	C-N	5.14	1.40	1.33
10	J	828	ASP	C-N	5.14	1.40	1.33
10	J	394	TYR	CZ-OH	5.14	1.48	1.38
10	J	359	SER	N-CA	-5.13	1.39	1.46
10	J	692	GLY	C-N	5.13	1.39	1.33
9	I	148	LEU	CA-C	5.13	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	93	LYS	CA-CB	5.13	1.61	1.53
1	A	28	ARG	CA-C	-5.13	1.46	1.53
2	B	64	GLN	C-N	5.13	1.40	1.33
9	I	150	ARG	CZ-NH1	5.13	1.40	1.32
2	B	3	ARG	NE-CZ	5.13	1.38	1.33
6	F	94	SER	N-CA	-5.12	1.39	1.46
8	H	10	ARG	CA-C	-5.12	1.45	1.52
10	J	675	ARG	CZ-NH1	5.12	1.40	1.32
3	C	150	THR	C-O	-5.12	1.17	1.24
5	E	216	SER	N-CA	-5.12	1.39	1.45
10	J	160	ARG	CZ-NH1	5.12	1.40	1.32
10	J	88	VAL	CA-CB	-5.12	1.48	1.54
10	J	275	GLN	N-CA	-5.12	1.39	1.45
10	J	291	SER	C-N	5.12	1.41	1.33
8	H	99	PRO	CA-C	-5.11	1.46	1.52
9	I	150	ARG	CA-C	-5.11	1.46	1.52
10	J	42	ARG	CA-C	-5.11	1.46	1.52
4	D	109	LEU	N-CA	-5.11	1.40	1.46
10	J	26	ARG	NE-CZ	5.11	1.38	1.33
10	J	150	ASN	N-CA	-5.11	1.39	1.46
10	J	623	ALA	CA-C	-5.11	1.46	1.52
3	C	295	SER	C-N	5.11	1.40	1.33
7	G	55	ALA	C-N	5.11	1.39	1.33
7	G	135	GLU	CA-C	-5.11	1.46	1.52
4	D	41	GLU	CA-C	-5.11	1.46	1.52
5	E	119	LYS	CA-C	-5.11	1.46	1.52
9	I	52	THR	C-O	-5.10	1.17	1.23
1	A	102	VAL	CA-C	-5.10	1.46	1.52
9	I	134	LYS	N-CA	-5.10	1.39	1.45
10	J	487	GLU	C-N	5.10	1.40	1.33
4	D	210	ARG	CD-NE	5.10	1.53	1.46
6	F	197	ASN	C-N	5.10	1.40	1.33
9	I	217	ARG	CZ-NH2	5.10	1.40	1.33
9	I	287	LYS	CA-C	-5.10	1.46	1.52
11	P	88	ILE	C-N	5.10	1.40	1.33
6	F	42	SER	N-CA	5.09	1.55	1.46
9	I	238	GLY	C-N	5.09	1.40	1.33
2	B	45	GLY	N-CA	-5.09	1.37	1.46
6	F	233	GLN	CA-C	-5.09	1.46	1.52
6	F	168	LEU	CA-CB	5.09	1.62	1.53
7	G	27	CYS	C-N	5.09	1.40	1.33
3	C	372	GLU	N-CA	-5.08	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	192	GLY	C-N	5.08	1.40	1.33
8	H	212	ASN	N-CA	-5.08	1.39	1.45
10	J	289	SER	C-O	-5.08	1.17	1.23
3	C	207	ARG	CZ-NH2	5.08	1.40	1.33
7	G	89	GLN	N-CA	-5.08	1.39	1.46
7	G	120	TYR	N-CA	-5.08	1.39	1.46
8	H	123	ARG	NE-CZ	5.08	1.38	1.33
1	A	48	SER	N-CA	-5.08	1.40	1.46
8	H	84	VAL	CA-C	-5.08	1.48	1.52
10	J	144	ARG	NE-CZ	5.07	1.38	1.33
10	J	302	VAL	CA-C	-5.07	1.46	1.52
10	J	99	ILE	CA-CB	-5.07	1.48	1.54
5	E	178	VAL	CA-C	-5.07	1.46	1.52
3	C	225	PRO	C-N	5.07	1.39	1.33
3	C	285	MET	N-CA	-5.07	1.40	1.46
7	G	123	VAL	N-CA	-5.07	1.40	1.46
7	G	227	ALA	CA-C	-5.07	1.46	1.52
10	J	905	GLN	N-CA	-5.07	1.40	1.46
5	E	230	ALA	CA-C	-5.06	1.46	1.52
10	J	422	VAL	CA-CB	-5.06	1.50	1.55
8	H	2	SER	CA-C	-5.06	1.42	1.52
8	H	291	ASN	CA-C	-5.06	1.46	1.52
8	H	293	ILE	C-N	5.06	1.40	1.33
10	J	287	GLU	CA-CB	5.06	1.60	1.53
3	C	52	VAL	N-CA	-5.06	1.39	1.46
5	E	145	ILE	C-N	5.06	1.40	1.33
8	H	98	ILE	CA-C	-5.06	1.49	1.52
10	J	672	MET	N-CA	5.06	1.52	1.46
10	J	788	ASP	C-N	5.05	1.41	1.33
3	C	362	LEU	CA-CB	5.05	1.62	1.53
6	F	105	TYR	CA-C	-5.05	1.46	1.52
9	I	258	ARG	CA-C	-5.05	1.46	1.52
10	J	152	PHE	C-O	-5.05	1.16	1.24
10	J	804	LEU	CA-CB	5.05	1.61	1.53
8	H	63	ASP	CA-CB	5.05	1.61	1.53
10	J	888	HIS	N-CA	-5.05	1.40	1.46
11	P	24	LEU	CA-C	-5.05	1.46	1.52
10	J	568	VAL	C-N	5.05	1.41	1.33
3	C	170	LEU	CA-C	-5.04	1.45	1.52
6	F	132	LYS	N-CA	5.04	1.52	1.46
10	J	647	ARG	NE-CZ	5.04	1.38	1.33
10	J	872	ARG	NE-CZ	5.04	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	233	ASP	C-N	5.04	1.39	1.33
1	A	188	GLY	C-N	5.04	1.40	1.33
2	B	68	SER	C-O	-5.04	1.17	1.24
4	D	108	GLU	N-CA	-5.04	1.40	1.46
10	J	982	GLN	CA-C	-5.04	1.46	1.52
2	B	233	ARG	CA-C	-5.04	1.45	1.52
10	J	890	ASN	C-N	5.04	1.40	1.33
10	J	453	ILE	CA-C	-5.04	1.46	1.52
8	H	292	ASN	N-CA	-5.03	1.39	1.46
10	J	23	VAL	CA-CB	5.03	1.60	1.54
1	A	22	ASN	CA-C	-5.03	1.46	1.52
10	J	425	ILE	C-N	5.03	1.40	1.33
10	J	883	ASN	CG-ND2	5.03	1.43	1.33
4	D	119	ALA	CA-C	-5.03	1.46	1.52
7	G	181	HIS	ND1-CE1	5.03	1.37	1.32
4	D	178	LEU	N-CA	5.02	1.52	1.46
4	D	59	ALA	N-CA	-5.02	1.39	1.46
2	B	101	GLN	CA-CB	5.02	1.61	1.53
8	H	119	VAL	CA-C	5.02	1.58	1.52
8	H	323	TYR	CZ-OH	5.02	1.48	1.38
10	J	984	ARG	CZ-NH1	5.02	1.39	1.32
10	J	514	THR	N-CA	-5.02	1.39	1.46
11	P	82	LYS	CA-C	5.02	1.59	1.52
3	C	62	TYR	N-CA	-5.01	1.40	1.46
5	E	147	SER	C-N	5.01	1.40	1.33
10	J	146	ILE	N-CA	-5.01	1.40	1.46
10	J	882	ARG	CZ-NH2	5.01	1.40	1.33
1	A	17	GLU	N-CA	-5.01	1.39	1.46
7	G	172	PHE	CA-C	-5.01	1.47	1.52
10	J	626	VAL	CA-CB	-5.00	1.47	1.53
10	J	909	ASN	N-CA	-5.00	1.40	1.46

All (1825) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	641	PHE	CA-CB-CG	-14.26	99.54	113.80
10	J	225	LEU	CA-C-O	-12.16	108.32	119.75
2	B	132	ASP	N-CA-C	-11.84	96.52	112.03
1	A	125	ILE	N-CA-C	-11.41	100.84	111.45
1	A	252	GLY	N-CA-C	-11.36	100.45	112.04
5	E	200	ASP	CA-CB-CG	-11.09	101.51	112.60
10	J	842	PHE	CA-CB-CG	11.05	124.85	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ASP	CA-CB-CG	-10.99	101.61	112.60
7	G	38	ASN	CA-CB-CG	-10.98	101.62	112.60
3	C	187	VAL	N-CA-C	-10.81	91.97	107.75
10	J	543	ASP	CA-C-N	10.74	131.44	120.38
10	J	543	ASP	C-N-CA	10.74	131.44	120.38
6	F	126	ASN	OD1-CG-ND2	10.53	133.12	122.60
10	J	637	VAL	N-CA-C	-10.49	102.79	111.81
3	C	393	ASN	CA-CB-CG	-10.37	102.23	112.60
5	E	172	PHE	CA-CB-CG	-10.32	103.48	113.80
6	F	101	LEU	N-CA-C	-10.29	100.27	112.92
1	A	205	ASP	CA-C-N	10.21	133.72	120.44
1	A	205	ASP	C-N-CA	10.21	133.72	120.44
1	A	81	THR	N-CA-C	-10.19	98.21	110.44
10	J	762	ASN	CA-CB-CG	-10.16	102.44	112.60
3	C	42	CYS	CA-C-N	10.15	137.29	122.36
3	C	42	CYS	C-N-CA	10.15	137.29	122.36
8	H	227	VAL	N-CA-C	-10.08	103.22	112.90
2	B	6	ILE	N-CA-C	-10.06	103.67	113.53
3	C	26	SER	CA-C-N	9.88	129.54	119.56
3	C	26	SER	C-N-CA	9.88	129.54	119.56
10	J	421	ASN	OD1-CG-ND2	9.85	132.45	122.60
5	E	71	VAL	N-CA-C	-9.85	103.37	112.43
5	E	161	PHE	CA-CB-CG	-9.77	104.03	113.80
9	I	271	ASP	N-CA-C	-9.71	94.42	108.60
4	D	81	HIS	CA-CB-CG	-9.53	104.27	113.80
8	H	203	PRO	N-CA-CB	9.52	112.18	103.33
9	I	13	PRO	N-CA-CB	9.50	111.74	103.19
9	I	150	ARG	NE-CZ-NH2	9.49	127.74	119.20
6	F	53	ILE	O-C-N	-9.45	112.61	123.00
5	E	153	TYR	N-CA-C	-9.43	94.62	109.72
8	H	286	ASP	CA-CB-CG	-9.38	103.22	112.60
1	A	254	LEU	CA-C-O	-9.35	110.45	119.80
10	J	798	ASP	CB-CA-C	-9.35	97.73	110.16
10	J	277	ASN	CA-C-O	-9.33	109.98	120.43
11	P	57	VAL	CA-C-N	9.31	132.76	120.28
11	P	57	VAL	C-N-CA	9.31	132.76	120.28
10	J	730	PHE	CA-CB-CG	-9.23	104.57	113.80
10	J	666	GLN	N-CA-C	-9.23	93.37	108.41
10	J	652	PHE	CA-CB-CG	-9.22	104.58	113.80
6	F	231	LYS	CA-C-N	9.22	132.99	120.54
6	F	231	LYS	C-N-CA	9.22	132.99	120.54
4	D	197	LEU	CA-C-N	9.19	130.18	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	197	LEU	C-N-CA	9.19	130.18	119.98
9	I	231	ARG	O-C-N	-9.14	112.80	123.22
5	E	88	ASP	CA-CB-CG	9.13	121.73	112.60
10	J	335	ASP	CA-CB-CG	9.12	121.72	112.60
10	J	98	ALA	CA-C-N	9.05	132.86	120.46
10	J	98	ALA	C-N-CA	9.05	132.86	120.46
10	J	297	LYS	CA-C-N	9.02	129.10	119.90
10	J	297	LYS	C-N-CA	9.02	129.10	119.90
6	F	247	ASN	N-CA-C	-8.98	102.45	113.50
10	J	758	PRO	N-CA-C	8.97	121.64	110.70
10	J	943	ASN	CA-CB-CG	-8.92	103.68	112.60
8	H	98	ILE	CA-C-O	-8.92	113.98	119.51
8	H	349	LEU	CA-C-N	8.87	132.52	120.54
8	H	349	LEU	C-N-CA	8.87	132.52	120.54
3	C	385	ALA	CA-C-N	8.86	132.52	120.38
3	C	385	ALA	C-N-CA	8.86	132.52	120.38
3	C	123	ILE	N-CA-C	-8.82	95.56	108.71
2	B	116	ILE	N-CA-C	-8.82	102.60	111.77
10	J	897	ALA	CA-C-O	8.81	129.89	120.55
1	A	44	PHE	CA-CB-CG	-8.81	104.99	113.80
3	C	11	GLU	CA-C-N	8.79	137.79	121.97
3	C	11	GLU	C-N-CA	8.79	137.79	121.97
7	G	229	ARG	N-CA-C	8.78	120.93	111.36
10	J	804	LEU	N-CA-C	8.74	120.81	111.28
8	H	303	VAL	CA-C-O	8.74	129.91	120.47
10	J	428	ASP	CA-CB-CG	8.73	121.33	112.60
7	G	92	SER	CA-C-N	8.68	134.25	121.31
7	G	92	SER	C-N-CA	8.68	134.25	121.31
10	J	413	ASP	CA-C-N	8.68	128.31	118.85
10	J	413	ASP	C-N-CA	8.68	128.31	118.85
10	J	599	LYS	CA-C-O	8.64	130.03	120.70
4	D	169	ASN	CA-CB-CG	-8.64	103.96	112.60
10	J	865	GLU	N-CA-C	-8.63	97.11	110.58
1	A	213	GLU	CA-C-O	8.63	128.01	118.52
9	I	62	GLY	CA-C-N	8.62	133.74	121.42
9	I	62	GLY	C-N-CA	8.62	133.74	121.42
6	F	98	LYS	O-C-N	8.61	133.39	123.31
5	E	136	HIS	CA-CB-CG	-8.58	105.22	113.80
7	G	84	TYR	N-CA-C	-8.57	96.23	109.52
2	B	215	ALA	N-CA-C	-8.57	102.02	111.36
6	F	195	GLU	CA-C-O	8.57	129.58	120.33
10	J	552	ASP	CA-CB-CG	8.55	121.16	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	277	ASP	CA-CB-CG	-8.53	104.07	112.60
1	A	8	SER	CA-C-N	8.53	132.06	120.38
1	A	8	SER	C-N-CA	8.53	132.06	120.38
1	A	46	ASP	CA-CB-CG	-8.52	104.08	112.60
8	H	53	GLN	O-C-N	8.51	133.40	122.93
5	E	136	HIS	CE1-NE2-CD2	-8.50	100.50	109.00
4	D	203	GLN	OE1-CD-NE2	8.48	131.08	122.60
6	F	79	GLY	O-C-N	-8.47	113.30	121.77
2	B	220	GLY	CA-C-N	8.46	131.62	120.28
2	B	220	GLY	C-N-CA	8.46	131.62	120.28
5	E	125	PHE	CA-CB-CG	-8.43	105.37	113.80
8	H	282	SER	CA-C-O	8.40	129.61	120.71
2	B	7	TYR	CB-CG-CD2	8.39	133.39	120.80
10	J	278	ILE	CA-C-O	8.39	131.10	120.95
10	J	770	LEU	CA-C-N	8.37	132.43	120.79
10	J	770	LEU	C-N-CA	8.37	132.43	120.79
10	J	84	GLY	CA-C-N	8.34	132.58	120.82
10	J	84	GLY	C-N-CA	8.34	132.58	120.82
9	I	235	LEU	CA-C-O	8.34	129.47	120.55
10	J	141	ASP	CA-CB-CG	-8.28	104.32	112.60
3	C	27	PRO	N-CA-C	-8.28	103.52	113.86
10	J	763	PHE	CA-CB-CG	-8.27	105.53	113.80
6	F	88	THR	CA-C-N	8.27	131.36	120.28
6	F	88	THR	C-N-CA	8.27	131.36	120.28
5	E	54	ASP	CA-CB-CG	8.26	120.86	112.60
11	P	10	ILE	CA-C-O	-8.24	112.44	121.17
7	G	4	PHE	CA-CB-CG	-8.23	105.57	113.80
1	A	216	SER	CA-C-N	8.23	132.40	120.71
1	A	216	SER	C-N-CA	8.23	132.40	120.71
10	J	321	LEU	CA-C-N	8.23	130.13	119.84
10	J	321	LEU	C-N-CA	8.23	130.13	119.84
3	C	181	GLU	N-CA-C	-8.23	102.80	113.17
10	J	338	HIS	CE1-NE2-CD2	-8.21	100.79	109.00
4	D	151	ALA	CA-C-N	8.21	131.11	120.44
4	D	151	ALA	C-N-CA	8.21	131.11	120.44
6	F	189	ASP	N-CA-C	-8.21	95.80	108.76
7	G	123	VAL	N-CA-C	-8.15	96.84	108.58
8	H	192	GLY	N-CA-C	-8.15	101.36	112.52
10	J	184	HIS	CE1-NE2-CD2	-8.13	100.87	109.00
10	J	167	ASN	CA-CB-CG	-8.10	104.50	112.60
10	J	875	ASN	CA-CB-CG	-8.07	104.53	112.60
5	E	209	ALA	CA-C-N	8.05	131.38	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	209	ALA	C-N-CA	8.05	131.38	120.44
7	G	149	ILE	N-CA-C	-8.01	96.89	108.11
10	J	212	ASN	OD1-CG-ND2	8.01	130.61	122.60
6	F	55	ASN	OD1-CG-ND2	8.00	130.60	122.60
10	J	923	ASN	N-CA-C	-8.00	103.52	113.28
10	J	899	ILE	CB-CA-C	-8.00	101.19	112.22
10	J	230	ASP	N-CA-C	-7.98	101.72	114.09
2	B	46	ASN	CA-CB-CG	-7.92	104.67	112.60
6	F	190	MET	CG-SD-CE	-7.92	83.49	100.90
8	H	61	VAL	N-CA-C	-7.91	103.54	110.74
3	C	182	ASP	N-CA-C	-7.89	103.55	113.02
8	H	241	LEU	N-CA-C	-7.89	103.47	113.72
5	E	193	VAL	N-CA-C	-7.86	96.06	107.78
5	E	13	ASP	N-CA-C	7.86	120.83	111.33
10	J	499	VAL	O-C-N	7.85	129.48	121.87
6	F	54	GLU	CA-C-N	7.84	136.52	121.54
6	F	54	GLU	C-N-CA	7.84	136.52	121.54
1	A	177	HIS	CA-CB-CG	-7.83	105.97	113.80
2	B	58	GLU	CB-CA-C	7.81	120.75	109.26
3	C	33	ARG	NE-CZ-NH2	7.81	126.23	119.20
10	J	110	ASP	CA-CB-CG	-7.80	104.80	112.60
3	C	273	GLU	N-CA-C	-7.80	95.42	108.75
10	J	488	HIS	CA-CB-CG	-7.79	106.00	113.80
1	A	72	PRO	N-CA-C	-7.79	104.70	114.68
4	D	144	ASP	CA-C-N	7.79	131.00	120.63
4	D	144	ASP	C-N-CA	7.79	131.00	120.63
10	J	763	PHE	CA-C-N	7.78	130.56	120.44
10	J	763	PHE	C-N-CA	7.78	130.56	120.44
10	J	701	VAL	CA-C-N	7.78	130.55	120.44
10	J	701	VAL	C-N-CA	7.78	130.55	120.44
8	H	76	LEU	N-CA-C	-7.77	95.60	108.34
3	C	262	ARG	CA-C-N	7.74	136.58	121.41
3	C	262	ARG	C-N-CA	7.74	136.58	121.41
3	C	134	VAL	N-CA-C	-7.73	97.29	108.11
10	J	198	ASP	N-CA-C	-7.73	96.81	109.40
4	D	190	GLN	OE1-CD-NE2	-7.72	114.88	122.60
10	J	39	HIS	CA-CB-CG	7.72	121.52	113.80
3	C	296	ASN	OD1-CG-ND2	7.71	130.31	122.60
10	J	303	GLY	CA-C-N	7.70	130.60	120.28
10	J	303	GLY	C-N-CA	7.70	130.60	120.28
6	F	189	ASP	CA-C-O	7.69	129.35	120.89
6	F	178	LEU	CA-C-N	7.69	130.59	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	178	LEU	C-N-CA	7.69	130.59	120.28
11	P	3	ASP	CA-CB-CG	-7.69	104.91	112.60
10	J	95	VAL	N-CA-CB	7.68	119.54	110.55
10	J	855	HIS	CA-CB-CG	7.65	121.45	113.80
7	G	220	THR	N-CA-C	7.62	120.48	111.71
10	J	545	PRO	CA-C-O	-7.62	113.02	121.32
10	J	487	GLU	O-C-N	-7.61	114.05	122.12
4	D	114	ASN	CB-CA-C	-7.61	97.92	110.85
7	G	161	ASN	CA-CB-CG	-7.58	105.02	112.60
3	C	44	ARG	NE-CZ-NH2	-7.58	112.38	119.20
5	E	14	SER	O-C-N	7.57	129.90	122.03
10	J	527	LEU	N-CA-C	-7.56	103.62	112.92
1	A	200	PHE	CA-CB-CG	-7.56	106.24	113.80
9	I	137	ASP	CA-CB-CG	-7.54	105.06	112.60
4	D	185	ASP	CA-CB-CG	-7.53	105.07	112.60
5	E	255	ALA	CA-C-O	-7.52	112.21	119.13
9	I	268	TYR	N-CA-C	-7.51	97.99	109.41
2	B	205	ILE	N-CA-C	-7.51	98.67	107.61
2	B	106	ARG	N-CA-C	-7.50	103.18	111.36
10	J	458	THR	N-CA-C	-7.50	104.16	113.38
5	E	161	PHE	CA-C-O	7.49	129.42	120.81
2	B	114	LEU	N-CA-C	-7.48	103.74	113.17
7	G	77	ILE	N-CA-C	-7.47	105.73	112.90
6	F	240	LEU	N-CA-C	-7.47	103.07	111.14
10	J	429	LYS	N-CA-C	-7.47	102.41	112.94
5	E	7	GLU	N-CA-CB	7.45	121.05	109.94
10	J	321	LEU	CA-C-O	-7.45	113.14	120.97
10	J	548	VAL	CA-C-O	-7.45	112.20	120.25
3	C	242	LYS	N-CA-C	-7.45	97.98	109.52
6	F	133	SER	CA-C-N	-7.43	116.60	121.65
6	F	133	SER	C-N-CA	-7.43	116.60	121.65
2	B	58	GLU	N-CA-C	-7.43	100.72	109.93
10	J	674	MET	N-CA-C	7.43	119.37	111.28
9	I	247	THR	CA-C-N	7.42	130.09	120.44
9	I	247	THR	C-N-CA	7.42	130.09	120.44
4	D	12	HIS	ND1-CE1-NE2	7.42	115.82	108.40
10	J	968	ASP	CA-CB-CG	-7.40	105.20	112.60
11	P	69	ASP	CA-CB-CG	-7.40	105.20	112.60
6	F	49	HIS	ND1-CE1-NE2	7.38	115.78	108.40
8	H	196	ASN	O-C-N	-7.38	114.33	122.67
10	J	754	ARG	NE-CZ-NH1	-7.37	114.13	121.50
2	B	15	ASP	N-CA-C	-7.36	104.27	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	202	VAL	CA-C-N	7.36	127.29	119.85
8	H	202	VAL	C-N-CA	7.36	127.29	119.85
8	H	7	ILE	N-CA-C	-7.36	97.42	108.17
9	I	214	ASP	CA-CB-CG	-7.36	105.24	112.60
10	J	773	ARG	NE-CZ-NH1	-7.36	114.14	121.50
2	B	93	ASN	CA-CB-CG	7.34	119.94	112.60
8	H	219	GLY	CA-C-N	7.34	132.54	122.34
8	H	219	GLY	C-N-CA	7.34	132.54	122.34
10	J	156	THR	N-CA-C	-7.34	101.60	113.19
1	A	177	HIS	CB-CA-C	-7.33	100.83	109.47
5	E	136	HIS	ND1-CE1-NE2	7.33	115.73	108.40
10	J	923	ASN	CA-CB-CG	-7.32	105.28	112.60
10	J	169	ARG	NE-CZ-NH2	-7.32	112.61	119.20
4	D	110	SER	N-CA-C	-7.30	103.26	111.07
10	J	699	PRO	O-C-N	7.29	130.98	122.23
1	A	24	ARG	CA-C-N	7.29	130.04	120.28
1	A	24	ARG	C-N-CA	7.29	130.04	120.28
3	C	215	ALA	N-CA-CB	7.28	122.79	110.71
7	G	172	PHE	CA-C-O	-7.27	112.53	119.80
1	A	191	HIS	CA-CB-CG	-7.27	106.53	113.80
11	P	4	PHE	CB-CA-C	-7.27	99.47	110.88
11	P	59	ILE	CA-C-N	7.27	130.02	120.28
11	P	59	ILE	C-N-CA	7.27	130.02	120.28
10	J	284	ASN	CA-CB-CG	7.26	119.86	112.60
10	J	488	HIS	CE1-NE2-CD2	-7.26	101.74	109.00
4	D	22	GLN	CA-C-N	7.26	131.35	120.31
4	D	22	GLN	C-N-CA	7.26	131.35	120.31
10	J	116	ILE	O-C-N	7.26	129.00	121.89
2	B	192	LYS	CA-C-N	7.25	133.12	120.87
2	B	192	LYS	C-N-CA	7.25	133.12	120.87
4	D	109	LEU	N-CA-CB	7.24	120.51	110.01
6	F	238	ARG	CA-C-N	7.24	131.32	120.31
6	F	238	ARG	C-N-CA	7.24	131.32	120.31
10	J	191	ASN	OD1-CG-ND2	-7.24	115.36	122.60
2	B	123	ASP	CA-CB-CG	-7.24	105.36	112.60
10	J	11	LYS	CA-C-N	7.24	132.85	121.56
10	J	11	LYS	C-N-CA	7.24	132.85	121.56
3	C	236	TYR	N-CA-C	-7.23	103.43	111.82
10	J	53	THR	N-CA-C	-7.23	104.09	113.12
3	C	341	THR	N-CA-C	7.22	119.16	111.28
1	A	281	GLN	CA-C-N	7.22	129.95	120.28
1	A	281	GLN	C-N-CA	7.22	129.95	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ASP	CA-CB-CG	-7.21	105.39	112.60
10	J	519	PRO	CA-C-N	7.21	129.94	120.28
10	J	519	PRO	C-N-CA	7.21	129.94	120.28
7	G	141	THR	N-CA-C	-7.20	102.84	111.69
9	I	186	ALA	N-CA-C	-7.18	105.70	114.75
8	H	147	ILE	N-CA-CB	7.18	123.08	111.23
6	F	69	HIS	CE1-NE2-CD2	-7.18	101.82	109.00
5	E	75	LEU	N-CA-C	-7.17	105.45	114.56
1	A	136	ALA	N-CA-C	-7.17	97.52	109.07
3	C	235	MET	CB-CA-C	-7.17	98.89	110.79
5	E	240	LYS	CA-C-N	7.17	127.49	119.32
5	E	240	LYS	C-N-CA	7.17	127.49	119.32
2	B	111	ASN	CA-C-N	7.16	130.86	120.91
2	B	111	ASN	C-N-CA	7.16	130.86	120.91
10	J	235	ILE	CA-C-N	7.16	128.78	119.84
10	J	235	ILE	C-N-CA	7.16	128.78	119.84
10	J	739	ALA	N-CA-C	-7.16	103.41	111.07
7	G	155	ILE	N-CA-CB	7.15	118.33	110.53
9	I	130	ASN	N-CA-C	-7.15	103.77	114.64
10	J	175	ARG	CA-C-N	7.15	130.44	120.29
10	J	175	ARG	C-N-CA	7.15	130.44	120.29
2	B	52	LEU	N-CA-C	-7.14	98.21	109.50
2	B	142	GLY	CA-C-N	7.14	129.69	120.56
2	B	142	GLY	C-N-CA	7.14	129.69	120.56
1	A	137	ASP	CA-CB-CG	-7.13	105.47	112.60
3	C	263	GLY	CA-C-N	7.13	134.53	121.70
3	C	263	GLY	C-N-CA	7.13	134.53	121.70
2	B	156	ASP	CA-CB-CG	7.13	119.73	112.60
10	J	868	SER	CA-C-N	7.12	129.81	120.28
10	J	868	SER	C-N-CA	7.12	129.81	120.28
2	B	165	LEU	CA-C-O	7.11	128.15	120.32
5	E	136	HIS	CG-CD2-NE2	7.11	114.31	107.20
3	C	76	GLY	CA-C-O	-7.11	114.72	121.19
10	J	161	LEU	CA-C-N	7.11	127.03	119.85
10	J	161	LEU	C-N-CA	7.11	127.03	119.85
3	C	157	ASP	CA-C-O	-7.10	112.89	120.42
11	P	88	ILE	N-CA-C	7.10	117.86	110.62
6	F	147	LEU	N-CA-C	-7.09	104.65	113.38
8	H	309	PHE	O-C-N	7.09	129.37	122.07
11	P	41	LEU	N-CA-C	-7.08	104.51	113.72
9	I	206	ARG	CA-C-N	7.08	130.48	120.28
9	I	206	ARG	C-N-CA	7.08	130.48	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	28	ARG	CA-C-N	7.07	132.41	122.36
10	J	28	ARG	C-N-CA	7.07	132.41	122.36
10	J	277	ASN	O-C-N	7.07	131.26	123.13
7	G	75	VAL	N-CA-C	-7.07	97.96	108.85
6	F	138	PHE	CA-CB-CG	-7.07	106.73	113.80
9	I	38	GLY	N-CA-C	-7.07	97.92	112.34
10	J	39	HIS	ND1-CE1-NE2	7.07	115.47	108.40
7	G	168	PHE	N-CA-C	-7.06	103.78	112.88
10	J	698	SER	CA-C-N	7.06	126.88	119.05
10	J	698	SER	C-N-CA	7.06	126.88	119.05
10	J	374	ALA	CA-C-O	-7.05	113.02	120.63
2	B	12	LEU	CA-C-N	7.04	132.65	122.23
2	B	12	LEU	C-N-CA	7.04	132.65	122.23
8	H	67	TRP	CB-CG-CD2	-7.04	116.94	126.80
8	H	118	GLU	N-CA-C	-7.04	97.94	108.99
5	E	6	ALA	N-CA-C	7.02	118.93	111.28
3	C	67	ASN	OD1-CG-ND2	-7.02	115.58	122.60
10	J	788	ASP	CB-CA-C	-7.02	98.92	110.85
4	D	18	GLU	N-CA-C	-7.01	96.62	108.26
11	P	91	VAL	N-CA-CB	7.01	115.92	110.45
3	C	17	PHE	CA-CB-CG	-7.00	106.80	113.80
6	F	129	ARG	NE-CZ-NH2	7.00	125.50	119.20
10	J	67	LEU	N-CA-C	-7.00	100.97	109.72
10	J	852	VAL	CB-CA-C	-6.99	102.57	112.22
3	C	159	ILE	CB-CA-C	6.99	121.58	112.14
7	G	161	ASN	OD1-CG-ND2	6.99	129.59	122.60
2	B	139	LEU	CB-CA-C	-6.99	97.26	110.67
10	J	482	GLU	N-CA-C	6.99	118.55	111.07
11	P	8	ASN	O-C-N	6.98	129.26	122.07
8	H	111	HIS	CE1-NE2-CD2	-6.98	102.02	109.00
9	I	140	LEU	N-CA-CB	6.97	121.50	110.55
10	J	189	ASP	CA-CB-CG	-6.97	105.63	112.60
1	A	198	PHE	N-CA-C	-6.96	97.86	109.07
11	P	66	SER	CA-C-O	-6.96	111.91	118.73
10	J	508	HIS	CE1-NE2-CD2	-6.96	102.04	109.00
10	J	161	LEU	O-C-N	-6.96	114.94	121.20
3	C	379	LEU	CA-C-N	6.96	129.60	120.28
3	C	379	LEU	C-N-CA	6.96	129.60	120.28
10	J	679	LYS	N-CA-C	6.95	118.94	111.36
10	J	226	PRO	N-CA-C	-6.94	105.79	114.68
1	A	24	ARG	NE-CZ-NH2	6.94	125.44	119.20
7	G	35	ARG	CA-C-N	6.94	127.11	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	35	ARG	C-N-CA	6.94	127.11	120.31
10	J	211	SER	N-CA-C	-6.92	102.96	112.03
6	F	47	SER	N-CA-C	-6.92	97.06	108.76
10	J	283	TYR	N-CA-C	-6.92	104.50	114.12
10	J	406	GLN	CB-CG-CD	-6.91	100.84	112.60
10	J	200	LEU	CA-C-O	-6.91	112.02	119.97
8	H	150	ARG	NE-CZ-NH1	-6.91	114.59	121.50
10	J	815	ALA	O-C-N	-6.90	114.68	122.75
1	A	155	VAL	N-CA-C	6.90	117.04	110.42
10	J	34	LYS	N-CA-C	-6.90	99.30	110.20
6	F	124	VAL	N-CA-C	6.89	117.51	110.82
10	J	64	GLN	OE1-CD-NE2	-6.89	115.71	122.60
10	J	622	PHE	CB-CA-C	-6.89	96.78	109.46
10	J	928	VAL	CA-C-O	6.89	127.62	120.39
5	E	55	GLY	N-CA-C	-6.88	105.33	115.72
10	J	356	ASN	CA-CB-CG	-6.87	105.73	112.60
10	J	931	PRO	N-CA-C	-6.87	105.89	114.68
10	J	272	VAL	N-CA-C	-6.87	105.94	113.43
4	D	209	ILE	CA-C-N	6.87	129.48	120.28
4	D	209	ILE	C-N-CA	6.87	129.48	120.28
10	J	857	GLN	OE1-CD-NE2	6.87	129.47	122.60
2	B	147	LEU	CA-C-O	-6.86	113.15	120.42
11	P	44	ILE	N-CA-C	-6.86	98.60	108.48
1	A	180	ASN	CB-CG-ND2	-6.86	106.12	116.40
2	B	186	THR	CA-C-O	-6.86	112.71	120.32
9	I	106	ILE	N-CA-C	-6.85	97.75	107.75
11	P	18	LEU	CA-C-N	6.85	129.34	120.44
11	P	18	LEU	C-N-CA	6.85	129.34	120.44
8	H	215	HIS	CE1-NE2-CD2	-6.84	102.16	109.00
10	J	396	GLN	N-CA-C	-6.84	103.90	111.36
1	A	212	GLY	N-CA-C	-6.84	102.14	112.60
2	B	141	ASN	N-CA-CB	6.84	120.17	110.12
3	C	78	ASN	OD1-CG-ND2	6.84	129.44	122.60
4	D	183	ASN	CA-C-N	6.83	131.97	122.06
4	D	183	ASN	C-N-CA	6.83	131.97	122.06
10	J	152	PHE	CA-CB-CG	-6.83	106.97	113.80
10	J	342	ASN	N-CA-C	-6.83	102.56	111.71
1	A	91	PHE	N-CA-C	-6.82	97.78	108.90
3	C	133	VAL	N-CA-C	-6.82	98.56	108.11
1	A	49	VAL	CA-C-O	6.82	127.48	120.39
10	J	488	HIS	CG-CD2-NE2	6.82	114.02	107.20
1	A	264	CYS	CA-C-N	6.82	129.41	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	CYS	C-N-CA	6.82	129.41	120.28
3	C	96	ILE	CA-C-O	6.82	127.58	120.36
7	G	177	VAL	CA-C-N	6.82	129.41	120.28
7	G	177	VAL	C-N-CA	6.82	129.41	120.28
5	E	139	SER	CA-C-N	6.81	129.97	120.29
5	E	139	SER	C-N-CA	6.81	129.97	120.29
3	C	96	ILE	O-C-N	-6.81	115.85	123.20
8	H	152	SER	CB-CA-C	-6.81	98.51	109.13
6	F	197	ASN	O-C-N	-6.80	114.42	122.58
9	I	111	LEU	N-CA-C	-6.80	101.25	110.36
4	D	60	THR	CA-C-N	6.80	130.07	120.28
4	D	60	THR	C-N-CA	6.80	130.07	120.28
1	A	300	GLU	CB-CG-CD	-6.79	101.06	112.60
9	I	127	ASP	N-CA-CB	6.79	120.77	110.11
8	H	125	LYS	CA-C-N	6.79	132.43	123.06
8	H	125	LYS	C-N-CA	6.79	132.43	123.06
6	F	49	HIS	CE1-NE2-CD2	-6.78	102.22	109.00
6	F	191	ALA	O-C-N	-6.78	115.26	123.19
10	J	201	ASN	CA-CB-CG	-6.78	105.82	112.60
9	I	290	LYS	O-C-N	-6.78	117.37	121.71
10	J	44	ASP	CA-CB-CG	-6.77	105.83	112.60
4	D	132	ALA	N-CA-C	-6.77	99.31	108.86
8	H	113	VAL	O-C-N	-6.77	115.95	123.26
5	E	181	ASP	CA-CB-CG	-6.77	105.83	112.60
3	C	131	TYR	CA-C-N	6.76	126.70	120.21
3	C	131	TYR	C-N-CA	6.76	126.70	120.21
1	A	180	ASN	CA-C-N	6.76	129.22	120.44
1	A	180	ASN	C-N-CA	6.76	129.22	120.44
5	E	24	ASP	CA-CB-CG	-6.75	105.85	112.60
8	H	121	ASN	CA-CB-CG	-6.75	105.85	112.60
8	H	292	ASN	CA-C-N	6.74	129.19	120.56
8	H	292	ASN	C-N-CA	6.74	129.19	120.56
10	J	303	GLY	CA-C-O	-6.74	116.38	122.24
5	E	73	ASN	CA-C-N	6.74	133.04	122.94
5	E	73	ASN	C-N-CA	6.74	133.04	122.94
1	A	57	HIS	ND1-CE1-NE2	6.73	115.13	108.40
10	J	240	SER	N-CA-C	-6.73	102.39	113.50
7	G	90	ASN	CA-CB-CG	-6.73	105.87	112.60
8	H	215	HIS	ND1-CE1-NE2	6.73	115.13	108.40
10	J	907	MET	N-CA-CB	6.73	120.01	110.12
10	J	527	LEU	CA-C-N	6.72	130.52	120.31
10	J	527	LEU	C-N-CA	6.72	130.52	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	466	HIS	CA-C-N	6.71	130.40	120.87
10	J	466	HIS	C-N-CA	6.71	130.40	120.87
10	J	791	ASP	N-CA-CB	6.70	119.92	109.94
3	C	69	ASP	CA-CB-CG	-6.70	105.90	112.60
10	J	791	ASP	CA-C-O	-6.70	113.73	120.90
11	P	26	SER	CA-C-N	6.70	133.76	121.70
11	P	26	SER	C-N-CA	6.70	133.76	121.70
3	C	22	LEU	O-C-N	-6.70	115.17	122.07
9	I	237	LEU	N-CA-C	-6.70	104.06	111.36
3	C	12	ILE	CB-CA-C	6.69	122.27	111.29
4	D	75	THR	CA-C-O	-6.69	111.85	118.34
10	J	696	LEU	N-CA-C	-6.69	104.47	114.64
6	F	141	LEU	CB-CA-C	-6.69	102.57	111.74
1	A	53	ASN	N-CA-C	6.68	120.69	112.54
10	J	278	ILE	O-C-N	-6.67	114.99	122.66
1	A	69	GLU	N-CA-C	6.67	119.38	111.71
7	G	110	ARG	NE-CZ-NH1	6.67	128.16	121.50
3	C	70	THR	O-C-N	6.66	131.87	122.41
4	D	187	ASN	N-CA-C	-6.66	99.28	109.41
3	C	258	THR	CA-C-N	6.66	130.26	120.74
3	C	258	THR	C-N-CA	6.66	130.26	120.74
8	H	286	ASP	N-CA-CB	6.65	120.53	110.02
10	J	896	ARG	N-CA-CB	6.65	120.11	110.20
10	J	76	PRO	CA-C-N	6.65	131.22	121.31
10	J	76	PRO	C-N-CA	6.65	131.22	121.31
10	J	749	THR	CA-C-O	6.64	126.42	119.51
1	A	229	LEU	O-C-N	6.64	129.72	122.15
10	J	344	ASN	CA-CB-CG	6.63	119.23	112.60
10	J	452	SER	N-CA-CB	6.63	120.99	111.05
3	C	237	ALA	CA-C-N	6.63	129.16	120.28
3	C	237	ALA	C-N-CA	6.63	129.16	120.28
3	C	262	ARG	NE-CZ-NH1	6.62	128.12	121.50
7	G	65	ILE	CA-C-N	6.62	128.11	119.84
7	G	65	ILE	C-N-CA	6.62	128.11	119.84
10	J	765	ILE	CA-C-O	-6.62	113.83	120.85
10	J	624	PHE	N-CA-C	-6.61	97.74	108.52
10	J	403	TYR	CA-C-N	6.61	130.40	120.75
10	J	403	TYR	C-N-CA	6.61	130.40	120.75
2	B	47	ASN	N-CA-CB	6.61	120.44	109.60
3	C	78	ASN	CA-C-N	6.60	131.38	123.19
3	C	78	ASN	C-N-CA	6.60	131.38	123.19
3	C	68	ILE	N-CA-C	-6.60	95.77	107.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	281	TYR	CB-CA-C	-6.60	100.89	111.18
10	J	717	ILE	N-CA-CB	6.59	119.66	110.56
4	D	9	ILE	CA-CB-CG1	6.59	121.60	110.40
3	C	372	GLU	CA-C-N	6.59	129.64	120.29
3	C	372	GLU	C-N-CA	6.59	129.64	120.29
8	H	314	ILE	CA-CB-CG1	-6.58	99.21	110.40
5	E	42	PRO	N-CA-C	-6.58	103.56	114.75
1	A	243	ARG	N-CA-CB	6.58	121.61	110.49
10	J	184	HIS	CG-CD2-NE2	6.58	113.78	107.20
4	D	114	ASN	CA-C-N	6.57	129.09	120.28
4	D	114	ASN	C-N-CA	6.57	129.09	120.28
5	E	144	ALA	CB-CA-C	-6.57	99.51	110.68
11	P	42	LEU	N-CA-C	-6.57	105.23	112.72
3	C	247	PHE	CA-CB-CG	-6.57	107.23	113.80
10	J	525	ASP	N-CA-C	-6.57	98.89	109.40
10	J	75	SER	CA-C-O	-6.57	113.66	120.09
10	J	167	ASN	CB-CA-C	-6.57	99.52	110.68
3	C	255	LEU	CA-C-O	-6.56	113.57	121.05
10	J	248	ASP	CA-C-N	6.56	132.28	121.39
10	J	248	ASP	C-N-CA	6.56	132.28	121.39
7	G	25	ILE	N-CA-C	-6.56	98.99	108.17
1	A	288	GLU	N-CA-C	6.55	119.25	111.71
6	F	145	LYS	N-CA-CB	6.55	121.81	110.81
8	H	111	HIS	N-CA-C	-6.54	97.70	108.76
4	D	219	PRO	N-CA-C	-6.54	105.09	114.18
10	J	434	VAL	CB-CA-C	-6.54	100.86	110.81
10	J	908	ARG	CA-C-O	-6.54	113.55	120.55
10	J	269	LYS	O-C-N	6.52	129.14	122.09
8	H	53	GLN	CA-C-O	-6.52	113.31	120.81
10	J	270	ASN	OD1-CG-ND2	6.51	129.11	122.60
10	J	50	ARG	CD-NE-CZ	-6.50	115.29	124.40
2	B	230	GLU	CA-C-N	6.50	128.99	120.28
2	B	230	GLU	C-N-CA	6.50	128.99	120.28
3	C	145	THR	O-C-N	-6.50	115.69	123.03
10	J	66	GLU	N-CA-C	-6.49	98.42	108.42
2	B	127	HIS	CG-CD2-NE2	6.49	113.69	107.20
10	J	838	ILE	CA-CB-CG1	6.49	121.43	110.40
3	C	12	ILE	N-CA-C	6.49	122.83	109.34
2	B	47	ASN	CA-CB-CG	-6.48	106.12	112.60
10	J	72	LEU	N-CA-CB	6.48	121.20	110.63
4	D	152	GLU	CA-C-N	6.47	129.48	120.29
4	D	152	GLU	C-N-CA	6.47	129.48	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	171	LYS	CA-C-N	6.47	131.77	122.45
3	C	171	LYS	C-N-CA	6.47	131.77	122.45
10	J	849	TYR	CA-C-N	6.47	129.24	120.38
10	J	849	TYR	C-N-CA	6.47	129.24	120.38
9	I	204	ILE	N-CA-CB	6.47	122.64	111.39
10	J	765	ILE	CA-C-N	6.46	128.84	120.44
10	J	765	ILE	C-N-CA	6.46	128.84	120.44
3	C	58	THR	N-CA-C	-6.46	103.68	113.89
10	J	906	VAL	CA-C-N	6.46	128.94	120.28
10	J	906	VAL	C-N-CA	6.46	128.94	120.28
6	F	215	LYS	N-CA-CB	6.46	120.91	110.77
2	B	41	TYR	N-CA-C	-6.45	98.88	109.40
7	G	129	GLU	N-CA-C	-6.45	105.57	113.50
11	P	86	LEU	N-CA-CB	6.45	119.36	110.01
10	J	79	LEU	N-CA-CB	6.44	122.75	111.55
10	J	619	VAL	N-CA-C	-6.44	99.45	108.27
8	H	106	PRO	N-CA-C	6.43	121.31	111.34
4	D	195	LEU	CB-CA-C	-6.43	100.11	110.79
8	H	71	HIS	CG-CD2-NE2	6.43	113.63	107.20
10	J	868	SER	N-CA-C	-6.43	100.09	110.32
1	A	303	ARG	NE-CZ-NH1	-6.43	115.07	121.50
8	H	86	GLY	O-C-N	-6.43	117.60	123.96
9	I	208	GLN	N-CA-C	6.43	120.38	112.54
8	H	121	ASN	N-CA-C	-6.42	104.70	113.30
6	F	115	SER	N-CA-CB	6.42	119.66	110.16
7	G	191	ASN	CA-CB-CG	-6.42	106.18	112.60
10	J	367	ASP	N-CA-CB	6.42	119.38	110.07
3	C	156	HIS	CB-CG-ND1	6.42	132.32	122.70
10	J	208	GLU	CA-C-N	6.41	133.51	121.97
10	J	208	GLU	C-N-CA	6.41	133.51	121.97
2	B	32	HIS	CA-CB-CG	-6.41	107.39	113.80
7	G	32	GLN	CA-C-O	6.41	128.91	121.28
10	J	608	LEU	N-CA-C	6.41	118.27	111.28
10	J	67	LEU	CA-C-N	6.41	127.85	119.84
10	J	67	LEU	C-N-CA	6.41	127.85	119.84
10	J	882	ARG	NE-CZ-NH2	6.41	124.97	119.20
8	H	324	GLU	N-CA-C	6.40	118.25	111.28
10	J	831	HIS	N-CA-C	-6.39	98.19	109.06
6	F	234	TYR	CB-CA-C	-6.39	100.84	110.88
9	I	213	THR	CA-CB-OG1	6.39	119.19	109.60
1	A	202	ASN	CA-C-O	-6.39	114.42	119.66
10	J	796	PRO	CA-C-N	6.39	129.36	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	796	PRO	C-N-CA	6.39	129.36	120.29
11	P	93	LYS	O-C-N	6.39	128.99	122.09
4	D	71	ARG	CA-C-O	-6.38	113.78	120.55
10	J	926	ILE	N-CA-C	-6.38	99.29	108.42
1	A	21	GLN	CB-CA-C	-6.37	99.02	110.37
10	J	218	LEU	N-CA-C	-6.37	104.25	111.07
5	E	39	ASP	N-CA-C	6.37	120.18	111.39
11	P	80	ASN	CB-CA-C	-6.37	100.22	110.79
10	J	387	GLN	O-C-N	-6.36	117.00	121.65
8	H	281	TYR	CB-CG-CD2	-6.36	111.26	120.80
4	D	119	ALA	O-C-N	6.36	129.40	122.15
5	E	242	HIS	CE1-NE2-CD2	-6.36	102.64	109.00
6	F	53	ILE	CA-C-O	6.35	127.73	121.19
8	H	185	HIS	CE1-NE2-CD2	-6.35	102.65	109.00
2	B	118	PRO	N-CA-C	-6.35	101.92	111.57
3	C	21	VAL	CA-C-N	6.35	128.69	120.44
3	C	21	VAL	C-N-CA	6.35	128.69	120.44
4	D	92	CYS	N-CA-C	-6.35	97.93	108.34
5	E	157	LEU	CA-C-N	6.35	129.48	120.53
5	E	157	LEU	C-N-CA	6.35	129.48	120.53
4	D	78	ILE	N-CA-C	-6.34	99.29	108.36
3	C	125	ALA	O-C-N	6.34	129.95	122.34
11	P	64	ARG	O-C-N	-6.34	114.75	120.71
10	J	510	TRP	CB-CG-CD1	6.33	136.40	126.90
1	A	199	SER	N-CA-C	-6.33	98.58	108.90
10	J	184	HIS	ND1-CE1-NE2	6.33	114.73	108.40
4	D	23	ASP	N-CA-CB	6.33	120.08	110.28
1	A	134	VAL	CA-C-O	6.32	127.03	120.39
6	F	116	PHE	CA-C-N	6.32	128.75	120.28
6	F	116	PHE	C-N-CA	6.32	128.75	120.28
6	F	43	GLU	N-CA-C	-6.32	104.13	113.61
11	P	86	LEU	CA-C-N	6.32	129.27	120.29
11	P	86	LEU	C-N-CA	6.32	129.27	120.29
3	C	62	TYR	CA-C-O	6.32	128.30	120.15
3	C	86	ILE	CA-C-O	6.32	127.03	120.39
6	F	180	LEU	N-CA-C	-6.31	104.48	111.36
6	F	177	THR	CA-C-N	6.30	129.05	120.54
6	F	177	THR	C-N-CA	6.30	129.05	120.54
10	J	265	MET	CA-C-N	6.30	128.22	120.22
10	J	265	MET	C-N-CA	6.30	128.22	120.22
3	C	34	HIS	CA-C-N	6.29	128.71	120.28
3	C	34	HIS	C-N-CA	6.29	128.71	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	126	VAL	CB-CA-C	-6.29	103.11	110.91
11	P	88	ILE	CA-C-N	6.29	129.22	120.29
11	P	88	ILE	C-N-CA	6.29	129.22	120.29
3	C	27	PRO	N-CA-CB	6.29	109.54	103.51
1	A	74	GLU	O-C-N	6.28	130.77	123.17
5	E	250	MET	N-CA-CB	6.28	119.46	110.16
4	D	40	GLN	CB-CA-C	-6.28	100.72	111.46
10	J	755	HIS	CB-CG-CD2	-6.28	123.03	131.20
3	C	15	ILE	CA-C-N	6.28	129.74	120.95
3	C	15	ILE	C-N-CA	6.28	129.74	120.95
8	H	236	THR	N-CA-CB	6.28	119.58	109.28
1	A	279	ILE	CA-C-O	-6.28	114.42	120.95
10	J	641	PHE	CB-CA-C	-6.27	99.75	110.16
10	J	257	GLU	CA-C-O	6.26	129.11	121.72
5	E	242	HIS	CB-CG-ND1	6.26	132.09	122.70
4	D	136	ILE	N-CA-C	-6.26	99.11	108.12
10	J	105	PRO	N-CA-C	-6.26	106.67	114.68
3	C	392	PHE	O-C-N	6.26	129.76	122.19
10	J	155	HIS	CA-C-O	6.26	125.53	119.08
10	J	216	LYS	CA-C-N	6.25	129.58	120.71
10	J	216	LYS	C-N-CA	6.25	129.58	120.71
11	P	10	ILE	O-C-N	6.24	128.03	121.91
9	I	145	ARG	NH1-CZ-NH2	6.24	127.42	119.30
5	E	127	ASP	CB-CA-C	-6.24	100.53	110.14
4	D	213	ILE	CB-CA-C	-6.24	103.61	112.22
7	G	52	VAL	N-CA-CB	6.23	121.67	111.45
6	F	164	GLN	N-CA-C	-6.23	105.81	113.41
2	B	234	LYS	O-C-N	-6.23	115.52	122.12
8	H	138	LEU	N-CA-C	6.23	119.98	112.38
7	G	234	ILE	CA-C-O	6.22	127.15	119.43
8	H	317	GLN	N-CA-CB	6.22	119.80	110.22
10	J	33	THR	N-CA-CB	6.22	120.56	110.42
2	B	4	LEU	N-CA-CB	6.22	121.00	110.49
1	A	162	PHE	N-CA-C	6.22	118.81	110.35
6	F	229	ARG	NE-CZ-NH1	6.22	127.72	121.50
5	E	22	ARG	O-C-N	-6.22	114.17	121.32
5	E	228	SER	N-CA-CB	6.22	119.90	110.45
10	J	884	ILE	CA-C-N	6.22	128.52	120.44
10	J	884	ILE	C-N-CA	6.22	128.52	120.44
6	F	106	ASN	CA-C-N	6.21	128.61	120.28
6	F	106	ASN	C-N-CA	6.21	128.61	120.28
9	I	211	ARG	CA-C-O	-6.21	112.85	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	242	HIS	CB-CG-CD2	-6.21	123.13	131.20
5	E	244	LEU	N-CA-C	6.21	118.05	111.28
10	J	746	PHE	CA-C-O	-6.20	111.66	120.16
7	G	232	LYS	CA-C-N	6.20	128.59	120.28
7	G	232	LYS	C-N-CA	6.20	128.59	120.28
1	A	173	GLN	CB-CG-CD	-6.20	102.07	112.60
11	P	4	PHE	CA-C-N	6.20	128.58	120.28
11	P	4	PHE	C-N-CA	6.20	128.58	120.28
10	J	634	ALA	N-CA-CB	6.19	120.96	110.49
2	B	94	GLU	CA-C-N	6.19	128.58	120.28
2	B	94	GLU	C-N-CA	6.19	128.58	120.28
10	J	905	GLN	N-CA-C	6.19	117.69	111.07
7	G	146	GLY	N-CA-C	-6.19	106.70	115.30
10	J	533	ASP	CA-CB-CG	-6.18	106.42	112.60
10	J	995	LYS	O-C-N	-6.18	116.34	123.33
9	I	141	THR	CA-CB-OG1	6.18	118.87	109.60
10	J	748	GLN	OE1-CD-NE2	6.18	128.78	122.60
10	J	249	THR	O-C-N	-6.17	115.98	122.96
6	F	184	GLY	CA-C-O	6.17	125.52	118.98
10	J	920	LYS	N-CA-C	-6.16	99.32	108.99
3	C	151	ILE	CA-C-N	6.16	128.53	120.28
3	C	151	ILE	C-N-CA	6.16	128.53	120.28
3	C	186	SER	CA-C-N	-6.16	114.91	123.10
3	C	186	SER	C-N-CA	-6.16	114.91	123.10
3	C	382	ARG	N-CA-CB	-6.16	100.74	110.28
5	E	2	SER	N-CA-C	-6.16	105.60	113.23
5	E	6	ALA	CA-C-N	6.16	128.85	120.54
5	E	6	ALA	C-N-CA	6.16	128.85	120.54
8	H	196	ASN	OD1-CG-ND2	6.15	128.75	122.60
3	C	335	ASP	N-CA-C	-6.15	107.61	114.62
1	A	276	THR	CA-CB-OG1	6.15	118.83	109.60
7	G	170	ASN	N-CA-C	-6.15	104.94	112.88
9	I	239	ASP	O-C-N	-6.15	114.41	122.59
1	A	246	VAL	N-CA-C	-6.15	105.73	111.45
4	D	158	LEU	N-CA-C	-6.15	106.10	113.97
6	F	174	THR	CB-CA-C	-6.15	101.23	110.88
8	H	185	HIS	CB-CG-CD2	-6.15	123.21	131.20
4	D	120	LEU	CB-CA-C	-6.15	100.58	110.79
3	C	163	ARG	CA-C-N	6.15	130.38	120.55
3	C	163	ARG	C-N-CA	6.15	130.38	120.55
5	E	204	ASN	CA-CB-CG	-6.14	106.46	112.60
8	H	79	MET	N-CA-C	-6.14	99.26	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	GLY	N-CA-C	-6.14	106.85	115.32
5	E	173	HIS	N-CA-C	-6.14	101.84	110.50
10	J	493	ARG	CA-C-O	-6.14	114.12	120.87
10	J	789	SER	CA-C-N	6.14	128.50	120.28
10	J	789	SER	C-N-CA	6.14	128.50	120.28
7	G	11	PHE	CA-C-N	-6.13	113.95	120.94
7	G	11	PHE	C-N-CA	-6.13	113.95	120.94
8	H	84	VAL	CA-C-N	6.13	131.78	122.65
8	H	84	VAL	C-N-CA	6.13	131.78	122.65
4	D	58	VAL	CA-C-N	6.13	129.54	120.90
4	D	58	VAL	C-N-CA	6.13	129.54	120.90
5	E	98	LEU	N-CA-CB	6.12	118.89	110.01
10	J	506	GLU	N-CA-C	-6.12	101.22	110.28
4	D	12	HIS	CE1-NE2-CD2	-6.12	102.88	109.00
1	A	62	CYS	N-CA-CB	6.11	121.10	111.20
10	J	742	ILE	CA-C-O	-6.11	114.03	120.57
8	H	343	SER	CB-CA-C	-6.11	101.28	110.88
5	E	111	SER	N-CA-C	-6.11	101.33	110.06
5	E	30	GLN	N-CA-CB	6.11	120.21	111.05
7	G	231	PHE	CA-CB-CG	-6.11	107.69	113.80
6	F	58	GLY	N-CA-C	-6.10	101.81	110.91
10	J	468	VAL	CA-C-O	-6.10	113.15	120.78
9	I	223	CYS	O-C-N	6.10	128.13	121.85
5	E	103	LEU	N-CA-C	-6.09	105.42	112.92
9	I	258	ARG	N-CA-C	-6.09	99.47	109.40
7	G	186	VAL	CA-C-N	6.09	131.40	122.39
7	G	186	VAL	C-N-CA	6.09	131.40	122.39
8	H	288	SER	N-CA-C	-6.09	105.14	113.30
3	C	131	TYR	O-C-N	-6.08	114.32	121.32
4	D	182	SER	N-CA-C	-6.08	97.38	108.02
7	G	139	SER	N-CA-C	-6.08	105.90	113.38
1	A	75	GLY	O-C-N	6.08	128.75	122.79
6	F	181	ALA	CA-C-N	6.08	128.92	120.29
6	F	181	ALA	C-N-CA	6.08	128.92	120.29
5	E	106	GLY	CA-C-O	6.08	126.54	119.13
10	J	963	VAL	CA-C-N	6.08	126.92	120.11
10	J	963	VAL	C-N-CA	6.08	126.92	120.11
10	J	819	PHE	CA-C-O	6.08	127.26	120.94
1	A	291	ASN	N-CA-CB	6.07	119.48	110.49
5	E	183	ASN	O-C-N	-6.07	114.16	121.02
8	H	352	GLU	N-CA-CB	6.06	118.86	110.07
10	J	155	HIS	CG-CD2-NE2	6.06	113.26	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	LEU	N-CA-C	6.06	117.89	111.28
8	H	291	ASN	CA-CB-CG	-6.06	106.54	112.60
3	C	154	LYS	CA-C-N	6.06	128.32	120.44
3	C	154	LYS	C-N-CA	6.06	128.32	120.44
10	J	374	ALA	O-C-N	6.06	128.54	122.12
1	A	222	ASP	CA-CB-CG	6.06	118.66	112.60
2	B	143	ILE	CA-C-O	6.06	127.77	121.05
4	D	178	LEU	N-CA-CB	6.06	119.89	110.44
7	G	170	ASN	OD1-CG-ND2	6.06	128.66	122.60
11	P	77	ASN	N-CA-C	6.06	118.67	111.71
1	A	14	PHE	CA-CB-CG	6.06	119.86	113.80
4	D	113	ILE	CA-C-N	6.05	128.89	120.29
4	D	113	ILE	C-N-CA	6.05	128.89	120.29
2	B	146	ALA	N-CA-C	6.05	117.88	111.28
10	J	963	VAL	CB-CA-C	-6.05	103.90	111.04
8	H	178	GLN	CA-C-N	6.04	128.87	120.29
8	H	178	GLN	C-N-CA	6.04	128.87	120.29
1	A	259	LEU	CA-C-N	6.04	128.38	120.28
1	A	259	LEU	C-N-CA	6.04	128.38	120.28
6	F	237	TYR	CA-C-N	6.04	129.19	120.79
6	F	237	TYR	C-N-CA	6.04	129.19	120.79
10	J	216	LYS	O-C-N	-6.04	115.81	123.24
1	A	68	TYR	CA-C-N	6.04	128.98	120.28
1	A	68	TYR	C-N-CA	6.04	128.98	120.28
9	I	239	ASP	CA-C-O	6.04	129.15	120.51
1	A	177	HIS	ND1-CE1-NE2	6.04	114.44	108.40
10	J	39	HIS	CE1-NE2-CD2	-6.03	102.97	109.00
1	A	223	ALA	N-CA-C	6.03	118.08	110.24
2	B	32	HIS	CA-C-O	-6.03	111.90	120.16
8	H	237	SER	CA-C-N	6.03	129.86	120.82
8	H	237	SER	C-N-CA	6.03	129.86	120.82
7	G	91	PHE	CA-CB-CG	6.03	119.83	113.80
3	C	287	ASN	CA-C-N	6.03	128.85	120.29
3	C	287	ASN	C-N-CA	6.03	128.85	120.29
10	J	570	ILE	N-CA-CB	6.03	120.50	110.86
11	P	38	ASN	N-CA-CB	6.02	118.80	110.07
10	J	870	THR	CA-CB-CG2	-6.02	100.27	110.50
1	A	190	LEU	N-CA-C	-6.01	106.07	113.41
7	G	12	PRO	CA-C-O	-6.01	112.52	118.29
10	J	343	ASP	N-CA-C	-6.01	100.82	110.14
3	C	227	PHE	CA-C-N	6.01	129.45	120.31
3	C	227	PHE	C-N-CA	6.01	129.45	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	VAL	CA-C-O	-6.01	114.20	120.27
4	D	89	GLN	CA-C-O	6.01	126.93	120.32
10	J	323	GLN	OE1-CD-NE2	6.01	128.61	122.60
10	J	140	ASP	CA-CB-CG	6.00	118.60	112.60
7	G	46	ALA	CA-C-N	6.00	131.01	120.87
7	G	46	ALA	C-N-CA	6.00	131.01	120.87
10	J	762	ASN	O-C-N	6.00	128.25	122.07
10	J	198	ASP	CA-CB-CG	6.00	118.60	112.60
2	B	166	TYR	CA-C-N	6.00	132.99	121.54
2	B	166	TYR	C-N-CA	6.00	132.99	121.54
10	J	415	GLN	O-C-N	5.99	128.47	122.12
10	J	473	THR	CA-C-N	5.99	130.47	120.64
10	J	473	THR	C-N-CA	5.99	130.47	120.64
9	I	128	PHE	N-CA-C	-5.99	105.15	112.88
5	E	126	VAL	CA-CB-CG2	-5.99	100.22	110.40
9	I	45	GLN	OE1-CD-NE2	5.99	128.59	122.60
10	J	648	SER	N-CA-C	-5.99	100.43	109.95
10	J	737	SER	O-C-N	5.99	128.46	122.12
3	C	374	ILE	N-CA-C	-5.98	104.68	110.72
4	D	75	THR	O-C-N	-5.98	115.09	120.71
8	H	156	GLU	CA-C-N	5.98	128.22	120.44
8	H	156	GLU	C-N-CA	5.98	128.22	120.44
1	A	64	ILE	N-CA-CB	-5.98	104.01	110.53
8	H	127	ASP	N-CA-CB	5.98	120.39	110.47
6	F	188	VAL	O-C-N	5.97	128.11	121.90
10	J	166	ILE	CA-C-N	5.97	128.57	120.38
10	J	166	ILE	C-N-CA	5.97	128.57	120.38
5	E	97	SER	CA-C-N	5.97	128.20	120.44
5	E	97	SER	C-N-CA	5.97	128.20	120.44
10	J	1001	LYS	CG-CD-CE	5.97	125.04	111.30
1	A	86	MET	N-CA-C	-5.97	103.65	113.50
10	J	687	LYS	N-CA-C	5.97	118.57	111.71
4	D	104	PHE	N-CA-C	-5.96	99.68	109.40
1	A	163	LYS	CA-C-O	-5.96	114.15	121.06
4	D	101	GLU	CA-C-O	-5.95	114.18	120.55
6	F	71	THR	CA-CB-OG1	5.95	118.53	109.60
6	F	117	LEU	CB-CA-C	-5.95	100.91	110.79
4	D	9	ILE	N-CA-C	-5.95	104.52	111.00
10	J	928	VAL	N-CA-C	-5.95	99.78	108.11
10	J	604	LEU	CA-C-N	5.95	127.28	119.84
10	J	604	LEU	C-N-CA	5.95	127.28	119.84
1	A	78	VAL	N-CA-C	-5.95	99.65	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	57	ASN	O-C-N	5.95	129.93	122.55
4	D	120	LEU	CA-C-N	5.95	128.61	120.46
4	D	120	LEU	C-N-CA	5.95	128.61	120.46
6	F	135	ILE	N-CA-C	-5.95	99.92	108.48
5	E	49	ARG	N-CA-C	-5.94	98.72	108.76
7	G	229	ARG	NE-CZ-NH1	-5.94	115.56	121.50
7	G	196	VAL	CA-CB-CG1	5.94	120.50	110.40
10	J	252	ASP	CB-CA-C	-5.94	100.17	110.09
4	D	208	ASN	CA-C-O	-5.94	114.12	120.42
10	J	810	THR	N-CA-CB	5.94	119.44	110.30
9	I	107	LEU	N-CA-C	-5.93	101.70	110.48
1	A	42	LYS	N-CA-C	-5.93	105.35	113.30
1	A	169	VAL	N-CA-C	-5.93	99.93	108.53
9	I	62	GLY	N-CA-C	5.93	119.25	110.42
9	I	148	LEU	N-CA-C	5.93	118.51	111.33
2	B	157	TYR	N-CA-CB	5.93	120.09	110.43
4	D	189	ASP	CB-CA-C	-5.92	99.30	110.67
5	E	170	PRO	CA-C-O	-5.92	114.69	121.56
8	H	185	HIS	CA-C-N	5.92	131.34	122.99
8	H	185	HIS	C-N-CA	5.92	131.34	122.99
1	A	293	TYR	CA-C-N	5.92	128.70	120.29
1	A	293	TYR	C-N-CA	5.92	128.70	120.29
8	H	301	ALA	CA-C-N	5.92	128.14	120.44
8	H	301	ALA	C-N-CA	5.92	128.14	120.44
8	H	101	LYS	CA-C-O	-5.92	114.90	121.23
10	J	429	LYS	CA-C-N	5.92	132.12	122.65
10	J	429	LYS	C-N-CA	5.92	132.12	122.65
10	J	531	ARG	N-CA-C	-5.92	98.64	108.34
11	P	32	LEU	CA-C-O	-5.91	114.15	120.42
1	A	33	PHE	CA-CB-CG	5.91	119.71	113.80
10	J	323	GLN	N-CA-CB	5.91	119.32	110.22
8	H	73	THR	CA-C-N	5.91	131.56	121.87
8	H	73	THR	C-N-CA	5.91	131.56	121.87
7	G	152	ASP	CA-C-N	5.90	130.00	121.44
7	G	152	ASP	C-N-CA	5.90	130.00	121.44
10	J	505	ALA	CA-C-N	5.90	129.25	120.87
10	J	505	ALA	C-N-CA	5.90	129.25	120.87
10	J	744	ASP	N-CA-CB	5.90	118.63	110.07
5	E	99	LEU	CA-C-N	5.90	128.19	120.28
5	E	99	LEU	C-N-CA	5.90	128.19	120.28
10	J	797	GLU	N-CA-C	-5.90	104.93	111.36
3	C	337	GLU	CA-C-N	5.90	128.18	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	337	GLU	C-N-CA	5.90	128.18	120.28
6	F	67	LEU	CA-C-O	5.90	126.77	120.70
10	J	155	HIS	CE1-NE2-CD2	-5.90	103.10	109.00
10	J	814	MET	CA-C-N	5.90	130.83	120.87
10	J	814	MET	C-N-CA	5.90	130.83	120.87
10	J	657	ALA	CB-CA-C	-5.89	101.01	110.79
5	E	70	HIS	N-CA-C	-5.89	105.28	112.88
5	E	233	ASP	N-CA-C	-5.89	107.08	114.56
2	B	182	MET	CA-C-N	5.89	129.19	120.95
2	B	182	MET	C-N-CA	5.89	129.19	120.95
4	D	54	PRO	N-CA-CB	5.89	108.86	103.15
1	A	87	ALA	N-CA-C	-5.88	107.09	114.56
3	C	266	ALA	N-CA-CB	-5.88	103.21	111.62
3	C	290	ASN	CA-CB-CG	-5.88	106.72	112.60
5	E	244	LEU	CA-C-N	5.88	128.16	120.28
5	E	244	LEU	C-N-CA	5.88	128.16	120.28
8	H	71	HIS	CA-C-N	5.88	131.60	121.07
8	H	71	HIS	C-N-CA	5.88	131.60	121.07
10	J	841	HIS	CA-CB-CG	5.88	119.68	113.80
1	A	200	PHE	CB-CA-C	-5.88	99.54	109.72
1	A	205	ASP	N-CA-C	-5.88	100.36	109.24
3	C	161	HIS	CA-CB-CG	-5.88	107.92	113.80
5	E	82	ILE	N-CA-C	-5.88	99.17	107.75
3	C	154	LYS	O-C-N	5.88	128.35	122.12
2	B	11	GLY	CA-C-O	5.88	125.82	119.06
9	I	246	THR	N-CA-C	-5.87	99.08	109.06
10	J	806	ARG	O-C-N	5.87	128.34	122.12
10	J	421	ASN	CB-CG-OD1	-5.87	109.06	120.80
10	J	979	VAL	O-C-N	-5.87	116.55	123.00
3	C	180	ASN	CA-CB-CG	-5.86	106.74	112.60
10	J	929	LEU	O-C-N	-5.86	116.64	123.27
8	H	238	GLN	CA-C-N	5.86	129.98	120.60
8	H	238	GLN	C-N-CA	5.86	129.98	120.60
10	J	116	ILE	CA-C-O	-5.86	114.95	121.05
4	D	59	ALA	CA-C-N	5.86	130.91	122.23
4	D	59	ALA	C-N-CA	5.86	130.91	122.23
10	J	617	PRO	CA-C-O	-5.86	114.45	121.48
10	J	548	VAL	O-C-N	5.85	129.84	121.82
10	J	86	HIS	CG-CD2-NE2	5.85	113.05	107.20
3	C	46	TYR	CB-CA-C	-5.85	101.08	110.79
6	F	182	ASP	CA-C-O	5.85	126.62	120.42
8	H	134	ALA	N-CA-C	-5.85	101.08	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	348	ILE	N-CA-CB	5.85	118.49	110.54
1	A	116	GLY	N-CA-C	-5.85	97.95	111.04
11	P	37	HIS	CE1-NE2-CD2	-5.85	103.15	109.00
2	B	235	HIS	ND1-CE1-NE2	5.84	114.24	108.40
10	J	564	TRP	CB-CG-CD2	-5.84	118.62	126.80
3	C	226	VAL	N-CA-C	-5.84	107.06	113.43
10	J	644	SER	CA-C-O	5.84	127.55	121.36
11	P	85	ASN	CA-CB-CG	-5.84	106.76	112.60
3	C	220	LEU	N-CA-CB	5.84	119.75	110.65
10	J	192	VAL	N-CA-C	-5.84	100.00	108.17
3	C	272	TYR	N-CA-C	-5.83	100.78	110.17
4	D	111	CYS	N-CA-C	5.83	117.64	111.28
9	I	7	PHE	CA-C-N	5.83	126.29	119.99
9	I	7	PHE	C-N-CA	5.83	126.29	119.99
10	J	760	SER	CA-C-O	-5.83	114.69	120.82
1	A	261	LEU	CA-C-O	5.83	126.94	120.82
4	D	67	GLU	CB-CG-CD	-5.83	102.69	112.60
5	E	242	HIS	CG-CD2-NE2	5.83	113.03	107.20
10	J	755	HIS	CE1-NE2-CD2	-5.83	103.17	109.00
10	J	498	LYS	N-CA-C	5.83	118.41	111.71
3	C	20	GLU	CB-CG-CD	-5.82	102.70	112.60
10	J	194	LEU	CA-C-O	5.82	126.81	120.58
10	J	492	TYR	N-CA-C	-5.82	105.95	114.39
3	C	275	ILE	N-CA-CB	5.82	120.83	111.23
8	H	322	ALA	N-CA-C	5.82	117.62	111.28
10	J	324	SER	N-CA-C	5.82	117.62	111.28
10	J	359	SER	N-CA-C	5.82	119.88	111.56
7	G	147	PHE	N-CA-CB	5.81	118.60	109.83
11	P	93	LYS	CA-C-N	5.81	128.06	120.28
11	P	93	LYS	C-N-CA	5.81	128.06	120.28
1	A	221	ILE	N-CA-C	-5.81	101.04	109.29
10	J	182	SER	CA-C-N	5.81	127.99	120.44
10	J	182	SER	C-N-CA	5.81	127.99	120.44
9	I	194	SER	N-CA-C	-5.80	100.31	108.96
9	I	270	THR	N-CA-C	-5.80	104.90	113.61
11	P	5	ALA	CA-C-O	-5.80	114.40	120.55
4	D	75	THR	CA-C-N	5.80	126.68	120.47
4	D	75	THR	C-N-CA	5.80	126.68	120.47
5	E	126	VAL	CA-C-O	-5.80	114.16	120.71
9	I	259	ALA	CA-C-O	-5.80	115.48	122.03
1	A	58	CYS	CB-CA-C	5.80	119.79	109.65
2	B	237	GLN	N-CA-C	5.79	117.60	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	188	GLY	CA-C-O	5.79	126.68	121.47
2	B	242	ASN	CA-CB-CG	-5.79	106.81	112.60
8	H	137	MET	O-C-N	-5.79	116.44	123.10
10	J	167	ASN	OD1-CG-ND2	5.79	128.39	122.60
7	G	143	ARG	NE-CZ-NH2	-5.79	113.99	119.20
3	C	255	LEU	N-CA-C	-5.79	101.05	110.20
6	F	222	ASP	CB-CA-C	5.79	119.76	110.09
10	J	86	HIS	CE1-NE2-CD2	-5.79	103.21	109.00
1	A	177	HIS	CE1-NE2-CD2	-5.79	103.22	109.00
3	C	207	ARG	CG-CD-NE	-5.79	99.27	112.00
1	A	279	ILE	N-CA-CB	5.78	118.40	110.54
1	A	198	PHE	CA-C-O	5.78	126.68	120.38
10	J	37	ARG	CB-CG-CD	5.78	124.59	111.30
10	J	899	ILE	CA-C-N	5.78	127.95	120.44
10	J	899	ILE	C-N-CA	5.78	127.95	120.44
2	B	138	SER	CA-C-O	-5.77	113.58	120.10
9	I	31	ILE	N-CA-C	-5.77	97.54	107.24
1	A	20	ARG	CA-C-O	-5.77	114.76	120.82
3	C	135	GLU	N-CA-C	-5.77	99.49	108.90
8	H	346	SER	N-CA-C	5.77	117.57	111.28
10	J	732	LEU	N-CA-C	5.77	118.04	111.11
1	A	301	ASN	N-CA-C	-5.77	100.54	109.14
5	E	49	ARG	NE-CZ-NH2	-5.77	114.01	119.20
9	I	262	GLY	O-C-N	-5.77	115.20	122.70
3	C	30	SER	O-C-N	-5.77	116.01	122.12
5	E	203	ALA	CA-C-N	5.77	127.94	120.44
5	E	203	ALA	C-N-CA	5.77	127.94	120.44
5	E	179	LYS	CA-C-N	-5.76	115.11	122.77
5	E	179	LYS	C-N-CA	-5.76	115.11	122.77
1	A	170	HIS	CE1-NE2-CD2	-5.76	103.24	109.00
1	A	182	ARG	N-CA-C	-5.76	100.55	109.24
3	C	17	PHE	N-CA-C	-5.76	101.63	110.32
8	H	340	VAL	O-C-N	-5.76	115.90	121.83
9	I	69	GLU	N-CA-C	-5.76	106.88	114.31
1	A	134	VAL	N-CA-C	-5.75	100.05	108.11
4	D	117	PHE	N-CA-C	5.75	117.22	111.07
6	F	87	PHE	N-CA-C	-5.75	100.33	109.76
8	H	111	HIS	ND1-CE1-NE2	5.75	114.15	108.40
7	G	162	PHE	N-CA-C	-5.75	104.93	111.14
1	A	39	THR	N-CA-CB	5.74	120.16	110.46
7	G	15	PRO	CA-C-N	5.74	129.03	120.31
7	G	15	PRO	C-N-CA	5.74	129.03	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	251	SER	N-CA-C	-5.74	100.33	109.23
3	C	156	HIS	CB-CG-CD2	-5.74	123.74	131.20
4	D	151	ALA	N-CA-C	5.74	117.53	111.28
7	G	163	ALA	CB-CA-C	-5.74	101.09	110.85
5	E	219	ASN	OD1-CG-ND2	5.74	128.34	122.60
8	H	228	ASN	N-CA-C	-5.74	105.00	113.61
1	A	154	ALA	CA-C-O	-5.74	114.47	120.55
8	H	121	ASN	OD1-CG-ND2	5.74	128.34	122.60
1	A	57	HIS	CE1-NE2-CD2	-5.73	103.27	109.00
10	J	585	ALA	CA-C-O	5.73	126.63	120.55
1	A	290	ARG	N-CA-CB	5.73	119.74	110.40
3	C	156	HIS	CA-C-N	5.73	128.43	120.29
3	C	156	HIS	C-N-CA	5.73	128.43	120.29
8	H	218	PRO	N-CA-C	5.73	119.52	111.33
10	J	383	SER	N-CA-CB	5.73	118.42	110.17
10	J	578	LYS	O-C-N	-5.73	117.08	121.55
3	C	307	GLN	OE1-CD-NE2	-5.72	116.88	122.60
4	D	110	SER	N-CA-CB	5.72	118.31	110.01
6	F	126	ASN	CA-C-N	5.72	131.22	122.29
6	F	126	ASN	C-N-CA	5.72	131.22	122.29
4	D	71	ARG	O-C-N	5.72	128.19	122.12
5	E	7	GLU	CA-C-N	5.72	127.95	120.28
5	E	7	GLU	C-N-CA	5.72	127.95	120.28
10	J	54	LYS	N-CA-C	-5.72	106.30	113.28
1	A	90	GLN	CA-C-O	5.72	125.99	119.18
3	C	72	ASN	OD1-CG-ND2	-5.71	116.89	122.60
10	J	627	ILE	O-C-N	-5.71	117.09	123.26
10	J	836	VAL	CA-CB-CG2	5.71	120.11	110.40
10	J	704	HIS	CA-CB-CG	5.71	119.51	113.80
10	J	905	GLN	CA-C-N	5.71	128.53	120.42
10	J	905	GLN	C-N-CA	5.71	128.53	120.42
6	F	238	ARG	NE-CZ-NH2	-5.71	114.06	119.20
10	J	155	HIS	CB-CG-CD2	-5.71	123.78	131.20
10	J	873	ASP	CA-C-N	5.71	128.18	120.65
10	J	873	ASP	C-N-CA	5.71	128.18	120.65
10	J	635	ASN	CA-C-N	5.71	129.74	121.18
10	J	635	ASN	C-N-CA	5.71	129.74	121.18
11	P	73	SER	N-CA-C	-5.70	106.09	113.16
3	C	392	PHE	CB-CA-C	-5.70	100.83	110.64
8	H	103	ARG	NE-CZ-NH2	-5.70	114.07	119.20
1	A	93	ASN	N-CA-C	5.70	119.11	111.24
2	B	7	TYR	CB-CG-CD1	-5.70	112.25	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	887	LYS	CA-C-N	5.70	127.91	120.28
10	J	887	LYS	C-N-CA	5.70	127.91	120.28
5	E	31	PHE	N-CA-C	-5.69	100.40	109.23
2	B	57	LYS	CA-C-O	-5.69	115.18	121.33
10	J	601	ILE	CA-C-N	5.69	129.79	121.31
10	J	601	ILE	C-N-CA	5.69	129.79	121.31
1	A	185	VAL	N-CA-CB	5.69	118.44	111.21
6	F	185	ILE	CA-C-N	5.69	129.34	120.75
6	F	185	ILE	C-N-CA	5.69	129.34	120.75
5	E	197	MET	CA-C-O	5.69	126.39	120.30
9	I	280	THR	N-CA-C	-5.69	106.69	113.97
10	J	517	ASP	CA-C-N	5.69	128.29	120.67
10	J	517	ASP	C-N-CA	5.69	128.29	120.67
10	J	673	GLY	CA-C-N	5.69	127.90	120.28
10	J	673	GLY	C-N-CA	5.69	127.90	120.28
10	J	79	LEU	CA-C-N	5.69	131.07	120.95
10	J	79	LEU	C-N-CA	5.69	131.07	120.95
11	P	62	PHE	N-CA-CB	5.68	118.25	110.01
1	A	115	SER	N-CA-C	-5.68	104.55	112.45
3	C	161	HIS	O-C-N	-5.68	114.81	122.43
4	D	203	GLN	CB-CA-C	-5.68	99.76	110.67
6	F	124	VAL	CA-C-O	-5.68	114.20	120.96
3	C	155	LEU	CA-C-O	-5.68	114.86	120.82
4	D	189	ASP	N-CA-C	-5.68	105.23	111.82
2	B	54	LYS	N-CA-C	-5.68	99.65	108.90
2	B	99	GLU	N-CA-C	5.68	117.47	111.28
10	J	726	LEU	CB-CA-C	-5.67	101.98	110.88
3	C	347	ILE	N-CA-C	-5.67	99.96	108.12
2	B	195	LYS	CA-C-N	5.67	130.18	122.19
2	B	195	LYS	C-N-CA	5.67	130.18	122.19
7	G	181	HIS	CE1-NE2-CD2	-5.67	103.33	109.00
3	C	284	LEU	CA-C-O	5.66	127.38	120.92
10	J	855	HIS	CE1-NE2-CD2	-5.66	103.34	109.00
10	J	758	PRO	N-CA-CB	5.66	108.57	103.08
10	J	285	PHE	CB-CA-C	-5.66	99.34	109.24
10	J	808	MET	CA-C-O	5.66	126.49	120.10
1	A	277	ASP	N-CA-C	5.66	117.44	111.28
4	D	62	ARG	N-CA-C	-5.66	105.02	111.07
10	J	848	ARG	NE-CZ-NH1	5.66	127.16	121.50
4	D	44	THR	N-CA-C	-5.65	106.37	113.72
2	B	215	ALA	CA-C-O	-5.65	114.43	120.42
2	B	208	ASP	CB-CA-C	-5.65	98.50	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	394	ILE	CA-CB-CG1	-5.65	100.79	110.40
4	D	189	ASP	CA-CB-CG	-5.65	106.95	112.60
10	J	228	ALA	CA-C-N	5.65	129.29	120.82
10	J	228	ALA	C-N-CA	5.65	129.29	120.82
3	C	33	ARG	N-CA-C	5.65	117.44	111.28
7	G	35	ARG	O-C-N	-5.65	117.90	121.85
1	A	177	HIS	CG-CD2-NE2	5.65	112.85	107.20
10	J	896	ARG	O-C-N	5.65	129.57	122.23
2	B	136	MET	CA-C-N	5.64	127.45	120.34
2	B	136	MET	C-N-CA	5.64	127.45	120.34
3	C	58	THR	N-CA-CB	5.64	119.08	110.95
9	I	286	ARG	NE-CZ-NH2	5.64	124.28	119.20
3	C	222	ARG	CB-CA-C	-5.64	102.03	110.16
5	E	181	ASP	N-CA-CB	5.64	119.88	110.85
9	I	7	PHE	CA-CB-CG	-5.64	108.16	113.80
1	A	226	LYS	CA-C-N	5.64	127.84	120.28
1	A	226	LYS	C-N-CA	5.64	127.84	120.28
10	J	359	SER	CB-CA-C	-5.64	104.60	111.82
10	J	397	ARG	NE-CZ-NH2	5.64	124.28	119.20
7	G	64	TYR	CB-CG-CD2	5.64	129.25	120.80
8	H	137	MET	CA-C-O	5.64	127.48	121.45
10	J	219	VAL	CA-C-O	-5.64	115.09	120.95
10	J	191	ASN	CA-CB-CG	-5.63	106.97	112.60
9	I	39	PRO	O-C-N	-5.63	116.80	123.10
6	F	20	PHE	CA-CB-CG	-5.63	108.17	113.80
7	G	212	MET	CA-C-N	5.63	127.82	120.28
7	G	212	MET	C-N-CA	5.63	127.82	120.28
6	F	70	GLN	N-CA-C	-5.62	100.61	109.50
1	A	139	HIS	N-CA-C	-5.62	98.74	108.69
3	C	209	TRP	CA-C-O	5.62	127.07	120.89
10	J	257	GLU	N-CA-C	-5.62	102.20	110.52
4	D	61	THR	OG1-CB-CG2	-5.62	98.06	109.30
10	J	815	ALA	CA-C-O	5.62	128.05	121.87
5	E	264	ASN	CA-C-O	-5.62	114.35	120.36
5	E	65	LYS	N-CA-C	-5.61	100.18	108.99
2	B	158	ILE	N-CA-C	-5.61	100.35	108.87
3	C	370	THR	CA-CB-OG1	5.60	118.01	109.60
10	J	937	GLY	O-C-N	5.60	127.53	123.27
10	J	460	HIS	N-CA-CB	-5.60	102.12	111.20
10	J	813	MET	CA-C-O	-5.60	115.61	121.55
6	F	234	TYR	CA-CB-CG	5.60	123.98	113.90
3	C	56	ASN	CA-C-O	-5.60	114.79	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	64	ASP	N-CA-C	-5.59	100.80	109.14
9	I	68	GLU	CA-C-N	5.59	131.02	122.24
9	I	68	GLU	C-N-CA	5.59	131.02	122.24
10	J	789	SER	N-CA-CB	5.59	118.54	110.20
2	B	83	LYS	CA-C-N	5.59	128.81	120.31
2	B	83	LYS	C-N-CA	5.59	128.81	120.31
7	G	28	ASP	N-CA-CB	5.59	118.76	109.98
9	I	141	THR	CA-C-N	5.59	131.35	122.74
9	I	141	THR	C-N-CA	5.59	131.35	122.74
10	J	115	GLN	N-CA-C	5.59	117.37	111.28
10	J	564	TRP	CB-CG-CD1	5.59	135.28	126.90
2	B	226	ASP	CA-CB-CG	-5.58	107.02	112.60
5	E	85	GLN	N-CA-C	-5.58	101.03	109.85
8	H	84	VAL	N-CA-C	-5.58	101.72	108.53
10	J	573	VAL	N-CA-C	-5.58	107.54	112.90
5	E	36	ILE	N-CA-C	-5.58	100.36	108.17
4	D	54	PRO	CA-C-N	5.58	128.03	120.44
4	D	54	PRO	C-N-CA	5.58	128.03	120.44
5	E	169	LEU	CA-C-N	5.58	125.53	119.78
5	E	169	LEU	C-N-CA	5.58	125.53	119.78
6	F	111	LYS	N-CA-CB	5.58	118.41	110.16
10	J	940	ARG	CA-C-N	5.58	128.02	120.38
10	J	940	ARG	C-N-CA	5.58	128.02	120.38
10	J	39	HIS	N-CA-CB	5.57	119.34	110.65
10	J	738	VAL	CA-C-N	5.57	127.68	120.44
10	J	738	VAL	C-N-CA	5.57	127.68	120.44
10	J	898	SER	CA-C-O	5.57	126.45	120.55
2	B	142	GLY	O-C-N	-5.57	116.22	122.28
10	J	386	ILE	N-CA-C	-5.57	102.34	109.30
8	H	203	PRO	CB-CA-C	-5.56	103.69	110.98
2	B	34	HIS	CE1-NE2-CD2	-5.56	103.44	109.00
1	A	300	GLU	N-CA-CB	5.56	119.54	110.37
6	F	92	THR	CA-C-N	5.56	130.72	122.99
6	F	92	THR	C-N-CA	5.56	130.72	122.99
10	J	27	SER	CA-C-O	5.56	126.25	120.30
3	C	127	TYR	CA-CB-CG	-5.56	103.90	113.90
3	C	286	ILE	CA-C-O	5.56	127.13	121.63
7	G	52	VAL	CA-C-N	5.56	128.99	120.82
7	G	52	VAL	C-N-CA	5.56	128.99	120.82
8	H	243	ARG	N-CA-C	-5.56	105.85	113.30
1	A	95	ASN	OD1-CG-ND2	5.56	128.16	122.60
2	B	219	ALA	CA-C-N	5.55	127.27	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	219	ALA	C-N-CA	5.55	127.27	120.22
5	E	263	GLU	CB-CG-CD	-5.55	103.16	112.60
10	J	389	THR	CA-C-O	-5.55	114.77	120.99
3	C	254	ASP	N-CA-CB	5.55	120.71	111.49
8	H	186	THR	N-CA-CB	5.55	120.01	110.68
2	B	120	THR	N-CA-C	-5.55	100.86	109.24
7	G	62	LYS	N-CA-C	-5.55	104.75	113.02
10	J	510	TRP	CB-CG-CD2	-5.55	119.03	126.80
10	J	460	HIS	CE1-NE2-CD2	-5.55	103.45	109.00
10	J	536	ASP	N-CA-C	-5.54	106.51	113.72
8	H	51	ASP	CA-CB-CG	5.54	118.14	112.60
9	I	135	GLU	N-CA-C	5.54	118.06	110.24
7	G	14	ASP	N-CA-C	-5.54	102.64	110.29
8	H	14	PHE	N-CA-C	5.54	117.32	111.28
6	F	126	ASN	CA-C-O	5.54	127.29	120.92
6	F	90	GLN	CA-C-N	5.54	128.26	121.06
6	F	90	GLN	C-N-CA	5.54	128.26	121.06
8	H	128	ILE	CB-CA-C	-5.54	104.33	111.20
5	E	10	TYR	CA-CB-CG	-5.54	103.94	113.90
9	I	145	ARG	NE-CZ-NH1	-5.54	115.96	121.50
1	A	221	ILE	O-C-N	5.53	127.83	122.69
9	I	253	GLY	N-CA-C	-5.53	103.30	110.38
10	J	504	PRO	CA-C-O	-5.53	114.67	121.31
10	J	654	TYR	CA-C-N	5.53	127.63	120.44
10	J	654	TYR	C-N-CA	5.53	127.63	120.44
2	B	36	ALA	CA-C-N	5.53	128.14	120.29
2	B	36	ALA	C-N-CA	5.53	128.14	120.29
6	F	139	VAL	N-CA-C	-5.53	99.68	107.75
3	C	28	GLU	N-CA-C	-5.53	105.34	111.36
3	C	257	MET	CA-C-N	5.53	129.46	120.23
3	C	257	MET	C-N-CA	5.53	129.46	120.23
7	G	68	VAL	O-C-N	5.53	129.52	122.61
10	J	262	ALA	N-CA-CB	5.53	118.81	110.30
1	A	142	ASP	CA-CB-CG	-5.52	107.08	112.60
10	J	232	ARG	N-CA-CB	5.52	121.00	111.00
10	J	285	PHE	N-CA-C	-5.52	106.67	113.41
10	J	402	GLN	CA-C-O	-5.52	114.46	120.81
7	G	151	GLU	N-CA-C	-5.52	100.68	109.07
10	J	1001	LYS	CA-CB-CG	5.52	125.14	114.10
5	E	29	HIS	ND1-CE1-NE2	5.52	113.92	108.40
7	G	79	THR	CA-CB-OG1	5.52	117.87	109.60
7	G	162	PHE	CA-C-N	5.51	128.12	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	162	PHE	C-N-CA	5.51	128.12	120.29
1	A	44	PHE	CA-C-O	-5.51	114.41	120.69
5	E	172	PHE	CA-C-O	5.51	128.38	121.66
4	D	113	ILE	O-C-N	-5.51	116.17	121.90
10	J	93	ASN	N-CA-CB	5.51	118.70	110.22
8	H	60	LEU	N-CA-CB	5.51	118.75	109.94
10	J	419	THR	CA-C-O	5.51	127.35	121.02
11	P	65	PRO	N-CA-C	5.51	120.78	113.57
7	G	98	SER	CA-C-N	5.50	127.66	120.28
7	G	98	SER	C-N-CA	5.50	127.66	120.28
9	I	187	THR	N-CA-C	-5.50	99.31	108.34
10	J	20	THR	N-CA-C	-5.50	100.71	109.07
1	A	207	GLU	N-CA-C	5.50	117.28	111.28
3	C	146	ASP	CA-C-N	5.50	127.59	120.44
3	C	146	ASP	C-N-CA	5.50	127.59	120.44
2	B	13	ARG	N-CA-C	-5.50	100.49	108.07
9	I	191	SER	CA-C-N	5.50	128.66	120.31
9	I	191	SER	C-N-CA	5.50	128.66	120.31
4	D	150	THR	CA-C-N	5.49	127.64	120.28
4	D	150	THR	C-N-CA	5.49	127.64	120.28
5	E	146	TYR	N-CA-CB	5.49	117.97	110.01
8	H	240	ASP	CB-CA-C	-5.49	100.90	110.17
3	C	298	GLY	CA-C-N	5.49	130.33	123.14
3	C	298	GLY	C-N-CA	5.49	130.33	123.14
1	A	77	PHE	N-CA-C	-5.49	99.49	108.76
3	C	125	ALA	CB-CA-C	-5.49	101.29	110.56
9	I	192	GLN	CA-C-N	5.49	128.50	120.71
9	I	192	GLN	C-N-CA	5.49	128.50	120.71
10	J	725	SER	CA-C-N	5.49	127.57	120.44
10	J	725	SER	C-N-CA	5.49	127.57	120.44
2	B	188	GLY	O-C-N	-5.48	118.48	123.36
1	A	105	SER	CA-C-N	5.48	127.63	120.28
1	A	105	SER	C-N-CA	5.48	127.63	120.28
3	C	63	ALA	N-CA-CB	5.48	119.49	110.39
11	P	34	LEU	CA-C-O	-5.48	114.61	120.42
5	E	213	LEU	CA-C-O	5.48	126.05	120.24
6	F	69	HIS	ND1-CE1-NE2	5.48	113.88	108.40
7	G	110	ARG	O-C-N	-5.48	115.51	121.53
5	E	46	GLY	O-C-N	-5.47	117.22	123.51
9	I	272	TRP	CB-CG-CD1	5.47	135.11	126.90
9	I	246	THR	CB-CA-C	5.47	120.49	109.38
10	J	81	ALA	N-CA-C	5.47	116.59	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	103	GLU	CA-C-O	-5.47	114.75	120.55
10	J	954	ASP	CA-C-N	5.47	132.24	122.06
10	J	954	ASP	C-N-CA	5.47	132.24	122.06
5	E	97	SER	O-C-N	5.47	127.70	122.07
5	E	255	ALA	CA-C-N	5.47	125.55	119.32
5	E	255	ALA	C-N-CA	5.47	125.55	119.32
8	H	210	ALA	CA-C-N	5.47	128.05	120.29
8	H	210	ALA	C-N-CA	5.47	128.05	120.29
10	J	338	HIS	CA-C-N	-5.47	112.97	122.37
10	J	338	HIS	C-N-CA	-5.47	112.97	122.37
4	D	120	LEU	CA-C-O	-5.46	114.76	120.55
10	J	590	ARG	N-CA-CB	5.46	118.25	110.16
3	C	26	SER	O-C-N	-5.46	115.04	121.32
2	B	32	HIS	O-C-N	5.46	127.60	121.32
10	J	958	TYR	N-CA-CB	5.46	119.72	110.49
10	J	972	ASP	CB-CA-C	-5.46	100.30	109.53
10	J	320	LEU	CA-C-O	5.46	127.51	121.56
4	D	185	ASP	CB-CA-C	-5.46	101.16	109.89
10	J	92	THR	O-C-N	-5.46	116.45	122.07
2	B	9	PRO	N-CA-CB	5.46	108.54	103.41
8	H	355	ARG	N-CA-C	5.46	117.03	111.14
11	P	61	ASN	CA-C-N	5.46	127.53	120.44
11	P	61	ASN	C-N-CA	5.46	127.53	120.44
7	G	57	ILE	CA-C-N	5.46	129.63	121.72
7	G	57	ILE	C-N-CA	5.46	129.63	121.72
10	J	416	SER	N-CA-CB	5.45	118.40	109.95
7	G	99	TYR	CA-C-N	5.45	131.50	122.73
7	G	99	TYR	C-N-CA	5.45	131.50	122.73
4	D	34	ILE	N-CA-C	-5.45	99.86	108.90
11	P	46	VAL	O-C-N	5.45	127.31	121.10
6	F	245	LEU	CA-C-N	5.45	131.53	122.54
6	F	245	LEU	C-N-CA	5.45	131.53	122.54
6	F	224	LEU	CB-CA-C	-5.45	101.59	110.85
8	H	324	GLU	CA-C-N	5.45	128.12	120.28
8	H	324	GLU	C-N-CA	5.45	128.12	120.28
2	B	130	GLU	CA-C-O	-5.44	114.65	120.75
10	J	18	SER	N-CA-C	-5.44	100.80	109.07
10	J	421	ASN	O-C-N	-5.44	117.02	123.22
11	P	84	GLU	CB-CA-C	-5.44	101.75	110.79
2	B	235	HIS	CG-CD2-NE2	5.44	112.64	107.20
3	C	142	GLY	O-C-N	-5.44	118.47	122.71
3	C	347	ILE	O-C-N	-5.44	117.33	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	55	ALA	N-CA-C	5.44	117.11	108.79
3	C	146	ASP	CA-C-O	-5.44	114.79	120.55
11	P	67	PRO	O-C-N	5.44	129.61	122.27
1	A	56	VAL	CA-C-O	-5.43	116.25	121.63
10	J	451	ILE	CA-CB-CG2	-5.43	101.26	110.50
9	I	138	ILE	CB-CA-C	5.43	119.77	111.68
5	E	233	ASP	CA-C-O	5.43	124.74	118.55
7	G	221	ALA	CA-C-N	5.43	127.55	120.28
7	G	221	ALA	C-N-CA	5.43	127.55	120.28
10	J	744	ASP	N-CA-C	-5.43	105.28	111.14
10	J	95	VAL	CB-CA-C	-5.42	105.03	111.97
2	B	106	ARG	N-CA-CB	5.42	118.19	110.16
2	B	235	HIS	CE1-NE2-CD2	-5.42	103.58	109.00
3	C	146	ASP	CA-CB-CG	-5.42	107.18	112.60
6	F	16	LYS	O-C-N	-5.42	117.14	121.80
7	G	44	VAL	O-C-N	5.42	128.90	123.10
3	C	279	THR	CA-CB-OG1	5.42	117.73	109.60
3	C	165	LEU	CA-C-N	5.42	125.88	120.14
3	C	165	LEU	C-N-CA	5.42	125.88	120.14
8	H	159	MET	CA-C-N	5.42	127.98	120.29
8	H	159	MET	C-N-CA	5.42	127.98	120.29
5	E	29	HIS	CE1-NE2-CD2	-5.42	103.58	109.00
7	G	6	PHE	CA-CB-CG	-5.42	108.38	113.80
10	J	442	ALA	CA-C-N	5.42	127.54	120.28
10	J	442	ALA	C-N-CA	5.42	127.54	120.28
1	A	164	LYS	O-C-N	-5.41	117.14	121.80
10	J	262	ALA	CA-C-N	5.41	127.98	120.29
10	J	262	ALA	C-N-CA	5.41	127.98	120.29
2	B	34	HIS	ND1-CE1-NE2	5.41	113.81	108.40
10	J	440	ARG	CD-NE-CZ	-5.41	116.83	124.40
2	B	232	LEU	N-CA-CB	5.41	118.17	110.16
4	D	208	ASN	CB-CA-C	-5.41	101.66	110.85
7	G	32	GLN	OE1-CD-NE2	5.41	128.01	122.60
8	H	183	SER	N-CA-CB	5.41	118.69	109.87
9	I	187	THR	CA-C-O	5.41	125.97	120.24
10	J	872	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	A	19	LEU	N-CA-C	5.41	117.25	111.36
2	B	240	VAL	N-CA-C	-5.41	108.01	113.20
3	C	339	GLU	CA-C-O	-5.41	115.13	120.70
7	G	97	LEU	N-CA-C	-5.41	99.29	108.26
8	H	350	THR	CA-C-N	5.41	127.52	120.28
8	H	350	THR	C-N-CA	5.41	127.52	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	497	LYS	N-CA-CB	-5.41	102.17	110.12
1	A	80	SER	N-CA-C	-5.40	99.71	108.52
8	H	227	VAL	CB-CA-C	5.40	117.90	111.20
10	J	253	PHE	N-CA-CB	5.40	118.16	110.44
5	E	153	TYR	N-CA-CB	5.40	120.31	111.08
10	J	854	ALA	CA-C-N	5.40	127.78	120.44
10	J	854	ALA	C-N-CA	5.40	127.78	120.44
7	G	213	GLU	N-CA-C	5.40	117.16	111.28
10	J	744	ASP	CA-C-O	5.40	126.26	120.70
1	A	135	ARG	CA-C-O	-5.39	114.53	120.36
10	J	490	VAL	CA-CB-CG2	-5.39	101.23	110.40
10	J	811	ARG	O-C-N	-5.39	116.00	122.15
1	A	237	VAL	CA-C-O	5.39	126.71	120.67
3	C	250	GLU	CB-CA-C	-5.39	101.49	109.90
9	I	235	LEU	O-C-N	-5.39	115.65	122.17
10	J	966	ASN	CA-C-O	5.39	128.21	120.51
10	J	15	ASP	CA-C-N	5.39	128.24	120.11
10	J	15	ASP	C-N-CA	5.39	128.24	120.11
3	C	90	SER	N-CA-C	-5.38	99.91	109.06
10	J	258	TYR	CA-C-N	5.38	128.49	120.95
10	J	258	TYR	C-N-CA	5.38	128.49	120.95
10	J	943	ASN	O-C-N	5.38	129.07	122.34
10	J	85	LYS	O-C-N	-5.38	116.28	122.95
8	H	144	PRO	N-CA-CB	-5.38	97.73	103.38
8	H	98	ILE	CA-C-N	5.38	125.37	119.89
8	H	98	ILE	C-N-CA	5.38	125.37	119.89
8	H	179	ASP	O-C-N	5.38	128.28	122.15
10	J	421	ASN	N-CA-CB	5.38	119.03	110.16
10	J	660	ARG	NE-CZ-NH1	-5.38	116.12	121.50
4	D	64	LYS	CA-C-N	5.37	127.44	120.56
4	D	64	LYS	C-N-CA	5.37	127.44	120.56
7	G	218	ASN	OD1-CG-ND2	5.37	127.97	122.60
10	J	668	ASP	CA-C-N	5.37	127.48	120.28
10	J	668	ASP	C-N-CA	5.37	127.48	120.28
4	D	107	ARG	N-CA-CB	5.37	118.20	110.20
10	J	831	HIS	ND1-CE1-NE2	5.37	113.77	108.40
1	A	111	SER	CB-CA-C	-5.37	102.42	110.90
8	H	196	ASN	CB-CA-C	-5.37	104.95	111.82
8	H	132	GLN	N-CA-C	-5.37	101.69	108.45
10	J	315	GLN	CA-C-O	-5.36	114.27	120.49
10	J	338	HIS	CG-CD2-NE2	5.36	112.56	107.20
11	P	21	SER	CB-CA-C	-5.36	103.21	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	138	ARG	NE-CZ-NH2	5.36	124.03	119.20
4	D	104	PHE	CA-CB-CG	-5.36	108.44	113.80
6	F	214	TRP	CA-CB-CG	5.36	123.78	113.60
10	J	810	THR	N-CA-C	-5.36	105.47	112.23
1	A	284	LYS	N-CA-C	5.36	117.12	111.28
2	B	17	ARG	NE-CZ-NH2	5.36	124.02	119.20
10	J	51	SER	N-CA-C	-5.36	106.91	113.50
10	J	508	HIS	CG-CD2-NE2	5.36	112.56	107.20
4	D	179	LEU	CA-C-O	-5.36	114.99	120.99
6	F	116	PHE	N-CA-C	5.36	116.92	111.14
8	H	201	GLN	CA-C-O	-5.35	115.00	120.89
10	J	361	ASN	OD1-CG-ND2	5.35	127.95	122.60
8	H	54	ILE	N-CA-C	5.35	120.47	109.34
10	J	502	CYS	CA-C-O	5.35	126.15	119.78
10	J	754	ARG	NE-CZ-NH2	5.35	124.02	119.20
11	P	39	ASN	OD1-CG-ND2	-5.35	117.25	122.60
4	D	14	ASP	CA-CB-CG	-5.35	107.25	112.60
7	G	212	MET	N-CA-C	5.35	117.53	111.11
3	C	139	GLY	N-CA-C	-5.35	107.83	115.64
9	I	236	SER	CA-C-N	5.35	127.88	120.29
9	I	236	SER	C-N-CA	5.35	127.88	120.29
1	A	135	ARG	O-C-N	5.35	129.66	123.30
8	H	181	SER	O-C-N	5.34	129.38	122.81
10	J	667	ASN	N-CA-C	-5.34	104.04	110.88
10	J	735	ASN	CA-C-N	5.34	127.78	120.46
10	J	735	ASN	C-N-CA	5.34	127.78	120.46
3	C	263	GLY	N-CA-C	-5.34	100.52	113.18
7	G	234	ILE	O-C-N	-5.34	115.16	122.26
1	A	260	THR	CA-C-N	5.34	127.38	120.44
1	A	260	THR	C-N-CA	5.34	127.38	120.44
4	D	105	SER	CB-CA-C	-5.34	101.47	110.44
5	E	51	ILE	N-CA-C	-5.34	100.63	108.11
9	I	54	GLU	N-CA-C	-5.34	100.32	109.24
10	J	215	THR	N-CA-C	-5.34	99.58	108.34
7	G	208	TYR	O-C-N	5.34	127.64	122.09
1	A	126	VAL	CA-C-N	5.34	128.34	120.82
1	A	126	VAL	C-N-CA	5.34	128.34	120.82
8	H	230	TYR	N-CA-C	-5.34	101.01	109.76
10	J	561	ASN	OD1-CG-ND2	5.33	127.94	122.60
4	D	152	GLU	N-CA-CB	5.33	117.75	110.01
6	F	70	GLN	OE1-CD-NE2	5.33	127.93	122.60
8	H	179	ASP	N-CA-CB	5.33	118.05	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	881	CYS	N-CA-CB	5.33	117.89	109.94
5	E	226	ILE	N-CA-C	-5.33	100.80	108.48
10	J	812	CYS	CA-C-N	5.33	128.80	120.75
10	J	812	CYS	C-N-CA	5.33	128.80	120.75
6	F	14	ALA	CA-C-N	5.33	128.80	120.75
6	F	14	ALA	C-N-CA	5.33	128.80	120.75
8	H	342	GLU	O-C-N	-5.33	116.47	122.12
9	I	218	VAL	CA-C-N	5.33	128.80	120.75
9	I	218	VAL	C-N-CA	5.33	128.80	120.75
10	J	979	VAL	N-CA-C	-5.33	100.80	108.42
10	J	756	ALA	CA-C-N	5.33	128.75	120.60
10	J	756	ALA	C-N-CA	5.33	128.75	120.60
2	B	32	HIS	CB-CG-CD2	-5.32	124.28	131.20
9	I	278	PRO	N-CA-C	-5.32	107.25	114.80
10	J	113	VAL	N-CA-C	-5.32	102.28	107.55
1	A	136	ALA	N-CA-CB	5.32	118.92	110.57
7	G	38	ASN	CA-C-N	5.32	130.66	123.11
7	G	38	ASN	C-N-CA	5.32	130.66	123.11
10	J	87	TYR	N-CA-CB	5.32	118.84	110.23
10	J	464	LEU	N-CA-C	-5.32	100.51	109.07
4	D	203	GLN	N-CA-CB	5.31	118.52	110.28
8	H	276	SER	N-CA-C	-5.31	101.22	109.24
10	J	129	TYR	N-CA-CB	5.31	117.90	109.82
8	H	152	SER	N-CA-CB	5.31	118.06	111.00
11	P	69	ASP	CB-CA-C	-5.31	100.98	110.70
1	A	100	ASP	N-CA-C	5.31	117.15	111.36
8	H	280	ILE	O-C-N	-5.31	116.36	121.83
10	J	314	ASP	N-CA-CB	5.30	117.84	110.26
10	J	593	SER	N-CA-C	-5.30	100.25	108.90
7	G	86	VAL	N-CA-C	-5.30	100.83	108.89
5	E	202	ALA	CA-C-N	5.30	127.69	120.54
5	E	202	ALA	C-N-CA	5.30	127.69	120.54
7	G	89	GLN	CA-C-O	5.30	126.96	120.60
10	J	177	THR	CB-CA-C	-5.30	101.99	110.79
11	P	64	ARG	N-CA-CB	5.30	118.64	110.43
3	C	254	ASP	N-CA-C	-5.30	105.10	112.30
7	G	76	ILE	CA-CB-CG1	-5.30	101.40	110.40
3	C	271	THR	N-CA-C	-5.29	100.69	108.79
5	E	195	ASN	CA-CB-CG	-5.29	107.31	112.60
9	I	192	GLN	CA-C-O	5.29	126.06	119.97
1	A	10	SER	N-CA-CB	5.29	117.99	110.16
10	J	462	TYR	CA-C-N	5.29	126.45	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	462	TYR	C-N-CA	5.29	126.45	119.84
1	A	298	THR	CA-CB-OG1	5.29	117.53	109.60
10	J	154	GLU	N-CA-C	-5.29	106.69	112.72
1	A	147	PHE	N-CA-C	5.29	116.73	110.97
6	F	52	PHE	CA-CB-CG	5.29	119.08	113.80
10	J	217	SER	CA-C-N	5.29	127.31	120.44
10	J	217	SER	C-N-CA	5.29	127.31	120.44
11	P	19	SER	O-C-N	5.28	127.51	122.07
10	J	376	ASP	N-CA-CB	5.28	117.67	110.01
8	H	285	ASN	CA-C-N	5.28	127.99	120.49
8	H	285	ASN	C-N-CA	5.28	127.99	120.49
10	J	967	SER	N-CA-C	-5.28	100.71	108.79
3	C	130	VAL	CA-C-O	-5.28	116.16	121.59
11	P	64	ARG	NE-CZ-NH2	5.28	123.95	119.20
7	G	22	GLY	CA-C-N	5.27	126.43	119.84
7	G	22	GLY	C-N-CA	5.27	126.43	119.84
6	F	104	LYS	O-C-N	-5.27	117.15	123.27
6	F	143	TYR	CA-CB-CG	5.27	123.39	113.90
8	H	67	TRP	CD2-CE2-CZ2	-5.27	117.13	122.40
10	J	425	ILE	N-CA-C	-5.27	99.66	107.51
10	J	677	LEU	N-CA-CB	5.27	117.65	110.01
3	C	240	SER	CA-C-N	5.27	128.24	120.91
3	C	240	SER	C-N-CA	5.27	128.24	120.91
10	J	97	GLN	CA-C-O	5.27	125.86	119.38
1	A	133	ALA	N-CA-C	-5.27	100.32	108.90
10	J	544	PRO	CA-C-O	-5.27	112.92	120.56
7	G	139	SER	CB-CA-C	-5.26	100.49	109.65
7	G	179	ALA	N-CA-C	5.26	117.76	111.71
10	J	108	PHE	CA-CB-CG	-5.26	108.53	113.80
7	G	207	CYS	CA-C-N	5.26	127.64	120.54
7	G	207	CYS	C-N-CA	5.26	127.64	120.54
10	J	97	GLN	N-CA-C	5.26	118.96	112.54
5	E	156	LYS	CA-C-N	5.26	128.57	121.05
5	E	156	LYS	C-N-CA	5.26	128.57	121.05
3	C	288	ALA	CA-C-O	5.26	125.99	120.42
5	E	94	THR	CA-C-O	-5.26	114.98	120.55
2	B	43	GLU	N-CA-CB	5.26	118.85	110.65
3	C	358	LYS	CB-CA-C	-5.26	101.60	110.64
1	A	208	GLU	CA-C-N	5.25	127.59	120.44
1	A	208	GLU	C-N-CA	5.25	127.59	120.44
4	D	66	LEU	CA-C-O	-5.25	114.98	120.55
9	I	50	GLY	O-C-N	5.25	128.84	122.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	831	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
11	P	86	LEU	CB-CA-C	-5.25	102.63	110.88
10	J	406	GLN	N-CA-C	-5.25	101.31	109.24
10	J	155	HIS	CB-CG-ND1	5.24	130.56	122.70
10	J	726	LEU	N-CA-C	5.24	116.68	111.07
2	B	50	ILE	CA-CB-CG1	5.24	119.31	110.40
3	C	261	THR	CA-CB-OG1	5.24	117.46	109.60
1	A	48	SER	O-C-N	-5.24	117.11	123.13
10	J	888	HIS	CA-CB-CG	5.24	119.04	113.80
2	B	148	ILE	N-CA-C	5.24	117.59	111.05
10	J	714	GLU	O-C-N	5.24	128.80	122.94
4	D	148	ASP	CA-CB-CG	-5.23	107.37	112.60
7	G	129	GLU	CA-C-N	5.23	130.73	122.36
7	G	129	GLU	C-N-CA	5.23	130.73	122.36
11	P	61	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	147	PHE	CA-C-N	5.23	127.63	120.46
1	A	147	PHE	C-N-CA	5.23	127.63	120.46
5	E	20	SER	O-C-N	-5.23	116.76	122.67
5	E	181	ASP	N-CA-C	-5.23	101.64	109.95
10	J	142	HIS	CE1-NE2-CD2	-5.23	103.77	109.00
1	A	167	ILE	CA-CB-CG1	5.23	119.29	110.40
4	D	166	GLU	CB-CG-CD	-5.23	103.71	112.60
5	E	152	THR	N-CA-C	-5.23	101.45	109.76
8	H	315	THR	N-CA-C	-5.23	101.59	109.85
8	H	311	GLU	N-CA-CB	5.23	119.44	111.70
9	I	32	ILE	N-CA-C	-5.22	102.85	109.80
1	A	13	LYS	O-C-N	5.22	128.10	122.15
6	F	98	LYS	CA-C-N	5.22	128.13	120.71
6	F	98	LYS	C-N-CA	5.22	128.13	120.71
9	I	256	PHE	CA-CB-CG	5.22	119.02	113.80
10	J	421	ASN	CA-C-O	5.22	126.44	120.54
10	J	909	ASN	N-CA-C	5.22	116.97	111.28
2	B	71	LEU	N-CA-C	-5.22	101.19	109.96
10	J	379	ILE	CA-C-N	5.22	127.27	120.28
10	J	379	ILE	C-N-CA	5.22	127.27	120.28
3	C	30	SER	CA-C-O	5.22	126.27	120.63
10	J	10	ARG	CD-NE-CZ	-5.22	117.09	124.40
9	I	49	ASN	CA-CB-CG	5.22	117.82	112.60
7	G	90	ASN	CA-C-N	5.21	131.50	121.54
7	G	90	ASN	C-N-CA	5.21	131.50	121.54
10	J	51	SER	CA-C-N	5.21	128.25	120.95
10	J	51	SER	C-N-CA	5.21	128.25	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	260	ARG	NE-CZ-NH2	-5.21	114.51	119.20
9	I	67	GLU	O-C-N	-5.21	117.11	123.10
10	J	479	ALA	CA-C-O	-5.21	114.90	120.42
10	J	874	LYS	CA-C-O	5.21	126.47	121.00
10	J	876	LYS	O-C-N	5.21	128.68	122.27
2	B	80	LYS	CA-C-O	-5.21	113.13	119.43
5	E	98	LEU	CB-CA-C	-5.21	102.71	110.88
8	H	8	THR	N-CA-C	-5.21	100.03	108.52
8	H	287	PRO	N-CA-C	-5.21	108.72	114.92
11	P	34	LEU	CA-C-N	5.21	128.22	120.31
11	P	34	LEU	C-N-CA	5.21	128.22	120.31
8	H	286	ASP	O-C-N	5.20	127.26	121.43
11	P	70	ILE	N-CA-C	5.20	117.59	111.09
5	E	182	ILE	N-CA-C	-5.20	98.52	109.34
8	H	213	HIS	CE1-NE2-CD2	-5.20	103.80	109.00
11	P	64	ARG	CA-C-N	5.20	124.70	119.19
11	P	64	ARG	C-N-CA	5.20	124.70	119.19
6	F	239	ASP	CA-C-N	5.20	127.51	120.44
6	F	239	ASP	C-N-CA	5.20	127.51	120.44
10	J	147	VAL	CG1-CB-CG2	5.20	122.24	110.80
4	D	158	LEU	CA-C-O	5.20	124.53	118.97
2	B	69	LYS	CA-C-N	5.20	128.60	120.75
2	B	69	LYS	C-N-CA	5.20	128.60	120.75
8	H	216	ASN	OD1-CG-ND2	5.20	127.80	122.60
10	J	312	ASN	OD1-CG-ND2	5.20	127.80	122.60
5	E	205	GLU	N-CA-CB	-5.19	102.47	110.16
10	J	658	GLN	O-C-N	5.19	127.42	122.07
10	J	788	ASP	N-CA-CB	5.19	117.85	110.16
6	F	83	ILE	CA-C-N	5.19	131.45	121.54
6	F	83	ILE	C-N-CA	5.19	131.45	121.54
7	G	211	ILE	N-CA-C	-5.19	105.48	110.72
9	I	8	PRO	N-CA-C	-5.19	102.44	111.32
7	G	138	ASP	N-CA-CB	5.19	118.88	110.42
3	C	19	PRO	N-CA-C	5.19	123.16	112.47
6	F	204	ILE	CA-C-O	-5.19	116.22	121.67
1	A	257	ASP	CA-C-N	5.19	127.23	120.28
1	A	257	ASP	C-N-CA	5.19	127.23	120.28
9	I	133	PRO	CB-CA-C	5.18	118.22	111.64
10	J	102	LEU	CB-CA-C	-5.18	102.74	110.88
10	J	639	VAL	CA-CB-CG1	5.18	119.21	110.40
4	D	4	GLN	OE1-CD-NE2	5.18	127.78	122.60
4	D	19	PHE	CA-CB-CG	-5.18	108.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	93	GLU	CB-CG-CD	-5.18	103.79	112.60
5	E	251	VAL	CA-C-N	5.18	127.22	120.28
5	E	251	VAL	C-N-CA	5.18	127.22	120.28
7	G	103	PRO	N-CA-CB	5.18	107.93	103.27
7	G	137	PHE	N-CA-C	-5.18	99.52	108.69
9	I	255	VAL	CA-C-O	-5.18	115.30	121.05
4	D	67	GLU	CA-CB-CG	5.18	124.46	114.10
4	D	7	ILE	CA-C-O	-5.18	116.23	121.67
5	E	195	ASN	CA-C-O	5.18	125.70	119.59
10	J	950	SER	N-CA-C	-5.18	106.27	112.59
6	F	128	SER	CA-C-O	5.18	124.75	119.05
6	F	195	GLU	CB-CG-CD	5.18	121.40	112.60
10	J	735	ASN	CB-CA-C	-5.18	101.88	110.68
7	G	131	GLU	CB-CA-C	-5.18	99.93	109.46
8	H	331	ASN	CA-C-N	5.18	129.13	120.64
8	H	331	ASN	C-N-CA	5.18	129.13	120.64
10	J	242	ASP	N-CA-C	-5.18	100.26	109.06
10	J	356	ASN	O-C-N	-5.18	116.42	123.15
10	J	836	VAL	CA-CB-CG1	-5.18	101.60	110.40
10	J	672	MET	CA-C-N	5.17	131.55	121.41
10	J	672	MET	C-N-CA	5.17	131.55	121.41
10	J	764	GLU	CA-C-N	5.17	127.77	120.42
10	J	764	GLU	C-N-CA	5.17	127.77	120.42
10	J	898	SER	N-CA-C	5.17	116.92	111.28
3	C	48	GLU	CA-C-O	-5.17	115.99	121.94
2	B	31	THR	N-CA-C	-5.17	106.21	112.88
4	D	22	GLN	CB-CG-CD	-5.17	103.81	112.60
6	F	65	ARG	CD-NE-CZ	-5.17	117.16	124.40
4	D	180	LEU	O-C-N	-5.17	116.42	123.24
4	D	161	HIS	CE1-NE2-CD2	-5.17	103.83	109.00
4	D	180	LEU	CA-C-N	5.17	130.62	123.07
4	D	180	LEU	C-N-CA	5.17	130.62	123.07
10	J	195	VAL	N-CA-C	-5.17	100.44	107.99
10	J	243	LYS	CA-C-N	5.17	128.13	120.17
10	J	243	LYS	C-N-CA	5.17	128.13	120.17
1	A	181	GLU	N-CA-C	5.17	116.60	111.07
3	C	276	CYS	CA-C-O	-5.17	115.12	120.70
5	E	222	ILE	CB-CA-C	-5.17	103.98	111.68
9	I	229	ILE	O-C-N	-5.17	116.64	122.94
10	J	371	ARG	N-CA-C	5.17	117.81	111.82
2	B	224	VAL	CA-C-O	-5.16	115.38	120.85
10	J	142	HIS	ND1-CE1-NE2	5.16	113.56	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	HIS	N-CA-C	-5.16	99.55	108.69
7	G	9	ASP	CA-CB-CG	-5.16	107.44	112.60
10	J	447	LYS	CA-C-O	-5.16	115.13	120.70
2	B	101	GLN	N-CA-CB	5.16	117.66	109.82
7	G	22	GLY	CA-C-O	-5.16	114.14	121.52
9	I	35	TYR	CA-C-N	5.16	128.95	121.68
9	I	35	TYR	C-N-CA	5.16	128.95	121.68
10	J	92	THR	CA-C-N	5.16	127.70	120.28
10	J	92	THR	C-N-CA	5.16	127.70	120.28
8	H	213	HIS	CG-CD2-NE2	5.15	112.35	107.20
10	J	83	ILE	O-C-N	5.15	126.96	121.91
10	J	678	LEU	CA-C-O	-5.15	114.28	120.10
11	P	49	ASN	CB-CA-C	-5.15	100.17	110.42
4	D	145	ILE	N-CA-C	5.15	116.32	109.37
8	H	8	THR	N-CA-CB	5.15	118.64	110.55
11	P	91	VAL	CA-CB-CG1	5.15	119.15	110.40
1	A	191	HIS	N-CA-CB	5.15	119.81	111.21
1	A	234	VAL	CA-C-N	5.15	130.03	122.77
1	A	234	VAL	C-N-CA	5.15	130.03	122.77
5	E	73	ASN	CB-CA-C	-5.15	100.90	109.75
10	J	946	GLU	CB-CA-C	-5.15	100.70	109.65
4	D	114	ASN	N-CA-C	5.14	116.97	111.36
1	A	66	GLN	OE1-CD-NE2	5.14	127.74	122.60
2	B	29	ILE	CA-C-N	5.14	131.36	121.54
2	B	29	ILE	C-N-CA	5.14	131.36	121.54
10	J	34	LYS	N-CA-CB	5.14	117.82	110.06
4	D	210	ARG	CA-C-N	5.14	127.58	120.29
4	D	210	ARG	C-N-CA	5.14	127.58	120.29
8	H	71	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
10	J	431	LEU	CA-C-N	5.14	126.26	119.84
10	J	431	LEU	C-N-CA	5.14	126.26	119.84
3	C	32	GLN	N-CA-C	5.13	116.88	111.28
5	E	218	SER	N-CA-CB	5.13	119.44	110.81
1	A	295	ALA	CA-C-N	5.13	127.16	120.28
1	A	295	ALA	C-N-CA	5.13	127.16	120.28
6	F	231	LYS	CB-CG-CD	5.13	123.11	111.30
9	I	156	LEU	N-CA-CB	-5.13	103.80	110.88
3	C	221	SER	CB-CA-C	-5.13	104.62	112.11
7	G	217	LYS	O-C-N	5.13	128.00	122.15
5	E	21	ILE	N-CA-CB	5.13	119.46	110.49
10	J	287	GLU	N-CA-CB	5.13	118.98	110.47
1	A	285	GLU	N-CA-CB	5.12	118.19	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	P	64	ARG	NE-CZ-NH1	-5.12	116.38	121.50
10	J	43	SER	CB-CA-C	-5.12	101.94	110.81
1	A	156	MET	CA-C-O	-5.12	114.99	120.42
2	B	92	LYS	N-CA-C	-5.12	107.54	112.97
10	J	177	THR	N-CA-CB	5.12	117.65	110.12
10	J	237	GLN	N-CA-C	5.12	116.94	111.36
6	F	188	VAL	N-CA-CB	5.12	117.12	110.57
10	J	45	ILE	CA-C-N	5.12	125.10	120.03
10	J	45	ILE	C-N-CA	5.12	125.10	120.03
11	P	60	GLU	CA-C-O	-5.12	115.12	120.55
8	H	125	LYS	N-CA-CB	5.12	118.60	110.57
1	A	191	HIS	CA-C-O	5.12	126.78	121.36
6	F	43	GLU	N-CA-CB	5.12	118.42	110.80
8	H	334	GLU	N-CA-C	-5.12	106.82	113.16
11	P	20	THR	CA-C-O	-5.12	113.19	120.51
2	B	65	MET	N-CA-CB	5.11	117.78	110.06
4	D	13	VAL	O-C-N	5.11	128.30	122.98
6	F	96	GLN	N-CA-C	-5.11	100.84	109.07
4	D	140	LYS	N-CA-C	-5.11	107.04	113.28
10	J	255	PHE	CA-CB-CG	-5.11	108.69	113.80
10	J	495	PHE	N-CA-C	5.11	117.84	110.28
1	A	148	ILE	CA-C-N	5.11	127.08	120.44
1	A	148	ILE	C-N-CA	5.11	127.08	120.44
1	A	299	SER	O-C-N	5.11	128.42	122.24
3	C	177	ARG	CA-C-N	5.11	130.20	123.00
3	C	177	ARG	C-N-CA	5.11	130.20	123.00
2	B	209	ARG	N-CA-C	-5.11	106.29	112.88
7	G	187	ALA	CA-C-O	-5.11	113.97	120.20
4	D	6	GLU	CA-C-O	-5.11	115.14	121.06
10	J	201	ASN	CA-C-O	-5.11	113.93	120.31
6	F	87	PHE	CA-C-N	5.10	131.00	122.73
6	F	87	PHE	C-N-CA	5.10	131.00	122.73
8	H	353	LYS	N-CA-CB	-5.10	102.61	110.01
10	J	342	ASN	CA-CB-CG	-5.10	107.50	112.60
10	J	578	LYS	CA-C-N	-5.10	114.73	120.14
10	J	578	LYS	C-N-CA	-5.10	114.73	120.14
3	C	96	ILE	N-CA-CB	5.10	118.97	111.52
3	C	39	ILE	N-CA-C	-5.10	101.04	108.99
3	C	370	THR	N-CA-C	-5.10	103.25	110.29
7	G	171	ASP	N-CA-CB	5.10	118.47	110.46
10	J	58	ILE	CA-C-O	-5.10	115.44	120.85
11	P	33	SER	N-CA-C	5.10	117.57	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	159	SER	CA-C-N	5.10	127.31	122.36
2	B	159	SER	C-N-CA	5.10	127.31	122.36
4	D	198	GLY	CA-C-O	5.10	126.00	120.75
7	G	54	THR	N-CA-C	-5.10	100.59	108.90
10	J	939	ILE	O-C-N	-5.10	117.14	123.10
11	P	84	GLU	CA-C-N	5.10	127.11	120.28
11	P	84	GLU	C-N-CA	5.10	127.11	120.28
6	F	85	GLY	N-CA-C	-5.10	108.29	115.32
5	E	15	LEU	CB-CA-C	-5.09	102.19	110.85
10	J	319	GLU	N-CA-C	-5.09	101.39	109.59
8	H	288	SER	CA-C-N	5.09	127.91	120.98
8	H	288	SER	C-N-CA	5.09	127.91	120.98
2	B	166	TYR	N-CA-C	-5.09	101.88	109.11
8	H	347	ASP	CA-CB-CG	-5.09	107.51	112.60
2	B	83	LYS	O-C-N	5.09	129.00	122.23
10	J	913	THR	O-C-N	-5.09	117.15	123.36
2	B	176	SER	N-CA-C	5.09	116.82	111.28
4	D	61	THR	CA-C-N	5.09	127.05	120.44
4	D	61	THR	C-N-CA	5.09	127.05	120.44
4	D	170	GLY	N-CA-C	-5.09	108.05	115.63
10	J	187	PRO	CA-C-O	-5.09	111.91	119.18
3	C	287	ASN	CA-CB-CG	5.08	117.69	112.60
4	D	51	ILE	N-CA-C	-5.08	100.75	108.17
5	E	36	ILE	CA-C-N	5.08	130.57	122.74
5	E	36	ILE	C-N-CA	5.08	130.57	122.74
1	A	143	CYS	O-C-N	5.08	129.36	123.41
6	F	81	ARG	CD-NE-CZ	5.08	131.51	124.40
8	H	95	LEU	N-CA-C	-5.08	101.47	109.25
10	J	567	GLY	N-CA-C	-5.08	102.57	111.46
10	J	992	SER	N-CA-C	-5.08	105.78	112.94
10	J	318	VAL	CA-CB-CG2	5.08	119.03	110.40
11	P	15	LYS	CA-C-O	5.08	125.93	120.55
10	J	555	HIS	CB-CG-ND1	5.08	130.31	122.70
3	C	370	THR	CA-CB-CG2	-5.07	101.88	110.50
8	H	318	ARG	CG-CD-NE	-5.07	100.84	112.00
4	D	144	ASP	CA-CB-CG	5.07	117.67	112.60
9	I	271	ASP	CA-CB-CG	-5.07	107.53	112.60
3	C	356	ASN	CA-C-N	5.07	130.94	122.73
3	C	356	ASN	C-N-CA	5.07	130.94	122.73
1	A	57	HIS	CG-CD2-NE2	5.07	112.27	107.20
4	D	49	GLU	N-CA-C	-5.07	99.04	107.80
7	G	181	HIS	ND1-CE1-NE2	5.07	113.47	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	385	LYS	N-CA-CB	5.06	119.05	110.49
10	J	681	SER	N-CA-C	5.06	116.80	111.28
10	J	164	GLU	O-C-N	-5.06	117.58	122.99
10	J	82	PRO	CA-C-N	5.06	126.94	120.56
10	J	82	PRO	C-N-CA	5.06	126.94	120.56
10	J	476	SER	CA-C-N	5.06	127.06	120.28
10	J	476	SER	C-N-CA	5.06	127.06	120.28
7	G	19	VAL	CA-CB-CG1	-5.06	101.80	110.40
8	H	294	ARG	CA-C-N	5.06	127.06	120.28
8	H	294	ARG	C-N-CA	5.06	127.06	120.28
11	P	67	PRO	CA-C-O	-5.06	111.91	119.34
10	J	828	ASP	CA-CB-CG	-5.06	107.54	112.60
10	J	906	VAL	CB-CA-C	5.06	119.20	112.22
3	C	177	ARG	N-CA-C	-5.05	100.17	108.41
5	E	175	TYR	CA-C-N	5.05	127.95	120.82
5	E	175	TYR	C-N-CA	5.05	127.95	120.82
6	F	187	LEU	CA-C-N	5.05	127.03	120.56
6	F	187	LEU	C-N-CA	5.05	127.03	120.56
8	H	77	ASP	N-CA-CB	5.05	119.03	110.49
8	H	353	LYS	CA-C-O	-5.05	115.51	120.82
10	J	181	TYR	CA-C-N	5.05	127.05	120.28
10	J	181	TYR	C-N-CA	5.05	127.05	120.28
10	J	375	LYS	CA-C-N	5.05	127.01	120.44
10	J	375	LYS	C-N-CA	5.05	127.01	120.44
5	E	248	LEU	CA-C-N	5.05	127.05	120.28
5	E	248	LEU	C-N-CA	5.05	127.05	120.28
10	J	137	ARG	CB-CA-C	-5.05	102.26	110.85
5	E	69	HIS	O-C-N	5.05	128.30	122.19
7	G	203	ASN	CA-C-N	5.05	127.05	120.28
7	G	203	ASN	C-N-CA	5.05	127.05	120.28
3	C	380	LEU	CA-C-N	5.05	127.46	120.29
3	C	380	LEU	C-N-CA	5.05	127.46	120.29
10	J	362	THR	CA-C-N	5.05	131.19	121.54
10	J	362	THR	C-N-CA	5.05	131.19	121.54
10	J	720	LEU	N-CA-C	-5.05	101.87	109.85
7	G	228	LYS	CA-C-O	-5.05	115.07	120.42
10	J	479	ALA	N-CA-CB	5.05	117.63	110.16
7	G	31	THR	N-CA-CB	5.04	117.71	110.20
10	J	995	LYS	CG-CD-CE	5.04	122.90	111.30
2	B	164	GLY	O-C-N	-5.04	119.16	123.80
2	B	233	ARG	CA-C-O	-5.04	113.84	119.79
4	D	136	ILE	CA-CB-CG1	5.04	118.97	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	132	LEU	CB-CA-C	-5.04	101.37	109.08
9	I	238	GLY	CA-C-N	5.04	131.17	121.54
9	I	238	GLY	C-N-CA	5.04	131.17	121.54
10	J	308	ASN	CA-C-O	-5.04	115.40	121.40
10	J	615	LEU	N-CA-C	-5.04	102.61	109.71
3	C	184	THR	CA-CB-OG1	5.04	117.16	109.60
9	I	286	ARG	NH1-CZ-NH2	-5.04	112.75	119.30
1	A	95	ASN	CA-C-N	5.03	131.03	121.97
1	A	95	ASN	C-N-CA	5.03	131.03	121.97
9	I	287	LYS	N-CA-C	-5.03	101.49	109.59
10	J	232	ARG	N-CA-C	-5.03	100.84	109.24
1	A	33	PHE	CA-C-N	5.03	128.34	120.75
1	A	33	PHE	C-N-CA	5.03	128.34	120.75
11	P	60	GLU	O-C-N	5.03	127.45	122.12
10	J	172	ARG	CB-CA-C	-5.03	102.31	110.85
10	J	600	ARG	CB-CA-C	5.03	118.91	109.71
10	J	730	PHE	N-CA-CB	5.03	117.96	110.22
5	E	34	ILE	CB-CA-C	-5.03	103.66	110.90
2	B	108	PHE	CA-C-N	5.02	127.26	120.38
2	B	108	PHE	C-N-CA	5.02	127.26	120.38
3	C	292	ALA	CA-C-O	-5.02	115.75	121.68
6	F	48	LEU	CA-C-O	-5.02	115.48	121.56
10	J	271	GLY	CA-C-N	-5.02	115.83	122.16
10	J	271	GLY	C-N-CA	-5.02	115.83	122.16
3	C	139	GLY	CA-C-O	5.02	124.38	118.96
3	C	283	PRO	CB-CA-C	-5.02	102.33	110.21
11	P	92	PRO	O-C-N	5.02	128.96	122.24
6	F	114	SER	CA-C-N	5.02	127.41	120.29
6	F	114	SER	C-N-CA	5.02	127.41	120.29
1	A	53	ASN	CB-CA-C	-5.01	99.83	110.31
10	J	842	PHE	CB-CA-C	5.01	117.94	110.62
8	H	231	ILE	N-CA-C	-5.01	100.85	108.17
9	I	69	GLU	O-C-N	5.01	127.85	122.34
7	G	168	PHE	CA-CB-CG	-5.01	108.79	113.80
10	J	10	ARG	O-C-N	-5.01	116.74	122.95
1	A	150	ALA	CA-C-N	5.01	126.99	120.28
1	A	150	ALA	C-N-CA	5.01	126.99	120.28
6	F	106	ASN	CA-CB-CG	-5.01	107.59	112.60
6	F	130	TYR	CA-C-N	5.01	125.02	120.21
6	F	130	TYR	C-N-CA	5.01	125.02	120.21
2	B	96	ARG	CA-C-O	5.01	125.86	120.55
10	J	922	PHE	N-CA-C	-5.01	102.48	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	322	ALA	O-C-N	5.01	127.43	122.12
10	J	743	TYR	CB-CG-CD1	5.00	128.31	120.80
10	J	851	ASP	CA-C-N	5.00	127.53	120.42
10	J	851	ASP	C-N-CA	5.00	127.53	120.42
1	A	86	MET	CG-SD-CE	-5.00	89.89	100.90
8	H	67	TRP	CE2-CD2-CE3	5.00	123.80	118.80
2	B	11	GLY	CA-C-N	5.00	131.32	122.67
2	B	11	GLY	C-N-CA	5.00	131.32	122.67
4	D	215	ASP	CA-CB-CG	-5.00	107.60	112.60
5	E	52	ALA	CA-C-N	5.00	129.89	121.14
5	E	52	ALA	C-N-CA	5.00	129.89	121.14
7	G	73	ILE	CB-CA-C	-5.00	103.21	110.81

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	TYR	Sidechain
1	A	303	ARG	Sidechain
1	A	44	PHE	Sidechain
2	B	106	ARG	Sidechain
2	B	155	PHE	Sidechain
2	B	225	ARG	Sidechain
2	B	23	ARG	Sidechain
2	B	3	ARG	Sidechain
2	B	41	TYR	Sidechain
2	B	96	ARG	Sidechain
3	C	127	TYR	Sidechain
3	C	131	TYR	Sidechain
3	C	222	ARG	Sidechain
3	C	236	TYR	Sidechain
3	C	256	ARG	Sidechain
3	C	269	ARG	Sidechain
3	C	382	ARG	Sidechain
3	C	40	ARG	Sidechain
3	C	44	ARG	Sidechain
3	C	46	TYR	Sidechain
4	D	36	PRO	Peptide
4	D	71	ARG	Sidechain
5	E	12	TYR	Sidechain
5	E	175	TYR	Sidechain
5	E	22	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	E	40	PHE	Sidechain
6	F	138	PHE	Sidechain
6	F	140	TYR	Sidechain
6	F	20	PHE	Sidechain
6	F	222	ASP	Peptide
6	F	84	ARG	Sidechain
7	G	120	TYR	Sidechain
7	G	143	ARG	Sidechain
7	G	147	PHE	Sidechain
7	G	231	PHE	Sidechain
7	G	26	TYR	Sidechain
7	G	35	ARG	Sidechain
7	G	59	TYR	Sidechain
8	H	10	ARG	Sidechain
8	H	104	TYR	Sidechain
8	H	209	ARG	Sidechain
8	H	294	ARG	Sidechain
8	H	71	HIS	Sidechain
9	I	21	TYR	Sidechain
9	I	215	ARG	Sidechain
9	I	217	ARG	Sidechain
9	I	244	TYR	Sidechain
9	I	46	TYR	Sidechain
9	I	51	ARG	Sidechain
10	J	109	PHE	Sidechain
10	J	12	ARG	Sidechain
10	J	133	ARG	Sidechain
10	J	137	ARG	Sidechain
10	J	175	ARG	Sidechain
10	J	221	TYR	Sidechain
10	J	247	ARG	Sidechain
10	J	250	PHE	Sidechain
10	J	26	ARG	Sidechain
10	J	37	ARG	Sidechain
10	J	50	ARG	Sidechain
10	J	595	TYR	Sidechain
10	J	600	ARG	Sidechain
10	J	633	SER	Peptide
10	J	660	ARG	Sidechain
10	J	675	ARG	Sidechain
10	J	72	LEU	Peptide
10	J	740	ARG	Sidechain

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Mol	Chain	Res	Type	Group
10	J	773	ARG	Sidechain
10	J	800	TYR	Sidechain
10	J	806	ARG	Sidechain
10	J	818	TYR	Sidechain
10	J	830	ARG	Sidechain
10	J	832	TYR	Sidechain
10	J	865	GLU	Peptide
10	J	889	ARG	Sidechain
11	P	4	PHE	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2350	0	2345	6	0
2	B	1890	0	1943	7	0
3	C	2622	0	2688	25	0
4	D	1707	0	1766	4	0
5	E	2048	0	2079	4	0
6	F	1627	0	1607	51	0
7	G	1831	0	1829	2	0
8	H	2277	0	2283	9	0
9	I	1750	0	1755	46	0
10	J	7942	0	7947	13	0
11	P	750	0	759	113	0
All	All	26794	0	27001	164	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 3.

All (164) 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)
6:F:49:HIS:NE2	11:P:36:LYS:HD2	1.28	1.43
3:C:51:ASP:CB	11:P:47:PRO:HD3	1.49	1.41
9:I:250:ASN:OD1	11:P:86:LEU:CD1	1.71	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:LYS:HE2	11:P:35:LYS:CB	1.45	1.38
6:F:52:PHE:CD2	11:P:32:LEU:HD22	1.61	1.34
3:C:51:ASP:HB2	11:P:47:PRO:CD	1.56	1.33
3:C:81:LYS:CE	11:P:35:LYS:HB3	1.65	1.27
9:I:272:TRP:CZ3	11:P:86:LEU:HD21	1.72	1.24
6:F:52:PHE:CE2	11:P:32:LEU:HD22	1.76	1.21
9:I:250:ASN:CG	11:P:86:LEU:CD1	2.17	1.18
6:F:61:LEU:HD22	11:P:32:LEU:HD13	1.23	1.15
9:I:250:ASN:ND2	11:P:86:LEU:HD13	1.63	1.14
9:I:272:TRP:CD1	11:P:82:LYS:HE2	1.80	1.13
6:F:49:HIS:NE2	11:P:36:LYS:CD	2.12	1.12
9:I:272:TRP:HZ3	11:P:86:LEU:HD21	0.96	1.10
9:I:250:ASN:OD1	11:P:86:LEU:HD11	0.92	1.10
6:F:52:PHE:CE2	11:P:32:LEU:CD2	2.38	1.06
9:I:250:ASN:CG	11:P:86:LEU:HD13	1.82	1.04
6:F:239:ASP:CG	11:P:19:SER:HA	1.82	1.03
9:I:272:TRP:CD1	11:P:82:LYS:CE	2.27	1.02
9:I:272:TRP:CZ3	11:P:86:LEU:CD2	2.42	1.02
6:F:238:ARG:HD3	11:P:18:LEU:CD2	1.89	1.01
6:F:206:ASN:OD1	11:P:18:LEU:HD22	1.62	0.99
9:I:250:ASN:CG	11:P:86:LEU:HD11	1.84	0.98
3:C:37:LEU:HD13	11:P:61:ASN:HD22	1.26	0.98
9:I:291:PRO:HD2	11:P:79:PHE:HE2	1.30	0.96
6:F:239:ASP:HB3	11:P:19:SER:O	1.65	0.95
6:F:61:LEU:HD22	11:P:32:LEU:CD1	1.95	0.95
6:F:239:ASP:CB	11:P:19:SER:HA	1.96	0.95
6:F:52:PHE:CD2	11:P:32:LEU:CD2	2.49	0.95
6:F:239:ASP:OD1	11:P:19:SER:HA	1.67	0.94
9:I:48:HIS:CD2	11:P:11:ILE:HD11	2.03	0.93
9:I:19:PRO:HB3	11:P:8:ASN:HD21	1.35	0.91
9:I:272:TRP:HZ3	11:P:86:LEU:CD2	1.78	0.90
6:F:52:PHE:HE2	11:P:32:LEU:CD2	1.84	0.90
6:F:239:ASP:OD2	11:P:18:LEU:O	1.94	0.85
6:F:239:ASP:CG	11:P:18:LEU:O	2.20	0.85
9:I:291:PRO:HB2	11:P:73:SER:HB2	1.59	0.84
6:F:52:PHE:HE2	11:P:32:LEU:HD21	1.43	0.84
6:F:52:PHE:HD2	11:P:32:LEU:HD22	1.39	0.83
6:F:238:ARG:HD3	11:P:18:LEU:HD21	1.60	0.83
6:F:238:ARG:HD3	11:P:18:LEU:HD23	1.61	0.82
6:F:238:ARG:NH1	11:P:18:LEU:HD23	1.94	0.82
3:C:37:LEU:HD13	11:P:61:ASN:ND2	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:206:ASN:OD1	11:P:18:LEU:CD2	2.27	0.81
6:F:239:ASP:CG	11:P:19:SER:CA	2.53	0.81
6:F:239:ASP:OD1	11:P:18:LEU:C	2.24	0.81
9:I:250:ASN:HD21	11:P:86:LEU:HD13	1.43	0.80
9:I:19:PRO:HB3	11:P:8:ASN:ND2	1.97	0.78
6:F:238:ARG:CD	11:P:18:LEU:HD21	2.14	0.77
6:F:239:ASP:HB3	11:P:19:SER:C	2.08	0.77
6:F:61:LEU:CD2	11:P:32:LEU:CD1	2.62	0.77
6:F:239:ASP:HB3	11:P:19:SER:CA	2.16	0.76
3:C:48:GLU:HB3	11:P:49:ASN:ND2	1.86	0.76
3:C:81:LYS:HE2	11:P:35:LYS:HB3	0.78	0.75
6:F:239:ASP:OD1	11:P:19:SER:N	2.20	0.75
3:C:81:LYS:HB3	11:P:35:LYS:NZ	2.02	0.75
6:F:61:LEU:CD2	11:P:32:LEU:HD13	2.10	0.75
9:I:291:PRO:HD2	11:P:79:PHE:CE2	2.20	0.74
9:I:272:TRP:HB3	11:P:82:LYS:HE3	1.66	0.74
6:F:239:ASP:HB3	11:P:19:SER:HA	1.69	0.74
3:C:51:ASP:OD2	11:P:47:PRO:HB3	1.87	0.74
6:F:239:ASP:OD1	11:P:19:SER:CA	2.34	0.73
6:F:238:ARG:CD	11:P:18:LEU:CD2	2.65	0.73
3:C:51:ASP:CG	11:P:47:PRO:HD3	2.15	0.71
9:I:16:LEU:HG	11:P:15:LYS:NZ	2.06	0.71
6:F:238:ARG:HH11	11:P:18:LEU:HD23	1.56	0.71
9:I:291:PRO:HG2	11:P:73:SER:O	1.90	0.70
2:B:42:MET:HE3	2:B:44:GLN:HB2	1.74	0.70
10:J:831:HIS:CD2	10:J:836:VAL:HG23	2.26	0.70
6:F:239:ASP:CB	11:P:19:SER:CA	2.70	0.69
3:C:37:LEU:CD1	11:P:61:ASN:HD22	2.03	0.68
10:J:991:THR:HG22	10:J:992:SER:H	1.59	0.67
6:F:239:ASP:CB	11:P:19:SER:O	2.42	0.65
9:I:15:LYS:NZ	11:P:16:ASN:HD21	1.97	0.63
10:J:628:TRP:HB3	10:J:639:VAL:HG23	1.80	0.63
6:F:239:ASP:CG	11:P:18:LEU:C	2.68	0.61
10:J:694:LEU:HD23	10:J:694:LEU:H	1.66	0.61
9:I:254:VAL:HG12	9:I:275:MET:HE1	1.83	0.60
9:I:272:TRP:CH2	11:P:86:LEU:HD23	2.36	0.60
6:F:49:HIS:CD2	11:P:36:LYS:HD2	2.28	0.60
6:F:61:LEU:CD2	11:P:32:LEU:HD12	2.32	0.60
3:C:81:LYS:HB3	11:P:35:LYS:HZ1	1.65	0.59
6:F:49:HIS:CE1	11:P:36:LYS:HB2	2.39	0.58
9:I:272:TRP:CB	11:P:82:LYS:HE3	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:67:TRP:CD2	8:H:95:LEU:HD12	2.38	0.57
3:C:11:GLU:HG2	11:P:79:PHE:HD2	1.69	0.56
9:I:15:LYS:CE	11:P:16:ASN:ND2	2.68	0.56
6:F:238:ARG:CZ	11:P:18:LEU:HD23	2.35	0.56
3:C:81:LYS:CE	11:P:35:LYS:CB	2.39	0.56
9:I:19:PRO:CB	11:P:8:ASN:HD21	2.12	0.56
9:I:272:TRP:CH2	11:P:86:LEU:CD2	2.88	0.56
3:C:51:ASP:HB2	11:P:47:PRO:HD3	0.67	0.56
6:F:61:LEU:HD21	11:P:32:LEU:HD12	1.88	0.55
8:H:128:ILE:H	8:H:128:ILE:HD13	1.70	0.55
5:E:21:ILE:HD13	5:E:21:ILE:H	1.72	0.54
2:B:79:THR:HG21	5:E:129:LEU:HD22	1.91	0.53
9:I:19:PRO:CB	11:P:8:ASN:ND2	2.71	0.53
3:C:81:LYS:HB3	11:P:35:LYS:HZ2	1.74	0.53
9:I:16:LEU:HD12	11:P:11:ILE:CG2	2.39	0.53
6:F:242:ILE:HD13	11:P:19:SER:OG	2.08	0.52
9:I:16:LEU:CD1	11:P:11:ILE:HG21	2.39	0.52
6:F:49:HIS:HE1	11:P:36:LYS:HB2	1.75	0.51
10:J:573:VAL:HG21	10:J:845:PRO:HB2	1.93	0.51
10:J:869:LEU:HA	10:J:872:ARG:HE	1.76	0.50
1:A:86:MET:HE1	1:A:141:LEU:HD12	1.94	0.50
9:I:15:LYS:HD2	11:P:15:LYS:HE3	1.93	0.50
6:F:236:ARG:HH12	11:P:22:ILE:HD12	1.77	0.49
1:A:34:ARG:HH21	1:A:51:MET:HE3	1.77	0.49
6:F:238:ARG:CD	11:P:18:LEU:HD23	2.35	0.49
9:I:272:TRP:NE1	11:P:82:LYS:CE	2.70	0.49
9:I:15:LYS:NZ	11:P:16:ASN:ND2	2.61	0.48
8:H:145:GLY:HA3	8:H:150:ARG:HG2	1.95	0.48
5:E:154:LEU:HD11	5:E:180:LEU:HD13	1.94	0.48
10:J:856:ARG:HB2	10:J:871:HIS:CE1	2.48	0.47
3:C:263:GLY:HA2	3:C:264:ARG:HB2	1.96	0.47
7:G:99:TYR:CD2	7:G:111:PRO:HD2	2.50	0.47
2:B:108:PHE:CE1	2:B:158:ILE:HD12	2.50	0.47
9:I:16:LEU:HD12	11:P:11:ILE:HG22	1.97	0.47
1:A:12:SER:HA	1:A:230:LEU:HD21	1.97	0.47
9:I:16:LEU:HG	11:P:15:LYS:CE	2.44	0.46
8:H:107:GLU:HA	8:H:176:LEU:HD22	1.98	0.46
6:F:239:ASP:CB	11:P:19:SER:C	2.85	0.46
9:I:16:LEU:HD11	11:P:11:ILE:HG21	1.98	0.46
7:G:224:LYS:HD2	7:G:224:LYS:H	1.81	0.46
9:I:272:TRP:CZ3	11:P:86:LEU:HD23	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:424:VAL:HG21	10:J:451:ILE:HG21	1.97	0.45
8:H:106:PRO:HB2	8:H:176:LEU:HD13	1.98	0.45
4:D:50:ILE:HB	4:D:67:GLU:HG3	1.98	0.45
11:P:59:ILE:HA	11:P:62:PHE:CD2	2.51	0.45
3:C:48:GLU:CB	11:P:49:ASN:ND2	2.66	0.45
3:C:39:ILE:HD12	3:C:43:LEU:HA	1.99	0.45
6:F:102:LEU:O	6:F:102:LEU:HG	2.17	0.45
9:I:272:TRP:NE1	11:P:82:LYS:HE2	2.26	0.45
6:F:52:PHE:CE2	11:P:32:LEU:HD21	2.24	0.44
11:P:20:THR:HG22	11:P:21:SER:H	1.82	0.44
3:C:81:LYS:CB	11:P:35:LYS:NZ	2.75	0.44
8:H:160:ARG:HH12	9:I:240:GLY:H	1.63	0.44
3:C:87:VAL:HG22	3:C:219:VAL:HG22	2.00	0.44
1:A:303:ARG:HH22	10:J:715:VAL:HG13	1.83	0.43
8:H:62:THR:HG21	8:H:68:MET:SD	2.58	0.43
9:I:16:LEU:HG	11:P:15:LYS:HE2	2.00	0.43
4:D:46:LEU:HD23	4:D:78:ILE:HG21	2.00	0.43
9:I:46:TYR:HB2	9:I:53:LEU:HB3	2.00	0.43
3:C:51:ASP:OD2	11:P:47:PRO:CB	2.62	0.42
9:I:143:VAL:HG22	9:I:153:VAL:HG12	2.00	0.42
10:J:408:ALA:HA	10:J:425:ILE:HD11	2.00	0.42
1:A:120:VAL:HA	1:A:123:LEU:HG	2.02	0.42
1:A:179:VAL:HG12	1:A:184:PRO:HB3	2.01	0.42
2:B:171:LEU:HD12	2:B:182:MET:HE1	2.02	0.42
3:C:269:ARG:HG2	3:C:270:GLU:H	1.85	0.42
5:E:255:ALA:HB3	5:E:256:PRO:HD3	2.02	0.42
8:H:213:HIS:CE1	8:H:316:GLN:HE21	2.38	0.41
2:B:20:ASN:H	2:B:20:ASN:HD22	1.68	0.41
2:B:169:THR:HG23	10:J:63:ALA:CB	2.50	0.41
10:J:451:ILE:C	10:J:451:ILE:HD12	2.46	0.41
4:D:202:CYS:O	4:D:206:VAL:HG23	2.20	0.41
8:H:214:THR:HG23	8:H:224:VAL:HA	2.02	0.41
10:J:91:ASP:HB2	10:J:196:THR:HA	2.03	0.41
3:C:24:ARG:HG3	9:I:156:LEU:HB3	2.03	0.41
6:F:52:PHE:HD2	11:P:32:LEU:CD2	2.12	0.40
2:B:156:ASP:HB2	2:B:190:VAL:HG22	2.03	0.40
9:I:15:LYS:HE2	11:P:16:ASN:ND2	2.37	0.40
4:D:28:CYS:HB2	4:D:115:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/305 (98%)	278 (93%)	18 (6%)	4 (1%)	9	41
2	B	238/246 (97%)	223 (94%)	11 (5%)	4 (2%)	7	35
3	C	327/394 (83%)	294 (90%)	22 (7%)	11 (3%)	3	21
4	D	221/223 (99%)	211 (96%)	9 (4%)	1 (0%)	24	62
5	E	263/265 (99%)	248 (94%)	10 (4%)	5 (2%)	6	32
6	F	205/250 (82%)	194 (95%)	8 (4%)	3 (2%)	8	38
7	G	234/240 (98%)	219 (94%)	14 (6%)	1 (0%)	30	66
8	H	287/359 (80%)	263 (92%)	15 (5%)	9 (3%)	3	23
9	I	219/292 (75%)	200 (91%)	14 (6%)	5 (2%)	5	29
10	J	991/1001 (99%)	905 (91%)	68 (7%)	18 (2%)	6	33
11	P	93/747 (12%)	82 (88%)	9 (10%)	2 (2%)	5	29
All	All	3378/4322 (78%)	3117 (92%)	198 (6%)	63 (2%)	8	32

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	251	ALA
3	C	10	ILE
3	C	11	GLU
3	C	12	ILE
3	C	143	ALA
3	C	191	ASP
5	E	182	ILE
6	F	55	ASN
6	F	80	PRO
8	H	54	ILE
8	H	148	LEU
10	J	238	MET
10	J	838	ILE

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Mol	Chain	Res	Type
10	J	966	ASN
3	C	73	ASN
3	C	353	PRO
5	E	29	HIS
5	E	166	VAL
6	F	84	ARG
8	H	92	ASN
8	H	147	ILE
9	I	4	ASN
10	J	385	LYS
10	J	508	HIS
10	J	634	ALA
1	A	117	ALA
2	B	35	ALA
2	B	167	ASP
5	E	112	SER
5	E	134	HIS
8	H	77	ASP
9	I	217	ARG
9	I	251	ASP
10	J	150	ASN
10	J	833	GLY
11	P	53	THR
1	A	242	ASN
3	C	190	PRO
3	C	359	GLN
7	G	145	ALA
8	H	122	LYS
8	H	151	LYS
8	H	187	ARG
8	H	277	SER
9	I	215	ARG
10	J	107	CYS
10	J	246	GLU
10	J	363	THR
10	J	507	GLY
10	J	605	PRO
11	P	20	THR
3	C	8	GLU
3	C	366	GLY
9	I	212	SER
10	J	228	ALA

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Mol	Chain	Res	Type
10	J	364	VAL
10	J	844	SER
1	A	96	ILE
2	B	93	ASN
2	B	33	PRO
10	J	322	PRO
4	D	135	PRO
10	J	432	PRO

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	263/266 (99%)	260 (99%)	3 (1%)	65	73
2	B	214/218 (98%)	206 (96%)	8 (4%)	30	51
3	C	294/349 (84%)	283 (96%)	11 (4%)	30	51
4	D	197/197 (100%)	194 (98%)	3 (2%)	57	70
5	E	240/240 (100%)	231 (96%)	9 (4%)	29	51
6	F	181/219 (83%)	175 (97%)	6 (3%)	33	55
7	G	205/209 (98%)	197 (96%)	8 (4%)	28	50
8	H	252/311 (81%)	247 (98%)	5 (2%)	48	65
9	I	190/240 (79%)	186 (98%)	4 (2%)	47	65
10	J	895/901 (99%)	862 (96%)	33 (4%)	30	51
11	P	89/702 (13%)	88 (99%)	1 (1%)	65	73
All	All	3020/3852 (78%)	2929 (97%)	91 (3%)	37	57

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	A	96	ILE
1	A	167	ILE

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Mol	Chain	Res	Type
2	B	20	ASN
2	B	34	HIS
2	B	124	ILE
2	B	173	ASP
2	B	180	ASN
2	B	187	LEU
2	B	192	LYS
2	B	225	ARG
3	C	10	ILE
3	C	24	ARG
3	C	58	THR
3	C	80	LEU
3	C	88	ILE
3	C	159	ILE
3	C	212	VAL
3	C	274	ILE
3	C	275	ILE
3	C	289	LYS
3	C	349	ILE
4	D	9	ILE
4	D	136	ILE
4	D	193	SER
5	E	21	ILE
5	E	54	ASP
5	E	66	VAL
5	E	76	LEU
5	E	86	ARG
5	E	90	LEU
5	E	232	ASN
5	E	253	LYS
5	E	259	VAL
6	F	43	GLU
6	F	52	PHE
6	F	80	PRO
6	F	175	SER
6	F	188	VAL
6	F	189	ASP
7	G	29	PRO
7	G	68	VAL
7	G	96	SER
7	G	99	TYR
7	G	108	LYS

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Mol	Chain	Res	Type
7	G	119	VAL
7	G	152	ASP
7	G	234	ILE
8	H	80	THR
8	H	128	ILE
8	H	207	ILE
8	H	225	LEU
8	H	312	ILE
9	I	52	THR
9	I	53	LEU
9	I	161	LYS
9	I	215	ARG
10	J	68	PRO
10	J	72	LEU
10	J	107	CYS
10	J	135	LEU
10	J	137	ARG
10	J	140	ASP
10	J	208	GLU
10	J	251	SER
10	J	254	THR
10	J	294	ARG
10	J	364	VAL
10	J	366	SER
10	J	421	ASN
10	J	422	VAL
10	J	486	LEU
10	J	570	ILE
10	J	602	ASP
10	J	628	TRP
10	J	642	MET
10	J	671	THR
10	J	694	LEU
10	J	709	THR
10	J	713	ASN
10	J	817	GLN
10	J	820	TYR
10	J	830	ARG
10	J	841	HIS
10	J	870	THR
10	J	902	TYR
10	J	935	VAL

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Mol	Chain	Res	Type
10	J	959	LYS
10	J	993	LYS
10	J	1001	LYS
11	P	46	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	66	GLN
1	A	90	GLN
1	A	93	ASN
1	A	161	HIS
1	A	291	ASN
2	B	20	ASN
2	B	32	HIS
2	B	34	HIS
2	B	127	HIS
2	B	212	ASN
2	B	242	ASN
3	C	56	ASN
3	C	57	ASN
3	C	78	ASN
3	C	278	GLN
3	C	287	ASN
3	C	356	ASN
4	D	45	GLN
5	E	29	HIS
5	E	77	GLN
5	E	173	HIS
5	E	232	ASN
5	E	235	ASN
6	F	70	GLN
6	F	96	GLN
6	F	99	ASN
6	F	171	HIS
6	F	235	ASN
7	G	38	ASN
7	G	104	ASN
7	G	170	ASN
7	G	230	GLN
8	H	121	ASN

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Mol	Chain	Res	Type
8	H	142	ASN
8	H	185	HIS
8	H	196	ASN
8	H	201	GLN
8	H	302	ASN
8	H	316	GLN
8	H	357	ASN
9	I	25	ASN
10	J	150	ASN
10	J	155	HIS
10	J	163	ASN
10	J	179	GLN
10	J	184	HIS
10	J	212	ASN
10	J	237	GLN
10	J	306	ASN
10	J	308	ASN
10	J	369	GLN
10	J	421	ASN
10	J	555	HIS
10	J	704	HIS
10	J	724	ASN
10	J	755	HIS
10	J	771	ASN
10	J	831	HIS
10	J	841	HIS
10	J	871	HIS
10	J	890	ASN
10	J	909	ASN
11	P	8	ASN
11	P	16	ASN
11	P	37	HIS
11	P	61	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

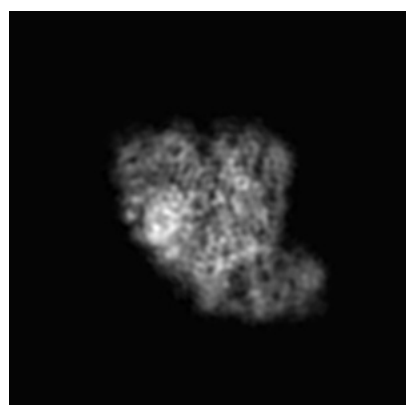
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3366. These allow visual inspection of the internal detail of the map and identification of artifacts.

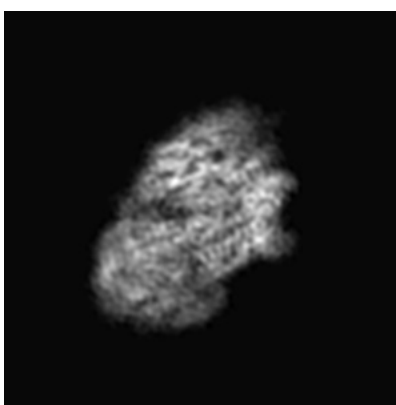
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

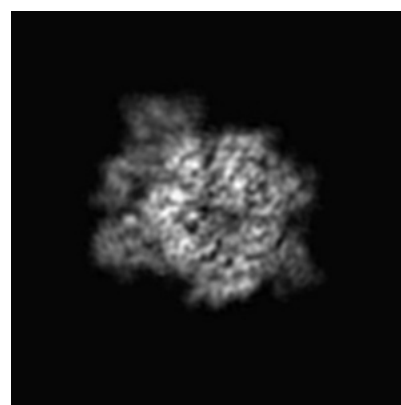
6.1.1 Primary map



X



Y

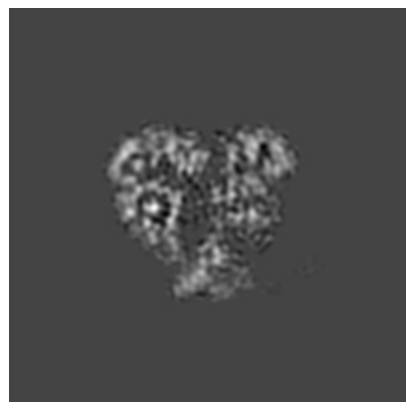


Z

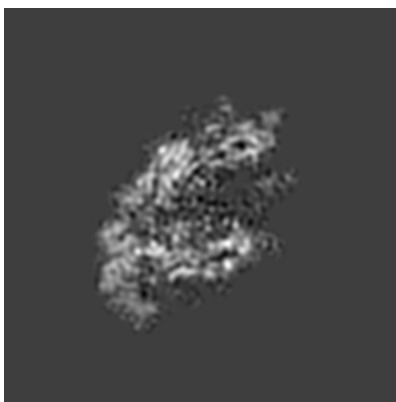
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

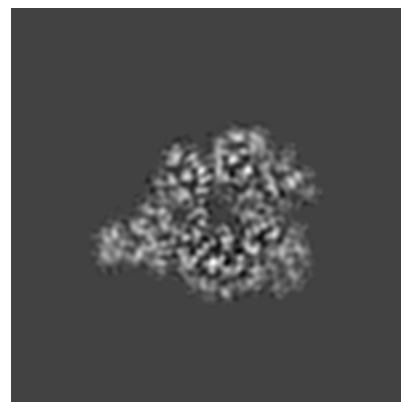
6.2.1 Primary map



X Index: 90



Y Index: 90

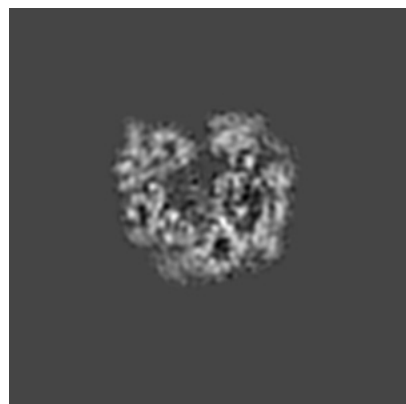


Z Index: 90

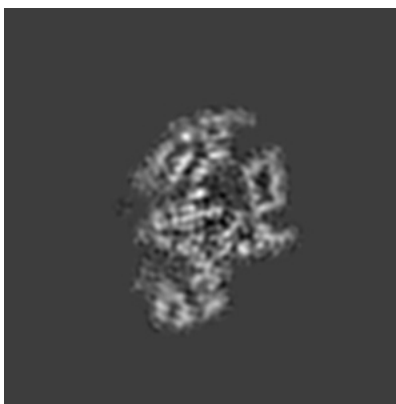
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

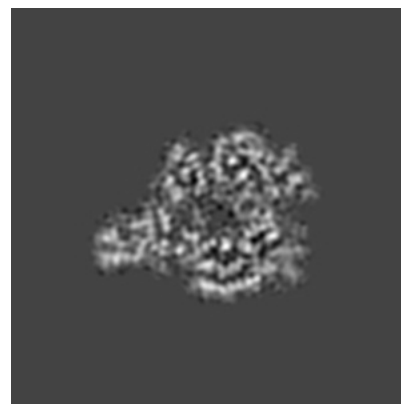
6.3.1 Primary map



X Index: 103



Y Index: 72

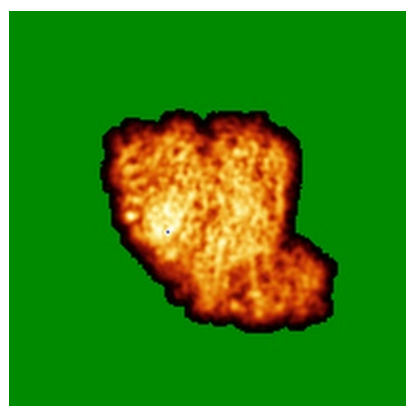


Z Index: 88

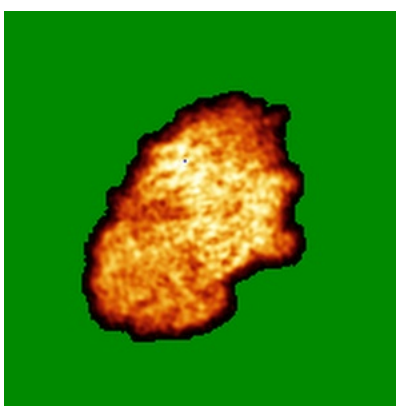
The images above show the largest variance slices of the map in three orthogonal directions.

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

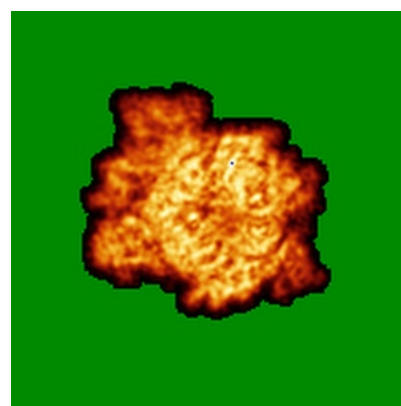
6.4.1 Primary map



X



Y

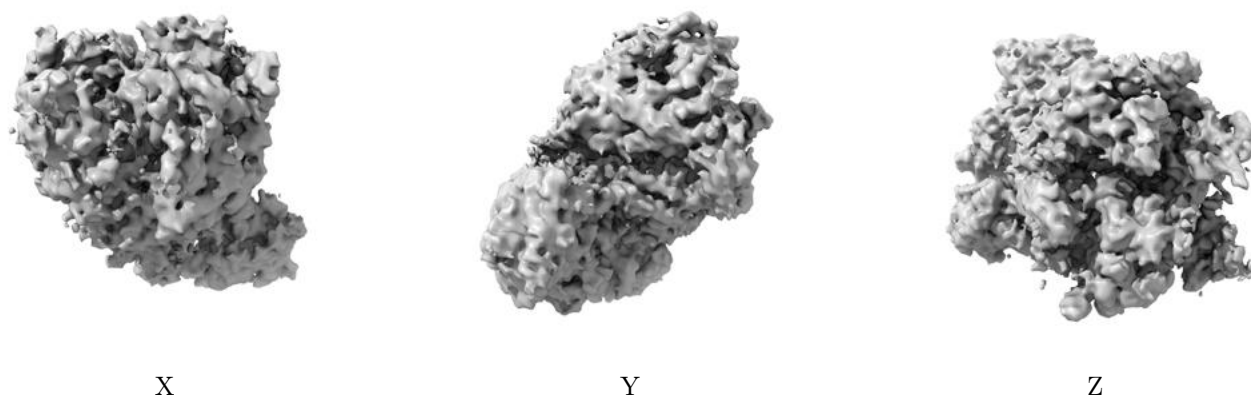


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

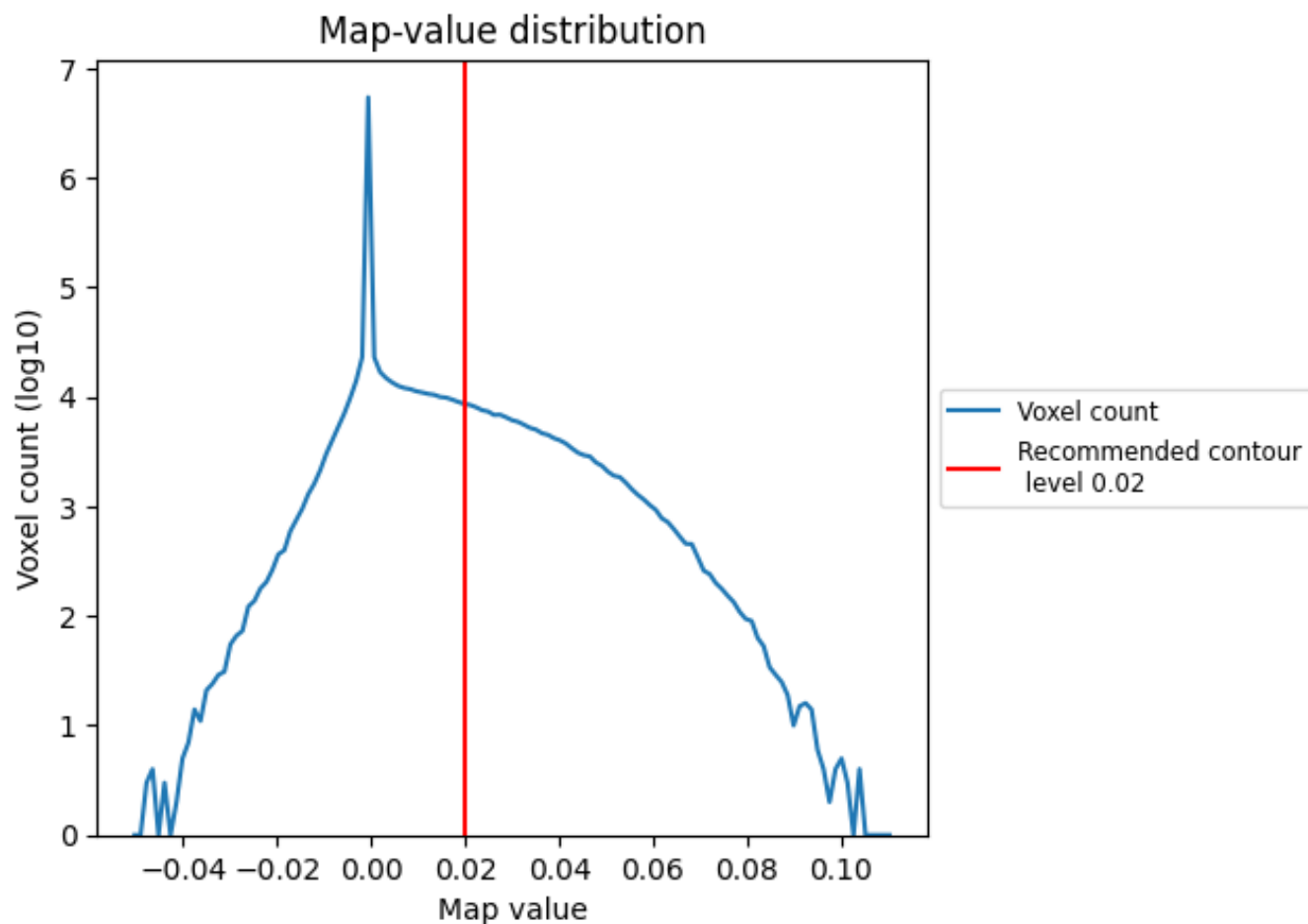
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

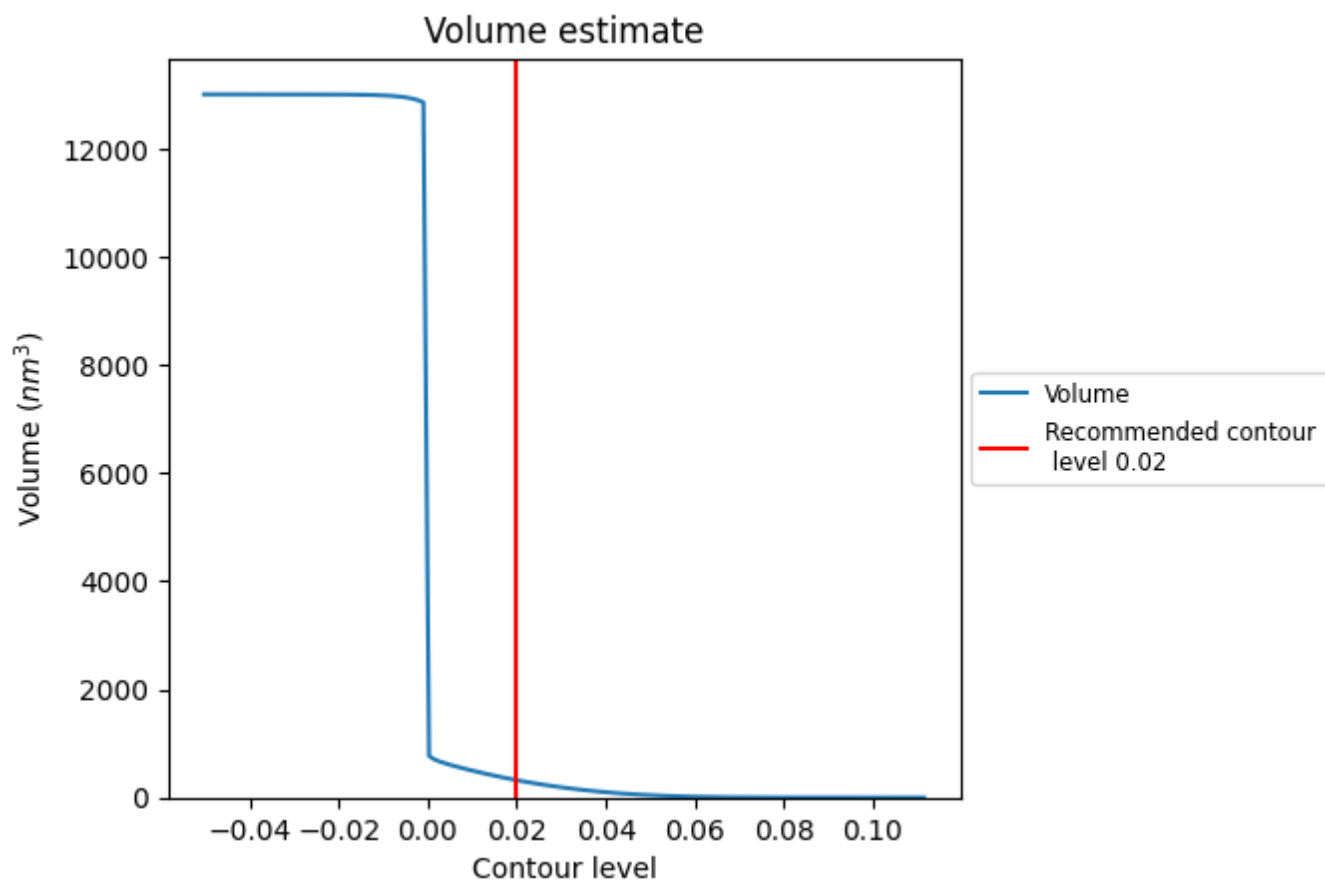
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

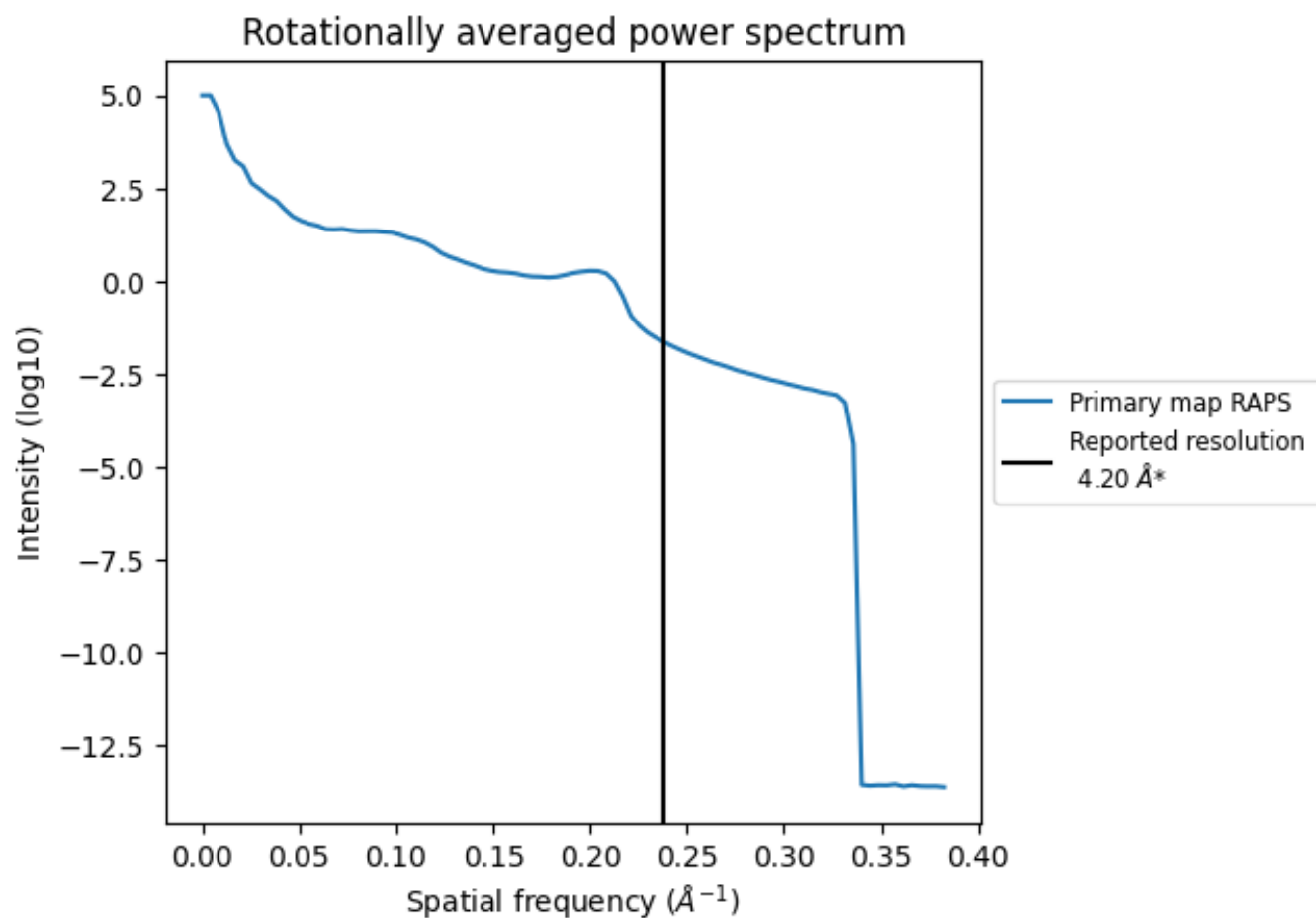
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 321 nm^3 ; this corresponds to an approximate mass of 290 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 0.238 Å⁻¹

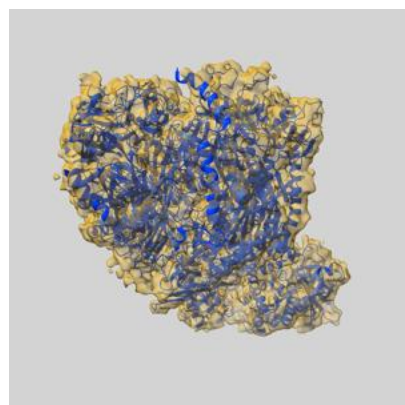
8 Fourier-Shell correlation ⓘ

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

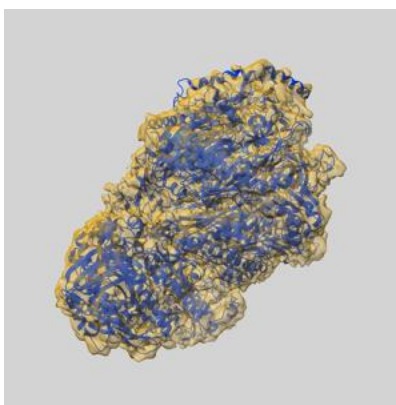
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3366 and PDB model 5G06. Per-residue inclusion information can be found in section [3](#) on page [7](#).

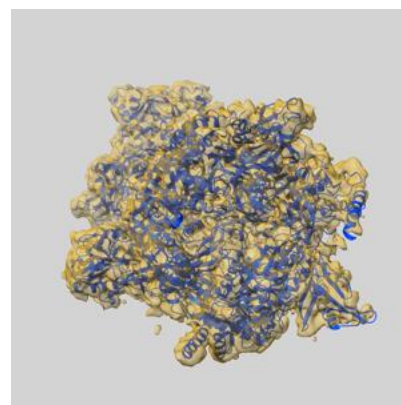
9.1 Map-model overlay [i](#)



X



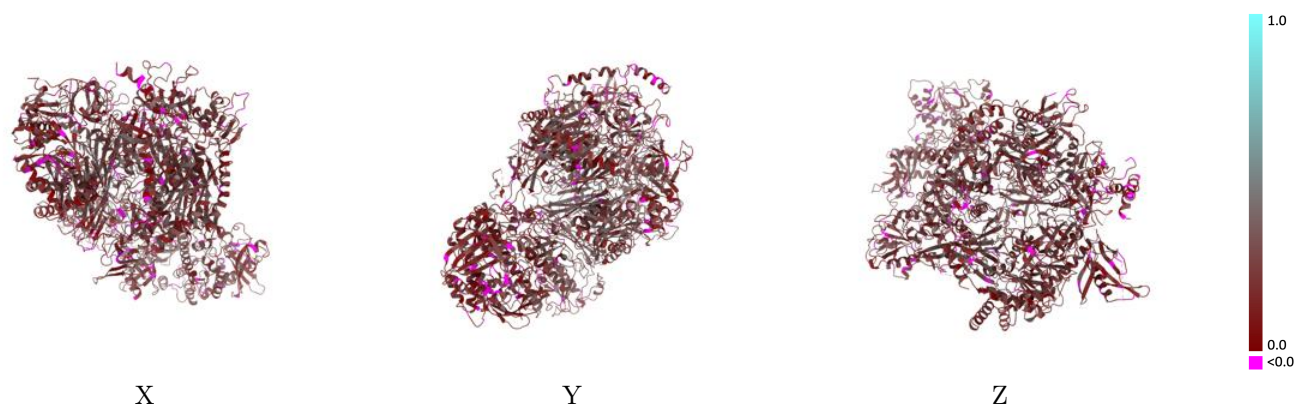
Y



Z

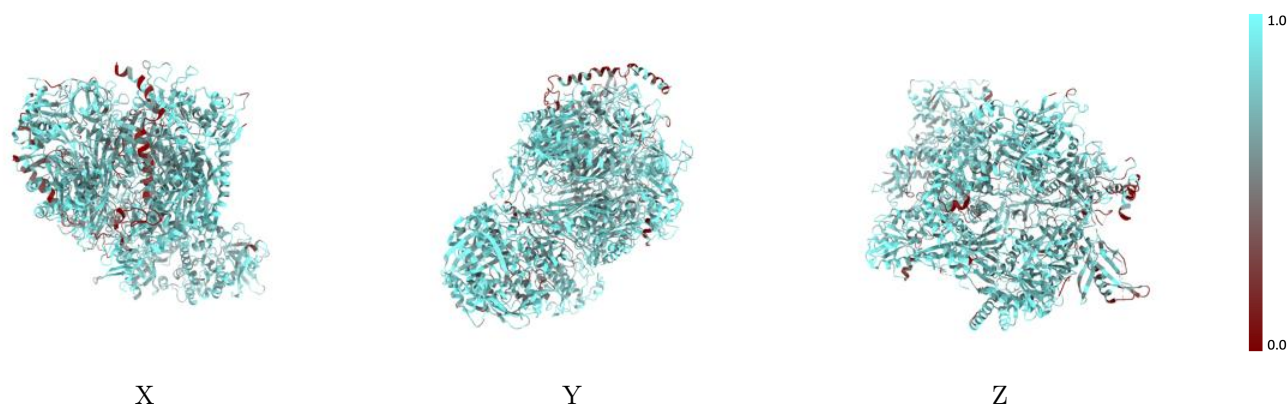
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



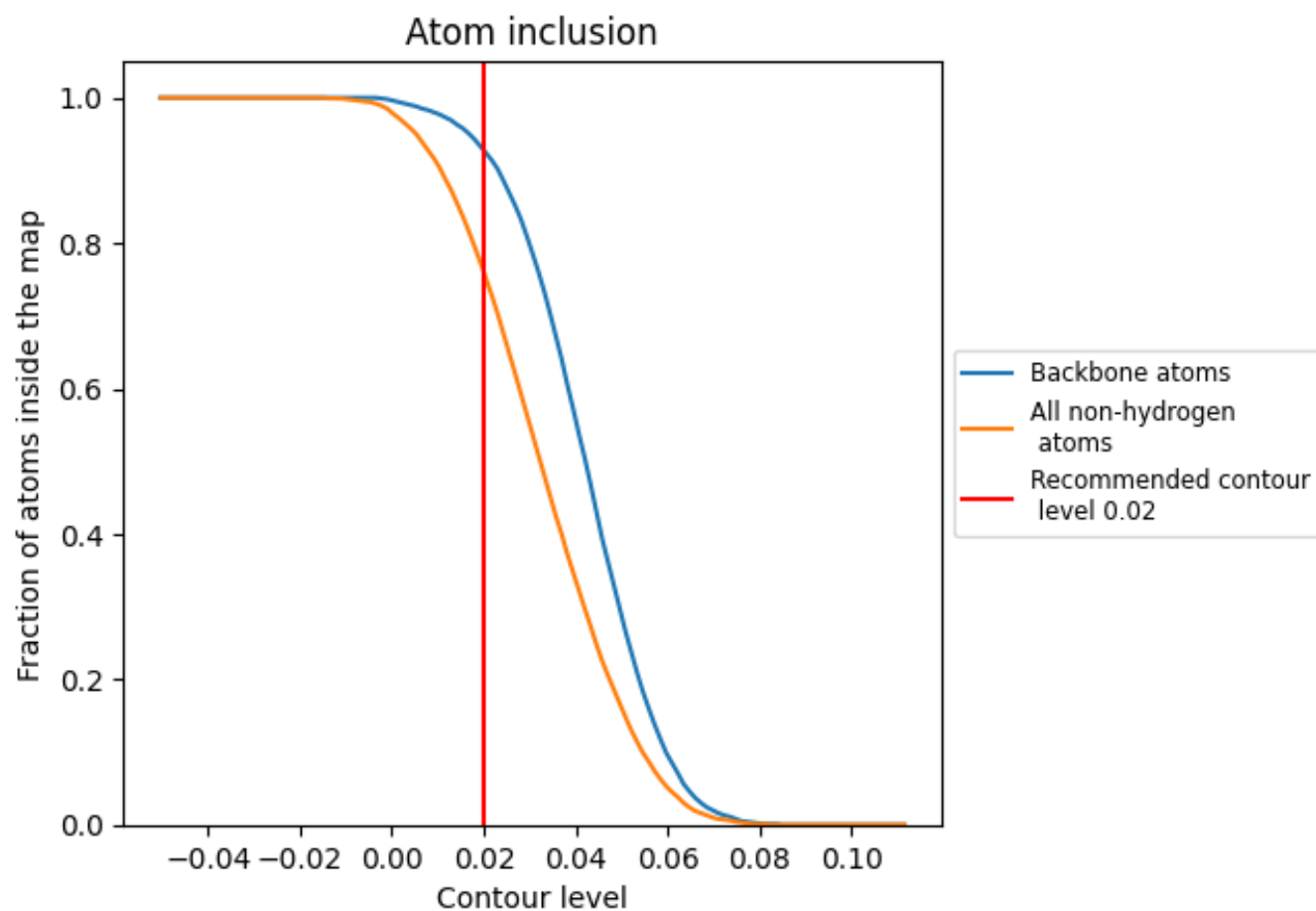
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 76% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7610	 0.2210
A	 0.7730	 0.2500
B	 0.7970	 0.2640
C	 0.7610	 0.2210
D	 0.7870	 0.2500
E	 0.7830	 0.2560
F	 0.7890	 0.2430
G	 0.8120	 0.2240
H	 0.7980	 0.2180
I	 0.6840	 0.1960
J	 0.7690	 0.1990
P	 0.3070	 0.1120

