



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 07:24 PM UTC

PDB ID : 6EQC / pdb_00006eqc
EMDB ID : EMD-3821
Title : Cryo-EM reconstruction of a complex of a binding protein and human adenovirus C5 hexon
Authors : Schmid, M.; Ernst, P.; Honegger, A.; Suomalainen, M.; Zimmermann, M.; Braun, L.; Stauffer, S.; Thom, C.; Dreier, B.; Eibauer, M.; Kipar, A.; Vogel, V.; Greber, U.F.; Medalia, O.; Plueckthun, A.
Deposited on : 2017-10-12
Resolution : 7.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

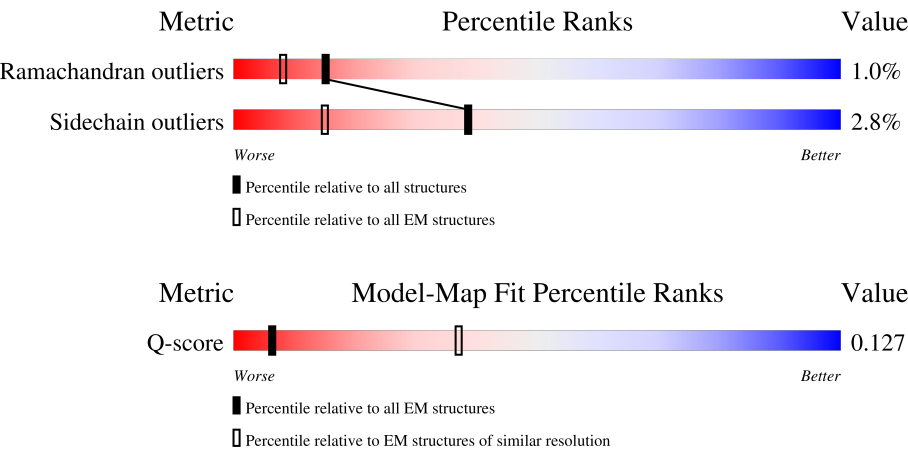
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 7.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	412 (6.90 - 7.90)

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

Mol	Chain	Length	Quality of chain
1	A	952	48% 45% . .
1	B	952	51% 43% . .
1	C	952	51% 42% . .
2	D	254	54% 34% . 8%
2	E	254	47% 43% . 8%

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Mol	Chain	Length	Quality of chain
2	F	254	48% 41% 8%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 53964 atoms, of which 26442 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 Hexon protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	921	Total	C	H	N	O	S	0	0
			14445	4686	7070	1250	1404	35		
1	B	921	Total	C	H	N	O	S	0	0
			14445	4686	7070	1250	1404	35		
1	C	921	Total	C	H	N	O	S	0	0
			14445	4686	7070	1250	1404	35		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	ALA	THR	conflict	UNP P04133
A	420	GLY	ILE	conflict	UNP P04133
A	422	ASN	THR	conflict	UNP P04133
A	423	SER	GLU	conflict	UNP P04133
A	425	TYR	LEU	conflict	UNP P04133
B	272	ALA	THR	conflict	UNP P04133
B	420	GLY	ILE	conflict	UNP P04133
B	422	ASN	THR	conflict	UNP P04133
B	423	SER	GLU	conflict	UNP P04133
B	425	TYR	LEU	conflict	UNP P04133
C	272	ALA	THR	conflict	UNP P04133
C	420	GLY	ILE	conflict	UNP P04133
C	422	ASN	THR	conflict	UNP P04133
C	423	SER	GLU	conflict	UNP P04133
C	425	TYR	LEU	conflict	UNP P04133

- Molecule 2 is a protein called scFv of 9C12 antibody.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	233	Total	C	H	N	O	S	0	0
			3543	1130	1744	306	356	7		
2	E	233	Total	C	H	N	O	S	0	0
			3543	1130	1744	306	356	7		

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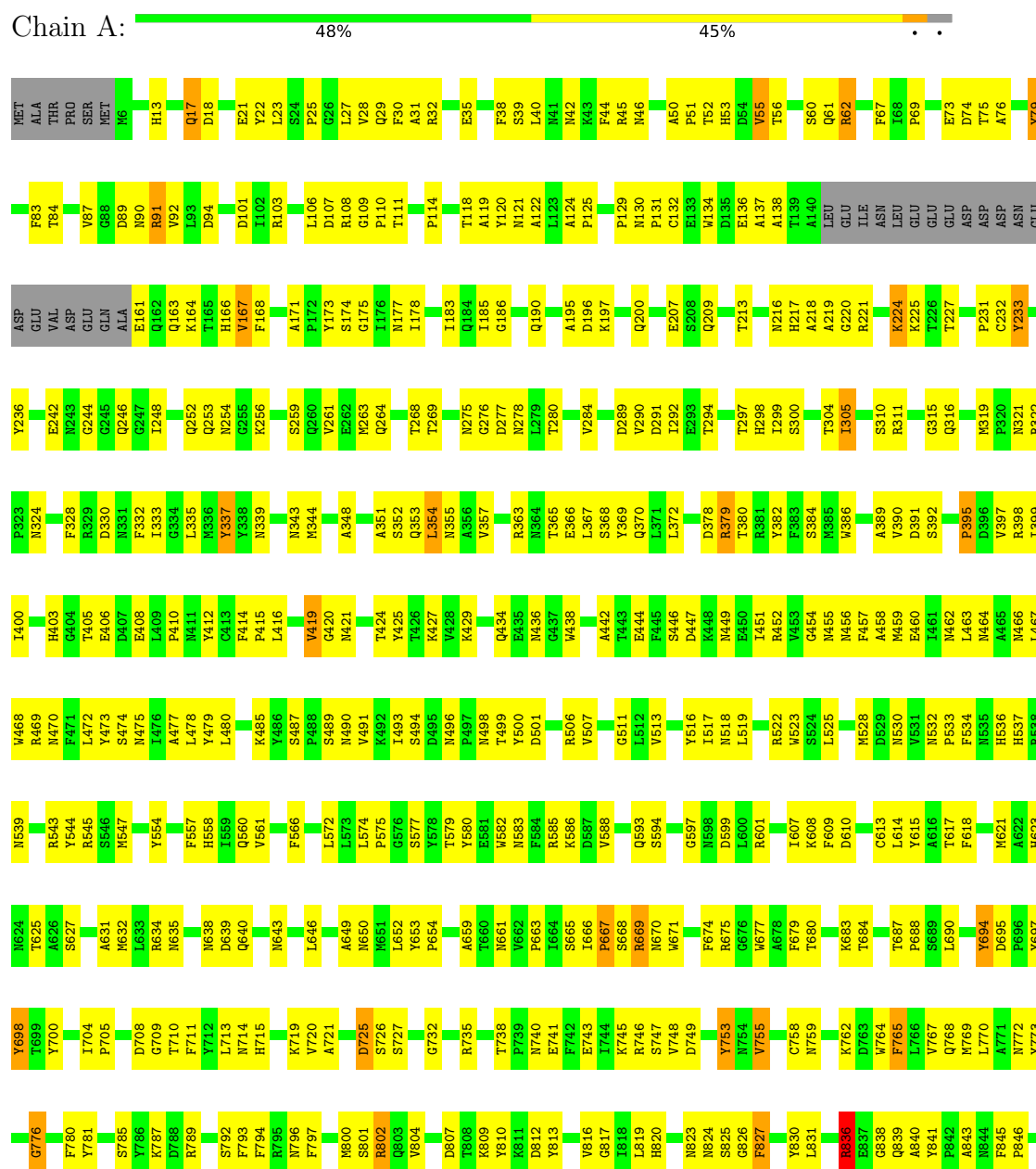
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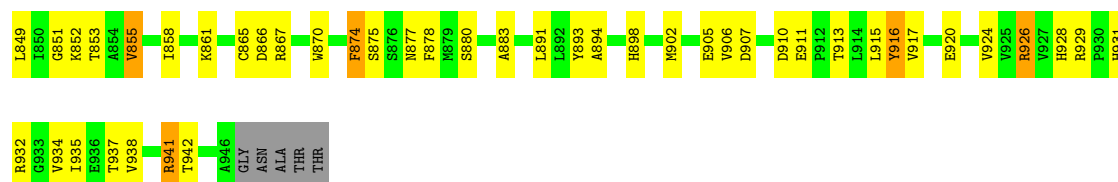
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	F	233	3543	1130	1744	306	356	7	0	0

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: Hexon protein



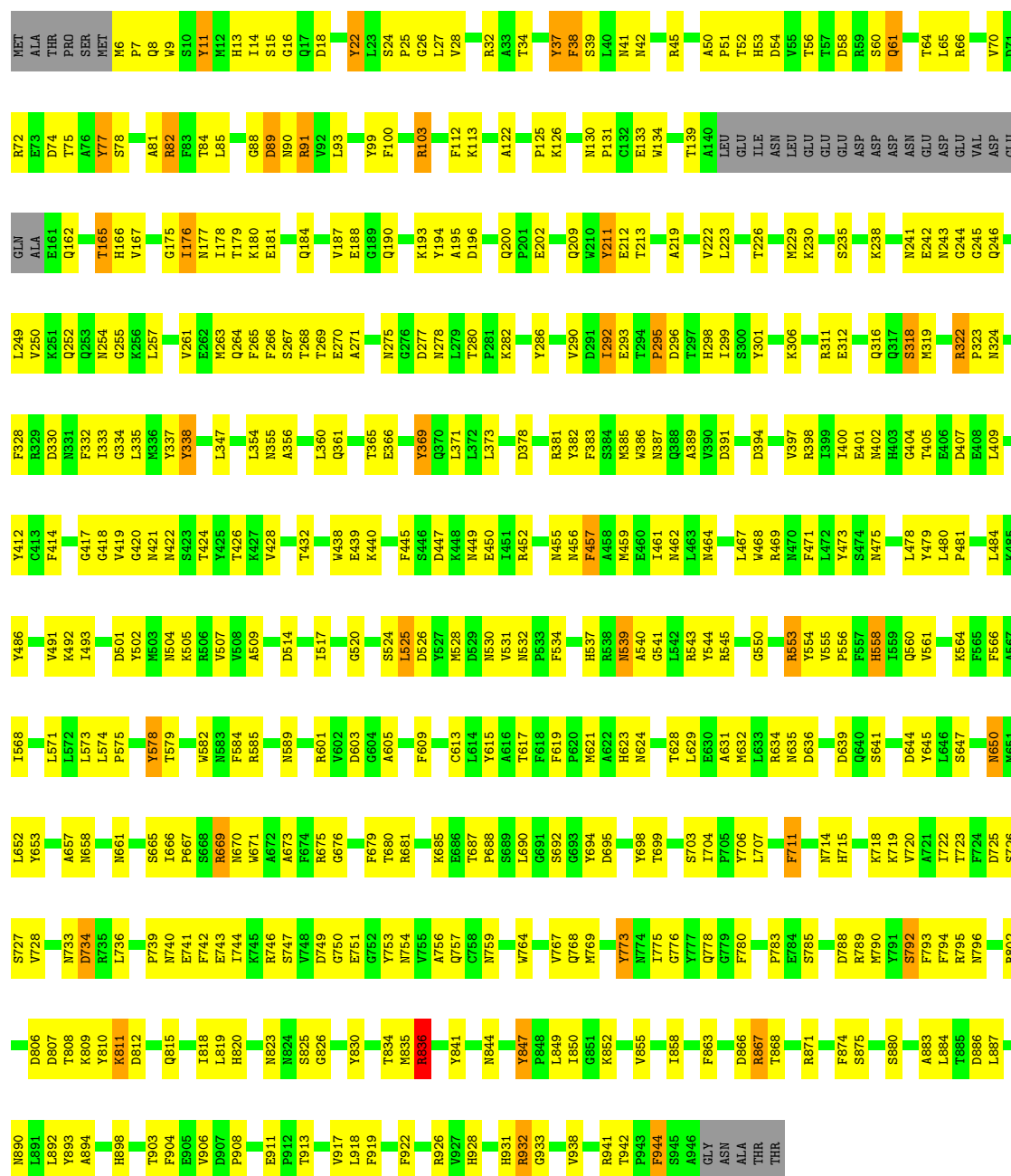


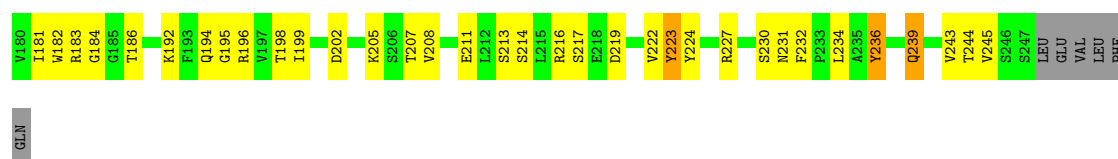
• Molecule 1: Hexon protein

Chain B:

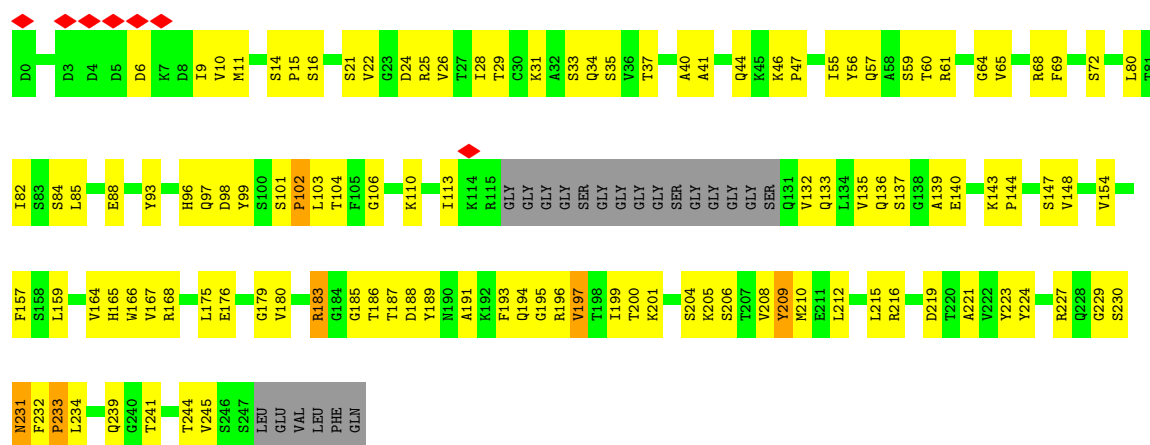
• Molecule 1: Hexon protein

Chain C:  51% 42%

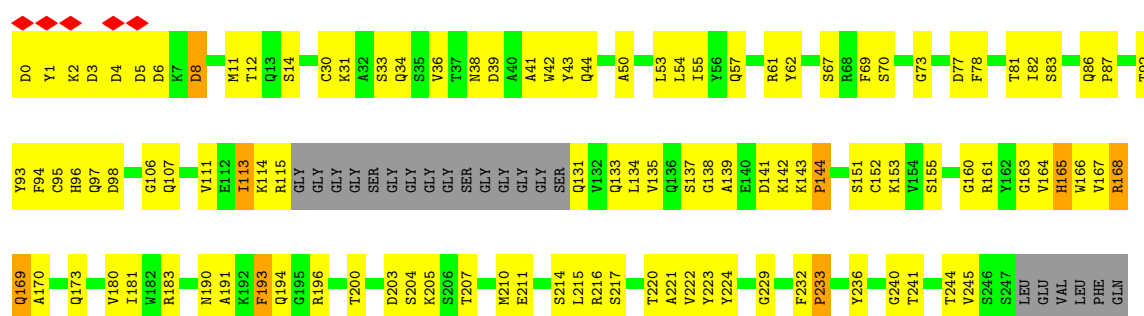




- Molecule 2: scFv of 9C12 antibody



- Molecule 2: scFv of 9C12 antibody



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1880	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.014	Depositor
Map size ($\text{\AA}$)	1568.0, 1568.0, 1568.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.96, 1.96, 1.96	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	2.15	234/7574 (3.1%)	2.39	465/10299 (4.5%)
1	B	2.12	207/7574 (2.7%)	2.35	421/10299 (4.1%)
1	C	2.14	214/7574 (2.8%)	2.32	388/10299 (3.8%)
2	D	2.20	61/1839 (3.3%)	2.23	81/2490 (3.3%)
2	E	2.20	56/1839 (3.0%)	2.36	112/2490 (4.5%)
2	F	2.22	57/1839 (3.1%)	2.33	98/2490 (3.9%)
All	All	2.15	829/28239 (2.9%)	2.34	1565/38367 (4.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	26
1	B	0	28
1	C	0	33
2	D	0	10
2	E	0	6
2	F	0	4
All	All	0	107

All (829) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	GLY	CA-C	12.08	1.65	1.51
1	A	715	HIS	ND1-CE1	11.70	1.44	1.32
1	C	680	THR	CA-C	11.28	1.67	1.52
2	E	11	MET	CA-CB	11.16	1.67	1.53
1	A	84	THR	CA-C	-10.35	1.40	1.52
1	C	560	GLN	C-N	10.15	1.40	1.33
1	A	53	HIS	CA-C	-9.73	1.40	1.52
1	C	704	ILE	CA-C	9.66	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	187	THR	CA-C	-9.25	1.40	1.52
1	C	112	PHE	CA-C	9.23	1.64	1.52
1	B	655	ILE	N-CA	9.17	1.53	1.46
1	C	561	VAL	N-CA	9.09	1.54	1.46
1	C	855	VAL	CA-C	9.04	1.64	1.52
1	C	188	GLU	CA-C	-9.00	1.42	1.53
1	B	702	GLY	N-CA	8.90	1.55	1.45
2	F	39	ASP	CA-C	8.83	1.63	1.53
1	A	163	GLN	CA-C	8.75	1.63	1.52
1	C	585	ARG	CD-NE	8.72	1.58	1.46
2	F	169	GLN	CA-C	-8.72	1.42	1.52
1	B	292	ILE	CA-CB	8.60	1.62	1.54
2	F	207	THR	N-CA	8.48	1.56	1.46
1	C	229	MET	C-N	8.47	1.43	1.33
1	A	343	ASN	CA-CB	8.43	1.64	1.53
1	A	496	ASN	CA-C	8.41	1.61	1.52
1	C	880	SER	CA-CB	8.38	1.63	1.52
1	A	632	MET	CA-C	8.26	1.63	1.52
2	D	59	SER	CA-C	8.19	1.63	1.52
1	C	219	ALA	CA-C	8.08	1.62	1.52
1	A	506	ARG	C-N	8.05	1.43	1.33
2	E	40	ALA	N-CA	-8.02	1.36	1.46
2	E	159	LEU	CA-C	8.02	1.63	1.52
1	B	480	LEU	N-CA	8.01	1.56	1.45
2	D	194	GLN	CA-CB	7.99	1.66	1.53
2	D	131	GLN	N-CA	7.97	1.61	1.46
1	C	24	SER	CA-CB	7.95	1.64	1.53
1	A	669	ARG	CA-C	-7.91	1.43	1.52
1	B	388	GLN	C-N	7.86	1.44	1.33
1	B	413	CYS	N-CA	7.85	1.55	1.46
1	C	213	THR	CA-C	-7.84	1.43	1.52
1	C	66	ARG	CD-NE	7.82	1.57	1.46
1	A	883	ALA	N-CA	-7.79	1.36	1.46
1	A	770	LEU	CA-CB	7.78	1.65	1.53
2	D	54	LEU	CA-CB	-7.77	1.41	1.53
1	C	440	LYS	N-CA	7.75	1.55	1.46
1	A	55	VAL	CA-CB	7.71	1.65	1.54
1	B	681	ARG	N-CA	-7.70	1.36	1.46
1	C	428	VAL	N-CA	-7.69	1.37	1.46
1	C	311	ARG	CA-CB	7.68	1.65	1.53
1	B	570	ASN	CA-C	7.68	1.63	1.52
1	C	694	TYR	C-N	7.67	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	86	GLN	C-N	7.66	1.41	1.33
2	F	114	LYS	CA-C	7.62	1.62	1.52
2	F	152	CYS	CA-CB	7.61	1.62	1.52
1	A	916	TYR	CA-CB	7.60	1.63	1.53
1	B	168	PHE	C-N	7.59	1.41	1.33
1	B	931	HIS	ND1-CE1	7.58	1.40	1.32
1	A	617	THR	N-CA	7.56	1.55	1.46
1	C	196	ASP	CA-CB	7.55	1.62	1.53
1	A	747	SER	N-CA	7.52	1.56	1.46
1	A	175	GLY	CA-C	-7.50	1.43	1.52
1	C	412	TYR	CA-C	7.50	1.61	1.52
1	C	397	VAL	C-N	7.49	1.43	1.33
2	D	65	VAL	CA-C	-7.48	1.46	1.52
1	C	645	TYR	CA-C	7.43	1.62	1.52
1	B	609	PHE	CA-CB	7.43	1.63	1.53
1	A	659	ALA	CA-CB	7.42	1.62	1.53
1	B	844	ASN	C-N	7.41	1.42	1.33
1	B	50	ALA	CA-C	7.41	1.61	1.53
1	C	269	THR	CA-C	7.41	1.62	1.52
1	A	277	ASP	C-N	7.41	1.43	1.33
1	B	217	HIS	ND1-CE1	7.41	1.40	1.32
1	B	199	PHE	CA-CB	7.39	1.64	1.54
1	B	549	LEU	CA-C	7.38	1.62	1.52
2	E	80	LEU	N-CA	-7.37	1.37	1.46
1	A	28	VAL	CA-CB	7.36	1.63	1.54
1	A	442	ALA	CA-C	7.35	1.62	1.53
1	A	475	ASN	CA-CB	7.35	1.65	1.53
2	E	244	THR	C-N	7.33	1.43	1.33
1	B	651	MET	CA-C	-7.32	1.43	1.52
1	B	275	ASN	CA-CB	7.32	1.64	1.53
1	B	730	TRP	NE1-CE2	-7.32	1.29	1.37
1	C	792	SER	CA-C	-7.31	1.43	1.52
1	A	410	PRO	CA-C	7.30	1.60	1.52
1	C	64	THR	CA-C	7.30	1.61	1.52
1	C	573	LEU	CA-CB	7.30	1.62	1.53
2	D	208	VAL	N-CA	-7.30	1.37	1.46
1	C	631	ALA	N-CA	-7.30	1.37	1.46
2	F	106	GLY	CA-C	-7.29	1.42	1.51
1	B	708	ASP	C-N	7.28	1.43	1.33
2	E	209	TYR	C-N	7.27	1.43	1.33
2	E	25	ARG	CD-NE	7.27	1.56	1.46
1	A	720	VAL	CA-C	7.26	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	745	LYS	CA-C	7.25	1.61	1.52
1	B	798	GLN	CA-CB	7.25	1.63	1.53
1	B	383	PHE	N-CA	-7.24	1.37	1.46
1	C	277	ASP	CA-CB	7.22	1.64	1.53
2	F	194	GLN	CA-CB	7.22	1.65	1.53
1	A	277	ASP	N-CA	-7.20	1.37	1.46
1	A	575	PRO	CA-C	-7.20	1.44	1.52
1	C	692	SER	CA-C	7.19	1.62	1.52
1	C	61	GLN	CA-CB	7.19	1.65	1.53
2	F	8	ASP	CA-CB	7.18	1.65	1.53
2	F	190	ASN	CA-C	7.17	1.62	1.52
1	A	324	ASN	CA-C	7.16	1.61	1.52
1	A	849	LEU	CA-CB	7.16	1.63	1.53
1	B	800	MET	CA-C	7.15	1.61	1.52
1	C	687	THR	C-N	7.15	1.42	1.33
2	F	2	LYS	CA-C	7.13	1.61	1.52
2	F	62	TYR	C-N	7.12	1.43	1.33
2	E	201	LYS	CA-C	7.11	1.61	1.52
1	A	577	SER	N-CA	-7.10	1.37	1.45
1	C	788	ASP	CA-C	7.10	1.60	1.53
2	F	163	GLY	CA-C	-7.10	1.45	1.52
2	E	98	ASP	N-CA	-7.07	1.36	1.46
1	A	39	SER	CA-CB	7.06	1.63	1.53
1	A	244	GLY	C-N	7.05	1.42	1.33
1	A	109	GLY	N-CA	7.05	1.54	1.44
1	B	175	GLY	C-O	-7.04	1.15	1.23
2	E	183	ARG	CA-C	7.04	1.62	1.52
1	C	381	ARG	C-N	7.01	1.43	1.33
1	C	775	ILE	CA-CB	-7.00	1.46	1.54
2	F	168	ARG	CD-NE	7.00	1.56	1.46
2	E	201	LYS	CA-CB	6.99	1.65	1.53
2	E	164	VAL	CA-CB	-6.99	1.46	1.54
1	A	614	LEU	CA-CB	6.98	1.61	1.53
1	A	106	LEU	CA-CB	6.97	1.65	1.53
2	E	167	VAL	N-CA	6.96	1.54	1.46
1	A	670	ASN	CA-CB	6.96	1.63	1.53
1	B	278	ASN	CA-C	6.96	1.62	1.52
1	B	507	VAL	C-O	6.96	1.31	1.24
2	F	222	VAL	CA-C	6.95	1.61	1.52
1	A	46	ASN	CA-CB	6.94	1.63	1.53
1	A	493	ILE	C-N	6.94	1.42	1.33
1	B	103	ARG	N-CA	-6.93	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	743	GLU	N-CA	-6.93	1.37	1.46
1	C	318	SER	N-CA	6.93	1.53	1.45
1	C	928	HIS	N-CA	6.92	1.54	1.46
1	A	275	ASN	N-CA	6.90	1.55	1.46
2	F	77	ASP	C-N	6.89	1.42	1.33
1	B	748	VAL	CA-CB	6.89	1.63	1.54
1	B	130	ASN	CA-CB	6.89	1.63	1.53
1	C	51	PRO	N-CD	6.88	1.57	1.47
2	E	180	VAL	CA-C	-6.88	1.44	1.52
1	A	738	THR	N-CA	6.88	1.54	1.46
2	D	161	ARG	CD-NE	6.87	1.55	1.46
1	C	673	ALA	CA-C	6.85	1.61	1.52
1	B	704	ILE	N-CA	6.84	1.51	1.46
2	E	104	THR	CA-C	-6.84	1.44	1.52
1	A	392	SER	CA-C	-6.82	1.44	1.52
1	B	458	ALA	CA-C	6.82	1.61	1.52
1	A	94	ASP	CA-C	6.82	1.61	1.52
1	B	415	PRO	CA-C	6.81	1.62	1.52
1	C	743	GLU	CA-CB	6.80	1.61	1.53
1	C	34	THR	N-CA	6.80	1.54	1.46
1	C	582	TRP	N-CA	6.79	1.54	1.45
2	D	166	TRP	N-CA	-6.79	1.38	1.46
2	F	33	SER	CA-CB	6.78	1.65	1.53
1	B	493	ILE	N-CA	-6.75	1.39	1.46
1	A	704	ILE	CA-C	6.75	1.59	1.52
1	B	202	GLU	C-N	6.75	1.42	1.34
1	A	634	ARG	CA-C	6.75	1.61	1.52
1	B	600	LEU	N-CA	-6.74	1.37	1.46
1	C	334	GLY	N-CA	6.74	1.55	1.45
1	B	932	ARG	NE-CZ	-6.73	1.25	1.33
1	A	713	LEU	C-N	6.73	1.43	1.34
1	B	227	THR	CA-C	6.69	1.60	1.52
1	B	889	GLN	CA-C	-6.69	1.44	1.52
1	B	170	GLN	CA-C	6.69	1.60	1.52
1	C	623	HIS	ND1-CE1	6.68	1.39	1.32
2	F	43	TYR	CA-C	-6.68	1.44	1.52
1	B	860	GLN	CA-C	-6.66	1.44	1.52
1	A	663	PRO	CA-CB	6.66	1.61	1.54
2	E	245	VAL	CA-CB	-6.66	1.45	1.54
1	C	613	CYS	CA-C	6.65	1.60	1.52
1	A	639	ASP	CA-C	6.65	1.61	1.52
1	A	53	HIS	ND1-CE1	6.65	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	545	ARG	N-CA	-6.64	1.37	1.46
1	C	32	ARG	CD-NE	6.63	1.55	1.46
2	D	245	VAL	CA-C	6.62	1.60	1.52
1	A	167	VAL	CA-C	-6.61	1.44	1.52
1	B	714	ASN	CA-C	6.61	1.61	1.52
1	B	328	PHE	CA-CB	6.60	1.63	1.53
1	B	45	ARG	CD-NE	6.59	1.55	1.46
1	A	661	ASN	CA-CB	6.58	1.62	1.53
1	C	751	GLU	C-O	-6.58	1.16	1.24
2	E	61	ARG	CD-NE	6.58	1.55	1.46
2	F	165	HIS	CA-C	6.57	1.61	1.52
1	A	136	GLU	CA-C	-6.56	1.44	1.52
1	B	558	HIS	CG-CD2	6.56	1.43	1.35
2	F	229	GLY	CA-C	-6.56	1.42	1.51
1	A	558	HIS	CA-C	-6.55	1.44	1.52
1	B	212	GLU	CA-CB	6.55	1.61	1.53
1	B	466	ASN	CA-CB	6.54	1.63	1.53
2	F	210	MET	C-N	6.54	1.42	1.33
1	B	822	HIS	CA-CB	6.53	1.62	1.53
1	B	81	ALA	N-CA	-6.53	1.38	1.46
2	E	14	SER	CA-C	6.53	1.58	1.52
2	F	165	HIS	CG-CD2	6.53	1.43	1.35
1	A	755	VAL	N-CA	-6.52	1.39	1.46
1	B	621	MET	CA-C	6.52	1.61	1.52
1	C	634	ARG	CD-NE	6.51	1.55	1.46
1	B	620	PRO	C-N	6.51	1.42	1.33
2	D	214	SER	CA-C	-6.51	1.45	1.53
1	A	668	SER	CA-C	6.50	1.61	1.52
1	B	496	ASN	CA-CB	6.50	1.63	1.52
1	A	207	GLU	CA-CB	6.50	1.64	1.53
1	A	419	VAL	CA-C	-6.49	1.44	1.52
1	C	306	LYS	C-N	6.49	1.42	1.33
2	F	211	GLU	CA-CB	6.49	1.63	1.53
2	D	25	ARG	N-CA	-6.48	1.38	1.46
2	D	96	HIS	ND1-CE1	6.48	1.39	1.32
1	B	910	ASP	N-CA	-6.47	1.37	1.46
2	E	96	HIS	CG-CD2	6.45	1.43	1.35
1	B	909	MET	CA-C	-6.45	1.45	1.52
1	A	720	VAL	N-CA	6.45	1.53	1.46
1	C	266	PHE	CA-C	6.45	1.60	1.52
1	B	174	SER	CA-CB	6.45	1.61	1.53
1	C	734	ASP	CA-CB	6.44	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	675	ARG	CA-CB	6.43	1.63	1.54
1	A	800	MET	CA-C	6.41	1.60	1.52
1	B	426	THR	C-N	6.41	1.41	1.33
1	B	741	GLU	CA-C	6.41	1.60	1.52
1	B	905	GLU	CA-CB	6.40	1.62	1.53
1	B	414	PHE	CA-C	6.39	1.58	1.52
1	A	464	ASN	N-CA	-6.39	1.38	1.46
1	C	806	ASP	CA-C	6.39	1.61	1.52
1	A	915	LEU	N-CA	-6.39	1.38	1.46
1	C	398	ARG	CD-NE	6.39	1.55	1.46
1	C	944	PHE	CA-CB	6.38	1.62	1.53
1	B	379	ARG	CA-C	-6.38	1.43	1.52
1	B	897	ALA	CA-C	6.38	1.60	1.52
1	A	416	LEU	C-N	6.37	1.42	1.33
1	B	519	LEU	C-N	6.37	1.43	1.33
1	A	560	GLN	CA-CB	6.37	1.62	1.53
1	C	400	ILE	CA-CB	6.36	1.61	1.54
1	C	624	ASN	CA-CB	6.35	1.63	1.53
2	E	194	GLN	CA-CB	6.34	1.62	1.54
1	C	387	ASN	CA-CB	6.34	1.62	1.53
1	B	349	GLY	C-N	6.33	1.41	1.33
1	C	361	GLN	CA-CB	6.33	1.63	1.53
1	B	424	THR	N-CA	6.33	1.53	1.46
1	A	735	ARG	CD-NE	6.32	1.55	1.46
1	A	929	ARG	CA-C	6.32	1.59	1.52
1	B	752	GLY	N-CA	6.31	1.54	1.45
2	E	24	ASP	C-N	6.31	1.42	1.33
2	F	12	THR	CA-CB	6.30	1.61	1.53
2	D	231	ASN	CA-C	-6.29	1.43	1.52
1	B	838	GLY	C-N	6.29	1.42	1.33
1	A	259	SER	CA-C	6.28	1.60	1.52
1	A	623	HIS	CA-CB	6.28	1.63	1.53
1	C	641	SER	C-N	6.28	1.42	1.33
1	B	450	GLU	N-CA	-6.28	1.38	1.46
1	B	190	GLN	CA-CB	6.28	1.63	1.53
1	B	732	GLY	C-N	6.28	1.42	1.33
1	B	863	PHE	CA-CB	6.28	1.64	1.53
1	B	298	HIS	ND1-CE1	6.27	1.38	1.32
1	B	718	LYS	CA-C	6.27	1.58	1.52
1	B	129	PRO	N-CA	-6.27	1.39	1.47
1	C	250	VAL	CA-C	6.26	1.60	1.52
1	C	866	ASP	CA-CB	6.26	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	GLU	CA-C	6.25	1.61	1.52
1	B	361	GLN	C-N	6.25	1.42	1.34
1	B	489	SER	CA-CB	6.25	1.61	1.53
1	B	408	GLU	N-CA	-6.25	1.38	1.46
1	C	808	THR	C-N	6.25	1.43	1.33
1	A	652	LEU	CA-C	6.25	1.59	1.52
1	A	661	ASN	CA-C	6.24	1.60	1.52
1	A	935	ILE	CA-C	-6.23	1.44	1.52
1	C	554	TYR	CA-C	6.23	1.60	1.52
2	D	86	GLN	N-CA	6.23	1.52	1.45
1	A	354	LEU	CA-C	-6.23	1.44	1.52
1	B	429	LYS	CA-C	6.22	1.60	1.52
1	C	720	VAL	CA-CB	-6.22	1.46	1.54
2	E	22	VAL	C-N	6.22	1.42	1.33
1	B	921	VAL	C-N	6.22	1.41	1.33
1	B	574	LEU	CA-C	6.22	1.60	1.53
1	C	360	LEU	CA-C	6.21	1.60	1.52
2	D	93	TYR	N-CA	6.21	1.53	1.46
1	A	891	LEU	CA-CB	6.21	1.62	1.53
1	A	741	GLU	CA-C	-6.21	1.44	1.52
1	B	176	ILE	N-CA	-6.20	1.39	1.46
1	A	421	ASN	C-N	6.19	1.41	1.33
1	B	47	PRO	CA-C	6.19	1.61	1.52
1	B	891	LEU	CA-CB	6.19	1.63	1.53
1	B	822	HIS	ND1-CE1	6.18	1.38	1.32
1	B	316	GLN	C-N	6.18	1.42	1.33
1	A	390	VAL	N-CA	6.18	1.54	1.46
1	A	929	ARG	C-O	-6.18	1.17	1.24
1	B	302	MET	CA-C	6.17	1.59	1.52
1	B	537	HIS	ND1-CE1	6.17	1.38	1.32
1	C	673	ALA	C-N	6.17	1.41	1.33
1	B	442	ALA	CA-C	6.16	1.60	1.53
2	D	21	SER	C-N	6.16	1.42	1.33
1	A	378	ASP	N-CA	6.16	1.53	1.46
1	B	638	ASN	C-N	6.16	1.41	1.33
1	A	196	ASP	CA-CB	6.14	1.61	1.53
2	E	148	VAL	C-N	6.14	1.41	1.33
1	B	920	GLU	N-CA	-6.13	1.38	1.46
1	A	29	GLN	CA-C	6.13	1.60	1.52
1	A	545	ARG	CD-NE	6.12	1.54	1.46
2	E	101	SER	CA-CB	6.12	1.62	1.53
2	D	60	THR	N-CA	6.11	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	621	MET	C-N	6.11	1.41	1.33
2	F	113	ILE	CA-C	6.11	1.59	1.52
1	A	414	PHE	CA-CB	6.11	1.61	1.54
1	C	447	ASP	CA-C	6.11	1.61	1.52
1	B	208	SER	CA-C	6.10	1.62	1.52
1	A	87	VAL	N-CA	-6.09	1.39	1.46
1	A	583	ASN	CA-C	-6.09	1.45	1.52
1	A	781	TYR	CA-C	-6.08	1.45	1.52
1	A	753	TYR	CA-CB	6.08	1.63	1.54
1	A	219	ALA	N-CA	6.08	1.53	1.45
1	A	451	ILE	CA-CB	6.07	1.62	1.54
1	A	910	ASP	CA-CB	6.07	1.62	1.53
1	A	924	VAL	CA-C	6.07	1.60	1.52
1	B	735	ARG	CA-C	6.07	1.58	1.52
1	C	695	ASP	C-O	-6.07	1.20	1.25
1	C	51	PRO	CA-CB	6.06	1.61	1.53
1	A	667	PRO	N-CA	-6.06	1.39	1.47
1	B	336	MET	N-CA	-6.06	1.38	1.46
1	C	257	LEU	CA-C	6.06	1.60	1.52
2	F	70	SER	CA-CB	6.06	1.63	1.53
1	A	507	VAL	CA-C	6.05	1.60	1.52
2	F	4	ASP	N-CA	6.04	1.53	1.46
1	A	298	HIS	ND1-CE1	6.04	1.38	1.32
1	B	93	LEU	CA-C	6.04	1.59	1.52
1	C	871	ARG	C-N	6.04	1.40	1.33
1	B	719	LYS	CA-C	6.04	1.59	1.52
1	A	369	TYR	CA-CB	6.03	1.62	1.53
1	A	107	ASP	CA-CB	6.03	1.63	1.53
2	D	9	ILE	N-CA	-6.02	1.38	1.46
2	E	166	TRP	NE1-CE2	-6.02	1.30	1.37
1	A	480	LEU	CB-CG	6.02	1.65	1.53
2	F	61	ARG	C-N	6.01	1.41	1.33
1	C	311	ARG	CA-C	-6.00	1.45	1.52
1	C	249	LEU	CA-C	6.00	1.60	1.52
1	A	874	PHE	CA-C	6.00	1.60	1.53
1	C	486	TYR	CA-C	6.00	1.60	1.52
1	B	278	ASN	CA-CB	5.99	1.64	1.53
2	D	61	ARG	CA-C	-5.99	1.45	1.52
1	A	121	ASN	CA-CB	5.99	1.62	1.53
1	A	824	ASN	N-CA	5.98	1.55	1.46
2	D	30	CYS	CA-C	-5.98	1.45	1.52
1	B	291	ASP	CA-C	5.98	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	CYS	CA-CB	5.98	1.62	1.53
1	B	809	LYS	CA-C	5.98	1.60	1.52
1	A	534	PHE	CA-C	5.97	1.60	1.52
1	A	557	PHE	CA-C	-5.97	1.45	1.52
1	B	197	LYS	CA-CB	5.97	1.62	1.53
2	E	15	PRO	C-N	5.97	1.41	1.33
2	E	179	GLY	N-CA	5.96	1.52	1.45
1	B	531	VAL	N-CA	-5.96	1.39	1.46
1	B	580	TYR	CA-C	-5.96	1.45	1.53
2	E	144	PRO	N-CA	5.95	1.54	1.47
1	A	819	LEU	N-CA	-5.95	1.38	1.46
1	C	892	LEU	CA-CB	5.95	1.62	1.53
1	A	938	VAL	CA-CB	-5.94	1.46	1.54
2	F	44	GLN	CA-C	-5.94	1.45	1.52
1	A	518	ASN	CA-CB	5.93	1.62	1.53
1	A	674	PHE	N-CA	-5.93	1.38	1.46
1	C	366	GLU	CA-CB	-5.93	1.44	1.53
1	C	524	SER	CA-C	-5.93	1.45	1.52
1	A	17	GLN	N-CA	-5.93	1.38	1.46
1	C	89	ASP	CA-C	-5.93	1.44	1.52
1	C	7	PRO	C-N	5.92	1.42	1.33
1	A	131	PRO	N-CA	5.92	1.54	1.47
1	C	282	LYS	N-CA	-5.92	1.38	1.46
1	B	608	LYS	N-CA	-5.92	1.38	1.46
1	B	875	SER	CA-CB	5.92	1.64	1.53
1	C	391	ASP	CA-C	5.92	1.60	1.52
1	C	419	VAL	CA-C	-5.92	1.45	1.52
1	C	918	LEU	N-CA	5.91	1.53	1.46
1	C	193	LYS	CA-CB	5.91	1.62	1.53
1	B	899	ALA	CA-C	-5.90	1.45	1.52
2	D	156	GLY	C-N	5.90	1.40	1.33
2	D	99	TYR	CA-C	5.90	1.60	1.52
1	B	588	VAL	CA-CB	5.89	1.61	1.54
1	B	243	ASN	CA-C	5.89	1.60	1.52
1	C	333	ILE	CA-C	5.89	1.60	1.52
1	B	52	THR	CA-C	-5.89	1.45	1.52
1	A	452	ARG	CZ-NH2	-5.89	1.25	1.33
1	B	18	ASP	CA-C	-5.89	1.45	1.52
1	B	941	ARG	CD-NE	5.89	1.54	1.46
1	C	77	TYR	CA-CB	5.88	1.62	1.54
1	A	231	PRO	N-CA	-5.88	1.40	1.47
1	B	219	ALA	CA-C	-5.88	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45	ARG	N-CA	5.88	1.53	1.46
1	B	662	VAL	CA-CB	-5.88	1.49	1.54
1	C	720	VAL	N-CA	5.86	1.52	1.46
2	D	82	ILE	CA-C	5.86	1.60	1.52
1	A	769	MET	CA-C	5.86	1.60	1.52
1	C	928	HIS	CB-CG	5.85	1.58	1.50
1	B	823	ASN	CA-C	5.85	1.60	1.52
2	D	1	TYR	CA-CB	5.85	1.61	1.53
1	C	369	TYR	N-CA	-5.83	1.39	1.46
1	A	171	ALA	CA-CB	5.82	1.60	1.53
1	A	687	THR	C-N	5.82	1.41	1.33
2	D	50	ALA	C-N	5.82	1.41	1.33
2	F	73	GLY	N-CA	5.82	1.52	1.45
1	C	926	ARG	CZ-NH2	-5.81	1.25	1.33
1	A	166	HIS	N-CA	5.81	1.53	1.46
1	A	178	ILE	C-O	-5.81	1.17	1.24
1	A	434	GLN	C-N	5.80	1.42	1.34
1	A	83	PHE	C-N	5.79	1.41	1.33
2	F	36	VAL	CA-CB	-5.79	1.47	1.54
1	B	675	ARG	N-CA	5.78	1.53	1.46
1	A	200	GLN	CA-CB	5.78	1.61	1.53
1	A	277	ASP	CA-CB	5.78	1.62	1.53
1	B	933	GLY	CA-C	-5.78	1.43	1.51
1	B	29	GLN	N-CA	-5.77	1.39	1.46
2	D	214	SER	N-CA	5.77	1.55	1.46
1	B	565	PHE	CA-C	5.77	1.60	1.52
1	A	801	SER	CA-CB	5.76	1.64	1.53
1	C	26	GLY	CA-C	-5.76	1.45	1.52
1	A	372	LEU	CA-C	-5.76	1.45	1.52
2	E	208	VAL	CA-C	-5.76	1.46	1.52
1	A	101	ASP	C-N	-5.76	1.26	1.33
1	A	337	TYR	CA-C	-5.76	1.45	1.52
2	E	193	PHE	CA-C	5.76	1.61	1.52
1	A	458	ALA	CA-C	5.75	1.59	1.52
1	C	27	LEU	C-N	5.75	1.41	1.33
1	A	468	TRP	CA-C	5.75	1.60	1.52
1	C	811	LYS	CA-CB	5.75	1.62	1.53
1	C	866	ASP	C-N	5.75	1.41	1.33
1	B	491	VAL	C-N	5.75	1.41	1.33
1	C	14	ILE	CA-CB	-5.74	1.47	1.54
1	A	586	LYS	CA-CB	5.73	1.62	1.53
1	A	825	SER	CA-CB	5.73	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15	SER	CA-CB	5.73	1.64	1.53
1	A	363	ARG	CA-C	5.72	1.60	1.52
1	A	554	TYR	CA-C	5.72	1.60	1.52
2	E	186	THR	C-N	5.72	1.41	1.33
1	B	509	ALA	CA-C	5.72	1.59	1.52
2	D	55	ILE	N-CA	5.72	1.52	1.46
1	C	670	ASN	C-O	-5.72	1.17	1.23
1	C	502	TYR	CA-C	5.72	1.60	1.52
2	F	241	THR	CA-C	-5.72	1.45	1.52
1	A	487	SER	C-N	5.71	1.41	1.33
1	C	16	GLY	C-N	5.71	1.41	1.33
1	C	703	SER	C-N	5.71	1.39	1.33
1	A	328	PHE	CA-CB	5.71	1.62	1.53
1	A	665	SER	C-N	5.71	1.37	1.32
1	B	332	PHE	CA-CB	5.70	1.62	1.53
1	B	365	THR	CA-CB	5.70	1.62	1.53
2	D	178	MET	CA-C	-5.70	1.45	1.53
1	B	248	ILE	CA-C	5.70	1.58	1.52
1	A	268	THR	CA-CB	5.69	1.62	1.53
1	C	292	ILE	N-CA	5.69	1.53	1.46
1	C	426	THR	C-N	5.69	1.41	1.33
1	A	278	ASN	CA-CB	5.68	1.61	1.53
1	B	707	LEU	CA-C	5.68	1.59	1.52
1	C	386	TRP	NE1-CE2	5.68	1.43	1.37
1	C	355	ASN	C-N	5.68	1.42	1.33
1	A	429	LYS	CA-CB	5.67	1.62	1.54
1	C	759	ASN	CA-C	-5.67	1.44	1.52
2	D	236	TYR	N-CA	5.67	1.52	1.46
2	E	244	THR	N-CA	5.67	1.52	1.46
1	A	470	ASN	C-N	5.67	1.41	1.33
1	B	555	VAL	CA-CB	-5.67	1.49	1.54
1	A	638	ASN	CA-CB	5.66	1.60	1.53
1	B	717	PHE	CA-CB	5.66	1.62	1.53
1	C	671	TRP	CA-CB	5.66	1.60	1.53
2	F	139	ALA	C-N	5.66	1.40	1.33
2	F	144	PRO	CA-CB	5.66	1.61	1.53
1	A	768	GLN	CA-C	-5.66	1.45	1.52
2	E	175	LEU	CA-CB	5.66	1.61	1.53
1	C	459	MET	C-N	5.65	1.41	1.33
2	D	16	SER	CA-C	5.65	1.60	1.52
1	A	787	LYS	N-CA	-5.65	1.38	1.46
2	D	30	CYS	C-N	5.65	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	781	TYR	N-CA	-5.65	1.39	1.46
1	C	575	PRO	CA-CB	5.65	1.61	1.53
1	A	300	SER	N-CA	5.64	1.53	1.46
1	A	412	TYR	C-N	5.64	1.41	1.33
1	C	165	THR	CA-C	-5.64	1.45	1.52
2	E	224	TYR	CB-CG	-5.64	1.39	1.51
2	F	96	HIS	CG-CD2	-5.64	1.29	1.35
1	B	403	HIS	ND1-CE1	5.63	1.38	1.32
1	B	183	ILE	CA-CB	5.63	1.61	1.54
1	C	675	ARG	C-N	5.63	1.38	1.32
1	B	491	VAL	N-CA	5.62	1.52	1.46
1	B	795	ARG	CA-C	5.62	1.60	1.52
1	C	875	SER	C-N	5.62	1.41	1.33
1	A	367	LEU	N-CA	-5.61	1.39	1.46
2	F	96	HIS	CG-ND1	5.61	1.44	1.38
1	C	619	PHE	CA-C	5.61	1.59	1.53
1	A	305	ILE	C-N	5.60	1.41	1.33
1	A	924	VAL	C-N	5.60	1.41	1.33
1	C	9	TRP	C-O	5.60	1.30	1.24
1	A	710	THR	CA-CB	5.60	1.60	1.52
1	C	617	THR	CA-CB	5.59	1.62	1.53
2	F	114	LYS	N-CA	5.59	1.53	1.46
1	A	781	TYR	CA-CB	5.59	1.63	1.53
1	B	13	HIS	CA-C	5.59	1.60	1.52
2	F	161	ARG	N-CA	5.59	1.53	1.46
1	A	812	ASP	N-CA	5.59	1.53	1.46
1	C	471	PHE	CA-CB	5.59	1.62	1.53
2	D	217	SER	CA-C	5.59	1.60	1.52
1	A	242	GLU	C-N	5.58	1.40	1.33
1	A	478	LEU	CA-C	5.58	1.60	1.52
1	A	23	LEU	CA-C	-5.58	1.45	1.52
1	C	635	ASN	CA-CB	5.58	1.62	1.53
1	B	403	HIS	CG-CD2	5.57	1.42	1.35
2	F	224	TYR	CA-CB	5.56	1.61	1.53
1	C	809	LYS	CA-C	5.56	1.60	1.52
1	B	646	LEU	CA-CB	5.56	1.62	1.53
1	A	561	VAL	C-O	-5.55	1.17	1.24
2	D	194	GLN	C-N	5.55	1.40	1.33
1	B	776	GLY	CA-C	-5.55	1.44	1.51
2	F	30	CYS	CA-CB	5.55	1.63	1.53
2	F	93	TYR	CZ-OH	5.55	1.49	1.38
2	E	132	VAL	CA-C	5.54	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	721	ALA	N-CA	-5.54	1.39	1.46
1	A	880	SER	CA-CB	5.54	1.60	1.52
1	A	522	ARG	CD-NE	5.54	1.54	1.46
1	A	652	LEU	C-N	5.54	1.41	1.33
1	C	893	TYR	CA-CB	5.53	1.62	1.53
1	A	671	TRP	C-N	5.53	1.41	1.33
1	B	925	VAL	CA-CB	5.53	1.61	1.54
2	D	166	TRP	CA-C	-5.53	1.46	1.52
1	A	931	HIS	ND1-CE1	5.52	1.38	1.32
1	B	917	VAL	CA-C	-5.52	1.45	1.52
1	C	810	TYR	N-CA	5.52	1.53	1.46
1	A	469	ARG	CD-NE	5.52	1.53	1.46
1	B	243	ASN	C-N	5.52	1.40	1.33
1	B	127	GLY	CA-C	-5.52	1.42	1.51
2	D	175	LEU	N-CA	-5.52	1.39	1.46
2	F	87	PRO	N-CA	5.52	1.53	1.47
1	B	320	PRO	CA-C	5.51	1.59	1.52
2	E	216	ARG	N-CA	-5.51	1.38	1.45
1	C	178	ILE	CA-CB	5.51	1.61	1.54
1	B	830	TYR	CA-CB	5.51	1.59	1.52
2	E	176	GLU	N-CA	-5.51	1.39	1.46
1	A	536	HIS	ND1-CE1	5.50	1.38	1.32
1	B	510	PRO	C-N	5.50	1.40	1.33
1	B	614	LEU	CA-CB	5.50	1.61	1.53
1	C	793	PHE	CA-CB	5.50	1.62	1.53
1	B	406	GLU	CA-C	5.50	1.59	1.52
1	C	703	SER	N-CA	5.50	1.52	1.46
1	C	928	HIS	ND1-CE1	5.50	1.38	1.32
1	A	177	ASN	CA-CB	5.49	1.62	1.53
1	B	480	LEU	CA-CB	5.49	1.61	1.53
2	D	167	VAL	C-N	5.49	1.40	1.33
1	A	607	ILE	CA-CB	-5.49	1.47	1.54
2	F	95	CYS	CA-C	5.49	1.60	1.52
1	C	918	LEU	CA-C	5.48	1.59	1.52
1	A	444	GLU	CA-CB	5.48	1.62	1.53
1	C	11	TYR	CA-CB	5.48	1.61	1.53
2	D	211	GLU	N-CA	5.48	1.52	1.46
1	B	28	VAL	CA-C	-5.48	1.46	1.52
1	B	648	ALA	N-CA	-5.47	1.39	1.46
2	D	167	VAL	N-CA	5.47	1.52	1.46
1	A	339	ASN	CA-C	-5.47	1.45	1.52
1	A	870	TRP	N-CA	-5.47	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	242	GLU	CA-C	5.47	1.60	1.52
1	C	286	TYR	CA-CB	5.47	1.59	1.52
1	C	409	LEU	C-O	5.47	1.31	1.24
1	C	890	ASN	CA-CB	5.47	1.62	1.53
2	D	243	VAL	CA-CB	-5.47	1.47	1.54
1	A	773	TYR	CA-C	5.46	1.59	1.52
1	B	856	ASP	CA-C	5.46	1.59	1.52
1	B	855	VAL	C-N	5.46	1.40	1.33
1	B	707	LEU	CA-CB	5.46	1.62	1.53
1	C	246	GLN	CA-C	5.46	1.60	1.52
2	D	239	GLN	N-CA	5.46	1.52	1.46
1	B	918	LEU	C-N	5.45	1.41	1.33
2	D	244	THR	N-CA	5.45	1.52	1.45
1	B	133	GLU	CA-C	5.45	1.59	1.52
1	A	809	LYS	C-N	5.44	1.41	1.33
1	A	666	ILE	C-N	5.44	1.40	1.33
1	C	725	ASP	CA-CB	5.43	1.62	1.53
1	A	926	ARG	CA-CB	5.43	1.61	1.53
2	F	151	SER	CA-C	-5.43	1.46	1.52
1	B	476	ILE	N-CA	-5.43	1.39	1.46
1	B	109	GLY	C-N	-5.43	1.29	1.33
1	A	168	PHE	N-CA	-5.43	1.40	1.46
1	A	867	ARG	CD-NE	5.43	1.53	1.46
1	B	194	TYR	C-N	5.43	1.40	1.33
1	C	299	ILE	CA-CB	5.42	1.60	1.54
1	C	517	ILE	CA-C	5.42	1.58	1.52
1	C	88	GLY	C-N	5.42	1.41	1.33
2	D	198	THR	CA-CB	-5.42	1.45	1.53
1	B	403	HIS	CD2-NE2	5.41	1.43	1.37
1	A	408	GLU	CA-CB	5.41	1.62	1.53
1	B	465	ALA	CA-C	5.41	1.59	1.52
1	C	166	HIS	ND1-CE1	5.41	1.38	1.32
1	B	783	PRO	C-N	5.41	1.40	1.33
1	C	290	VAL	CA-C	-5.41	1.46	1.52
1	C	657	ALA	CA-C	5.41	1.60	1.52
1	A	768	GLN	CA-CB	5.40	1.61	1.53
2	F	180	VAL	CA-CB	-5.40	1.50	1.55
1	A	111	THR	N-CA	5.40	1.53	1.46
1	A	532	ASN	CA-C	5.40	1.59	1.52
1	B	663	PRO	CA-C	5.40	1.58	1.52
1	C	789	ARG	CZ-NH2	-5.40	1.26	1.33
1	A	462	ASN	CA-CB	5.40	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	820	HIS	ND1-CE1	5.40	1.38	1.32
1	B	813	TYR	CA-CB	5.40	1.62	1.53
2	E	47	PRO	C-N	-5.40	1.25	1.33
2	E	188	ASP	CA-CB	5.40	1.62	1.53
1	B	737	LEU	C-N	5.39	1.39	1.33
1	C	75	THR	CA-C	-5.39	1.45	1.53
1	B	832	ALA	N-CA	-5.39	1.40	1.45
1	B	759	ASN	C-O	-5.39	1.17	1.24
2	F	98	ASP	CA-CB	5.39	1.60	1.53
1	A	714	ASN	C-N	5.39	1.41	1.33
1	B	105	VAL	CA-C	-5.38	1.46	1.52
1	C	190	GLN	N-CA	-5.38	1.39	1.46
1	C	420	GLY	C-N	5.37	1.40	1.33
2	F	83	SER	N-CA	5.37	1.52	1.46
1	C	296	ASP	C-N	5.37	1.40	1.33
1	A	817	GLY	CA-C	-5.37	1.46	1.52
1	B	775	ILE	CA-C	-5.37	1.46	1.52
1	C	113	LYS	CA-C	-5.37	1.46	1.52
2	F	170	ALA	CA-C	5.36	1.59	1.53
1	B	587	ASP	CA-CB	5.36	1.59	1.53
1	B	112	PHE	CA-C	5.35	1.59	1.52
1	C	445	PHE	CA-CB	5.35	1.61	1.53
1	C	481	PRO	CA-CB	-5.35	1.46	1.53
1	C	295	PRO	CA-C	5.34	1.59	1.52
1	B	525	LEU	N-CA	5.34	1.52	1.46
1	C	767	VAL	CA-CB	-5.34	1.48	1.54
1	A	688	PRO	C-O	-5.33	1.17	1.23
1	B	590	MET	C-N	5.33	1.40	1.33
1	C	133	GLU	CA-C	5.33	1.59	1.52
1	A	705	PRO	CA-CB	5.33	1.61	1.53
1	B	322	ARG	CD-NE	5.33	1.53	1.46
1	B	777	TYR	CA-C	5.33	1.59	1.52
1	C	715	HIS	ND1-CE1	-5.33	1.27	1.32
2	D	182	TRP	CA-CB	5.33	1.61	1.53
2	D	223	TYR	CA-CB	5.33	1.61	1.53
1	C	826	GLY	CA-C	-5.33	1.44	1.51
1	A	457	PHE	C-N	5.32	1.40	1.33
2	D	183	ARG	C-N	5.32	1.40	1.33
2	F	233	PRO	CA-C	5.32	1.59	1.52
1	C	397	VAL	CA-CB	-5.32	1.46	1.54
1	A	32	ARG	CA-CB	5.31	1.61	1.53
1	B	377	GLY	CA-C	-5.31	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	SER	C-O	-5.31	1.18	1.24
1	A	536	HIS	CD2-NE2	5.31	1.43	1.37
1	B	649	ALA	CA-C	-5.31	1.46	1.52
1	C	584	PHE	C-N	5.31	1.41	1.33
2	E	6	ASP	N-CA	5.31	1.54	1.46
2	F	244	THR	CA-C	-5.31	1.46	1.52
1	C	312	GLU	C-N	5.31	1.41	1.33
2	D	196	ARG	CD-NE	5.31	1.53	1.46
1	A	28	VAL	C-O	-5.30	1.18	1.24
1	B	310	SER	CA-C	5.29	1.58	1.52
1	A	715	HIS	N-CA	-5.29	1.39	1.46
1	B	471	PHE	C-N	-5.29	1.27	1.33
1	C	180	LYS	CA-C	5.29	1.60	1.52
1	C	780	PHE	CA-C	5.29	1.59	1.52
2	E	35	SER	N-CA	5.29	1.52	1.46
2	E	9	ILE	CA-C	5.29	1.58	1.52
1	C	575	PRO	C-N	5.29	1.38	1.32
1	C	455	ASN	C-N	5.28	1.40	1.33
2	D	153	LYS	CA-C	5.28	1.59	1.52
1	B	51	PRO	N-CD	5.28	1.55	1.47
1	B	86	ALA	C-N	5.28	1.40	1.33
1	C	874	PHE	N-CA	5.28	1.52	1.46
1	A	785	SER	CA-CB	5.27	1.61	1.53
1	A	820	HIS	CD2-NE2	5.27	1.43	1.37
1	B	368	SER	N-CA	5.26	1.52	1.46
1	A	25	PRO	N-CA	-5.26	1.40	1.47
1	C	941	ARG	CD-NE	5.26	1.53	1.46
2	D	186	THR	N-CA	5.26	1.52	1.46
1	A	124	ALA	CA-CB	5.25	1.62	1.53
1	C	323	PRO	CA-CB	5.25	1.60	1.53
1	C	652	LEU	CA-C	5.25	1.58	1.52
1	C	688	PRO	CA-C	5.25	1.58	1.52
1	C	783	PRO	CA-CB	5.25	1.60	1.53
1	A	13	HIS	CB-CG	5.25	1.57	1.50
1	A	741	GLU	C-N	5.25	1.41	1.33
1	C	70	VAL	N-CA	-5.25	1.40	1.46
1	B	363	ARG	CD-NE	5.25	1.53	1.46
1	B	213	THR	CA-C	-5.25	1.45	1.53
1	C	222	VAL	N-CA	5.24	1.52	1.46
1	C	461	ILE	CA-CB	-5.24	1.47	1.54
1	B	29	GLN	CA-CB	5.24	1.61	1.53
1	B	629	LEU	N-CA	-5.24	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	GLN	CA-C	-5.24	1.46	1.52
1	C	623	HIS	CE1-NE2	-5.24	1.27	1.32
2	D	168	ARG	CA-C	-5.24	1.46	1.52
1	A	79	TYR	CA-CB	5.24	1.63	1.53
1	B	527	TYR	CZ-OH	5.24	1.49	1.38
1	B	402	ASN	CA-CB	5.23	1.59	1.52
1	A	161	GLU	C-N	5.23	1.40	1.33
1	B	130	ASN	C-N	5.22	1.39	1.33
1	C	467	LEU	N-CA	-5.22	1.40	1.46
2	D	149	LYS	N-CA	-5.22	1.40	1.46
1	A	399	ILE	C-N	5.22	1.41	1.33
1	C	6	MET	N-CA	5.22	1.56	1.46
2	F	86	GLN	CA-CB	5.22	1.61	1.53
1	A	92	VAL	CA-C	5.21	1.59	1.52
1	B	733	ASN	CA-CB	5.21	1.61	1.53
1	C	493	ILE	CA-CB	-5.21	1.46	1.54
1	A	460	GLU	CA-C	-5.21	1.46	1.52
1	B	22	TYR	CA-CB	5.21	1.62	1.53
1	A	893	TYR	N-CA	-5.21	1.39	1.46
1	B	329	ARG	CD-NE	5.20	1.53	1.46
1	A	22	TYR	CA-CB	5.20	1.61	1.53
1	C	904	PHE	N-CA	-5.19	1.39	1.46
2	D	192	LYS	CA-CB	5.19	1.61	1.53
1	A	635	ASN	CA-C	5.19	1.59	1.52
1	B	82	ARG	N-CA	-5.19	1.39	1.46
1	C	734	ASP	C-N	5.19	1.40	1.33
1	C	242	GLU	C-N	5.18	1.41	1.33
2	E	144	PRO	C-N	5.18	1.39	1.33
1	A	224	LYS	C-N	5.17	1.41	1.33
1	C	636	ASP	C-N	5.17	1.41	1.33
1	C	685	LYS	N-CA	5.17	1.52	1.46
1	B	644	ASP	CA-CB	5.17	1.62	1.53
1	C	747	SER	C-N	5.17	1.40	1.33
2	F	155	SER	N-CA	-5.17	1.39	1.45
1	A	467	LEU	N-CA	-5.17	1.40	1.46
1	A	708	ASP	C-N	-5.17	1.26	1.33
1	A	79	TYR	N-CA	-5.17	1.40	1.46
1	A	875	SER	N-CA	5.17	1.52	1.45
1	C	601	ARG	NE-CZ	-5.17	1.27	1.33
1	B	567	ALA	C-N	5.17	1.40	1.33
1	C	903	THR	N-CA	5.17	1.52	1.46
1	B	209	GLN	C-N	5.16	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	354	LEU	CA-C	5.16	1.58	1.52
1	C	484	LEU	N-CA	5.16	1.52	1.46
2	F	31	LYS	CA-CB	5.16	1.61	1.53
1	A	838	GLY	CA-C	-5.15	1.46	1.52
1	C	400	ILE	CA-C	-5.15	1.46	1.52
2	D	105	PHE	N-CA	-5.15	1.39	1.45
1	C	564	LYS	CA-CB	5.14	1.61	1.54
2	D	66	PRO	CA-C	5.14	1.58	1.52
1	A	269	THR	C-O	-5.14	1.18	1.24
1	A	378	ASP	CA-C	5.14	1.59	1.52
1	C	230	LYS	N-CA	-5.14	1.39	1.46
1	C	555	VAL	CA-CB	-5.14	1.47	1.54
1	B	27	LEU	CA-C	5.14	1.59	1.52
2	D	219	ASP	CA-C	5.14	1.60	1.52
1	B	10	SER	C-N	5.13	1.41	1.33
1	B	901	ASP	C-O	-5.13	1.18	1.24
1	C	360	LEU	C-N	5.13	1.40	1.33
1	B	569	LYS	CA-C	5.13	1.59	1.52
1	B	632	MET	N-CA	-5.13	1.40	1.46
1	C	338	TYR	CZ-OH	5.13	1.48	1.38
2	D	5	ASP	CA-CB	5.13	1.61	1.53
1	A	523	TRP	CA-CB	5.13	1.62	1.53
1	A	867	ARG	C-O	-5.13	1.17	1.23
1	C	628	THR	N-CA	5.13	1.52	1.46
2	E	55	ILE	C-N	5.12	1.40	1.33
1	B	532	ASN	C-N	-5.12	1.28	1.34
1	C	825	SER	CA-CB	5.12	1.62	1.53
1	C	764	TRP	N-CA	-5.12	1.40	1.46
2	E	191	ALA	CA-C	5.12	1.60	1.52
1	A	294	THR	N-CA	5.12	1.52	1.46
2	E	31	LYS	CA-C	5.12	1.58	1.52
2	E	93	TYR	CA-CB	5.11	1.62	1.53
1	C	478	LEU	CB-CG	5.11	1.63	1.53
1	C	582	TRP	CA-C	-5.11	1.46	1.52
1	C	324	ASN	CA-C	5.11	1.58	1.52
2	D	207	THR	CA-C	5.11	1.58	1.52
1	A	221	ARG	CD-NE	5.11	1.53	1.46
1	A	400	ILE	C-O	5.11	1.30	1.24
1	B	892	LEU	CA-CB	5.11	1.61	1.53
2	D	195	GLY	N-CA	5.11	1.52	1.45
1	C	356	ALA	C-N	5.10	1.40	1.33
1	A	185	ILE	C-N	5.10	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	10	VAL	CA-C	-5.10	1.47	1.52
2	E	197	VAL	CA-CB	5.10	1.61	1.54
1	C	28	VAL	CA-CB	-5.10	1.48	1.54
1	A	406	GLU	N-CA	5.09	1.52	1.46
1	C	263	MET	C-N	5.09	1.40	1.33
2	F	164	VAL	N-CA	-5.09	1.40	1.46
1	B	767	VAL	C-O	-5.09	1.18	1.24
1	C	707	LEU	CA-CB	5.09	1.61	1.53
1	B	814	GLN	CA-C	5.08	1.58	1.52
2	E	9	ILE	N-CA	-5.08	1.40	1.46
1	B	32	ARG	C-N	5.08	1.40	1.33
1	B	684	THR	C-N	5.08	1.40	1.33
1	C	82	ARG	C-N	5.08	1.40	1.33
1	C	369	TYR	C-O	5.08	1.30	1.24
2	E	189	TYR	CB-CG	-5.08	1.40	1.51
1	A	494	SER	N-CA	5.07	1.52	1.46
1	B	207	GLU	CA-CB	5.07	1.60	1.53
1	C	139	THR	C-O	-5.07	1.17	1.23
1	C	167	VAL	CA-C	-5.07	1.46	1.52
1	C	571	LEU	N-CA	5.07	1.52	1.45
1	C	718	LYS	CA-C	-5.07	1.47	1.52
2	E	140	GLU	CA-CB	5.07	1.61	1.53
1	A	631	ALA	CA-CB	-5.07	1.45	1.53
1	B	904	PHE	N-CA	-5.07	1.39	1.46
1	B	906	VAL	CA-C	-5.06	1.46	1.52
1	C	871	ARG	NE-CZ	5.06	1.38	1.33
2	F	131	GLN	N-CA	5.06	1.55	1.46
1	A	277	ASP	CA-C	5.06	1.59	1.52
1	A	40	LEU	CA-C	5.05	1.59	1.52
1	B	536	HIS	CG-ND1	5.05	1.43	1.38
1	C	293	GLU	C-N	5.05	1.39	1.33
1	A	516	TYR	C-N	5.05	1.39	1.33
2	E	16	SER	CA-CB	5.05	1.61	1.53
1	A	351	ALA	C-N	5.05	1.40	1.33
1	C	669	ARG	CZ-NH2	-5.05	1.26	1.33
1	A	894	ALA	CA-C	5.05	1.59	1.52
1	C	742	PHE	CA-C	-5.05	1.46	1.52
1	A	395	PRO	N-CA	-5.04	1.40	1.47
2	E	210	MET	CA-C	-5.04	1.46	1.52
1	C	847	TYR	CA-C	5.04	1.58	1.53
1	A	73	GLU	CA-CB	5.04	1.65	1.53
1	A	920	GLU	C-N	5.04	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	328	PHE	C-N	5.03	1.40	1.33
2	D	179	GLY	N-CA	-5.03	1.38	1.45
1	A	810	TYR	CA-CB	5.03	1.61	1.53
2	E	206	SER	CA-CB	5.03	1.61	1.53
1	B	719	LYS	N-CA	5.03	1.52	1.46
2	D	2	LYS	CA-CB	5.03	1.62	1.53
1	C	324	ASN	C-O	-5.02	1.18	1.24
1	C	50	ALA	C-N	-5.02	1.27	1.33
1	A	907	ASP	C-N	-5.02	1.28	1.33
2	F	211	GLU	CA-C	-5.02	1.46	1.52
1	A	386	TRP	NE1-CE2	-5.02	1.31	1.37
1	A	291	ASP	CA-C	5.01	1.59	1.53
1	B	243	ASN	CA-CB	5.01	1.62	1.53
1	A	855	VAL	CA-C	5.01	1.58	1.52
1	A	333	ILE	CA-CB	5.01	1.60	1.54
2	E	65	VAL	CA-C	-5.01	1.49	1.53
1	A	220	GLY	CA-C	5.01	1.57	1.51
1	C	665	SER	C-N	5.01	1.39	1.33
1	C	757	GLN	C-N	5.01	1.39	1.33
2	F	137	SER	CA-C	-5.00	1.46	1.52
1	C	736	LEU	N-CA	5.00	1.52	1.45
1	A	330	ASP	C-N	5.00	1.40	1.33
2	D	96	HIS	N-CA	-5.00	1.40	1.46

All (1565) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	ARG	NE-CZ-NH2	-13.91	106.68	119.20
2	E	183	ARG	NE-CZ-NH2	-12.82	107.66	119.20
1	A	836	ARG	NE-CZ-NH1	-12.61	108.89	121.50
1	C	280	THR	O-C-N	-12.59	113.04	121.85
1	C	82	ARG	NE-CZ-NH2	12.12	130.11	119.20
2	E	196	ARG	NE-CZ-NH1	11.87	133.37	121.50
2	F	168	ARG	NE-CZ-NH2	-11.76	108.61	119.20
1	A	836	ARG	NE-CZ-NH2	11.62	129.66	119.20
1	B	746	ARG	NE-CZ-NH2	-11.41	108.93	119.20
1	C	558	HIS	CA-CB-CG	11.39	125.19	113.80
1	B	746	ARG	NE-CZ-NH1	10.76	132.26	121.50
1	C	749	ASP	CA-CB-CG	10.59	123.19	112.60
1	A	69	PRO	CA-C-N	10.52	134.87	120.46
1	A	69	PRO	C-N-CA	10.52	134.87	120.46
2	F	138	GLY	N-CA-C	10.47	123.85	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	797	PHE	CA-CB-CG	10.46	124.26	113.80
1	A	534	PHE	CA-CB-CG	-10.43	103.37	113.80
1	B	749	ASP	CA-CB-CG	10.41	123.02	112.60
1	C	841	TYR	CA-C-N	10.37	130.46	119.78
1	C	841	TYR	C-N-CA	10.37	130.46	119.78
1	B	52	THR	N-CA-C	10.35	122.14	111.07
1	B	384	SER	N-CA-C	10.34	122.55	111.28
1	C	449	ASN	CA-CB-CG	-10.11	102.49	112.60
2	F	69	PHE	CA-CB-CG	-10.03	103.77	113.80
1	B	836	ARG	NE-CZ-NH2	10.00	128.20	119.20
1	C	756	ALA	N-CA-C	9.93	125.05	111.54
1	B	643	ASN	CA-CB-CG	9.91	122.51	112.60
1	C	553	ARG	NE-CZ-NH1	-9.86	111.64	121.50
1	A	45	ARG	NE-CZ-NH1	-9.84	111.66	121.50
2	F	142	LYS	O-C-N	-9.83	112.94	123.26
1	B	498	ASN	CA-CB-CG	-9.80	102.80	112.60
1	B	409	LEU	CA-C-N	9.56	129.60	119.76
1	B	409	LEU	C-N-CA	9.56	129.60	119.76
1	A	846	PRO	CA-C-N	9.51	133.58	120.65
1	A	846	PRO	C-N-CA	9.51	133.58	120.65
1	A	289	ASP	CA-CB-CG	9.43	122.03	112.60
1	C	405	THR	N-CA-C	9.43	124.14	110.10
1	C	931	HIS	CA-CB-CG	9.42	123.22	113.80
1	B	217	HIS	CA-CB-CG	-9.29	104.50	113.80
1	A	738	THR	O-C-N	-9.25	113.74	121.23
1	C	836	ARG	NE-CZ-NH2	9.22	127.50	119.20
1	B	475	ASN	CA-CB-CG	-9.21	103.39	112.60
1	A	941	ARG	NE-CZ-NH2	9.12	127.41	119.20
2	E	68	ARG	NE-CZ-NH1	9.12	130.62	121.50
1	C	785	SER	N-CA-C	9.10	121.19	111.28
1	B	49	VAL	CA-C-O	9.01	129.37	120.27
1	A	942	THR	O-C-N	-8.98	112.51	121.94
1	B	813	TYR	N-CA-C	8.98	123.53	110.42
1	C	750	GLY	CA-C-N	8.98	132.12	120.44
1	C	750	GLY	C-N-CA	8.98	132.12	120.44
1	A	390	VAL	O-C-N	-8.96	113.39	122.62
1	A	280	THR	CA-C-O	-8.93	110.11	119.22
1	A	601	ARG	NE-CZ-NH2	-8.92	111.17	119.20
1	B	274	GLY	CA-C-N	8.91	132.56	120.54
1	B	274	GLY	C-N-CA	8.91	132.56	120.54
1	B	771	ALA	N-CA-CB	-8.90	97.04	110.12
1	A	195	ALA	O-C-N	-8.89	111.99	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	844	ASN	CA-CB-CG	8.86	121.46	112.60
1	A	103	ARG	NE-CZ-NH2	8.85	127.16	119.20
2	E	216	ARG	NE-CZ-NH1	-8.81	112.69	121.50
1	C	545	ARG	NH1-CZ-NH2	-8.79	107.88	119.30
1	A	311	ARG	NE-CZ-NH2	-8.76	111.31	119.20
1	B	311	ARG	NE-CZ-NH2	-8.74	111.33	119.20
1	B	285	LEU	CA-C-O	8.74	129.90	120.38
1	B	378	ASP	CA-CB-CG	8.74	121.34	112.60
1	B	574	LEU	CA-C-N	8.70	130.71	119.84
1	B	574	LEU	C-N-CA	8.70	130.71	119.84
1	A	38	PHE	CA-CB-CG	-8.68	105.12	113.80
1	C	306	LYS	N-CA-C	8.66	121.49	110.24
1	B	877	ASN	OD1-CG-ND2	-8.65	113.95	122.60
1	B	534	PHE	CA-CB-CG	-8.65	105.15	113.80
1	A	845	PHE	O-C-N	-8.64	115.10	121.84
1	B	418	GLY	CA-C-N	8.61	131.47	120.70
1	B	418	GLY	C-N-CA	8.61	131.47	120.70
1	A	130	ASN	OD1-CG-ND2	-8.58	114.02	122.60
1	C	241	ASN	OD1-CG-ND2	-8.58	114.02	122.60
1	C	543	ARG	NE-CZ-NH1	8.54	130.04	121.50
1	C	609	PHE	CA-CB-CG	-8.52	105.28	113.80
1	B	670	ASN	CA-CB-CG	8.51	121.11	112.60
2	E	110	LYS	CA-C-N	8.50	134.06	122.93
2	E	110	LYS	C-N-CA	8.50	134.06	122.93
2	E	216	ARG	NE-CZ-NH2	8.47	126.82	119.20
2	D	87	PRO	N-CA-CB	8.43	111.53	103.52
1	A	601	ARG	NE-CZ-NH1	8.42	129.92	121.50
1	B	312	GLU	N-CA-C	8.40	120.44	111.28
1	A	643	ASN	CA-CB-CG	8.38	120.98	112.60
1	C	823	ASN	OD1-CG-ND2	-8.35	114.25	122.60
1	B	408	GLU	N-CA-C	8.33	120.36	111.28
1	A	487	SER	CA-C-O	-8.33	113.19	120.19
2	F	217	SER	CA-C-N	8.33	132.97	120.31
2	F	217	SER	C-N-CA	8.33	132.97	120.31
1	B	694	TYR	O-C-N	-8.32	113.67	123.41
1	C	568	ILE	N-CA-C	-8.32	101.93	111.00
2	E	196	ARG	NH1-CZ-NH2	-8.32	108.49	119.30
1	A	22	TYR	N-CA-C	8.31	121.46	111.82
1	A	561	VAL	N-CA-C	8.31	117.85	108.05
1	B	920	GLU	N-CA-C	8.30	122.33	109.96
1	A	561	VAL	CA-C-O	-8.28	113.81	119.19
1	A	793	PHE	N-CA-C	8.28	120.00	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	115	ARG	NE-CZ-NH1	8.26	129.76	121.50
1	A	62	ARG	NE-CZ-NH2	-8.24	111.78	119.20
2	F	236	TYR	CA-C-O	8.24	129.12	120.30
1	C	545	ARG	NE-CZ-NH2	8.22	126.60	119.20
1	A	269	THR	N-CA-C	8.21	120.23	111.28
2	F	215	LEU	N-CA-C	8.17	121.78	110.35
1	A	477	ALA	N-CA-C	8.14	120.88	111.11
1	A	588	VAL	CA-CB-CG2	8.12	124.20	110.40
1	C	175	GLY	O-C-N	-8.12	116.03	123.42
1	A	30	PHE	N-CA-C	8.11	120.11	111.28
1	A	537	HIS	CB-CG-CD2	-8.10	120.67	131.20
1	A	574	LEU	CA-C-N	8.09	128.16	119.90
1	A	574	LEU	C-N-CA	8.09	128.16	119.90
1	B	243	ASN	CA-CB-CG	-8.06	104.53	112.60
1	A	35	GLU	N-CA-C	8.05	119.69	111.07
1	C	894	ALA	N-CA-C	8.05	120.06	111.28
1	B	609	PHE	CA-CB-CG	-8.03	105.77	113.80
1	C	93	LEU	O-C-N	-8.03	112.53	123.12
1	C	9	TRP	CA-C-N	8.02	131.03	120.28
1	C	9	TRP	C-N-CA	8.02	131.03	120.28
1	C	122	ALA	O-C-N	8.02	130.33	122.07
1	B	559	ILE	O-C-N	-8.02	114.42	122.76
1	C	278	ASN	CA-CB-CG	-8.01	104.59	112.60
1	C	749	ASP	N-CA-C	7.99	121.50	110.24
2	D	82	ILE	CA-C-N	7.98	130.81	120.44
2	D	82	ILE	C-N-CA	7.98	130.81	120.44
1	A	410	PRO	N-CA-C	7.98	123.87	110.95
1	C	650	ASN	CA-CB-CG	7.97	120.57	112.60
1	A	823	ASN	N-CA-C	-7.96	96.49	108.99
1	A	517	ILE	N-CA-CB	7.96	119.65	110.82
1	B	687	THR	CA-C-N	7.93	127.93	119.76
1	B	687	THR	C-N-CA	7.93	127.93	119.76
1	A	708	ASP	CA-CB-CG	7.93	120.53	112.60
1	C	532	ASN	OD1-CG-ND2	-7.93	114.67	122.60
1	C	312	GLU	N-CA-C	7.93	119.92	111.28
1	C	867	ARG	N-CA-C	7.90	127.63	110.80
1	B	26	GLY	CA-C-N	7.89	131.50	120.29
1	B	26	GLY	C-N-CA	7.89	131.50	120.29
1	B	733	ASN	CA-CB-CG	-7.89	104.71	112.60
1	B	436	ASN	CA-C-N	7.88	127.01	121.65
1	B	436	ASN	C-N-CA	7.88	127.01	121.65
1	A	929	ARG	NE-CZ-NH2	7.87	126.28	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	634	ARG	CD-NE-CZ	7.84	135.37	124.40
1	A	519	LEU	CA-C-O	-7.82	112.43	120.96
1	A	599	ASP	CA-C-N	7.82	131.54	120.28
1	A	599	ASP	C-N-CA	7.82	131.54	120.28
1	C	531	VAL	CA-C-O	7.80	128.58	120.39
2	E	196	ARG	N-CA-C	7.80	121.89	112.38
1	B	688	PRO	N-CA-CB	7.77	110.22	103.31
1	C	456	ASN	CA-CB-CG	7.75	120.35	112.60
1	B	681	ARG	NE-CZ-NH1	7.74	129.24	121.50
1	C	579	THR	CA-C-O	7.74	129.51	120.69
1	C	619	PHE	CA-CB-CG	-7.72	106.08	113.80
1	A	671	TRP	CB-CG-CD2	7.72	137.60	126.80
1	C	657	ALA	CA-C-N	7.71	133.74	122.63
1	C	657	ALA	C-N-CA	7.71	133.74	122.63
1	A	704	ILE	CA-C-N	7.70	128.10	119.32
1	A	704	ILE	C-N-CA	7.70	128.10	119.32
1	A	367	LEU	N-CA-C	7.70	119.67	111.28
1	C	271	ALA	N-CA-CB	-7.69	98.77	110.16
1	A	867	ARG	N-CA-C	7.69	121.99	111.54
1	C	543	ARG	NE-CZ-NH2	-7.69	112.28	119.20
2	D	63	THR	CA-C-N	7.67	132.15	121.26
2	D	63	THR	C-N-CA	7.67	132.15	121.26
1	C	778	GLN	N-CA-C	-7.66	102.14	112.94
1	C	347	LEU	O-C-N	-7.62	114.35	123.27
1	A	357	VAL	N-CA-C	7.60	119.59	107.73
1	B	649	ALA	O-C-N	-7.59	114.69	123.27
1	C	727	SER	N-CA-C	7.57	121.84	111.54
1	A	583	ASN	CA-CB-CG	7.57	120.17	112.60
1	A	635	ASN	OD1-CG-ND2	-7.57	115.03	122.60
2	E	68	ARG	NE-CZ-NH2	-7.57	112.39	119.20
1	C	793	PHE	CA-CB-CG	7.56	121.36	113.80
1	A	732	GLY	O-C-N	-7.55	114.75	122.60
1	B	171	ALA	O-C-N	-7.55	115.23	121.27
1	C	330	ASP	CB-CA-C	7.54	121.66	109.90
2	F	223	TYR	N-CA-CB	7.54	122.41	110.65
1	A	200	GLN	O-C-N	-7.54	112.50	121.39
1	A	44	PHE	CA-CB-CG	-7.53	106.27	113.80
1	B	456	ASN	CA-CB-CG	7.53	120.13	112.60
1	A	830	TYR	CA-C-N	7.52	133.04	122.36
1	A	830	TYR	C-N-CA	7.52	133.04	122.36
1	A	937	THR	O-C-N	-7.52	114.23	123.33
1	B	708	ASP	CA-CB-CG	7.51	120.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	ASN	O-C-N	-7.50	112.69	121.99
2	F	133	GLN	OE1-CD-NE2	-7.50	115.10	122.60
1	A	122	ALA	N-CA-C	7.49	120.32	111.71
1	A	498	ASN	OD1-CG-ND2	-7.47	115.13	122.60
1	A	545	ARG	NH1-CZ-NH2	-7.46	109.60	119.30
1	C	394	ASP	CB-CA-C	7.46	120.12	109.38
2	E	232	PHE	CA-C-N	7.45	129.16	119.84
2	E	232	PHE	C-N-CA	7.45	129.16	119.84
1	A	539	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	A	579	THR	N-CA-CB	7.45	121.49	109.95
1	B	444	GLU	N-CA-C	-7.44	103.33	113.30
2	F	67	SER	N-CA-C	7.40	121.57	112.54
1	B	553	ARG	NE-CZ-NH1	-7.39	114.11	121.50
1	C	746	ARG	NE-CZ-NH1	7.39	128.89	121.50
2	E	199	ILE	CA-C-O	7.39	128.31	120.48
1	B	280	THR	O-C-N	-7.39	116.07	121.83
1	B	570	ASN	CA-C-N	7.38	131.34	120.87
1	B	570	ASN	C-N-CA	7.38	131.34	120.87
2	D	181	ILE	CA-C-O	7.38	128.06	120.39
1	B	565	PHE	CA-CB-CG	-7.37	106.43	113.80
1	B	790	MET	N-CA-C	7.37	119.31	111.28
1	A	796	ASN	OD1-CG-ND2	7.35	129.95	122.60
1	C	922	PHE	CA-CB-CG	-7.35	106.45	113.80
2	F	220	THR	N-CA-CB	7.35	121.30	110.35
1	B	378	ASP	CA-C-N	7.35	132.36	120.60
1	B	378	ASP	C-N-CA	7.35	132.36	120.60
1	A	101	ASP	CA-CB-CG	-7.34	105.26	112.60
2	F	203	ASP	CA-C-N	7.34	131.47	120.31
2	F	203	ASP	C-N-CA	7.34	131.47	120.31
1	C	394	ASP	O-C-N	-7.33	114.61	121.35
1	A	575	PRO	CB-CA-C	7.33	120.86	111.56
2	E	205	LYS	CA-C-N	7.32	133.21	122.82
2	E	205	LYS	C-N-CA	7.32	133.21	122.82
1	B	895	ASN	OD1-CG-ND2	-7.31	115.29	122.60
1	C	82	ARG	NH1-CZ-NH2	-7.31	109.80	119.30
1	B	187	VAL	CA-C-N	7.31	134.22	123.12
1	B	187	VAL	C-N-CA	7.31	134.22	123.12
2	E	188	ASP	CA-CB-CG	7.30	119.90	112.60
1	B	636	ASP	N-CA-C	7.30	118.88	111.07
1	A	31	ALA	N-CA-C	-7.29	103.26	111.07
1	B	574	LEU	CA-C-O	-7.29	114.04	120.60
2	F	164	VAL	O-C-N	-7.29	115.39	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	HIS	CE1-NE2-CD2	-7.29	101.71	109.00
1	A	13	HIS	CA-CB-CG	-7.28	106.52	113.80
1	A	511	GLY	CA-C-N	7.28	133.06	120.68
1	A	511	GLY	C-N-CA	7.28	133.06	120.68
1	B	464	ASN	N-CA-C	7.28	119.29	111.36
1	B	553	ARG	N-CA-C	7.27	120.25	111.82
1	C	578	TYR	O-C-N	-7.27	114.53	123.33
1	A	53	HIS	CE1-NE2-CD2	-7.26	101.74	109.00
1	B	779	GLY	CA-C-N	7.25	132.23	121.72
1	B	779	GLY	C-N-CA	7.25	132.23	121.72
1	C	629	LEU	O-C-N	-7.24	113.90	122.15
1	C	917	VAL	CA-C-O	7.24	128.15	120.48
1	A	675	ARG	NE-CZ-NH1	7.24	128.74	121.50
1	B	391	ASP	CA-CB-CG	-7.22	105.38	112.60
1	C	908	PRO	CB-CA-C	7.22	119.56	111.11
1	C	644	ASP	CA-CB-CG	7.21	119.81	112.60
2	F	196	ARG	NE-CZ-NH2	7.21	125.69	119.20
2	D	231	ASN	N-CA-CB	7.20	120.42	111.79
1	C	246	GLN	OE1-CD-NE2	-7.19	115.41	122.60
2	D	167	VAL	O-C-N	-7.18	115.31	123.00
1	C	90	ASN	CA-CB-CG	-7.18	105.42	112.60
1	A	310	SER	CA-C-O	-7.17	113.21	121.10
1	B	470	ASN	CA-C-N	7.17	129.76	120.44
1	B	470	ASN	C-N-CA	7.17	129.76	120.44
1	C	332	PHE	CA-CB-CG	-7.16	106.64	113.80
1	A	530	ASN	OD1-CG-ND2	7.16	129.75	122.60
2	D	14	SER	CB-CA-C	7.15	119.95	108.87
1	A	608	LYS	CA-C-N	7.14	130.94	120.95
1	A	608	LYS	C-N-CA	7.14	130.94	120.95
1	B	39	SER	O-C-N	-7.13	114.50	123.06
1	A	765	PHE	CA-C-N	7.13	129.71	120.44
1	A	765	PHE	C-N-CA	7.13	129.71	120.44
1	A	898	HIS	CA-CB-CG	7.11	120.91	113.80
1	B	402	ASN	OD1-CG-ND2	-7.11	115.49	122.60
1	A	209	GLN	O-C-N	-7.11	114.56	123.17
1	B	553	ARG	NE-CZ-NH2	7.11	125.60	119.20
1	B	44	PHE	O-C-N	-7.11	114.60	123.27
2	D	115	ARG	NE-CZ-NH2	-7.11	112.80	119.20
1	A	447	ASP	CA-CB-CG	7.11	119.71	112.60
1	B	29	GLN	OE1-CD-NE2	7.09	129.69	122.60
1	C	890	ASN	N-CA-C	7.09	120.77	110.28
1	A	62	ARG	NE-CZ-NH1	7.08	128.58	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	TRP	CB-CG-CD2	7.08	136.71	126.80
1	A	459	MET	CA-C-O	-7.07	113.16	121.44
1	A	479	TYR	CA-C-O	7.07	127.83	119.56
1	A	137	ALA	N-CA-C	7.07	119.98	109.59
1	A	248	ILE	N-CA-C	7.06	119.80	109.63
1	B	599	ASP	CA-C-N	7.06	131.04	120.31
1	B	599	ASP	C-N-CA	7.06	131.04	120.31
1	C	561	VAL	O-C-N	-7.06	113.98	121.11
2	D	86	GLN	O-C-N	-7.06	115.35	121.35
1	C	361	GLN	N-CA-C	7.05	118.97	111.28
1	C	711	PHE	CA-CB-CG	7.05	120.85	113.80
1	C	783	PRO	CA-C-N	7.05	130.72	120.71
1	C	783	PRO	C-N-CA	7.05	130.72	120.71
2	F	44	GLN	O-C-N	-7.05	114.98	123.29
1	C	932	ARG	NE-CZ-NH2	7.04	125.54	119.20
1	A	264	GLN	OE1-CD-NE2	-7.04	115.56	122.60
1	B	580	TYR	CA-C-O	7.04	129.44	120.57
2	F	143	LYS	O-C-N	-7.04	113.08	121.39
1	A	434	GLN	O-C-N	-7.03	114.30	123.16
1	C	81	ALA	CA-C-O	-7.03	113.10	120.70
2	F	97	GLN	CA-C-N	7.03	133.61	122.86
2	F	97	GLN	C-N-CA	7.03	133.61	122.86
1	C	18	ASP	CA-CB-CG	7.02	119.62	112.60
1	B	39	SER	N-CA-CB	7.02	120.36	109.48
1	B	809	LYS	CA-C-O	7.02	126.77	119.05
1	C	13	HIS	CA-C-N	7.01	130.38	120.42
1	C	13	HIS	C-N-CA	7.01	130.38	120.42
1	A	820	HIS	CE1-NE2-CD2	-7.01	101.99	109.00
1	B	496	ASN	CB-CA-C	7.01	119.48	109.38
1	C	378	ASP	CA-CB-CG	7.00	119.60	112.60
1	C	715	HIS	CE1-NE2-CD2	-7.00	102.00	109.00
1	A	276	GLY	CA-C-N	7.00	129.99	120.54
1	A	276	GLY	C-N-CA	7.00	129.99	120.54
2	D	107	GLN	N-CA-C	7.00	118.99	111.36
2	F	61	ARG	NE-CZ-NH1	6.99	128.49	121.50
1	A	907	ASP	N-CA-C	6.98	118.51	109.64
1	B	43	LYS	CA-C-O	6.98	127.96	119.38
1	C	39	SER	N-CA-CB	6.98	120.30	109.48
1	A	177	ASN	CA-CB-CG	6.97	119.58	112.60
1	A	343	ASN	CA-C-N	6.97	130.60	120.71
1	A	343	ASN	C-N-CA	6.97	130.60	120.71
1	B	192	PRO	CA-C-N	6.97	132.33	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	PRO	C-N-CA	6.97	132.33	122.72
1	B	217	HIS	CG-CD2-NE2	6.96	114.16	107.20
1	B	690	LEU	N-CA-C	6.96	120.47	110.10
1	C	794	PHE	CA-C-N	6.96	129.91	120.38
1	C	794	PHE	C-N-CA	6.96	129.91	120.38
1	B	115	TYR	O-C-N	-6.96	115.47	123.33
1	B	681	ARG	NE-CZ-NH2	-6.95	112.94	119.20
2	F	215	LEU	CA-C-O	-6.95	113.56	121.07
1	A	384	SER	N-CA-C	6.95	118.86	111.28
2	F	34	GLN	N-CA-C	-6.95	98.08	108.99
1	C	883	ALA	N-CA-C	6.95	118.93	111.36
2	E	231	ASN	OD1-CG-ND2	-6.94	115.66	122.60
1	C	41	ASN	OD1-CG-ND2	-6.94	115.66	122.60
1	B	35	GLU	N-CA-C	6.94	118.49	111.07
2	E	143	LYS	CA-C-O	-6.94	113.40	120.96
1	B	791	TYR	O-C-N	-6.93	113.68	122.34
1	A	941	ARG	NE-CZ-NH1	-6.93	114.57	121.50
1	B	784	GLU	O-C-N	-6.93	114.35	122.87
1	C	58	ASP	CA-C-O	6.92	127.56	119.32
1	C	532	ASN	O-C-N	-6.92	115.29	121.31
1	B	121	ASN	CA-C-N	6.92	129.85	120.38
1	B	121	ASN	C-N-CA	6.92	129.85	120.38
1	B	785	SER	N-CA-C	6.91	118.47	111.07
1	A	190	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	C	464	ASN	CA-CB-CG	-6.91	105.69	112.60
1	B	805	VAL	N-CA-C	6.90	119.57	109.63
1	A	683	LYS	CA-C-N	6.90	130.22	120.28
1	A	683	LYS	C-N-CA	6.90	130.22	120.28
1	C	886	ASP	CA-CB-CG	6.89	119.49	112.60
1	B	909	MET	CA-C-N	6.89	132.23	120.72
1	B	909	MET	C-N-CA	6.89	132.23	120.72
1	B	865	CYS	CA-C-O	6.89	127.86	120.63
2	E	57	GLN	CA-C-N	6.89	133.35	122.61
2	E	57	GLN	C-N-CA	6.89	133.35	122.61
1	A	826	GLY	CA-C-O	6.88	126.82	119.04
1	A	389	ALA	N-CA-CB	-6.88	100.09	110.35
1	C	743	GLU	CA-C-N	6.88	131.56	120.55
1	C	743	GLU	C-N-CA	6.88	131.56	120.55
1	A	221	ARG	NE-CZ-NH1	6.88	128.38	121.50
1	C	491	VAL	O-C-N	-6.87	116.03	123.18
1	C	639	ASP	O-C-N	-6.87	114.59	122.97
1	A	91	ARG	NE-CZ-NH1	6.87	128.37	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	464	ASN	OD1-CG-ND2	-6.86	115.74	122.60
1	C	134	TRP	O-C-N	-6.85	116.07	123.26
1	B	939	TYR	O-C-N	-6.84	115.18	123.19
1	B	197	LYS	N-CA-C	6.84	119.60	111.33
1	B	738	THR	CA-C-O	-6.84	114.26	119.59
2	D	138	GLY	N-CA-C	6.83	119.78	111.93
1	A	324	ASN	CB-CA-C	6.83	120.93	110.62
1	A	594	SER	CA-C-N	6.83	129.31	120.44
1	A	594	SER	C-N-CA	6.83	129.31	120.44
1	A	762	LYS	N-CA-C	6.82	118.71	111.28
1	A	715	HIS	CG-CD2-NE2	6.81	114.01	107.20
1	B	521	ALA	CA-C-N	6.81	132.32	122.85
1	B	521	ALA	C-N-CA	6.81	132.32	122.85
1	C	525	LEU	CB-CA-C	6.81	120.53	109.90
1	C	526	ASP	N-CA-CB	-6.81	99.84	110.06
2	F	135	VAL	O-C-N	-6.81	115.98	123.20
2	D	159	LEU	CA-C-N	6.79	128.84	120.22
2	D	159	LEU	C-N-CA	6.79	128.84	120.22
1	B	554	TYR	CA-C-O	6.79	127.62	120.36
1	C	202	GLU	CA-C-N	6.79	126.41	119.56
1	C	202	GLU	C-N-CA	6.79	126.41	119.56
1	A	322	ARG	O-C-N	-6.77	114.32	121.30
1	C	574	LEU	CA-C-N	6.77	128.30	119.84
1	C	574	LEU	C-N-CA	6.77	128.30	119.84
2	E	183	ARG	NH1-CZ-NH2	6.77	128.10	119.30
1	A	511	GLY	N-CA-C	6.76	121.91	114.40
1	A	794	PHE	CA-C-N	6.76	130.25	120.38
1	A	794	PHE	C-N-CA	6.76	130.25	120.38
1	B	507	VAL	N-CA-CB	6.75	119.11	111.21
1	B	346	VAL	CA-C-O	6.75	127.79	120.43
2	E	196	ARG	CA-C-N	6.75	133.29	122.50
2	E	196	ARG	C-N-CA	6.75	133.29	122.50
1	B	700	TYR	O-C-N	-6.74	115.45	123.27
1	C	414	PHE	CA-C-N	6.74	127.66	120.11
1	C	414	PHE	C-N-CA	6.74	127.66	120.11
1	C	768	GLN	N-CA-C	6.74	118.28	111.07
1	C	187	VAL	O-C-N	-6.74	115.28	123.09
1	C	230	LYS	CA-C-O	-6.74	113.04	119.91
1	A	501	ASP	O-C-N	-6.73	114.98	122.12
1	C	658	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	B	235	SER	N-CA-C	6.73	120.05	109.96
1	A	315	GLY	CA-C-N	6.72	130.30	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	GLY	C-N-CA	6.72	130.30	120.82
2	E	24	ASP	N-CA-C	6.72	119.97	110.23
1	A	597	GLY	CA-C-O	6.71	128.07	119.68
2	E	168	ARG	NE-CZ-NH1	6.71	128.21	121.50
1	B	866	ASP	O-C-N	-6.71	115.55	123.06
1	B	515	CYS	CA-C-N	6.70	133.37	122.65
1	B	515	CYS	C-N-CA	6.70	133.37	122.65
1	A	827	PHE	CA-CB-CG	-6.70	107.10	113.80
1	C	209	GLN	O-C-N	-6.70	115.32	123.30
1	C	507	VAL	N-CA-CB	6.70	119.03	110.99
1	A	506	ARG	NE-CZ-NH2	-6.70	113.17	119.20
1	A	76	ALA	N-CA-CB	-6.69	99.91	110.22
1	A	236	TYR	O-C-N	-6.69	115.24	123.33
1	A	30	PHE	CA-C-N	6.69	129.13	120.44
1	A	30	PHE	C-N-CA	6.69	129.13	120.44
2	E	46	LYS	CA-C-O	-6.68	113.76	120.64
1	A	711	PHE	CA-CB-CG	-6.68	107.12	113.80
1	B	166	HIS	CA-C-O	6.68	127.79	120.71
1	B	227	THR	O-C-N	-6.67	115.21	121.35
1	B	453	VAL	CA-CB-CG1	6.67	121.74	110.40
1	B	11	TYR	CA-C-O	6.67	127.49	120.42
1	C	893	TYR	CA-CB-CG	-6.67	101.90	113.90
1	C	270	GLU	O-C-N	-6.67	115.06	122.12
1	C	631	ALA	N-CA-C	6.67	118.55	111.28
1	A	767	VAL	O-C-N	6.66	128.44	121.91
2	D	115	ARG	CD-NE-CZ	-6.66	115.08	124.40
1	C	624	ASN	OD1-CG-ND2	-6.65	115.95	122.60
1	C	445	PHE	CA-CB-CG	-6.65	107.15	113.80
1	B	332	PHE	CA-CB-CG	-6.64	107.16	113.80
2	F	11	MET	CA-C-O	6.64	127.44	120.54
1	A	125	PRO	O-C-N	6.63	131.31	122.89
1	C	532	ASN	CB-CG-OD1	6.62	134.05	120.80
2	F	143	LYS	CA-C-N	6.62	127.01	119.93
2	F	143	LYS	C-N-CA	6.62	127.01	119.93
1	B	502	TYR	CA-C-N	6.61	129.80	120.28
1	B	502	TYR	C-N-CA	6.61	129.80	120.28
2	D	205	LYS	N-CA-C	-6.61	104.52	112.59
1	B	305	ILE	N-CA-C	-6.61	106.35	112.43
1	B	750	GLY	CA-C-N	6.61	129.80	120.28
1	B	750	GLY	C-N-CA	6.61	129.80	120.28
1	A	807	ASP	CA-CB-CG	6.60	119.20	112.60
1	C	378	ASP	N-CA-C	6.60	119.29	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	571	LEU	N-CA-C	6.59	119.80	110.50
1	C	812	ASP	CA-C-O	6.59	127.48	119.31
1	B	719	LYS	CA-C-O	-6.58	113.86	121.10
1	A	561	VAL	CA-C-N	6.57	127.83	120.66
1	A	561	VAL	C-N-CA	6.57	127.83	120.66
2	E	84	SER	CA-C-N	6.56	131.96	120.87
2	E	84	SER	C-N-CA	6.56	131.96	120.87
1	A	661	ASN	CA-CB-CG	-6.56	106.04	112.60
1	C	894	ALA	O-C-N	-6.56	115.17	122.12
1	B	434	GLN	OE1-CD-NE2	-6.56	116.04	122.60
1	C	863	PHE	CA-CB-CG	6.56	120.36	113.80
1	A	108	ARG	CA-C-O	6.55	127.20	119.28
1	C	202	GLU	O-C-N	-6.54	114.10	121.43
1	A	720	VAL	O-C-N	-6.54	116.11	123.18
1	C	195	ALA	N-CA-C	6.54	119.85	110.10
2	F	191	ALA	CA-C-N	6.54	129.69	120.28
2	F	191	ALA	C-N-CA	6.54	129.69	120.28
1	A	408	GLU	N-CA-C	6.53	124.72	110.80
1	C	679	PHE	N-CA-C	6.53	119.08	108.76
1	A	762	LYS	CA-C-N	6.53	128.92	120.44
1	A	762	LYS	C-N-CA	6.53	128.92	120.44
1	B	587	ASP	N-CA-C	6.53	118.55	109.15
1	C	601	ARG	CA-C-N	6.53	130.99	120.55
1	C	601	ARG	C-N-CA	6.53	130.99	120.55
1	A	27	LEU	CA-C-N	6.52	128.77	120.56
1	A	27	LEU	C-N-CA	6.52	128.77	120.56
2	E	209	TYR	O-C-N	-6.52	114.93	123.21
1	C	457	PHE	CA-CB-CG	-6.51	107.29	113.80
1	B	341	THR	N-CA-C	6.51	118.45	111.36
2	D	16	SER	CA-CB-OG	6.51	124.11	111.10
1	B	585	ARG	NE-CZ-NH2	6.50	125.06	119.20
1	B	816	VAL	CA-C-N	6.50	127.88	120.53
1	B	816	VAL	C-N-CA	6.50	127.88	120.53
1	B	13	HIS	O-C-N	-6.50	113.88	122.00
1	C	539	ASN	CA-C-N	6.49	128.98	120.28
1	C	539	ASN	C-N-CA	6.49	128.98	120.28
1	B	46	ASN	CA-CB-CG	-6.49	106.11	112.60
1	A	740	ASN	CA-CB-CG	-6.49	106.11	112.60
2	D	232	PHE	CA-C-N	6.49	127.95	119.84
2	D	232	PHE	C-N-CA	6.49	127.95	119.84
1	B	363	ARG	NE-CZ-NH1	6.48	127.98	121.50
1	C	37	TYR	N-CA-C	-6.48	103.89	113.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	591	VAL	N-CA-C	6.48	120.12	111.44
1	B	322	ARG	N-CA-C	6.48	118.81	109.48
1	C	756	ALA	N-CA-CB	-6.48	102.19	111.84
2	F	107	GLN	CA-C-O	-6.48	111.77	119.35
1	C	898	HIS	ND1-CE1-NE2	6.47	114.88	108.40
2	D	98	ASP	CA-CB-CG	6.47	119.07	112.60
2	F	12	THR	O-C-N	-6.47	115.35	123.05
1	C	99	TYR	N-CA-C	6.47	118.98	108.76
1	B	704	ILE	CA-C-N	6.46	126.69	119.32
1	B	704	ILE	C-N-CA	6.46	126.69	119.32
1	C	243	ASN	N-CA-CB	6.46	121.27	110.41
1	B	89	ASP	CA-CB-CG	6.46	119.06	112.60
1	B	690	LEU	O-C-N	-6.45	114.95	122.95
1	C	74	ASP	CA-CB-CG	6.45	119.05	112.60
1	C	818	ILE	O-C-N	6.45	128.38	121.87
1	C	835	MET	CA-C-N	6.44	133.85	121.54
1	C	835	MET	C-N-CA	6.44	133.85	121.54
1	A	566	PHE	N-CA-C	6.44	118.30	111.28
1	B	727	SER	N-CA-C	6.44	120.55	111.92
1	B	222	VAL	O-C-N	-6.43	115.92	123.00
1	A	625	THR	CA-C-N	6.43	128.89	120.28
1	A	625	THR	C-N-CA	6.43	128.89	120.28
1	A	715	HIS	CE1-NE2-CD2	-6.43	102.57	109.00
1	B	59	ARG	CA-C-N	6.43	129.96	120.90
1	B	59	ARG	C-N-CA	6.43	129.96	120.90
1	B	232	CYS	CA-C-N	6.42	130.48	121.24
1	B	232	CYS	C-N-CA	6.42	130.48	121.24
1	C	667	PRO	O-C-N	-6.42	115.17	123.00
1	A	794	PHE	CA-C-O	6.41	127.34	120.55
2	E	212	LEU	O-C-N	-6.41	114.90	123.23
1	A	635	ASN	N-CA-CB	6.41	119.39	110.17
1	C	265	PHE	O-C-N	-6.40	115.73	123.10
1	A	638	ASN	O-C-N	-6.40	114.01	122.20
2	E	110	LYS	O-C-N	-6.40	114.67	123.12
1	B	632	MET	N-CA-C	6.40	118.33	111.36
2	D	96	HIS	CE1-NE2-CD2	-6.39	102.61	109.00
1	A	485	LYS	N-CA-C	6.38	119.91	110.46
1	B	69	PRO	N-CA-CB	6.38	108.40	103.30
1	C	296	ASP	CA-CB-CG	6.38	118.98	112.60
1	B	903	THR	CB-CA-C	-6.38	100.99	110.62
1	B	399	ILE	O-C-N	-6.38	114.86	122.77
1	C	514	ASP	CA-C-N	6.38	128.82	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	514	ASP	C-N-CA	6.38	128.82	120.28
1	B	865	CYS	O-C-N	-6.37	117.64	123.50
1	C	65	LEU	N-CA-CB	6.37	120.55	110.23
1	B	621	MET	CG-SD-CE	-6.37	86.88	100.90
2	D	199	ILE	CA-C-O	6.37	127.23	120.48
1	A	425	TYR	N-CA-C	6.37	119.78	109.40
1	C	815	GLN	CA-CB-CG	6.37	126.84	114.10
1	A	849	LEU	N-CA-C	-6.36	104.83	112.59
1	C	715	HIS	ND1-CE1-NE2	6.36	114.76	108.40
1	B	92	VAL	CB-CA-C	6.36	118.77	110.12
1	B	249	LEU	CA-C-N	6.36	131.30	123.10
1	B	249	LEU	C-N-CA	6.36	131.30	123.10
2	F	33	SER	N-CA-CB	6.35	120.44	110.46
1	C	389	ALA	CA-C-O	6.34	129.58	120.51
2	D	79	THR	CA-CB-OG1	6.34	119.11	109.60
1	A	275	ASN	N-CA-C	-6.33	104.82	113.30
1	B	555	VAL	CA-C-O	-6.33	114.54	119.98
1	C	560	GLN	O-C-N	-6.33	115.81	123.27
2	F	55	ILE	O-C-N	-6.32	116.35	123.18
1	A	213	THR	CA-CB-OG1	6.32	119.07	109.60
1	A	523	TRP	O-C-N	-6.32	115.67	123.44
1	A	906	VAL	CA-C-N	6.32	129.17	120.39
1	A	906	VAL	C-N-CA	6.32	129.17	120.39
1	B	41	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	A	263	MET	CG-SD-CE	-6.31	87.03	100.90
1	C	931	HIS	ND1-CE1-NE2	6.30	114.70	108.40
1	C	543	ARG	CA-C-O	6.30	127.44	120.82
1	C	711	PHE	N-CA-C	6.30	119.13	110.24
1	C	223	LEU	O-C-N	-6.30	116.04	123.22
1	A	852	LYS	CA-C-O	6.30	127.23	120.55
1	A	623	HIS	N-CA-C	6.29	118.14	111.28
1	A	446	SER	N-CA-C	6.29	119.10	110.24
2	E	6	ASP	CA-C-N	6.29	131.85	122.99
2	E	6	ASP	C-N-CA	6.29	131.85	122.99
1	C	130	ASN	CA-C-N	6.28	127.27	119.98
1	C	130	ASN	C-N-CA	6.28	127.27	119.98
1	C	275	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	B	480	LEU	CA-C-N	6.27	127.68	119.84
1	B	480	LEU	C-N-CA	6.27	127.68	119.84
1	A	710	THR	CA-C-N	6.27	129.78	120.87
1	A	710	THR	C-N-CA	6.27	129.78	120.87
1	A	694	TYR	CB-CG-CD2	-6.27	111.40	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	ARG	O-C-N	-6.27	115.47	122.12
1	C	268	THR	O-C-N	-6.27	115.10	122.81
1	A	638	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	C	405	THR	CB-CA-C	-6.27	100.13	109.90
1	B	545	ARG	N-CA-CB	6.26	119.98	110.28
2	D	16	SER	N-CA-C	6.25	118.10	111.28
1	B	82	ARG	NE-CZ-NH2	-6.25	113.58	119.20
2	E	102	PRO	N-CA-CB	6.25	109.47	102.60
1	C	492	LYS	N-CA-CB	6.25	119.22	110.04
1	A	537	HIS	CB-CG-ND1	6.24	132.07	122.70
1	B	919	PHE	N-CA-C	6.24	118.98	107.99
2	F	221	ALA	CA-C-O	6.24	128.00	121.38
1	A	768	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	A	462	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	C	537	HIS	CE1-NE2-CD2	-6.23	102.77	109.00
1	A	209	GLN	OE1-CD-NE2	-6.23	116.37	122.60
1	B	245	GLY	CA-C-O	-6.23	114.61	121.71
1	C	796	ASN	N-CA-CB	-6.23	101.07	110.73
2	F	92	THR	CA-C-O	6.23	126.97	120.30
1	B	817	GLY	CA-C-N	6.23	130.31	120.47
1	B	817	GLY	C-N-CA	6.23	130.31	120.47
1	A	216	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	A	454	GLY	O-C-N	-6.22	116.99	122.90
1	B	248	ILE	N-CA-C	6.22	117.08	109.30
1	C	690	LEU	CA-C-N	6.22	131.60	120.77
1	C	690	LEU	C-N-CA	6.22	131.60	120.77
2	D	145	GLY	CA-C-N	6.22	133.42	121.54
2	D	145	GLY	C-N-CA	6.22	133.42	121.54
1	C	605	ALA	O-C-N	-6.22	115.94	122.96
1	C	235	SER	N-CA-CB	6.21	119.10	109.85
1	C	480	LEU	CA-C-N	6.21	127.60	119.84
1	C	480	LEU	C-N-CA	6.21	127.60	119.84
1	C	541	GLY	O-C-N	-6.21	116.23	122.19
2	E	28	ILE	O-C-N	-6.21	116.36	123.00
2	F	50	ALA	CA-C-N	6.21	126.16	119.76
2	F	50	ALA	C-N-CA	6.21	126.16	119.76
1	B	525	LEU	O-C-N	-6.21	115.30	122.93
1	C	162	GLN	CA-C-O	6.21	127.21	120.32
1	C	277	ASP	CA-CB-CG	6.21	118.81	112.60
2	F	36	VAL	CA-C-O	6.20	127.08	120.26
1	C	332	PHE	N-CA-CB	6.20	121.49	112.13
2	F	245	VAL	CA-C-O	6.20	126.38	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	GLY	O-C-N	-6.19	115.63	122.50
2	F	216	ARG	NE-CZ-NH2	6.19	124.77	119.20
2	D	24	ASP	CA-C-N	6.19	130.15	121.24
2	D	24	ASP	C-N-CA	6.19	130.15	121.24
2	E	159	LEU	O-C-N	-6.18	114.99	122.22
1	A	671	TRP	CB-CG-CD1	-6.18	117.63	126.90
1	B	602	VAL	CA-C-O	6.17	127.39	120.85
1	B	908	PRO	N-CA-C	6.17	120.11	110.80
1	B	316	GLN	N-CA-C	6.16	118.92	110.24
1	A	174	SER	N-CA-CB	6.16	120.45	110.42
1	B	585	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	C	773	TYR	CA-C-O	6.15	126.12	118.43
2	D	84	SER	N-CA-CB	6.15	120.34	110.86
1	A	764	TRP	CA-C-N	6.15	128.52	120.28
1	A	764	TRP	C-N-CA	6.15	128.52	120.28
1	B	111	THR	CA-CB-OG1	6.15	118.83	109.60
1	C	93	LEU	CA-C-O	6.15	126.86	120.40
2	F	57	GLN	CG-CD-NE2	6.15	125.63	116.40
1	B	32	ARG	NE-CZ-NH1	6.15	127.65	121.50
1	A	928	HIS	CA-CB-CG	6.15	119.95	113.80
1	B	772	ASN	CA-CB-CG	-6.14	106.46	112.60
2	E	137	SER	CA-C-N	6.14	133.45	121.41
2	E	137	SER	C-N-CA	6.14	133.45	121.41
1	C	688	PRO	O-C-N	-6.14	115.25	122.86
1	A	905	GLU	O-C-N	-6.13	116.03	123.27
1	A	479	TYR	O-C-N	-6.13	114.98	122.34
1	A	715	HIS	CA-CB-CG	6.13	119.93	113.80
1	B	258	GLU	O-C-N	-6.13	115.91	123.33
1	C	531	VAL	CA-CB-CG2	-6.13	99.98	110.40
1	A	477	ALA	O-C-N	-6.13	115.72	122.09
1	A	726	SER	CA-C-N	6.12	133.36	123.93
1	A	726	SER	C-N-CA	6.12	133.36	123.93
1	A	877	ASN	CA-C-N	6.12	131.55	122.74
1	A	877	ASN	C-N-CA	6.12	131.55	122.74
1	A	491	VAL	CA-C-O	-6.10	114.21	120.25
1	C	669	ARG	NH1-CZ-NH2	-6.10	111.37	119.30
1	A	501	ASP	CA-C-N	6.10	128.74	120.44
1	A	501	ASP	C-N-CA	6.10	128.74	120.44
1	A	366	GLU	CA-C-O	6.10	127.22	120.82
1	A	380	THR	CA-C-N	6.10	130.88	122.77
1	A	380	THR	C-N-CA	6.10	130.88	122.77
1	A	836	ARG	CB-CG-CD	6.10	125.33	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	TYR	CB-CG-CD1	-6.10	111.65	120.80
2	E	44	GLN	CA-C-O	6.10	126.95	120.36
2	F	0	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	67	PHE	CA-CB-CG	-6.10	107.70	113.80
1	A	363	ARG	NE-CZ-NH2	6.10	124.69	119.20
1	A	865	CYS	CB-CA-C	-6.10	102.43	111.70
2	F	142	LYS	CA-C-O	6.10	127.84	121.38
1	C	944	PHE	N-CA-C	6.10	118.04	110.91
1	B	565	PHE	O-C-N	6.09	130.32	122.89
1	A	735	ARG	NE-CZ-NH2	-6.09	113.72	119.20
1	A	518	ASN	CA-C-N	6.09	129.76	121.05
1	A	518	ASN	C-N-CA	6.09	129.76	121.05
1	B	810	TYR	CB-CG-CD1	6.09	129.93	120.80
1	C	373	LEU	N-CA-C	6.09	118.70	111.33
1	C	680	THR	O-C-N	-6.09	114.88	122.73
1	A	438	TRP	N-CA-C	6.08	118.66	109.23
1	A	225	LYS	CA-C-O	6.08	126.89	119.11
1	A	319	MET	O-C-N	-6.07	114.99	122.16
1	B	858	ILE	O-C-N	6.07	128.34	122.69
1	A	780	PHE	N-CA-C	6.07	119.15	110.10
1	A	679	PHE	CA-CB-CG	-6.07	107.73	113.80
1	A	877	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	A	623	HIS	CE1-NE2-CD2	-6.07	102.93	109.00
1	A	62	ARG	N-CA-C	6.06	119.02	110.23
1	C	579	THR	O-C-N	-6.06	115.95	123.04
1	B	385	MET	CG-SD-CE	-6.06	87.57	100.90
1	C	56	THR	O-C-N	-6.06	115.59	122.68
1	B	593	GLN	O-C-N	-6.06	116.22	123.31
2	F	78	PHE	CA-CB-CG	-6.06	107.74	113.80
2	F	38	ASN	N-CA-C	-6.05	105.07	112.88
1	C	807	ASP	CB-CA-C	6.05	120.20	110.09
1	C	365	THR	O-C-N	-6.05	115.25	122.15
2	E	215	LEU	CA-C-N	6.05	132.00	122.21
2	E	215	LEU	C-N-CA	6.05	132.00	122.21
1	A	474	SER	CA-C-O	6.04	126.83	120.42
1	A	164	LYS	CA-C-O	6.04	127.01	120.43
1	A	178	ILE	O-C-N	-6.04	117.54	122.97
1	A	545	ARG	NE-CZ-NH1	6.04	127.54	121.50
1	C	378	ASP	CB-CA-C	6.04	119.31	110.26
1	C	790	MET	N-CA-C	6.03	117.85	111.28
1	C	932	ARG	NH1-CZ-NH2	-6.02	111.47	119.30
1	A	370	GLN	CA-C-N	6.02	128.35	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	GLN	C-N-CA	6.02	128.35	120.28
1	A	816	VAL	CA-C-N	6.02	127.00	120.44
1	A	816	VAL	C-N-CA	6.02	127.00	120.44
1	C	632	MET	O-C-N	-6.02	115.29	122.15
1	B	350	GLN	N-CA-C	6.02	118.33	111.11
2	E	230	SER	O-C-N	6.01	128.49	122.12
1	A	42	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	A	324	ASN	CA-CB-CG	-6.01	106.59	112.60
1	C	200	GLN	CA-C-O	-6.01	115.19	120.60
1	C	687	THR	CA-CB-CG2	6.01	120.71	110.50
1	A	610	ASP	CA-CB-CG	6.00	118.61	112.60
1	B	370	GLN	O-C-N	-5.99	115.90	122.07
1	B	773	TYR	CA-C-O	5.99	125.92	118.43
2	D	98	ASP	O-C-N	-5.99	114.95	122.19
1	A	547	MET	N-CA-C	5.98	120.31	112.89
2	F	241	THR	O-C-N	-5.98	116.27	123.27
1	C	788	ASP	O-C-N	-5.98	115.79	122.55
2	E	72	SER	CA-C-O	5.98	127.72	121.38
1	A	772	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	B	115	TYR	N-CA-C	5.98	118.37	108.99
1	A	740	ASN	N-CA-C	-5.97	106.03	113.38
1	A	114	PRO	N-CA-CB	-5.97	96.98	103.25
2	D	137	SER	CA-C-N	5.97	125.77	120.10
2	D	137	SER	C-N-CA	5.97	125.77	120.10
1	A	469	ARG	NE-CZ-NH1	5.97	127.47	121.50
1	C	475	ASN	OD1-CG-ND2	-5.96	116.64	122.60
2	D	34	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	C	125	PRO	CB-CA-C	5.96	118.85	111.23
1	A	688	PRO	O-C-N	-5.95	115.71	122.91
2	F	244	THR	CA-C-O	-5.95	114.38	121.11
1	A	781	TYR	O-C-N	-5.95	117.01	123.26
2	E	34	GLN	O-C-N	-5.95	114.79	122.94
2	F	44	GLN	N-CA-CB	5.95	119.91	110.57
1	C	316	GLN	N-CA-C	5.95	118.96	110.10
1	C	795	ARG	N-CA-C	5.95	118.53	111.33
1	A	489	SER	O-C-N	-5.95	116.40	123.06
1	C	468	TRP	CA-C-N	5.94	128.17	120.44
1	C	468	TRP	C-N-CA	5.94	128.17	120.44
2	E	223	TYR	CA-CB-CG	-5.94	103.20	113.90
2	D	184	GLY	O-C-N	-5.94	115.95	122.84
1	B	49	VAL	O-C-N	-5.94	117.00	123.18
1	B	421	ASN	N-CA-C	5.94	119.07	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	MET	N-CA-C	5.94	119.62	112.38
1	C	670	ASN	O-C-N	-5.93	116.28	123.16
1	C	809	LYS	CA-C-O	5.93	126.66	119.31
1	B	272	ALA	N-CA-C	5.93	120.12	113.01
1	B	465	ALA	N-CA-C	5.92	117.74	111.28
1	A	290	VAL	O-C-N	-5.92	116.82	122.98
1	C	530	ASN	CA-CB-CG	-5.92	106.68	112.60
1	A	536	HIS	O-C-N	-5.92	116.85	123.48
1	B	286	TYR	CA-C-O	5.92	127.23	120.84
1	B	649	ALA	CB-CA-C	5.92	119.51	109.75
1	B	777	TYR	O-C-N	-5.92	114.99	122.27
1	A	746	ARG	NE-CZ-NH1	5.92	127.42	121.50
1	A	902	MET	O-C-N	-5.92	115.70	123.21
1	B	270	GLU	N-CA-C	5.91	117.72	111.28
1	C	9	TRP	N-CA-C	5.91	117.39	111.07
1	B	108	ARG	NE-CZ-NH1	5.91	127.41	121.50
2	E	232	PHE	CA-C-O	-5.90	113.39	120.41
1	A	397	VAL	CA-C-N	5.90	128.44	120.65
1	A	397	VAL	C-N-CA	5.90	128.44	120.65
2	D	141	ASP	O-C-N	-5.90	116.53	123.25
1	A	804	VAL	O-C-N	-5.89	116.29	123.00
1	A	455	ASN	CA-CB-CG	5.89	118.49	112.60
1	A	337	TYR	CA-C-N	5.88	131.42	122.65
1	A	337	TYR	C-N-CA	5.88	131.42	122.65
1	C	526	ASP	N-CA-C	5.88	118.45	111.33
1	A	45	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	B	684	THR	CA-C-N	5.88	128.15	120.28
1	B	684	THR	C-N-CA	5.88	128.15	120.28
2	E	183	ARG	N-CA-C	5.88	119.27	111.75
1	B	364	ASN	O-C-N	-5.87	116.47	123.28
1	A	451	ILE	CB-CA-C	-5.87	101.00	110.28
1	A	466	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	A	695	ASP	CA-CB-CG	5.87	118.47	112.60
2	E	82	ILE	CA-C-N	5.87	128.47	120.54
2	E	82	ILE	C-N-CA	5.87	128.47	120.54
1	B	321	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	C	858	ILE	O-C-N	-5.87	117.23	122.69
1	B	364	ASN	CA-C-N	5.86	128.62	120.29
1	B	364	ASN	C-N-CA	5.86	128.62	120.29
1	B	491	VAL	CA-C-N	5.86	129.60	120.75
1	B	491	VAL	C-N-CA	5.86	129.60	120.75
1	B	799	PRO	N-CA-C	5.86	120.70	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	421	ASN	OD1-CG-ND2	5.86	128.46	122.60
1	C	520	GLY	O-C-N	-5.85	115.48	122.33
1	B	526	ASP	CA-CB-CG	-5.85	106.75	112.60
1	C	922	PHE	CA-C-N	5.85	132.24	123.23
1	C	922	PHE	C-N-CA	5.85	132.24	123.23
2	E	139	ALA	N-CA-C	5.85	118.25	110.53
1	A	84	THR	N-CA-C	-5.85	98.88	108.41
1	A	300	SER	N-CA-C	-5.85	105.24	112.90
1	A	787	LYS	CA-C-O	5.84	126.69	119.79
1	C	371	LEU	O-C-N	-5.84	115.92	122.12
2	F	183	ARG	NE-CZ-NH2	-5.84	113.94	119.20
1	B	635	ASN	CB-CG-ND2	-5.84	107.64	116.40
1	A	680	THR	CA-CB-OG1	5.84	118.36	109.60
1	A	698	TYR	CA-C-O	5.84	126.71	120.46
2	F	204	SER	CA-C-N	5.84	132.18	122.54
2	F	204	SER	C-N-CA	5.84	132.18	122.54
1	B	206	GLY	O-C-N	-5.84	118.70	123.14
1	A	233	TYR	CB-CA-C	5.84	118.56	110.16
1	A	246	GLN	CA-C-O	5.84	125.22	118.97
1	A	528	MET	CA-C-N	5.84	128.10	120.28
1	A	528	MET	C-N-CA	5.84	128.10	120.28
1	B	82	ARG	NE-CZ-NH1	5.84	127.34	121.50
1	C	740	ASN	CB-CG-ND2	-5.84	107.65	116.40
2	E	229	GLY	CA-C-N	5.84	128.10	120.28
2	E	229	GLY	C-N-CA	5.84	128.10	120.28
1	A	841	TYR	N-CA-CB	5.83	117.23	111.10
1	B	768	GLN	O-C-N	-5.83	115.50	122.15
1	C	252	GLN	CA-C-N	5.83	128.10	120.28
1	C	252	GLN	C-N-CA	5.83	128.10	120.28
1	C	324	ASN	CA-C-O	5.83	126.63	120.33
1	A	519	LEU	CB-CA-C	5.83	118.58	109.84
1	C	361	GLN	CA-C-O	5.83	126.73	120.55
2	D	43	TYR	CA-C-N	5.83	131.04	123.00
2	D	43	TYR	C-N-CA	5.83	131.04	123.00
2	F	181	ILE	CA-C-O	5.83	126.45	120.39
1	A	89	ASP	N-CA-CB	5.82	119.15	109.60
1	A	278	ASN	CB-CG-OD1	5.82	132.45	120.80
2	D	135	VAL	CA-C-O	5.82	126.50	120.39
1	A	640	GLN	O-C-N	-5.82	116.15	123.01
1	B	528	MET	CA-C-O	5.82	125.78	119.15
1	C	184	GLN	CA-C-O	5.82	127.32	120.69
1	A	608	LYS	CB-CA-C	5.81	119.40	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	851	GLY	CA-C-N	5.81	128.07	120.28
1	A	851	GLY	C-N-CA	5.81	128.07	120.28
2	F	92	THR	O-C-N	-5.81	116.53	123.27
1	B	828	VAL	CA-C-N	5.80	126.77	120.44
1	B	828	VAL	C-N-CA	5.80	126.77	120.44
1	B	885	THR	O-C-N	-5.80	115.81	122.89
1	A	60	SER	N-CA-CB	5.80	119.33	109.87
1	C	176	ILE	N-CA-C	5.80	116.54	110.62
1	C	238	LYS	N-CA-C	5.80	117.90	109.84
1	B	266	PHE	N-CA-C	5.80	118.21	109.23
1	A	585	ARG	CA-C-O	-5.79	114.81	121.47
1	B	53	HIS	CA-C-N	5.79	130.36	122.07
1	B	53	HIS	C-N-CA	5.79	130.36	122.07
2	E	233	PRO	CA-C-N	5.79	129.34	121.05
2	E	233	PRO	C-N-CA	5.79	129.34	121.05
1	C	715	HIS	CA-CB-CG	-5.79	108.01	113.80
2	E	219	ASP	N-CA-C	5.79	120.34	113.16
1	A	275	ASN	CA-CB-CG	5.79	118.39	112.60
1	B	177	ASN	CA-CB-CG	5.79	118.39	112.60
1	C	293	GLU	O-C-N	-5.79	117.23	123.42
2	F	82	ILE	N-CA-CB	5.79	118.96	111.67
1	B	379	ARG	CA-C-N	5.78	128.35	120.54
1	B	379	ARG	C-N-CA	5.78	128.35	120.54
1	A	932	ARG	NH1-CZ-NH2	-5.78	111.78	119.30
1	B	451	ILE	N-CA-CB	5.78	120.94	111.58
1	C	54	ASP	CA-C-O	5.78	125.97	119.78
1	C	792	SER	N-CA-C	5.78	119.03	110.48
1	A	442	ALA	N-CA-C	-5.78	103.72	111.87
1	B	116	SER	CA-C-O	-5.78	114.90	121.72
1	B	184	GLN	CA-C-O	5.77	127.19	120.49
1	A	789	ARG	NE-CZ-NH1	5.77	127.27	121.50
1	A	372	LEU	N-CA-C	5.77	117.24	111.07
1	A	499	THR	N-CA-C	5.77	118.63	110.50
1	B	753	TYR	O-C-N	-5.77	115.26	122.35
1	C	793	PHE	N-CA-C	5.76	117.25	110.97
1	C	133	GLU	N-CA-C	5.76	118.86	109.59
1	A	278	ASN	CB-CG-ND2	-5.76	107.76	116.40
1	B	52	THR	CA-C-O	-5.76	114.78	120.82
1	C	418	GLY	N-CA-C	-5.76	107.70	115.36
1	C	200	GLN	N-CA-C	5.75	118.23	110.29
2	E	195	GLY	CA-C-N	5.75	129.81	120.60
2	E	195	GLY	C-N-CA	5.75	129.81	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	215	LEU	N-CA-CB	5.75	118.52	109.83
2	F	163	GLY	O-C-N	-5.75	117.23	122.93
1	A	543	ARG	CA-C-N	5.75	127.99	120.28
1	A	543	ARG	C-N-CA	5.75	127.99	120.28
1	C	337	TYR	CA-C-N	5.75	132.15	121.62
1	C	337	TYR	C-N-CA	5.75	132.15	121.62
1	A	802	ARG	NE-CZ-NH2	5.75	124.37	119.20
1	A	870	TRP	N-CA-CB	5.75	118.86	109.95
1	C	41	ASN	CB-CG-ND2	5.75	125.02	116.40
1	A	506	ARG	NE-CZ-NH1	5.74	127.24	121.50
1	B	302	MET	CA-CB-CG	5.74	125.59	114.10
1	B	463	LEU	N-CA-C	5.74	117.22	111.07
1	B	636	ASP	CA-C-O	5.74	126.85	120.82
1	A	449	ASN	CA-CB-CG	-5.74	106.86	112.60
1	B	262	GLU	CB-CG-CD	-5.74	102.84	112.60
1	B	47	PRO	N-CA-C	-5.74	100.65	112.47
1	B	932	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	A	29	GLN	N-CA-CB	5.73	118.48	109.94
1	A	843	ALA	N-CA-CB	-5.73	101.91	110.17
1	A	898	HIS	CE1-NE2-CD2	-5.73	103.27	109.00
1	B	74	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	161	GLU	CA-C-N	5.73	130.04	122.42
1	B	161	GLU	C-N-CA	5.73	130.04	122.42
1	B	357	VAL	O-C-N	-5.73	116.41	122.83
1	B	824	ASN	CA-CB-CG	-5.73	106.87	112.60
1	B	488	PRO	N-CA-CB	5.73	108.33	103.35
1	C	402	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	B	783	PRO	N-CA-C	5.73	120.22	111.34
1	C	166	HIS	CA-C-N	5.73	130.43	122.93
1	C	166	HIS	C-N-CA	5.73	130.43	122.93
2	D	194	GLN	N-CA-C	5.73	119.85	112.86
1	A	129	PRO	CA-C-N	5.72	128.35	120.39
1	A	129	PRO	C-N-CA	5.72	128.35	120.39
1	B	661	ASN	CA-C-N	5.72	129.54	123.25
1	B	661	ASN	C-N-CA	5.72	129.54	123.25
2	E	230	SER	N-CA-C	-5.72	105.04	111.28
1	A	316	GLN	CB-CG-CD	-5.72	102.88	112.60
2	D	223	TYR	CA-C-O	5.72	126.42	120.30
1	B	875	SER	CA-C-O	-5.72	114.59	120.99
1	C	504	ASN	CA-CB-CG	5.72	118.32	112.60
1	B	177	ASN	CA-C-N	5.71	131.41	122.84
1	B	177	ASN	C-N-CA	5.71	131.41	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	537	HIS	CE1-NE2-CD2	-5.71	103.28	109.00
1	C	558	HIS	N-CA-CB	5.71	120.19	110.71
1	C	741	GLU	CA-C-O	5.71	127.92	120.21
2	E	113	ILE	CA-C-N	5.71	130.00	121.72
2	E	113	ILE	C-N-CA	5.71	130.00	121.72
1	A	52	THR	O-C-N	5.71	129.48	122.34
2	F	31	LYS	CG-CD-CE	5.71	124.43	111.30
2	D	227	ARG	CA-C-O	5.71	127.56	120.54
1	B	924	VAL	O-C-N	-5.71	116.83	122.76
1	B	337	TYR	N-CA-C	5.70	117.75	108.63
1	B	810	TYR	CB-CG-CD2	-5.70	112.24	120.80
1	B	334	GLY	CA-C-O	5.70	125.31	119.10
1	C	746	ARG	NH1-CZ-NH2	-5.70	111.89	119.30
1	A	456	ASN	CA-CB-CG	5.69	118.29	112.60
1	A	480	LEU	N-CA-CB	5.69	118.62	110.03
1	B	657	ALA	CA-C-N	5.69	130.65	122.40
1	B	657	ALA	C-N-CA	5.69	130.65	122.40
1	B	45	ARG	N-CA-C	5.68	118.47	110.23
1	B	636	ASP	O-C-N	-5.68	116.22	122.07
1	B	814	GLN	O-C-N	-5.67	116.67	123.31
2	F	173	GLN	OE1-CD-NE2	-5.67	116.93	122.60
1	A	543	ARG	O-C-N	-5.67	116.23	122.07
1	C	422	ASN	N-CA-C	-5.67	100.79	109.41
1	C	928	HIS	CE1-NE2-CD2	-5.67	103.33	109.00
1	C	264	GLN	OE1-CD-NE2	5.67	128.27	122.60
1	A	932	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	C	573	LEU	N-CA-C	5.67	117.53	108.41
2	F	3	ASP	CA-C-N	5.66	129.39	121.24
2	F	3	ASP	C-N-CA	5.66	129.39	121.24
1	A	276	GLY	N-CA-C	5.66	121.81	115.08
1	A	335	LEU	N-CA-C	-5.66	105.19	111.36
2	E	44	GLN	O-C-N	-5.66	116.56	123.30
2	F	193	PHE	CA-C-N	5.66	130.16	122.07
2	F	193	PHE	C-N-CA	5.66	130.16	122.07
1	A	90	ASN	N-CA-C	5.66	119.48	112.24
1	B	227	THR	N-CA-CB	5.66	117.64	110.23
1	B	754	ASN	CA-CB-CG	-5.66	106.94	112.60
1	C	531	VAL	O-C-N	-5.66	117.15	123.26
1	A	348	ALA	CA-C-N	5.65	126.31	120.60
1	A	348	ALA	C-N-CA	5.65	126.31	120.60
1	B	692	SER	N-CA-C	5.65	120.24	113.23
1	C	919	PHE	CA-CB-CG	-5.65	108.15	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	TYR	N-CA-CB	5.65	118.80	109.88
1	B	558	HIS	CA-CB-CG	5.65	119.45	113.80
2	F	36	VAL	O-C-N	-5.65	114.77	122.11
1	C	369	TYR	CA-C-N	5.64	128.10	120.65
1	C	369	TYR	C-N-CA	5.64	128.10	120.65
1	B	286	TYR	O-C-N	-5.64	115.93	122.87
2	F	205	LYS	CA-C-N	5.64	130.37	122.36
2	F	205	LYS	C-N-CA	5.64	130.37	122.36
1	A	261	VAL	N-CA-CB	5.64	117.69	110.13
2	E	185	GLY	CA-C-O	5.64	125.29	118.86
1	A	284	VAL	O-C-N	-5.64	116.98	123.07
1	C	267	SER	CA-C-N	5.63	129.26	120.75
1	C	267	SER	C-N-CA	5.63	129.26	120.75
1	C	450	GLU	CB-CG-CD	5.63	122.18	112.60
1	B	17	GLN	CB-CG-CD	5.63	122.17	112.60
1	B	250	VAL	CA-C-N	5.63	129.89	121.72
1	B	250	VAL	C-N-CA	5.63	129.89	121.72
1	B	455	ASN	O-C-N	-5.63	116.10	122.68
2	D	86	GLN	CA-C-N	5.62	125.33	119.82
2	D	86	GLN	C-N-CA	5.62	125.33	119.82
1	B	659	ALA	CA-C-O	5.62	126.67	120.71
2	F	240	GLY	N-CA-C	-5.62	105.68	112.48
1	A	108	ARG	NE-CZ-NH2	-5.62	114.14	119.20
1	A	299	ILE	N-CA-C	5.62	116.82	108.23
1	B	217	HIS	ND1-CE1-NE2	5.61	114.01	108.40
1	A	496	ASN	OD1-CG-ND2	-5.61	116.99	122.60
1	C	244	GLY	CA-C-N	5.61	125.43	120.10
1	C	244	GLY	C-N-CA	5.61	125.43	120.10
1	B	6	MET	O-C-N	-5.61	114.03	123.00
1	C	621	MET	CA-C-N	5.61	128.73	120.82
1	C	621	MET	C-N-CA	5.61	128.73	120.82
1	A	759	ASN	OD1-CG-ND2	-5.61	116.99	122.60
1	C	715	HIS	ND1-CG-CD2	-5.61	100.49	106.10
1	A	725	ASP	O-C-N	-5.60	115.14	122.59
1	A	403	HIS	CA-CB-CG	5.60	119.40	113.80
1	C	261	VAL	CA-CB-CG2	-5.60	100.88	110.40
2	D	222	VAL	CA-C-O	-5.60	113.91	121.02
1	A	929	ARG	NE-CZ-NH1	-5.60	115.90	121.50
1	B	221	ARG	NE-CZ-NH2	-5.60	114.16	119.20
1	B	26	GLY	CA-C-O	5.59	126.51	120.75
1	B	273	ALA	CA-C-N	5.59	126.53	120.44
1	B	273	ALA	C-N-CA	5.59	126.53	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	PHE	CA-CB-CG	-5.59	108.21	113.80
1	B	99	TYR	N-CA-C	5.59	117.68	109.24
1	A	254	ASN	CA-CB-CG	5.58	118.18	112.60
1	A	452	ARG	NH1-CZ-NH2	-5.58	112.04	119.30
1	A	831	LEU	CA-C-N	5.58	132.29	122.08
1	A	831	LEU	C-N-CA	5.58	132.29	122.08
2	E	157	PHE	CA-C-N	5.58	130.06	122.19
2	E	157	PHE	C-N-CA	5.58	130.06	122.19
1	A	21	GLU	N-CA-C	-5.58	106.60	113.41
2	D	132	VAL	N-CA-C	5.58	116.80	109.21
1	B	649	ALA	N-CA-CB	-5.57	101.34	110.43
1	A	920	GLU	CB-CG-CD	5.57	122.07	112.60
1	C	382	TYR	CB-CG-CD1	5.57	129.16	120.80
1	A	801	SER	N-CA-CB	5.57	121.88	111.52
1	B	383	PHE	N-CA-C	5.57	117.50	108.26
1	A	649	ALA	CA-C-O	5.56	126.50	120.43
1	A	843	ALA	O-C-N	-5.56	116.30	122.86
1	C	61	GLN	CA-C-N	5.56	129.37	121.42
1	C	61	GLN	C-N-CA	5.56	129.37	121.42
1	C	566	PHE	N-CA-C	5.56	117.79	111.11
2	F	164	VAL	N-CA-C	5.56	115.90	108.11
1	C	254	ASN	CA-C-O	5.56	126.43	119.59
1	A	840	ALA	CA-C-O	-5.56	114.90	120.96
1	B	452	ARG	NE-CZ-NH1	5.56	127.06	121.50
1	C	507	VAL	CA-C-O	5.56	126.52	120.57
1	A	709	GLY	O-C-N	-5.56	115.95	122.45
1	B	870	TRP	CA-C-O	-5.56	114.94	121.16
1	A	666	ILE	N-CA-CB	5.55	117.55	111.61
1	B	585	ARG	N-CA-C	5.55	118.04	110.55
1	B	781	TYR	CA-C-O	-5.55	115.51	121.45
1	A	582	TRP	CE3-CZ3-CH2	5.55	128.31	121.10
1	B	600	LEU	CA-C-N	5.54	127.64	120.44
1	B	600	LEU	C-N-CA	5.54	127.64	120.44
1	C	51	PRO	CA-C-O	-5.54	115.28	121.32
1	C	84	THR	CA-C-O	5.54	126.39	120.46
2	E	93	TYR	CA-CB-CG	-5.54	103.92	113.90
1	A	275	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	C	699	THR	N-CA-C	5.54	117.32	111.28
1	A	929	ARG	O-C-N	-5.53	115.62	121.04
1	C	371	LEU	CA-C-O	5.53	126.41	120.55
1	B	517	ILE	CA-C-N	5.53	129.97	122.07
1	B	517	ILE	C-N-CA	5.53	129.97	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	554	TYR	CB-CG-CD1	5.53	129.09	120.80
1	A	53	HIS	ND1-CE1-NE2	5.52	113.92	108.40
1	A	755	VAL	N-CA-C	5.52	117.00	108.44
1	B	166	HIS	CA-C-N	5.52	130.37	123.14
1	B	166	HIS	C-N-CA	5.52	130.37	123.14
2	F	111	VAL	CA-CB-CG2	5.52	119.79	110.40
1	B	525	LEU	CA-C-N	5.52	127.68	120.28
1	B	525	LEU	C-N-CA	5.52	127.68	120.28
1	C	439	GLU	CA-C-N	5.52	128.55	120.71
1	C	439	GLU	C-N-CA	5.52	128.55	120.71
1	C	670	ASN	CB-CA-C	5.52	118.64	109.53
2	E	159	LEU	CA-C-O	5.52	126.34	120.10
1	C	322	ARG	CA-C-N	5.52	125.79	119.83
1	C	322	ARG	C-N-CA	5.52	125.79	119.83
1	C	675	ARG	CA-C-O	5.52	124.89	118.77
2	F	42	TRP	CB-CG-CD1	5.52	135.18	126.90
1	B	554	TYR	CB-CG-CD2	-5.51	112.53	120.80
1	B	601	ARG	N-CA-CB	5.51	118.00	110.01
1	A	472	LEU	N-CA-C	5.51	117.29	111.28
1	A	42	ASN	CA-C-N	5.51	130.78	121.14
1	A	42	ASN	C-N-CA	5.51	130.78	121.14
1	A	353	GLN	CA-C-N	5.51	132.06	121.54
1	A	353	GLN	C-N-CA	5.51	132.06	121.54
2	F	115	ARG	NH1-CZ-NH2	-5.51	112.14	119.30
1	B	694	TYR	CA-CB-CG	5.51	123.81	113.90
1	A	593	GLN	CA-CB-CG	5.50	125.11	114.10
1	C	645	TYR	CA-C-O	5.50	126.37	120.70
1	B	119	ALA	N-CA-C	-5.50	106.07	112.89
1	B	369	TYR	N-CA-C	5.50	117.27	111.28
1	B	791	TYR	CA-C-O	5.50	125.78	119.35
1	A	613	CYS	CA-C-O	5.49	127.64	120.11
1	C	676	GLY	O-C-N	-5.49	118.52	123.96
1	A	419	VAL	CA-CB-CG2	-5.49	101.07	110.40
2	E	133	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	A	103	ARG	NH1-CZ-NH2	-5.49	112.17	119.30
1	B	289	ASP	N-CA-C	-5.49	101.59	110.32
1	A	490	ASN	CA-C-N	5.49	131.09	122.70
1	A	490	ASN	C-N-CA	5.49	131.09	122.70
2	E	98	ASP	CA-C-N	5.49	127.57	120.44
2	E	98	ASP	C-N-CA	5.49	127.57	120.44
2	D	16	SER	N-CA-CB	5.48	118.18	110.12
2	D	13	GLN	OE1-CD-NE2	-5.48	117.12	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	THR	CB-CA-C	-5.48	104.09	110.17
1	B	530	ASN	CA-C-O	5.48	126.12	119.11
2	F	200	THR	N-CA-CB	5.48	120.14	111.43
1	A	911	GLU	CA-C-N	5.47	125.48	119.90
1	A	911	GLU	C-N-CA	5.47	125.48	119.90
1	A	138	ALA	CA-C-N	5.47	129.95	122.34
1	A	138	ALA	C-N-CA	5.47	129.95	122.34
2	D	165	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	A	609	PHE	CA-CB-CG	-5.46	108.34	113.80
1	B	39	SER	CB-CA-C	-5.46	101.65	109.84
1	A	124	ALA	CA-C-O	-5.46	114.35	120.25
1	A	905	GLU	N-CA-C	5.46	117.42	108.52
1	A	91	ARG	NE-CZ-NH2	-5.46	114.29	119.20
1	A	332	PHE	O-C-N	-5.46	115.25	122.40
1	C	126	LYS	CA-C-N	5.46	127.21	120.34
1	C	126	LYS	C-N-CA	5.46	127.21	120.34
1	C	883	ALA	O-C-N	-5.46	115.93	122.15
2	E	60	THR	N-CA-CB	5.46	119.16	110.16
1	C	911	GLU	O-C-N	-5.45	118.03	121.85
1	A	666	ILE	CA-C-N	5.45	125.75	119.92
1	A	666	ILE	C-N-CA	5.45	125.75	119.92
1	C	589	ASN	OD1-CG-ND2	-5.45	117.15	122.60
2	D	230	SER	CA-C-O	5.45	126.52	120.90
2	E	200	THR	CA-CB-OG1	5.45	117.78	109.60
1	B	120	TYR	N-CA-C	5.45	117.56	108.02
1	B	471	PHE	CA-CB-CG	5.45	119.25	113.80
1	C	269	THR	CA-CB-OG1	5.45	117.77	109.60
1	C	553	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	B	701	SER	CA-C-O	5.44	125.08	119.97
1	C	263	MET	N-CA-CB	5.44	119.05	110.23
1	C	884	LEU	CA-C-O	5.44	126.53	120.43
1	A	134	TRP	CB-CG-CD1	-5.44	118.74	126.90
1	C	424	THR	CA-C-O	5.44	126.69	120.54
1	C	812	ASP	CA-C-N	5.44	129.07	121.02
1	C	812	ASP	C-N-CA	5.44	129.07	121.02
2	F	5	ASP	CA-C-O	-5.43	115.07	121.16
1	C	714	ASN	CA-CB-CG	-5.43	107.17	112.60
1	B	230	LYS	CA-C-N	5.43	125.35	119.76
1	B	230	LYS	C-N-CA	5.43	125.35	119.76
1	C	852	LYS	N-CA-C	5.43	117.20	111.28
1	B	432	THR	N-CA-C	5.43	119.16	112.54
1	C	266	PHE	CA-C-O	5.42	127.35	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	216	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	C	386	TRP	CZ3-CH2-CZ2	-5.42	114.46	121.50
1	B	202	GLU	N-CA-C	5.41	117.55	110.08
1	B	466	ASN	CA-C-O	5.41	126.28	120.55
1	A	506	ARG	N-CA-C	5.41	118.16	110.10
2	E	16	SER	O-C-N	-5.41	116.50	122.07
1	A	167	VAL	O-C-N	-5.40	117.35	123.18
2	E	61	ARG	N-CA-C	5.40	117.51	109.25
1	C	407	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	792	SER	N-CA-CB	5.40	117.97	110.04
2	E	97	GLN	OE1-CD-NE2	-5.40	117.20	122.60
2	F	183	ARG	CA-C-O	5.40	126.24	120.20
1	A	379	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	B	262	GLU	O-C-N	-5.39	116.22	123.23
1	B	836	ARG	NH1-CZ-NH2	-5.39	112.29	119.30
2	F	14	SER	CA-C-O	-5.39	114.37	120.46
2	E	33	SER	N-CA-C	5.39	117.85	111.33
1	A	643	ASN	CB-CG-ND2	5.38	124.48	116.40
1	B	364	ASN	CA-C-O	5.38	127.73	120.89
1	A	420	GLY	CA-C-N	5.38	129.77	122.07
1	A	420	GLY	C-N-CA	5.38	129.77	122.07
1	A	627	SER	N-CA-CB	5.38	118.03	110.12
1	B	802	ARG	NE-CZ-NH1	-5.38	116.12	121.50
2	D	232	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	297	THR	O-C-N	-5.38	116.67	123.17
1	C	520	GLY	CA-C-O	5.38	124.94	118.97
1	C	537	HIS	ND1-CE1-NE2	5.37	113.77	108.40
1	C	849	LEU	CA-C-O	5.37	125.78	119.28
1	C	933	GLY	CA-C-O	5.37	124.93	118.97
1	A	322	ARG	N-CA-C	5.37	116.46	109.64
1	C	177	ASN	CA-CB-CG	5.37	117.97	112.60
1	B	80	LYS	CA-C-O	5.37	126.40	120.71
2	F	134	LEU	O-C-N	-5.37	116.99	123.27
1	A	580	TYR	CB-CA-C	5.36	119.43	111.17
2	D	202	ASP	O-C-N	-5.36	116.04	123.12
2	D	213	SER	O-C-N	-5.36	115.92	123.11
1	B	941	ARG	NE-CZ-NH2	5.36	124.02	119.20
2	F	181	ILE	O-C-N	-5.36	117.52	123.20
1	B	699	THR	N-CA-C	5.36	118.93	112.93
1	A	118	THR	N-CA-CB	5.36	119.42	110.85
1	A	108	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	C	741	GLU	O-C-N	-5.36	116.85	123.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	THR	N-CA-CB	5.35	119.00	110.65
2	D	219	ASP	CA-C-O	5.35	125.91	119.43
1	B	394	ASP	CA-C-O	5.35	125.15	119.80
1	C	78	SER	O-C-N	-5.35	116.22	122.96
1	C	887	LEU	CA-C-N	5.35	129.94	120.74
1	C	887	LEU	C-N-CA	5.35	129.94	120.74
2	E	205	LYS	N-CA-C	-5.35	105.46	112.41
1	B	832	ALA	CB-CA-C	5.35	118.26	109.97
2	F	166	TRP	CG-CD2-CE3	5.35	139.25	133.90
2	F	214	SER	N-CA-C	5.35	118.81	111.54
2	F	236	TYR	O-C-N	-5.34	117.07	123.27
1	B	168	PHE	O-C-N	-5.34	116.75	123.27
1	A	217	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
1	A	659	ALA	N-CA-CB	5.34	118.36	109.60
1	B	386	TRP	CB-CG-CD1	-5.34	118.89	126.90
1	B	737	LEU	CA-C-O	5.34	126.14	120.10
1	B	861	LYS	O-C-N	-5.34	116.43	123.16
1	C	818	ILE	CA-C-N	5.34	129.15	120.60
1	C	818	ILE	C-N-CA	5.34	129.15	120.60
2	D	211	GLU	CA-C-O	5.34	126.13	120.36
1	B	108	ARG	NH1-CZ-NH2	-5.34	112.36	119.30
1	C	298	HIS	ND1-CE1-NE2	5.34	113.74	108.40
1	B	97	SER	CA-C-N	5.34	129.87	122.77
1	B	97	SER	C-N-CA	5.34	129.87	122.77
1	B	719	LYS	O-C-N	5.34	128.74	123.46
2	E	224	TYR	N-CA-C	5.33	117.66	109.07
1	B	363	ARG	N-CA-C	5.33	118.41	110.52
1	C	603	ASP	O-C-N	-5.33	115.51	122.39
2	E	103	LEU	CA-C-O	-5.33	115.33	121.19
1	B	482	ASP	N-CA-C	5.33	118.88	112.38
2	E	21	SER	CA-C-N	5.33	127.71	120.63
2	E	21	SER	C-N-CA	5.33	127.71	120.63
1	B	908	PRO	CA-C-O	-5.32	114.96	121.03
2	F	94	PHE	CA-CB-CG	-5.32	108.48	113.80
1	A	337	TYR	CA-C-O	5.32	126.73	120.98
1	C	58	ASP	CA-CB-CG	-5.32	107.28	112.60
2	D	159	LEU	O-C-N	-5.32	114.66	122.43
1	A	330	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	614	LEU	N-CA-C	5.32	116.92	108.67
1	C	338	TYR	CA-C-N	5.32	129.92	122.36
1	C	338	TYR	C-N-CA	5.32	129.92	122.36
1	C	550	GLY	CA-C-O	-5.32	116.85	122.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	942	THR	CB-CA-C	-5.32	101.73	109.45
1	B	452	ARG	NE-CZ-NH2	-5.32	114.41	119.20
1	A	452	ARG	CA-C-O	5.32	126.45	120.92
1	B	355	ASN	CB-CA-C	5.32	118.74	109.65
1	A	75	THR	N-CA-CB	5.32	119.03	111.05
1	B	280	THR	CA-C-O	-5.32	114.60	119.76
1	C	356	ALA	O-C-N	-5.32	114.52	122.39
1	C	417	GLY	N-CA-C	5.32	121.25	114.66
2	F	3	ASP	CA-CB-CG	-5.32	107.28	112.60
1	C	211	TYR	CA-C-N	5.31	131.69	121.54
1	C	211	TYR	C-N-CA	5.31	131.69	121.54
1	C	534	PHE	CA-CB-CG	-5.31	108.49	113.80
1	A	51	PRO	N-CA-C	5.31	123.41	112.47
1	B	916	TYR	O-C-N	-5.30	117.03	123.13
1	A	935	ILE	O-C-N	-5.30	115.94	122.57
1	B	316	GLN	O-C-N	-5.30	116.50	122.97
1	C	501	ASP	N-CA-CB	-5.30	102.33	110.12
2	F	160	GLY	O-C-N	-5.30	116.69	122.68
1	B	901	ASP	CA-CB-CG	-5.30	107.30	112.60
1	A	27	LEU	N-CA-C	5.30	117.13	111.36
1	A	233	TYR	N-CA-CB	-5.30	101.14	109.51
1	A	618	PHE	CA-CB-CG	-5.30	108.50	113.80
1	C	528	MET	CA-C-O	-5.30	113.11	119.15
1	C	806	ASP	CA-C-O	5.30	126.72	120.58
2	F	133	GLN	CG-CD-OE1	5.29	131.39	120.80
1	B	545	ARG	CB-CA-C	-5.29	100.51	110.67
1	B	912	PRO	CB-CA-C	5.29	118.01	111.23
1	A	866	ASP	CA-C-O	-5.29	115.70	121.89
1	C	45	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	650	ASN	CA-CB-CG	-5.29	107.31	112.60
1	A	820	HIS	ND1-CE1-NE2	5.29	113.69	108.40
1	B	570	ASN	CA-CB-CG	-5.28	107.32	112.60
1	C	75	THR	CA-CB-OG1	5.28	117.53	109.60
2	E	167	VAL	O-C-N	-5.28	117.32	122.97
1	C	319	MET	CG-SD-CE	-5.28	89.28	100.90
1	C	452	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	A	218	ALA	CA-C-O	5.28	127.64	121.46
1	C	11	TYR	CA-C-O	5.28	126.01	120.42
1	C	820	HIS	O-C-N	-5.28	115.55	122.20
1	A	825	SER	N-CA-C	5.28	116.75	109.15
1	B	190	GLN	CB-CG-CD	5.28	121.57	112.60
2	F	233	PRO	N-CA-C	5.28	123.34	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	ASN	CB-CG-ND2	-5.27	108.49	116.40
1	A	32	ARG	CA-C-N	5.27	127.78	120.29
1	A	32	ARG	C-N-CA	5.27	127.78	120.29
1	B	244	GLY	CA-C-N	5.27	125.11	120.10
1	B	244	GLY	C-N-CA	5.27	125.11	120.10
1	B	367	LEU	N-CA-C	5.27	117.03	111.28
1	A	74	ASP	CA-C-O	5.27	126.72	120.66
1	B	598	ASN	CA-C-O	5.27	128.03	121.81
1	C	298	HIS	CE1-NE2-CD2	-5.27	103.73	109.00
1	C	756	ALA	CA-C-N	5.27	129.62	122.19
1	C	756	ALA	C-N-CA	5.27	129.62	122.19
1	A	50	ALA	CA-C-N	5.27	126.42	119.84
1	A	50	ALA	C-N-CA	5.27	126.42	119.84
1	B	13	HIS	CA-C-O	5.26	126.49	119.59
1	B	530	ASN	O-C-N	-5.26	114.74	122.43
1	C	85	LEU	N-CA-C	5.26	117.29	108.23
1	C	385	MET	N-CA-C	5.26	117.02	111.28
1	B	658	ASN	CB-CG-OD1	5.26	131.33	120.80
1	A	776	GLY	CA-C-N	5.26	127.33	120.28
1	A	776	GLY	C-N-CA	5.26	127.33	120.28
1	B	416	LEU	N-CA-C	5.26	117.76	111.71
1	C	8	GLN	OE1-CD-NE2	-5.26	117.34	122.60
2	E	65	VAL	N-CA-C	5.26	113.07	107.76
1	A	119	ALA	CB-CA-C	5.26	120.24	109.67
1	B	625	THR	O-C-N	-5.26	116.16	122.15
1	A	684	THR	CA-C-N	5.26	127.75	120.29
1	A	684	THR	C-N-CA	5.26	127.75	120.29
1	C	836	ARG	CB-CG-CD	5.26	123.39	111.30
1	C	753	TYR	CB-CG-CD1	5.25	128.68	120.80
1	B	537	HIS	CG-CD2-NE2	5.25	112.45	107.20
1	C	728	VAL	O-C-N	-5.25	115.04	122.76
2	D	91	ALA	CA-C-O	5.25	126.55	121.14
2	F	1	TYR	N-CA-CB	5.25	117.85	110.24
2	F	61	ARG	NH1-CZ-NH2	-5.25	112.48	119.30
1	C	401	GLU	CB-CG-CD	5.25	121.52	112.60
1	A	928	HIS	CG-CD2-NE2	5.24	112.44	107.20
1	B	733	ASN	CA-C-N	5.24	131.55	121.54
1	B	733	ASN	C-N-CA	5.24	131.55	121.54
2	E	10	VAL	N-CA-CB	-5.24	105.08	111.21
2	D	4	ASP	N-CA-C	5.24	117.29	109.59
2	D	51	PRO	N-CA-C	5.24	119.43	111.15
1	C	698	TYR	CA-CB-CG	-5.24	104.48	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	208	VAL	CA-C-N	5.24	130.52	122.93
2	E	208	VAL	C-N-CA	5.24	130.52	122.93
1	B	395	PRO	N-CA-CB	5.23	109.04	103.39
1	A	700	TYR	O-C-N	-5.23	117.12	123.29
2	E	196	ARG	CA-C-O	5.23	125.82	119.49
1	A	414	PHE	CA-C-N	5.23	125.52	119.92
1	A	414	PHE	C-N-CA	5.23	125.52	119.92
1	C	462	ASN	CA-CB-CG	5.23	117.83	112.60
2	E	22	VAL	CA-C-N	5.23	132.63	121.18
2	E	22	VAL	C-N-CA	5.23	132.63	121.18
1	A	525	LEU	N-CA-CB	5.23	117.64	109.85
1	A	533	PRO	CA-C-N	5.22	128.25	120.31
1	A	533	PRO	C-N-CA	5.22	128.25	120.31
1	B	903	THR	O-C-N	-5.22	116.22	123.12
1	C	868	THR	N-CA-CB	5.22	118.36	110.42
1	A	183	ILE	O-C-N	-5.22	116.56	122.72
1	C	255	GLY	N-CA-C	5.22	121.99	115.21
1	C	898	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
1	C	195	ALA	N-CA-CB	-5.22	101.71	109.69
2	D	234	LEU	N-CA-CB	5.22	117.56	109.48
1	B	248	ILE	O-C-N	-5.21	116.99	122.67
2	E	88	GLU	CA-C-O	5.21	125.80	119.49
1	C	556	PRO	N-CA-CB	5.21	106.72	103.23
1	B	309	ASN	N-CA-CB	5.21	118.67	110.23
2	F	115	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	A	839	GLN	CA-C-N	5.21	128.50	121.05
1	A	839	GLN	C-N-CA	5.21	128.50	121.05
1	C	531	VAL	CA-CB-CG1	5.21	119.25	110.40
1	C	53	HIS	CB-CG-CD2	-5.21	124.43	131.20
2	E	241	THR	N-CA-CB	5.21	118.94	110.77
2	D	66	PRO	CA-C-O	-5.20	115.42	122.08
2	D	141	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	415	PRO	CA-C-N	5.20	127.77	120.28
1	A	415	PRO	C-N-CA	5.20	127.77	120.28
2	D	46	LYS	N-CA-CB	5.20	116.31	109.55
2	E	64	GLY	CA-C-N	-5.20	118.85	122.59
2	E	64	GLY	C-N-CA	-5.20	118.85	122.59
1	A	120	TYR	N-CA-CB	5.20	119.09	110.47
1	C	740	ASN	CB-CG-OD1	5.20	131.19	120.80
1	C	334	GLY	O-C-N	-5.19	115.58	122.28
1	C	335	LEU	CA-C-O	-5.19	114.92	120.42
1	A	344	MET	CA-C-O	-5.19	115.48	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	TYR	CA-C-O	5.19	125.92	120.42
2	F	82	ILE	N-CA-C	-5.19	99.69	107.37
1	B	702	GLY	CA-C-N	5.19	129.08	120.94
1	B	702	GLY	C-N-CA	5.19	129.08	120.94
2	F	165	HIS	ND1-CE1-NE2	5.19	113.59	108.40
1	A	355	ASN	CA-CB-CG	5.18	117.78	112.60
1	B	689	SER	N-CA-C	5.18	116.61	109.15
1	C	179	THR	N-CA-CB	5.18	118.70	110.87
2	E	136	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	A	305	ILE	O-C-N	-5.18	117.11	122.14
1	B	198	THR	OG1-CB-CG2	-5.18	98.93	109.30
2	D	141	ASP	CB-CG-OD1	5.18	130.32	118.40
2	F	153	LYS	CB-CG-CD	5.18	123.21	111.30
1	A	268	THR	N-CA-CB	5.18	117.76	110.36
1	A	197	LYS	CA-C-N	5.17	127.47	120.38
1	A	197	LYS	C-N-CA	5.17	127.47	120.38
2	D	43	TYR	CB-CA-C	-5.17	99.14	109.33
1	B	38	PHE	O-C-N	-5.17	115.71	122.59
1	A	125	PRO	CA-C-O	-5.17	115.52	121.36
1	A	275	ASN	CA-C-O	-5.17	113.17	119.32
1	B	224	LYS	N-CA-CB	5.17	117.61	110.17
1	C	209	GLN	CA-C-O	5.17	125.94	120.36
1	A	469	ARG	N-CA-C	5.17	116.91	111.28
2	D	157	PHE	CA-C-N	5.17	129.73	122.09
2	D	157	PHE	C-N-CA	5.17	129.73	122.09
1	A	792	SER	CA-C-O	-5.16	116.08	121.55
1	C	769	MET	CA-C-N	5.16	127.46	120.44
1	C	769	MET	C-N-CA	5.16	127.46	120.44
1	B	43	LYS	CG-CD-CE	5.16	123.17	111.30
2	E	135	VAL	CB-CA-C	5.16	118.27	110.63
2	F	41	ALA	O-C-N	-5.16	116.97	123.27
1	A	46	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	C	56	THR	CA-CB-OG1	5.16	117.34	109.60
1	C	834	THR	CA-CB-CG2	-5.16	101.73	110.50
1	A	623	HIS	ND1-CE1-NE2	5.16	113.56	108.40
1	B	198	THR	CA-CB-OG1	5.16	117.33	109.60
1	C	464	ASN	CA-C-N	5.15	127.18	120.28
1	C	464	ASN	C-N-CA	5.15	127.18	120.28
2	D	51	PRO	CA-C-N	5.15	130.25	122.99
2	D	51	PRO	C-N-CA	5.15	130.25	122.99
1	A	934	VAL	O-C-N	-5.15	117.62	123.18
1	A	166	HIS	N-CA-C	-5.15	101.30	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	896	SER	O-C-N	-5.15	116.21	123.11
1	A	390	VAL	CA-CB-CG1	5.15	119.15	110.40
1	B	221	ARG	CD-NE-CZ	-5.15	117.19	124.40
1	C	687	THR	OG1-CB-CG2	-5.15	99.01	109.30
1	A	32	ARG	N-CA-C	5.14	116.89	111.28
1	A	861	LYS	CA-C-O	-5.14	115.35	121.16
1	B	44	PHE	CA-CB-CG	-5.14	108.66	113.80
1	B	576	GLY	N-CA-C	-5.14	105.71	111.63
1	B	599	ASP	CA-C-O	5.14	126.74	120.62
1	B	776	GLY	N-CA-C	5.14	125.37	113.18
1	C	245	GLY	N-CA-C	5.14	117.85	111.93
1	B	875	SER	CA-C-N	5.14	127.94	120.79
1	B	875	SER	C-N-CA	5.14	127.94	120.79
1	C	462	ASN	CA-C-N	5.14	127.13	120.44
1	C	462	ASN	C-N-CA	5.14	127.13	120.44
1	A	421	ASN	CA-C-N	5.14	129.01	120.94
1	A	421	ASN	C-N-CA	5.14	129.01	120.94
1	B	660	THR	N-CA-C	5.14	119.63	112.90
1	B	24	SER	CA-C-N	5.14	125.18	119.32
1	B	24	SER	C-N-CA	5.14	125.18	119.32
1	A	537	HIS	ND1-CE1-NE2	5.14	113.54	108.40
1	A	708	ASP	O-C-N	-5.13	115.29	122.37
1	B	376	ILE	CA-CB-CG2	5.13	119.22	110.50
1	B	497	PRO	CA-C-N	5.13	131.67	122.38
1	B	497	PRO	C-N-CA	5.13	131.67	122.38
2	E	165	HIS	CE1-NE2-CD2	-5.13	103.87	109.00
2	E	224	TYR	CA-CB-CG	-5.13	104.66	113.90
1	A	171	ALA	CB-CA-C	-5.13	105.10	110.33
1	B	539	ASN	CA-C-N	5.13	127.15	120.28
1	B	539	ASN	C-N-CA	5.13	127.15	120.28
1	B	836	ARG	N-CA-C	5.13	121.72	110.80
1	C	783	PRO	O-C-N	-5.13	116.75	123.06
1	A	61	GLN	CA-C-N	5.13	127.99	120.71
1	A	61	GLN	C-N-CA	5.13	127.99	120.71
1	B	468	TRP	CG-CD1-NE1	-5.13	103.53	110.20
2	E	88	GLU	CB-CA-C	5.13	121.14	110.32
1	B	346	VAL	N-CA-C	5.12	115.65	108.17
1	C	722	ILE	O-C-N	-5.12	116.20	122.97
1	A	588	VAL	CA-C-O	-5.12	115.62	120.95
1	A	677	TRP	CZ3-CH2-CZ2	-5.12	114.84	121.50
1	B	856	ASP	N-CA-CB	5.12	117.56	109.83
2	F	141	ASP	CA-CB-CG	5.12	117.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	43	TYR	CB-CG-CD2	-5.12	113.12	120.80
1	C	509	ALA	CA-C-N	5.12	124.78	119.56
1	C	509	ALA	C-N-CA	5.12	124.78	119.56
2	D	164	VAL	O-C-N	-5.12	117.81	123.18
2	F	53	LEU	N-CA-C	5.12	117.11	109.59
1	A	507	VAL	CA-C-N	-5.12	116.50	123.10
1	A	507	VAL	C-N-CA	-5.12	116.50	123.10
1	B	655	ILE	N-CA-CB	5.12	118.20	111.40
1	A	132	CYS	N-CA-C	5.11	116.84	109.07
1	A	415	PRO	CA-C-O	-5.11	115.56	121.95
1	B	890	ASN	N-CA-C	5.11	117.30	110.35
2	F	54	LEU	O-C-N	5.11	128.22	122.19
1	C	734	ASP	O-C-N	-5.11	115.79	122.59
2	E	221	ALA	CB-CA-C	-5.11	101.75	110.95
1	B	840	ALA	CA-C-O	-5.11	115.59	121.47
1	B	911	GLU	CA-C-N	5.11	125.04	119.78
1	B	911	GLU	C-N-CA	5.11	125.04	119.78
2	E	168	ARG	NH1-CZ-NH2	-5.11	112.66	119.30
1	A	177	ASN	OD1-CG-ND2	5.11	127.71	122.60
1	B	452	ARG	O-C-N	-5.11	117.24	123.27
1	A	382	TYR	CB-CG-CD2	-5.11	113.14	120.80
1	B	624	ASN	CA-C-N	5.11	127.54	120.29
1	B	624	ASN	C-N-CA	5.11	127.54	120.29
1	C	60	SER	N-CA-C	5.11	117.63	110.23
1	A	18	ASP	CA-CB-CG	-5.10	107.50	112.60
1	A	427	LYS	N-CA-C	5.10	117.43	110.24
1	B	268	THR	O-C-N	-5.10	116.84	122.86
1	A	764	TRP	N-CA-C	5.10	116.84	111.28
2	D	216	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A	297	THR	CA-C-N	5.09	130.73	122.53
1	A	297	THR	C-N-CA	5.09	130.73	122.53
1	A	898	HIS	CB-CA-C	5.09	119.77	109.68
1	B	130	ASN	OD1-CG-ND2	-5.09	117.50	122.60
1	B	903	THR	CA-C-N	5.09	129.75	122.72
1	B	903	THR	C-N-CA	5.09	129.75	122.72
1	C	666	ILE	O-C-N	-5.09	115.29	121.10
2	D	51	PRO	O-C-N	-5.09	116.42	122.89
1	C	501	ASP	CA-CB-CG	5.09	117.69	112.60
2	D	165	HIS	CE1-NE2-CD2	-5.09	103.91	109.00
2	F	50	ALA	N-CA-C	5.09	117.53	110.20
1	B	88	GLY	CA-C-N	5.09	131.26	121.54
1	B	88	GLY	C-N-CA	5.09	131.26	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	432	THR	CA-C-O	5.09	125.64	119.38
1	B	747	SER	CB-CA-C	5.09	118.14	109.84
1	C	806	ASP	CB-CA-C	5.09	117.90	110.26
1	A	253	GLN	N-CA-C	5.09	117.49	111.33
1	C	455	ASN	O-C-N	-5.09	116.99	122.79
2	E	204	SER	O-C-N	-5.09	115.51	122.33
1	A	56	THR	N-CA-CB	5.09	119.78	111.08
1	A	391	ASP	N-CA-C	5.09	117.67	110.50
1	A	917	VAL	CA-C-O	5.08	125.68	120.39
1	B	573	LEU	CA-C-O	5.08	125.80	120.36
2	E	60	THR	O-C-N	-5.08	117.43	123.22
1	A	498	ASN	CA-CB-CG	-5.08	107.52	112.60
2	E	194	GLN	OE1-CD-NE2	5.08	127.68	122.60
1	C	892	LEU	CA-C-N	5.08	127.35	120.44
1	C	892	LEU	C-N-CA	5.08	127.35	120.44
1	B	729	SER	O-C-N	-5.08	117.02	123.01
1	C	505	LYS	N-CA-CB	5.08	118.10	110.53
1	C	386	TRP	CA-CB-CG	5.08	123.25	113.60
1	A	823	ASN	CA-CB-CG	5.08	117.67	112.60
1	B	236	TYR	CG-CD1-CE1	-5.08	113.59	121.20
1	B	317	GLN	O-C-N	-5.08	116.63	123.23
1	B	563	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	C	540	ALA	CA-C-N	5.08	125.47	119.94
1	C	540	ALA	C-N-CA	5.08	125.47	119.94
2	E	26	VAL	O-C-N	-5.08	117.70	123.18
1	C	103	ARG	NE-CZ-NH1	5.07	126.57	121.50
1	B	581	GLU	CA-C-N	-5.07	114.25	122.36
1	B	581	GLU	C-N-CA	-5.07	114.25	122.36
1	C	699	THR	CA-C-O	5.07	125.92	120.55
1	C	37	TYR	CA-C-O	-5.07	113.20	119.18
1	C	42	ASN	O-C-N	-5.07	115.69	122.43
1	A	304	THR	N-CA-C	5.07	116.95	108.99
1	B	771	ALA	N-CA-C	5.07	116.81	111.28
1	C	754	ASN	N-CA-C	5.07	117.07	110.53
2	F	142	LYS	N-CA-C	5.07	116.00	108.60
1	B	235	SER	O-C-N	-5.06	116.70	122.93
1	C	428	VAL	CB-CA-C	5.06	118.79	110.69
1	C	545	ARG	CB-CG-CD	5.06	122.95	111.30
1	A	405	THR	N-CA-C	5.06	117.64	110.50
1	A	928	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
1	B	456	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	C	471	PHE	CA-C-N	5.06	127.02	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	471	PHE	C-N-CA	5.06	127.02	120.44
2	D	11	MET	CG-SD-CE	-5.06	89.77	100.90
1	A	22	TYR	CA-C-N	5.06	128.39	120.75
1	A	22	TYR	C-N-CA	5.06	128.39	120.75
1	B	358	VAL	N-CA-CB	5.06	118.91	111.52
1	C	690	LEU	N-CA-C	5.06	117.76	110.28
1	A	749	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	365	THR	CB-CA-C	-5.05	102.26	110.85
1	A	758	CYS	O-C-N	-5.05	116.21	122.73
1	B	455	ASN	CA-C-N	5.05	128.38	120.75
1	B	455	ASN	C-N-CA	5.05	128.38	120.75
2	E	41	ALA	O-C-N	-5.05	117.03	123.24
1	B	469	ARG	NE-CZ-NH1	5.05	126.55	121.50
2	F	39	ASP	N-CA-C	5.05	117.01	110.65
1	C	759	ASN	N-CA-C	5.04	118.47	112.72
2	E	147	SER	CA-C-N	5.04	130.71	122.69
2	E	147	SER	C-N-CA	5.04	130.71	122.69
1	A	480	LEU	CA-C-O	-5.04	114.99	120.69
1	B	715	HIS	ND1-CE1-NE2	5.04	113.44	108.40
1	A	403	HIS	CE1-NE2-CD2	-5.04	103.96	109.00
1	B	172	PRO	CA-C-O	-5.04	111.42	120.60
1	B	917	VAL	O-C-N	-5.04	117.86	123.20
1	C	775	ILE	N-CA-C	5.04	115.27	110.53
2	E	106	GLY	N-CA-C	5.04	121.64	112.27
1	A	252	GLN	N-CA-CB	-5.04	102.78	110.49
1	B	359	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	218	ALA	O-C-N	-5.04	116.36	123.11
1	A	469	ARG	CA-C-N	5.04	127.03	120.28
1	A	469	ARG	C-N-CA	5.04	127.03	120.28
1	B	376	ILE	CA-CB-CG1	-5.04	101.84	110.40
1	B	441	ASP	CA-C-O	5.04	125.85	120.46
1	C	25	PRO	CA-C-N	5.04	125.57	119.98
1	C	25	PRO	C-N-CA	5.04	125.57	119.98
1	A	321	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	A	650	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	C	52	THR	CA-C-O	5.03	125.45	119.56
2	E	37	THR	N-CA-CB	5.03	119.00	110.49
1	A	928	HIS	CB-CG-CD2	5.03	137.74	131.20
1	C	166	HIS	ND1-CE1-NE2	5.03	113.43	108.40
2	D	222	VAL	N-CA-C	-5.03	101.22	108.87
1	A	436	ASN	CA-C-O	5.03	126.43	121.20
1	B	243	ASN	OD1-CG-ND2	-5.03	117.57	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	540	ALA	O-C-N	-5.03	116.79	122.12
2	F	41	ALA	CA-C-O	5.03	126.44	120.66
1	A	332	PHE	CB-CG-CD2	-5.03	112.16	120.70
1	B	204	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	B	278	ASN	OD1-CG-ND2	-5.03	117.57	122.60
1	C	661	ASN	CB-CA-C	5.03	118.04	109.75
2	D	1	TYR	O-C-N	-5.03	117.35	123.13
1	A	94	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	442	ALA	O-C-N	-5.02	115.47	122.20
1	A	727	SER	N-CA-C	5.02	120.79	113.40
1	C	432	THR	CA-CB-OG1	-5.02	102.06	109.60
1	C	438	TRP	O-C-N	-5.02	117.44	123.27
1	C	543	ARG	O-C-N	-5.02	116.90	122.07
1	B	592	LEU	CA-C-O	5.02	127.79	121.66
1	B	929	ARG	O-C-N	-5.02	116.12	121.04
1	C	22	TYR	N-CA-C	5.02	118.55	112.23
1	C	383	PHE	CA-CB-CG	5.02	118.82	113.80
1	B	898	HIS	ND1-CE1-NE2	5.01	113.41	108.40
1	A	646	LEU	CA-C-N	5.01	131.12	121.54
1	A	646	LEU	C-N-CA	5.01	131.12	121.54
1	B	481	PRO	N-CA-CB	5.01	108.51	103.25
1	A	634	ARG	NE-CZ-NH2	-5.01	114.69	119.20
2	D	65	VAL	N-CA-C	5.01	113.96	108.05
2	D	157	PHE	CA-C-O	-5.01	115.87	121.23
2	E	234	LEU	CA-C-N	5.01	130.24	121.52
2	E	234	LEU	C-N-CA	5.01	130.24	121.52
1	C	131	PRO	O-C-N	5.01	128.44	122.98
1	C	400	ILE	N-CA-CB	5.01	116.56	110.95
1	A	572	LEU	O-C-N	-5.01	117.38	123.29
1	A	463	LEU	N-CA-C	5.01	116.43	111.07
2	F	5	ASP	O-C-N	5.01	129.00	122.89
1	C	38	PHE	CA-C-N	5.00	128.21	121.05
1	C	38	PHE	C-N-CA	5.00	128.21	121.05
1	A	227	THR	CA-C-N	5.00	126.09	119.84
1	A	227	THR	C-N-CA	5.00	126.09	119.84
1	A	638	ASN	CB-CG-OD1	5.00	130.81	120.80
1	B	531	VAL	O-C-N	-5.00	117.93	123.18
2	E	29	THR	CA-CB-OG1	5.00	117.10	109.60

There are no chirality outliers.

All (107) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	TYR	Sidechain
1	A	233	TYR	Sidechain
1	A	337	TYR	Sidechain
1	A	379	ARG	Sidechain
1	A	398	ARG	Sidechain
1	A	500	TYR	Sidechain
1	A	544	TYR	Sidechain
1	A	615	TYR	Sidechain
1	A	62	ARG	Sidechain
1	A	653	TYR	Sidechain
1	A	669	ARG	Sidechain
1	A	694	TYR	Sidechain
1	A	697	TYR	Sidechain
1	A	698	TYR	Sidechain
1	A	753	TYR	Sidechain
1	A	765	PHE	Sidechain
1	A	79	TYR	Sidechain
1	A	802	ARG	Sidechain
1	A	813	TYR	Sidechain
1	A	827	PHE	Sidechain
1	A	874	PHE	Sidechain
1	A	878	PHE	Sidechain
1	A	91	ARG	Sidechain
1	A	916	TYR	Sidechain
1	A	926	ARG	Sidechain
1	A	941	ARG	Sidechain
1	B	103	ARG	Sidechain
1	B	120	TYR	Sidechain
1	B	286	TYR	Sidechain
1	B	329	ARG	Sidechain
1	B	338	TYR	Sidechain
1	B	379	ARG	Sidechain
1	B	381	ARG	Sidechain
1	B	45	ARG	Sidechain
1	B	500	TYR	Sidechain
1	B	543	ARG	Sidechain
1	B	554	TYR	Sidechain
1	B	585	ARG	Sidechain
1	B	601	ARG	Sidechain
1	B	62	ARG	Sidechain
1	B	669	ARG	Sidechain
1	B	697	TYR	Sidechain
1	B	77	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	773	TYR	Sidechain
1	B	786	TYR	Sidechain
1	B	79	TYR	Sidechain
1	B	794	PHE	Sidechain
1	B	810	TYR	Sidechain
1	B	813	TYR	Sidechain
1	B	82	ARG	Sidechain
1	B	847	TYR	Sidechain
1	B	91	ARG	Sidechain
1	B	929	ARG	Sidechain
1	B	932	ARG	Sidechain
1	C	103	ARG	Sidechain
1	C	11	TYR	Sidechain
1	C	194	TYR	Sidechain
1	C	211	TYR	Sidechain
1	C	22	TYR	Sidechain
1	C	301	TYR	Sidechain
1	C	322	ARG	Sidechain
1	C	338	TYR	Sidechain
1	C	369	TYR	Sidechain
1	C	38	PHE	Sidechain
1	C	457	PHE	Sidechain
1	C	469	ARG	Sidechain
1	C	473	TYR	Sidechain
1	C	479	TYR	Sidechain
1	C	544	TYR	Sidechain
1	C	553	ARG	Sidechain
1	C	578	TYR	Sidechain
1	C	615	TYR	Sidechain
1	C	653	TYR	Sidechain
1	C	669	ARG	Sidechain
1	C	681	ARG	Sidechain
1	C	706	TYR	Sidechain
1	C	72	ARG	Sidechain
1	C	77	TYR	Sidechain
1	C	773	TYR	Sidechain
1	C	802	ARG	Sidechain
1	C	82	ARG	Sidechain
1	C	830	TYR	Sidechain
1	C	836	ARG	Sidechain
1	C	847	TYR	Sidechain
1	C	91	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	932	ARG	Sidechain
1	C	944	PHE	Sidechain
2	D	115	ARG	Sidechain
2	D	161	ARG	Sidechain
2	D	168	ARG	Sidechain
2	D	223	TYR	Sidechain
2	D	224	TYR	Sidechain
2	D	236	TYR	Sidechain
2	D	25	ARG	Sidechain
2	D	43	TYR	Sidechain
2	D	68	ARG	Sidechain
2	D	99	TYR	Sidechain
2	E	183	ARG	Sidechain
2	E	209	TYR	Sidechain
2	E	227	ARG	Sidechain
2	E	56	TYR	Sidechain
2	E	69	PHE	Sidechain
2	E	99	TYR	Sidechain
2	F	165	HIS	Sidechain
2	F	168	ARG	Sidechain
2	F	193	PHE	Sidechain
2	F	232	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	7375	7070	7068	0	0
1	B	7375	7070	7068	0	0
1	C	7375	7070	7068	0	0
2	D	1799	1744	1743	0	0
2	E	1799	1744	1743	0	0
2	F	1799	1744	1743	0	0
All	All	27522	26442	26433	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	917/952 (96%)	866 (94%)	43 (5%)	8 (1%)	14	51
1	B	917/952 (96%)	863 (94%)	47 (5%)	7 (1%)	16	54
1	C	917/952 (96%)	853 (93%)	51 (6%)	13 (1%)	9	40
2	D	229/254 (90%)	213 (93%)	15 (7%)	1 (0%)	30	67
2	E	229/254 (90%)	207 (90%)	18 (8%)	4 (2%)	7	36
2	F	229/254 (90%)	211 (92%)	16 (7%)	2 (1%)	14	51
All	All	3438/3618 (95%)	3213 (94%)	190 (6%)	35 (1%)	15	48

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	295	PRO
1	C	539	ASN
2	E	231	ASN
1	C	61	GLN
1	C	734	ASP
1	C	776	GLY
1	C	836	ARG
2	D	59	SER
1	A	725	ASP
1	A	836	ARG
1	B	443	THR
1	C	647	SER
1	C	726	SER
1	C	867	ARG
2	E	59	SER
2	F	233	PRO
1	A	354	LEU

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Mol	Chain	Res	Type
1	A	419	VAL
1	B	748	VAL
1	B	824	ASN
1	A	224	LYS
1	A	748	VAL
1	B	739	PRO
1	C	733	ASN
2	F	6	ASP
1	A	352	SER
1	B	61	GLN
1	C	212	GLU
2	E	233	PRO
1	B	7	PRO
1	A	776	GLY
1	B	575	PRO
1	C	404	GLY
1	C	739	PRO
2	E	102	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	800/827 (97%)	779 (97%)	21 (3%)	40	62
1	B	800/827 (97%)	772 (96%)	28 (4%)	32	53
1	C	800/827 (97%)	778 (97%)	22 (3%)	38	59
2	D	197/206 (96%)	194 (98%)	3 (2%)	57	72
2	E	197/206 (96%)	193 (98%)	4 (2%)	48	66
2	F	197/206 (96%)	191 (97%)	6 (3%)	36	57
All	All	2991/3099 (96%)	2907 (97%)	84 (3%)	38	59

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	55	VAL
1	A	110	PRO
1	A	167	VAL
1	A	256	LYS
1	A	292	ILE
1	A	305	ILE
1	A	395	PRO
1	A	424	THR
1	A	513	VAL
1	A	654	PRO
1	A	667	PRO
1	A	690	LEU
1	A	719	LYS
1	A	743	GLU
1	A	755	VAL
1	A	836	ARG
1	A	853	THR
1	A	855	VAL
1	A	858	ILE
1	A	913	THR
1	B	161	GLU
1	B	180	LYS
1	B	191	THR
1	B	226	THR
1	B	238	LYS
1	B	248	ILE
1	B	269	THR
1	B	297	THR
1	B	305	ILE
1	B	330	ASP
1	B	352	SER
1	B	415	PRO
1	B	513	VAL
1	B	517	ILE
1	B	595	SER
1	B	643	ASN
1	B	719	LYS
1	B	729	SER
1	B	741	GLU
1	B	755	VAL
1	B	828	VAL
1	B	836	ARG

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Mol	Chain	Res	Type
1	B	857	SER
1	B	861	LYS
1	B	868	THR
1	B	907	ASP
1	B	913	THR
1	B	925	VAL
1	C	37	TYR
1	C	89	ASP
1	C	91	ARG
1	C	165	THR
1	C	176	ILE
1	C	226	THR
1	C	292	ILE
1	C	318	SER
1	C	525	LEU
1	C	558	HIS
1	C	650	ASN
1	C	711	PHE
1	C	719	LYS
1	C	723	THR
1	C	744	ILE
1	C	792	SER
1	C	811	LYS
1	C	819	LEU
1	C	850	ILE
1	C	906	VAL
1	C	913	THR
1	C	938	VAL
2	D	2	LYS
2	D	28	ILE
2	D	239	GLN
2	E	85	LEU
2	E	154	VAL
2	E	197	VAL
2	E	239	GLN
2	F	8	ASP
2	F	81	THR
2	F	113	ILE
2	F	144	PRO
2	F	167	VAL
2	F	169	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

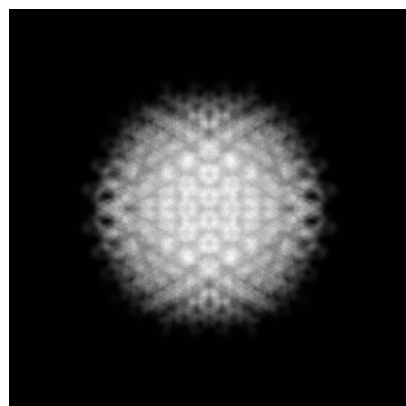
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3821. These allow visual inspection of the internal detail of the map and identification of artifacts.

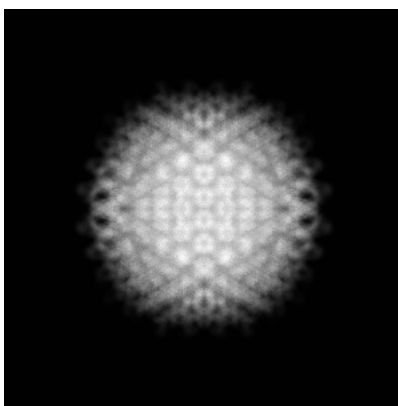
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

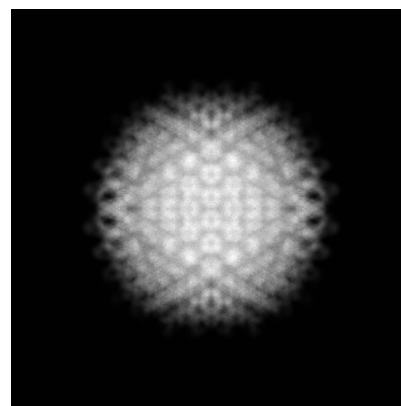
6.1.1 Primary map



X

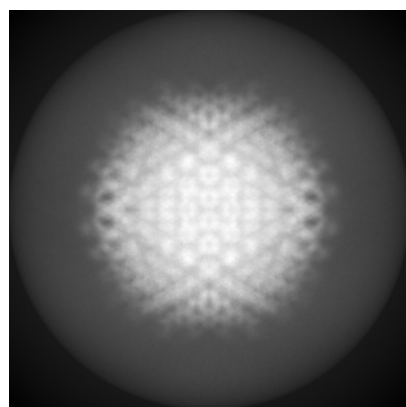


Y

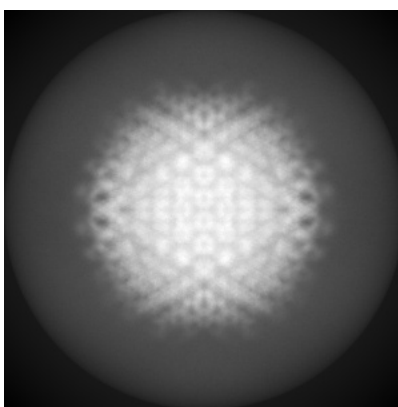


Z

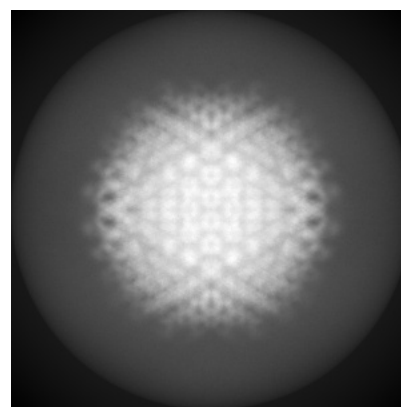
6.1.2 Raw map



X



Y

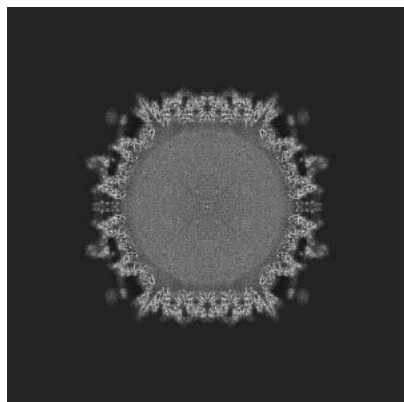


Z

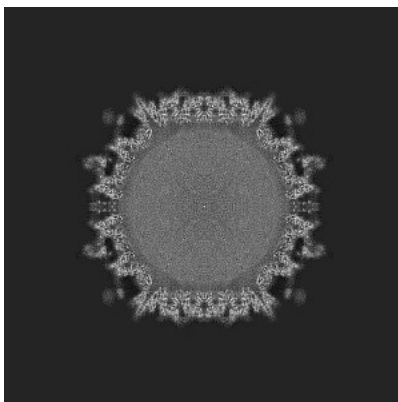
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

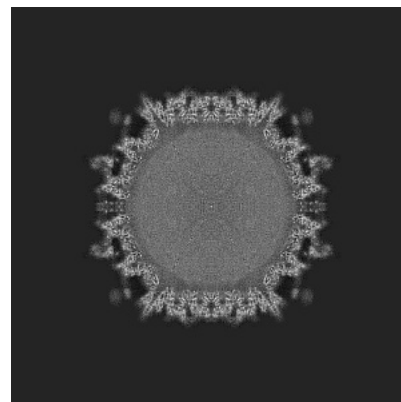
6.2.1 Primary map



X Index: 400

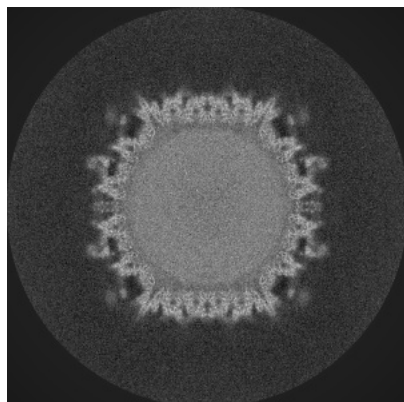


Y Index: 400

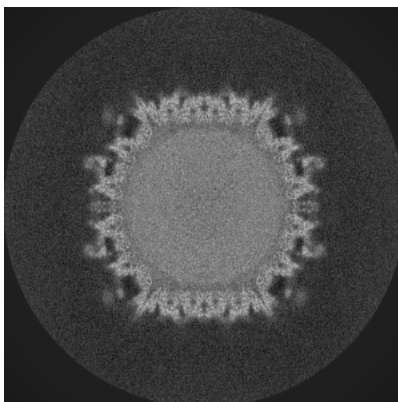


Z Index: 400

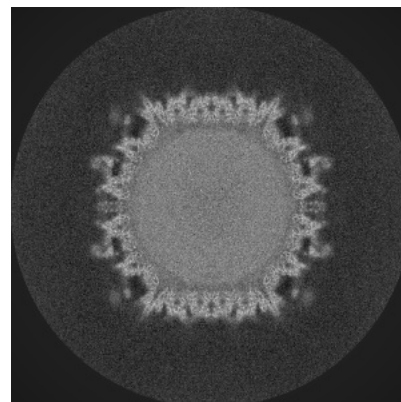
6.2.2 Raw map



X Index: 400



Y Index: 400

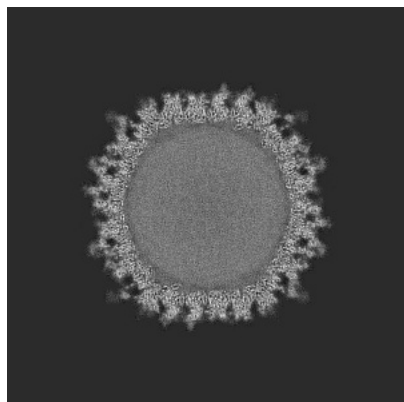


Z Index: 400

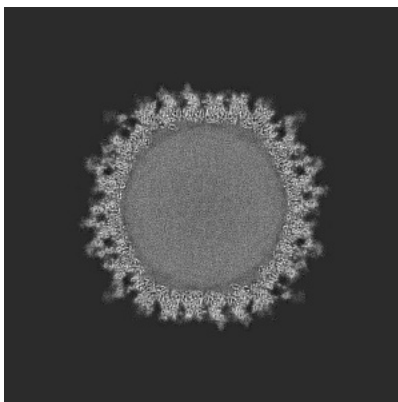
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

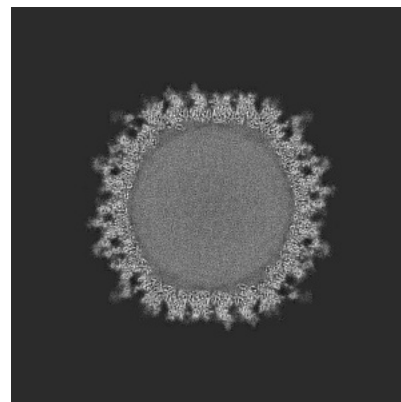
6.3.1 Primary map



X Index: 391

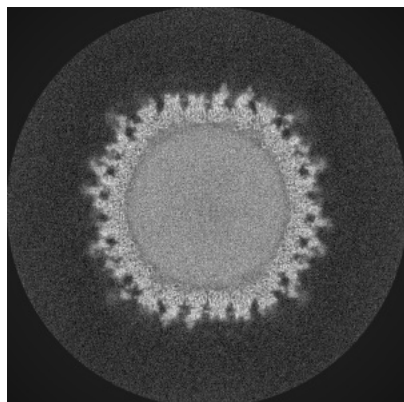


Y Index: 409

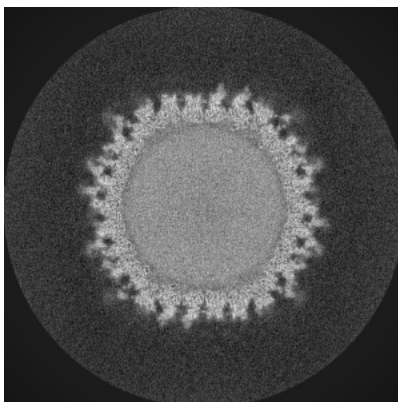


Z Index: 409

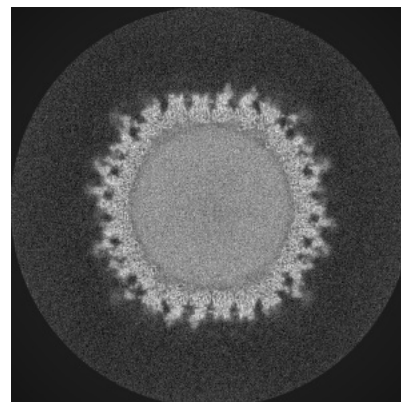
6.3.2 Raw map



X Index: 390



Y Index: 390

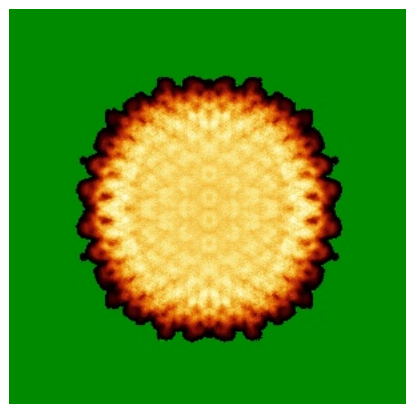


Z Index: 390

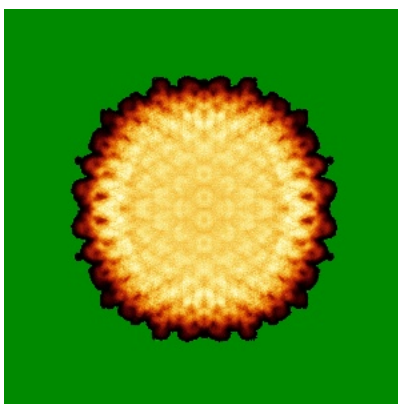
The images above show the largest variance slices of the map in three orthogonal directions.

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

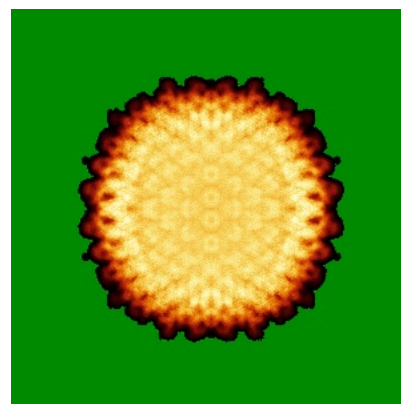
6.4.1 Primary map



X

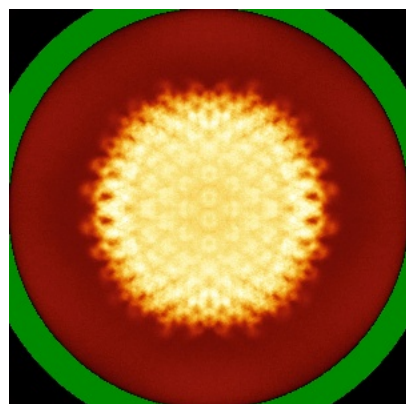


Y

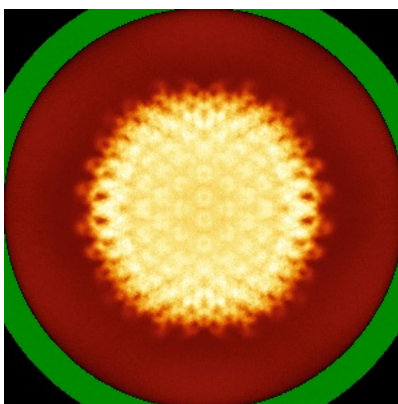


Z

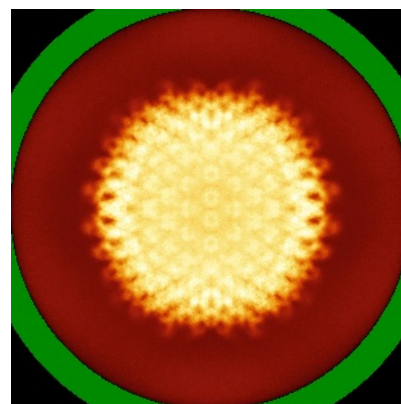
6.4.2 Raw map



X



Y

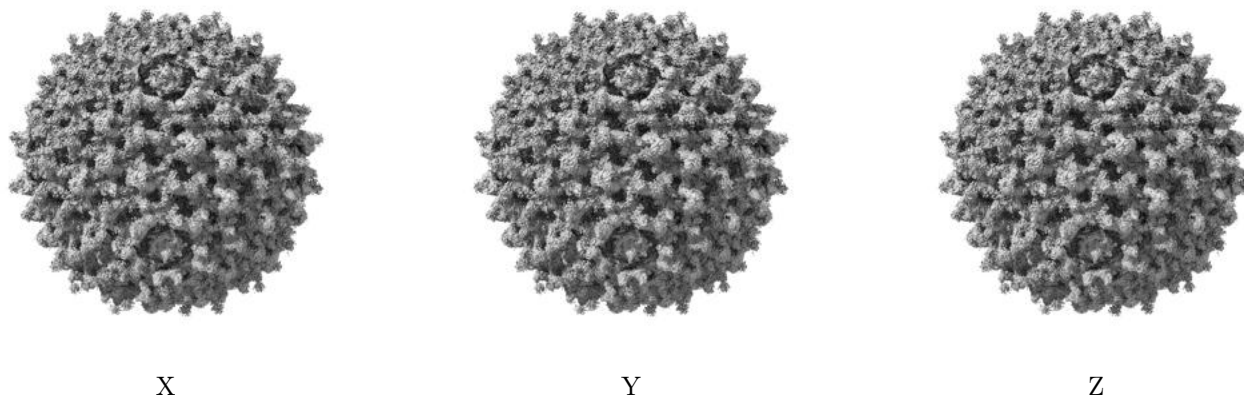


Z

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

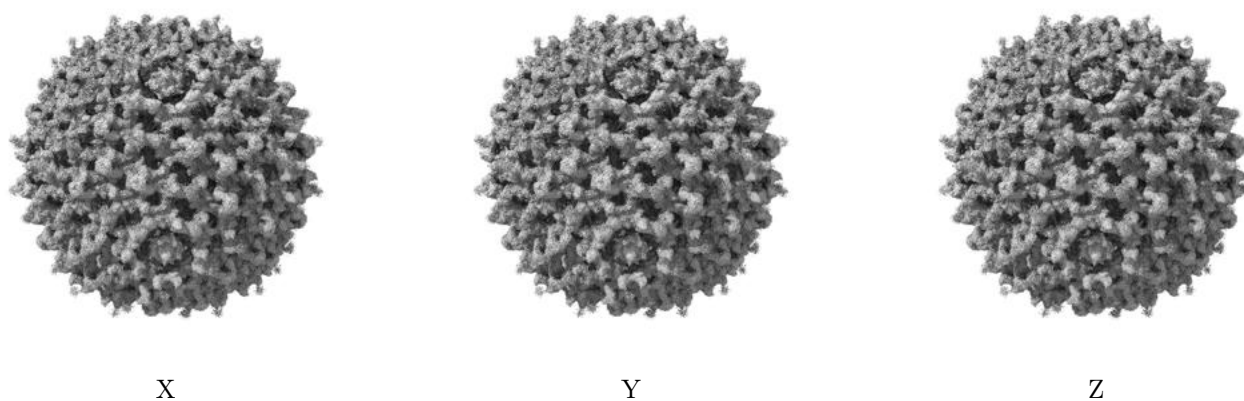
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

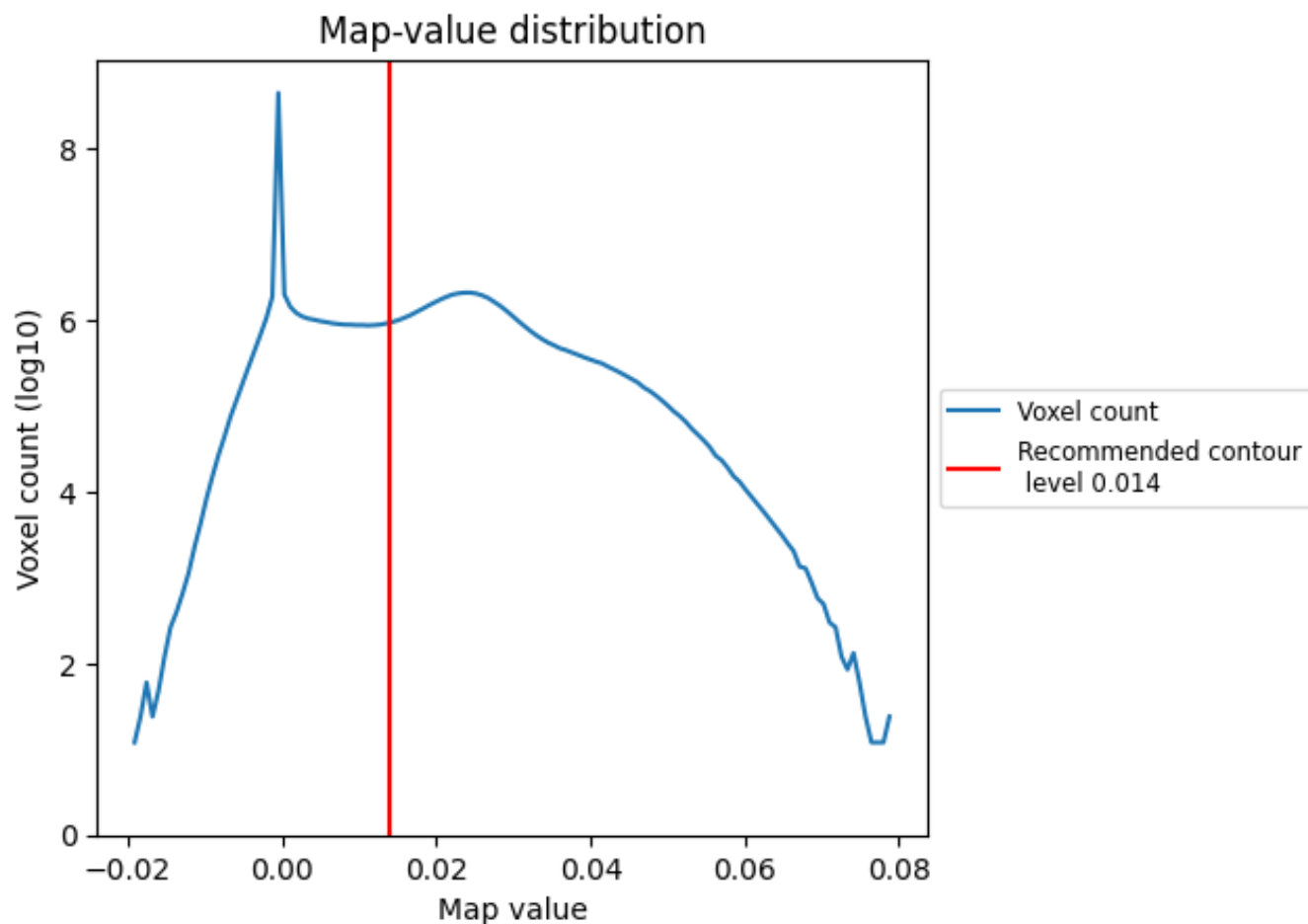
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

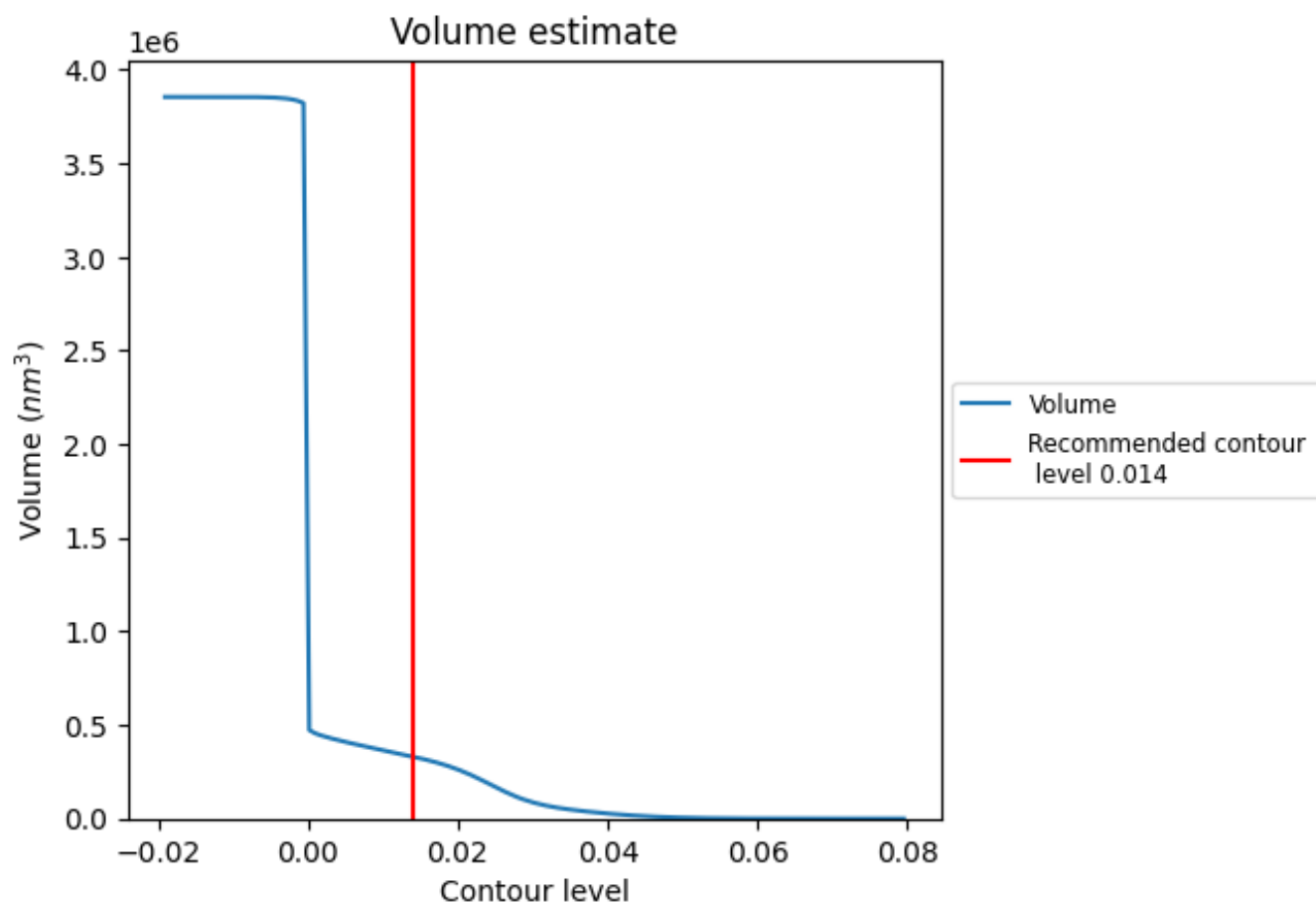
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

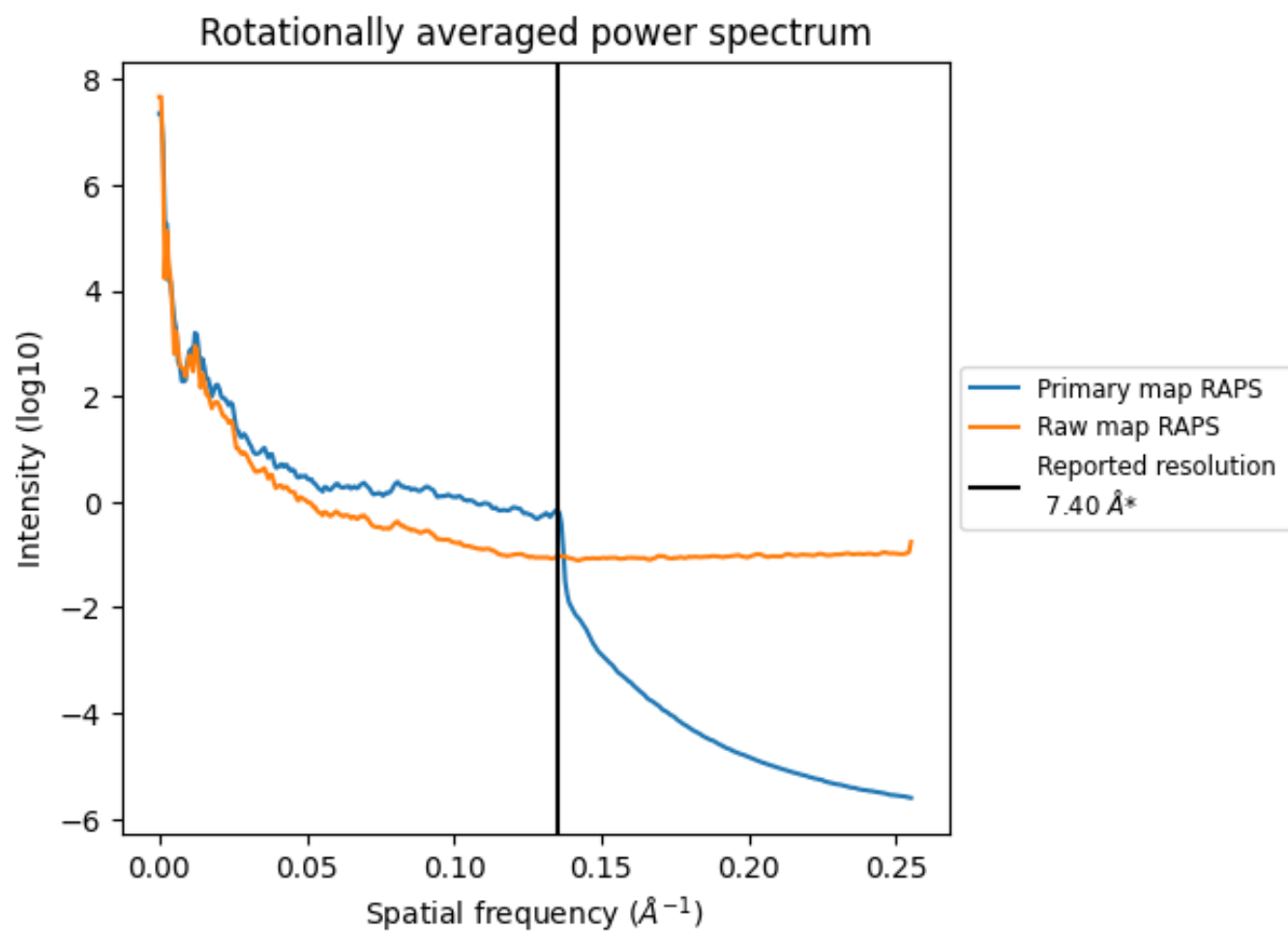
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 330949 nm³; this corresponds to an approximate mass of 298955 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 ⓘ

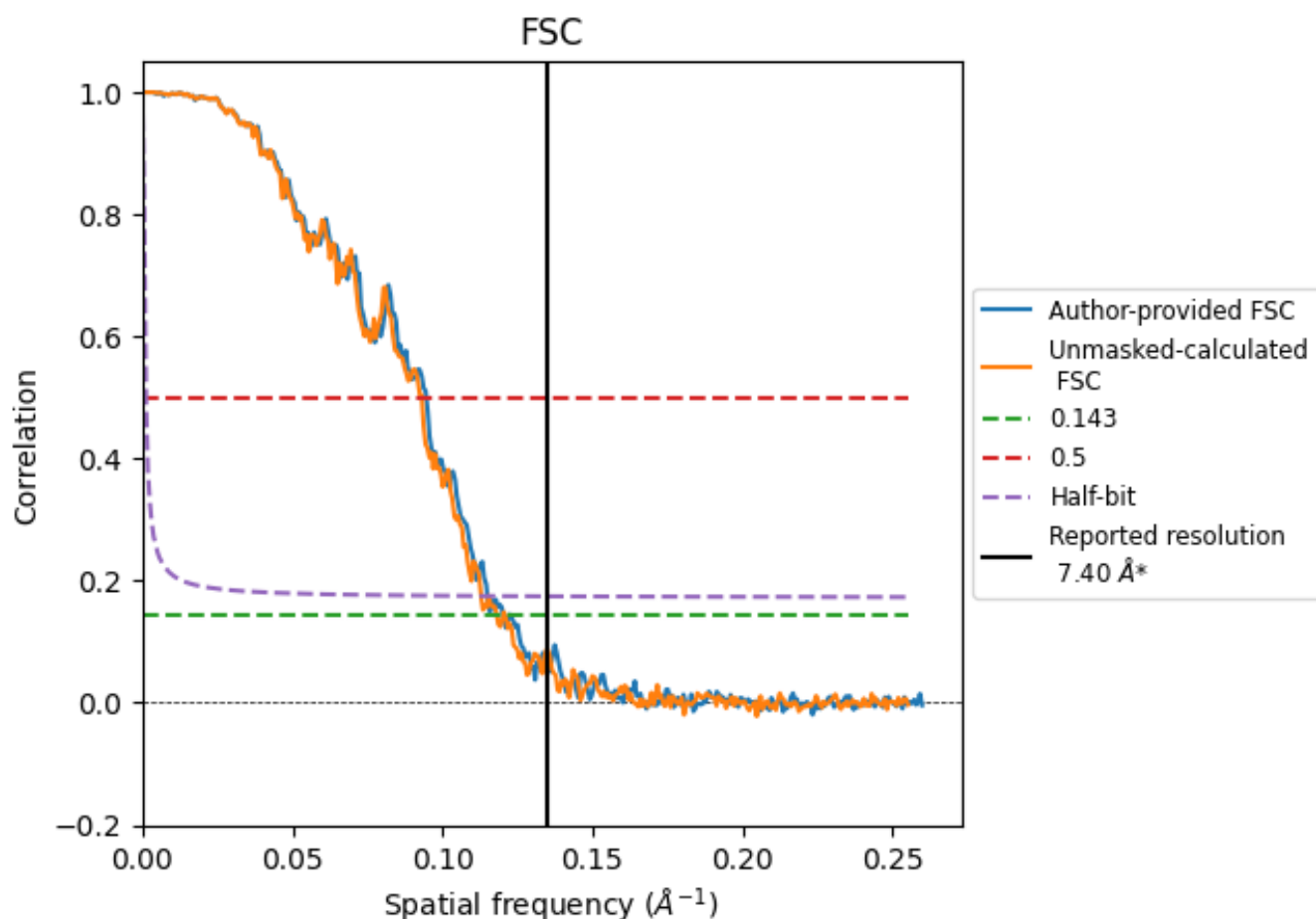


*Reported resolution corresponds to spatial frequency of 0.135 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.135 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.40	-	-
Author-provided FSC curve	8.32	10.57	8.70
Unmasked-calculated*	8.47	10.73	8.86

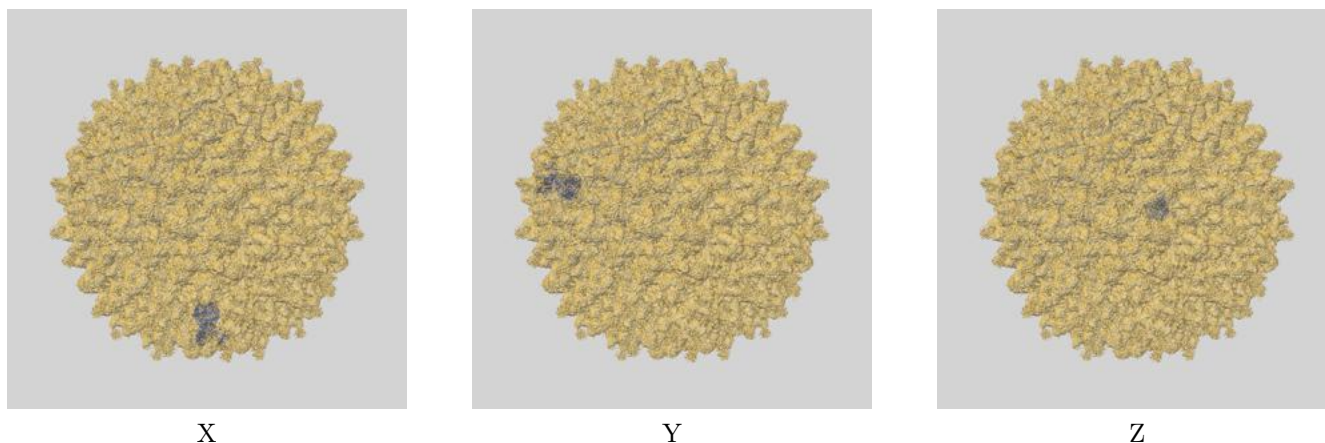
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.32 differs from the reported value 7.4 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.47 differs from the reported value 7.4 by more than 10 %

9 Map-model fit [i](#)

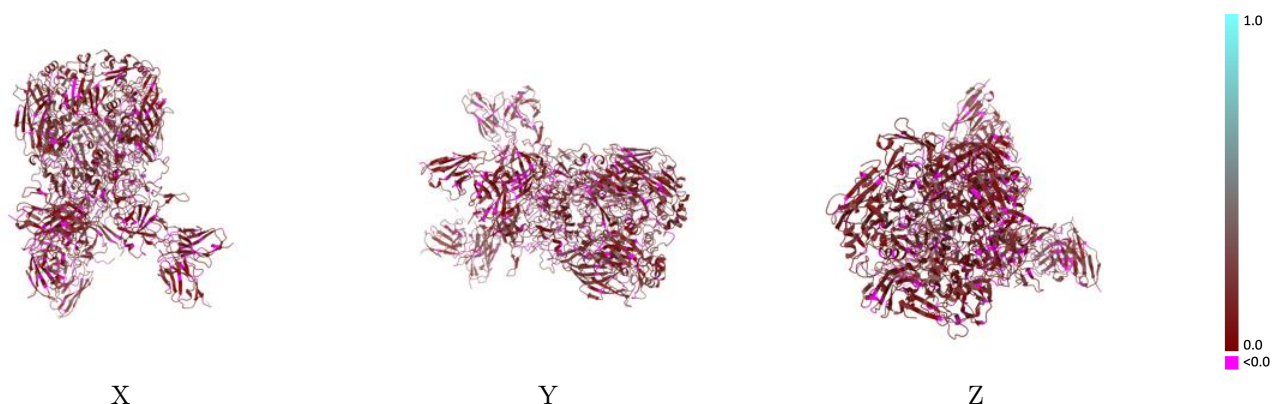
This section contains information regarding the fit between EMDB map EMD-3821 and PDB model 6EQC. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



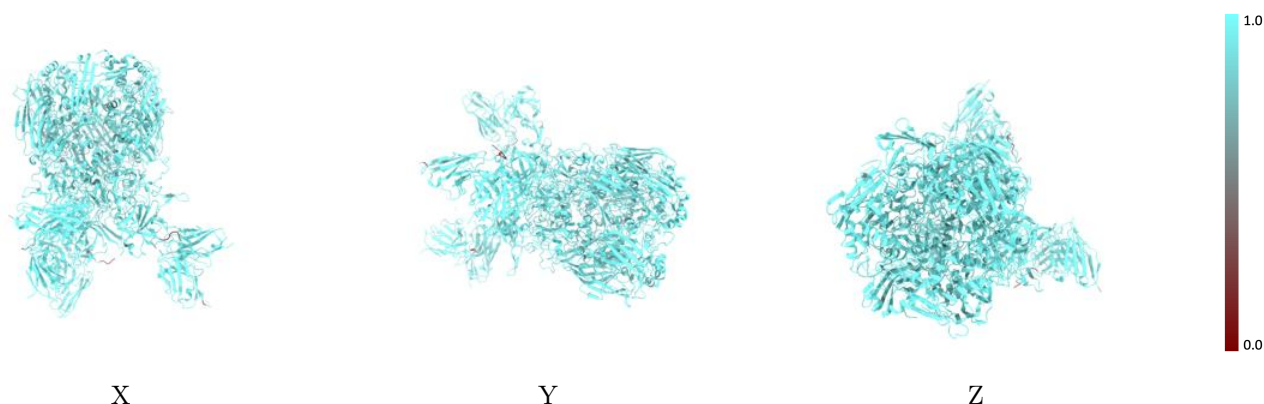
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



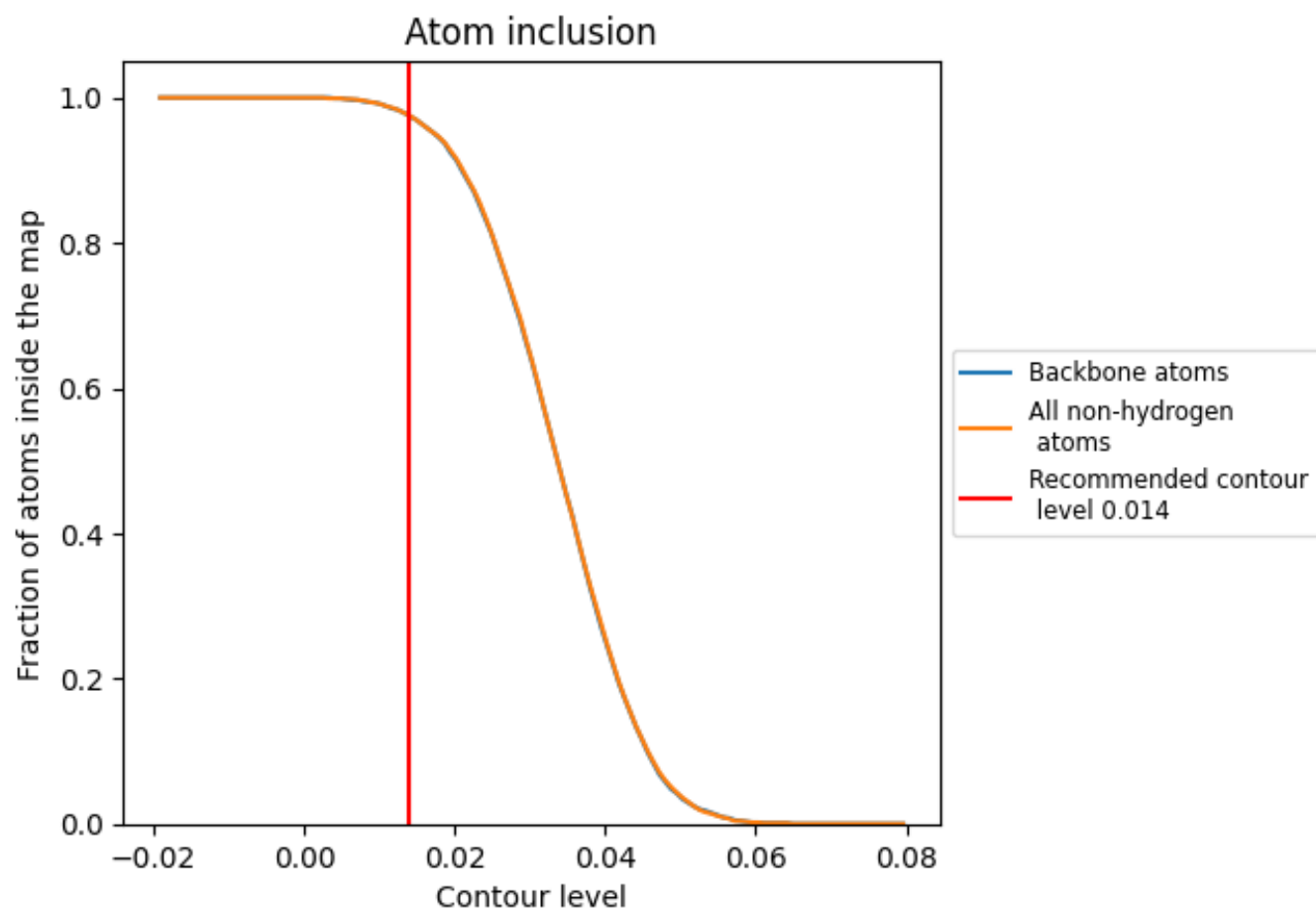
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9750	0.1270
A	0.9820	0.1340
B	0.9780	0.1310
C	0.9780	0.1240
D	0.9670	0.1200
E	0.9500	0.1120
F	0.9680	0.1250

1.0

0.0

<0.0