



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 05:35 AM UTC

PDB ID : 8W4F / pdb_00008w4f
EMDB ID : EMD-36904
Title : SARS-CoV-2 spike protein in complex with a trivalent nanobody
Authors : Jiang, X.Y.; Qian, J.Q.; Zhu, H.X.; Qin, Q.; Huang, Q.
Deposited on : 2023-08-24
Resolution : 4.20 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

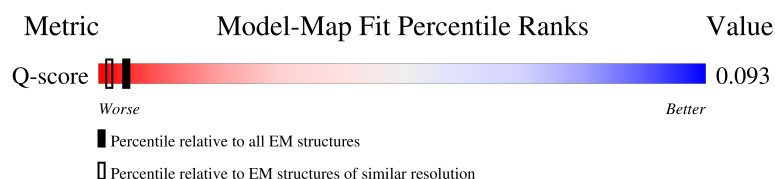
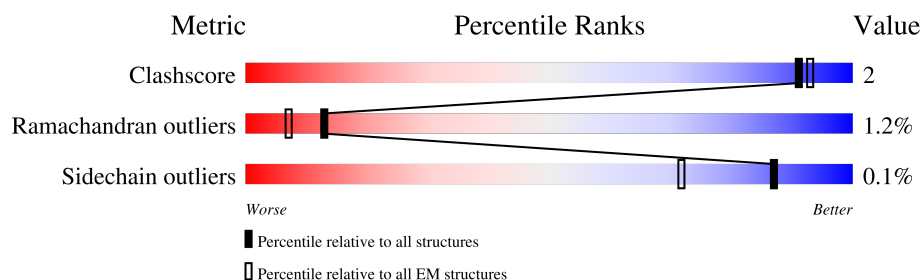
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1120	31% 56% 42% .
1	B	1120	30% 52% 46% .
1	C	1120	36% 56% 42% .
2	D	197	65% 54% 40% 6% .

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Mol	Chain	Length	Quality of chain
2	E	197	71% 52% 46% .
2	F	197	67% 54% 45% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 60429 atoms, of which 29841 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1120	Total	C	H	N	O	S	0	0
			17237	5560	8509	1460	1669	39		
1	B	1120	Total	C	H	N	O	S	0	0
			17237	5560	8509	1460	1669	39		
1	C	1120	Total	C	H	N	O	S	0	0
			17237	5560	8509	1460	1669	39		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	683	ALA	ARG	engineered mutation	UNP P0DTC2
A	685	ALA	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	683	ALA	ARG	engineered mutation	UNP P0DTC2
B	685	ALA	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	683	ALA	ARG	engineered mutation	UNP P0DTC2
C	685	ALA	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Tribody.

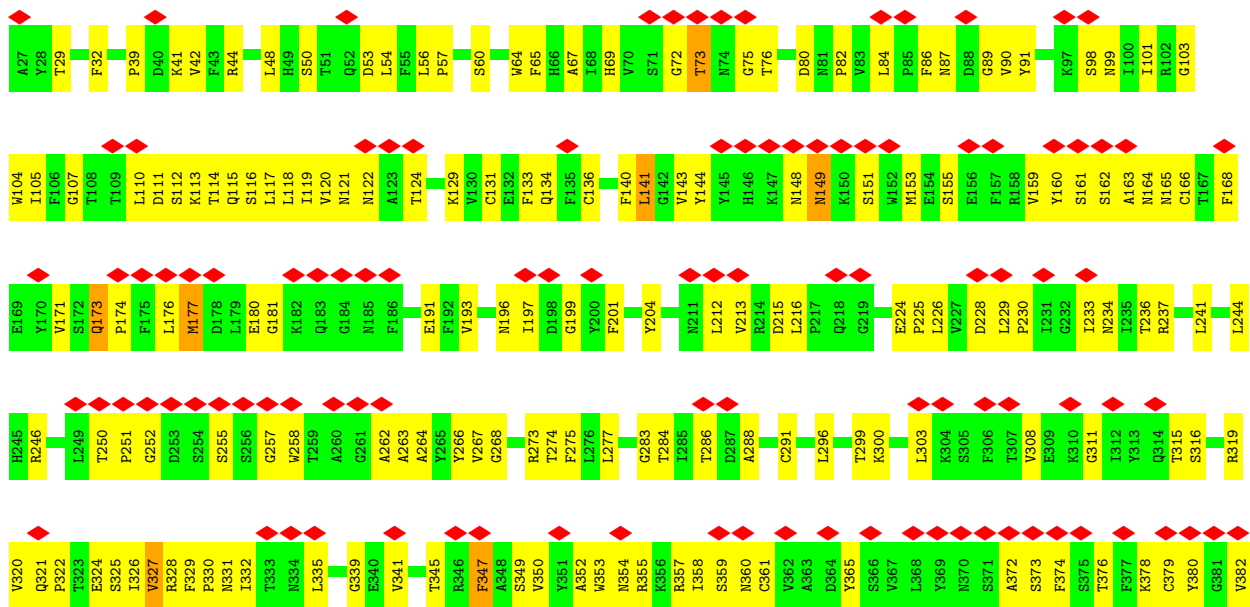
Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	197	Total	C	H	N	O	S	0	0
			2906	917	1438	259	286	6		
2	E	197	Total	C	H	N	O	S	0	0
			2906	917	1438	259	286	6		
2	F	197	Total	C	H	N	O	S	0	0
			2906	917	1438	259	286	6		

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.

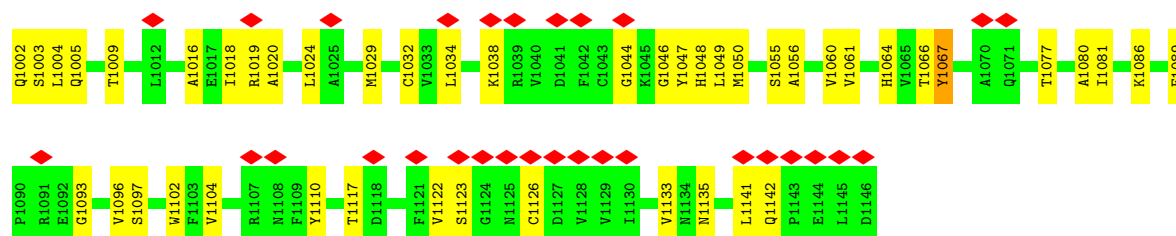
• Molecule 1: Spike glycoprotein



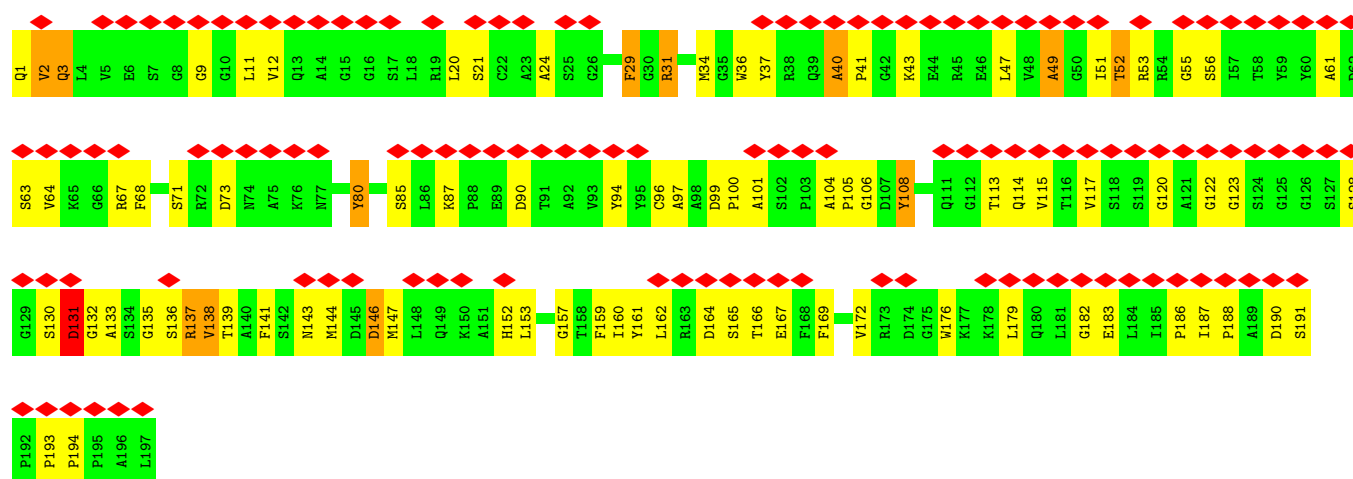




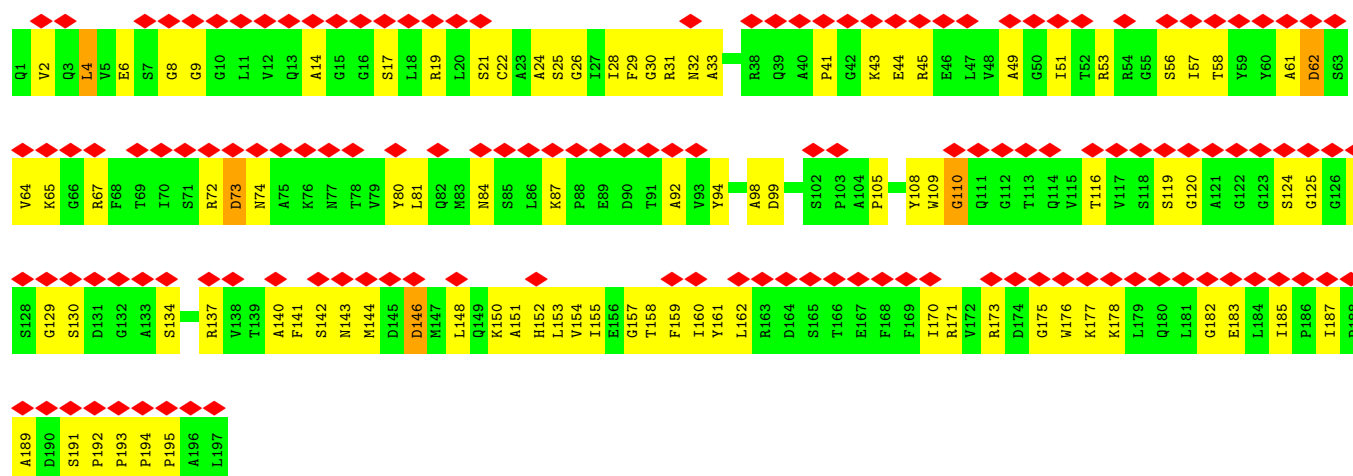




• Molecule 2: Tribody

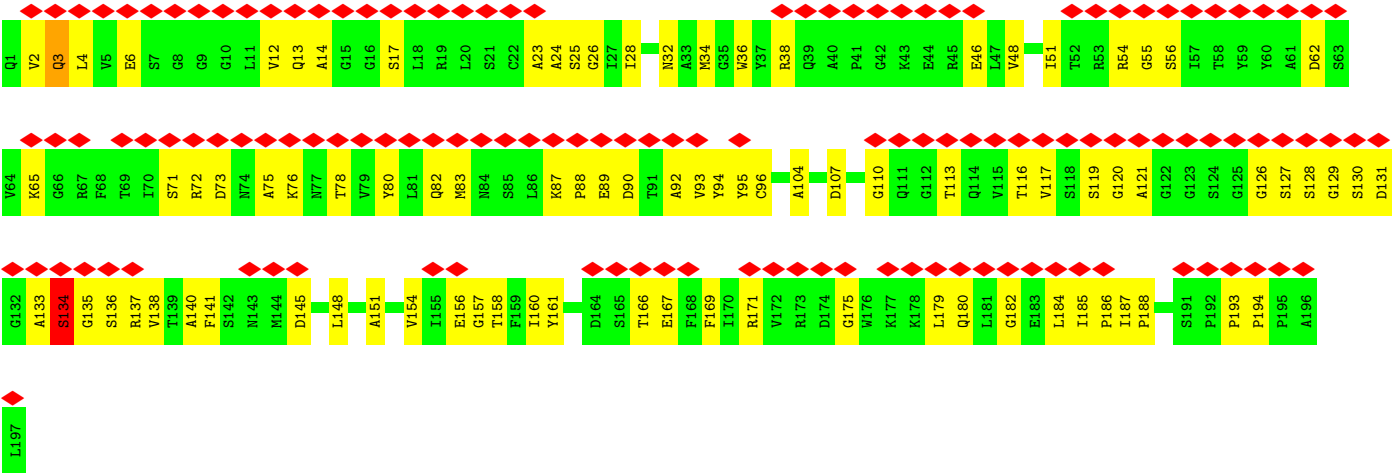


• Molecule 2: Tribody



• Molecule 2: Tribody





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	262855	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.175	Depositor
Minimum map value	-0.506	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.116	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	401.92, 401.92, 401.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.57, 1.57, 1.57	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	1.92	253/8937 (2.8%)	2.00	425/12174 (3.5%)
1	B	1.97	292/8937 (3.3%)	2.03	465/12174 (3.8%)
1	C	1.90	232/8937 (2.6%)	1.96	420/12174 (3.4%)
2	D	1.95	45/1499 (3.0%)	2.10	83/2029 (4.1%)
2	E	2.07	49/1499 (3.3%)	2.01	81/2029 (4.0%)
2	F	1.99	41/1499 (2.7%)	2.08	85/2029 (4.2%)
All	All	1.94	912/31308 (2.9%)	2.01	1559/42609 (3.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	3
2	D	0	2
2	F	0	1
All	All	0	11

All (912) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	ASP	CA-C	-12.18	1.38	1.52
1	B	713	ALA	C-N	12.13	1.42	1.33
1	A	896	ILE	CA-C	-11.57	1.43	1.52
1	B	1018	ILE	CA-C	-11.14	1.38	1.52
2	E	154	VAL	CA-C	-10.79	1.42	1.53
2	E	137	ARG	CA-C	10.70	1.63	1.53
1	B	166	CYS	CA-C	-10.63	1.39	1.52
1	A	241	LEU	CA-C	-10.49	1.39	1.52
1	A	60	SER	CA-C	-10.39	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	VAL	CA-C	-10.09	1.40	1.52
1	B	165	ASN	CA-C	-9.92	1.40	1.52
1	A	160	TYR	CA-C	-9.69	1.41	1.52
2	D	162	LEU	CA-C	-9.68	1.40	1.53
1	C	397	ALA	CA-C	-9.55	1.41	1.52
2	F	56	SER	C-N	9.52	1.44	1.33
1	B	911	VAL	CA-C	-9.36	1.41	1.52
1	B	664	ILE	CA-C	9.35	1.61	1.52
1	B	1039	ARG	C-N	9.30	1.44	1.33
1	C	196	ASN	CA-C	-9.21	1.41	1.52
1	C	875	SER	N-CA	-9.20	1.35	1.46
2	E	153	LEU	C-N	9.16	1.42	1.33
1	A	699	LEU	CA-C	-9.08	1.43	1.53
1	A	230	PRO	CA-C	-9.04	1.44	1.52
1	B	559	PHE	N-CA	-9.03	1.34	1.45
1	C	749	CYS	CA-C	9.02	1.64	1.52
1	C	288	ALA	C-N	8.97	1.44	1.33
1	A	639	GLY	C-N	8.90	1.46	1.33
1	B	537	LYS	CA-C	-8.87	1.41	1.52
2	E	92	ALA	CA-C	-8.83	1.41	1.52
1	B	447	GLY	CA-C	-8.79	1.43	1.52
1	B	44	ARG	N-CA	-8.79	1.34	1.45
1	B	445	VAL	CA-C	-8.79	1.42	1.52
1	C	542	ASN	N-CA	-8.79	1.35	1.46
1	B	710	ASN	N-CA	-8.78	1.36	1.46
1	C	992	GLN	N-CA	-8.71	1.35	1.46
1	A	826	VAL	CA-C	-8.70	1.41	1.52
2	E	158	THR	CA-C	-8.45	1.42	1.52
2	E	158	THR	N-CA	-8.32	1.35	1.46
1	C	416	GLY	CA-C	-8.31	1.44	1.52
1	A	268	GLY	CA-C	-8.31	1.45	1.52
1	A	594	GLY	CA-C	-8.29	1.44	1.52
1	B	215	ASP	CA-C	-8.28	1.42	1.52
1	C	620	VAL	CA-C	8.28	1.61	1.52
2	D	9	GLY	CA-C	-8.25	1.42	1.52
1	B	672	ALA	CA-C	-8.21	1.43	1.52
1	C	456	PHE	CA-C	-8.20	1.42	1.52
1	C	505	TYR	N-CA	-8.19	1.36	1.46
1	B	361	CYS	C-N	8.17	1.44	1.33
1	C	359	SER	C-N	8.14	1.44	1.33
1	B	104	TRP	C-N	8.11	1.43	1.33
1	A	43	PHE	CA-C	-8.10	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	GLY	N-CA	8.09	1.52	1.44
1	C	83	VAL	CA-C	-8.07	1.43	1.52
1	A	1071	GLN	CA-C	-8.02	1.42	1.52
1	C	439	ASN	C-N	8.02	1.44	1.33
2	F	120	GLY	C-N	8.01	1.43	1.33
1	B	573	THR	CA-C	-7.99	1.43	1.52
1	B	626	ALA	CA-C	-7.95	1.42	1.52
2	E	108	TYR	CA-C	-7.94	1.43	1.52
1	B	29	THR	CA-C	-7.92	1.43	1.52
1	C	121	ASN	CA-C	-7.91	1.44	1.52
1	B	431	GLY	CA-C	-7.91	1.43	1.51
1	B	1056	ALA	C-N	7.90	1.43	1.33
1	B	116	SER	C-N	7.89	1.44	1.33
1	B	171	VAL	N-CA	-7.89	1.36	1.46
1	C	65	PHE	CA-C	-7.88	1.43	1.52
1	A	170	TYR	N-CA	-7.87	1.37	1.46
1	A	190	ARG	CA-C	-7.86	1.43	1.52
1	C	849	LEU	CA-C	-7.79	1.43	1.52
1	B	112	SER	CA-C	-7.72	1.43	1.53
1	A	509	ARG	CA-C	-7.72	1.43	1.52
1	B	84	LEU	CA-C	-7.70	1.43	1.52
1	C	1032	CYS	C-N	7.69	1.41	1.33
2	E	192	PRO	CA-C	7.68	1.59	1.52
1	A	602	THR	N-CA	7.66	1.55	1.46
1	B	1103	PHE	CA-C	-7.65	1.43	1.52
1	B	257	GLY	CA-C	-7.62	1.41	1.51
1	A	463	PRO	C-N	7.62	1.42	1.33
1	A	930	ALA	C-N	7.60	1.43	1.33
1	C	143	VAL	N-CA	-7.60	1.37	1.46
1	A	692	ILE	N-CA	-7.59	1.37	1.46
2	E	161	TYR	N-CA	-7.58	1.36	1.46
1	B	181	GLY	C-N	7.58	1.44	1.33
1	A	1110	TYR	C-N	7.57	1.40	1.33
1	C	825	LYS	C-N	7.55	1.42	1.33
1	C	382	VAL	C-N	7.53	1.40	1.33
1	C	723	THR	CA-C	-7.51	1.43	1.52
1	A	687	VAL	N-CA	-7.50	1.38	1.46
1	B	823	PHE	C-N	7.50	1.44	1.34
2	E	22	CYS	N-CA	-7.49	1.36	1.45
1	B	547	THR	C-N	7.48	1.41	1.33
1	A	397	ALA	CA-C	-7.48	1.43	1.52
1	A	834	ILE	N-CA	-7.47	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	642	VAL	N-CA	-7.46	1.37	1.46
1	B	1104	VAL	C-N	7.45	1.42	1.33
1	B	151	SER	C-N	7.43	1.42	1.33
1	B	159	VAL	C-N	7.39	1.43	1.33
1	B	779	GLN	CA-C	-7.38	1.43	1.52
1	C	611	LEU	N-CA	-7.35	1.37	1.46
1	B	462	LYS	N-CA	-7.34	1.39	1.45
1	B	495	TYR	C-N	7.33	1.41	1.33
1	C	636	TYR	N-CA	-7.33	1.37	1.46
1	A	82	PRO	N-CA	7.33	1.55	1.47
1	A	216	LEU	N-CA	-7.33	1.39	1.45
2	D	36	TRP	CA-C	-7.32	1.43	1.52
1	A	119	ILE	C-N	7.31	1.42	1.33
1	C	511	VAL	CA-C	-7.27	1.44	1.52
1	B	1077	THR	C-N	7.27	1.42	1.33
1	B	857	GLY	C-N	7.26	1.44	1.33
2	F	186	PRO	N-CA	-7.26	1.38	1.47
1	A	291	CYS	N-CA	7.25	1.55	1.46
1	B	663	ASP	C-N	7.24	1.41	1.33
1	B	770	ILE	N-CA	-7.24	1.38	1.46
2	E	148	LEU	CA-C	-7.23	1.42	1.52
1	C	195	LYS	CA-C	-7.22	1.43	1.52
1	A	177	MET	N-CA	-7.22	1.36	1.46
1	B	349	SER	N-CA	-7.21	1.36	1.46
1	C	168	PHE	CA-C	-7.18	1.43	1.52
1	B	597	VAL	C-O	-7.18	1.15	1.24
1	A	1045	LYS	N-CA	7.18	1.54	1.45
1	B	324	GLU	CA-C	-7.17	1.44	1.52
1	B	844	ILE	N-CA	-7.16	1.37	1.46
2	E	61	ALA	CA-C	-7.14	1.43	1.53
2	E	185	ILE	N-CA	-7.13	1.37	1.46
1	C	254	SER	CA-C	-7.12	1.44	1.52
1	A	169	GLU	C-N	7.11	1.45	1.34
1	B	355	ARG	CA-C	-7.09	1.44	1.52
1	C	587	ILE	CA-C	-7.08	1.43	1.52
1	A	1065	VAL	N-CA	-7.08	1.37	1.46
2	F	14	ALA	CA-C	-7.07	1.44	1.52
1	B	345	THR	CA-C	-7.06	1.44	1.52
1	A	818	ILE	CA-C	-7.06	1.44	1.52
1	C	192	PHE	CA-C	-7.05	1.44	1.52
1	B	1114	ILE	C-N	7.02	1.40	1.33
2	F	193	PRO	CA-C	7.02	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	626	ALA	CA-C	-7.00	1.44	1.52
1	B	642	VAL	C-N	7.00	1.42	1.33
1	C	581	THR	CA-C	-7.00	1.43	1.53
1	B	1066	THR	CA-C	-6.99	1.44	1.52
1	A	411	ALA	CA-C	-6.99	1.45	1.53
1	A	276	LEU	CA-C	-6.98	1.44	1.53
1	C	406	GLU	CA-C	-6.97	1.43	1.52
1	C	289	VAL	N-CA	-6.97	1.37	1.46
1	A	1098	ASN	C-N	6.97	1.43	1.33
1	C	202	LYS	N-CA	-6.95	1.37	1.45
1	C	454	ARG	CA-C	-6.95	1.44	1.52
1	A	280	ASN	C-N	6.94	1.43	1.33
1	A	364	ASP	C-N	6.94	1.42	1.33
2	F	83	MET	CA-C	-6.94	1.43	1.52
1	B	372	ALA	CA-C	-6.93	1.43	1.52
1	C	436	TRP	CA-C	-6.93	1.44	1.52
1	C	430	THR	C-N	6.93	1.40	1.32
1	C	213	VAL	CA-C	-6.93	1.44	1.52
1	B	1049	LEU	N-CA	-6.92	1.37	1.46
1	A	1055	SER	CA-C	-6.92	1.43	1.53
1	B	939	SER	CA-C	-6.91	1.44	1.52
1	A	516	GLU	C-N	6.91	1.43	1.33
1	B	524	VAL	CA-C	-6.91	1.43	1.52
1	B	619	GLU	C-N	6.90	1.41	1.33
1	B	274	THR	N-CA	6.89	1.54	1.46
1	C	120	VAL	CA-C	-6.89	1.43	1.52
1	A	282	ASN	C-N	6.89	1.43	1.33
1	B	615	VAL	N-CA	-6.89	1.38	1.46
1	A	62	VAL	CA-C	-6.85	1.44	1.52
1	A	386	LYS	C-N	6.85	1.43	1.33
1	B	379	CYS	CA-C	-6.85	1.44	1.52
1	A	342	PHE	C-N	6.84	1.42	1.33
1	B	275	PHE	N-CA	-6.84	1.37	1.46
1	B	1020	ALA	CA-C	-6.83	1.44	1.52
1	A	594	GLY	C-N	6.82	1.42	1.33
1	A	904	TYR	CA-C	-6.82	1.44	1.52
1	B	299	THR	C-O	6.81	1.32	1.24
1	B	163	ALA	C-N	6.79	1.43	1.33
1	B	833	PHE	CA-C	-6.79	1.43	1.52
1	A	261	GLY	CA-C	-6.79	1.42	1.51
1	B	935	GLN	N-CA	-6.79	1.38	1.46
2	E	141	PHE	CA-C	-6.79	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	25	SER	C-N	6.78	1.41	1.33
1	C	235	ILE	C-N	6.77	1.43	1.33
1	C	1142	GLN	CA-C	6.77	1.61	1.52
1	C	509	ARG	NE-CZ	6.76	1.40	1.33
1	C	666	ILE	CA-C	-6.75	1.44	1.52
1	C	946	GLY	N-CA	-6.75	1.36	1.45
1	B	1051	SER	CA-C	-6.74	1.44	1.52
1	A	510	VAL	CA-C	-6.72	1.44	1.52
1	C	924	ALA	CA-C	-6.72	1.44	1.52
1	A	130	VAL	C-O	-6.71	1.16	1.24
1	A	213	VAL	CA-C	-6.70	1.42	1.52
1	B	424	LYS	N-CA	-6.69	1.38	1.46
1	A	1102	TRP	C-N	6.69	1.42	1.33
1	C	395	VAL	CA-C	-6.69	1.44	1.52
1	A	740	MET	C-N	6.69	1.42	1.33
1	A	720	ILE	CA-C	6.68	1.61	1.52
1	B	303	LEU	C-N	6.68	1.43	1.33
2	E	175	GLY	C-N	6.68	1.43	1.33
1	A	788	ILE	CA-C	-6.67	1.44	1.52
1	A	92	PHE	CA-C	-6.66	1.44	1.52
1	A	34	ARG	NE-CZ	6.64	1.40	1.33
2	E	8	GLY	CA-C	-6.64	1.43	1.52
1	A	985	ASP	C-N	-6.63	1.25	1.33
1	A	101	ILE	CA-C	-6.62	1.44	1.52
1	B	165	ASN	C-N	6.61	1.42	1.33
2	D	133	ALA	CA-C	-6.59	1.47	1.52
1	C	1049	LEU	N-CA	-6.59	1.38	1.46
1	C	459	SER	C-N	6.58	1.42	1.33
1	C	257	GLY	C-N	6.58	1.42	1.33
1	B	477	SER	C-N	6.58	1.42	1.33
2	E	14	ALA	CA-C	-6.57	1.44	1.52
1	A	28	TYR	C-N	6.57	1.42	1.33
1	A	192	PHE	N-CA	-6.56	1.37	1.45
2	E	49	ALA	CA-C	-6.56	1.44	1.52
2	E	72	ARG	CD-NE	6.55	1.55	1.46
1	A	717	ASN	CA-C	-6.54	1.44	1.52
1	C	622	VAL	C-N	6.54	1.42	1.33
1	C	703	ASN	CA-C	-6.54	1.44	1.52
1	B	213	VAL	N-CA	-6.54	1.37	1.46
1	B	1000	ARG	CD-NE	6.54	1.55	1.46
1	B	140	PHE	N-CA	-6.53	1.38	1.46
1	C	617	CYS	CA-CB	6.53	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	157	GLY	C-N	6.53	1.41	1.33
1	A	1092	GLU	CA-C	-6.53	1.44	1.52
1	B	107	GLY	N-CA	-6.53	1.39	1.45
2	E	124	SER	N-CA	-6.53	1.38	1.46
1	A	1122	VAL	CA-C	-6.53	1.44	1.52
2	F	140	ALA	CA-C	-6.53	1.45	1.53
1	C	93	ALA	CA-C	-6.52	1.46	1.53
1	A	393	THR	CA-C	-6.51	1.43	1.52
1	A	851	CYS	N-CA	-6.51	1.38	1.46
2	E	157	GLY	C-N	6.51	1.42	1.33
1	A	1006	THR	CA-C	-6.51	1.44	1.52
1	B	54	LEU	CA-C	-6.51	1.44	1.52
2	F	3	GLN	C-N	6.51	1.41	1.33
2	F	175	GLY	CA-C	-6.51	1.42	1.51
2	D	40	ALA	C-N	6.50	1.41	1.33
1	A	166	CYS	N-CA	-6.50	1.37	1.45
1	B	924	ALA	N-CA	-6.50	1.38	1.46
1	A	120	VAL	C-N	6.49	1.42	1.33
1	B	54	LEU	N-CA	-6.49	1.38	1.46
1	A	944	ALA	CA-C	-6.48	1.43	1.52
1	C	1077	THR	C-N	6.48	1.43	1.33
1	B	335	LEU	CA-C	-6.48	1.44	1.52
1	B	623	ALA	N-CA	-6.48	1.38	1.46
1	C	357	ARG	CA-C	-6.48	1.45	1.52
1	B	174	PRO	C-N	6.47	1.42	1.33
2	E	21	SER	C-N	6.45	1.41	1.33
1	A	314	GLN	CA-C	-6.45	1.44	1.52
1	B	376	THR	N-CA	-6.44	1.38	1.46
1	A	123	ALA	CA-C	-6.44	1.44	1.53
1	A	38	TYR	CA-C	-6.43	1.45	1.52
1	C	205	SER	CA-C	6.43	1.60	1.52
1	C	371	SER	CA-C	-6.43	1.43	1.52
1	A	552	LEU	C-N	6.43	1.40	1.33
1	C	827	THR	CA-C	-6.42	1.45	1.52
1	B	894	LEU	N-CA	-6.42	1.38	1.46
1	B	228	ASP	CA-C	-6.42	1.46	1.53
1	B	960	ASN	CA-C	-6.42	1.44	1.52
1	B	113	LYS	N-CA	-6.41	1.38	1.46
1	C	549	THR	C-N	6.40	1.40	1.33
1	A	926	GLN	N-CA	-6.39	1.38	1.46
1	A	916	LEU	C-N	6.39	1.42	1.33
1	C	306	PHE	N-CA	-6.38	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	THR	N-CA	-6.38	1.37	1.46
1	A	1138	TYR	C-N	6.38	1.39	1.33
1	B	89	GLY	CA-C	-6.38	1.44	1.52
1	C	988	GLU	CA-C	-6.37	1.45	1.52
1	A	135	PHE	CA-C	-6.37	1.44	1.52
1	B	449	TYR	N-CA	-6.36	1.37	1.46
1	A	355	ARG	N-CA	-6.34	1.37	1.46
1	A	863	PRO	CA-C	6.34	1.59	1.52
1	B	704	SER	N-CA	-6.33	1.38	1.45
2	D	144	MET	N-CA	-6.33	1.38	1.46
1	B	122	ASN	C-N	6.33	1.42	1.33
1	C	596	SER	N-CA	-6.32	1.38	1.46
2	F	2	VAL	C-N	6.31	1.42	1.33
1	A	651	ILE	CA-C	-6.31	1.44	1.52
1	C	190	ARG	CA-C	-6.31	1.45	1.52
1	B	575	ALA	CA-C	-6.31	1.44	1.52
1	C	848	ASP	C-N	6.31	1.42	1.33
1	B	435	ALA	CA-C	-6.29	1.45	1.52
1	A	1052	PHE	CA-C	-6.29	1.45	1.52
1	C	280	ASN	N-CA	-6.28	1.38	1.45
1	C	896	ILE	N-CA	-6.28	1.38	1.46
1	A	214	ARG	C-N	6.26	1.42	1.33
1	B	168	PHE	CA-C	-6.26	1.45	1.52
1	B	731	MET	CA-C	-6.26	1.45	1.52
1	B	129	LYS	CA-C	-6.26	1.44	1.52
1	A	414	GLN	CA-C	-6.26	1.44	1.52
1	B	354	ASN	C-N	6.25	1.41	1.33
1	B	291	CYS	C-N	6.24	1.41	1.33
1	A	451	TYR	N-CA	-6.23	1.39	1.46
1	B	42	VAL	CA-C	-6.23	1.44	1.52
2	D	182	GLY	C-N	6.22	1.41	1.33
1	A	705	VAL	N-CA	-6.22	1.39	1.46
1	B	494	SER	N-CA	6.21	1.54	1.46
2	F	46	GLU	CA-C	6.21	1.60	1.52
1	B	827	THR	CA-C	6.21	1.60	1.52
1	C	557	LYS	CA-C	-6.20	1.45	1.52
1	B	326	ILE	CA-C	-6.20	1.44	1.52
1	C	167	THR	C-N	6.20	1.41	1.33
1	C	399	SER	C-N	6.20	1.41	1.33
1	C	1002	GLN	CA-C	-6.20	1.44	1.52
1	B	884	SER	N-CA	-6.19	1.39	1.46
1	C	1049	LEU	CA-C	6.19	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	838	GLY	C-N	6.19	1.42	1.33
2	D	97	ALA	CA-C	-6.18	1.45	1.52
2	D	49	ALA	CA-C	-6.18	1.45	1.52
2	F	55	GLY	CA-C	6.17	1.59	1.52
1	B	161	SER	CA-C	6.16	1.61	1.52
1	B	556	ASN	C-N	6.15	1.41	1.33
2	F	73	ASP	N-CA	-6.14	1.38	1.46
1	C	86	PHE	C-N	6.13	1.42	1.33
1	B	877	LEU	N-CA	-6.13	1.38	1.46
1	B	1064	HIS	ND1-CE1	6.13	1.38	1.32
1	B	860	VAL	N-CA	-6.13	1.39	1.46
2	F	17	SER	N-CA	-6.12	1.38	1.45
1	C	634	ARG	C-N	6.12	1.41	1.33
1	B	614	ASP	N-CA	-6.11	1.37	1.46
1	A	80	ASP	N-CA	-6.11	1.37	1.45
1	B	176	LEU	CA-C	-6.11	1.47	1.53
1	C	623	ALA	C-N	6.11	1.39	1.33
1	A	1058	HIS	C-N	6.11	1.40	1.33
2	D	56	SER	N-CA	-6.11	1.38	1.46
2	F	6	GLU	C-N	6.10	1.40	1.33
1	A	1067	TYR	CA-C	-6.10	1.45	1.52
1	C	101	ILE	CA-C	6.09	1.59	1.52
1	C	509	ARG	CD-NE	6.09	1.54	1.46
1	C	953	ASN	C-N	6.09	1.42	1.33
1	B	311	GLY	N-CA	6.08	1.50	1.45
1	C	465	GLU	N-CA	-6.08	1.38	1.46
1	B	263	ALA	N-CA	-6.07	1.39	1.46
1	B	444	LYS	C-N	6.07	1.39	1.33
1	A	452	LEU	CA-C	-6.07	1.45	1.52
2	E	84	ASN	CA-C	-6.07	1.45	1.52
1	A	831	ALA	C-N	6.07	1.43	1.33
1	B	862	PRO	C-O	-6.07	1.19	1.24
1	B	723	THR	CA-C	-6.07	1.45	1.52
1	A	188	ASN	CA-C	-6.06	1.45	1.52
1	B	388	ASN	C-N	6.06	1.41	1.33
2	E	57	ILE	N-CA	-6.06	1.39	1.46
1	A	169	GLU	N-CA	-6.05	1.38	1.46
1	C	400	PHE	C-N	6.05	1.41	1.33
1	B	101	ILE	C-N	6.05	1.41	1.33
1	C	433	VAL	CA-C	-6.05	1.45	1.52
1	B	748	GLU	CA-C	-6.05	1.45	1.52
1	C	82	PRO	N-CA	-6.04	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	785	VAL	C-N	6.04	1.42	1.33
1	B	480	CYS	C-N	6.03	1.42	1.33
1	A	364	ASP	N-CA	-6.03	1.38	1.46
1	A	585	LEU	C-O	-6.03	1.16	1.23
1	C	750	SER	CA-C	-6.03	1.45	1.52
1	B	684	ALA	CA-CB	6.02	1.63	1.53
1	B	1049	LEU	C-N	6.02	1.40	1.33
1	A	550	GLY	N-CA	-6.02	1.39	1.45
1	B	201	PHE	CA-C	-6.02	1.45	1.52
1	B	645	THR	N-CA	-6.02	1.37	1.45
1	B	572	THR	C-N	6.01	1.41	1.33
1	B	692	ILE	CA-C	-6.01	1.46	1.52
1	B	631	PRO	N-CA	-6.01	1.39	1.47
1	C	1133	VAL	CA-C	-6.01	1.45	1.52
1	A	407	VAL	C-N	6.01	1.42	1.33
1	A	617	CYS	CA-C	-6.01	1.45	1.53
1	B	921	LYS	CA-C	6.00	1.60	1.52
1	B	760	CYS	CA-CB	6.00	1.62	1.53
1	B	829	ALA	N-CA	-6.00	1.41	1.46
1	B	859	THR	C-N	6.00	1.42	1.33
1	B	67	ALA	CA-C	-5.99	1.44	1.52
1	B	193	VAL	CA-C	-5.98	1.45	1.52
1	C	148	ASN	C-N	-5.98	1.25	1.33
1	B	1072	GLU	N-CA	-5.98	1.38	1.45
1	B	781	VAL	CA-C	-5.98	1.44	1.52
1	A	1060	VAL	CA-C	-5.98	1.45	1.52
1	A	514	SER	N-CA	-5.97	1.38	1.46
1	B	738	CYS	CA-CB	5.97	1.62	1.53
1	A	901	GLN	CA-C	-5.97	1.45	1.52
1	C	165	ASN	CA-C	-5.97	1.46	1.52
1	A	968	SER	CA-C	-5.97	1.45	1.52
1	A	192	PHE	CA-C	-5.96	1.45	1.52
1	B	695	TYR	CA-C	-5.96	1.45	1.52
1	B	512	VAL	CA-C	-5.96	1.45	1.52
2	F	3	GLN	N-CA	5.96	1.53	1.46
1	B	453	TYR	C-N	5.96	1.41	1.33
2	D	120	GLY	C-N	5.95	1.40	1.33
1	A	1102	TRP	N-CA	-5.94	1.38	1.45
1	C	424	LYS	N-CA	-5.94	1.38	1.46
2	E	143	ASN	CA-C	-5.94	1.45	1.52
1	A	755	GLN	CA-C	-5.94	1.44	1.52
1	B	666	ILE	C-N	5.94	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1016	ALA	CA-C	-5.94	1.45	1.52
1	A	455	LEU	C-N	5.93	1.41	1.33
1	A	72	GLY	C-N	5.92	1.41	1.33
1	A	669	GLY	CA-C	-5.92	1.43	1.51
1	B	328	ARG	CA-C	-5.92	1.45	1.52
1	C	299	THR	C-N	5.92	1.41	1.33
1	C	339	GLY	CA-C	-5.92	1.43	1.51
1	A	63	THR	N-CA	-5.91	1.38	1.46
1	C	909	ILE	N-CA	5.91	1.52	1.46
1	C	700	GLY	N-CA	-5.90	1.40	1.45
1	B	262	ALA	N-CA	-5.90	1.40	1.46
1	A	359	SER	CA-C	-5.90	1.45	1.52
1	C	303	LEU	C-N	5.89	1.42	1.33
1	A	970	PHE	CA-C	-5.89	1.45	1.53
2	F	71	SER	CA-C	-5.89	1.45	1.52
2	D	152	HIS	CA-C	-5.89	1.45	1.52
1	B	1061	VAL	CA-C	-5.89	1.45	1.52
1	B	1112	PRO	CA-C	-5.88	1.44	1.52
1	B	1101	HIS	N-CA	-5.88	1.38	1.45
1	B	131	CYS	CA-CB	5.88	1.61	1.53
1	C	411	ALA	CA-C	5.88	1.59	1.53
1	C	595	VAL	N-CA	-5.88	1.38	1.46
1	A	331	ASN	C-N	5.88	1.41	1.33
2	D	96	CYS	C-N	5.87	1.41	1.33
1	A	158	ARG	C-N	5.87	1.41	1.33
2	E	183	GLU	N-CA	-5.87	1.38	1.46
1	B	528	LYS	CA-C	-5.87	1.45	1.52
1	B	729	VAL	CA-C	-5.87	1.47	1.52
1	B	994	ASP	C-N	5.87	1.41	1.33
1	C	458	LYS	N-CA	-5.87	1.37	1.46
2	E	45	ARG	CA-C	-5.87	1.45	1.52
1	A	715	PRO	CA-C	-5.87	1.45	1.52
1	B	160	TYR	C-N	5.87	1.42	1.33
1	C	146	HIS	CA-CB	5.86	1.63	1.53
1	A	52	GLN	C-N	5.86	1.41	1.33
1	A	903	ALA	CA-CB	5.85	1.62	1.53
1	C	42	VAL	C-N	5.85	1.41	1.33
1	C	162	SER	CA-C	-5.85	1.45	1.52
1	C	219	GLY	N-CA	-5.85	1.39	1.44
2	D	12	VAL	CA-C	-5.85	1.45	1.52
1	B	1127	ASP	C-N	5.84	1.41	1.33
1	C	864	LEU	N-CA	-5.84	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	956	ALA	C-N	5.84	1.41	1.33
1	C	347	PHE	CA-C	-5.83	1.45	1.52
1	A	221	SER	CA-C	-5.83	1.45	1.52
1	B	105	ILE	CA-C	-5.83	1.45	1.52
1	C	86	PHE	N-CA	-5.82	1.39	1.45
1	C	757	GLY	CA-C	-5.82	1.43	1.52
1	B	927	PHE	C-N	5.81	1.41	1.33
1	A	98	SER	N-CA	-5.81	1.41	1.46
1	B	73	THR	N-CA	-5.81	1.39	1.46
1	C	204	TYR	C-N	5.81	1.41	1.33
1	C	1122	VAL	CA-C	-5.81	1.45	1.52
1	A	71	SER	C-N	5.80	1.40	1.33
1	A	526	GLY	C-N	5.80	1.40	1.34
2	F	38	ARG	N-CA	5.80	1.53	1.45
2	E	99	ASP	N-CA	-5.79	1.41	1.46
1	B	1025	ALA	CA-CB	5.79	1.62	1.53
1	C	483	VAL	CA-C	-5.79	1.45	1.52
1	A	726	ILE	N-CA	-5.79	1.39	1.46
1	C	396	TYR	CA-C	-5.78	1.45	1.52
1	A	617	CYS	N-CA	5.78	1.52	1.46
1	B	427	ASP	CA-C	-5.78	1.44	1.52
1	B	153	MET	CA-C	5.78	1.60	1.52
1	C	541	PHE	CA-C	-5.78	1.45	1.52
1	A	111	ASP	CA-C	-5.78	1.44	1.52
1	B	807	PRO	CA-C	-5.78	1.45	1.52
1	A	379	CYS	CA-C	-5.77	1.45	1.52
1	A	905	ARG	N-CA	-5.77	1.39	1.46
1	C	211	ASN	C-N	5.76	1.41	1.33
1	C	159	VAL	N-CA	-5.76	1.39	1.46
1	B	64	TRP	N-CA	-5.75	1.38	1.46
1	B	576	VAL	CA-C	-5.75	1.46	1.52
1	A	879	ALA	N-CA	-5.75	1.39	1.46
1	B	983	ARG	N-CA	-5.75	1.38	1.46
2	E	192	PRO	C-O	-5.75	1.18	1.24
1	C	1080	ALA	CA-CB	-5.75	1.44	1.53
2	D	41	PRO	C-N	5.74	1.39	1.34
1	B	714	ILE	N-CA	-5.74	1.41	1.46
1	C	240	THR	C-N	5.74	1.41	1.33
1	C	117	LEU	CA-C	-5.74	1.45	1.52
1	B	651	ILE	CA-C	-5.73	1.45	1.52
1	C	187	LYS	CA-C	-5.73	1.48	1.53
1	A	600	PRO	N-CA	5.73	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	570	ALA	C-N	5.73	1.41	1.33
1	B	373	SER	C-N	5.72	1.40	1.33
1	B	353	TRP	CA-C	5.72	1.60	1.52
1	C	1123	SER	CA-C	-5.72	1.46	1.52
1	A	759	PHE	N-CA	-5.72	1.39	1.46
1	C	980	ILE	CA-C	-5.72	1.45	1.52
1	B	769	GLY	N-CA	-5.71	1.38	1.45
1	B	499	PRO	C-N	5.71	1.41	1.33
1	C	1097	SER	C-N	5.71	1.41	1.33
1	A	1097	SER	N-CA	-5.71	1.39	1.46
2	D	49	ALA	C-N	5.71	1.39	1.33
2	F	28	ILE	C-N	5.70	1.41	1.33
1	A	997	ILE	N-CA	-5.70	1.40	1.46
1	B	517	LEU	CA-C	-5.70	1.45	1.53
1	C	981	LEU	CA-C	-5.70	1.45	1.52
1	B	473	TYR	N-CA	-5.69	1.39	1.46
1	B	571	ASP	N-CA	5.68	1.53	1.46
1	B	814	LYS	N-CA	-5.68	1.39	1.46
1	A	764	ASN	C-N	5.68	1.41	1.33
1	B	277	LEU	C-N	-5.68	1.25	1.33
1	B	266	TYR	C-N	5.68	1.41	1.33
2	D	94	TYR	N-CA	-5.67	1.39	1.45
1	B	862	PRO	C-N	-5.67	1.26	1.33
1	A	918	GLU	N-CA	5.67	1.53	1.46
1	B	841	LEU	C-N	5.67	1.41	1.33
2	E	140	ALA	N-CA	-5.67	1.39	1.46
1	A	41	LYS	N-CA	-5.67	1.40	1.46
1	C	515	PHE	CA-C	-5.66	1.46	1.52
1	A	61	ASN	C-N	5.66	1.40	1.33
1	A	305	SER	C-N	5.66	1.41	1.33
1	A	767	LEU	CA-C	-5.66	1.45	1.52
2	F	89	GLU	N-CA	-5.66	1.38	1.46
1	C	734	THR	C-N	5.66	1.41	1.33
1	A	395	VAL	CA-C	-5.65	1.45	1.52
1	C	1055	SER	C-N	5.65	1.39	1.33
1	A	358	ILE	N-CA	-5.65	1.39	1.46
1	A	925	ASN	CA-C	-5.65	1.45	1.52
1	A	377	PHE	CA-C	-5.65	1.46	1.53
1	A	322	PRO	CA-C	5.64	1.59	1.52
1	C	895	GLN	C-N	5.64	1.39	1.33
1	C	784	GLN	C-N	5.64	1.40	1.33
2	F	136	SER	C-O	-5.64	1.20	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	664	ILE	C-O	-5.64	1.18	1.24
1	B	697	MET	C-N	5.64	1.41	1.33
2	E	171	ARG	CD-NE	5.64	1.54	1.46
1	C	819	GLU	CA-C	-5.64	1.45	1.52
2	E	49	ALA	N-CA	-5.64	1.39	1.46
1	B	623	ALA	C-N	5.63	1.40	1.33
1	B	65	PHE	CA-C	-5.63	1.45	1.52
2	D	161	TYR	CZ-OH	5.63	1.49	1.38
2	F	169	PHE	CA-C	-5.63	1.45	1.52
1	C	76	THR	N-CA	-5.63	1.38	1.45
1	A	88	ASP	N-CA	-5.62	1.38	1.46
1	C	794	ILE	C-N	5.62	1.40	1.33
1	C	1110	TYR	C-N	-5.62	1.27	1.33
2	E	19	ARG	N-CA	-5.62	1.39	1.46
1	C	731	MET	N-CA	-5.62	1.38	1.45
2	D	190	ASP	CA-C	-5.62	1.45	1.52
1	A	1023	ASN	CA-C	5.62	1.60	1.52
1	A	1131	GLY	CA-C	5.61	1.59	1.51
1	B	714	ILE	C-N	5.61	1.41	1.33
2	E	142	SER	N-CA	5.61	1.53	1.46
2	F	26	GLY	C-N	5.61	1.41	1.33
1	A	600	PRO	N-CD	5.61	1.55	1.47
1	B	597	VAL	CA-C	-5.61	1.45	1.52
1	A	362	VAL	CA-C	-5.61	1.45	1.52
1	B	859	THR	N-CA	5.61	1.53	1.45
1	B	685	ALA	CA-C	-5.60	1.45	1.52
1	C	483	VAL	C-N	5.60	1.41	1.33
1	B	382	VAL	N-CA	5.60	1.52	1.46
2	E	67	ARG	C-O	-5.60	1.17	1.23
1	A	186	PHE	CA-C	-5.60	1.45	1.53
1	C	1048	HIS	C-N	5.60	1.40	1.33
1	A	146	HIS	CA-C	-5.59	1.45	1.52
1	B	404	GLY	CA-C	-5.59	1.44	1.51
1	C	765	ARG	C-N	5.59	1.41	1.33
1	A	984	LEU	C-O	-5.59	1.16	1.23
1	C	91	TYR	CA-C	-5.59	1.45	1.52
1	C	546	LEU	CA-C	-5.59	1.45	1.52
1	A	839	ASP	N-CA	5.58	1.53	1.46
1	C	902	MET	N-CA	-5.58	1.39	1.46
1	B	688	ALA	CA-C	-5.57	1.45	1.52
1	A	597	VAL	CA-C	-5.57	1.46	1.52
2	E	177	LYS	C-N	5.57	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	451	TYR	C-N	5.57	1.41	1.33
1	B	898	PHE	CA-C	5.57	1.59	1.52
1	B	899	PRO	CA-C	-5.57	1.43	1.52
1	C	262	ALA	C-N	5.57	1.41	1.33
1	B	612	TYR	CA-C	-5.56	1.45	1.52
1	A	657	ASN	C-N	5.56	1.42	1.33
1	A	366	SER	C-N	5.56	1.40	1.34
2	E	109	TRP	CA-C	-5.56	1.46	1.52
1	B	991	VAL	C-N	5.56	1.41	1.33
1	C	590	CYS	C-O	-5.55	1.17	1.23
1	B	118	LEU	N-CA	-5.55	1.39	1.46
1	B	736	VAL	CA-C	-5.55	1.45	1.52
1	C	901	GLN	N-CA	-5.55	1.39	1.46
1	C	657	ASN	C-N	5.55	1.41	1.33
1	A	487	ASN	CA-C	-5.55	1.46	1.53
1	A	621	PRO	N-CA	-5.54	1.40	1.47
1	B	839	ASP	CA-C	-5.54	1.46	1.53
1	C	491	PRO	CA-C	5.54	1.57	1.52
1	C	617	CYS	CA-C	5.54	1.60	1.53
1	C	1004	LEU	N-CA	-5.54	1.39	1.46
1	A	733	LYS	N-CA	-5.54	1.39	1.46
1	B	162	SER	C-N	5.54	1.41	1.33
1	A	154	GLU	N-CA	-5.53	1.39	1.45
1	B	286	THR	C-N	5.53	1.40	1.33
1	C	560	LEU	C-N	5.53	1.38	1.33
1	A	586	ASP	C-O	-5.52	1.17	1.24
1	B	843	ASP	N-CA	-5.52	1.39	1.46
2	D	176	TRP	CA-C	-5.52	1.45	1.52
2	E	134	SER	N-CA	-5.52	1.39	1.46
2	D	159	PHE	C-N	5.52	1.41	1.33
1	B	522	ALA	N-CA	-5.51	1.39	1.46
1	A	531	THR	C-N	5.51	1.41	1.33
1	C	479	PRO	N-CA	-5.51	1.40	1.47
1	A	148	ASN	CA-C	-5.51	1.46	1.52
1	B	264	ALA	CA-C	-5.51	1.46	1.52
1	B	804	GLN	N-CA	-5.51	1.39	1.46
1	B	869	MET	N-CA	-5.51	1.39	1.46
1	B	852	ALA	CA-C	-5.51	1.47	1.53
2	D	114	GLN	N-CA	-5.50	1.39	1.46
2	D	152	HIS	N-CA	-5.50	1.40	1.46
2	F	110	GLY	CA-C	-5.50	1.43	1.52
1	C	760	CYS	C-N	5.50	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	32	ASN	C-N	5.50	1.41	1.33
1	A	75	GLY	C-N	5.49	1.41	1.33
1	C	356	LYS	C-N	5.49	1.41	1.33
2	D	179	LEU	C-N	5.49	1.39	1.33
1	A	540	ASN	N-CA	-5.49	1.39	1.46
1	B	423	TYR	CA-CB	5.49	1.62	1.53
1	B	464	PHE	C-N	5.48	1.41	1.33
1	B	483	VAL	N-CA	5.48	1.53	1.46
2	E	41	PRO	C-N	5.48	1.41	1.33
1	B	802	PHE	CA-C	-5.48	1.46	1.53
1	B	56	LEU	C-N	5.47	1.40	1.33
1	A	1142	GLN	C-O	-5.47	1.19	1.24
1	C	854	LYS	N-CA	5.47	1.52	1.46
2	D	67	ARG	N-CA	-5.47	1.39	1.46
2	F	129	GLY	C-O	-5.47	1.19	1.24
2	E	2	VAL	C-N	5.46	1.40	1.33
1	B	684	ALA	CA-C	-5.46	1.45	1.53
1	C	606	ASN	CA-C	5.46	1.59	1.52
1	C	627	ASP	N-CA	-5.46	1.39	1.45
1	A	656	VAL	N-CA	5.46	1.52	1.46
1	A	952	VAL	C-N	5.46	1.40	1.33
1	C	273	ARG	N-CA	-5.45	1.39	1.45
1	A	436	TRP	CA-C	-5.45	1.45	1.52
1	A	813	SER	CA-C	5.45	1.59	1.52
1	B	677	GLN	CA-C	-5.45	1.43	1.52
1	A	684	ALA	N-CA	-5.45	1.38	1.45
1	C	1080	ALA	CA-C	-5.45	1.46	1.52
2	E	44	GLU	CA-C	-5.45	1.45	1.52
1	B	795	LYS	N-CA	5.44	1.52	1.46
1	C	244	LEU	CA-C	-5.44	1.45	1.52
1	B	874	THR	CA-C	-5.44	1.45	1.52
1	C	160	TYR	N-CA	-5.44	1.39	1.46
1	B	196	ASN	CA-C	-5.43	1.46	1.52
1	B	844	ILE	C-N	5.43	1.40	1.33
1	B	252	GLY	N-CA	-5.43	1.38	1.45
1	C	457	ARG	N-CA	-5.43	1.39	1.46
1	B	671	CYS	CA-C	-5.43	1.46	1.52
1	C	316	SER	C-N	5.42	1.40	1.33
1	C	685	ALA	N-CA	-5.42	1.38	1.45
1	C	937	SER	CA-C	-5.42	1.46	1.52
1	C	719	THR	C-N	5.42	1.40	1.33
1	A	1025	ALA	CA-C	-5.42	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	832	GLY	N-CA	-5.42	1.36	1.45
2	D	96	CYS	CA-C	-5.42	1.46	1.53
2	D	133	ALA	CA-CB	5.42	1.60	1.53
1	B	225	PRO	CA-C	5.41	1.59	1.52
1	C	980	ILE	C-N	5.41	1.41	1.33
2	D	24	ALA	N-CA	-5.41	1.40	1.46
1	B	401	VAL	C-N	5.41	1.41	1.33
1	B	448	ASN	CA-C	-5.41	1.46	1.52
1	B	558	LYS	C-N	5.41	1.40	1.33
1	A	519	HIS	N-CA	-5.40	1.39	1.46
1	A	806	LEU	CA-C	5.40	1.60	1.53
1	B	439	ASN	CA-C	-5.40	1.45	1.52
1	A	401	VAL	N-CA	-5.40	1.40	1.46
1	C	53	ASP	N-CA	-5.40	1.40	1.46
1	B	696	THR	CA-C	-5.39	1.45	1.52
1	C	993	ILE	CA-C	-5.39	1.46	1.52
1	A	573	THR	C-N	5.38	1.40	1.33
1	C	340	GLU	CA-C	-5.38	1.45	1.52
2	D	191	SER	N-CA	-5.38	1.40	1.46
1	B	48	LEU	CA-C	-5.38	1.46	1.52
1	C	940	SER	CA-C	-5.38	1.45	1.52
1	A	180	GLU	C-N	5.38	1.40	1.33
1	B	776	LYS	N-CA	-5.38	1.40	1.46
1	A	672	ALA	N-CA	5.37	1.52	1.45
1	B	143	VAL	CA-C	-5.37	1.45	1.52
1	C	642	VAL	N-CA	-5.37	1.39	1.46
1	C	238	PHE	N-CA	-5.37	1.39	1.45
1	B	585	LEU	N-CA	-5.37	1.39	1.46
1	C	431	GLY	N-CA	-5.37	1.40	1.45
1	C	433	VAL	C-N	5.37	1.40	1.33
1	B	471	GLU	CA-C	-5.36	1.46	1.52
1	A	1106	GLN	C-N	5.35	1.41	1.33
2	F	90	ASP	N-CA	-5.35	1.39	1.46
2	D	147	MET	CA-C	-5.35	1.46	1.52
2	D	52	THR	CA-C	-5.35	1.45	1.52
1	A	283	GLY	N-CA	-5.34	1.36	1.45
1	C	358	ILE	N-CA	-5.34	1.39	1.46
2	F	184	LEU	C-N	5.34	1.39	1.33
1	C	1067	TYR	C-N	5.34	1.39	1.33
1	A	1007	TYR	N-CA	-5.34	1.40	1.46
1	C	638	THR	CA-C	-5.34	1.45	1.52
1	A	435	ALA	CA-C	-5.33	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	406	GLU	N-CA	5.33	1.53	1.46
1	C	1093	GLY	C-O	5.33	1.29	1.23
2	E	109	TRP	C-N	5.33	1.40	1.33
1	A	783	ALA	C-N	5.33	1.41	1.33
1	B	551	VAL	CA-C	-5.32	1.45	1.52
1	B	1050	MET	CA-C	5.32	1.59	1.52
1	A	699	LEU	N-CA	-5.32	1.40	1.46
1	C	184	GLY	CA-C	-5.32	1.45	1.52
1	C	843	ASP	N-CA	-5.32	1.39	1.46
1	A	761	THR	C-N	5.32	1.41	1.33
1	B	850	ILE	C-N	5.32	1.41	1.33
1	A	473	TYR	CA-C	-5.31	1.46	1.52
1	A	165	ASN	CA-C	-5.31	1.46	1.52
2	E	81	LEU	C-O	-5.31	1.18	1.24
1	A	713	ALA	C-N	5.31	1.37	1.33
1	B	151	SER	N-CA	-5.31	1.39	1.46
1	C	819	GLU	C-N	5.31	1.40	1.33
1	C	1141	LEU	C-N	5.31	1.40	1.33
1	C	680	SER	CA-C	5.30	1.59	1.52
2	E	29	PHE	CA-C	-5.30	1.45	1.52
1	C	734	THR	CA-C	-5.30	1.45	1.52
1	B	995	ARG	C-N	5.30	1.41	1.33
1	C	527	PRO	C-N	5.29	1.40	1.33
1	A	995	ARG	C-N	5.29	1.41	1.33
1	C	1061	VAL	C-N	5.29	1.40	1.33
1	A	948	LEU	CA-C	-5.29	1.45	1.52
1	C	460	ASN	C-N	5.29	1.40	1.33
2	F	137	ARG	C-N	5.29	1.40	1.33
1	B	288	ALA	C-N	5.28	1.40	1.33
1	A	589	PRO	C-N	5.28	1.40	1.33
2	E	151	ALA	CA-C	-5.28	1.45	1.52
1	A	316	SER	N-CA	-5.27	1.39	1.46
1	A	994	ASP	N-CA	5.27	1.52	1.46
2	D	115	VAL	CA-C	-5.27	1.45	1.52
1	A	49	HIS	N-CA	-5.27	1.39	1.45
1	A	1051	SER	CA-C	-5.27	1.46	1.52
1	B	141	LEU	C-O	-5.27	1.17	1.24
1	B	492	LEU	C-N	5.27	1.40	1.33
1	A	560	LEU	C-O	-5.27	1.16	1.23
1	B	1141	LEU	C-N	5.27	1.40	1.33
1	A	782	PHE	C-N	5.27	1.41	1.33
1	B	580	GLN	N-CA	-5.27	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	707	TYR	CA-CB	5.27	1.60	1.53
1	C	797	PHE	N-CA	-5.27	1.40	1.46
1	A	34	ARG	CD-NE	5.27	1.53	1.46
1	A	297	SER	C-N	5.27	1.40	1.33
1	A	919	ASN	C-N	5.27	1.40	1.33
1	C	975	SER	C-N	5.27	1.40	1.33
1	A	51	THR	C-N	5.26	1.40	1.33
1	B	1058	HIS	C-N	5.26	1.38	1.33
1	B	357	ARG	CA-C	-5.26	1.46	1.52
1	A	232	GLY	CA-C	-5.26	1.44	1.51
1	A	100	ILE	C-N	5.25	1.40	1.33
1	A	898	PHE	CA-C	-5.25	1.46	1.52
1	A	368	LEU	C-N	5.25	1.40	1.33
1	C	1080	ALA	N-CA	-5.25	1.39	1.46
1	B	837	TYR	N-CA	-5.25	1.39	1.45
1	A	714	ILE	N-CA	5.25	1.50	1.46
1	A	472	ILE	CA-C	5.25	1.59	1.52
2	E	187	ILE	CA-C	-5.25	1.47	1.52
1	A	631	PRO	CA-CB	-5.25	1.46	1.53
1	B	155	SER	N-CA	-5.24	1.39	1.45
1	B	957	GLN	N-CA	-5.24	1.40	1.46
1	B	1123	SER	C-N	5.24	1.40	1.33
1	A	663	ASP	C-N	5.24	1.37	1.33
1	C	830	ASP	C-O	-5.24	1.18	1.23
1	B	378	LYS	C-N	5.24	1.40	1.33
1	C	927	PHE	CA-C	5.24	1.59	1.52
1	C	81	ASN	CA-C	-5.23	1.47	1.52
1	C	412	PRO	N-CA	-5.23	1.40	1.47
1	C	1135	ASN	C-O	-5.23	1.18	1.23
2	D	61	ALA	CA-CB	5.23	1.61	1.53
2	D	146	ASP	CA-C	-5.23	1.46	1.52
1	A	279	TYR	CA-C	-5.22	1.46	1.52
1	A	199	GLY	CA-C	5.22	1.59	1.51
1	A	911	VAL	N-CA	-5.22	1.39	1.46
1	C	36	VAL	CA-C	-5.22	1.46	1.52
1	C	310	LYS	C-N	5.22	1.39	1.33
1	C	443	SER	N-CA	-5.22	1.38	1.45
1	C	465	GLU	CA-C	-5.22	1.46	1.52
1	C	900	MET	N-CA	-5.22	1.39	1.46
2	F	138	VAL	C-N	5.22	1.40	1.33
1	B	316	SER	N-CA	-5.21	1.40	1.46
1	C	834	ILE	CA-C	-5.21	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	85	SER	C-O	-5.21	1.16	1.23
1	C	495	TYR	CA-C	-5.21	1.46	1.52
1	C	1018	ILE	CA-C	-5.21	1.46	1.52
1	A	883	THR	C-N	5.20	1.41	1.33
1	A	1010	GLN	N-CA	-5.20	1.40	1.46
1	C	919	ASN	CA-C	-5.20	1.46	1.53
1	A	1047	TYR	CA-C	-5.20	1.46	1.52
1	C	661	GLU	C-N	5.20	1.41	1.33
1	B	650	LEU	CA-C	-5.19	1.46	1.52
1	B	727	LEU	C-O	-5.19	1.20	1.24
1	B	1113	GLN	CA-C	-5.19	1.46	1.52
1	A	95	THR	C-N	5.19	1.41	1.33
1	B	901	GLN	N-CA	5.19	1.52	1.46
1	B	1075	PHE	C-N	5.19	1.40	1.33
1	A	734	THR	CA-C	-5.19	1.46	1.53
2	D	87	LYS	CA-C	-5.19	1.45	1.52
1	A	1141	LEU	CA-C	-5.18	1.46	1.53
1	C	263	ALA	C-O	-5.18	1.17	1.24
1	B	647	ALA	CA-C	-5.18	1.45	1.52
1	C	735	SER	N-CA	-5.18	1.39	1.46
2	D	193	PRO	CA-C	5.18	1.56	1.52
1	A	1034	LEU	CA-C	-5.18	1.46	1.52
1	C	401	VAL	CA-C	-5.18	1.46	1.52
2	F	38	ARG	C-N	5.18	1.40	1.33
2	F	160	ILE	N-CA	-5.18	1.40	1.46
1	A	423	TYR	C-O	-5.17	1.17	1.24
1	B	131	CYS	C-N	5.17	1.40	1.33
1	B	829	ALA	C-N	5.17	1.41	1.33
1	C	265	TYR	N-CA	-5.17	1.39	1.46
1	C	481	ASN	N-CA	-5.17	1.39	1.46
1	C	811	LYS	CA-C	-5.17	1.46	1.52
2	D	31	ARG	C-N	5.17	1.41	1.33
1	B	526	GLY	C-N	5.17	1.38	1.33
1	B	751	ASN	CA-C	5.17	1.59	1.52
1	C	1003	SER	CA-C	-5.17	1.46	1.52
2	F	156	GLU	C-N	5.17	1.41	1.33
1	B	133	PHE	N-CA	-5.16	1.39	1.45
1	B	1090	PRO	C-O	5.16	1.29	1.23
1	A	395	VAL	C-N	5.16	1.40	1.33
1	B	635	VAL	N-CA	-5.16	1.40	1.46
1	B	889	GLY	C-N	5.16	1.40	1.33
1	A	918	GLU	C-O	-5.16	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	832	GLY	C-N	5.16	1.41	1.33
2	F	116	THR	N-CA	5.16	1.52	1.46
1	A	372	ALA	CA-CB	5.15	1.62	1.53
1	B	114	THR	C-N	5.15	1.40	1.33
1	A	132	GLU	N-CA	-5.15	1.40	1.46
1	A	128	ILE	N-CA	-5.14	1.39	1.46
1	B	497	PHE	C-N	5.14	1.38	1.33
1	B	657	ASN	CA-C	-5.14	1.45	1.52
2	D	161	TYR	CA-CB	5.14	1.61	1.53
1	C	852	ALA	N-CA	5.14	1.52	1.46
1	A	54	LEU	N-CA	-5.14	1.40	1.46
1	A	434	ILE	N-CA	-5.14	1.39	1.46
1	A	455	LEU	CA-C	-5.14	1.47	1.53
1	B	1120	THR	CA-C	-5.14	1.46	1.52
1	A	413	GLY	N-CA	-5.14	1.38	1.45
1	B	652	GLY	C-N	5.14	1.39	1.33
1	C	277	LEU	CA-C	-5.14	1.46	1.52
1	C	461	LEU	CA-C	-5.14	1.46	1.52
1	C	882	ILE	C-N	5.14	1.41	1.33
1	A	538	CYS	C-N	5.13	1.40	1.33
1	C	355	ARG	CA-C	-5.13	1.46	1.52
2	E	30	GLY	C-N	5.13	1.41	1.33
1	C	464	PHE	N-CA	5.13	1.52	1.46
1	C	979	ASP	C-O	-5.13	1.18	1.24
1	B	241	LEU	CA-C	-5.13	1.46	1.52
2	F	95	TYR	CA-C	-5.13	1.46	1.52
2	D	138	VAL	N-CA	-5.13	1.40	1.46
2	F	154	VAL	C-N	5.12	1.39	1.33
1	C	888	PHE	C-N	5.12	1.41	1.33
1	A	93	ALA	CA-CB	5.12	1.62	1.53
1	B	701	ALA	CA-C	-5.11	1.46	1.52
1	B	237	ARG	N-CA	-5.11	1.39	1.45
1	C	676	THR	CA-CB	5.11	1.61	1.53
1	A	93	ALA	CA-C	-5.11	1.46	1.52
2	F	48	VAL	C-N	5.11	1.39	1.33
1	B	750	SER	C-N	-5.10	1.27	1.33
1	A	587	ILE	N-CA	-5.10	1.40	1.46
1	C	697	MET	C-N	5.10	1.40	1.33
1	B	504	GLY	C-O	-5.09	1.17	1.24
1	B	1122	VAL	N-CA	5.09	1.52	1.46
1	A	909	ILE	N-CA	-5.09	1.40	1.46
2	D	94	TYR	C-N	5.09	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	CYS	C-O	-5.08	1.19	1.24
1	B	914	ASN	N-CA	-5.08	1.40	1.46
1	A	638	THR	N-CA	-5.08	1.39	1.45
1	A	1121	PHE	CA-C	5.08	1.58	1.52
1	C	357	ARG	C-N	5.08	1.39	1.33
1	A	1027	THR	CA-C	-5.08	1.46	1.52
1	B	867	ASP	CA-C	-5.08	1.45	1.52
1	A	938	LEU	CA-C	-5.07	1.45	1.52
2	E	72	ARG	CZ-NH2	5.07	1.40	1.33
1	B	653	ALA	C-O	5.07	1.29	1.23
1	C	1047	TYR	C-O	-5.07	1.17	1.24
1	A	904	TYR	C-N	5.07	1.40	1.33
2	F	12	VAL	C-N	5.07	1.40	1.33
1	C	651	ILE	CA-C	-5.07	1.46	1.52
1	A	64	TRP	N-CA	5.07	1.52	1.46
1	B	633	TRP	N-CA	-5.07	1.39	1.46
2	E	24	ALA	CA-C	-5.07	1.46	1.52
1	C	963	VAL	C-O	-5.06	1.18	1.24
1	B	229	LEU	CA-C	-5.06	1.48	1.52
1	B	359	SER	CA-C	-5.06	1.46	1.52
1	B	852	ALA	CA-CB	5.06	1.58	1.53
1	C	606	ASN	N-CA	-5.06	1.40	1.46
1	A	1028	LYS	N-CA	-5.05	1.40	1.46
1	C	265	TYR	CA-C	-5.05	1.46	1.52
1	C	1066	THR	C-N	5.05	1.40	1.33
1	A	717	ASN	C-N	5.05	1.40	1.33
1	A	789	TYR	C-N	5.05	1.40	1.33
2	D	73	ASP	C-N	5.04	1.40	1.33
1	C	129	LYS	C-N	5.04	1.39	1.33
2	D	80	TYR	CA-C	-5.04	1.46	1.52
1	B	579	PRO	C-N	5.04	1.40	1.33
1	B	679	ASN	CA-C	-5.04	1.46	1.52
1	B	1036	GLN	N-CA	-5.04	1.40	1.46
1	B	433	VAL	C-O	-5.03	1.18	1.24
2	F	96	CYS	C-N	5.03	1.39	1.33
1	A	727	LEU	CA-C	5.03	1.58	1.52
1	B	705	VAL	N-CA	-5.03	1.40	1.46
1	A	362	VAL	C-N	5.03	1.40	1.33
1	C	111	ASP	CA-C	5.03	1.59	1.53
1	B	300	LYS	CA-C	5.02	1.59	1.52
1	B	500	THR	C-O	-5.02	1.17	1.23
1	B	789	TYR	CA-C	-5.02	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1020	ALA	CA-C	-5.02	1.46	1.52
1	B	103	GLY	CA-C	-5.02	1.43	1.51
1	B	141	LEU	N-CA	-5.02	1.39	1.46
1	A	413	GLY	C-N	5.02	1.40	1.33
1	C	98	SER	C-N	5.02	1.40	1.33
1	A	852	ALA	N-CA	-5.01	1.39	1.46
1	B	610	VAL	C-N	5.01	1.40	1.33
1	C	378	LYS	CA-C	-5.01	1.46	1.52
1	B	110	LEU	CA-C	-5.01	1.47	1.53
1	B	320	VAL	N-CA	-5.01	1.40	1.46
1	B	826	VAL	C-N	5.01	1.40	1.33
1	B	1092	GLU	CA-C	-5.01	1.46	1.52
1	A	865	LEU	N-CA	-5.01	1.40	1.46
1	B	421	TYR	N-CA	-5.01	1.39	1.46
1	B	741	TYR	C-N	5.01	1.39	1.33
2	D	20	LEU	C-N	5.01	1.40	1.33
2	D	11	LEU	CA-C	-5.01	1.46	1.52
1	A	741	TYR	CA-C	-5.01	1.46	1.52
1	A	1084	ASP	C-N	5.00	1.41	1.33
1	A	596	SER	CA-C	-5.00	1.46	1.52
1	C	484	GLU	CA-C	-5.00	1.46	1.52

All (1559) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	862	PRO	N-CA-CB	13.95	110.48	103.22
1	A	497	PHE	CA-CB-CG	13.78	127.58	113.80
2	F	193	PRO	N-CA-C	13.45	127.10	110.70
1	B	565	PHE	CA-C-N	12.88	132.34	120.10
1	B	565	PHE	C-N-CA	12.88	132.34	120.10
1	A	375	SER	N-CA-C	-12.17	100.75	114.62
1	A	1056	ALA	N-CA-C	-11.70	97.69	108.22
1	A	844	ILE	N-CA-C	-11.60	101.15	112.17
1	A	236	THR	N-CA-C	-11.39	101.63	114.62
1	B	236	THR	N-CA-C	-11.11	101.96	114.62
1	B	424	LYS	N-CA-C	-10.91	91.98	108.46
2	D	193	PRO	N-CA-C	10.89	123.99	110.70
1	C	862	PRO	O-C-N	-10.89	116.03	121.15
1	B	1110	TYR	CA-C-N	10.87	133.73	122.00
1	B	1110	TYR	C-N-CA	10.87	133.73	122.00
1	B	1117	THR	CA-C-N	10.81	135.85	120.28
1	B	1117	THR	C-N-CA	10.81	135.85	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	SER	N-CA-C	-10.77	101.17	114.75
2	D	55	GLY	N-CA-C	-10.67	96.50	111.76
1	B	685	ALA	N-CA-C	10.62	125.47	110.50
2	D	153	LEU	N-CA-C	-10.38	99.49	112.88
2	D	63	SER	N-CA-C	-10.36	101.69	114.75
1	A	943	SER	CA-C-N	10.33	135.16	120.28
1	A	943	SER	C-N-CA	10.33	135.16	120.28
1	B	811	LYS	N-CA-C	-10.30	96.91	110.40
1	C	562	PHE	N-CA-C	-10.22	99.92	114.12
2	D	1	GLN	CA-C-N	10.21	134.18	120.50
2	D	1	GLN	C-N-CA	10.21	134.18	120.50
1	B	520	ALA	CA-C-N	10.14	130.21	119.76
1	B	520	ALA	C-N-CA	10.14	130.21	119.76
1	A	805	ILE	N-CA-C	-10.12	103.25	113.47
2	E	194	PRO	N-CA-C	10.11	123.04	110.70
1	B	986	PRO	N-CA-C	10.05	122.96	110.70
2	D	179	LEU	N-CA-C	-9.93	99.47	112.68
1	C	791	THR	CA-C-N	9.92	130.60	120.38
1	C	791	THR	C-N-CA	9.92	130.60	120.38
1	A	621	PRO	CA-C-N	9.91	134.04	120.46
1	A	621	PRO	C-N-CA	9.91	134.04	120.46
1	C	805	ILE	N-CA-C	-9.87	103.53	113.10
1	C	1034	LEU	N-CA-C	-9.85	101.90	112.93
2	F	194	PRO	N-CA-C	9.79	122.64	110.70
1	B	429	PHE	CA-C-O	9.70	130.83	120.36
1	A	833	PHE	N-CA-C	-9.58	101.48	113.55
1	B	471	GLU	CA-C-N	9.58	134.01	120.98
1	B	471	GLU	C-N-CA	9.58	134.01	120.98
1	A	462	LYS	N-CA-C	-9.57	97.10	110.31
1	B	560	LEU	N-CA-C	-9.57	97.76	109.72
2	F	107	ASP	N-CA-C	-9.51	99.03	110.44
2	E	191	SER	CA-C-N	9.49	130.16	120.38
2	E	191	SER	C-N-CA	9.49	130.16	120.38
1	C	218	GLN	N-CA-C	-9.44	101.28	113.17
1	C	417	LYS	N-CA-C	-9.41	101.49	113.16
1	B	806	LEU	CA-C-N	9.40	129.49	119.90
1	B	806	LEU	C-N-CA	9.40	129.49	119.90
1	B	498	GLN	CA-C-N	9.37	131.55	119.84
1	B	498	GLN	C-N-CA	9.37	131.55	119.84
1	A	986	PRO	N-CA-C	9.36	122.12	110.70
1	B	164	ASN	CA-CB-CG	-9.32	103.28	112.60
1	B	498	GLN	O-C-N	-9.25	115.79	121.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	92	ALA	CA-C-N	9.25	134.30	122.37
2	F	92	ALA	C-N-CA	9.25	134.30	122.37
2	F	185	ILE	CA-C-N	9.24	129.18	119.85
2	F	185	ILE	C-N-CA	9.24	129.18	119.85
1	B	1064	HIS	CE1-NE2-CD2	-9.19	99.81	109.00
1	B	729	VAL	N-CA-C	-9.18	104.41	112.12
1	B	772	VAL	CA-C-N	9.17	133.49	120.28
1	B	772	VAL	C-N-CA	9.17	133.49	120.28
1	B	386	LYS	N-CA-C	-9.16	100.71	114.64
1	B	250	THR	CA-C-O	-9.14	113.35	119.29
1	A	192	PHE	CA-CB-CG	-9.11	104.69	113.80
1	A	162	SER	CA-C-N	9.11	135.03	122.19
1	A	162	SER	C-N-CA	9.11	135.03	122.19
1	A	382	VAL	CA-C-O	-9.04	112.67	121.63
1	A	316	SER	CA-C-O	8.89	130.18	120.94
1	A	355	ARG	N-CA-C	-8.86	94.75	109.46
1	A	603	ASN	N-CA-C	-8.83	102.06	112.92
1	C	502	GLY	N-CA-C	-8.79	98.99	110.69
1	A	630	THR	CA-C-O	-8.78	110.95	119.91
2	E	51	ILE	CA-C-O	8.74	128.26	121.09
1	B	630	THR	CA-C-N	8.74	130.76	119.84
1	B	630	THR	C-N-CA	8.74	130.76	119.84
1	C	306	PHE	N-CA-C	-8.73	102.17	113.17
2	E	183	GLU	CA-C-O	8.72	130.78	121.19
1	C	797	PHE	N-CA-C	-8.65	100.83	112.26
1	B	1122	VAL	CA-C-O	8.62	129.80	120.57
1	A	364	ASP	N-CA-C	-8.60	99.01	111.30
1	A	294	ASP	CA-CB-CG	8.59	121.19	112.60
2	E	124	SER	CA-C-N	8.58	128.16	119.92
2	E	124	SER	C-N-CA	8.58	128.16	119.92
1	A	72	GLY	CA-C-N	8.58	132.12	120.54
1	A	72	GLY	C-N-CA	8.58	132.12	120.54
1	A	138	ASP	O-C-N	-8.57	113.52	121.32
1	A	216	LEU	CA-C-O	-8.54	112.18	120.64
1	A	113	LYS	N-CA-C	-8.47	100.36	111.71
1	C	204	TYR	N-CA-C	-8.46	96.18	109.72
1	A	389	ASP	N-CA-C	-8.43	102.58	113.12
1	A	216	LEU	CA-C-N	8.41	128.48	119.90
1	A	216	LEU	C-N-CA	8.41	128.48	119.90
1	B	352	ALA	CA-C-N	8.41	133.46	120.75
1	B	352	ALA	C-N-CA	8.41	133.46	120.75
1	B	654	GLU	CA-C-N	8.41	132.82	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	654	GLU	C-N-CA	8.41	132.82	120.87
1	C	970	PHE	CA-CB-CG	-8.41	105.39	113.80
1	A	548	GLY	N-CA-C	-8.40	98.62	110.63
1	C	64	TRP	N-CA-C	-8.39	96.95	110.20
1	B	614	ASP	CA-C-O	-8.38	111.75	122.14
1	B	72	GLY	CA-C-N	8.37	131.83	120.54
1	B	72	GLY	C-N-CA	8.37	131.83	120.54
1	B	1064	HIS	ND1-CE1-NE2	8.31	116.71	108.40
1	C	123	ALA	N-CA-CB	8.31	125.29	112.41
1	C	624	ILE	CA-C-N	8.30	133.90	122.19
1	C	624	ILE	C-N-CA	8.30	133.90	122.19
1	A	401	VAL	CA-C-O	-8.27	111.71	120.39
1	B	524	VAL	O-C-N	-8.21	114.50	123.20
1	B	515	PHE	N-CA-C	-8.20	95.15	108.52
1	C	630	THR	CA-C-N	8.19	128.26	119.90
1	C	630	THR	C-N-CA	8.19	128.26	119.90
1	A	218	GLN	CA-C-N	8.19	130.74	122.30
1	A	218	GLN	C-N-CA	8.19	130.74	122.30
1	C	891	GLY	CA-C-N	8.18	128.24	119.90
1	C	891	GLY	C-N-CA	8.18	128.24	119.90
1	A	417	LYS	N-CA-C	-8.17	103.83	113.88
2	D	104	ALA	CA-C-N	8.16	128.09	119.85
2	D	104	ALA	C-N-CA	8.16	128.09	119.85
2	F	187	ILE	N-CA-C	8.12	115.96	107.76
1	A	1033	VAL	N-CA-C	-8.11	103.96	111.67
1	C	891	GLY	O-C-N	-8.11	113.66	121.77
1	C	932	GLY	CA-C-N	8.10	131.13	120.28
1	C	932	GLY	C-N-CA	8.10	131.13	120.28
1	C	701	ALA	CA-C-O	8.09	130.12	121.55
1	C	317	ASN	N-CA-C	-8.07	95.11	108.34
1	B	251	PRO	CA-C-N	8.03	130.18	120.14
1	B	251	PRO	C-N-CA	8.03	130.18	120.14
2	D	172	VAL	N-CA-C	-8.03	99.03	108.82
1	B	949	GLN	CA-C-N	8.03	131.03	120.28
1	B	949	GLN	C-N-CA	8.03	131.03	120.28
1	C	833	PHE	N-CA-C	-8.02	103.63	113.41
1	C	957	GLN	N-CA-C	8.01	120.02	111.28
1	A	193	VAL	N-CA-C	-7.99	96.56	108.46
1	C	660	TYR	N-CA-C	-7.96	97.87	109.18
2	E	99	ASP	O-C-N	-7.94	113.01	120.55
1	A	602	THR	N-CA-C	-7.93	102.91	112.59
1	A	1006	THR	CA-C-O	-7.92	112.50	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	23	ALA	CA-C-N	7.92	132.75	121.02
2	F	23	ALA	C-N-CA	7.92	132.75	121.02
1	A	556	ASN	N-CA-C	-7.89	104.13	114.31
2	F	76	LYS	CA-C-N	7.86	133.82	121.56
2	F	76	LYS	C-N-CA	7.86	133.82	121.56
1	B	478	THR	N-CA-C	-7.85	96.85	109.40
1	B	464	PHE	N-CA-C	-7.84	100.34	111.56
1	A	762	GLN	N-CA-C	7.84	119.82	111.28
1	B	57	PRO	CA-C-O	-7.82	112.42	121.34
1	B	177	MET	N-CA-C	-7.82	103.73	113.20
1	C	1056	ALA	CA-C-O	-7.82	113.15	120.34
1	C	1086	LYS	CA-C-O	-7.81	111.71	120.54
2	D	157	GLY	CA-C-O	7.75	127.75	119.07
1	A	867	ASP	CA-C-N	7.74	131.28	120.29
1	A	867	ASP	C-N-CA	7.74	131.28	120.29
1	B	861	LEU	CA-C-N	7.74	125.23	119.66
1	B	861	LEU	C-N-CA	7.74	125.23	119.66
1	A	266	TYR	N-CA-C	-7.73	96.33	109.24
1	C	72	GLY	N-CA-C	-7.71	103.92	115.32
1	C	267	VAL	CA-C-O	-7.70	112.20	120.36
1	B	905	ARG	CA-C-N	7.70	130.91	120.44
1	B	905	ARG	C-N-CA	7.70	130.91	120.44
1	A	445	VAL	N-CA-C	-7.69	106.00	113.53
1	A	922	LEU	CA-C-N	7.67	130.22	120.56
1	A	922	LEU	C-N-CA	7.67	130.22	120.56
1	B	847	ARG	N-CA-C	-7.66	100.99	111.56
1	B	448	ASN	CA-C-O	7.63	128.63	120.46
1	A	290	ASP	CA-C-N	7.58	130.29	120.44
1	A	290	ASP	C-N-CA	7.58	130.29	120.44
1	C	293	LEU	CA-C-O	-7.57	112.85	120.80
1	C	1089	PHE	N-CA-C	-7.56	99.58	110.40
2	E	170	ILE	N-CA-C	-7.56	97.20	108.46
1	A	986	PRO	N-CA-CB	7.55	110.41	103.08
1	B	506	GLN	CA-C-N	7.55	127.71	120.31
1	B	506	GLN	C-N-CA	7.55	127.71	120.31
2	D	137	ARG	CA-C-N	7.55	135.56	121.97
2	D	137	ARG	C-N-CA	7.55	135.56	121.97
1	C	986	PRO	CA-C-O	-7.54	109.62	120.56
1	A	669	GLY	N-CA-C	-7.54	105.34	115.36
1	C	689	SER	N-CA-C	-7.53	98.22	108.38
1	C	692	ILE	N-CA-C	-7.52	95.99	107.73
1	B	406	GLU	CA-C-O	-7.51	110.82	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	636	TYR	N-CA-C	-7.50	98.34	109.81
1	B	941	THR	CA-C-N	7.49	127.13	119.56
1	B	941	THR	C-N-CA	7.49	127.13	119.56
1	B	199	GLY	N-CA-C	-7.49	105.19	114.92
1	A	537	LYS	N-CA-C	-7.48	97.94	109.24
1	A	856	ASN	N-CA-C	-7.48	103.46	112.59
1	A	986	PRO	CA-C-O	-7.47	109.73	120.56
1	B	263	ALA	N-CA-C	-7.47	102.70	112.41
1	A	701	ALA	CA-C-O	7.46	130.49	121.68
1	C	259	THR	N-CA-C	-7.46	103.77	113.17
1	B	798	GLY	N-CA-C	-7.46	104.45	115.72
1	C	113	LYS	CA-C-O	7.44	127.02	118.77
1	C	1142	GLN	CA-C-N	7.43	129.12	119.84
1	C	1142	GLN	C-N-CA	7.43	129.12	119.84
1	A	526	GLY	CA-C-N	7.42	127.59	119.87
1	A	526	GLY	C-N-CA	7.42	127.59	119.87
1	B	358	ILE	O-C-N	7.39	131.75	123.10
1	C	680	SER	CA-C-O	-7.39	110.03	120.16
2	F	24	ALA	CA-C-N	7.38	132.53	120.94
2	F	24	ALA	C-N-CA	7.38	132.53	120.94
1	A	177	MET	N-CA-C	-7.35	104.20	113.02
2	E	9	GLY	N-CA-C	-7.33	102.47	112.52
1	A	456	PHE	N-CA-C	-7.33	97.73	109.76
1	C	617	CYS	N-CA-C	-7.33	102.58	112.26
1	B	593	GLY	CA-C-N	7.33	127.30	120.34
1	B	593	GLY	C-N-CA	7.33	127.30	120.34
1	C	429	PHE	N-CA-C	-7.33	98.11	109.76
2	E	155	ILE	N-CA-C	-7.30	98.71	108.06
1	A	941	THR	CA-C-O	-7.29	111.69	121.02
1	B	992	GLN	CA-C-N	7.29	129.89	120.56
1	B	992	GLN	C-N-CA	7.29	129.89	120.56
1	A	938	LEU	CA-C-N	7.28	129.90	120.44
1	A	938	LEU	C-N-CA	7.28	129.90	120.44
1	A	1039	ARG	N-CA-C	-7.27	99.76	110.52
2	E	4	LEU	N-CA-C	-7.27	98.77	110.32
1	A	896	ILE	CA-C-N	7.26	127.30	119.90
1	A	896	ILE	C-N-CA	7.26	127.30	119.90
2	D	164	ASP	N-CA-C	-7.26	103.58	113.30
1	B	974	SER	O-C-N	-7.25	115.14	123.33
1	C	191	GLU	CA-C-O	-7.24	112.76	120.80
1	A	91	TYR	N-CA-C	-7.24	97.88	109.76
1	B	752	LEU	CA-C-N	7.24	130.95	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	752	LEU	C-N-CA	7.24	130.95	120.38
1	B	512	VAL	N-CA-C	-7.23	97.99	108.11
1	B	1064	HIS	CG-CD2-NE2	7.22	114.42	107.20
2	E	26	GLY	CA-C-N	7.22	131.88	120.47
2	E	26	GLY	C-N-CA	7.22	131.88	120.47
1	B	121	ASN	N-CA-C	-7.21	101.79	111.96
1	A	29	THR	N-CA-C	-7.21	99.31	109.69
1	B	975	SER	O-C-N	-7.20	113.53	122.24
1	B	854	LYS	N-CA-C	-7.18	102.54	112.30
1	B	550	GLY	CA-C-O	7.17	128.88	121.35
1	A	467	ASP	CA-C-O	-7.17	112.50	120.60
1	A	565	PHE	CA-CB-CG	-7.16	106.64	113.80
1	B	926	GLN	CA-C-N	7.16	129.75	120.44
1	B	926	GLN	C-N-CA	7.16	129.75	120.44
1	B	86	PHE	N-CA-C	-7.16	96.60	108.34
1	C	589	PRO	CA-C-O	-7.16	113.27	121.36
1	B	666	ILE	N-CA-C	-7.15	104.88	111.67
2	F	128	SER	N-CA-C	-7.15	106.47	114.62
1	B	548	GLY	CA-C-O	-7.14	114.47	121.75
1	C	834	ILE	N-CA-C	-7.12	98.32	108.58
1	A	173	GLN	CA-C-O	-7.12	112.58	119.13
1	A	316	SER	N-CA-C	-7.12	98.19	107.73
1	A	604	THR	N-CA-C	-7.12	97.90	108.79
1	B	234	ASN	N-CA-C	-7.12	97.65	108.96
1	A	839	ASP	CA-C-O	-7.11	113.05	122.44
2	F	121	ALA	CA-C-N	7.11	129.60	120.64
2	F	121	ALA	C-N-CA	7.11	129.60	120.64
1	A	453	TYR	CA-C-N	7.11	132.10	120.94
1	A	453	TYR	C-N-CA	7.11	132.10	120.94
1	A	630	THR	CA-C-N	7.11	128.72	119.84
1	A	630	THR	C-N-CA	7.11	128.72	119.84
1	B	1038	LYS	N-CA-C	-7.10	102.92	112.94
1	A	145	TYR	O-C-N	7.09	131.54	122.89
1	C	53	ASP	N-CA-C	-7.09	97.89	107.88
1	A	204	TYR	N-CA-C	-7.09	98.38	109.72
1	A	1116	THR	N-CA-C	-7.08	99.50	109.69
2	E	192	PRO	N-CA-C	7.08	119.33	110.70
1	B	117	LEU	CA-C-O	7.08	128.14	120.43
1	C	480	CYS	CA-C-N	7.08	135.05	121.54
1	C	480	CYS	C-N-CA	7.08	135.05	121.54
1	A	186	PHE	CA-C-N	7.07	132.68	122.35
1	A	186	PHE	C-N-CA	7.07	132.68	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	862	PRO	CA-C-N	7.07	127.49	119.92
1	C	862	PRO	C-N-CA	7.07	127.49	119.92
1	B	359	SER	CA-C-N	7.07	132.40	122.36
1	B	359	SER	C-N-CA	7.07	132.40	122.36
1	B	255	SER	N-CA-C	-7.05	103.92	114.64
1	A	832	GLY	CA-C-O	7.04	126.78	119.10
1	A	286	THR	O-C-N	-7.04	113.96	122.48
1	A	292	ALA	N-CA-C	-7.04	99.78	109.71
2	F	126	GLY	CA-C-N	7.04	132.00	120.94
2	F	126	GLY	C-N-CA	7.04	132.00	120.94
1	A	38	TYR	O-C-N	-7.03	115.33	121.31
1	A	1104	VAL	N-CA-C	-7.03	98.19	108.87
1	A	905	ARG	O-C-N	7.02	129.39	122.09
2	F	62	ASP	N-CA-C	-7.02	104.60	113.02
1	B	999	GLY	N-CA-C	7.01	121.15	112.73
1	C	1061	VAL	N-CA-C	-7.01	98.01	108.46
2	F	55	GLY	CA-C-N	7.01	133.87	122.65
2	F	55	GLY	C-N-CA	7.01	133.87	122.65
1	B	321	GLN	CA-C-O	-7.01	114.29	120.60
1	B	603	ASN	N-CA-C	-7.01	103.69	111.82
1	B	960	ASN	O-C-N	-6.97	114.56	122.09
1	A	477	SER	N-CA-C	-6.97	95.95	110.80
1	C	167	THR	N-CA-C	-6.97	98.47	109.07
1	C	729	VAL	CA-C-O	-6.97	114.60	120.80
1	B	864	LEU	CA-C-N	-6.96	113.16	122.42
1	B	864	LEU	C-N-CA	-6.96	113.16	122.42
2	E	162	LEU	N-CA-CB	6.96	120.80	110.49
1	B	484	GLU	CA-C-N	6.96	130.68	122.19
1	B	484	GLU	C-N-CA	6.96	130.68	122.19
1	A	677	GLN	N-CA-C	-6.96	104.78	112.72
1	C	72	GLY	CA-C-N	6.96	129.94	120.54
1	C	72	GLY	C-N-CA	6.96	129.94	120.54
1	A	165	ASN	CA-C-O	6.96	129.69	120.15
1	A	343	ASN	N-CA-C	-6.95	102.16	111.96
1	C	177	MET	N-CA-C	-6.95	104.37	112.92
1	C	878	LEU	O-C-N	6.93	129.21	122.07
1	B	329	PHE	CA-C-N	6.93	126.89	120.03
1	B	329	PHE	C-N-CA	6.93	126.89	120.03
2	D	71	SER	N-CA-C	-6.93	97.95	108.96
1	A	861	LEU	N-CA-C	-6.92	99.61	109.24
1	C	219	GLY	N-CA-C	-6.92	101.64	112.58
1	B	267	VAL	CA-C-N	6.91	128.32	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	VAL	C-N-CA	6.91	128.32	122.17
1	B	876	ALA	CA-C-N	6.91	130.10	120.29
1	B	876	ALA	C-N-CA	6.91	130.10	120.29
1	C	633	TRP	CD2-CE3-CZ3	6.90	127.57	118.60
2	D	29	PHE	CA-CB-CG	6.88	120.68	113.80
1	C	499	PRO	CA-C-N	6.87	131.88	122.19
1	C	499	PRO	C-N-CA	6.87	131.88	122.19
1	A	262	ALA	O-C-N	6.87	130.26	122.22
2	F	87	LYS	CA-C-N	6.87	128.43	119.84
2	F	87	LYS	C-N-CA	6.87	128.43	119.84
1	A	424	LYS	O-C-N	6.87	128.34	120.58
1	C	794	ILE	CA-C-O	-6.87	113.18	120.39
1	A	720	ILE	O-C-N	6.86	131.31	122.94
2	F	182	GLY	CA-C-N	6.86	130.45	120.71
2	F	182	GLY	C-N-CA	6.86	130.45	120.71
1	B	699	LEU	N-CA-C	-6.84	104.05	112.88
1	B	441	LEU	N-CA-C	6.84	120.99	112.24
1	C	332	ILE	N-CA-C	-6.84	98.64	108.42
1	C	457	ARG	NE-CZ-NH2	6.83	125.35	119.20
1	C	530	SER	CA-C-O	6.82	128.80	121.16
1	C	789	TYR	N-CA-C	-6.82	98.81	109.72
1	C	318	PHE	CA-C-O	-6.82	113.77	121.81
1	A	323	THR	N-CA-C	-6.82	105.25	113.97
2	E	25	SER	CA-C-N	6.81	128.65	120.14
2	E	25	SER	C-N-CA	6.81	128.65	120.14
2	E	182	GLY	CA-C-N	6.81	130.37	120.71
2	E	182	GLY	C-N-CA	6.81	130.37	120.71
1	B	268	GLY	CA-C-O	-6.80	115.28	121.47
1	A	142	GLY	CA-C-N	6.80	129.67	120.63
1	A	142	GLY	C-N-CA	6.80	129.67	120.63
1	B	433	VAL	CA-C-O	6.80	127.13	120.27
1	B	833	PHE	N-CA-C	-6.80	105.02	113.38
2	D	128	SER	N-CA-C	-6.80	95.78	107.61
1	C	811	LYS	CA-C-O	-6.79	113.28	120.88
2	F	131	ASP	N-CA-C	-6.79	102.30	113.50
1	B	80	ASP	CA-C-N	6.78	131.11	122.64
1	B	80	ASP	C-N-CA	6.78	131.11	122.64
1	B	901	GLN	CA-C-O	-6.78	113.37	120.55
1	C	697	MET	CA-C-N	6.78	131.11	121.42
1	C	697	MET	C-N-CA	6.78	131.11	121.42
1	A	418	ILE	N-CA-C	-6.77	106.90	113.53
1	A	1044	GLY	CA-C-O	-6.77	114.66	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	581	THR	N-CA-C	-6.77	99.94	109.69
1	C	665	PRO	CA-C-O	-6.77	113.71	121.56
1	B	121	ASN	O-C-N	6.76	130.17	122.19
2	F	119	SER	N-CA-C	-6.76	104.67	113.12
1	B	1099	GLY	N-CA-C	-6.76	106.65	114.69
1	A	950	ASP	N-CA-C	6.75	118.64	111.28
1	B	478	THR	CA-C-N	6.74	126.78	119.90
1	B	478	THR	C-N-CA	6.74	126.78	119.90
1	B	839	ASP	CA-CB-CG	-6.74	105.86	112.60
1	C	630	THR	O-C-N	-6.74	117.13	121.85
2	E	105	PRO	N-CA-C	-6.74	105.17	114.27
1	C	874	THR	CA-C-N	6.74	129.31	120.28
1	C	874	THR	C-N-CA	6.74	129.31	120.28
1	B	809	PRO	N-CA-C	-6.71	103.42	112.48
1	B	811	LYS	CA-C-N	6.71	126.47	119.76
1	B	811	LYS	C-N-CA	6.71	126.47	119.76
1	C	1020	ALA	CA-C-N	6.71	129.28	120.28
1	C	1020	ALA	C-N-CA	6.71	129.28	120.28
1	A	501	ASN	N-CA-C	-6.71	102.29	110.88
1	B	566	GLY	N-CA-C	6.70	119.64	111.93
1	A	957	GLN	CA-C-N	6.70	129.15	120.44
1	A	957	GLN	C-N-CA	6.70	129.15	120.44
1	A	361	CYS	CA-C-O	6.70	128.48	121.38
1	A	684	ALA	CA-C-N	6.70	131.45	120.94
1	A	684	ALA	C-N-CA	6.70	131.45	120.94
1	B	476	GLY	N-CA-C	6.69	121.11	112.54
1	A	1002	GLN	CA-C-N	6.69	129.24	120.28
1	A	1002	GLN	C-N-CA	6.69	129.24	120.28
1	C	41	LYS	N-CA-C	-6.69	105.65	113.88
1	C	217	PRO	CA-C-O	-6.69	113.72	121.34
1	A	773	GLU	N-CA-C	6.68	118.56	111.28
1	C	1038	LYS	N-CA-C	-6.68	104.26	112.88
1	B	513	LEU	N-CA-C	-6.67	97.64	108.52
1	C	968	SER	N-CA-C	-6.67	98.33	109.07
1	B	709	ASN	O-C-N	-6.66	114.33	122.25
1	B	411	ALA	CA-C-O	-6.66	113.43	120.88
1	C	107	GLY	N-CA-C	-6.65	101.60	110.58
1	B	300	LYS	CA-C-N	6.65	129.85	120.28
1	B	300	LYS	C-N-CA	6.65	129.85	120.28
1	B	452	LEU	N-CA-C	-6.65	97.78	108.55
1	C	986	PRO	N-CA-C	6.65	118.81	110.70
1	A	462	LYS	CA-C-N	6.64	127.04	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	462	LYS	C-N-CA	6.64	127.04	119.93
1	C	939	SER	CA-C-O	-6.64	113.86	120.70
2	E	43	LYS	CA-C-N	6.63	130.29	120.87
2	E	43	LYS	C-N-CA	6.63	130.29	120.87
1	A	986	PRO	CA-C-N	6.63	127.16	119.47
1	A	986	PRO	C-N-CA	6.63	127.16	119.47
1	B	252	GLY	O-C-N	-6.63	115.22	122.24
1	B	614	ASP	O-C-N	6.62	131.00	122.86
1	A	740	MET	N-CA-C	6.62	118.49	111.28
1	A	994	ASP	CA-C-N	6.62	129.15	120.28
1	A	994	ASP	C-N-CA	6.62	129.15	120.28
1	B	191	GLU	O-C-N	-6.62	115.45	123.19
1	A	410	ILE	CA-C-N	6.62	129.89	120.49
1	A	410	ILE	C-N-CA	6.62	129.89	120.49
1	A	1070	ALA	CA-C-O	-6.62	111.77	119.64
2	D	101	ALA	O-C-N	6.60	130.31	122.79
2	E	98	ALA	CA-C-N	6.60	130.74	120.97
2	E	98	ALA	C-N-CA	6.60	130.74	120.97
1	B	727	LEU	CA-C-O	-6.59	112.56	120.08
1	B	816	SER	CA-C-N	6.59	127.12	119.47
1	B	816	SER	C-N-CA	6.59	127.12	119.47
2	F	151	ALA	CA-C-O	6.59	127.47	119.49
1	B	951	VAL	CA-C-N	6.59	128.99	120.56
1	B	951	VAL	C-N-CA	6.59	128.99	120.56
1	B	89	GLY	N-CA-C	-6.58	104.92	112.29
1	B	736	VAL	N-CA-C	-6.58	98.64	108.12
2	E	129	GLY	N-CA-C	-6.58	106.03	115.64
2	D	193	PRO	CA-C-O	-6.58	111.02	120.56
1	B	1065	VAL	N-CA-C	-6.58	98.39	107.99
1	A	436	TRP	CA-C-N	6.57	131.79	121.99
1	A	436	TRP	C-N-CA	6.57	131.79	121.99
1	A	747	THR	CA-C-N	6.57	129.09	120.28
1	A	747	THR	C-N-CA	6.57	129.09	120.28
2	E	57	ILE	N-CA-C	6.57	118.29	108.23
1	C	246	ARG	N-CA-C	-6.57	99.32	109.24
1	A	770	ILE	CA-C-N	6.57	129.37	120.38
1	A	770	ILE	C-N-CA	6.57	129.37	120.38
1	B	224	GLU	CA-C-N	6.55	126.94	119.93
1	B	224	GLU	C-N-CA	6.55	126.94	119.93
1	C	700	GLY	N-CA-C	-6.55	105.47	112.08
2	F	87	LYS	O-C-N	-6.55	115.31	121.20
1	B	325	SER	O-C-N	-6.54	115.64	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	193	PRO	N-CA-C	6.54	118.68	110.70
1	B	663	ASP	N-CA-C	-6.54	96.88	110.80
1	B	803	SER	N-CA-C	-6.54	104.49	114.16
1	A	183	GLN	CA-C-N	6.53	128.30	120.14
1	A	183	GLN	C-N-CA	6.53	128.30	120.14
1	C	133	PHE	N-CA-C	-6.53	99.82	109.81
2	F	127	SER	N-CA-C	6.53	119.71	110.50
1	C	182	LYS	CA-C-O	6.53	128.30	120.99
1	B	758	SER	CA-C-N	6.52	129.34	120.54
1	B	758	SER	C-N-CA	6.52	129.34	120.54
1	C	199	GLY	N-CA-C	-6.51	106.74	115.21
1	C	831	ALA	CB-CA-C	-6.51	99.74	109.90
1	C	879	ALA	CA-C-N	6.51	127.17	119.94
1	C	879	ALA	C-N-CA	6.51	127.17	119.94
1	C	979	ASP	CA-C-N	6.51	128.89	120.56
1	C	979	ASP	C-N-CA	6.51	128.89	120.56
1	C	81	ASN	O-C-N	-6.51	114.66	121.04
1	B	991	VAL	CA-C-O	6.51	127.75	120.85
2	E	193	PRO	CA-C-O	-6.50	111.13	120.56
1	B	107	GLY	O-C-N	6.50	129.20	123.80
1	B	496	GLY	O-C-N	-6.50	115.97	122.86
1	C	44	ARG	N-CA-C	-6.50	99.16	109.23
1	A	614	ASP	N-CA-C	6.49	120.34	111.39
1	B	825	LYS	CA-C-O	6.49	127.15	119.56
1	B	1079	PRO	N-CA-C	-6.49	105.75	113.86
2	D	194	PRO	N-CA-C	6.48	118.61	110.70
1	C	758	SER	N-CA-C	-6.48	104.52	112.88
1	A	945	LEU	CA-C-N	6.48	127.29	120.03
1	A	945	LEU	C-N-CA	6.48	127.29	120.03
1	C	146	HIS	N-CA-C	-6.47	104.07	112.68
1	C	854	LYS	N-CA-C	-6.47	105.34	112.72
1	C	783	ALA	CA-C-O	6.47	127.26	119.43
1	C	1044	GLY	N-CA-C	6.47	124.05	112.02
2	F	134	SER	O-C-N	6.47	131.20	122.59
1	B	697	MET	O-C-N	6.47	130.76	122.81
1	B	173	GLN	CA-C-O	-6.46	111.30	120.16
2	E	17	SER	O-C-N	6.46	130.33	123.42
1	B	1027	THR	CA-C-N	6.46	128.93	120.28
1	B	1027	THR	C-N-CA	6.46	128.93	120.28
1	C	411	ALA	CA-C-N	6.45	126.42	120.03
1	C	411	ALA	C-N-CA	6.45	126.42	120.03
1	A	791	THR	CA-C-O	-6.45	113.67	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	ILE	O-C-N	6.43	130.15	123.20
1	C	811	LYS	CA-C-N	6.43	126.93	119.47
1	C	811	LYS	C-N-CA	6.43	126.93	119.47
1	A	892	PRO	N-CA-C	6.43	121.31	111.15
1	C	267	VAL	N-CA-CB	6.43	120.90	111.52
2	E	125	GLY	N-CA-C	-6.42	103.85	111.36
2	E	129	GLY	CA-C-O	6.42	125.89	118.96
1	C	388	ASN	CA-C-O	-6.41	112.85	120.10
1	C	468	ILE	N-CA-C	-6.41	99.13	108.11
1	C	942	PRO	CA-C-N	6.41	128.87	120.28
1	C	942	PRO	C-N-CA	6.41	128.87	120.28
2	D	143	ASN	CA-C-N	6.41	128.87	120.28
2	D	143	ASN	C-N-CA	6.41	128.87	120.28
1	C	982	SER	N-CA-C	6.41	120.30	112.23
1	A	86	PHE	N-CA-C	-6.40	97.98	108.41
1	B	244	LEU	N-CA-C	-6.40	105.11	113.17
1	B	115	GLN	CA-C-O	-6.40	113.37	120.60
1	B	374	PHE	CB-CA-C	-6.39	109.22	116.63
1	C	239	GLN	N-CA-C	-6.39	98.95	108.99
1	B	91	TYR	CA-C-O	-6.38	113.72	120.80
1	A	152	TRP	N-CA-C	-6.38	97.86	108.32
1	A	321	GLN	CA-C-N	6.37	126.40	119.90
1	A	321	GLN	C-N-CA	6.37	126.40	119.90
1	B	136	CYS	N-CA-C	-6.36	99.48	108.96
1	C	945	LEU	N-CA-C	-6.36	105.50	113.20
1	B	881	THR	CA-C-N	6.36	130.72	120.55
1	B	881	THR	C-N-CA	6.36	130.72	120.55
1	A	891	GLY	CA-C-N	6.36	126.38	119.90
1	A	891	GLY	C-N-CA	6.36	126.38	119.90
1	C	340	GLU	N-CA-C	6.35	118.21	111.28
1	B	998	THR	CA-C-N	6.35	127.03	119.98
1	B	998	THR	C-N-CA	6.35	127.03	119.98
1	A	795	LYS	CA-C-N	6.35	130.22	121.33
1	A	795	LYS	C-N-CA	6.35	130.22	121.33
1	B	643	PHE	CB-CA-C	6.35	120.69	110.16
1	C	540	ASN	N-CA-C	-6.34	98.88	108.96
1	B	354	ASN	N-CA-C	-6.34	98.20	108.41
2	E	24	ALA	O-C-N	-6.34	116.21	122.99
1	C	756	TYR	CA-C-N	6.34	129.55	119.98
1	C	756	TYR	C-N-CA	6.34	129.55	119.98
1	B	149	ASN	CA-CB-CG	-6.33	106.27	112.60
1	C	567	ARG	N-CA-C	-6.33	98.90	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	188	PRO	CA-C-O	-6.33	114.03	121.95
1	A	33	THR	CA-C-O	6.32	129.18	121.84
1	A	797	PHE	CA-C-O	-6.32	112.87	120.65
1	B	955	ASN	CA-C-N	6.32	128.75	120.28
1	B	955	ASN	C-N-CA	6.32	128.75	120.28
1	C	676	THR	N-CA-CB	6.32	121.52	111.91
2	E	194	PRO	CA-C-O	-6.32	111.39	120.56
1	B	1060	VAL	O-C-N	-6.32	116.34	123.10
1	C	389	ASP	N-CA-C	-6.31	105.16	112.92
1	A	898	PHE	CA-C-N	6.31	126.51	119.32
1	A	898	PHE	C-N-CA	6.31	126.51	119.32
1	B	946	GLY	CA-C-O	6.31	126.89	120.45
1	A	599	THR	CA-C-N	6.30	127.72	119.84
1	A	599	THR	C-N-CA	6.30	127.72	119.84
1	A	765	ARG	CA-C-N	6.30	128.72	120.28
1	A	765	ARG	C-N-CA	6.30	128.72	120.28
1	A	288	ALA	CB-CA-C	-6.30	98.64	110.16
1	A	778	THR	O-C-N	-6.29	115.59	122.07
2	F	171	ARG	N-CA-C	-6.29	99.02	109.46
2	D	101	ALA	CA-C-O	-6.29	114.58	121.87
1	C	283	GLY	CA-C-O	6.28	124.68	118.77
1	B	502	GLY	CA-C-O	-6.28	114.78	121.38
1	B	943	SER	CA-C-N	6.28	129.32	120.28
1	B	943	SER	C-N-CA	6.28	129.32	120.28
1	C	817	PRO	O-C-N	6.28	129.46	122.24
2	E	192	PRO	CA-C-O	-6.28	111.46	120.56
1	B	714	ILE	CA-C-O	-6.27	115.62	119.51
2	E	144	MET	CA-C-N	6.27	128.97	120.38
2	E	144	MET	C-N-CA	6.27	128.97	120.38
1	A	532	ASN	CA-C-N	6.27	129.66	120.82
1	A	532	ASN	C-N-CA	6.27	129.66	120.82
1	A	1129	VAL	N-CA-C	-6.27	99.33	108.11
1	C	237	ARG	N-CA-C	-6.27	99.88	109.41
1	B	599	THR	O-C-N	-6.26	115.36	121.94
2	D	141	PHE	N-CA-C	-6.26	100.68	109.69
1	A	705	VAL	N-CA-C	-6.25	98.75	108.44
1	B	315	THR	N-CA-C	-6.25	106.28	114.04
2	F	13	GLN	N-CA-C	-6.25	100.73	110.42
1	C	131	CYS	N-CA-C	-6.25	99.36	107.73
1	A	458	LYS	O-C-N	6.25	128.63	122.19
1	A	859	THR	CA-C-N	6.25	131.68	122.99
1	A	859	THR	C-N-CA	6.25	131.68	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	998	THR	CA-C-N	6.24	126.87	119.94
1	A	998	THR	C-N-CA	6.24	126.87	119.94
1	A	1136	THR	O-C-N	-6.24	115.28	123.21
1	C	462	LYS	CA-C-N	6.24	127.64	119.84
1	C	462	LYS	C-N-CA	6.24	127.64	119.84
1	A	58	PHE	CA-C-N	6.23	132.83	123.05
1	A	58	PHE	C-N-CA	6.23	132.83	123.05
1	A	584	ILE	N-CA-C	-6.23	99.42	108.71
1	C	146	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	C	184	GLY	CA-C-N	6.23	133.23	122.64
1	C	184	GLY	C-N-CA	6.23	133.23	122.64
1	A	849	LEU	CA-C-N	6.23	128.91	120.63
1	A	849	LEU	C-N-CA	6.23	128.91	120.63
1	B	396	TYR	CA-C-O	-6.22	114.11	120.71
1	B	39	PRO	N-CA-C	-6.22	107.52	114.92
2	D	183	GLU	CA-C-O	-6.22	113.78	120.75
1	A	1040	VAL	N-CA-C	-6.22	99.27	108.85
1	A	869	MET	CA-C-O	6.22	127.14	120.55
1	A	468	ILE	CA-C-N	6.21	133.41	121.54
1	A	468	ILE	C-N-CA	6.21	133.41	121.54
1	A	904	TYR	CA-C-N	6.21	128.93	120.54
1	A	904	TYR	C-N-CA	6.21	128.93	120.54
1	A	1020	ALA	N-CA-C	6.21	118.05	111.28
1	B	322	PRO	O-C-N	6.21	130.71	123.01
1	B	99	ASN	N-CA-C	6.21	119.98	111.54
1	C	586	ASP	CA-C-N	6.21	130.84	122.90
1	C	586	ASP	C-N-CA	6.21	130.84	122.90
1	A	1142	GLN	O-C-N	-6.20	114.75	120.51
1	A	471	GLU	N-CA-C	-6.19	98.88	108.42
1	B	515	PHE	CA-C-O	6.19	127.13	120.32
1	C	775	ASP	N-CA-C	6.19	118.03	111.28
1	B	246	ARG	N-CA-C	-6.19	99.66	109.07
2	E	62	ASP	N-CA-C	-6.19	105.49	113.16
2	E	192	PRO	O-C-N	-6.19	114.16	121.46
1	B	549	THR	CA-C-N	-6.18	112.38	120.91
1	B	549	THR	C-N-CA	-6.18	112.38	120.91
2	F	117	VAL	CA-C-O	-6.18	113.96	120.39
1	A	577	ARG	CA-C-N	6.18	128.95	120.67
1	A	577	ARG	C-N-CA	6.18	128.95	120.67
1	A	956	ALA	CA-C-O	-6.18	114.00	120.55
1	B	778	THR	N-CA-C	6.18	117.68	111.07
2	E	56	SER	N-CA-C	-6.17	105.58	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	972	ALA	N-CA-C	-6.17	102.54	110.19
2	F	104	ALA	N-CA-CB	6.17	121.34	110.37
1	A	948	LEU	CA-C-N	6.17	128.54	120.28
1	A	948	LEU	C-N-CA	6.17	128.54	120.28
1	A	84	LEU	CA-C-N	6.16	126.18	119.90
1	A	84	LEU	C-N-CA	6.16	126.18	119.90
1	C	366	SER	O-C-N	-6.16	115.72	122.07
1	A	951	VAL	CA-C-N	6.16	128.32	120.56
1	A	951	VAL	C-N-CA	6.16	128.32	120.56
1	A	995	ARG	N-CA-C	6.16	117.99	111.28
1	B	119	ILE	CA-C-O	-6.16	113.46	120.66
1	A	818	ILE	CA-C-N	6.16	128.53	120.28
1	A	818	ILE	C-N-CA	6.16	128.53	120.28
1	B	828	LEU	CA-C-N	6.16	130.51	120.23
1	B	828	LEU	C-N-CA	6.16	130.51	120.23
1	C	543	PHE	CA-C-N	6.16	131.32	122.40
1	C	543	PHE	C-N-CA	6.16	131.32	122.40
1	C	985	ASP	CA-C-O	-6.15	113.95	120.23
1	B	144	TYR	N-CA-C	-6.15	100.94	110.10
2	E	28	ILE	N-CA-C	-6.15	105.83	111.67
2	D	80	TYR	N-CA-C	-6.15	99.88	109.72
1	C	761	THR	CA-C-N	6.15	128.52	120.28
1	C	761	THR	C-N-CA	6.15	128.52	120.28
1	A	914	ASN	CA-C-N	6.14	129.15	120.42
1	A	914	ASN	C-N-CA	6.14	129.15	120.42
1	B	560	LEU	CA-C-O	-6.14	114.62	119.66
1	B	975	SER	N-CA-C	-6.14	105.07	113.30
1	C	863	PRO	CA-C-N	6.13	128.42	120.44
1	C	863	PRO	C-N-CA	6.13	128.42	120.44
2	E	189	ALA	N-CA-C	6.13	118.69	110.35
1	B	776	LYS	N-CA-C	6.13	117.63	111.07
1	B	704	SER	N-CA-C	-6.12	100.18	109.85
1	C	139	PRO	N-CA-C	-6.12	102.23	111.41
1	B	686	SER	N-CA-C	-6.11	99.39	108.99
1	B	955	ASN	CA-C-O	-6.11	114.40	120.82
2	E	130	SER	CA-C-O	6.11	125.72	119.97
1	C	1089	PHE	CA-C-N	6.11	126.02	119.85
1	C	1089	PHE	C-N-CA	6.11	126.02	119.85
2	F	72	ARG	CA-C-N	6.11	131.15	122.72
2	F	72	ARG	C-N-CA	6.11	131.15	122.72
1	A	641	ASN	CA-C-N	6.11	131.06	123.12
1	A	641	ASN	C-N-CA	6.11	131.06	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	920	GLN	N-CA-C	6.11	118.44	111.11
1	C	1117	THR	CA-C-N	6.10	129.07	120.28
1	C	1117	THR	C-N-CA	6.10	129.07	120.28
1	A	975	SER	CA-C-O	6.10	125.76	119.05
1	A	1023	ASN	N-CA-C	-6.10	104.63	111.28
1	B	421	TYR	CA-C-N	6.10	133.19	121.54
1	B	421	TYR	C-N-CA	6.10	133.19	121.54
2	D	193	PRO	O-C-N	-6.10	114.26	121.46
1	A	314	GLN	CA-C-O	-6.10	114.06	120.58
1	B	892	PRO	CA-C-N	6.09	129.52	120.87
1	B	892	PRO	C-N-CA	6.09	129.52	120.87
2	F	141	PHE	N-CA-C	6.09	118.87	110.35
1	B	986	PRO	CA-C-O	-6.08	111.74	120.56
1	B	705	VAL	CA-C-N	6.08	129.34	120.71
1	B	705	VAL	C-N-CA	6.08	129.34	120.71
1	B	936	ASP	CA-C-O	-6.08	114.11	120.55
1	C	138	ASP	O-C-N	-6.07	115.89	121.42
1	B	1006	THR	CA-C-O	-6.07	114.44	120.82
1	C	118	LEU	N-CA-C	-6.07	99.00	108.90
1	C	245	HIS	N-CA-C	-6.07	99.82	109.23
1	C	1060	VAL	O-C-N	-6.07	116.61	123.10
1	C	447	GLY	CA-C-O	6.07	126.66	119.50
2	F	138	VAL	CA-C-N	6.06	128.68	120.38
2	F	138	VAL	C-N-CA	6.06	128.68	120.38
1	A	543	PHE	CA-C-N	6.06	133.11	121.54
1	A	543	PHE	C-N-CA	6.06	133.11	121.54
1	A	829	ALA	CA-C-N	6.06	129.36	120.82
1	A	829	ALA	C-N-CA	6.06	129.36	120.82
1	B	339	GLY	N-CA-C	6.06	121.33	113.27
1	B	380	TYR	N-CA-C	-6.06	99.12	109.24
1	B	559	PHE	N-CA-C	6.06	118.39	109.24
1	A	146	HIS	N-CA-C	-6.05	97.90	110.80
1	B	589	PRO	CA-C-N	6.05	129.30	120.71
1	B	589	PRO	C-N-CA	6.05	129.30	120.71
1	C	683	ALA	N-CA-C	6.05	119.36	110.59
1	C	364	ASP	N-CA-C	-6.05	103.14	110.88
1	C	766	ALA	N-CA-CB	6.04	118.77	110.01
1	B	50	SER	O-C-N	6.03	130.08	123.27
1	B	388	ASN	N-CA-C	-6.03	105.42	112.89
1	C	925	ASN	O-C-N	6.03	128.28	122.07
1	A	176	LEU	O-C-N	-6.03	115.86	122.67
1	A	473	TYR	CA-C-N	6.03	131.69	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	TYR	C-N-CA	6.03	131.69	122.29
2	D	131	ASP	CA-C-N	6.02	129.18	122.55
2	D	131	ASP	C-N-CA	6.02	129.18	122.55
1	A	190	ARG	CA-C-N	6.02	131.62	122.65
1	A	190	ARG	C-N-CA	6.02	131.62	122.65
1	A	250	THR	O-C-N	-6.02	115.62	121.94
2	F	188	PRO	N-CA-C	-6.02	101.72	111.77
1	C	62	VAL	CA-C-N	6.01	131.02	122.72
1	C	62	VAL	C-N-CA	6.01	131.02	122.72
1	A	1069	PRO	CA-C-O	-6.01	114.34	121.67
1	A	1117	THR	CA-C-O	6.01	126.55	119.28
1	B	67	ALA	CA-C-N	6.01	128.62	120.63
1	B	67	ALA	C-N-CA	6.01	128.62	120.63
1	B	1131	GLY	CA-C-N	6.01	128.70	120.35
1	B	1131	GLY	C-N-CA	6.01	128.70	120.35
1	C	164	ASN	N-CA-C	-6.01	101.09	110.17
2	F	4	LEU	N-CA-C	-6.01	98.47	108.32
1	B	495	TYR	CA-C-N	6.00	127.77	122.43
1	B	495	TYR	C-N-CA	6.00	127.77	122.43
1	A	530	SER	O-C-N	6.00	130.25	122.87
1	B	713	ALA	O-C-N	-6.00	116.23	123.13
1	C	92	PHE	N-CA-C	-6.00	100.02	109.50
1	B	1098	ASN	CA-C-N	6.00	131.62	122.86
1	B	1098	ASN	C-N-CA	6.00	131.62	122.86
1	A	365	TYR	O-C-N	6.00	129.39	122.25
1	B	237	ARG	N-CA-C	-6.00	100.20	109.14
1	C	861	LEU	CA-C-O	-6.00	115.20	120.60
1	C	1050	MET	O-C-N	6.00	129.84	123.42
1	B	1121	PHE	CA-C-N	5.99	130.48	122.93
1	B	1121	PHE	C-N-CA	5.99	130.48	122.93
1	C	501	ASN	N-CA-C	-5.99	104.62	112.41
1	B	684	ALA	CA-C-O	-5.99	114.74	121.81
1	B	1108	ASN	N-CA-C	-5.99	105.93	113.72
1	C	794	ILE	CA-C-N	5.99	132.37	122.73
1	C	794	ILE	C-N-CA	5.99	132.37	122.73
1	C	531	THR	N-CA-C	-5.98	99.98	109.07
1	A	1131	GLY	CA-C-N	5.98	128.51	120.50
1	A	1131	GLY	C-N-CA	5.98	128.51	120.50
1	B	540	ASN	O-C-N	-5.98	116.26	123.13
1	A	1057	PRO	N-CA-CB	5.98	108.62	103.36
2	F	82	GLN	O-C-N	-5.97	116.07	123.36
2	F	82	GLN	CA-C-O	5.97	127.63	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	SER	N-CA-C	-5.97	102.49	110.55
1	A	1056	ALA	CA-C-O	5.96	125.93	120.26
1	B	906	PHE	CA-C-O	-5.96	114.56	120.70
2	E	146	ASP	CA-C-N	5.96	128.87	120.28
2	E	146	ASP	C-N-CA	5.96	128.87	120.28
1	C	90	VAL	O-C-N	5.96	129.50	123.07
1	C	621	PRO	CA-C-O	-5.95	114.66	121.56
1	A	931	ILE	N-CA-C	5.95	116.69	110.62
1	C	292	ALA	N-CA-C	-5.95	104.55	112.94
1	C	448	ASN	CA-C-N	5.95	132.56	122.26
1	C	448	ASN	C-N-CA	5.95	132.56	122.26
2	D	157	GLY	O-C-N	-5.95	115.52	122.60
1	B	114	THR	N-CA-C	-5.95	100.03	109.07
1	C	633	TRP	CB-CA-C	5.95	122.25	110.42
2	F	154	VAL	CA-C-N	5.95	128.62	120.35
2	F	154	VAL	C-N-CA	5.95	128.62	120.35
1	A	184	GLY	O-C-N	5.94	128.54	122.24
1	C	941	THR	O-C-N	5.94	126.63	121.34
1	C	635	VAL	N-CA-C	-5.94	106.96	112.43
1	A	791	THR	CA-C-N	5.94	126.50	120.38
1	A	791	THR	C-N-CA	5.94	126.50	120.38
1	B	961	THR	CA-C-N	5.94	128.16	120.44
1	B	961	THR	C-N-CA	5.94	128.16	120.44
1	A	571	ASP	CA-C-O	5.94	128.34	120.98
1	C	708	SER	N-CA-C	-5.94	100.75	109.18
1	A	178	ASP	CA-C-O	5.94	126.46	119.28
2	E	49	ALA	CB-CA-C	-5.94	99.58	110.62
1	A	555	SER	N-CA-C	5.93	119.42	110.64
1	B	802	PHE	CA-C-N	5.93	130.37	120.70
1	B	802	PHE	C-N-CA	5.93	130.37	120.70
1	C	1104	VAL	N-CA-C	-5.93	99.93	108.53
2	E	162	LEU	CA-C-N	5.93	128.82	120.28
2	E	162	LEU	C-N-CA	5.93	128.82	120.28
1	C	343	ASN	CA-C-N	5.93	130.58	122.34
1	C	343	ASN	C-N-CA	5.93	130.58	122.34
1	A	701	ALA	N-CA-C	-5.93	100.74	109.81
1	B	416	GLY	N-CA-C	-5.93	104.81	111.63
1	A	813	SER	CA-C-O	-5.92	114.13	120.46
1	C	555	SER	CA-C-N	5.92	133.99	123.34
1	C	555	SER	C-N-CA	5.92	133.99	123.34
1	B	618	THR	N-CA-C	-5.92	106.02	113.18
1	C	565	PHE	CA-C-N	5.92	129.41	121.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	565	PHE	C-N-CA	5.92	129.41	121.01
1	B	1056	ALA	CA-C-O	-5.91	114.64	120.26
1	C	895	GLN	N-CA-C	-5.91	98.89	108.52
1	A	562	PHE	N-CA-C	-5.90	106.04	113.72
2	D	146	ASP	O-C-N	-5.90	115.99	122.07
1	B	429	PHE	N-CA-C	-5.90	99.28	108.90
1	C	926	GLN	CA-C-O	5.90	127.02	120.82
1	A	1075	PHE	CA-C-N	5.90	129.21	120.95
1	A	1075	PHE	C-N-CA	5.90	129.21	120.95
1	B	438	SER	N-CA-C	-5.90	103.45	110.41
1	C	321	GLN	CA-C-O	-5.90	114.56	120.63
1	A	166	CYS	CA-C-O	-5.90	114.96	121.33
2	F	131	ASP	CA-C-N	5.90	129.61	120.00
2	F	131	ASP	C-N-CA	5.90	129.61	120.00
1	A	329	PHE	N-CA-C	-5.89	101.97	110.40
1	B	849	LEU	CA-C-N	5.89	128.47	120.63
1	B	849	LEU	C-N-CA	5.89	128.47	120.63
2	D	167	GLU	CA-C-O	-5.89	114.56	121.16
1	C	105	ILE	O-C-N	5.89	129.40	123.10
1	B	930	ALA	CA-C-N	5.89	128.53	120.46
1	B	930	ALA	C-N-CA	5.89	128.53	120.46
1	B	864	LEU	N-CA-C	-5.88	103.57	112.04
2	F	133	ALA	N-CA-C	-5.88	103.44	111.56
1	C	251	PRO	CA-C-N	5.88	131.08	120.79
1	C	251	PRO	C-N-CA	5.88	131.08	120.79
1	B	740	MET	N-CA-C	5.88	117.68	111.28
1	B	1123	SER	N-CA-C	-5.88	100.14	109.07
1	B	308	VAL	N-CA-C	-5.87	99.66	108.12
1	B	952	VAL	N-CA-C	-5.87	105.01	110.53
2	D	55	GLY	CA-C-O	-5.87	115.90	122.24
1	A	878	LEU	CA-C-N	5.87	128.15	120.28
1	A	878	LEU	C-N-CA	5.87	128.15	120.28
1	C	37	TYR	N-CA-C	5.87	117.89	109.14
1	C	1004	LEU	O-C-N	5.87	128.84	122.15
1	C	262	ALA	N-CA-C	-5.87	106.10	113.20
2	E	58	THR	N-CA-C	-5.87	100.50	109.41
1	A	252	GLY	O-C-N	5.86	128.45	122.24
1	A	1078	ALA	CA-C-N	5.86	125.47	119.56
1	A	1078	ALA	C-N-CA	5.86	125.47	119.56
1	B	921	LYS	O-C-N	5.85	128.32	122.12
2	E	110	GLY	O-C-N	-5.85	116.51	122.60
1	B	1032	CYS	CB-CA-C	-5.85	98.74	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	193	PRO	CA-C-O	-5.85	112.08	120.56
1	A	583	GLU	CA-C-O	-5.85	114.34	121.36
1	C	146	HIS	CE1-NE2-CD2	-5.85	103.15	109.00
1	C	827	THR	N-CA-C	-5.84	98.88	108.41
1	C	383	SER	CA-C-N	5.84	125.86	119.90
1	C	383	SER	C-N-CA	5.84	125.86	119.90
2	D	159	PHE	N-CA-C	-5.84	99.21	108.73
1	C	779	GLN	CA-C-N	5.84	128.10	120.28
1	C	779	GLN	C-N-CA	5.84	128.10	120.28
1	C	138	ASP	CA-C-N	5.83	125.81	120.03
1	C	138	ASP	C-N-CA	5.83	125.81	120.03
1	A	613	GLN	CA-C-N	5.83	130.65	122.36
1	A	613	GLN	C-N-CA	5.83	130.65	122.36
1	A	135	PHE	N-CA-C	-5.83	99.55	108.76
1	A	528	LYS	CA-C-N	5.83	128.99	120.71
1	A	528	LYS	C-N-CA	5.83	128.99	120.71
1	C	213	VAL	O-C-N	5.83	127.62	121.91
1	C	239	GLN	O-C-N	5.83	129.91	123.33
1	C	960	ASN	CA-C-N	5.83	128.01	120.44
1	C	960	ASN	C-N-CA	5.83	128.01	120.44
1	A	119	ILE	CA-C-N	-5.82	115.97	123.19
1	A	119	ILE	C-N-CA	-5.82	115.97	123.19
1	C	615	VAL	CA-C-O	-5.82	113.86	120.67
1	C	928	ASN	CA-C-N	5.82	128.56	120.29
1	C	928	ASN	C-N-CA	5.82	128.56	120.29
1	A	874	THR	CA-C-N	5.82	128.08	120.28
1	A	874	THR	C-N-CA	5.82	128.08	120.28
1	C	649	CYS	N-CA-C	-5.82	99.75	109.24
1	A	424	LYS	N-CA-C	-5.82	98.88	108.48
1	A	160	TYR	N-CA-C	-5.82	100.70	109.95
1	C	991	VAL	CA-C-N	5.82	128.07	120.28
1	C	991	VAL	C-N-CA	5.82	128.07	120.28
1	B	590	CYS	N-CA-C	5.81	118.66	110.23
1	C	592	PHE	O-C-N	-5.81	116.42	123.10
2	E	176	TRP	N-CA-C	-5.81	99.53	109.24
2	D	152	HIS	O-C-N	5.81	129.88	122.04
1	C	146	HIS	CA-C-O	5.81	128.26	120.13
2	D	183	GLU	N-CA-C	-5.81	99.69	108.52
1	B	361	CYS	N-CA-C	5.81	117.08	108.60
1	C	45	SER	N-CA-C	-5.80	99.91	108.79
1	A	980	ILE	CA-C-N	5.80	127.98	120.44
1	A	980	ILE	C-N-CA	5.80	127.98	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	ILE	N-CA-C	-5.80	99.28	107.75
2	F	93	VAL	N-CA-C	-5.80	100.23	108.58
1	B	1124	GLY	N-CA-C	5.80	121.58	111.50
1	B	212	LEU	N-CA-C	-5.79	100.69	109.85
1	A	758	SER	N-CA-C	-5.79	106.07	113.02
1	C	478	THR	O-C-N	5.79	126.94	121.38
1	C	1029	MET	N-CA-C	5.79	117.59	111.28
1	B	489	TYR	N-CA-C	-5.79	100.75	108.74
1	B	1135	ASN	N-CA-C	-5.79	99.72	108.46
1	A	330	PRO	N-CA-C	5.78	120.30	111.34
1	A	1015	ALA	CA-C-O	-5.78	114.42	120.55
1	B	499	PRO	CA-C-N	5.78	128.92	120.71
1	B	499	PRO	C-N-CA	5.78	128.92	120.71
1	B	809	PRO	CA-C-O	-5.78	114.92	121.97
1	B	866	THR	CA-C-N	5.78	128.30	120.38
1	B	866	THR	C-N-CA	5.78	128.30	120.38
1	C	119	ILE	CA-C-N	5.78	130.63	123.12
1	C	119	ILE	C-N-CA	5.78	130.63	123.12
2	D	122	GLY	CA-C-N	5.78	132.73	121.41
2	D	122	GLY	C-N-CA	5.78	132.73	121.41
1	C	804	GLN	N-CA-C	-5.77	106.09	113.02
1	A	428	ASP	N-CA-C	-5.77	105.82	112.92
1	B	395	VAL	CA-C-O	5.77	127.13	120.67
2	D	105	PRO	CA-C-N	5.77	129.54	123.08
2	D	105	PRO	C-N-CA	5.77	129.54	123.08
2	E	87	LYS	CA-C-N	5.77	126.16	119.47
2	E	87	LYS	C-N-CA	5.77	126.16	119.47
1	A	511	VAL	N-CA-C	-5.77	99.87	108.46
1	B	124	THR	CA-C-N	5.77	128.95	120.82
1	B	124	THR	C-N-CA	5.77	128.95	120.82
1	B	332	ILE	O-C-N	-5.77	117.03	123.26
1	C	666	ILE	O-C-N	5.77	127.11	121.98
1	B	267	VAL	N-CA-C	-5.76	99.82	108.12
1	C	213	VAL	CA-C-N	-5.76	114.92	123.11
1	C	213	VAL	C-N-CA	-5.76	114.92	123.11
1	C	914	ASN	O-C-N	5.76	128.23	122.12
1	C	903	ALA	CA-C-N	5.76	128.28	120.44
1	C	903	ALA	C-N-CA	5.76	128.28	120.44
1	A	244	LEU	N-CA-C	-5.76	106.42	113.50
1	A	1015	ALA	CA-C-N	5.76	128.00	120.28
1	A	1015	ALA	C-N-CA	5.76	128.00	120.28
1	B	82	PRO	CA-C-O	-5.76	114.71	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	HIS	N-CA-C	-5.76	99.27	109.06
1	A	539	VAL	N-CA-C	-5.76	100.30	108.65
1	C	69	HIS	O-C-N	5.76	129.80	123.01
1	A	609	ALA	N-CA-CB	5.75	119.95	110.69
1	B	416	GLY	CA-C-O	5.75	126.88	122.16
1	B	1095	PHE	O-C-N	5.75	129.83	123.16
1	A	653	ALA	N-CA-C	-5.75	99.96	108.99
1	C	192	PHE	CA-C-O	-5.75	114.40	121.06
1	C	643	PHE	CA-CB-CG	5.75	119.55	113.80
1	A	407	VAL	N-CA-C	-5.74	104.76	110.62
1	A	1092	GLU	N-CA-C	-5.74	99.69	108.76
1	B	997	ILE	O-C-N	5.74	127.53	121.91
1	C	279	TYR	CA-C-N	5.74	132.22	122.12
1	C	279	TYR	C-N-CA	5.74	132.22	122.12
2	F	148	LEU	CA-C-O	-5.74	112.83	119.78
1	B	230	PRO	O-C-N	5.74	126.80	122.73
1	C	398	ASP	CA-C-O	5.74	126.44	120.30
1	B	950	ASP	CA-C-N	5.74	128.57	120.42
1	B	950	ASP	C-N-CA	5.74	128.57	120.42
2	D	166	THR	N-CA-C	-5.74	105.58	113.56
1	B	69	HIS	CA-C-O	-5.73	114.74	121.16
1	B	90	VAL	O-C-N	5.73	129.40	123.04
1	B	445	VAL	N-CA-C	-5.73	107.68	113.47
1	B	684	ALA	O-C-N	5.73	129.38	122.85
1	C	49	HIS	N-CA-C	-5.73	100.35	109.23
1	B	969	ASN	CA-C-N	5.73	130.26	122.19
1	B	969	ASN	C-N-CA	5.73	130.26	122.19
1	A	211	ASN	N-CA-C	-5.73	106.64	113.97
1	C	964	LYS	CA-C-O	-5.72	114.48	120.55
2	E	24	ALA	CA-C-N	5.72	130.54	120.87
2	E	24	ALA	C-N-CA	5.72	130.54	120.87
1	A	976	VAL	N-CA-C	-5.72	98.18	106.88
1	B	962	LEU	CA-C-N	5.72	127.88	120.56
1	B	962	LEU	C-N-CA	5.72	127.88	120.56
1	C	539	VAL	CA-C-N	5.72	130.02	122.30
1	C	539	VAL	C-N-CA	5.72	130.02	122.30
1	B	760	CYS	O-C-N	5.72	128.67	122.15
1	C	371	SER	N-CA-C	-5.72	105.41	112.38
1	B	945	LEU	N-CA-C	-5.71	106.21	112.72
1	B	107	GLY	N-CA-C	-5.71	102.80	111.42
1	B	879	ALA	CA-C-O	-5.71	114.50	120.55
1	B	386	LYS	CA-C-O	5.71	125.56	118.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	187	ILE	O-C-N	-5.71	114.59	121.10
2	E	195	PRO	N-CA-CB	-5.71	98.25	102.25
1	A	968	SER	CA-C-N	5.71	133.49	122.53
1	A	968	SER	C-N-CA	5.71	133.49	122.53
1	A	1037	SER	N-CA-C	-5.71	101.25	110.32
2	F	78	THR	N-CA-C	-5.70	100.07	108.79
1	C	391	CYS	N-CA-C	-5.70	101.00	110.17
2	E	80	TYR	N-CA-C	-5.69	100.43	109.59
1	C	633	TRP	CG-CD2-CE3	5.69	139.59	133.90
1	A	590	CYS	N-CA-C	5.68	118.47	110.23
1	C	59	PHE	CA-CB-CG	5.68	119.48	113.80
1	C	737	ASP	CA-C-N	5.68	128.21	120.54
1	C	737	ASP	C-N-CA	5.68	128.21	120.54
1	A	1094	VAL	N-CA-C	-5.68	99.58	108.95
1	A	128	ILE	N-CA-C	-5.68	100.24	108.36
1	C	585	LEU	CA-C-O	-5.67	114.69	120.71
1	C	321	GLN	CA-C-N	5.67	125.58	119.85
1	C	321	GLN	C-N-CA	5.67	125.58	119.85
1	B	116	SER	N-CA-C	-5.67	101.35	110.14
1	A	935	GLN	CA-C-N	5.67	127.88	120.28
1	A	935	GLN	C-N-CA	5.67	127.88	120.28
1	A	600	PRO	CA-C-N	5.67	129.64	121.54
1	A	600	PRO	C-N-CA	5.67	129.64	121.54
1	B	620	VAL	CA-C-O	-5.67	112.36	119.95
1	C	838	GLY	O-C-N	5.67	128.68	122.56
2	D	188	PRO	O-C-N	5.67	129.76	122.91
1	A	1142	GLN	CA-C-O	-5.66	113.12	118.44
1	C	1102	TRP	N-CA-C	-5.66	100.94	109.95
1	C	183	GLN	CA-C-N	5.66	127.22	120.14
1	C	183	GLN	C-N-CA	5.66	127.22	120.14
1	C	291	CYS	CB-CA-C	-5.66	99.89	110.36
1	A	344	ALA	N-CA-CB	5.66	120.05	110.49
1	C	267	VAL	N-CA-C	-5.66	99.97	108.12
1	C	1064	HIS	CA-C-O	-5.66	114.09	120.43
2	F	26	GLY	CA-C-O	5.66	125.88	119.09
1	A	578	ASP	O-C-N	-5.66	115.62	121.28
1	A	69	HIS	CA-C-N	5.65	131.61	122.68
1	A	69	HIS	C-N-CA	5.65	131.61	122.68
1	B	391	CYS	N-CA-CB	5.65	119.89	110.85
1	B	423	TYR	CB-CA-C	5.65	121.67	110.42
1	C	842	GLY	CA-C-N	5.65	128.73	120.71
1	C	842	GLY	C-N-CA	5.65	128.73	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	113	THR	N-CA-C	-5.65	100.12	108.99
1	C	454	ARG	O-C-N	-5.64	116.61	123.10
1	A	907	ASN	CA-C-N	5.64	130.44	120.74
1	A	907	ASN	C-N-CA	5.64	130.44	120.74
1	B	41	LYS	N-CA-C	-5.64	107.03	114.31
1	B	216	LEU	N-CA-C	-5.64	100.39	109.58
1	C	836	GLN	O-C-N	5.64	129.22	122.79
2	D	164	ASP	CA-C-O	-5.64	112.61	119.32
1	A	240	THR	CA-C-N	-5.63	114.93	122.42
1	A	240	THR	C-N-CA	-5.63	114.93	122.42
1	B	504	GLY	N-CA-C	-5.63	107.49	115.43
1	C	976	VAL	N-CA-C	-5.63	99.76	107.99
1	B	669	GLY	N-CA-C	-5.63	107.49	115.43
1	A	123	ALA	CB-CA-C	5.63	120.40	111.51
1	B	382	VAL	N-CA-C	-5.63	100.58	108.80
1	A	887	THR	CA-C-N	5.62	132.28	121.54
1	A	887	THR	C-N-CA	5.62	132.28	121.54
1	A	876	ALA	CA-C-N	5.62	127.81	120.28
1	A	876	ALA	C-N-CA	5.62	127.81	120.28
1	B	80	ASP	N-CA-C	-5.62	100.54	109.59
2	F	34	MET	N-CA-C	-5.62	98.47	108.13
1	A	863	PRO	CA-C-N	5.62	127.74	120.44
1	A	863	PRO	C-N-CA	5.62	127.74	120.44
1	B	760	CYS	CA-C-O	-5.62	114.47	120.42
1	A	1061	VAL	CA-C-O	-5.61	114.50	120.39
2	F	113	THR	CA-C-N	5.61	130.10	122.19
2	F	113	THR	C-N-CA	5.61	130.10	122.19
1	C	633	TRP	CE2-CD2-CE3	-5.61	113.19	118.80
2	E	127	SER	CA-C-N	5.61	130.18	121.26
2	E	127	SER	C-N-CA	5.61	130.18	121.26
1	C	998	THR	N-CA-C	5.61	117.07	111.07
1	A	203	ILE	N-CA-C	-5.60	100.05	108.12
2	D	34	MET	CA-C-O	5.60	127.56	121.06
2	E	130	SER	N-CA-C	-5.60	104.69	112.03
1	C	244	LEU	N-CA-C	-5.60	103.30	111.30
1	C	1029	MET	O-C-N	5.60	128.05	122.12
2	E	192	PRO	CA-C-N	5.60	126.14	120.38
2	E	192	PRO	C-N-CA	5.60	126.14	120.38
2	D	165	SER	N-CA-C	-5.59	107.70	114.75
1	A	1011	GLN	CA-C-N	5.59	127.77	120.28
1	A	1011	GLN	C-N-CA	5.59	127.77	120.28
1	A	666	ILE	N-CA-C	-5.59	106.75	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	389	ASP	CA-C-N	-5.59	115.22	123.05
1	C	389	ASP	C-N-CA	-5.59	115.22	123.05
1	C	866	THR	CA-C-N	5.58	128.53	120.38
1	C	866	THR	C-N-CA	5.58	128.53	120.38
1	B	365	TYR	N-CA-C	-5.58	104.89	112.26
1	B	580	GLN	CA-C-O	5.58	126.09	119.67
1	C	99	ASN	CA-C-O	-5.58	115.07	121.54
1	A	251	PRO	N-CA-C	-5.57	106.89	113.86
1	C	172	SER	N-CA-C	-5.57	100.82	109.24
1	A	871	ALA	CA-C-N	5.57	128.20	120.29
1	A	871	ALA	C-N-CA	5.57	128.20	120.29
1	B	822	LEU	N-CA-C	5.57	118.12	111.71
1	B	159	VAL	N-CA-C	-5.57	107.31	112.83
1	C	319	ARG	CA-C-N	5.57	128.55	120.98
1	C	319	ARG	C-N-CA	5.57	128.55	120.98
2	E	178	LYS	CA-C-N	5.56	130.32	122.09
2	E	178	LYS	C-N-CA	5.56	130.32	122.09
1	B	483	VAL	CA-C-N	5.56	130.72	122.82
1	B	483	VAL	C-N-CA	5.56	130.72	122.82
1	B	834	ILE	N-CA-C	-5.56	100.32	108.11
1	A	286	THR	CA-C-O	5.56	124.92	118.97
1	C	482	GLY	CA-C-N	5.56	130.74	123.06
1	C	482	GLY	C-N-CA	5.56	130.74	123.06
1	C	989	ALA	CA-C-N	5.56	127.73	120.28
1	C	989	ALA	C-N-CA	5.56	127.73	120.28
1	C	366	SER	CA-C-O	5.56	126.65	120.82
2	D	37	TYR	CG-CD1-CE1	-5.56	112.86	121.20
1	C	125	ASN	N-CA-C	5.55	118.07	110.24
1	C	844	ILE	CA-C-N	5.55	129.13	120.75
1	C	844	ILE	C-N-CA	5.55	129.13	120.75
1	B	629	LEU	N-CA-C	-5.55	105.84	113.56
1	A	1105	THR	N-CA-C	-5.55	100.64	109.07
1	C	111	ASP	N-CA-C	-5.54	104.05	111.87
1	A	55	PHE	CA-C-O	-5.54	114.90	121.66
1	A	62	VAL	N-CA-C	-5.54	100.41	108.17
2	D	113	THR	CA-C-O	5.54	127.20	120.99
1	A	145	TYR	CA-C-O	-5.54	114.96	121.16
1	B	87	ASN	CA-C-N	5.54	130.22	122.36
1	B	87	ASN	C-N-CA	5.54	130.22	122.36
1	A	920	GLN	N-CA-C	5.54	118.03	111.33
2	D	176	TRP	CA-C-O	-5.54	114.96	121.44
2	E	151	ALA	N-CA-C	-5.53	106.11	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	633	TRP	N-CA-C	-5.53	99.02	110.80
1	C	525	CYS	N-CA-C	-5.53	101.06	108.86
1	C	707	TYR	CA-CB-CG	-5.53	103.95	113.90
2	E	73	ASP	N-CA-C	-5.53	102.57	110.59
1	A	190	ARG	O-C-N	-5.53	116.75	123.27
2	E	159	PHE	O-C-N	-5.53	116.30	122.93
1	B	822	LEU	CA-C-O	5.53	126.34	120.10
1	B	383	SER	N-CA-C	-5.52	100.54	109.82
1	B	463	PRO	CA-C-N	5.52	130.47	122.36
1	B	463	PRO	C-N-CA	5.52	130.47	122.36
1	B	633	TRP	O-C-N	-5.52	115.25	122.59
1	C	1005	GLN	CA-C-O	-5.52	115.03	120.82
1	B	938	LEU	CA-C-N	5.51	127.94	120.44
1	B	938	LEU	C-N-CA	5.51	127.94	120.44
1	C	146	HIS	CA-C-N	5.51	130.85	122.37
1	C	146	HIS	C-N-CA	5.51	130.85	122.37
1	A	49	HIS	CA-C-O	-5.51	114.67	121.06
1	C	669	GLY	N-CA-C	-5.51	107.67	115.43
1	C	977	LEU	CA-C-N	5.51	128.21	120.28
1	C	977	LEU	C-N-CA	5.51	128.21	120.28
1	C	1126	CYS	N-CA-CB	5.50	118.70	110.22
1	A	1136	THR	CA-C-O	5.50	126.54	120.71
1	A	769	GLY	N-CA-C	-5.50	105.99	112.64
1	C	294	ASP	CA-C-O	-5.50	114.30	119.91
2	D	136	SER	CA-C-N	5.50	130.14	121.56
2	D	136	SER	C-N-CA	5.50	130.14	121.56
1	C	335	LEU	O-C-N	-5.50	116.17	122.93
1	C	855	PHE	N-CA-CB	5.49	121.08	112.46
2	D	133	ALA	N-CA-C	-5.49	103.16	111.34
2	D	152	HIS	CA-C-O	-5.49	113.42	119.08
2	F	36	TRP	CB-CG-CD2	-5.49	119.11	126.80
1	C	658	ASN	CA-C-O	-5.49	114.97	121.66
1	A	228	ASP	O-C-N	5.48	129.88	122.59
1	A	919	ASN	N-CA-C	-5.48	105.90	112.59
1	C	692	ILE	O-C-N	5.48	129.56	122.77
1	B	756	TYR	N-CA-C	-5.47	105.96	113.30
1	C	733	LYS	CA-C-N	5.47	128.62	120.95
1	C	733	LYS	C-N-CA	5.47	128.62	120.95
1	B	296	LEU	O-C-N	5.47	127.92	122.12
2	F	193	PRO	CB-CA-C	-5.47	104.24	110.92
1	A	774	GLN	CA-C-N	5.47	128.06	120.29
1	A	774	GLN	C-N-CA	5.47	128.06	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	706	ALA	CA-C-O	-5.47	115.17	121.19
2	F	161	TYR	CA-C-N	5.46	129.69	122.42
2	F	161	TYR	C-N-CA	5.46	129.69	122.42
1	B	1006	THR	N-CA-C	-5.46	105.22	111.07
1	B	988	GLU	CA-C-N	5.46	127.54	120.44
1	B	988	GLU	C-N-CA	5.46	127.54	120.44
1	A	297	SER	CA-C-O	-5.46	114.76	120.55
1	B	580	GLN	N-CA-C	-5.46	106.67	113.55
1	B	893	ALA	CA-C-O	5.46	127.27	121.16
1	B	996	LEU	CA-C-N	5.46	127.44	120.56
1	B	996	LEU	C-N-CA	5.46	127.44	120.56
1	C	897	PRO	O-C-N	-5.46	115.96	122.89
1	B	805	ILE	N-CA-C	-5.46	107.66	112.90
1	B	546	LEU	N-CA-C	-5.45	100.81	109.59
1	B	790	LYS	CA-C-N	5.45	128.97	120.68
1	B	790	LYS	C-N-CA	5.45	128.97	120.68
1	B	111	ASP	CA-C-N	5.45	130.10	122.36
1	B	111	ASP	C-N-CA	5.45	130.10	122.36
1	C	549	THR	N-CA-C	-5.45	100.30	109.07
1	C	899	PRO	CA-C-O	-5.45	110.63	119.84
1	C	298	GLU	CA-C-O	-5.45	114.78	120.55
1	A	936	ASP	CA-C-N	5.45	127.52	120.44
1	A	936	ASP	C-N-CA	5.45	127.52	120.44
1	C	881	THR	CA-C-N	5.45	128.53	120.74
1	C	881	THR	C-N-CA	5.45	128.53	120.74
1	A	239	GLN	N-CA-C	-5.44	101.02	109.24
1	A	490	PHE	N-CA-C	-5.44	99.50	108.75
1	C	988	GLU	CA-C-N	5.44	127.57	120.28
1	C	988	GLU	C-N-CA	5.44	127.57	120.28
2	D	135	GLY	O-C-N	5.44	129.57	122.71
1	B	1066	THR	N-CA-C	-5.44	101.09	109.52
1	A	745	ASP	N-CA-C	-5.44	106.56	114.12
1	B	886	TRP	N-CA-C	-5.43	106.65	113.28
1	C	36	VAL	N-CA-C	-5.43	100.66	108.48
1	C	618	THR	N-CA-C	-5.43	106.82	113.50
1	C	636	TYR	N-CA-C	-5.43	101.05	108.38
1	A	973	ILE	N-CA-C	-5.43	106.12	111.88
1	C	352	ALA	CA-C-N	5.43	129.47	120.94
1	C	352	ALA	C-N-CA	5.43	129.47	120.94
1	A	736	VAL	N-CA-C	-5.43	100.41	108.45
1	B	1025	ALA	CA-C-N	5.43	127.56	120.28
1	B	1025	ALA	C-N-CA	5.43	127.56	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	129	GLY	O-C-N	-5.42	116.48	122.50
1	B	567	ARG	N-CA-C	-5.42	98.81	108.13
1	C	216	LEU	CA-C-O	-5.42	113.53	120.04
1	A	628	GLN	CA-C-N	5.42	130.26	122.40
1	A	628	GLN	C-N-CA	5.42	130.26	122.40
2	F	80	TYR	CA-C-O	-5.42	114.90	120.54
1	B	778	THR	O-C-N	5.42	127.65	122.07
1	C	1002	GLN	O-C-N	5.42	127.86	122.12
2	F	158	THR	CA-C-N	5.42	129.61	122.30
2	F	158	THR	C-N-CA	5.42	129.61	122.30
1	A	1110	TYR	O-C-N	-5.42	116.36	123.02
1	B	978	ASN	CA-C-N	5.42	129.84	120.58
1	B	978	ASN	C-N-CA	5.42	129.84	120.58
1	A	807	PRO	CA-C-O	-5.41	115.37	121.97
1	C	647	ALA	N-CA-C	-5.41	107.05	113.97
1	C	634	ARG	O-C-N	-5.41	115.40	122.59
1	C	851	CYS	CA-C-O	5.41	127.09	120.60
2	F	88	PRO	CA-C-N	5.41	129.75	120.72
2	F	88	PRO	C-N-CA	5.41	129.75	120.72
1	B	365	TYR	CA-C-N	5.40	127.78	120.38
1	B	365	TYR	C-N-CA	5.40	127.78	120.38
1	B	527	PRO	N-CA-C	-5.40	107.13	114.80
1	C	402	ILE	CA-C-O	-5.40	116.16	121.67
2	F	180	GLN	N-CA-C	5.40	118.11	110.50
1	A	520	ALA	N-CA-CB	5.40	119.97	110.37
1	C	917	TYR	N-CA-C	5.39	118.33	111.69
1	B	124	THR	N-CA-C	-5.39	101.23	108.19
1	B	469	SER	O-C-N	-5.39	116.30	122.93
1	C	456	PHE	O-C-N	5.39	129.87	123.24
1	B	605	SER	N-CA-C	-5.38	103.42	110.53
1	B	956	ALA	CA-C-N	5.38	127.50	120.28
1	B	956	ALA	C-N-CA	5.38	127.50	120.28
1	A	466	ARG	N-CA-C	-5.38	106.02	112.59
1	A	1128	VAL	CA-C-O	5.38	124.87	119.97
1	A	1089	PHE	CA-C-N	5.38	125.84	120.14
1	A	1089	PHE	C-N-CA	5.38	125.84	120.14
1	C	131	CYS	N-CA-CB	5.38	119.58	111.35
1	B	176	LEU	N-CA-C	5.38	117.20	110.91
1	B	441	LEU	CA-C-N	-5.38	115.22	123.07
1	B	441	LEU	C-N-CA	-5.38	115.22	123.07
1	A	726	ILE	N-CA-C	-5.38	100.38	108.12
1	B	737	ASP	CA-C-N	5.37	127.43	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	737	ASP	C-N-CA	5.37	127.43	120.44
2	E	6	GLU	CA-C-O	5.37	127.73	121.44
1	B	496	GLY	N-CA-C	-5.37	105.21	112.57
1	B	528	LYS	O-C-N	5.37	129.20	122.86
1	C	847	ARG	N-CA-C	-5.37	104.15	111.56
1	C	1002	GLN	CA-C-O	-5.37	114.86	120.55
1	B	1034	LEU	N-CA-C	-5.37	106.92	112.93
1	C	697	MET	N-CA-C	5.37	118.10	110.10
1	A	1130	ILE	CA-C-N	5.37	129.61	120.91
1	A	1130	ILE	C-N-CA	5.37	129.61	120.91
1	B	735	SER	CA-C-O	5.37	126.76	120.43
2	D	100	PRO	N-CA-C	-5.37	107.02	114.27
1	C	682	ARG	N-CA-C	-5.37	99.37	110.80
1	C	692	ILE	CA-C-O	-5.37	114.20	120.75
1	C	849	LEU	CA-C-N	5.37	128.28	120.98
1	C	849	LEU	C-N-CA	5.37	128.28	120.98
1	A	892	PRO	CA-C-N	5.36	128.32	120.71
1	A	892	PRO	C-N-CA	5.36	128.32	120.71
1	A	611	LEU	CA-C-O	5.36	126.60	120.54
1	C	629	LEU	CA-C-O	5.36	125.52	119.78
1	A	499	PRO	CA-C-N	5.36	128.96	121.02
1	A	499	PRO	C-N-CA	5.36	128.96	121.02
1	A	420	ASP	N-CA-C	-5.36	106.42	113.17
1	C	489	TYR	O-C-N	5.36	128.96	122.85
1	B	818	ILE	CA-C-N	5.36	127.46	120.28
1	B	818	ILE	C-N-CA	5.36	127.46	120.28
1	B	831	ALA	CA-C-N	5.36	130.72	122.20
1	B	831	ALA	C-N-CA	5.36	130.72	122.20
2	E	185	ILE	CA-C-N	5.36	125.30	119.78
2	E	185	ILE	C-N-CA	5.36	125.30	119.78
1	C	640	SER	CA-C-O	-5.35	115.18	121.44
1	A	475	ALA	CA-C-O	-5.35	114.50	120.54
1	A	142	GLY	O-C-N	5.35	128.37	122.27
1	C	703	ASN	N-CA-C	-5.35	99.39	108.26
1	A	202	LYS	CA-C-O	5.34	126.73	120.80
1	B	148	ASN	O-C-N	5.34	128.71	122.99
1	B	327	VAL	N-CA-C	-5.34	100.78	108.48
1	C	805	ILE	O-C-N	5.34	127.35	122.06
2	F	136	SER	N-CA-C	-5.34	100.86	108.23
1	B	418	ILE	CA-C-N	5.34	131.74	121.54
1	B	418	ILE	C-N-CA	5.34	131.74	121.54
1	B	360	ASN	CA-C-N	-5.34	112.67	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	ASN	C-N-CA	-5.34	112.67	121.80
1	A	946	GLY	CA-C-N	5.34	129.63	120.72
1	A	946	GLY	C-N-CA	5.34	129.63	120.72
1	C	792	PRO	CA-C-O	-5.34	112.82	120.56
1	B	695	TYR	CB-CG-CD2	5.33	128.80	120.80
1	C	938	LEU	CA-C-N	5.33	127.69	120.44
1	C	938	LEU	C-N-CA	5.33	127.69	120.44
2	D	108	TYR	CA-C-N	5.33	131.73	121.54
2	D	108	TYR	C-N-CA	5.33	131.73	121.54
2	E	49	ALA	N-CA-CB	5.33	119.82	111.56
1	A	737	ASP	CA-C-N	5.33	127.73	120.54
1	A	737	ASP	C-N-CA	5.33	127.73	120.54
1	B	793	PRO	N-CA-C	-5.33	107.08	114.27
1	A	899	PRO	O-C-N	5.33	128.37	122.24
1	A	1040	VAL	O-C-N	-5.33	117.44	123.03
1	B	60	SER	CA-C-N	5.33	129.49	122.30
1	B	60	SER	C-N-CA	5.33	129.49	122.30
1	B	529	LYS	N-CA-C	5.32	122.14	110.80
1	B	557	LYS	CA-C-O	5.32	127.08	121.33
1	C	471	GLU	CA-C-N	5.32	129.64	122.93
1	C	471	GLU	C-N-CA	5.32	129.64	122.93
2	D	21	SER	N-CA-C	-5.32	101.44	109.85
1	A	920	GLN	CA-C-O	5.32	126.38	120.63
1	B	783	ALA	CB-CA-C	-5.32	102.81	111.06
1	B	920	GLN	CA-C-N	5.32	127.41	120.28
1	B	920	GLN	C-N-CA	5.32	127.41	120.28
2	D	1	GLN	O-C-N	-5.32	114.49	123.00
1	B	582	LEU	N-CA-C	-5.32	106.02	112.88
1	C	146	HIS	CG-CD2-NE2	5.32	112.52	107.20
1	A	554	GLU	CA-C-N	5.32	131.17	121.97
1	A	554	GLU	C-N-CA	5.32	131.17	121.97
1	C	867	ASP	N-CA-C	5.32	118.56	111.75
1	C	412	PRO	N-CA-C	5.31	119.38	111.41
1	B	911	VAL	N-CA-C	-5.31	100.67	108.11
1	C	457	ARG	NH1-CZ-NH2	-5.31	112.39	119.30
1	A	155	SER	CA-C-N	5.31	128.38	120.95
1	A	155	SER	C-N-CA	5.31	128.38	120.95
1	B	319	ARG	CA-C-N	5.31	128.20	120.98
1	B	319	ARG	C-N-CA	5.31	128.20	120.98
1	B	868	GLU	N-CA-C	5.31	117.07	111.28
1	B	495	TYR	CA-C-O	-5.31	114.64	120.69
1	C	1009	THR	O-C-N	-5.31	116.49	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1019	ARG	O-C-N	5.31	127.54	122.07
1	B	523	THR	N-CA-C	-5.30	107.47	114.31
1	B	1015	ALA	CA-C-N	5.30	127.82	120.29
1	B	1015	ALA	C-N-CA	5.30	127.82	120.29
2	F	119	SER	CA-C-N	5.30	131.98	121.53
2	F	119	SER	C-N-CA	5.30	131.98	121.53
1	C	159	VAL	CA-C-N	5.30	131.32	121.62
1	C	159	VAL	C-N-CA	5.30	131.32	121.62
1	C	770	ILE	CA-C-N	5.30	127.64	120.38
1	C	770	ILE	C-N-CA	5.30	127.64	120.38
1	A	121	ASN	N-CA-C	-5.29	99.53	110.80
1	A	334	ASN	N-CA-C	-5.29	100.42	107.88
1	C	35	GLY	CA-C-O	5.29	126.30	119.68
1	C	400	PHE	N-CA-C	5.29	116.33	108.60
1	B	922	LEU	CA-C-N	5.29	127.23	120.56
1	B	922	LEU	C-N-CA	5.29	127.23	120.56
1	C	631	PRO	N-CA-C	5.29	119.51	111.15
1	C	753	LEU	N-CA-C	5.29	117.13	111.36
1	C	766	ALA	CB-CA-C	-5.29	102.57	110.88
1	C	919	ASN	CA-C-N	5.29	127.63	120.38
1	C	919	ASN	C-N-CA	5.29	127.63	120.38
1	A	422	ASN	CB-CA-C	-5.29	110.46	116.54
1	A	1129	VAL	O-C-N	-5.29	117.55	123.26
1	C	1024	LEU	CA-C-N	5.29	127.37	120.28
1	C	1024	LEU	C-N-CA	5.29	127.37	120.28
2	D	49	ALA	N-CA-C	-5.29	100.70	108.79
1	C	820	ASP	CA-C-O	5.29	126.34	120.63
2	D	51	ILE	CA-C-N	5.28	131.62	121.54
2	D	51	ILE	C-N-CA	5.28	131.62	121.54
1	A	336	CYS	CA-C-O	-5.28	114.85	120.23
1	A	122	ASN	CA-C-N	5.28	130.05	122.40
1	A	122	ASN	C-N-CA	5.28	130.05	122.40
1	B	1016	ALA	CA-C-N	5.28	127.35	120.28
1	B	1016	ALA	C-N-CA	5.28	127.35	120.28
1	B	851	CYS	N-CA-C	-5.27	101.38	109.76
1	B	1013	ILE	CA-C-N	5.27	127.66	120.54
1	B	1013	ILE	C-N-CA	5.27	127.66	120.54
1	C	488	CYS	O-C-N	5.27	128.93	122.34
2	E	152	HIS	CA-C-N	5.27	133.68	121.87
2	E	152	HIS	C-N-CA	5.27	133.68	121.87
1	A	790	LYS	CA-C-N	5.27	128.69	120.68
1	A	790	LYS	C-N-CA	5.27	128.69	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1096	VAL	CA-C-O	-5.27	115.17	121.28
1	C	183	GLN	OE1-CD-NE2	5.26	127.86	122.60
1	C	226	LEU	O-C-N	5.26	128.56	122.09
2	E	94	TYR	CA-C-N	-5.26	114.20	122.73
2	E	94	TYR	C-N-CA	-5.26	114.20	122.73
1	C	771	ALA	CA-C-N	5.26	127.19	120.56
1	C	771	ALA	C-N-CA	5.26	127.19	120.56
1	A	512	VAL	N-CA-C	-5.26	100.81	108.17
1	A	1078	ALA	CA-C-O	-5.26	114.35	120.03
1	A	1079	PRO	O-C-N	5.26	129.46	122.30
1	B	993	ILE	CA-C-N	5.26	127.33	120.28
1	B	993	ILE	C-N-CA	5.26	127.33	120.28
1	C	570	ALA	CA-C-N	5.26	130.03	122.40
1	C	570	ALA	C-N-CA	5.26	130.03	122.40
1	A	383	SER	CA-C-N	5.26	124.87	119.56
1	A	383	SER	C-N-CA	5.26	124.87	119.56
1	C	1016	ALA	N-CA-CB	5.26	117.85	110.12
1	C	457	ARG	N-CA-C	-5.25	100.47	108.76
1	A	850	ILE	CA-C-O	-5.25	115.04	121.13
1	B	770	ILE	CA-C-N	5.25	127.26	120.44
1	B	770	ILE	C-N-CA	5.25	127.26	120.44
1	C	115	GLN	CA-C-O	-5.25	115.28	121.16
1	A	809	PRO	CA-C-N	5.25	128.29	120.31
1	A	809	PRO	C-N-CA	5.25	128.29	120.31
1	B	415	THR	N-CA-C	-5.25	103.76	110.53
1	B	731	MET	CA-C-N	5.25	128.22	120.82
1	B	731	MET	C-N-CA	5.25	128.22	120.82
1	B	1135	ASN	CA-C-O	5.25	126.24	120.31
2	D	161	TYR	CB-CG-CD2	5.25	128.67	120.80
1	C	314	GLN	CA-C-O	-5.25	114.61	120.54
1	C	369	TYR	N-CA-CB	5.24	117.83	110.12
1	C	966	LEU	CA-C-N	5.24	130.62	122.49
1	C	966	LEU	C-N-CA	5.24	130.62	122.49
2	D	2	VAL	CA-C-O	5.24	127.13	121.36
1	B	927	PHE	CA-C-O	5.24	126.32	120.82
2	E	178	LYS	O-C-N	-5.24	116.55	122.84
1	A	246	ARG	CA-C-O	5.24	126.99	121.33
1	C	870	ILE	CA-C-N	5.24	127.30	120.28
1	C	870	ILE	C-N-CA	5.24	127.30	120.28
2	F	92	ALA	O-C-N	-5.24	118.06	123.29
1	B	226	LEU	N-CA-C	-5.23	106.03	112.72
1	C	729	VAL	O-C-N	5.23	126.01	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	THR	CA-C-N	5.23	131.26	123.05
1	A	73	THR	C-N-CA	5.23	131.26	123.05
1	A	831	ALA	CA-C-O	-5.23	115.44	121.19
1	A	294	ASP	O-C-N	-5.23	118.19	121.85
1	A	751	ASN	CA-C-O	5.22	126.08	120.55
1	B	703	ASN	CA-C-N	5.22	131.58	122.81
1	B	703	ASN	C-N-CA	5.22	131.58	122.81
1	B	283	GLY	CA-C-N	5.22	129.55	122.19
1	B	283	GLY	C-N-CA	5.22	129.55	122.19
2	D	56	SER	CA-C-O	-5.22	115.00	120.32
2	D	99	ASP	O-C-N	-5.22	115.66	120.51
1	B	705	VAL	O-C-N	-5.21	117.82	123.14
1	C	876	ALA	N-CA-C	5.21	116.96	111.28
1	C	148	ASN	N-CA-C	-5.21	101.27	109.50
2	D	31	ARG	N-CA-CB	5.21	117.93	110.06
2	F	141	PHE	CA-CB-CG	5.21	119.01	113.80
1	B	581	THR	CA-C-N	5.20	130.71	122.60
1	B	581	THR	C-N-CA	5.20	130.71	122.60
1	C	249	LEU	N-CA-C	-5.19	106.25	112.59
1	A	235	ILE	CA-C-O	5.19	125.86	120.36
1	A	1104	VAL	O-C-N	-5.19	116.81	122.83
1	A	424	LYS	CA-C-O	-5.19	116.00	119.68
2	F	167	GLU	CA-C-O	-5.19	115.39	121.46
1	C	353	TRP	CA-C-N	5.18	129.32	122.42
1	C	353	TRP	C-N-CA	5.18	129.32	122.42
1	C	437	ASN	CA-C-N	5.18	128.23	120.87
1	C	437	ASN	C-N-CA	5.18	128.23	120.87
1	C	741	TYR	CA-C-N	5.18	127.20	120.88
1	C	741	TYR	C-N-CA	5.18	127.20	120.88
2	F	65	LYS	N-CA-C	-5.18	106.36	113.30
1	B	1039	ARG	O-C-N	-5.18	116.90	123.01
1	A	347	PHE	CA-C-N	5.17	131.42	121.54
1	A	347	PHE	C-N-CA	5.17	131.42	121.54
1	C	523	THR	N-CA-C	-5.17	106.93	114.12
1	C	831	ALA	N-CA-CB	5.17	117.61	109.69
2	D	187	ILE	CA-C-N	5.17	125.45	119.92
2	D	187	ILE	C-N-CA	5.17	125.45	119.92
1	C	88	ASP	CA-C-N	5.17	128.93	121.44
1	C	88	ASP	C-N-CA	5.17	128.93	121.44
1	B	902	MET	N-CA-C	5.17	116.91	111.28
1	A	45	SER	CA-C-N	5.16	130.15	122.82
1	A	45	SER	C-N-CA	5.16	130.15	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	751	ASN	N-CA-C	5.16	116.90	111.28
1	B	151	SER	N-CA-C	-5.16	99.81	110.80
1	A	995	ARG	CA-C-O	-5.16	115.08	120.55
1	A	1062	PHE	CA-C-O	-5.16	115.25	120.71
1	C	170	TYR	N-CA-C	-5.16	100.61	108.76
1	C	989	ALA	CB-CA-C	-5.16	102.23	110.79
1	A	496	GLY	CA-C-N	5.15	131.08	122.73
1	A	496	GLY	C-N-CA	5.15	131.08	122.73
1	A	600	PRO	CA-N-CD	-5.15	104.79	112.00
1	C	1081	ILE	CA-C-O	-5.15	114.98	120.39
1	A	821	LEU	CA-C-N	5.15	127.18	120.28
1	A	821	LEU	C-N-CA	5.15	127.18	120.28
1	A	70	VAL	N-CA-C	-5.15	100.46	108.95
1	C	813	SER	CA-C-O	-5.15	115.09	121.06
1	A	837	TYR	N-CA-C	-5.14	99.22	108.48
1	C	800	PHE	N-CA-C	5.14	118.09	110.48
1	C	985	ASP	N-CA-C	-5.14	103.55	109.93
1	B	330	PRO	CA-C-N	5.14	127.42	120.38
1	B	330	PRO	C-N-CA	5.14	127.42	120.38
1	B	1142	GLN	CA-C-O	-5.14	113.36	118.34
2	D	47	LEU	N-CA-C	-5.13	98.90	107.99
1	B	701	ALA	CA-C-N	5.13	130.86	122.65
1	B	701	ALA	C-N-CA	5.13	130.86	122.65
1	B	376	THR	O-C-N	-5.13	117.10	123.36
1	C	386	LYS	O-C-N	-5.13	115.17	122.15
2	F	128	SER	CA-C-N	5.12	129.05	122.85
2	F	128	SER	C-N-CA	5.12	129.05	122.85
1	B	931	ILE	N-CA-C	-5.12	105.40	110.62
1	B	331	ASN	CA-C-N	-5.12	116.43	123.14
1	B	331	ASN	C-N-CA	-5.12	116.43	123.14
1	C	857	GLY	CA-C-O	5.12	125.96	119.72
1	B	1089	PHE	N-CA-C	-5.12	103.08	110.40
1	A	807	PRO	N-CA-C	5.12	119.39	112.48
2	F	51	ILE	CA-C-N	5.12	129.40	122.19
2	F	51	ILE	C-N-CA	5.12	129.40	122.19
1	B	53	ASP	N-CA-C	-5.11	100.88	107.73
1	B	1060	VAL	CA-C-O	5.11	126.40	120.67
1	C	1046	GLY	N-CA-C	-5.11	104.53	112.45
1	C	652	GLY	CA-C-N	-5.11	112.28	121.62
1	C	652	GLY	C-N-CA	-5.11	112.28	121.62
2	E	160	ILE	CA-C-O	5.10	126.64	120.67
1	A	137	ASN	CA-C-N	5.10	129.97	122.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	ASN	C-N-CA	5.10	129.97	122.98
1	A	787	GLN	CA-C-N	-5.10	116.00	122.37
1	A	787	GLN	C-N-CA	-5.10	116.00	122.37
1	B	913	GLN	N-CA-C	5.10	117.57	111.71
1	A	686	SER	N-CA-C	-5.10	100.99	108.99
1	B	73	THR	CA-C-N	5.10	131.27	121.54
1	B	73	THR	C-N-CA	5.10	131.27	121.54
1	B	98	SER	O-C-N	5.09	128.92	122.04
1	A	396	TYR	N-CA-C	-5.09	101.39	109.59
1	A	938	LEU	N-CA-C	5.09	117.73	111.82
1	B	576	VAL	O-C-N	-5.09	117.27	123.02
2	E	191	SER	CA-C-O	-5.09	114.11	119.50
1	C	752	LEU	CA-C-N	5.08	127.51	120.29
1	C	752	LEU	C-N-CA	5.08	127.51	120.29
1	A	589	PRO	O-C-N	-5.08	116.44	122.89
1	C	124	THR	CA-C-N	5.08	128.07	120.90
1	C	124	THR	C-N-CA	5.08	128.07	120.90
2	D	40	ALA	O-C-N	5.08	127.16	121.32
1	A	626	ALA	O-C-N	-5.08	117.93	123.26
1	A	798	GLY	N-CA-C	-5.08	101.14	113.18
1	A	1137	VAL	N-CA-C	-5.08	101.06	108.17
1	B	241	LEU	N-CA-C	-5.08	100.89	108.96
1	B	321	GLN	N-CA-C	-5.08	103.28	110.29
1	B	680	SER	CA-C-O	-5.08	113.20	120.16
1	A	714	ILE	CA-C-N	5.08	124.99	119.76
1	A	714	ILE	C-N-CA	5.08	124.99	119.76
1	B	134	GLN	CA-C-N	5.08	131.38	121.63
1	B	134	GLN	C-N-CA	5.08	131.38	121.63
1	B	648	GLY	CA-C-N	-5.08	115.83	122.99
1	B	648	GLY	C-N-CA	-5.08	115.83	122.99
1	B	862	PRO	N-CA-C	-5.07	105.15	110.58
1	B	347	PHE	N-CA-C	-5.07	101.43	109.59
1	C	153	MET	N-CA-C	-5.07	106.69	112.92
2	F	145	ASP	CA-C-N	5.07	127.49	120.29
2	F	145	ASP	C-N-CA	5.07	127.49	120.29
1	B	657	ASN	CA-C-N	5.07	128.06	120.87
1	B	657	ASN	C-N-CA	5.07	128.06	120.87
1	B	1101	HIS	O-C-N	-5.06	116.88	122.86
1	B	517	LEU	O-C-N	-5.06	116.43	123.01
1	B	862	PRO	CA-N-CD	-5.06	104.91	112.00
2	D	132	GLY	CA-C-N	-5.06	115.52	121.90
2	D	132	GLY	C-N-CA	-5.06	115.52	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	737	ASP	N-CA-C	-5.06	100.92	108.96
1	B	595	VAL	N-CA-C	-5.06	101.03	108.11
2	D	106	GLY	N-CA-C	-5.06	108.46	114.48
2	D	186	PRO	CA-C-N	5.06	131.49	122.13
2	D	186	PRO	C-N-CA	5.06	131.49	122.13
1	C	852	ALA	CA-C-N	5.05	131.20	121.54
1	C	852	ALA	C-N-CA	5.05	131.20	121.54
2	F	75	ALA	N-CA-C	-5.05	99.38	108.48
1	C	835	LYS	N-CA-C	-5.05	102.98	110.46
2	F	130	SER	CA-C-O	-5.05	115.55	121.46
1	A	961	THR	CA-C-N	5.05	127.36	120.54
1	A	961	THR	C-N-CA	5.05	127.36	120.54
1	B	554	GLU	CA-C-O	-5.05	115.51	121.16
1	C	934	ILE	O-C-N	5.05	126.86	121.91
1	C	506	GLN	CA-C-N	5.05	124.95	119.85
1	C	506	GLN	C-N-CA	5.05	124.95	119.85
1	A	66	HIS	N-CA-C	-5.04	101.70	109.52
1	B	613	GLN	CA-C-O	5.04	126.44	120.69
1	B	1049	LEU	N-CA-C	-5.04	106.23	112.93
2	E	6	GLU	O-C-N	-5.04	116.60	123.15
1	A	220	PHE	N-CA-C	-5.04	102.24	110.20
1	C	923	ILE	N-CA-C	5.04	115.26	110.42
1	A	715	PRO	CA-C-N	5.04	130.15	122.24
1	A	715	PRO	C-N-CA	5.04	130.15	122.24
1	B	868	GLU	CA-C-N	5.04	127.45	120.29
1	B	868	GLU	C-N-CA	5.04	127.45	120.29
1	B	551	VAL	O-C-N	5.04	128.99	123.10
2	F	179	LEU	CA-C-N	5.04	128.85	120.94
2	F	179	LEU	C-N-CA	5.04	128.85	120.94
1	A	622	VAL	N-CA-C	-5.03	105.49	110.62
1	A	870	ILE	CA-C-N	5.03	127.03	120.28
1	A	870	ILE	C-N-CA	5.03	127.03	120.28
1	A	61	ASN	CA-C-N	-5.03	116.95	123.19
1	A	61	ASN	C-N-CA	-5.03	116.95	123.19
1	A	887	THR	CA-C-O	5.03	125.76	120.33
1	C	470	THR	N-CA-C	-5.03	107.31	113.50
1	C	607	GLN	N-CA-C	-5.03	101.67	109.72
1	C	1016	ALA	CB-CA-C	-5.03	102.44	110.79
1	B	341	VAL	N-CA-C	-5.03	107.93	112.96
1	B	273	ARG	N-CA-C	-5.03	101.44	109.23
1	C	418	ILE	O-C-N	5.03	127.95	122.12
2	D	123	GLY	CA-C-N	5.03	129.33	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	123	GLY	C-N-CA	5.03	129.33	122.34
2	D	164	ASP	CA-C-N	5.03	130.27	121.52
2	D	164	ASP	C-N-CA	5.03	130.27	121.52
1	A	151	SER	N-CA-C	-5.03	100.09	110.80
1	B	425	LEU	CA-C-O	-5.03	115.39	121.22
2	D	133	ALA	CA-C-N	5.02	130.44	122.10
2	D	133	ALA	C-N-CA	5.02	130.44	122.10
1	C	565	PHE	CA-C-O	5.02	125.67	120.30
1	B	76	THR	CA-C-N	5.02	131.13	121.54
1	B	76	THR	C-N-CA	5.02	131.13	121.54
1	B	917	TYR	CA-C-N	5.02	127.01	120.28
1	B	917	TYR	C-N-CA	5.02	127.01	120.28
1	C	673	SER	CA-C-O	-5.02	115.24	121.06
1	B	204	TYR	N-CA-C	-5.02	101.92	109.85
1	B	350	VAL	CA-C-O	-5.01	115.20	120.57
1	B	393	THR	CA-C-O	-5.01	115.53	120.70
1	B	1036	GLN	CA-C-N	5.01	127.99	120.87
1	B	1036	GLN	C-N-CA	5.01	127.99	120.87
1	B	107	GLY	CA-C-O	-5.01	117.08	121.04
1	C	184	GLY	N-CA-C	5.01	119.81	113.24
1	A	1095	PHE	O-C-N	-5.01	117.51	123.22
1	B	674	TYR	N-CA-CB	5.01	118.85	110.59
1	B	1005	GLN	N-CA-C	5.01	116.74	111.28
1	C	753	LEU	CA-C-N	5.01	128.61	120.60
1	C	753	LEU	C-N-CA	5.01	128.61	120.60
1	B	376	THR	N-CA-C	-5.00	99.83	108.69
1	C	146	HIS	CB-CG-ND1	5.00	130.21	122.70
1	A	432	CYS	N-CA-CB	5.00	120.48	111.37
1	B	894	LEU	CA-C-O	5.00	126.35	120.80
1	C	539	VAL	N-CA-C	-5.00	101.40	108.65

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	400	PHE	Sidechain
1	A	565	PHE	Sidechain
1	A	695	TYR	Sidechain
1	B	1075	PHE	Sidechain
1	B	695	TYR	Sidechain
1	C	369	TYR	Sidechain
1	C	476	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	C	59	PHE	Sidechain
2	D	29	PHE	Sidechain
2	D	80	TYR	Sidechain
2	F	94	TYR	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	8728	8509	8506	31	0
1	B	8728	8509	8506	22	0
1	C	8728	8509	8506	28	0
2	D	1468	1438	1438	12	0
2	E	1468	1438	1438	10	0
2	F	1468	1438	1438	2	0
All	All	30588	29841	29832	98	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (98) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:VAL:N	1:A:621:PRO:CD	2.54	0.71
1:C:350:VAL:HG22	1:C:350:VAL:O	1.96	0.64
2:F:134:SER:OG	2:F:135:GLY:N	2.31	0.63
2:E:116:THR:OG1	2:E:119:SER:OG	2.16	0.62
1:C:41:LYS:NZ	1:C:228:ASP:OD2	2.34	0.60
1:A:682:ARG:O	1:A:682:ARG:HG2	2.03	0.59
1:A:878:LEU:C	1:A:878:LEU:HD23	2.28	0.59
1:A:469:SER:OG	1:A:470:THR:N	2.31	0.59
2:E:31:ARG:O	2:E:32:ASN:C	2.47	0.58
1:B:141:LEU:C	1:B:141:LEU:HD12	2.29	0.57
1:B:981:LEU:C	1:B:981:LEU:HD23	2.30	0.57
1:A:176:LEU:O	1:A:176:LEU:HG	2.05	0.56
2:E:173:ARG:N	2:F:166:THR:OG1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:LYS:NZ	2:D:90:ASP:OD1	2.38	0.55
1:C:442:ASP:OD2	2:E:150:LYS:NZ	2.37	0.55
1:B:627:ASP:OD1	1:B:627:ASP:C	2.49	0.54
1:A:916:LEU:HD13	1:A:916:LEU:C	2.33	0.54
1:C:975:SER:O	1:C:1000:ARG:NH2	2.41	0.54
1:C:197:ILE:O	1:C:197:ILE:HG23	2.07	0.53
2:D:2:VAL:O	2:D:3:GLN:CB	2.56	0.53
1:C:678:THR:O	1:C:679:ASN:HB2	2.09	0.53
1:B:73:THR:C	1:B:75:GLY:H	2.15	0.53
1:A:443:SER:OG	1:A:444:LYS:N	2.41	0.53
1:A:620:VAL:H	1:A:621:PRO:CD	2.22	0.52
2:D:52:THR:OG1	2:D:53:ARG:N	2.40	0.52
1:A:349:SER:OG	1:A:350:VAL:N	2.39	0.52
1:C:568:ASP:N	1:C:572:THR:O	2.42	0.52
1:A:620:VAL:H	1:A:621:PRO:HD3	1.75	0.52
1:B:425:LEU:C	1:B:425:LEU:HD23	2.36	0.51
1:A:43:PHE:CD1	1:A:43:PHE:C	2.86	0.51
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.42	0.51
2:E:62:ASP:OD1	2:E:65:LYS:NZ	2.36	0.50
1:B:233:ILE:O	1:C:457:ARG:NH1	2.44	0.50
1:A:678:THR:O	1:A:679:ASN:HB2	2.13	0.49
1:C:141:LEU:HD23	1:C:141:LEU:H	1.77	0.48
1:A:557:LYS:NZ	1:A:574:ASP:OD1	2.46	0.48
2:D:2:VAL:O	2:D:3:GLN:HB3	2.12	0.48
1:C:141:LEU:HD23	1:C:141:LEU:N	2.28	0.48
2:E:119:SER:OG	2:E:120:GLY:N	2.46	0.48
1:C:690:GLN:O	1:C:691:SER:CB	2.61	0.47
1:C:678:THR:O	1:C:679:ASN:CB	2.61	0.47
2:D:160:ILE:HB	2:D:169:PHE:CZ	2.48	0.47
1:A:678:THR:O	1:A:679:ASN:CB	2.63	0.47
1:A:620:VAL:N	1:A:621:PRO:HD2	2.28	0.47
1:A:43:PHE:C	1:A:43:PHE:HD1	2.23	0.46
2:E:64:VAL:HG13	2:E:64:VAL:O	2.13	0.46
1:A:898:PHE:N	1:A:899:PRO:CD	2.77	0.46
1:A:464:PHE:O	1:A:464:PHE:CD2	2.69	0.46
1:B:425:LEU:O	1:B:425:LEU:CD2	2.64	0.46
1:A:454:ARG:NH1	1:A:465:GLU:OE1	2.49	0.46
1:B:453:TYR:O	1:B:493:GLN:N	2.47	0.45
1:A:223:LEU:HD12	1:A:223:LEU:N	2.31	0.45
1:B:327:VAL:N	1:B:531:THR:OG1	2.49	0.45
1:A:444:LYS:NZ	2:D:146:ASP:OD1	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:PHE:HB3	1:A:899:PRO:HD3	1.99	0.44
1:A:592:PHE:CD1	1:A:592:PHE:C	2.95	0.44
1:C:391:CYS:HA	1:C:524:VAL:O	2.18	0.44
1:A:55:PHE:HB2	1:A:275:PHE:CE1	2.52	0.44
1:C:31:SER:OG	1:C:57:PRO:O	2.34	0.44
1:C:451:TYR:C	1:C:451:TYR:CD1	2.96	0.44
1:A:176:LEU:C	1:A:178:ASP:H	2.24	0.44
1:A:533:LEU:C	1:A:533:LEU:HD23	2.43	0.43
1:C:452:LEU:HD23	1:C:452:LEU:N	2.32	0.43
1:B:1028:LYS:O	1:B:1032:CYS:N	2.50	0.43
2:E:73:ASP:OD1	2:E:74:ASN:N	2.51	0.43
1:B:835:LYS:NZ	1:C:614:ASP:OD2	2.51	0.43
1:A:440:ASN:O	1:A:441:LEU:HB2	2.18	0.43
1:A:680:SER:HB3	1:A:681:PRO:CD	2.48	0.43
1:C:223:LEU:HD12	1:C:223:LEU:N	2.34	0.42
1:B:630:THR:OG1	1:B:631:PRO:HD2	2.19	0.42
1:B:896:ILE:O	1:B:896:ILE:HG23	2.18	0.42
1:C:598:ILE:N	1:C:598:ILE:HD12	2.34	0.42
2:D:117:VAL:HG12	2:D:117:VAL:O	2.19	0.42
1:C:887:THR:O	1:C:887:THR:HG22	2.17	0.42
2:E:4:LEU:H	2:E:110:GLY:CA	2.33	0.42
1:C:77:LYS:O	1:C:245:HIS:ND1	2.52	0.42
1:B:785:VAL:O	1:B:785:VAL:HG13	2.19	0.42
1:B:620:VAL:N	1:B:621:PRO:CD	2.83	0.42
1:B:73:THR:C	1:B:75:GLY:N	2.78	0.42
2:D:130:SER:O	2:D:131:ASP:CB	2.67	0.41
1:A:149:ASN:C	1:A:151:SER:H	2.27	0.41
1:A:234:ASN:ND2	1:B:468:ILE:H	2.18	0.41
1:C:440:ASN:O	1:C:441:LEU:HB2	2.20	0.41
1:B:258:TRP:C	1:B:258:TRP:CD1	2.98	0.41
1:C:76:THR:O	1:C:77:LYS:HB2	2.20	0.41
2:D:49:ALA:CB	2:D:68:PHE:H	2.33	0.41
1:B:1130:ILE:HD12	1:B:1130:ILE:N	2.35	0.41
1:C:162:SER:OG	1:C:163:ALA:N	2.49	0.41
1:A:620:VAL:N	1:A:621:PRO:HD3	2.32	0.41
1:B:494:SER:O	2:D:31:ARG:HA	2.21	0.41
1:B:177:MET:HE2	1:B:177:MET:HA	2.03	0.41
1:B:347:PHE:CD2	1:B:399:SER:HB2	2.56	0.41
1:C:280:ASN:OD1	1:C:280:ASN:C	2.64	0.41
2:E:146:ASP:OD1	2:E:146:ASP:O	2.38	0.40
1:C:726:ILE:N	1:C:726:ILE:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:941:THR:C	1:C:943:SER:H	2.29	0.40
2:D:64:VAL:O	2:D:64:VAL:HG12	2.21	0.40
2:D:137:ARG:O	2:D:139:THR:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1118/1120 (100%)	1029 (92%)	79 (7%)	10 (1%)	14	49
1	B	1118/1120 (100%)	1042 (93%)	61 (6%)	15 (1%)	9	41
1	C	1118/1120 (100%)	1043 (93%)	63 (6%)	12 (1%)	11	45
2	D	195/197 (99%)	162 (83%)	28 (14%)	5 (3%)	4	26
2	E	195/197 (99%)	180 (92%)	13 (7%)	2 (1%)	12	47
2	F	195/197 (99%)	180 (92%)	12 (6%)	3 (2%)	8	38
All	All	3939/3951 (100%)	3636 (92%)	256 (6%)	47 (1%)	13	42

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	SER
1	A	662	CYS
1	B	691	SER
1	C	180	GLU
2	D	3	GLN
2	D	40	ALA
2	D	131	ASP
2	D	138	VAL
1	A	349	SER

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Mol	Chain	Res	Type
1	A	414	GLN
1	C	691	SER
1	A	374	PHE
1	A	441	LEU
1	A	679	ASN
1	B	180	GLU
1	B	529	LYS
1	B	680	SER
1	C	173	GLN
1	C	446	GLY
1	C	662	CYS
1	C	680	SER
2	E	53	ARG
2	F	134	SER
1	A	373	SER
1	A	443	SER
1	A	680	SER
1	B	32	PHE
1	B	149	ASN
1	B	173	GLN
1	B	460	ASN
1	B	631	PRO
1	B	813	SER
1	B	1084	ASP
1	C	176	LEU
1	C	441	LEU
1	C	481	ASN
1	C	679	ASN
2	D	108	TYR
2	E	33	ALA
2	F	54	ARG
2	F	3	GLN
1	B	679	ASN
1	C	520	ALA
1	C	986	PRO
1	B	482	GLY
1	B	520	ALA
1	B	412	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	972/972 (100%)	972 (100%)	0	100	100
1	B	972/972 (100%)	971 (100%)	1 (0%)	88	88
1	C	972/972 (100%)	970 (100%)	2 (0%)	87	85
2	D	152/152 (100%)	152 (100%)	0	100	100
2	E	152/152 (100%)	152 (100%)	0	100	100
2	F	152/152 (100%)	152 (100%)	0	100	100
All	All	3372/3372 (100%)	3369 (100%)	3 (0%)	87	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	986	PRO
1	C	451	TYR
1	C	1067	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	99	ASN
1	A	115	GLN
1	A	218	GLN
1	A	234	ASN
1	A	414	GLN
1	A	506	GLN
1	A	641	ASN
1	A	913	GLN
1	A	1005	GLN
1	B	52	GLN
1	B	69	HIS
1	B	183	GLN
1	B	239	GLN

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Mol	Chain	Res	Type
1	B	625	HIS
1	B	755	GLN
1	B	872	GLN
1	B	1002	GLN
1	B	1011	GLN
1	B	1074	ASN
1	C	115	GLN
1	C	183	GLN
1	C	580	GLN
1	C	613	GLN
1	C	804	GLN
1	C	853	GLN
1	C	913	GLN
1	C	935	GLN
1	C	955	ASN
1	C	1011	GLN
1	C	1134	ASN
2	D	3	GLN
2	D	13	GLN
2	F	1	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

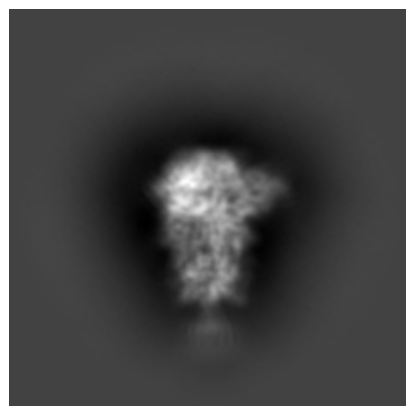
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36904. These allow visual inspection of the internal detail of the map and identification of artifacts.

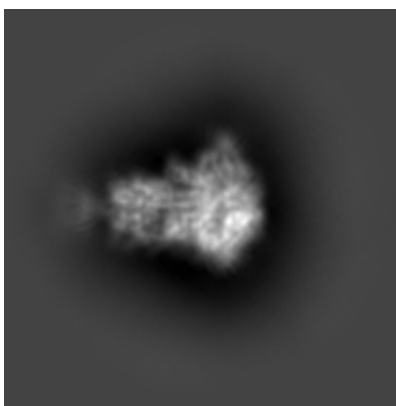
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

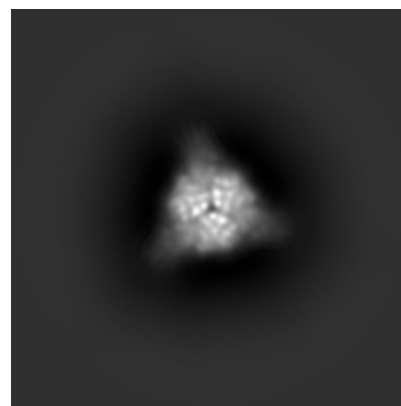
6.1.1 Primary map



X

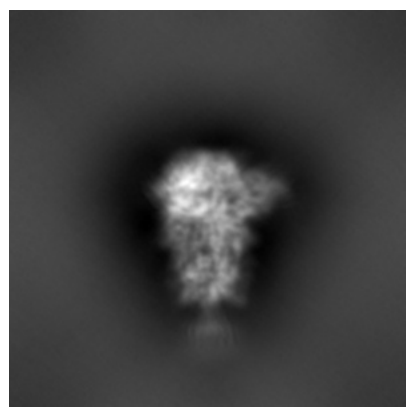


Y

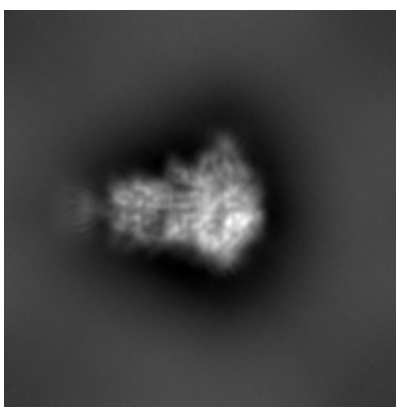


Z

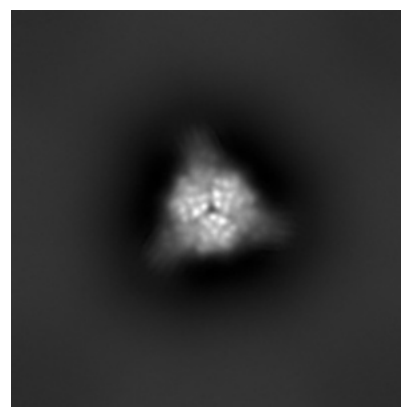
6.1.2 Raw map



X



Y

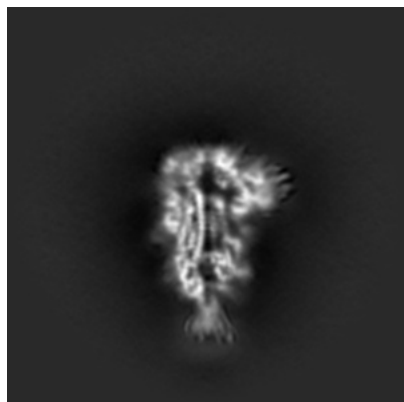


Z

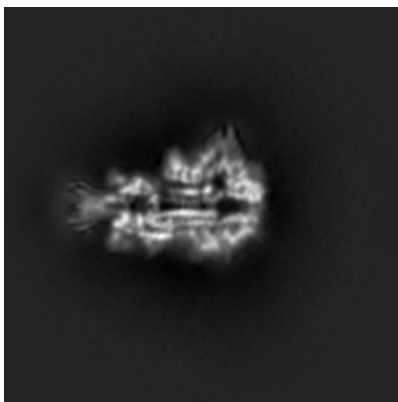
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

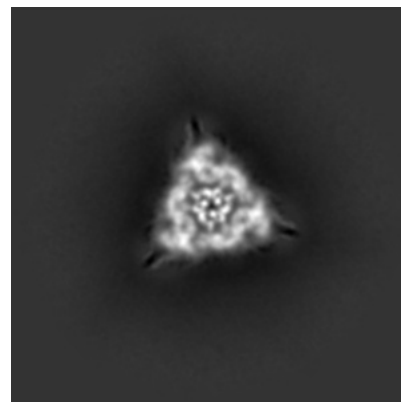
6.2.1 Primary map



X Index: 128

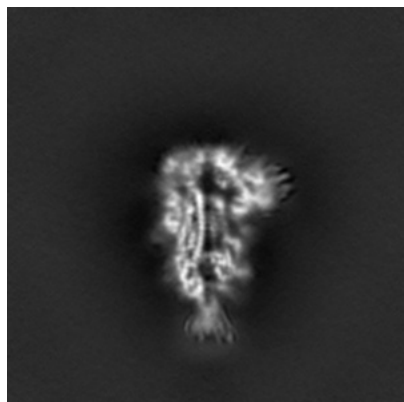


Y Index: 128

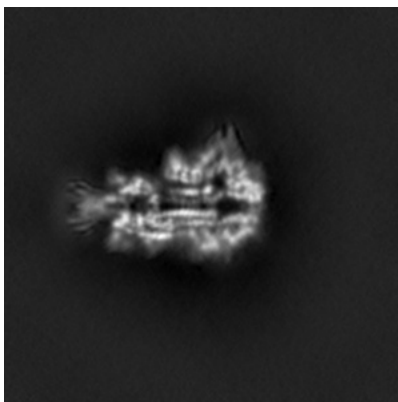


Z Index: 128

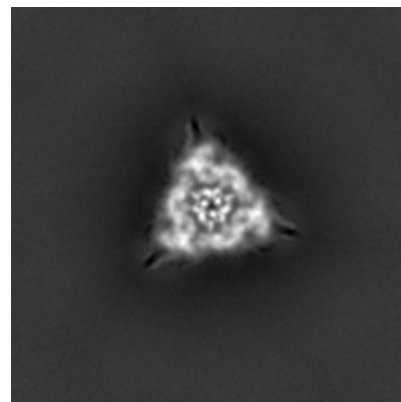
6.2.2 Raw map



X Index: 128



Y Index: 128

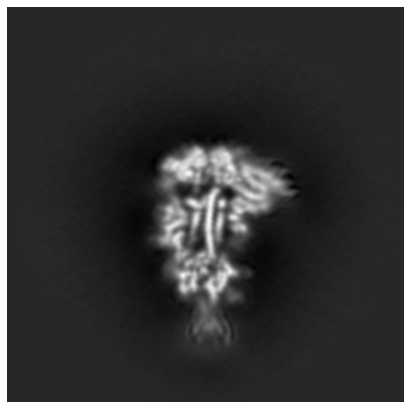


Z Index: 128

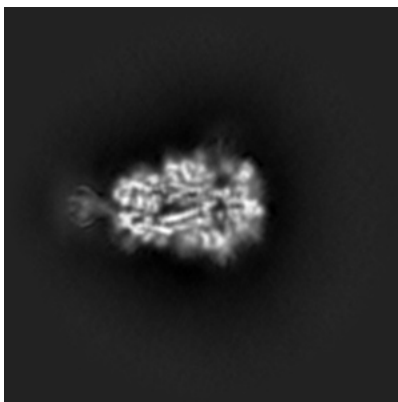
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

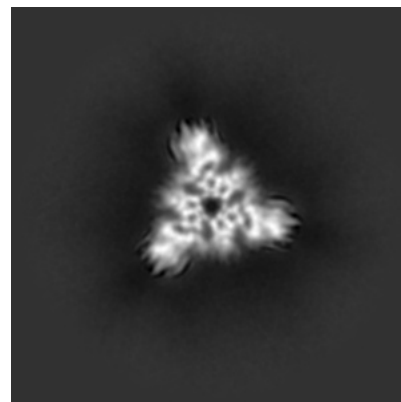
6.3.1 Primary map



X Index: 123

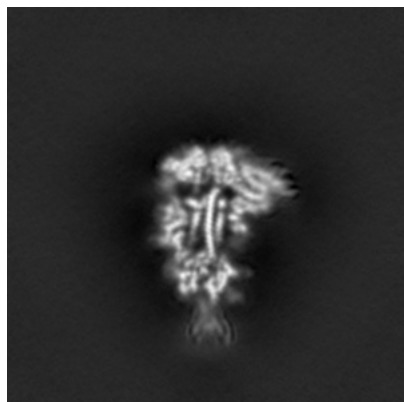


Y Index: 135

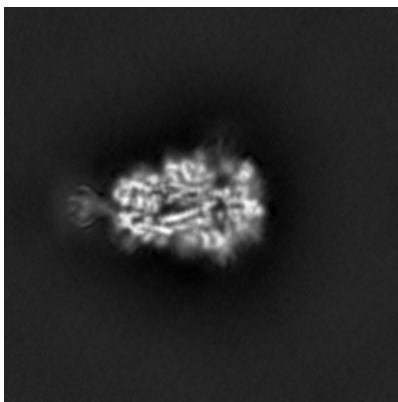


Z Index: 143

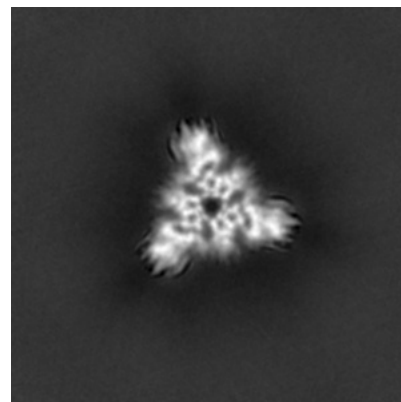
6.3.2 Raw map



X Index: 123



Y Index: 135

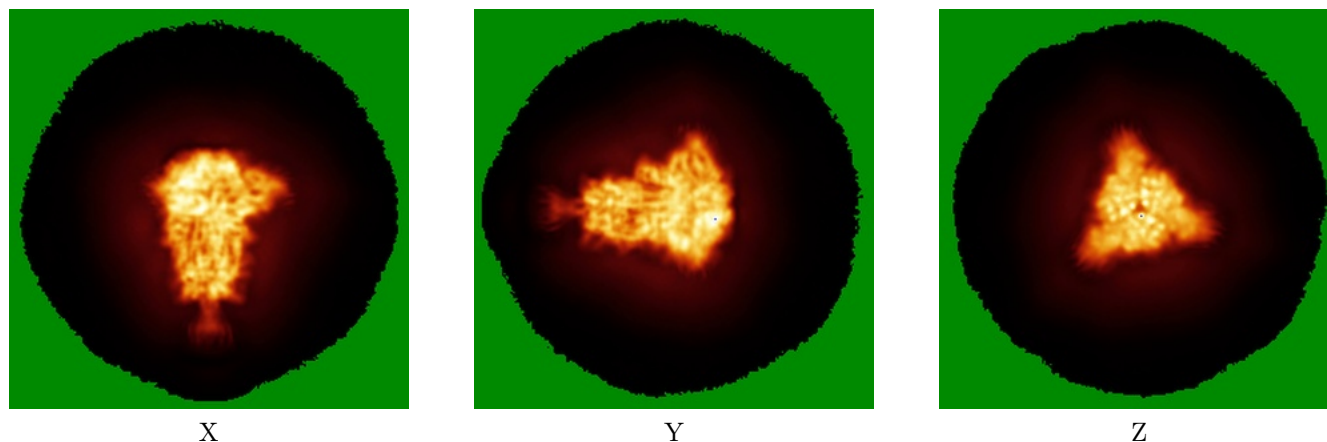


Z Index: 143

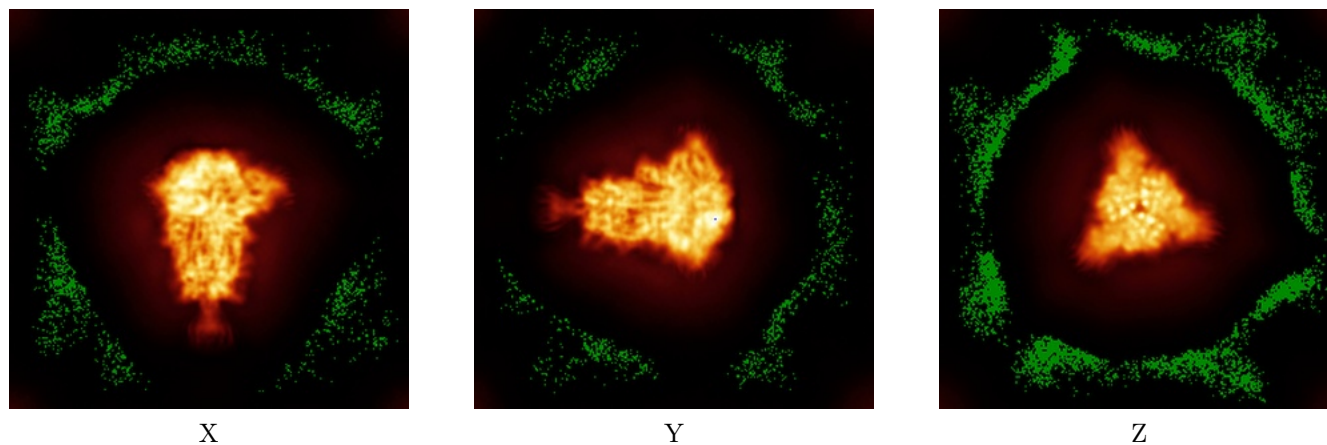
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

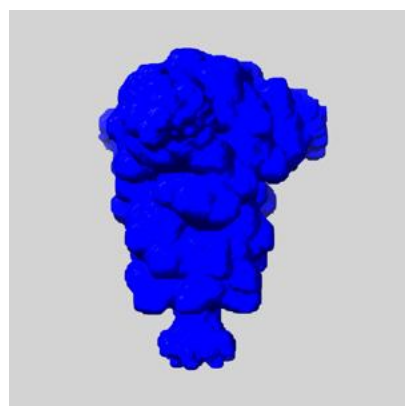
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

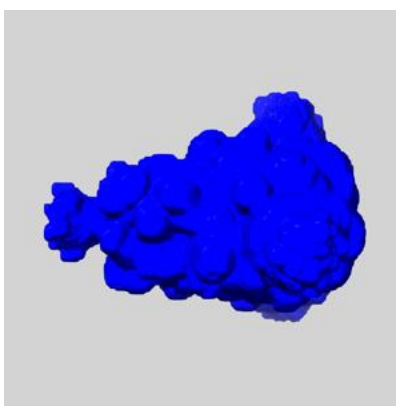
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

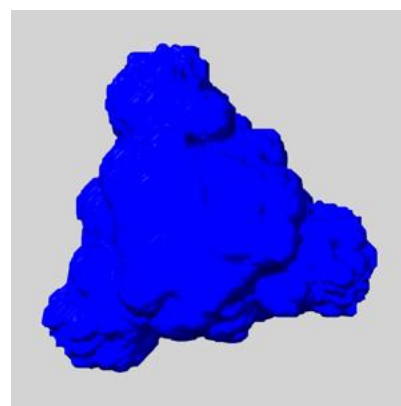
6.6.1 emd_36904_msk_1.map [i](#)



X



Y

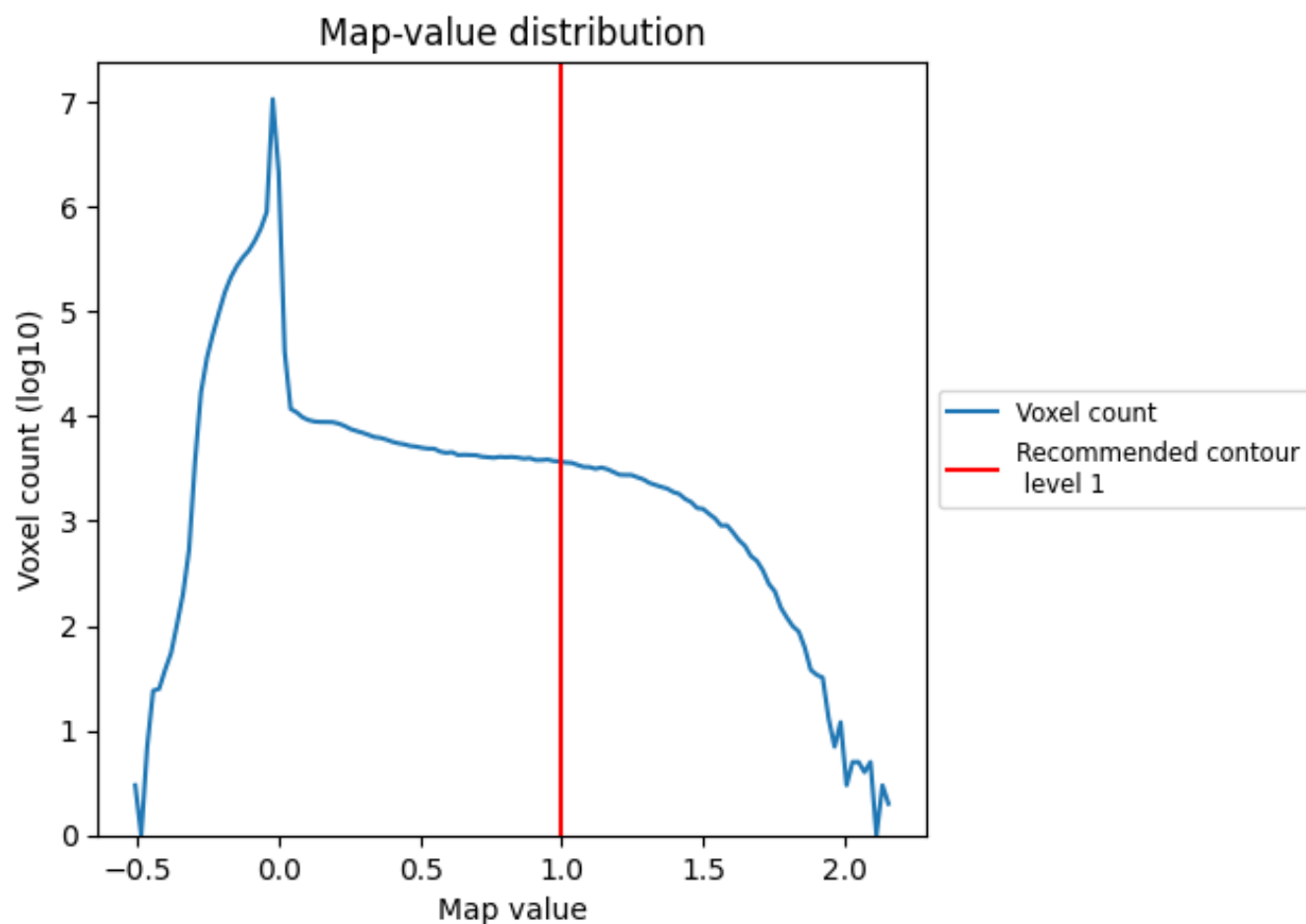


Z

7 Map analysis [i](#)

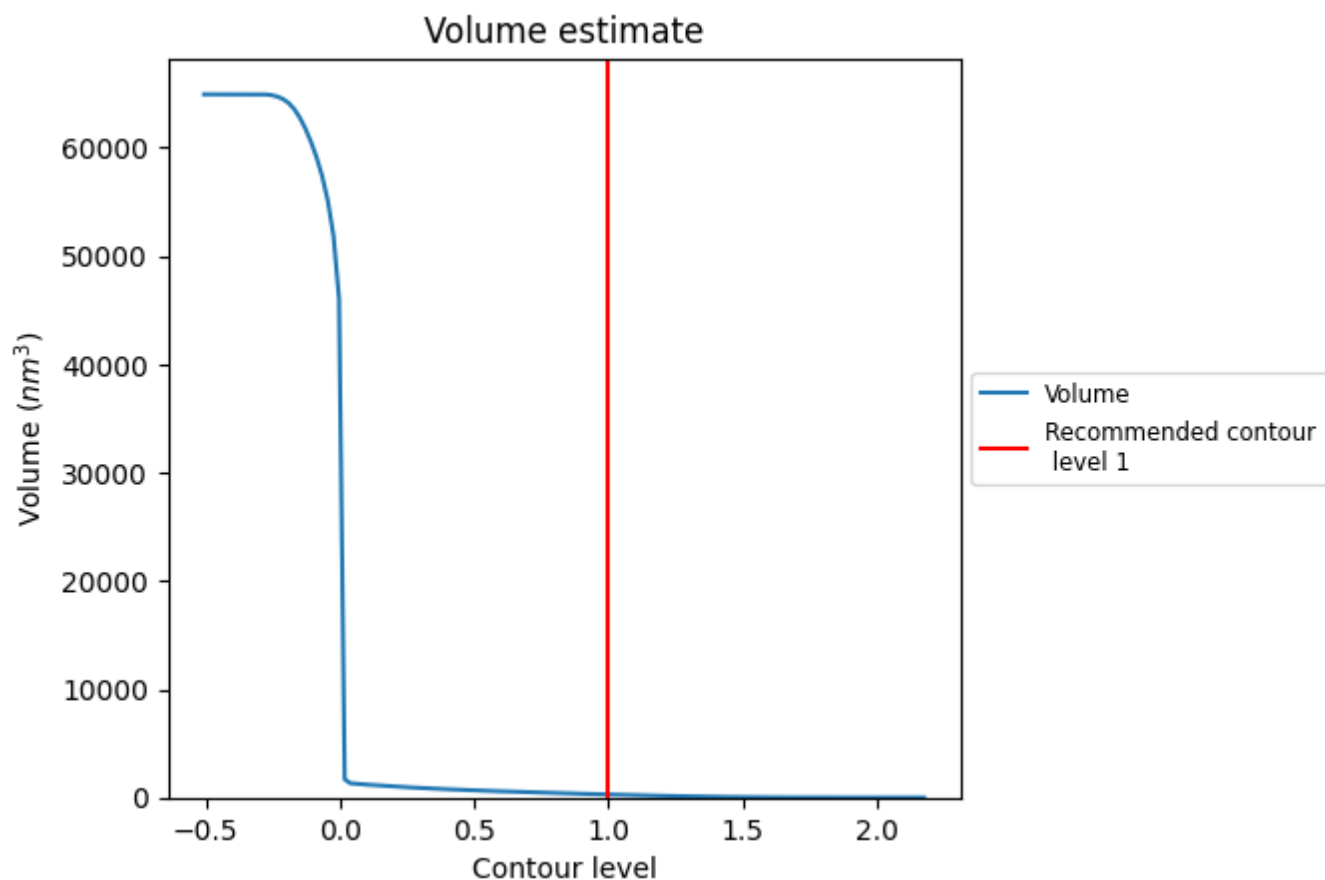
This section contains the results of statistical analysis of the map.

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.

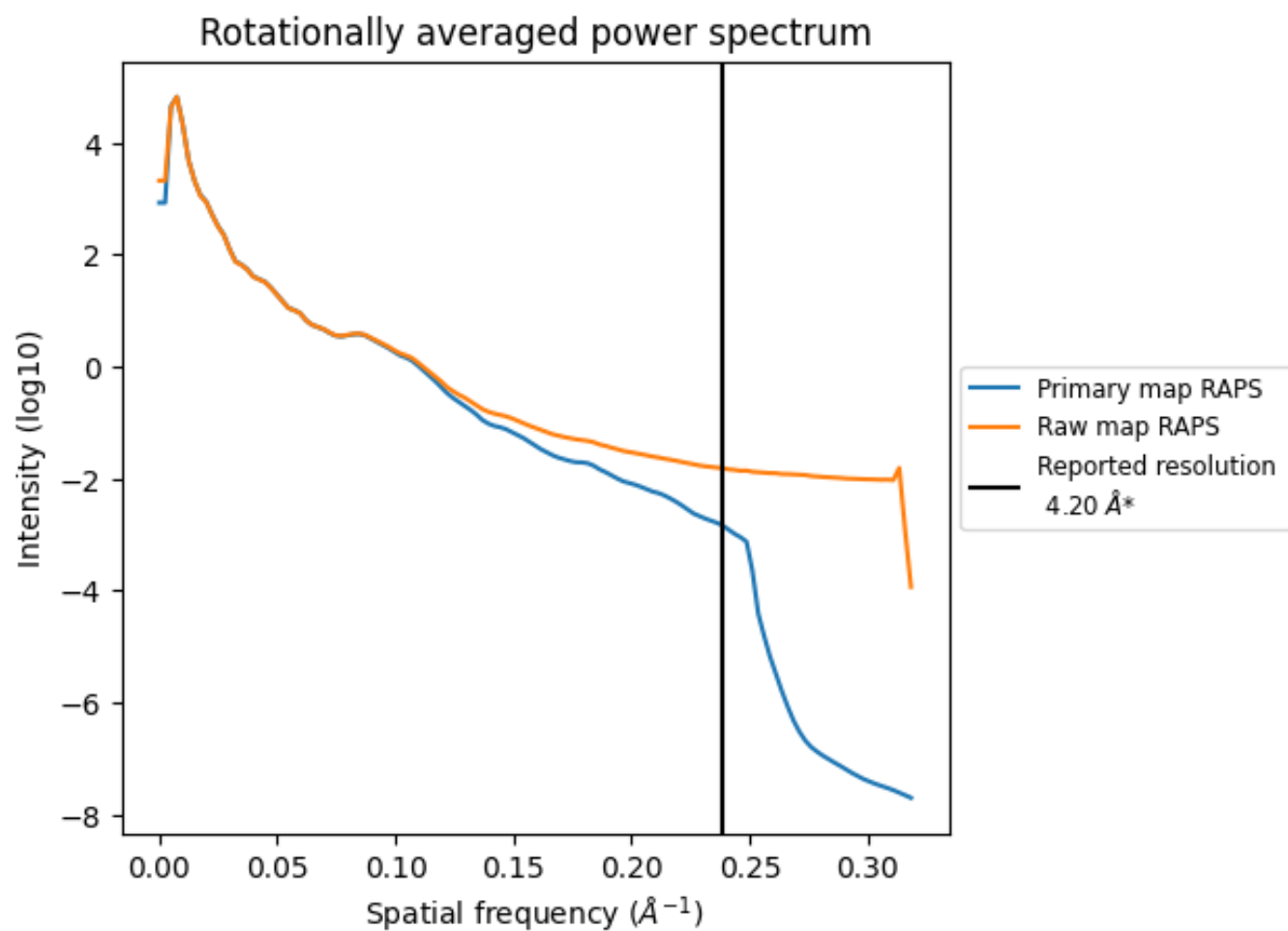
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 279 nm³; this corresponds to an approximate mass of 252 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

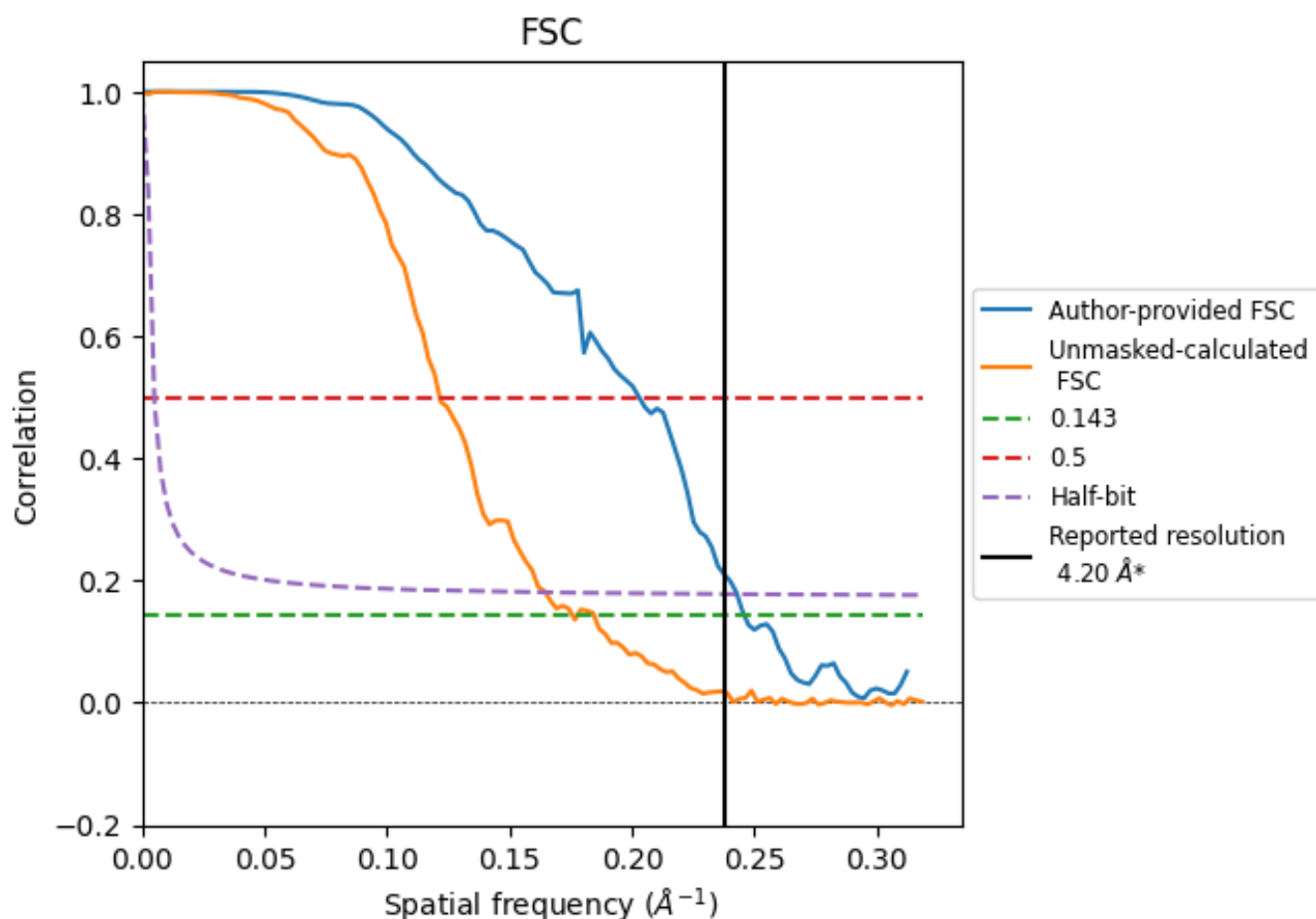


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

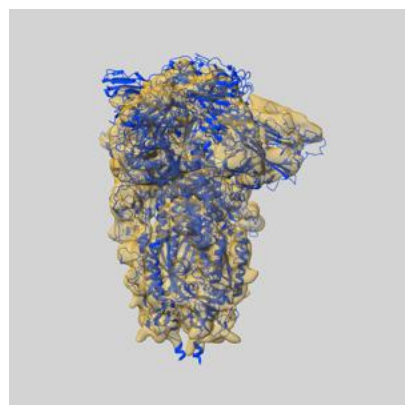
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.07	4.93	4.12
Unmasked-calculated*	5.69	8.23	6.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.69 differs from the reported value 4.2 by more than 10 %

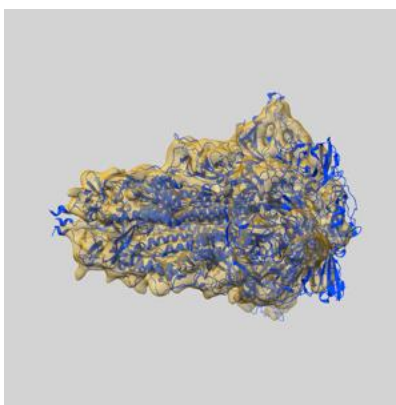
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36904 and PDB model 8W4F. Per-residue inclusion information can be found in section [3](#) on page [6](#).

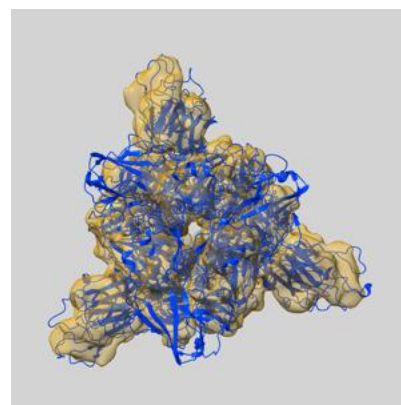
9.1 Map-model overlay [i](#)



X



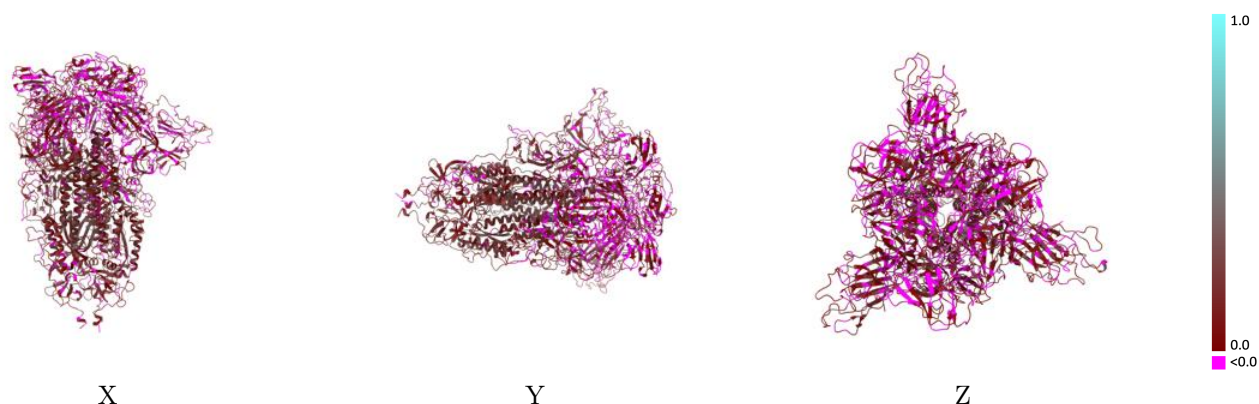
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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](#)

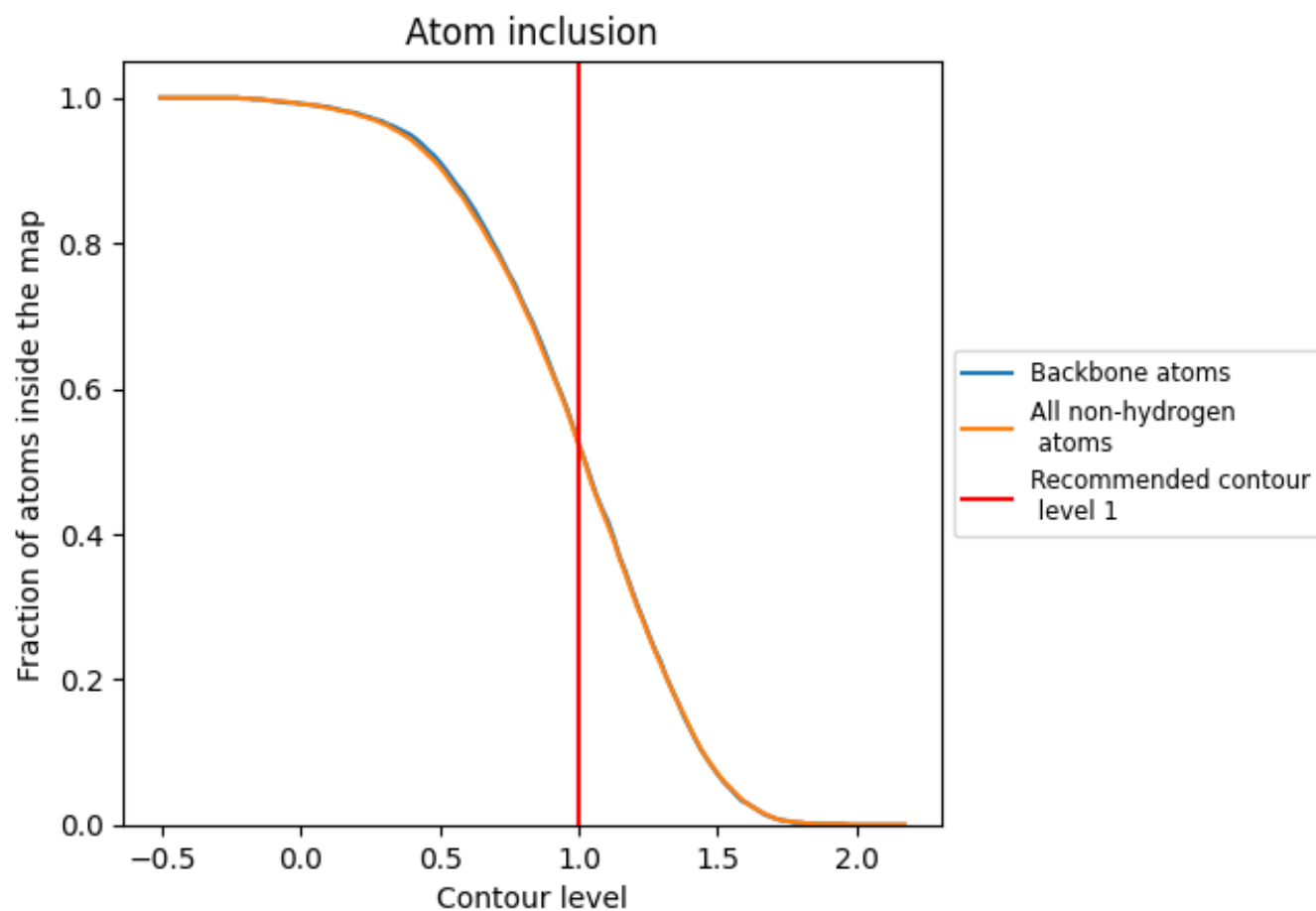


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5230	0.0930
A	0.5630	0.1030
B	0.5780	0.1200
C	0.5290	0.0870
D	0.3400	0.0320
E	0.2870	0.0230
F	0.2980	0.0340

1.0
0.0
-0.0