



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:07 PM UTC

PDB ID : 5Y60 / pdb_00005y60
EMDB ID : EMD-6813
Title : V/A-type ATPase/synthase from *Thermus thermophilus*, rotational state 3.
Authors : Nakanishi, A.; Kishikawa, J.; Tamakoshi, M.; Mitsuoka, K.; Yokoyama, K.
Deposited on : 2017-08-10
Resolution : 7.50 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

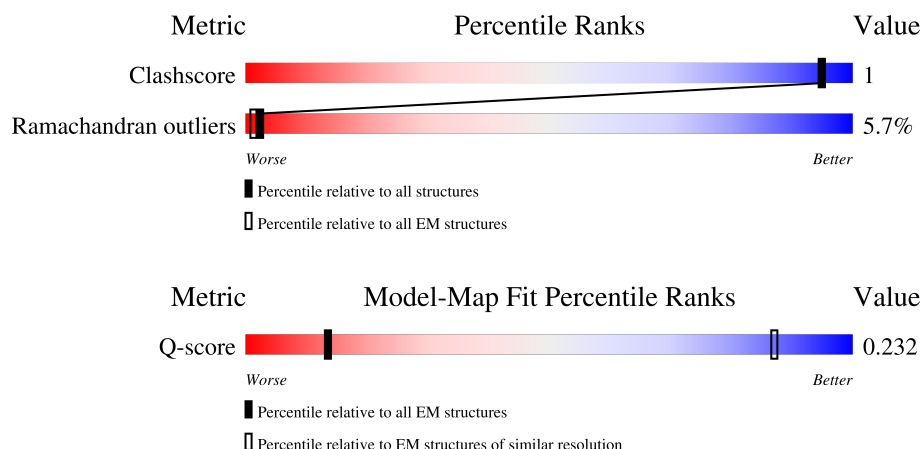
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 7.50 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.



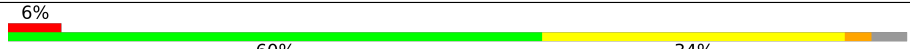
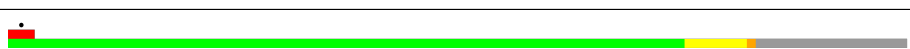
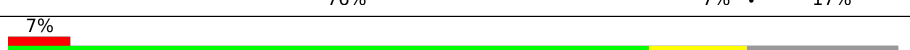
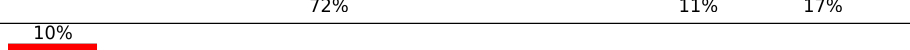
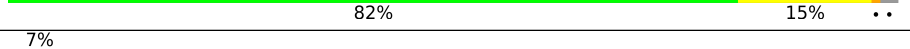
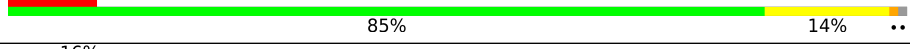
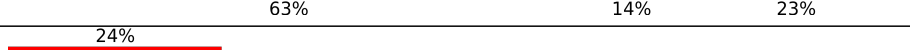
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	436 (7.00 - 8.00)

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	578	
1	B	578	
1	C	578	
2	D	478	
2	E	478	

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Mol	Chain	Length	Quality of chain
2	F	478	
3	G	223	
4	H	104	
5	I	120	
5	K	120	
6	J	188	
6	L	188	
7	M	323	
8	N	652	
9	O	99	
9	P	99	
9	Q	99	
9	R	99	
9	S	99	
9	T	99	
9	U	99	
9	V	99	
9	W	99	
9	X	99	
9	Y	99	
9	Z	99	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 23433 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	577	Total	C	N	O	0	0
			2307	1154	577	576		
1	B	577	Total	C	N	O	0	0
			2307	1154	577	576		
1	C	577	Total	C	N	O	0	0
			2307	1154	577	576		

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	459	Total	C	N	O	0	0
			1835	918	459	458		
2	E	459	Total	C	N	O	0	0
			1835	918	459	458		
2	F	459	Total	C	N	O	0	0
			1835	918	459	458		

- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	210	Total	C	N	O	0	0
			839	420	210	209		

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	100	Total	C	N	O	0	0
			399	200	100	99		

- Molecule 5 is a protein called V-type ATP synthase, subunit (VAPC-THERM).

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	100	Total	C	N	O	0	0
			399	200	100	99		
5	K	100	Total	C	N	O	0	0
			399	200	100	99		

- Molecule 6 is a protein called V-type ATP synthase subunit E.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	J	185	Total	C	N	O	0	0
			738	370	185	183		
6	L	185	Total	C	N	O	0	0
			738	370	185	183		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	134	MET	LEU	conflict	UNP P74901
J	171	MET	LEU	conflict	UNP P74901
J	178	MET	LEU	conflict	UNP P74901
L	134	MET	LEU	conflict	UNP P74901
L	171	MET	LEU	conflict	UNP P74901
L	178	MET	LEU	conflict	UNP P74901

- Molecule 7 is a protein called V-type ATP synthase subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	320	Total	C	N	O	0	0
			1279	640	320	319		

- Molecule 8 is a protein called V-type ATP synthase subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	N	632	Total	C	N	O	0	0
			2526	1264	632	630		

- Molecule 9 is a protein called V-type ATP synthase, subunit K.

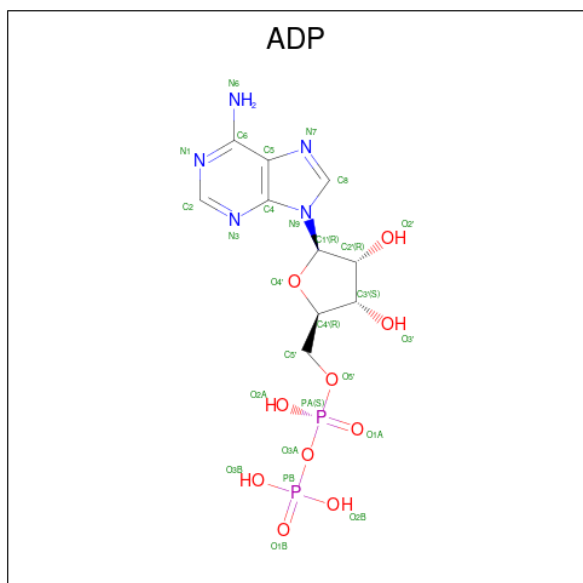
Mol	Chain	Residues	Atoms				AltConf	Trace
9	O	76	Total	C	N	O	0	0
			303	152	76	75		
9	P	76	Total	C	N	O	0	0
			303	152	76	75		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	76	Total	C	N	O	0	0
			303	152	76	75		
9	R	76	Total	C	N	O	0	0
			303	152	76	75		
9	S	76	Total	C	N	O	0	0
			303	152	76	75		
9	T	76	Total	C	N	O	0	0
			303	152	76	75		
9	U	76	Total	C	N	O	0	0
			303	152	76	75		
9	V	76	Total	C	N	O	0	0
			303	152	76	75		
9	W	76	Total	C	N	O	0	0
			303	152	76	75		
9	X	76	Total	C	N	O	0	0
			303	152	76	75		
9	Y	76	Total	C	N	O	0	0
			303	152	76	75		
9	Z	76	Total	C	N	O	0	0
			303	152	76	75		

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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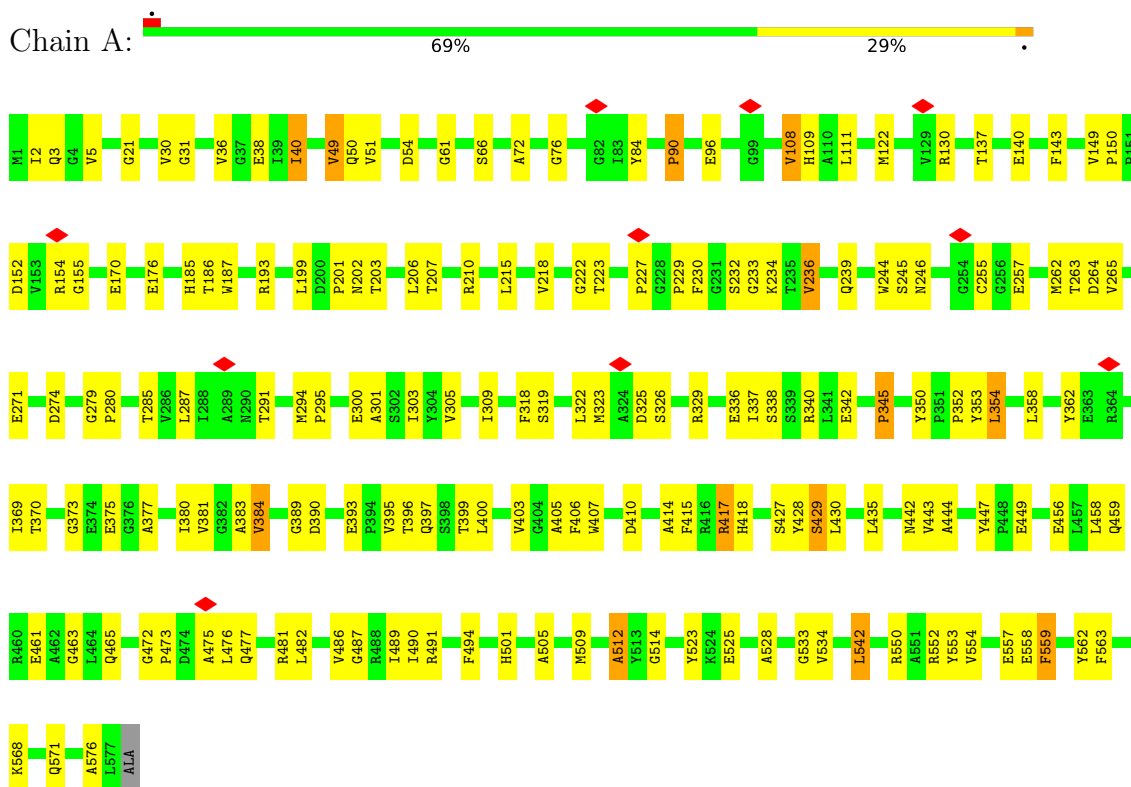
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	B	1	27	10	5	10	2	0

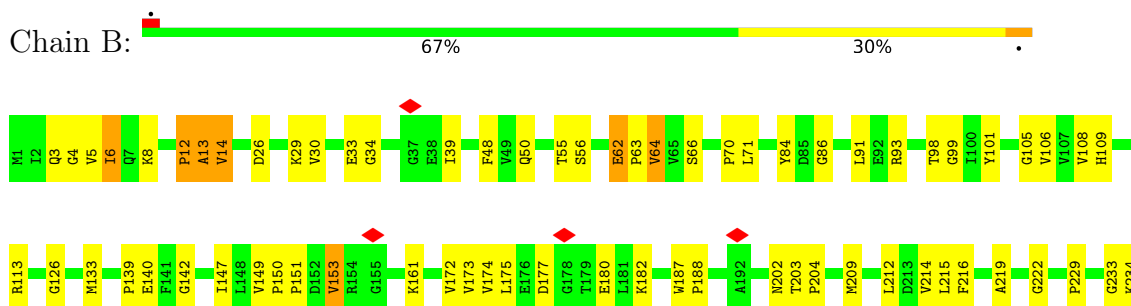
3 Residue-property plots

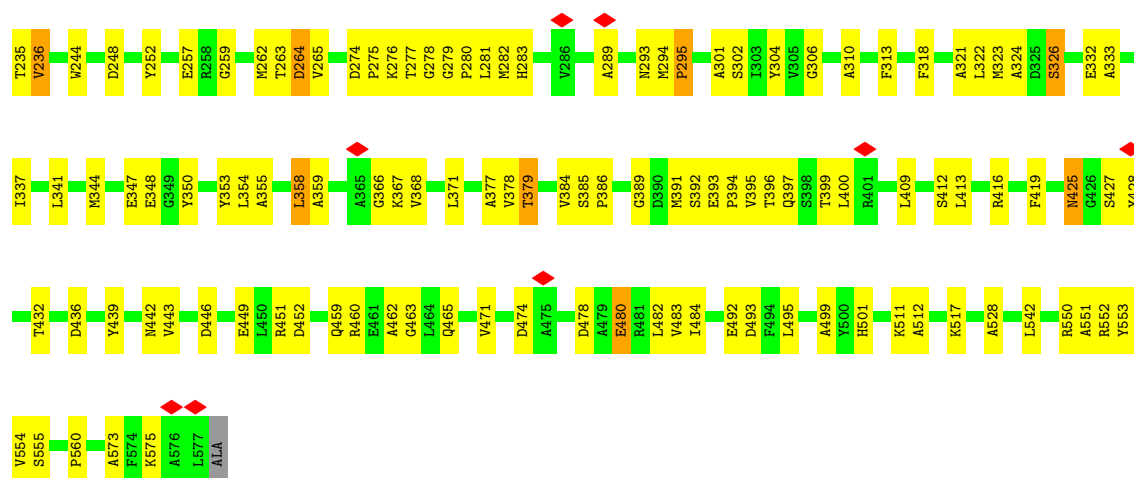
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: V-type ATP synthase alpha chain

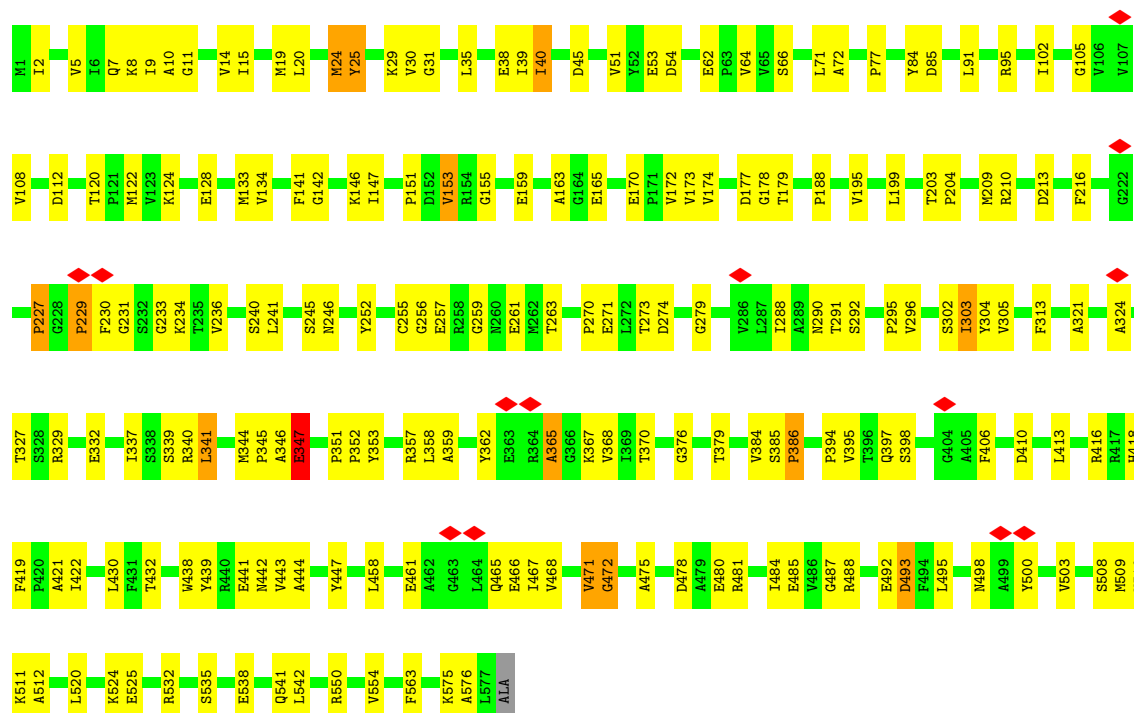


- Molecule 1: V-type ATP synthase alpha chain

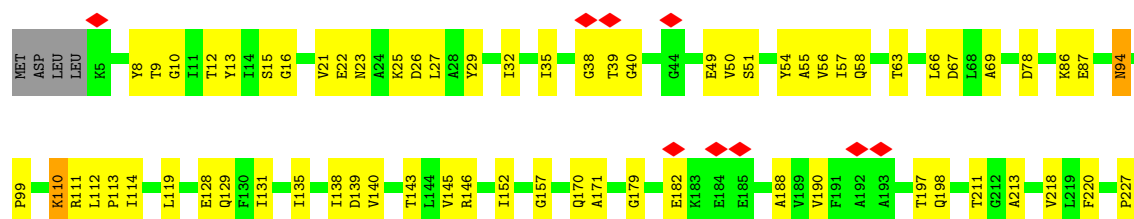


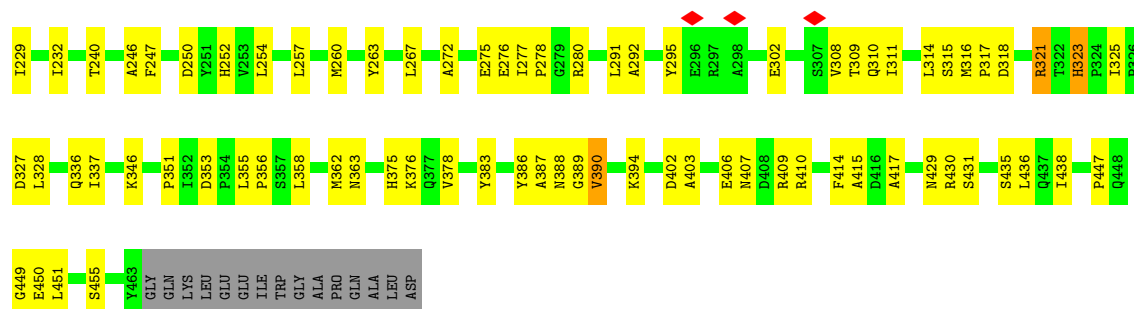


• Molecule 1: V-type ATP synthase alpha chain

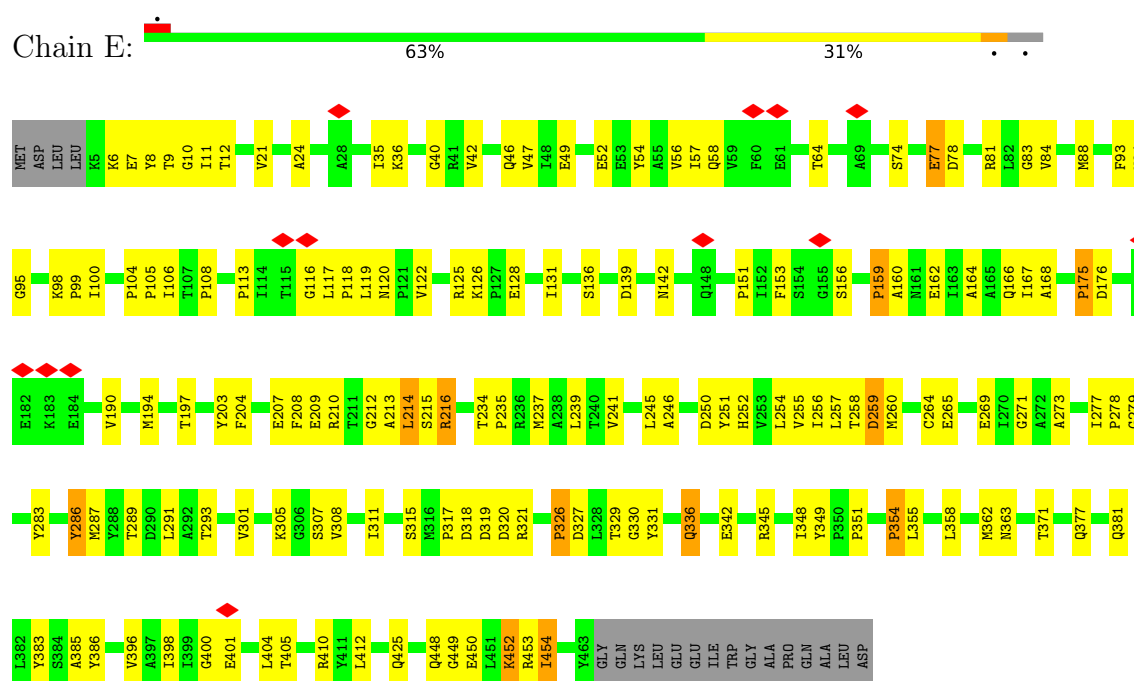


• Molecule 2: V-type ATP synthase beta chain

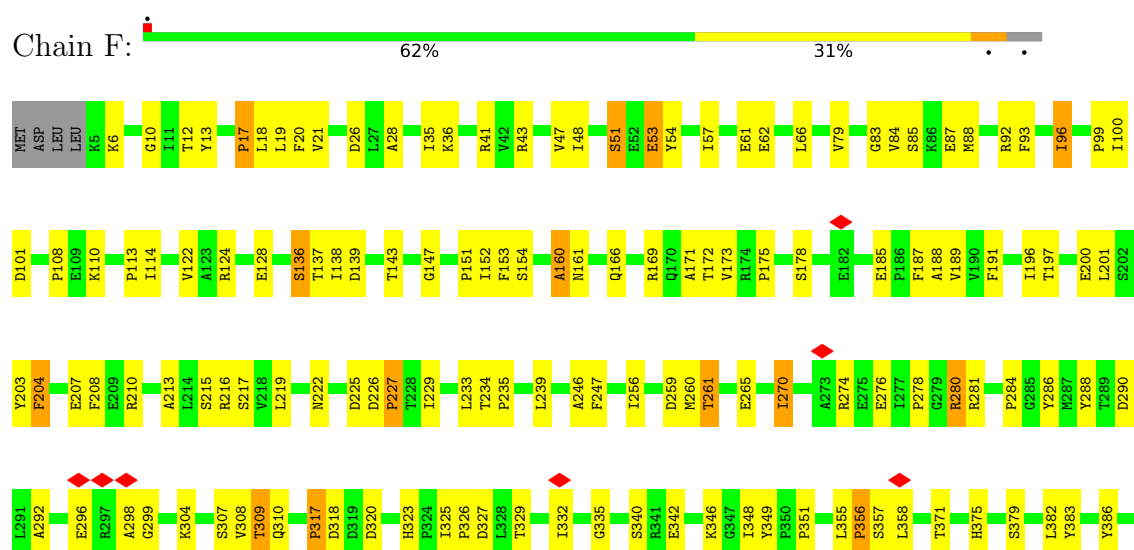




• Molecule 2: V-type ATP synthase beta chain

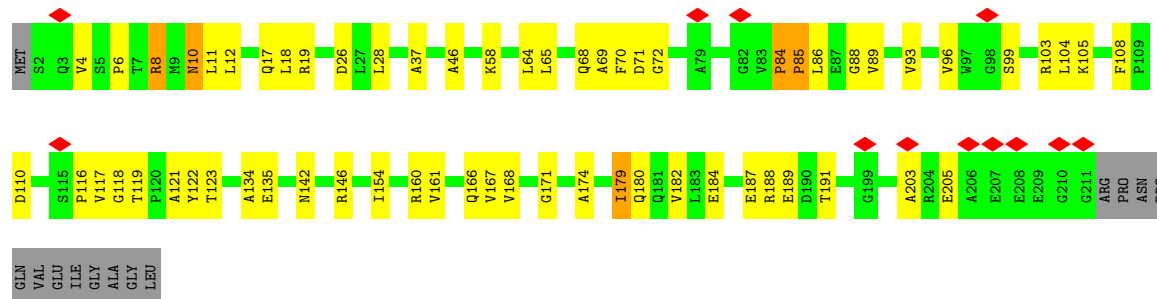


• Molecule 2: V-type ATP synthase beta chain

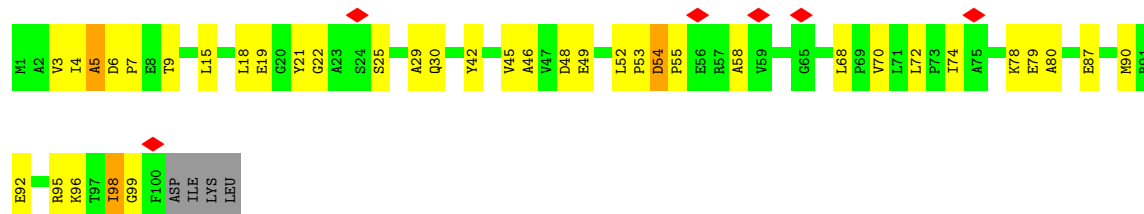




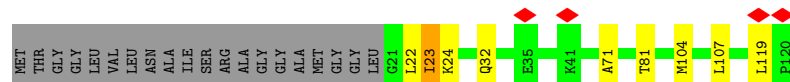
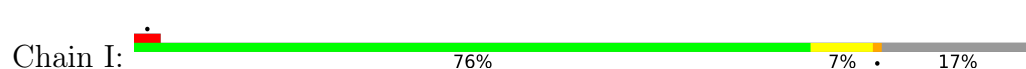
• Molecule 3: V-type ATP synthase subunit D



• Molecule 4: V-type ATP synthase subunit F



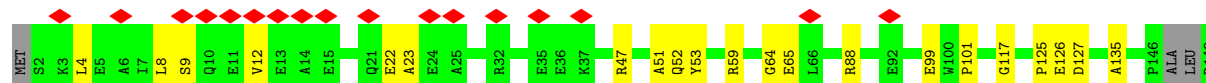
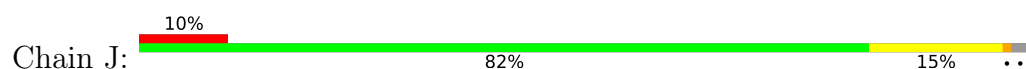
• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

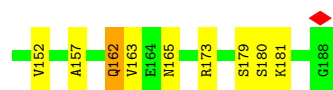


• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

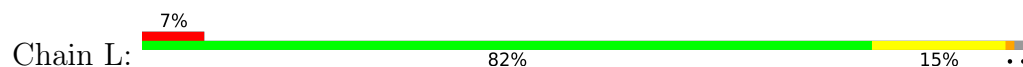


• Molecule 6: V-type ATP synthase subunit E

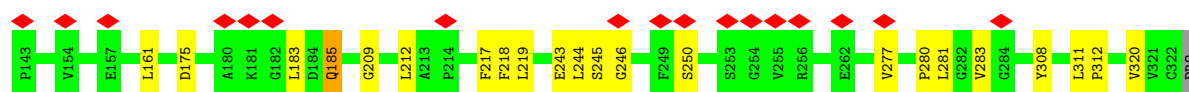
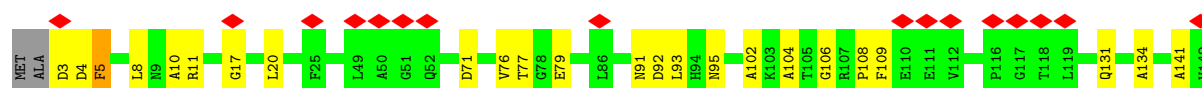
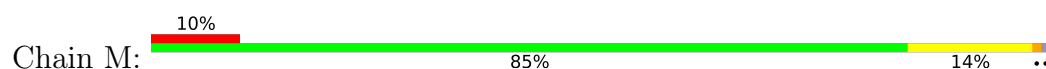




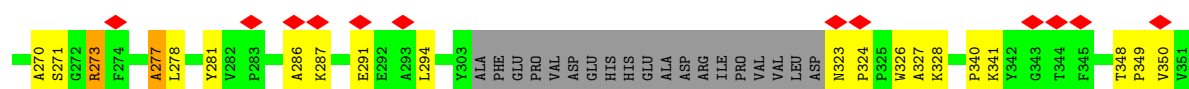
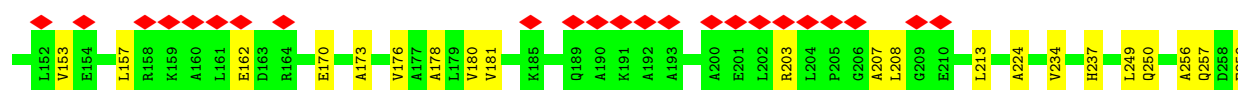
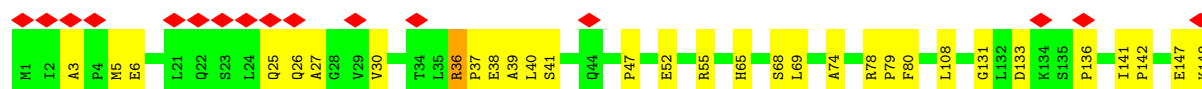
• Molecule 6: V-type ATP synthase subunit E



• Molecule 7: V-type ATP synthase subunit C

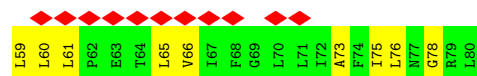


• Molecule 8: V-type ATP synthase subunit I

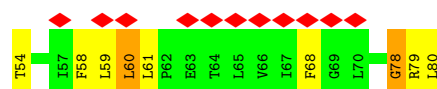




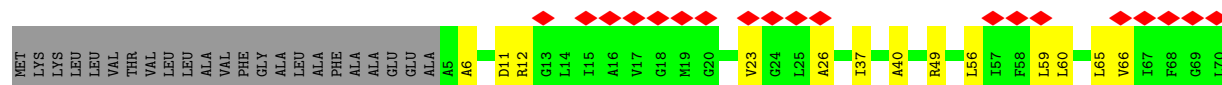
- Molecule 9: V-type ATP synthase, subunit K



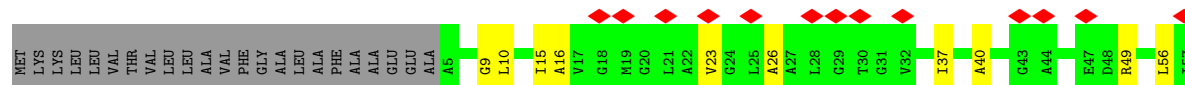
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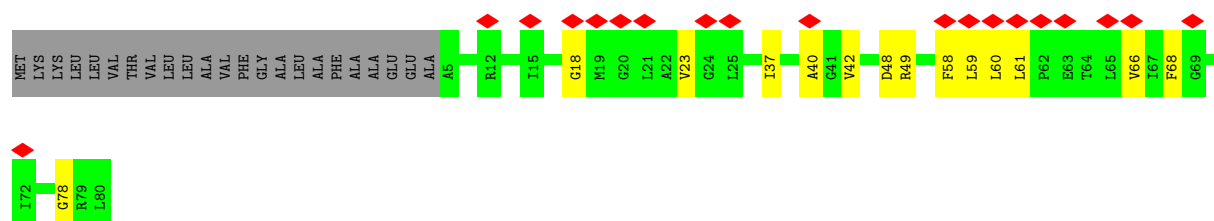
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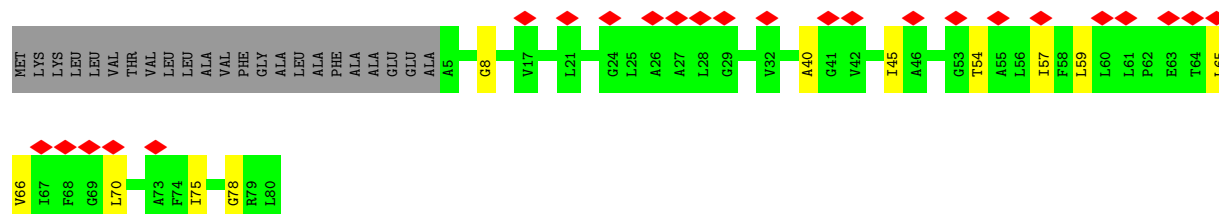
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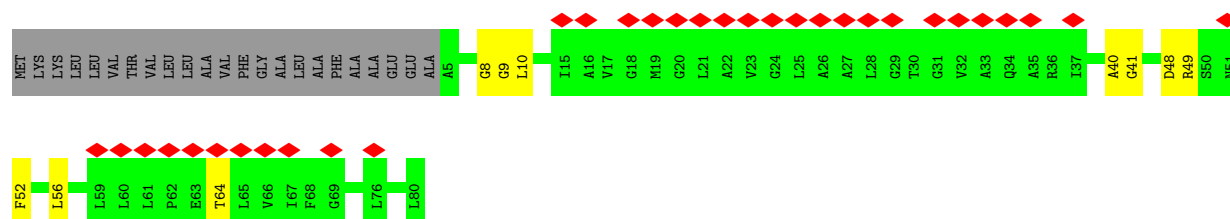
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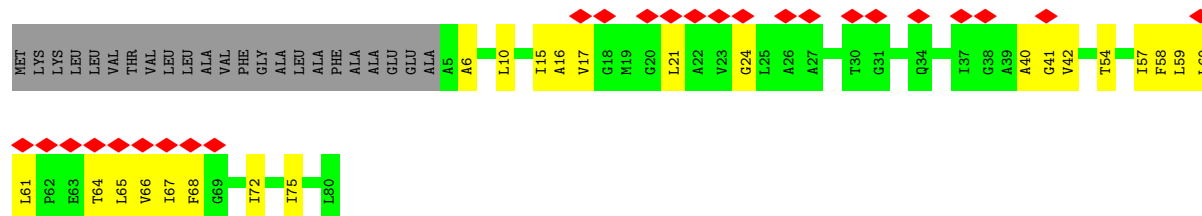
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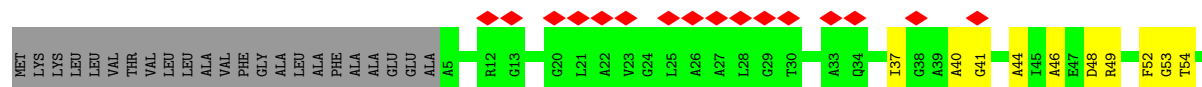
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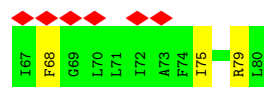
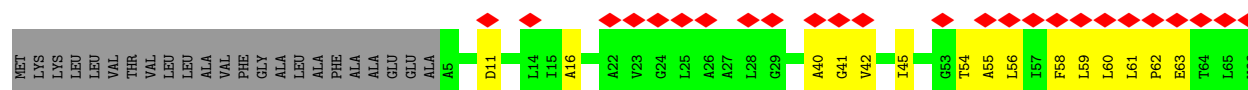


- Molecule 9: V-type ATP synthase, subunit K

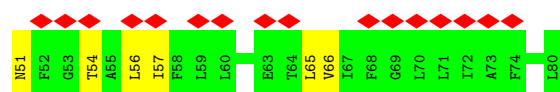
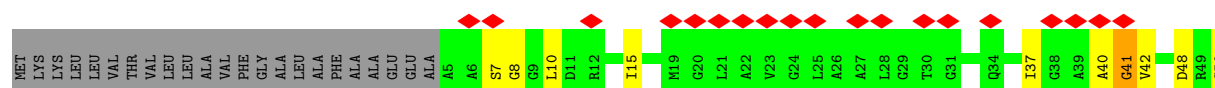




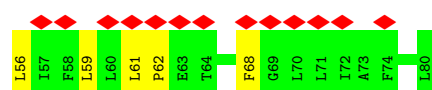
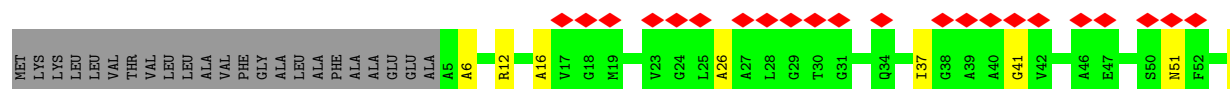
• Molecule 9: V-type ATP synthase, subunit K



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• Molecule 9: V-type ATP synthase, subunit K



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13851	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.203	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	330.4, 330.4, 330.4	wwPDB
Map dimensions	236, 236, 236	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	2.34	70/2306 (3.0%)	2.29	122/2881 (4.2%)
1	B	2.33	81/2306 (3.5%)	2.32	119/2881 (4.1%)
1	C	2.30	68/2306 (2.9%)	2.30	130/2881 (4.5%)
2	D	2.27	55/1834 (3.0%)	2.31	110/2291 (4.8%)
2	E	2.43	74/1834 (4.0%)	2.37	110/2291 (4.8%)
2	F	2.44	70/1834 (3.8%)	2.32	108/2291 (4.7%)
3	G	2.31	25/838 (3.0%)	2.37	41/1046 (3.9%)
4	H	2.11	12/398 (3.0%)	2.32	29/496 (5.8%)
5	I	1.76	0/398	2.27	15/496 (3.0%)
5	K	1.91	2/398 (0.5%)	2.24	16/496 (3.2%)
6	J	1.75	2/736 (0.3%)	2.11	31/917 (3.4%)
6	L	1.94	7/736 (1.0%)	2.10	24/917 (2.6%)
7	M	1.87	4/1278 (0.3%)	2.20	51/1596 (3.2%)
8	N	1.77	15/2524 (0.6%)	2.36	158/3152 (5.0%)
9	O	1.40	0/302	2.85	38/376 (10.1%)
9	P	1.49	0/302	2.74	32/376 (8.5%)
9	Q	1.49	0/302	2.54	23/376 (6.1%)
9	R	1.45	0/302	2.74	28/376 (7.4%)
9	S	1.50	2/302 (0.7%)	2.51	24/376 (6.4%)
9	T	1.45	0/302	2.44	19/376 (5.1%)
9	U	1.55	0/302	2.47	16/376 (4.3%)
9	V	1.57	0/302	3.13	36/376 (9.6%)
9	W	1.42	0/302	2.63	27/376 (7.2%)
9	X	1.48	0/302	2.67	30/376 (8.0%)
9	Y	1.44	1/302 (0.3%)	2.57	22/376 (5.9%)
9	Z	1.59	1/302 (0.3%)	2.60	19/376 (5.1%)
All	All	2.10	489/23350 (2.1%)	2.36	1378/29144 (4.7%)

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	2
1	B	0	3
1	C	0	1
2	F	0	2
7	M	0	3
9	P	0	1
9	U	0	1
9	Y	0	2
All	All	0	15

All (489) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	93	PHE	CA-C	-11.10	1.42	1.53
2	F	233	LEU	CA-C	-9.04	1.42	1.52
2	E	319	ASP	CA-C	-8.96	1.45	1.53
2	F	153	PHE	CA-C	-8.80	1.41	1.52
1	A	383	ALA	CA-C	-8.35	1.42	1.52
1	C	493	ASP	CA-C	-8.15	1.45	1.52
2	E	245	LEU	CA-C	-8.06	1.44	1.53
2	F	416	ASP	CA-C	-7.98	1.42	1.52
1	C	538	GLU	CA-C	-7.97	1.45	1.52
1	A	234	LYS	CA-C	-7.91	1.42	1.52
2	E	412	LEU	CA-C	-7.90	1.43	1.53
1	B	367	LYS	CA-C	-7.86	1.46	1.53
1	B	350	TYR	CA-C	-7.81	1.44	1.53
2	F	138	ILE	CA-C	-7.72	1.43	1.52
2	F	152	ILE	CA-C	-7.64	1.43	1.52
2	E	308	VAL	CA-C	-7.64	1.43	1.52
2	E	58	GLN	CA-C	-7.63	1.43	1.53
1	B	378	VAL	CA-C	-7.61	1.46	1.53
2	D	308	VAL	CA-C	-7.60	1.45	1.53
1	B	4	GLY	CA-C	-7.60	1.43	1.51
2	F	355	LEU	N-CA	-7.51	1.41	1.46
9	S	48	ASP	CA-C	-7.50	1.43	1.52
2	E	93	PHE	CA-C	-7.48	1.43	1.52
1	A	262	MET	CA-C	-7.47	1.42	1.52
1	B	98	THR	CA-C	-7.47	1.47	1.52
1	A	427	SER	CA-C	-7.45	1.43	1.52
1	A	442	ASN	CA-C	-7.44	1.46	1.52
1	A	456	GLU	CA-C	-7.33	1.43	1.52
2	E	257	LEU	CA-C	-7.33	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	LEU	CA-C	-7.29	1.47	1.52
1	C	8	LYS	CA-C	-7.28	1.43	1.52
2	E	162	GLU	CA-C	-7.26	1.43	1.52
2	E	209	GLU	CA-C	-7.21	1.42	1.52
1	A	291	THR	CA-C	-7.20	1.44	1.52
1	A	322	LEU	CA-C	-7.19	1.43	1.52
1	B	391	MET	CA-C	-7.16	1.45	1.53
2	E	349	TYR	CA-C	-7.12	1.44	1.52
2	E	264	CYS	CA-C	-7.08	1.43	1.52
1	A	481	ARG	CA-C	-7.05	1.43	1.52
1	A	449	GLU	CA-C	-7.04	1.45	1.52
2	D	112	LEU	N-CA	-7.03	1.41	1.46
2	F	201	LEU	CA-C	-7.00	1.44	1.52
1	A	559	PHE	N-CA	-7.00	1.40	1.46
2	E	12	THR	CA-C	-6.98	1.43	1.52
1	C	444	ALA	CA-C	-6.98	1.43	1.52
1	A	230	PHE	CA-C	-6.96	1.44	1.52
3	G	69	ALA	CA-C	-6.93	1.45	1.53
1	B	413	LEU	CA-C	-6.92	1.44	1.52
8	N	65	HIS	CA-C	-6.92	1.43	1.52
2	F	153	PHE	N-CA	-6.91	1.37	1.46
2	D	55	ALA	CA-C	-6.90	1.44	1.52
1	B	439	TYR	CA-C	-6.89	1.44	1.52
1	C	419	PHE	CA-C	-6.85	1.45	1.53
2	F	402	ASP	CA-C	-6.84	1.43	1.52
1	B	235	THR	CA-C	-6.84	1.44	1.52
1	C	245	SER	CA-C	-6.84	1.46	1.53
2	D	328	LEU	CA-C	-6.82	1.43	1.52
2	F	308	VAL	CA-C	-6.81	1.45	1.52
3	G	167	VAL	CA-C	-6.80	1.44	1.52
3	G	191	THR	N-CA	-6.80	1.38	1.46
2	F	430	ARG	CA-C	-6.79	1.44	1.52
2	E	377	GLN	CA-C	-6.77	1.43	1.52
2	F	154	SER	CA-C	-6.72	1.44	1.52
1	B	188	PRO	CA-C	-6.71	1.44	1.52
2	E	47	VAL	N-CA	-6.70	1.38	1.46
2	E	383	TYR	CA-C	-6.63	1.44	1.52
2	F	85	SER	CA-C	-6.63	1.50	1.53
1	C	439	TYR	CA-C	-6.62	1.44	1.52
2	E	12	THR	N-CA	-6.61	1.37	1.46
1	B	495	LEU	CA-C	-6.61	1.44	1.52
2	D	35	ILE	CA-C	-6.59	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	ILE	CA-C	-6.59	1.44	1.52
2	F	433	GLU	CA-C	-6.58	1.44	1.52
2	F	204	PHE	CA-C	-6.57	1.43	1.52
1	B	106	VAL	CA-C	-6.57	1.47	1.52
2	F	196	ILE	CA-C	-6.57	1.47	1.52
1	A	350	TYR	CA-C	-6.55	1.47	1.52
1	C	124	LYS	N-CA	-6.55	1.41	1.46
2	F	100	ILE	CA-C	-6.55	1.46	1.53
1	B	332	GLU	CA-C	-6.54	1.43	1.52
2	F	151	PRO	CA-C	-6.54	1.43	1.52
1	C	64	VAL	CA-C	-6.54	1.44	1.52
2	E	58	GLN	N-CA	-6.54	1.38	1.46
1	B	244	TRP	CA-C	-6.51	1.46	1.53
1	C	442	ASN	CA-C	-6.51	1.44	1.53
2	E	245	LEU	N-CA	-6.50	1.39	1.46
2	F	13	TYR	CA-C	-6.48	1.45	1.52
2	E	42	VAL	CA-C	-6.48	1.45	1.52
1	B	216	PHE	CA-C	-6.46	1.44	1.52
4	H	3	VAL	N-CA	-6.45	1.39	1.46
4	H	87	GLU	CA-C	-6.45	1.44	1.52
2	D	410	ARG	CA-C	-6.44	1.44	1.52
2	F	323	HIS	CA-C	-6.44	1.45	1.53
1	B	8	LYS	CA-C	-6.42	1.45	1.52
2	E	142	ASN	CA-C	-6.42	1.44	1.52
2	D	58	GLN	CA-C	-6.41	1.44	1.53
1	B	337	ILE	CA-C	-6.41	1.45	1.52
7	M	244	LEU	CA-C	-6.40	1.46	1.53
1	B	180	GLU	CA-C	-6.38	1.45	1.52
1	B	353	TYR	CA-C	-6.37	1.44	1.52
2	D	49	GLU	CA-C	-6.33	1.45	1.52
3	G	184	GLU	CA-C	-6.32	1.44	1.52
1	C	398	SER	CA-C	-6.31	1.45	1.53
1	B	313	PHE	CA-C	-6.30	1.44	1.52
6	L	154	ALA	CA-C	-6.30	1.45	1.52
9	Y	48	ASP	CA-C	-6.28	1.45	1.52
2	E	239	LEU	CA-C	-6.27	1.45	1.52
2	F	35	ILE	CA-C	-6.27	1.45	1.52
1	C	234	LYS	CA-C	-6.23	1.44	1.52
2	D	247	PHE	CA-C	-6.21	1.44	1.52
2	D	13	TYR	CA-C	-6.21	1.45	1.52
2	E	348	ILE	CA-C	-6.20	1.45	1.52
2	F	113	PRO	CA-C	-6.20	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	562	TYR	CA-C	-6.18	1.44	1.52
2	D	310	GLN	CA-C	-6.18	1.45	1.52
1	B	442	ASN	CA-C	-6.17	1.45	1.52
1	C	5	VAL	CA-C	-6.16	1.45	1.52
2	E	246	ALA	CA-C	-6.16	1.44	1.52
2	D	32	ILE	CA-C	-6.15	1.45	1.52
2	F	152	ILE	N-CA	-6.15	1.38	1.46
1	A	305	VAL	CA-C	-6.15	1.44	1.52
1	B	511	LYS	CA-C	-6.15	1.45	1.52
3	G	182	VAL	CA-C	-6.15	1.44	1.52
8	N	257	GLN	CA-C	-6.15	1.44	1.52
1	C	204	PRO	CA-C	-6.14	1.46	1.52
2	F	247	PHE	CA-C	-6.14	1.44	1.52
3	G	166	GLN	CA-C	-6.12	1.45	1.52
2	F	18	LEU	CA-C	-6.11	1.45	1.52
1	C	441	GLU	CA-C	-6.11	1.45	1.52
2	E	315	SER	CA-C	-6.10	1.45	1.52
3	G	184	GLU	N-CA	-6.09	1.39	1.46
1	A	90	PRO	CA-C	-6.09	1.43	1.52
2	E	7	GLU	CA-C	-6.08	1.45	1.52
1	A	509	MET	CA-C	-6.08	1.44	1.52
8	N	491	HIS	CA-C	-6.08	1.45	1.53
2	E	208	PHE	CA-C	-6.07	1.45	1.52
1	C	367	LYS	CA-C	-6.07	1.46	1.53
1	A	415	PHE	CA-C	-6.06	1.45	1.52
2	E	204	PHE	CA-C	-6.04	1.44	1.52
1	A	362	TYR	CA-C	-6.04	1.45	1.52
1	B	550	ARG	N-CA	-6.03	1.39	1.46
2	D	291	LEU	CA-C	-6.01	1.44	1.52
2	F	219	LEU	CA-C	-6.00	1.45	1.53
4	H	19	GLU	CA-C	-6.00	1.47	1.53
1	A	50	GLN	CA-C	-5.99	1.45	1.52
2	F	310	GLN	CA-C	-5.99	1.45	1.52
2	D	246	ALA	CA-C	-5.99	1.45	1.52
2	F	246	ALA	CA-C	-5.98	1.45	1.52
2	E	381	GLN	CA-C	-5.98	1.44	1.52
2	E	11	ILE	CA-C	-5.97	1.45	1.52
2	E	259	ASP	CA-C	-5.97	1.44	1.52
3	G	105	LYS	CA-C	-5.96	1.45	1.52
2	D	376	LYS	CA-C	-5.96	1.45	1.52
2	D	152	ILE	CA-C	-5.95	1.46	1.52
1	A	418	HIS	CA-C	-5.94	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	39	ILE	CA-C	-5.91	1.45	1.52
2	D	386	TYR	N-CA	-5.91	1.38	1.46
1	A	396	THR	CA-C	-5.90	1.44	1.52
2	E	151	PRO	CA-C	-5.90	1.46	1.52
2	D	292	ALA	CA-C	-5.90	1.47	1.53
2	E	410	ARG	CA-C	-5.90	1.45	1.52
1	C	14	VAL	CA-C	-5.89	1.45	1.52
1	A	109	HIS	CA-C	-5.89	1.45	1.52
2	D	388	ASN	CA-C	-5.87	1.44	1.52
2	F	307	SER	CA-C	-5.86	1.45	1.52
2	E	113	PRO	CA-C	-5.86	1.45	1.52
1	A	400	LEU	CA-C	-5.86	1.44	1.52
2	D	220	PHE	CA-C	-5.86	1.45	1.52
1	A	201	PRO	CA-C	-5.84	1.47	1.53
1	B	39	ILE	CA-C	-5.84	1.46	1.53
2	E	6	LYS	CA-C	-5.84	1.45	1.52
1	A	358	LEU	CA-C	-5.84	1.45	1.52
1	C	550	ARG	CA-C	-5.83	1.44	1.52
1	A	399	THR	CA-C	-5.83	1.45	1.52
2	E	203	TYR	CA-C	-5.83	1.44	1.52
3	G	26	ASP	N-CA	-5.83	1.39	1.46
1	B	482	LEU	CA-C	-5.81	1.45	1.52
1	A	380	ILE	CA-C	-5.81	1.45	1.52
8	N	237	HIS	CA-C	-5.80	1.45	1.52
3	G	6	PRO	CA-C	-5.80	1.44	1.52
1	A	295	PRO	CA-C	-5.80	1.45	1.52
2	F	47	VAL	CA-C	-5.80	1.45	1.52
6	L	161	THR	CA-C	-5.79	1.45	1.52
1	C	38	GLU	CA-C	-5.79	1.45	1.52
2	D	112	LEU	CA-C	-5.78	1.46	1.52
2	D	309	THR	CA-C	-5.78	1.45	1.52
1	C	511	LYS	CA-C	-5.78	1.46	1.53
1	B	358	LEU	N-CA	-5.77	1.40	1.46
1	A	384	VAL	CA-C	-5.77	1.45	1.52
4	H	95	ARG	CA-C	-5.77	1.45	1.52
2	E	326	PRO	CA-C	-5.77	1.44	1.52
1	A	553	TYR	N-CA	-5.76	1.40	1.46
1	C	353	TYR	CA-C	-5.76	1.47	1.53
2	F	171	ALA	CA-C	-5.76	1.45	1.52
1	B	84	TYR	CA-C	-5.75	1.45	1.52
2	E	311	ILE	CA-C	-5.74	1.46	1.52
1	B	368	VAL	CA-C	-5.74	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	416	ARG	CA-C	-5.74	1.44	1.52
7	M	308	TYR	CA-C	-5.73	1.45	1.52
8	N	142	PRO	CA-C	-5.73	1.46	1.52
2	E	167	ILE	CA-C	-5.73	1.45	1.52
2	E	190	VAL	CA-C	-5.73	1.45	1.52
2	E	289	THR	CA-C	-5.73	1.45	1.52
1	A	51	VAL	CA-C	-5.72	1.47	1.53
3	G	191	THR	CA-C	-5.72	1.45	1.52
2	D	277	ILE	CA-C	-5.72	1.46	1.52
1	B	212	LEU	CA-C	-5.72	1.45	1.52
1	A	395	VAL	N-CA	-5.70	1.39	1.46
4	H	96	LYS	CA-C	-5.70	1.45	1.53
1	B	147	ILE	CA-C	-5.69	1.45	1.52
1	B	175	LEU	CA-C	-5.69	1.45	1.52
1	B	354	LEU	CA-C	-5.69	1.45	1.52
2	F	325	ILE	N-CA	-5.68	1.39	1.46
3	G	19	ARG	CA-C	-5.68	1.45	1.52
1	B	3	GLN	CA-C	-5.68	1.45	1.52
8	N	181	VAL	CA-C	-5.68	1.46	1.52
1	B	209	MET	CA-C	-5.67	1.47	1.53
1	C	64	VAL	N-CA	-5.67	1.39	1.46
1	B	397	GLN	CA-C	-5.67	1.45	1.52
1	B	322	LEU	CA-C	-5.66	1.46	1.52
1	C	54	ASP	CA-C	-5.66	1.45	1.52
1	A	459	GLN	CA-C	-5.66	1.45	1.52
1	B	29	LYS	CA-C	-5.66	1.45	1.52
2	D	8	TYR	CA-C	-5.65	1.45	1.52
1	A	285	THR	CA-C	-5.64	1.45	1.52
1	B	385	SER	CA-C	-5.64	1.45	1.52
5	K	87	ARG	CA-C	-5.64	1.45	1.52
1	C	40	ILE	N-CA	-5.64	1.39	1.46
2	E	209	GLU	N-CA	-5.63	1.38	1.46
3	G	146	ARG	CA-C	-5.63	1.45	1.52
1	C	406	PHE	CA-C	-5.62	1.46	1.52
2	F	290	ASP	N-CA	-5.62	1.39	1.46
2	D	267	LEU	CA-C	-5.61	1.46	1.52
1	B	400	LEU	CA-C	-5.61	1.45	1.52
2	D	171	ALA	CA-C	-5.60	1.45	1.52
1	B	379	THR	N-CA	-5.60	1.39	1.46
2	F	19	LEU	CA-C	-5.60	1.45	1.52
2	F	318	ASP	CA-C	-5.58	1.46	1.53
1	B	30	VAL	N-CA	-5.57	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	187	GLU	N-CA	-5.57	1.38	1.46
2	F	88	MET	N-CA	-5.56	1.39	1.46
1	B	379	THR	CA-C	-5.56	1.46	1.52
1	B	396	THR	N-CA	-5.56	1.39	1.46
1	C	19	MET	CA-C	-5.56	1.45	1.52
2	F	83	GLY	CA-C	-5.56	1.45	1.52
2	F	349	TYR	CA-C	-5.56	1.46	1.52
1	A	96	GLU	CA-C	-5.55	1.46	1.52
2	F	342	GLU	N-CA	-5.55	1.39	1.46
1	A	407	TRP	CA-C	-5.55	1.45	1.52
1	B	465	GLN	CA-C	-5.55	1.44	1.52
2	E	342	GLU	CA-C	-5.54	1.45	1.52
2	F	265	GLU	CA-C	-5.54	1.45	1.52
1	C	487	GLY	CA-C	-5.54	1.45	1.52
1	A	458	LEU	CA-C	-5.53	1.45	1.52
1	B	6	ILE	CA-C	-5.53	1.46	1.52
2	F	92	ARG	CA-C	-5.53	1.46	1.52
3	G	179	ILE	CA-C	-5.53	1.45	1.52
2	E	254	LEU	CA-C	-5.53	1.46	1.52
3	G	11	LEU	CA-C	-5.53	1.44	1.52
1	B	550	ARG	CA-C	-5.52	1.46	1.52
1	C	313	PHE	CA-C	-5.51	1.45	1.52
2	D	309	THR	N-CA	-5.51	1.39	1.46
2	E	142	ASN	N-CA	-5.51	1.39	1.46
1	C	15	ILE	N-CA	-5.51	1.39	1.46
1	C	344	MET	N-CA	-5.51	1.41	1.46
2	F	392	ILE	CA-C	-5.51	1.46	1.52
1	C	62	GLU	CA-C	-5.50	1.47	1.53
4	H	96	LYS	N-CA	-5.50	1.39	1.46
5	K	80	GLU	CA-C	-5.50	1.45	1.52
1	B	161	LYS	CA-C	-5.50	1.47	1.53
3	G	11	LEU	N-CA	-5.49	1.39	1.46
2	F	20	PHE	CA-C	-5.49	1.45	1.52
2	F	348	ILE	CA-C	-5.49	1.46	1.52
2	F	349	TYR	N-CA	-5.49	1.41	1.46
1	B	64	VAL	CA-C	-5.48	1.45	1.52
2	D	13	TYR	N-CA	-5.48	1.39	1.46
2	D	317	PRO	CA-C	-5.48	1.46	1.52
7	M	311	LEU	CA-C	-5.48	1.46	1.52
1	A	40	ILE	CA-C	-5.48	1.45	1.52
3	G	12	LEU	CA-C	-5.48	1.45	1.52
2	E	54	TYR	CA-C	-5.47	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	50	VAL	CA-C	-5.46	1.47	1.52
1	A	461	GLU	CA-C	-5.46	1.45	1.52
3	G	135	GLU	CA-C	-5.46	1.45	1.52
1	C	362	TYR	CA-C	-5.45	1.45	1.52
2	D	26	ASP	N-CA	-5.45	1.40	1.46
1	A	244	TRP	CA-C	-5.45	1.46	1.52
1	C	498	ASN	CA-C	-5.45	1.45	1.53
2	E	241	VAL	CA-C	-5.45	1.45	1.52
2	E	166	GLN	N-CA	-5.45	1.40	1.46
1	A	318	PHE	CA-C	-5.45	1.46	1.52
1	B	400	LEU	N-CA	-5.45	1.39	1.46
2	E	47	VAL	CA-C	-5.44	1.46	1.52
2	F	154	SER	N-CA	-5.44	1.39	1.46
1	A	553	TYR	CA-C	-5.44	1.46	1.52
1	B	64	VAL	N-CA	-5.44	1.39	1.46
1	C	520	LEU	CA-C	-5.44	1.46	1.52
1	B	395	VAL	N-CA	-5.44	1.39	1.46
2	F	440	TRP	CA-C	-5.44	1.45	1.52
2	F	270	ILE	CA-C	-5.43	1.45	1.52
2	F	288	TYR	CA-C	-5.43	1.45	1.52
4	H	3	VAL	CA-C	-5.43	1.46	1.52
1	A	2	ILE	CA-C	-5.42	1.46	1.52
2	D	275	GLU	CA-C	-5.42	1.45	1.52
8	N	176	VAL	CA-C	-5.42	1.46	1.52
2	D	272	ALA	CA-C	-5.41	1.45	1.52
3	G	104	LEU	CA-C	-5.41	1.45	1.52
1	A	417	ARG	CA-C	-5.41	1.47	1.53
1	C	488	ARG	CA-C	-5.40	1.45	1.52
1	B	483	VAL	N-CA	-5.40	1.40	1.46
1	C	337	ILE	N-CA	-5.40	1.40	1.46
1	C	7	GLN	CA-C	-5.39	1.47	1.52
2	E	283	TYR	N-CA	-5.39	1.39	1.45
2	D	336	GLN	CA-C	-5.39	1.45	1.52
1	A	236	VAL	CA-C	-5.39	1.46	1.52
1	A	264	ASP	N-CA	-5.38	1.40	1.46
2	D	26	ASP	CA-C	-5.38	1.48	1.53
1	A	303	ILE	CA-C	-5.38	1.46	1.52
2	F	412	LEU	CA-C	-5.38	1.45	1.52
1	B	493	ASP	CA-C	-5.38	1.44	1.52
1	B	321	ALA	CA-C	-5.37	1.46	1.53
1	B	517	LYS	N-CA	-5.37	1.39	1.46
1	B	449	GLU	CA-C	-5.37	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	310	ALA	CA-C	-5.36	1.45	1.52
1	A	568	LYS	CA-C	-5.36	1.45	1.52
1	C	358	LEU	N-CA	-5.36	1.40	1.46
1	B	219	ALA	CA-C	-5.35	1.46	1.52
1	C	337	ILE	CA-C	-5.35	1.46	1.52
1	A	239	GLN	CA-C	-5.34	1.46	1.52
1	B	399	THR	CA-C	-5.34	1.45	1.52
7	M	218	PHE	CA-C	-5.34	1.46	1.52
2	D	138	ILE	CA-C	-5.34	1.46	1.52
1	C	31	GLY	CA-C	-5.34	1.45	1.52
1	C	45	ASP	N-CA	-5.34	1.42	1.47
1	A	512	ALA	CA-C	-5.34	1.45	1.52
1	C	173	VAL	CA-C	-5.34	1.46	1.53
6	L	82	GLU	CA-C	-5.33	1.46	1.52
1	A	336	GLU	CA-C	-5.33	1.46	1.52
1	A	340	ARG	CA-C	-5.33	1.45	1.52
2	D	257	LEU	CA-C	-5.33	1.46	1.52
2	E	251	TYR	CA-C	-5.32	1.46	1.52
8	N	108	LEU	CA-C	-5.32	1.45	1.52
1	B	318	PHE	CA-C	-5.32	1.45	1.52
1	A	482	LEU	CA-C	-5.31	1.45	1.52
1	B	463	GLY	CA-C	-5.31	1.45	1.52
2	F	217	SER	CA-C	-5.30	1.46	1.52
1	C	20	LEU	CA-C	-5.30	1.46	1.52
1	B	93	ARG	CA-C	-5.30	1.45	1.52
1	A	30	VAL	CA-C	-5.30	1.46	1.52
2	D	250	ASP	CA-C	-5.30	1.46	1.53
3	G	189	GLU	CA-C	-5.30	1.45	1.52
2	E	273	ALA	CA-C	-5.29	1.47	1.52
2	F	383	TYR	CA-C	-5.29	1.45	1.52
1	A	338	SER	CA-C	-5.29	1.46	1.52
1	C	273	THR	CA-C	-5.29	1.46	1.52
2	F	57	ILE	CA-C	-5.29	1.46	1.52
2	F	203	TYR	CA-C	-5.29	1.46	1.52
1	C	441	GLU	N-CA	-5.29	1.40	1.46
2	E	126	LYS	CA-C	-5.29	1.48	1.53
2	E	336	GLN	CA-C	-5.28	1.45	1.52
1	C	261	GLU	CA-C	-5.28	1.45	1.52
2	E	52	GLU	CA-C	-5.28	1.45	1.52
1	A	206	LEU	CA-C	-5.28	1.46	1.53
2	E	291	LEU	CA-C	-5.28	1.45	1.52
1	A	199	LEU	CA-C	-5.28	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	77	GLY	CA-C	-5.27	1.46	1.52
2	F	400	GLY	CA-C	-5.27	1.46	1.51
2	E	77	GLU	CA-C	-5.26	1.45	1.52
8	N	249	LEU	CA-C	-5.26	1.46	1.52
1	B	109	HIS	CA-C	-5.26	1.46	1.52
2	F	304	LYS	CA-C	-5.26	1.46	1.52
1	C	480	GLU	CA-C	-5.25	1.46	1.52
2	F	21	VAL	CA-C	-5.25	1.46	1.52
2	E	331	TYR	CA-C	-5.25	1.46	1.52
2	E	345	ARG	N-CA	-5.25	1.40	1.46
1	A	271	GLU	CA-C	-5.25	1.45	1.52
2	F	110	LYS	N-CA	-5.25	1.40	1.46
1	B	30	VAL	CA-C	-5.24	1.46	1.52
3	G	187	GLU	CA-C	-5.24	1.45	1.52
2	D	318	ASP	CA-C	-5.23	1.47	1.53
3	G	68	GLN	CA-C	-5.23	1.47	1.53
2	D	49	GLU	N-CA	-5.23	1.39	1.46
2	E	301	VAL	CA-C	-5.23	1.46	1.52
2	F	35	ILE	N-CA	-5.23	1.40	1.46
2	D	447	PRO	CA-C	-5.22	1.46	1.52
1	B	344	MET	CA-C	-5.22	1.46	1.52
2	D	57	ILE	CA-C	-5.22	1.46	1.52
2	D	337	ILE	CA-C	-5.21	1.46	1.52
1	A	49	VAL	CA-C	-5.21	1.47	1.52
4	H	29	ALA	CA-C	-5.21	1.48	1.53
1	C	484	ILE	CA-C	-5.21	1.46	1.52
2	D	311	ILE	CA-C	-5.21	1.47	1.52
1	A	215	LEU	CA-C	-5.20	1.46	1.53
1	A	406	PHE	CA-C	-5.20	1.46	1.52
2	E	153	PHE	CA-C	-5.19	1.46	1.52
1	C	329	ARG	CA-C	-5.19	1.45	1.52
1	B	554	VAL	CA-C	-5.19	1.45	1.52
2	D	119	LEU	CA-C	-5.19	1.46	1.52
6	J	47	ARG	CA-C	-5.19	1.46	1.52
9	Z	56	LEU	N-CA	-5.19	1.40	1.46
1	A	218	VAL	CA-C	-5.18	1.46	1.52
1	B	265	VAL	CA-C	-5.18	1.46	1.52
1	C	25	TYR	CA-C	-5.17	1.45	1.52
1	B	355	ALA	CA-C	-5.16	1.46	1.52
1	B	215	LEU	CA-C	-5.16	1.45	1.52
1	C	24	MET	CA-C	-5.16	1.46	1.52
2	D	430	ARG	CA-C	-5.16	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	261	THR	N-CA	-5.16	1.40	1.46
2	E	8	TYR	CA-C	-5.16	1.46	1.52
6	L	130	HIS	CA-C	-5.16	1.46	1.52
2	F	208	PHE	CA-C	-5.16	1.47	1.53
4	H	70	VAL	CA-C	-5.15	1.46	1.52
2	D	325	ILE	CA-C	-5.15	1.47	1.52
1	C	133	MET	CA-C	-5.15	1.46	1.52
1	C	447	TYR	N-CA	-5.14	1.42	1.46
2	D	295	TYR	CA-C	-5.14	1.46	1.52
1	B	384	VAL	CA-C	-5.14	1.46	1.52
8	N	362	ILE	N-CA	-5.14	1.40	1.46
1	B	175	LEU	N-CA	-5.14	1.39	1.45
1	C	485	GLU	CA-C	-5.14	1.46	1.52
1	A	287	LEU	CA-C	-5.14	1.46	1.52
2	F	99	PRO	CA-C	-5.13	1.47	1.53
1	C	216	PHE	N-CA	-5.13	1.41	1.46
2	F	309	THR	CA-C	-5.13	1.45	1.52
8	N	141	ILE	N-CA	-5.13	1.40	1.46
1	C	321	ALA	CA-C	-5.13	1.48	1.53
1	C	271	GLU	CA-C	-5.12	1.46	1.52
1	A	223	THR	CA-C	-5.12	1.46	1.52
1	C	481	ARG	N-CA	-5.12	1.40	1.46
1	C	295	PRO	CA-C	-5.12	1.46	1.52
1	C	40	ILE	CA-C	-5.12	1.46	1.52
8	N	178	ALA	CA-C	-5.12	1.46	1.52
1	A	342	GLU	N-CA	-5.11	1.39	1.46
2	E	256	ILE	CA-C	-5.11	1.46	1.52
2	E	355	LEU	N-CA	-5.11	1.41	1.46
1	B	460	ARG	CA-C	-5.11	1.45	1.52
2	D	12	THR	CA-C	-5.11	1.46	1.52
3	G	171	GLY	CA-C	-5.11	1.46	1.52
4	H	46	ALA	CA-C	-5.11	1.46	1.52
2	D	56	VAL	N-CA	-5.10	1.40	1.46
2	E	271	GLY	CA-C	-5.10	1.44	1.51
1	C	84	TYR	CA-C	-5.10	1.46	1.52
1	C	10	ALA	CA-C	-5.09	1.47	1.53
1	C	327	THR	CA-C	-5.09	1.46	1.52
2	D	66	LEU	CA-C	-5.09	1.46	1.52
2	F	187	PHE	CA-C	-5.09	1.46	1.53
1	A	301	ALA	CA-C	-5.09	1.46	1.52
1	A	487	GLY	CA-C	-5.09	1.46	1.51
1	B	301	ALA	CA-C	-5.09	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	377	ALA	CA-C	-5.09	1.46	1.52
2	D	406	GLU	CA-C	-5.09	1.45	1.52
2	E	255	VAL	CA-C	-5.09	1.46	1.52
2	F	327	ASP	CA-C	-5.09	1.46	1.52
1	C	467	ILE	CA-C	-5.08	1.46	1.52
8	N	250	GLN	N-CA	-5.08	1.40	1.46
6	J	165	ASN	CA-C	-5.08	1.48	1.53
6	L	53	TYR	CA-C	-5.08	1.48	1.52
2	E	386	TYR	N-CA	-5.08	1.40	1.46
2	D	277	ILE	N-CA	-5.08	1.40	1.46
2	F	161	ASN	CA-C	-5.08	1.46	1.52
2	F	292	ALA	CA-C	-5.08	1.46	1.52
4	H	92	GLU	CA-C	-5.08	1.46	1.53
8	N	55	ARG	CA-C	-5.07	1.46	1.52
1	C	188	PRO	CA-C	-5.07	1.46	1.52
2	E	307	SER	CA-C	-5.07	1.46	1.52
2	E	385	ALA	CA-C	-5.07	1.46	1.52
1	A	397	GLN	N-CA	-5.07	1.39	1.46
2	D	315	SER	CA-C	-5.06	1.47	1.53
1	B	151	PRO	CA-C	-5.06	1.46	1.52
2	E	349	TYR	N-CA	-5.05	1.41	1.46
2	E	235	PRO	CA-C	-5.05	1.45	1.52
1	A	38	GLU	CA-C	-5.05	1.46	1.52
1	B	236	VAL	N-CA	-5.05	1.39	1.46
6	L	61	GLU	CA-C	-5.04	1.46	1.52
8	N	259	GLU	CA-C	-5.04	1.46	1.52
3	G	17	GLN	CA-C	-5.03	1.46	1.52
2	F	234	THR	N-CA	-5.03	1.40	1.46
1	B	14	VAL	CA-C	-5.03	1.46	1.52
1	B	517	LYS	CA-C	-5.03	1.46	1.52
1	C	66	SER	CA-C	-5.02	1.46	1.52
4	H	78	LYS	CA-C	-5.02	1.46	1.52
1	B	26	ASP	CA-C	-5.02	1.46	1.52
2	F	229	ILE	N-CA	-5.02	1.40	1.46
2	E	254	LEU	N-CA	-5.02	1.40	1.46
9	S	49	ARG	N-CA	-5.01	1.39	1.46
2	E	398	ILE	CA-C	-5.01	1.46	1.52
1	B	101	TYR	CA-C	-5.00	1.46	1.52
2	D	302	GLU	CA-C	-5.00	1.46	1.52
2	E	318	ASP	CA-C	-5.00	1.46	1.52

All (1378) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	X	60	LEU	N-CA-C	14.94	127.57	111.28
9	V	58	PHE	N-CA-C	13.79	125.82	111.07
2	E	287	MET	N-CA-C	-12.96	97.14	111.14
9	P	58	PHE	N-CA-C	12.70	124.66	111.07
1	A	185	HIS	CA-C-N	12.36	140.94	121.66
1	A	185	HIS	C-N-CA	12.36	140.94	121.66
9	Y	41	GLY	N-CA-C	12.22	127.39	112.73
9	V	66	VAL	N-CA-C	11.54	121.37	110.53
2	D	12	THR	N-CA-C	-11.11	101.96	114.62
2	F	87	GLU	CA-C-N	11.10	136.59	120.38
2	F	87	GLU	C-N-CA	11.10	136.59	120.38
9	V	42	VAL	CA-C-N	11.02	132.21	119.98
9	V	42	VAL	C-N-CA	11.02	132.21	119.98
6	L	132	GLU	N-CA-C	-10.73	100.73	114.04
9	U	41	GLY	N-CA-C	10.42	125.23	112.73
2	F	101	ASP	N-CA-C	-10.38	96.87	112.54
2	F	222	ASN	N-CA-C	-10.36	101.14	113.88
1	B	493	ASP	N-CA-C	-10.26	101.32	114.04
1	B	5	VAL	N-CA-C	-10.23	96.04	108.53
9	Y	40	ALA	CA-C-N	10.20	131.30	119.98
9	Y	40	ALA	C-N-CA	10.20	131.30	119.98
1	B	56	SER	N-CA-C	-10.06	98.54	110.41
1	C	203	THR	N-CA-C	-10.02	95.09	109.62
2	E	139	ASP	N-CA-C	-10.01	102.13	114.75
1	B	295	PRO	CA-C-N	9.97	134.13	120.46
1	B	295	PRO	C-N-CA	9.97	134.13	120.46
2	D	292	ALA	N-CA-C	-9.90	97.99	111.96
5	I	107	LEU	CA-C-N	9.88	133.91	120.38
5	I	107	LEU	C-N-CA	9.88	133.91	120.38
1	A	149	VAL	N-CA-C	-9.85	99.86	109.02
1	B	462	ALA	CA-C-N	9.78	130.98	120.03
1	B	462	ALA	C-N-CA	9.78	130.98	120.03
8	N	327	ALA	N-CA-C	9.75	121.99	111.36
9	V	59	LEU	CA-C-N	9.74	133.33	120.28
9	V	59	LEU	C-N-CA	9.74	133.33	120.28
2	E	412	LEU	N-CA-C	-9.65	96.80	111.56
8	N	180	VAL	N-CA-C	-9.64	94.61	108.11
2	E	12	THR	N-CA-C	-9.63	93.16	109.24
9	R	40	ALA	CA-C-N	9.59	130.62	119.98
9	R	40	ALA	C-N-CA	9.59	130.62	119.98
1	C	461	GLU	N-CA-C	-9.48	101.60	113.55
2	E	207	GLU	N-CA-C	9.42	121.15	111.07
9	X	41	GLY	N-CA-C	9.31	123.90	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	471	VAL	CA-C-N	9.30	136.47	121.87
1	C	471	VAL	C-N-CA	9.30	136.47	121.87
2	F	260	MET	CA-C-N	9.24	132.45	120.44
2	F	260	MET	C-N-CA	9.24	132.45	120.44
8	N	25	GLN	N-CA-C	9.23	120.95	111.07
2	F	53	GLU	N-CA-C	-9.22	102.54	113.88
1	A	396	THR	N-CA-C	-9.15	102.63	113.88
9	R	37	ILE	CA-C-N	9.14	130.12	119.98
9	R	37	ILE	C-N-CA	9.14	130.12	119.98
2	E	98	LYS	N-CA-C	-9.10	96.39	110.14
2	F	51	SER	N-CA-C	-9.07	94.61	109.40
9	V	60	LEU	N-CA-C	9.07	121.17	111.28
9	W	59	LEU	CA-C-N	9.06	132.43	120.28
9	W	59	LEU	C-N-CA	9.06	132.43	120.28
1	A	369	ILE	N-CA-C	-9.04	95.45	108.11
1	B	552	ARG	N-CA-C	-8.99	102.03	113.72
9	V	41	GLY	N-CA-C	8.94	123.45	112.73
2	F	281	ARG	N-CA-C	-8.92	96.01	109.83
9	V	40	ALA	CA-C-N	8.89	129.85	119.98
9	V	40	ALA	C-N-CA	8.89	129.85	119.98
8	N	26	GLN	N-CA-C	8.87	122.11	111.82
2	D	63	THR	N-CA-C	-8.84	102.91	114.31
9	P	49	ARG	CA-C-N	8.79	132.06	120.28
9	P	49	ARG	C-N-CA	8.79	132.06	120.28
2	D	170	GLN	N-CA-C	-8.76	101.90	112.59
1	C	153	VAL	N-CA-C	-8.75	94.43	107.37
2	E	21	VAL	N-CA-C	-8.67	96.90	108.35
2	D	113	PRO	N-CA-C	-8.60	98.50	111.57
9	U	40	ALA	CA-C-N	8.58	129.50	119.98
9	U	40	ALA	C-N-CA	8.58	129.50	119.98
1	B	419	PHE	N-CA-C	-8.57	92.72	109.10
1	B	386	PRO	N-CA-C	-8.55	100.27	110.70
1	B	263	THR	N-CA-C	-8.53	102.79	113.02
4	H	21	TYR	N-CA-C	-8.53	99.67	112.54
7	M	8	LEU	N-CA-C	8.51	121.32	111.11
8	N	650	GLU	N-CA-C	8.49	121.60	111.33
8	N	281	TYR	N-CA-C	-8.48	95.57	109.40
1	B	173	VAL	N-CA-C	-8.45	97.20	108.35
2	D	213	ALA	CA-C-N	8.43	131.58	120.28
2	D	213	ALA	C-N-CA	8.43	131.58	120.28
9	O	40	ALA	CA-C-N	8.41	129.32	119.98
9	O	40	ALA	C-N-CA	8.41	129.32	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	363	ASN	CA-C-N	8.40	131.36	120.44
2	E	363	ASN	C-N-CA	8.40	131.36	120.44
9	O	76	LEU	N-CA-C	8.40	120.21	111.14
1	C	141	PHE	N-CA-C	-8.38	101.38	111.69
1	A	459	GLN	N-CA-C	-8.34	101.88	110.97
9	S	60	LEU	N-CA-C	8.33	120.36	111.28
9	W	49	ARG	CA-C-N	8.32	131.44	120.28
9	W	49	ARG	C-N-CA	8.32	131.44	120.28
1	C	563	PHE	CA-C-N	8.32	131.77	120.54
1	C	563	PHE	C-N-CA	8.32	131.77	120.54
1	A	435	LEU	CA-C-N	8.31	130.48	120.09
1	A	435	LEU	C-N-CA	8.31	130.48	120.09
2	E	9	THR	N-CA-C	-8.30	97.58	109.29
1	C	422	ILE	N-CA-C	8.29	120.12	108.93
2	D	387	ALA	CA-C-N	8.29	132.48	120.38
2	D	387	ALA	C-N-CA	8.29	132.48	120.38
9	P	59	LEU	CA-C-N	8.29	131.39	120.28
9	P	59	LEU	C-N-CA	8.29	131.39	120.28
1	A	501	HIS	CA-C-N	8.28	132.04	120.29
1	A	501	HIS	C-N-CA	8.28	132.04	120.29
9	W	41	GLY	N-CA-C	8.26	122.64	112.73
2	E	331	TYR	N-CA-C	-8.25	103.03	113.43
9	T	78	GLY	N-CA-C	-8.24	102.50	116.01
5	K	107	LEU	CA-C-N	8.23	131.65	120.54
5	K	107	LEU	C-N-CA	8.23	131.65	120.54
2	E	57	ILE	N-CA-C	-8.23	96.18	108.85
1	C	2	ILE	N-CA-C	-8.21	97.51	108.35
1	C	386	PRO	N-CA-C	8.21	120.71	110.70
1	B	289	ALA	N-CA-C	8.20	121.80	110.24
1	A	274	ASP	N-CA-C	-8.19	99.33	109.65
2	D	54	TYR	N-CA-C	-8.17	97.64	108.34
5	I	23	ILE	CA-C-N	8.17	133.07	120.82
5	I	23	ILE	C-N-CA	8.17	133.07	120.82
3	G	93	VAL	N-CA-C	-8.16	96.54	108.71
1	A	410	ASP	CA-C-N	8.16	131.05	120.44
1	A	410	ASP	C-N-CA	8.16	131.05	120.44
2	E	142	ASN	N-CA-C	-8.16	93.79	108.48
1	B	177	ASP	N-CA-C	-8.13	102.40	112.88
1	A	505	ALA	N-CA-C	-8.12	103.19	113.43
1	B	150	PRO	N-CA-C	-8.07	100.86	110.70
3	G	17	GLN	CA-C-N	8.05	131.41	120.54
3	G	17	GLN	C-N-CA	8.05	131.41	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	ASN	N-CA-C	-8.04	103.19	113.16
1	A	232	SER	CA-C-N	8.03	137.14	121.41
1	A	232	SER	C-N-CA	8.03	137.14	121.41
1	B	400	LEU	CA-C-N	7.99	133.46	122.19
1	B	400	LEU	C-N-CA	7.99	133.46	122.19
9	X	42	VAL	N-CA-C	7.99	121.04	111.05
9	T	40	ALA	CA-C-N	7.99	128.85	119.98
9	T	40	ALA	C-N-CA	7.99	128.85	119.98
9	Z	12	ARG	CA-C-N	7.99	128.85	119.98
9	Z	12	ARG	C-N-CA	7.99	128.85	119.98
2	D	450	GLU	N-CA-C	-7.98	100.60	110.65
1	B	13	ALA	CA-C-N	7.98	136.33	121.97
1	B	13	ALA	C-N-CA	7.98	136.33	121.97
9	Z	37	ILE	CA-C-N	7.97	128.82	119.98
9	Z	37	ILE	C-N-CA	7.97	128.82	119.98
1	A	542	LEU	CA-C-N	7.93	127.59	119.82
1	A	542	LEU	C-N-CA	7.93	127.59	119.82
9	R	58	PHE	N-CA-C	7.92	119.55	111.07
2	D	21	VAL	N-CA-C	-7.92	96.95	107.88
1	C	231	GLY	N-CA-C	-7.91	102.91	112.48
1	B	355	ALA	N-CA-C	-7.91	102.61	111.07
1	C	263	THR	N-CA-C	-7.90	104.24	114.04
8	N	39	ALA	N-CA-C	-7.90	103.20	112.92
7	M	243	GLU	N-CA-C	-7.90	104.12	114.31
3	G	88	GLY	N-CA-C	-7.89	103.36	115.66
3	G	121	ALA	N-CA-C	-7.88	103.27	113.12
8	N	601	ALA	CA-C-N	7.86	128.71	119.98
8	N	601	ALA	C-N-CA	7.86	128.71	119.98
1	B	451	ARG	N-CA-C	-7.85	103.50	113.23
2	F	210	ARG	N-CA-C	-7.84	102.63	112.90
1	C	542	LEU	CA-C-N	7.83	127.50	119.82
1	C	542	LEU	C-N-CA	7.83	127.50	119.82
2	F	36	LYS	CA-C-N	7.83	130.78	120.28
2	F	36	LYS	C-N-CA	7.83	130.78	120.28
3	G	46	ALA	N-CA-C	7.78	120.45	111.11
9	W	40	ALA	CA-C-N	7.78	128.62	119.98
9	W	40	ALA	C-N-CA	7.78	128.62	119.98
4	H	6	ASP	N-CA-C	-7.76	100.23	110.40
3	G	10	ASN	CA-C-N	7.76	132.46	120.82
3	G	10	ASN	C-N-CA	7.76	132.46	120.82
1	A	576	ALA	N-CA-C	-7.73	104.37	113.88
8	N	224	ALA	CA-C-N	7.71	130.93	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	224	ALA	C-N-CA	7.71	130.93	120.44
6	J	9	SER	CA-C-N	7.71	130.94	120.38
6	J	9	SER	C-N-CA	7.71	130.94	120.38
1	A	140	GLU	N-CA-C	-7.70	95.74	108.76
1	B	174	VAL	N-CA-C	-7.70	96.24	108.95
9	Z	59	LEU	N-CA-C	7.67	119.64	111.28
1	A	353	TYR	CA-C-N	7.66	136.18	121.54
1	A	353	TYR	C-N-CA	7.66	136.18	121.54
2	F	28	ALA	CA-C-N	7.66	131.58	120.71
2	F	28	ALA	C-N-CA	7.66	131.58	120.71
2	D	455	SER	CA-C-N	7.65	130.86	120.38
2	D	455	SER	C-N-CA	7.65	130.86	120.38
2	F	57	ILE	N-CA-C	7.65	118.88	108.17
9	R	16	ALA	CA-C-N	7.65	130.27	120.70
9	R	16	ALA	C-N-CA	7.65	130.27	120.70
6	J	12	VAL	N-CA-C	7.64	118.42	110.62
3	G	10	ASN	N-CA-C	-7.64	102.96	111.82
9	Q	60	LEU	N-CA-C	7.64	119.61	111.28
2	E	396	VAL	N-CA-C	7.63	117.60	110.42
1	A	449	GLU	N-CA-C	-7.63	102.78	112.93
8	N	350	VAL	N-CA-C	7.62	119.31	110.62
9	V	75	ILE	CA-C-N	7.62	130.49	120.28
9	V	75	ILE	C-N-CA	7.62	130.49	120.28
1	A	2	ILE	N-CA-C	-7.61	94.61	106.72
2	F	153	PHE	N-CA-C	-7.61	96.12	108.52
9	V	54	THR	CA-C-N	7.61	130.47	120.28
9	V	54	THR	C-N-CA	7.61	130.47	120.28
1	C	487	GLY	CA-C-N	7.60	130.80	120.54
1	C	487	GLY	C-N-CA	7.60	130.80	120.54
1	A	323	MET	CA-C-N	7.60	132.73	121.72
1	A	323	MET	C-N-CA	7.60	132.73	121.72
9	X	59	LEU	CA-C-N	7.59	130.46	120.28
9	X	59	LEU	C-N-CA	7.59	130.46	120.28
9	W	78	GLY	N-CA-C	-7.59	104.73	115.43
4	H	4	ILE	N-CA-C	-7.58	96.98	107.75
1	C	91	LEU	N-CA-C	7.57	122.19	112.34
9	V	24	GLY	N-CA-C	7.57	121.66	112.49
1	A	257	GLU	CA-C-N	7.56	131.44	120.71
1	A	257	GLU	C-N-CA	7.56	131.44	120.71
1	C	430	LEU	CA-C-N	7.56	130.74	120.54
1	C	430	LEU	C-N-CA	7.56	130.74	120.54
6	L	53	TYR	N-CA-C	-7.54	102.01	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Z	61	LEU	N-CA-C	7.54	123.01	112.75
2	E	197	THR	CA-C-N	7.54	132.12	120.82
2	E	197	THR	C-N-CA	7.54	132.12	120.82
1	A	329	ARG	CA-C-N	7.53	132.11	120.82
1	A	329	ARG	C-N-CA	7.53	132.11	120.82
8	N	649	ARG	N-CA-C	7.52	122.21	112.89
8	N	326	TRP	N-CA-C	-7.50	102.70	112.68
9	O	8	GLY	N-CA-C	-7.49	100.32	110.20
2	E	320	ASP	N-CA-C	-7.46	97.37	108.79
3	G	161	VAL	CA-C-N	7.46	131.16	120.79
3	G	161	VAL	C-N-CA	7.46	131.16	120.79
9	Q	59	LEU	CA-C-N	7.45	130.26	120.28
9	Q	59	LEU	C-N-CA	7.45	130.26	120.28
9	O	61	LEU	CA-C-N	7.44	127.46	119.28
9	O	61	LEU	C-N-CA	7.44	127.46	119.28
1	A	415	PHE	N-CA-C	-7.43	103.12	111.14
9	S	18	GLY	N-CA-C	7.43	123.15	114.16
9	U	49	ARG	CA-C-N	7.39	130.19	120.28
9	U	49	ARG	C-N-CA	7.39	130.19	120.28
1	C	385	SER	CA-C-N	7.39	127.99	120.38
1	C	385	SER	C-N-CA	7.39	127.99	120.38
9	P	40	ALA	CA-C-N	7.38	128.17	119.98
9	P	40	ALA	C-N-CA	7.38	128.17	119.98
1	B	62	GLU	CA-C-N	7.38	129.06	119.84
1	B	62	GLU	C-N-CA	7.38	129.06	119.84
2	E	354	PRO	CA-C-N	7.38	130.32	120.58
2	E	354	PRO	C-N-CA	7.38	130.32	120.58
3	G	121	ALA	CA-C-N	7.38	130.16	120.28
3	G	121	ALA	C-N-CA	7.38	130.16	120.28
1	B	203	THR	N-CA-C	-7.37	98.82	110.10
2	D	363	ASN	N-CA-C	7.37	118.96	111.07
2	F	348	ILE	N-CA-C	-7.37	97.48	108.46
2	D	78	ASP	N-CA-C	-7.35	104.45	113.50
1	B	50	GLN	N-CA-C	-7.35	97.26	109.24
2	F	346	LYS	N-CA-C	-7.34	104.86	113.88
2	F	320	ASP	CA-C-N	7.33	130.42	120.38
2	F	320	ASP	C-N-CA	7.33	130.42	120.38
9	V	57	ILE	CA-C-N	7.31	129.95	120.44
9	V	57	ILE	C-N-CA	7.31	129.95	120.44
9	Z	41	GLY	N-CA-C	7.31	121.50	112.73
1	B	385	SER	N-CA-C	-7.29	98.27	109.64
1	B	511	LYS	N-CA-C	-7.28	102.51	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	15	ILE	N-CA-C	-7.28	97.67	108.45
2	D	51	SER	N-CA-C	-7.28	98.69	108.74
1	A	309	ILE	N-CA-C	-7.28	103.07	111.00
9	S	42	VAL	N-CA-C	7.28	118.04	110.62
1	C	240	SER	N-CA-C	7.27	120.13	111.33
5	K	100	ARG	CA-C-N	7.27	130.02	120.28
5	K	100	ARG	C-N-CA	7.27	130.02	120.28
2	D	111	ARG	N-CA-C	-7.26	97.98	109.23
2	D	321	ARG	N-CA-C	-7.22	103.44	112.90
9	Z	16	ALA	CA-C-N	7.20	129.70	120.70
9	Z	16	ALA	C-N-CA	7.20	129.70	120.70
8	N	457	ALA	N-CA-C	7.20	119.74	111.11
2	E	405	THR	N-CA-C	-7.19	99.81	110.46
9	V	17	VAL	N-CA-C	7.19	117.28	110.30
2	E	64	THR	N-CA-C	-7.19	98.38	109.24
9	R	60	LEU	N-CA-C	7.19	119.12	111.28
2	D	394	LYS	N-CA-C	-7.16	101.87	111.96
1	B	393	GLU	CA-C-N	7.16	128.79	119.84
1	B	393	GLU	C-N-CA	7.16	128.79	119.84
2	F	178	SER	N-CA-C	-7.16	103.71	113.30
8	N	400	PRO	CA-C-N	7.14	129.85	120.28
8	N	400	PRO	C-N-CA	7.14	129.85	120.28
8	N	324	PRO	CA-C-N	7.14	127.75	119.47
8	N	324	PRO	C-N-CA	7.14	127.75	119.47
6	L	142	LEU	N-CA-C	-7.08	105.82	114.75
7	M	17	GLY	N-CA-C	7.08	122.73	114.16
7	M	5	PHE	N-CA-C	-7.08	104.25	113.17
9	V	16	ALA	CA-C-N	7.08	129.55	120.70
9	V	16	ALA	C-N-CA	7.08	129.55	120.70
8	N	447	ILE	N-CA-C	-7.08	100.03	107.60
1	B	359	ALA	N-CA-C	7.07	119.06	111.36
2	E	252	HIS	N-CA-C	-7.07	95.44	108.02
2	E	94	ASN	N-CA-C	-7.07	98.42	109.72
9	S	40	ALA	CA-C-N	7.07	127.82	119.98
9	S	40	ALA	C-N-CA	7.07	127.82	119.98
1	B	105	GLY	N-CA-C	-7.06	105.58	115.32
1	C	64	VAL	N-CA-C	-7.05	97.87	108.17
2	D	240	THR	N-CA-C	-7.04	104.84	113.50
1	A	552	ARG	N-CA-C	-7.03	104.27	112.92
2	D	87	GLU	CA-C-N	7.03	130.64	120.38
2	D	87	GLU	C-N-CA	7.03	130.64	120.38
2	E	283	TYR	CA-C-N	7.03	127.00	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	283	TYR	C-N-CA	7.03	127.00	119.76
9	O	59	LEU	CA-C-N	7.02	129.69	120.28
9	O	59	LEU	C-N-CA	7.02	129.69	120.28
2	F	390	VAL	N-CA-C	7.02	117.78	110.62
1	C	288	ILE	N-CA-C	-7.01	98.48	108.65
8	N	527	LEU	CA-C-N	7.01	132.60	120.68
8	N	527	LEU	C-N-CA	7.01	132.60	120.68
2	F	208	PHE	CA-C-N	7.01	134.93	121.54
2	F	208	PHE	C-N-CA	7.01	134.93	121.54
4	H	92	GLU	N-CA-C	-7.01	101.95	112.04
9	Q	66	VAL	CA-C-N	7.00	130.05	120.46
9	Q	66	VAL	C-N-CA	7.00	130.05	120.46
8	N	291	GLU	N-CA-C	7.00	119.94	111.82
1	C	520	LEU	N-CA-C	-6.99	102.22	111.24
8	N	524	LEU	N-CA-C	-6.97	104.52	113.16
1	B	293	ASN	N-CA-C	-6.97	103.12	111.69
9	O	42	VAL	CA-C-N	6.96	128.84	120.14
9	O	42	VAL	C-N-CA	6.96	128.84	120.14
1	A	389	GLY	CA-C-N	6.96	134.82	121.54
1	A	389	GLY	C-N-CA	6.96	134.82	121.54
1	A	558	GLU	N-CA-C	-6.95	105.60	112.97
1	C	524	LYS	N-CA-C	6.95	120.86	112.38
1	A	122	MET	N-CA-C	-6.94	106.00	114.75
9	P	68	PHE	CA-C-N	6.94	127.68	119.98
9	P	68	PHE	C-N-CA	6.94	127.68	119.98
9	Y	37	ILE	CA-C-N	6.93	127.67	119.98
9	Y	37	ILE	C-N-CA	6.93	127.67	119.98
1	C	511	LYS	N-CA-C	-6.92	100.97	111.56
1	A	553	TYR	N-CA-C	-6.92	102.26	113.19
9	Y	54	THR	N-CA-C	6.91	118.47	111.07
2	F	207	GLU	N-CA-C	6.90	121.30	112.34
1	A	465	GLN	CA-C-N	6.89	130.37	120.79
1	A	465	GLN	C-N-CA	6.89	130.37	120.79
2	E	251	TYR	N-CA-C	-6.89	98.69	108.96
2	F	335	GLY	CA-C-O	-6.89	117.49	122.45
1	B	555	SER	CA-C-N	6.89	129.82	120.38
1	B	555	SER	C-N-CA	6.89	129.82	120.38
2	F	379	SER	CA-C-N	6.89	130.07	120.29
2	F	379	SER	C-N-CA	6.89	130.07	120.29
9	T	66	VAL	CA-C-N	6.88	129.89	120.46
9	T	66	VAL	C-N-CA	6.88	129.89	120.46
9	Q	6	ALA	N-CA-C	-6.87	103.59	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	171	ALA	N-CA-C	-6.84	98.05	109.07
3	G	160	ARG	CA-C-N	6.84	129.73	120.77
3	G	160	ARG	C-N-CA	6.84	129.73	120.77
2	F	342	GLU	N-CA-C	-6.83	103.76	111.07
1	A	337	ILE	CA-C-N	6.83	129.31	120.44
1	A	337	ILE	C-N-CA	6.83	129.31	120.44
9	Q	12	ARG	CA-C-N	6.82	127.55	119.98
9	Q	12	ARG	C-N-CA	6.82	127.55	119.98
2	E	194	MET	N-CA-C	-6.82	98.64	108.60
2	F	114	ILE	N-CA-C	-6.82	106.08	112.83
2	D	26	ASP	N-CA-C	-6.81	100.66	108.49
1	C	213	ASP	N-CA-C	-6.81	103.65	112.23
3	G	205	GLU	N-CA-C	6.80	121.60	113.16
5	K	24	LYS	CA-C-N	6.80	130.24	120.79
5	K	24	LYS	C-N-CA	6.80	130.24	120.79
9	S	49	ARG	N-CA-C	-6.80	103.93	111.82
9	Q	23	VAL	CA-C-N	6.79	127.35	119.94
9	Q	23	VAL	C-N-CA	6.79	127.35	119.94
1	A	279	GLY	CA-C-N	6.78	128.32	119.84
1	A	279	GLY	C-N-CA	6.78	128.32	119.84
2	F	100	ILE	CA-C-N	6.78	133.70	121.15
2	F	100	ILE	C-N-CA	6.78	133.70	121.15
1	A	559	PHE	CA-C-O	-6.78	112.28	118.79
1	B	446	ASP	N-CA-C	-6.78	103.38	112.94
2	E	108	PRO	CA-C-N	6.78	129.37	120.28
2	E	108	PRO	C-N-CA	6.78	129.37	120.28
2	F	429	ASN	N-CA-C	-6.77	98.16	109.07
6	J	4	LEU	CA-C-N	6.77	132.03	120.72
6	J	4	LEU	C-N-CA	6.77	132.03	120.72
1	C	29	LYS	CA-C-N	6.76	134.14	121.97
1	C	29	LYS	C-N-CA	6.76	134.14	121.97
1	B	350	TYR	CA-C-O	-6.76	113.57	119.72
1	A	534	VAL	N-CA-C	-6.75	98.17	107.75
4	H	3	VAL	N-CA-C	-6.75	97.70	108.90
6	L	153	ARG	N-CA-C	-6.74	99.49	109.81
2	E	11	ILE	CA-C-O	6.74	128.53	120.65
9	Y	42	VAL	N-CA-C	6.73	119.47	111.05
9	P	54	THR	CA-C-N	6.73	129.30	120.28
9	P	54	THR	C-N-CA	6.73	129.30	120.28
9	V	57	ILE	N-CA-C	6.72	117.50	110.72
8	N	170	GLU	N-CA-C	-6.71	97.65	109.06
9	Y	51	ASN	CA-C-N	6.71	130.18	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Y	51	ASN	C-N-CA	6.71	130.18	120.38
4	H	29	ALA	CA-C-N	6.71	129.57	120.38
4	H	29	ALA	C-N-CA	6.71	129.57	120.38
9	X	40	ALA	CA-C-N	6.68	127.39	119.98
9	X	40	ALA	C-N-CA	6.68	127.39	119.98
9	T	59	LEU	CA-C-N	6.67	129.21	120.28
9	T	59	LEU	C-N-CA	6.67	129.21	120.28
1	A	66	SER	CA-C-N	6.66	129.74	120.29
1	A	66	SER	C-N-CA	6.66	129.74	120.29
1	A	486	VAL	CA-C-N	6.65	127.50	119.99
1	A	486	VAL	C-N-CA	6.65	127.50	119.99
2	E	176	ASP	CA-C-N	6.65	131.24	120.60
2	E	176	ASP	C-N-CA	6.65	131.24	120.60
4	H	6	ASP	CA-C-N	6.65	125.88	118.97
4	H	6	ASP	C-N-CA	6.65	125.88	118.97
8	N	323	ASN	CA-C-N	6.64	127.22	120.38
8	N	323	ASN	C-N-CA	6.64	127.22	120.38
1	C	257	GLU	CA-C-N	6.63	130.13	120.71
1	C	257	GLU	C-N-CA	6.63	130.13	120.71
9	O	60	LEU	CA-C-N	6.63	128.38	120.09
9	O	60	LEU	C-N-CA	6.63	128.38	120.09
2	D	16	GLY	CA-C-N	6.62	126.31	119.56
2	D	16	GLY	C-N-CA	6.62	126.31	119.56
1	A	494	PHE	CA-C-N	6.61	131.18	120.60
1	A	494	PHE	C-N-CA	6.61	131.18	120.60
8	N	324	PRO	N-CA-C	6.61	118.76	110.70
2	E	286	TYR	CA-C-N	6.60	129.42	120.44
2	E	286	TYR	C-N-CA	6.60	129.42	120.44
1	C	508	SER	N-CA-C	-6.60	99.12	108.96
8	N	273	ARG	N-CA-C	6.60	124.85	110.80
1	A	111	LEU	N-CA-C	-6.59	98.16	108.90
9	W	37	ILE	CA-C-N	6.59	127.29	119.98
9	W	37	ILE	C-N-CA	6.59	127.29	119.98
1	A	430	LEU	N-CA-C	-6.59	105.28	113.38
9	Q	56	LEU	N-CA-C	-6.58	104.18	111.36
2	E	265	GLU	N-CA-C	-6.58	103.00	111.02
5	I	119	LEU	N-CA-C	6.58	121.69	112.75
2	D	198	GLN	N-CA-C	-6.56	103.33	112.45
1	C	351	PRO	CA-C-N	6.55	128.03	119.84
1	C	351	PRO	C-N-CA	6.55	128.03	119.84
3	G	88	GLY	CA-C-N	6.55	133.77	121.97
3	G	88	GLY	C-N-CA	6.55	133.77	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	412	SER	CA-C-N	6.54	129.29	120.65
1	B	412	SER	C-N-CA	6.54	129.29	120.65
2	E	318	ASP	N-CA-C	-6.53	104.55	113.30
9	R	49	ARG	CA-C-N	6.53	129.04	120.28
9	R	49	ARG	C-N-CA	6.53	129.04	120.28
9	X	75	ILE	CA-C-N	6.53	128.93	120.44
9	X	75	ILE	C-N-CA	6.53	128.93	120.44
9	T	57	ILE	CA-C-N	6.53	129.03	120.28
9	T	57	ILE	C-N-CA	6.53	129.03	120.28
2	E	258	THR	N-CA-C	-6.53	98.45	108.76
1	B	48	PHE	CA-C-N	6.51	129.29	120.63
1	B	48	PHE	C-N-CA	6.51	129.29	120.63
1	A	84	TYR	N-CA-C	-6.51	103.76	112.94
2	F	408	ASP	N-CA-C	-6.51	105.23	113.43
9	O	45	ILE	CA-C-N	6.51	128.90	120.44
9	O	45	ILE	C-N-CA	6.51	128.90	120.44
9	O	21	LEU	CA-C-N	6.50	128.99	120.28
9	O	21	LEU	C-N-CA	6.50	128.99	120.28
9	X	63	GLU	CA-C-N	6.50	129.86	120.38
9	X	63	GLU	C-N-CA	6.50	129.86	120.38
6	J	126	GLU	N-CA-C	-6.49	103.86	113.40
9	W	48	ASP	CA-C-N	6.48	130.16	120.31
9	W	48	ASP	C-N-CA	6.48	130.16	120.31
1	B	409	LEU	N-CA-C	6.48	119.36	108.02
1	B	389	GLY	N-CA-C	-6.47	106.98	114.69
9	S	59	LEU	CA-C-N	6.47	128.96	120.28
9	S	59	LEU	C-N-CA	6.47	128.96	120.28
2	E	453	ARG	CA-C-N	6.47	133.62	121.97
2	E	453	ARG	C-N-CA	6.47	133.62	121.97
8	N	491	HIS	CA-C-N	6.47	128.95	120.28
8	N	491	HIS	C-N-CA	6.47	128.95	120.28
9	V	67	ILE	N-CA-C	6.47	117.22	110.62
1	A	397	GLN	N-CA-C	-6.45	104.10	112.23
7	M	312	PRO	CA-C-N	6.45	128.92	120.28
7	M	312	PRO	C-N-CA	6.45	128.92	120.28
9	Y	65	LEU	N-CA-C	6.45	117.97	111.07
1	C	95	ARG	N-CA-C	6.44	118.30	111.28
9	O	65	LEU	CA-C-N	6.42	129.26	120.46
9	O	65	LEU	C-N-CA	6.42	129.26	120.46
7	M	79	GLU	CA-C-N	6.42	128.89	120.28
7	M	79	GLU	C-N-CA	6.42	128.89	120.28
1	B	86	GLY	N-CA-C	-6.42	107.61	114.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	THR	N-CA-C	-6.41	99.40	108.96
1	C	122	MET	N-CA-C	-6.41	104.37	111.36
6	L	79	VAL	N-CA-C	-6.41	104.91	110.74
2	D	38	GLY	N-CA-C	6.40	123.25	115.31
2	F	43	ARG	N-CA-C	-6.39	99.92	108.74
2	E	213	ALA	N-CA-C	-6.39	104.02	113.61
9	V	6	ALA	CA-C-N	6.39	130.22	120.82
9	V	6	ALA	C-N-CA	6.39	130.22	120.82
9	T	75	ILE	CA-C-N	6.39	128.75	120.44
9	T	75	ILE	C-N-CA	6.39	128.75	120.44
9	O	78	GLY	CA-C-N	6.38	128.84	120.28
9	O	78	GLY	C-N-CA	6.38	128.84	120.28
9	S	23	VAL	CA-C-N	6.38	127.03	119.94
9	S	23	VAL	C-N-CA	6.38	127.03	119.94
4	H	99	GLY	N-CA-C	-6.38	98.06	113.18
2	E	46	GLN	CA-C-N	6.38	130.47	122.43
2	E	46	GLN	C-N-CA	6.38	130.47	122.43
8	N	505	LEU	N-CA-C	6.38	118.23	111.28
8	N	328	LYS	N-CA-C	6.37	121.42	112.75
8	N	3	ALA	CA-C-N	6.37	126.75	119.93
8	N	3	ALA	C-N-CA	6.37	126.75	119.93
1	B	99	GLY	N-CA-C	-6.37	101.98	110.58
9	P	78	GLY	N-CA-C	-6.36	106.45	115.30
1	C	108	VAL	N-CA-C	-6.36	99.55	108.27
1	B	187	TRP	CA-C-N	6.36	126.73	119.93
1	B	187	TRP	C-N-CA	6.36	126.73	119.93
2	F	17	PRO	CA-C-N	6.36	130.17	120.82
2	F	17	PRO	C-N-CA	6.36	130.17	120.82
9	Q	40	ALA	CA-C-N	6.36	127.04	119.98
9	Q	40	ALA	C-N-CA	6.36	127.04	119.98
3	G	71	ASP	N-CA-C	-6.36	104.68	112.88
6	J	99	GLU	N-CA-C	-6.35	105.40	113.02
1	C	227	PRO	N-CA-C	-6.35	99.40	112.47
2	F	261	THR	N-CA-C	-6.34	104.29	111.07
9	V	15	ILE	CA-C-N	6.34	128.78	120.28
9	V	15	ILE	C-N-CA	6.34	128.78	120.28
9	X	79	ARG	N-CA-C	-6.34	104.00	112.94
1	C	538	GLU	N-CA-C	-6.33	103.64	112.12
1	C	102	ILE	N-CA-C	-6.33	98.39	108.90
8	N	632	PHE	N-CA-C	-6.32	97.93	109.56
1	C	241	LEU	CA-C-N	6.32	129.38	120.28
1	C	241	LEU	C-N-CA	6.32	129.38	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	277	ILE	CA-C-N	6.32	127.74	119.84
2	E	277	ILE	C-N-CA	6.32	127.74	119.84
1	A	21	GLY	N-CA-C	-6.31	106.53	115.30
1	B	279	GLY	CA-C-N	6.31	127.73	119.84
1	B	279	GLY	C-N-CA	6.31	127.73	119.84
9	T	70	LEU	N-CA-C	6.31	118.16	111.28
1	B	550	ARG	N-CA-C	-6.31	96.98	108.02
2	E	160	ALA	CA-C-N	6.31	133.59	121.54
2	E	160	ALA	C-N-CA	6.31	133.59	121.54
2	F	280	ARG	N-CA-C	-6.31	97.36	110.80
2	F	446	LEU	N-CA-C	-6.31	98.02	108.23
1	B	394	PRO	CA-C-N	6.30	130.43	120.47
1	B	394	PRO	C-N-CA	6.30	130.43	120.47
1	B	326	SER	CA-C-N	6.30	131.24	120.72
1	B	326	SER	C-N-CA	6.30	131.24	120.72
2	D	114	ILE	CA-C-N	6.30	128.72	120.28
2	D	114	ILE	C-N-CA	6.30	128.72	120.28
2	E	305	LYS	N-CA-C	-6.29	105.58	113.18
2	F	401	GLU	N-CA-C	-6.29	104.67	112.90
1	A	246	ASN	N-CA-C	-6.28	104.86	114.16
1	A	533	GLY	CA-C-N	6.28	129.15	122.11
1	A	533	GLY	C-N-CA	6.28	129.15	122.11
1	C	178	GLY	N-CA-C	-6.28	101.40	112.77
8	N	356	PRO	CA-C-N	6.27	128.68	120.28
8	N	356	PRO	C-N-CA	6.27	128.68	120.28
2	D	145	VAL	CA-C-N	6.26	133.50	121.54
2	D	145	VAL	C-N-CA	6.26	133.50	121.54
2	D	211	THR	N-CA-C	-6.26	106.23	114.31
1	B	459	GLN	N-CA-C	-6.26	105.80	113.50
7	M	185	GLN	N-CA-C	-6.26	95.97	109.81
8	N	385	ARG	CA-C-N	6.24	129.74	120.87
8	N	385	ARG	C-N-CA	6.24	129.74	120.87
9	R	75	ILE	N-CA-C	6.24	116.99	110.62
2	E	10	GLY	N-CA-C	-6.23	104.86	115.08
3	G	84	PRO	N-CA-C	-6.23	103.10	110.70
1	B	341	LEU	N-CA-C	-6.23	105.32	113.17
1	A	429	SER	N-CA-C	-6.22	97.54	110.80
8	N	466	LEU	N-CA-C	6.22	117.73	111.07
9	W	53	GLY	CA-C-N	6.22	128.62	120.28
9	W	53	GLY	C-N-CA	6.22	128.62	120.28
2	D	353	ASP	N-CA-C	-6.22	98.77	109.15
2	E	159	PRO	CA-C-N	6.21	129.42	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	159	PRO	C-N-CA	6.21	129.42	120.79
2	E	35	ILE	N-CA-C	-6.20	99.47	108.71
1	B	108	VAL	N-CA-C	-6.20	99.75	108.80
1	A	325	ASP	CA-C-N	6.19	133.37	121.54
1	A	325	ASP	C-N-CA	6.19	133.37	121.54
2	D	394	LYS	CA-C-N	6.19	129.41	120.38
2	D	394	LYS	C-N-CA	6.19	129.41	120.38
1	C	51	VAL	CA-C-N	6.18	129.18	120.28
1	C	51	VAL	C-N-CA	6.18	129.18	120.28
2	F	160	ALA	CA-C-N	6.18	129.04	120.63
2	F	160	ALA	C-N-CA	6.18	129.04	120.63
1	B	501	HIS	N-CA-C	-6.18	97.12	107.99
2	E	100	ILE	N-CA-C	-6.17	104.61	113.07
8	N	133	ASP	N-CA-C	-6.17	105.75	113.28
9	Z	62	PRO	CA-C-N	6.17	130.47	120.60
9	Z	62	PRO	C-N-CA	6.17	130.47	120.60
1	B	153	VAL	N-CA-C	-6.17	96.52	109.34
8	N	40	LEU	N-CA-C	-6.17	105.40	113.17
2	E	104	PRO	CA-C-N	6.16	127.55	119.84
2	E	104	PRO	C-N-CA	6.16	127.55	119.84
5	I	32	GLN	CA-C-N	6.16	128.45	120.44
5	I	32	GLN	C-N-CA	6.16	128.45	120.44
2	E	214	LEU	N-CA-C	-6.15	105.75	113.20
8	N	460	ALA	CA-C-N	6.15	128.52	120.28
8	N	460	ALA	C-N-CA	6.15	128.52	120.28
8	N	277	ALA	N-CA-C	-6.15	97.70	110.80
8	N	6	GLU	N-CA-C	-6.14	98.88	108.90
1	A	435	LEU	N-CA-C	-6.14	105.74	113.72
2	D	94	ASN	N-CA-C	-6.13	97.74	110.80
3	G	122	TYR	N-CA-C	-6.12	104.61	111.28
7	M	93	LEU	N-CA-C	-6.11	104.62	111.28
9	U	49	ARG	N-CA-C	-6.11	104.74	111.82
1	C	279	GLY	CA-C-N	6.10	127.46	119.84
1	C	279	GLY	C-N-CA	6.10	127.46	119.84
2	D	409	ARG	CA-C-N	6.10	128.45	120.28
2	D	409	ARG	C-N-CA	6.10	128.45	120.28
1	A	512	ALA	CA-C-N	6.09	129.96	120.82
1	A	512	ALA	C-N-CA	6.09	129.96	120.82
9	O	37	ILE	CA-C-N	6.09	126.74	119.98
9	O	37	ILE	C-N-CA	6.09	126.74	119.98
9	P	60	LEU	N-CA-C	6.09	117.92	111.28
8	N	627	GLU	N-CA-C	-6.09	103.99	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	220	PHE	N-CA-C	-6.08	100.09	109.52
9	X	56	LEU	N-CA-C	-6.08	104.73	111.36
9	S	68	PHE	CA-C-N	6.08	126.73	119.98
9	S	68	PHE	C-N-CA	6.08	126.73	119.98
2	F	79	VAL	CA-C-N	6.08	129.47	120.90
2	F	79	VAL	C-N-CA	6.08	129.47	120.90
1	C	365	ALA	CA-C-N	6.07	133.31	121.41
1	C	365	ALA	C-N-CA	6.07	133.31	121.41
7	M	320	VAL	N-CA-C	-6.07	106.84	112.43
2	E	113	PRO	N-CA-C	-6.07	100.94	111.32
2	D	25	LYS	N-CA-C	-6.06	103.61	113.19
2	E	131	ILE	N-CA-C	-6.06	100.35	108.35
3	G	203	ALA	N-CA-C	6.06	117.55	111.07
1	B	492	GLU	N-CA-C	6.05	119.13	111.69
9	Y	50	SER	N-CA-C	6.05	117.95	111.36
1	C	554	VAL	CA-C-N	6.05	129.88	120.75
1	C	554	VAL	C-N-CA	6.05	129.88	120.75
1	C	472	GLY	N-CA-C	6.04	124.67	112.34
1	C	465	GLN	CA-C-N	6.04	133.08	121.54
1	C	465	GLN	C-N-CA	6.04	133.08	121.54
2	F	371	THR	N-CA-C	-6.04	100.23	108.38
1	B	553	TYR	N-CA-C	-6.03	105.50	112.92
7	M	109	PHE	CA-C-N	6.03	128.96	120.28
7	M	109	PHE	C-N-CA	6.03	128.96	120.28
1	B	34	GLY	N-CA-C	-6.02	107.01	115.32
8	N	147	GLU	CA-C-N	6.02	128.27	120.44
8	N	147	GLU	C-N-CA	6.02	128.27	120.44
1	A	525	GLU	N-CA-C	-6.02	104.06	111.40
2	D	417	ALA	CA-C-N	6.02	130.76	121.19
2	D	417	ALA	C-N-CA	6.02	130.76	121.19
1	C	421	ALA	CA-C-N	6.01	129.55	120.77
1	C	421	ALA	C-N-CA	6.01	129.55	120.77
2	E	400	GLY	CA-C-N	6.01	133.02	121.54
2	E	400	GLY	C-N-CA	6.01	133.02	121.54
8	N	408	HIS	CA-C-N	6.00	128.68	120.46
8	N	408	HIS	C-N-CA	6.00	128.68	120.46
2	D	323	HIS	N-CA-C	-6.00	102.22	109.72
8	N	27	ALA	N-CA-C	6.00	118.61	111.71
2	E	287	MET	CA-C-N	6.00	130.72	121.19
2	E	287	MET	C-N-CA	6.00	130.72	121.19
2	E	273	ALA	N-CA-C	-5.99	104.96	112.93
2	E	321	ARG	CA-C-N	5.99	128.59	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	321	ARG	C-N-CA	5.99	128.59	120.38
2	E	358	LEU	CA-C-N	5.99	130.91	121.99
2	E	358	LEU	C-N-CA	5.99	130.91	121.99
1	C	541	GLN	N-CA-C	-5.99	106.01	113.38
7	M	244	LEU	N-CA-C	-5.99	101.27	109.71
6	J	173	ARG	N-CA-C	-5.99	103.52	111.24
9	V	68	PHE	CA-C-N	5.98	126.62	119.98
9	V	68	PHE	C-N-CA	5.98	126.62	119.98
1	A	472	GLY	N-CA-C	-5.98	100.14	112.34
1	B	512	ALA	N-CA-C	-5.98	104.67	111.07
9	O	61	LEU	N-CA-C	5.98	121.65	113.16
1	C	173	VAL	N-CA-C	-5.98	101.53	108.82
1	A	155	GLY	CA-C-N	5.98	129.78	120.75
1	A	155	GLY	C-N-CA	5.98	129.78	120.75
5	K	33	LEU	CA-C-N	5.98	128.29	120.28
5	K	33	LEU	C-N-CA	5.98	128.29	120.28
8	N	208	LEU	CA-C-N	5.97	126.61	119.98
8	N	208	LEU	C-N-CA	5.97	126.61	119.98
8	N	581	VAL	N-CA-C	-5.97	106.49	112.17
2	F	356	PRO	CA-C-N	5.97	132.94	121.54
2	F	356	PRO	C-N-CA	5.97	132.94	121.54
2	D	309	THR	N-CA-C	-5.97	99.00	108.73
1	B	229	PRO	CA-C-N	5.97	132.94	121.54
1	B	229	PRO	C-N-CA	5.97	132.94	121.54
9	W	61	LEU	N-CA-C	5.97	120.86	112.75
1	C	9	ILE	N-CA-C	-5.96	96.94	109.34
4	H	45	VAL	N-CA-C	-5.96	99.83	108.89
1	A	373	GLY	N-CA-C	-5.96	107.03	115.43
2	D	218	VAL	N-CA-C	-5.96	99.63	108.45
1	A	245	SER	N-CA-C	-5.96	100.34	108.38
1	B	333	ALA	N-CA-C	-5.96	104.13	111.40
2	D	232	ILE	N-CA-C	-5.95	106.45	113.42
1	B	436	ASP	CA-C-N	5.95	127.28	119.84
1	B	436	ASP	C-N-CA	5.95	127.28	119.84
1	C	146	LYS	CA-C-N	5.95	129.81	122.37
1	C	146	LYS	C-N-CA	5.95	129.81	122.37
9	S	58	PHE	CA-C-N	5.95	128.84	120.28
9	S	58	PHE	C-N-CA	5.95	128.84	120.28
9	W	67	ILE	CA-C-N	5.94	128.25	120.28
9	W	67	ILE	C-N-CA	5.94	128.25	120.28
8	N	286	ALA	N-CA-C	5.94	118.71	111.82
9	U	52	PHE	N-CA-C	5.94	118.52	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	GLY	N-CA-C	-5.93	106.28	116.01
2	E	136	SER	CA-C-N	5.93	129.04	120.38
2	E	136	SER	C-N-CA	5.93	129.04	120.38
6	J	88	ARG	CA-C-N	5.93	128.51	120.38
6	J	88	ARG	C-N-CA	5.93	128.51	120.38
1	C	357	ARG	CA-C-N	5.93	128.50	120.44
1	C	357	ARG	C-N-CA	5.93	128.50	120.44
7	M	10	ALA	CA-C-N	5.92	128.70	120.29
7	M	10	ALA	C-N-CA	5.92	128.70	120.29
8	N	571	GLY	CA-C-N	5.92	126.51	119.94
8	N	571	GLY	C-N-CA	5.92	126.51	119.94
1	C	66	SER	N-CA-C	-5.92	100.02	109.96
2	F	296	GLU	N-CA-C	-5.91	104.96	111.82
2	F	136	SER	CA-C-N	5.91	132.82	121.54
2	F	136	SER	C-N-CA	5.91	132.82	121.54
9	P	39	ALA	CA-C-N	5.91	128.19	120.28
9	P	39	ALA	C-N-CA	5.91	128.19	120.28
9	Z	55	ALA	CA-C-N	5.91	128.47	120.44
9	Z	55	ALA	C-N-CA	5.91	128.47	120.44
7	M	20	LEU	N-CA-C	-5.90	95.36	107.70
9	X	16	ALA	CA-C-N	5.90	128.07	120.70
9	X	16	ALA	C-N-CA	5.90	128.07	120.70
2	D	390	VAL	CA-C-N	5.89	128.45	120.38
2	D	390	VAL	C-N-CA	5.89	128.45	120.38
1	C	347	GLU	N-CA-C	-5.88	98.27	110.80
9	Q	49	ARG	CA-C-N	5.88	128.16	120.28
9	Q	49	ARG	C-N-CA	5.88	128.16	120.28
1	C	376	GLY	CA-C-N	5.88	129.70	121.24
1	C	376	GLY	C-N-CA	5.88	129.70	121.24
1	C	174	VAL	N-CA-C	-5.87	99.42	107.75
6	L	56	ALA	N-CA-C	5.87	117.48	111.14
9	R	79	ARG	N-CA-C	-5.87	104.78	112.41
1	C	438	TRP	CA-C-N	5.87	128.95	120.79
1	C	438	TRP	C-N-CA	5.87	128.95	120.79
1	A	239	GLN	CA-C-N	5.86	128.13	120.28
1	A	239	GLN	C-N-CA	5.86	128.13	120.28
9	W	52	PHE	N-CA-C	5.86	118.42	111.33
7	M	250	SER	N-CA-C	5.84	118.43	111.71
1	C	332	GLU	CA-C-N	5.84	128.11	120.28
1	C	332	GLU	C-N-CA	5.84	128.11	120.28
2	D	86	LYS	CA-C-N	5.84	128.11	120.28
2	D	86	LYS	C-N-CA	5.84	128.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	435	SER	CA-C-N	5.84	128.11	120.28
2	F	435	SER	C-N-CA	5.84	128.11	120.28
9	O	35	ALA	N-CA-C	5.84	117.32	111.07
2	D	429	ASN	N-CA-C	-5.84	99.00	108.52
6	L	27	ALA	N-CA-C	-5.83	104.52	111.69
6	L	152	VAL	N-CA-C	-5.83	99.37	108.81
1	A	405	ALA	N-CA-C	-5.82	101.31	109.69
2	E	208	PHE	CA-C-N	5.82	130.43	120.72
2	E	208	PHE	C-N-CA	5.82	130.43	120.72
8	N	395	ALA	N-CA-C	5.82	119.58	111.90
9	Q	65	LEU	CA-C-N	5.82	128.43	120.46
9	Q	65	LEU	C-N-CA	5.82	128.43	120.46
9	R	78	GLY	N-CA-C	-5.82	107.36	114.92
1	B	528	ALA	N-CA-C	-5.81	106.23	113.38
1	A	244	TRP	N-CA-C	-5.81	99.71	109.07
2	D	22	GLU	CA-C-N	5.81	132.64	121.54
2	D	22	GLU	C-N-CA	5.81	132.64	121.54
2	D	40	GLY	N-CA-C	-5.81	107.22	115.30
2	D	254	LEU	N-CA-C	-5.81	99.26	108.73
2	F	143	THR	CA-C-N	5.81	128.96	120.71
2	F	143	THR	C-N-CA	5.81	128.96	120.71
1	B	306	GLY	N-CA-C	-5.80	106.61	115.66
1	B	182	LYS	N-CA-C	-5.80	100.95	109.18
9	Y	15	ILE	N-CA-C	5.79	116.57	110.72
1	A	345	PRO	N-CA-C	-5.79	100.54	112.47
1	A	370	THR	CA-C-N	5.79	128.31	120.38
1	A	370	THR	C-N-CA	5.79	128.31	120.38
2	D	29	TYR	N-CA-C	-5.79	100.55	109.76
7	M	71	ASP	CA-C-N	5.79	128.22	120.58
7	M	71	ASP	C-N-CA	5.79	128.22	120.58
2	E	398	ILE	N-CA-C	-5.78	105.48	110.74
2	F	84	VAL	N-CA-C	5.78	117.18	107.18
7	M	219	LEU	N-CA-C	-5.78	100.25	109.96
2	E	448	GLN	N-CA-C	-5.78	106.19	113.18
9	R	59	LEU	CA-C-N	5.77	128.02	120.28
9	R	59	LEU	C-N-CA	5.77	128.02	120.28
1	A	528	ALA	N-CA-C	-5.77	106.28	113.55
2	F	203	TYR	N-CA-C	-5.77	104.36	111.40
9	P	59	LEU	N-CA-C	5.77	118.34	111.71
1	C	209	MET	CA-C-N	5.77	132.55	121.54
1	C	209	MET	C-N-CA	5.77	132.55	121.54
8	N	549	PRO	CA-C-N	5.77	132.60	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	549	PRO	C-N-CA	5.77	132.60	121.18
9	O	46	ALA	N-CA-C	5.76	117.24	111.07
8	N	349	PRO	N-CA-C	5.76	121.33	113.84
8	N	580	ASP	N-CA-C	-5.76	106.38	113.41
1	A	550	ARG	N-CA-C	-5.76	105.84	112.92
1	A	554	VAL	N-CA-C	-5.75	103.78	110.05
9	Q	37	ILE	CA-C-N	5.75	126.37	119.98
9	Q	37	ILE	C-N-CA	5.75	126.37	119.98
9	W	44	ALA	CA-C-N	5.75	128.34	120.46
9	W	44	ALA	C-N-CA	5.75	128.34	120.46
7	M	11	ARG	N-CA-C	-5.75	105.09	111.36
4	H	72	LEU	CA-C-N	5.75	126.04	119.83
4	H	72	LEU	C-N-CA	5.75	126.04	119.83
9	O	26	ALA	CA-C-N	5.75	127.98	120.28
9	O	26	ALA	C-N-CA	5.75	127.98	120.28
9	X	62	PRO	CA-C-N	5.75	129.79	120.60
9	X	62	PRO	C-N-CA	5.75	129.79	120.60
1	C	105	GLY	CA-C-N	5.74	129.13	120.75
1	C	105	GLY	C-N-CA	5.74	129.13	120.75
9	O	44	ALA	N-CA-C	5.74	117.53	111.28
9	V	72	ILE	CA-C-N	5.73	127.95	120.28
9	V	72	ILE	C-N-CA	5.73	127.95	120.28
1	A	381	VAL	N-CA-C	-5.72	97.43	109.34
2	E	74	SER	N-CA-C	-5.72	99.19	108.41
1	A	143	PHE	CA-C-N	5.72	132.47	121.54
1	A	143	PHE	C-N-CA	5.72	132.47	121.54
1	C	398	SER	N-CA-C	-5.72	102.81	111.56
7	M	175	ASP	N-CA-C	-5.72	104.96	111.14
8	N	603	VAL	CA-C-N	5.72	127.94	120.28
8	N	603	VAL	C-N-CA	5.72	127.94	120.28
1	B	277	THR	N-CA-C	-5.72	98.62	110.80
9	O	19	MET	CA-C-N	5.71	126.29	120.00
9	O	19	MET	C-N-CA	5.71	126.29	120.00
1	B	276	LYS	N-CA-C	-5.71	106.27	113.18
5	K	32	GLN	CA-C-N	5.71	127.86	120.44
5	K	32	GLN	C-N-CA	5.71	127.86	120.44
1	C	444	ALA	N-CA-C	-5.70	100.03	108.99
7	M	108	PRO	CA-C-N	5.70	127.91	120.28
7	M	108	PRO	C-N-CA	5.70	127.91	120.28
9	Y	56	LEU	CA-C-N	5.70	128.26	120.46
9	Y	56	LEU	C-N-CA	5.70	128.26	120.46
1	B	264	ASP	N-CA-C	-5.69	104.58	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	180	SER	CA-C-N	5.69	128.47	120.28
6	L	180	SER	C-N-CA	5.69	128.47	120.28
9	Q	26	ALA	CA-C-N	5.69	127.90	120.28
9	Q	26	ALA	C-N-CA	5.69	127.90	120.28
3	G	65	LEU	N-CA-C	-5.68	106.20	113.02
8	N	495	PHE	CA-C-N	5.68	127.90	120.28
8	N	495	PHE	C-N-CA	5.68	127.90	120.28
8	N	207	ALA	N-CA-C	5.68	117.47	111.28
9	R	9	GLY	CA-C-N	5.68	127.89	120.28
9	R	9	GLY	C-N-CA	5.68	127.89	120.28
2	F	227	PRO	CA-C-N	5.67	129.33	120.82
2	F	227	PRO	C-N-CA	5.67	129.33	120.82
1	A	150	PRO	N-CA-C	-5.67	103.78	110.70
1	A	263	THR	CA-C-N	5.67	127.81	120.44
1	A	263	THR	C-N-CA	5.67	127.81	120.44
3	G	28	LEU	N-CA-C	5.67	119.71	112.34
2	E	125	ARG	CA-C-N	5.67	128.73	120.51
2	E	125	ARG	C-N-CA	5.67	128.73	120.51
2	E	234	THR	CA-C-N	5.67	124.86	118.97
2	E	234	THR	C-N-CA	5.67	124.86	118.97
2	D	378	VAL	N-CA-C	-5.67	105.09	110.42
1	B	324	ALA	CA-C-N	5.67	130.43	121.99
1	B	324	ALA	C-N-CA	5.67	130.43	121.99
8	N	605	HIS	CA-C-N	5.67	127.81	120.44
8	N	605	HIS	C-N-CA	5.67	127.81	120.44
1	C	384	VAL	N-CA-C	-5.66	104.63	112.50
2	E	265	GLU	CA-C-N	5.66	128.14	120.38
2	E	265	GLU	C-N-CA	5.66	128.14	120.38
2	D	129	GLN	CA-C-N	5.66	128.75	120.71
2	D	129	GLN	C-N-CA	5.66	128.75	120.71
2	D	263	TYR	CA-C-N	5.66	128.64	120.38
2	D	263	TYR	C-N-CA	5.66	128.64	120.38
2	D	407	ASN	N-CA-C	-5.66	104.75	111.03
2	F	62	GLU	N-CA-C	-5.66	100.76	109.76
1	C	503	VAL	N-CA-C	-5.65	104.65	112.50
2	F	299	GLY	N-CA-C	5.65	121.32	111.78
1	B	126	GLY	N-CA-C	-5.64	107.45	115.30
1	C	458	LEU	CA-C-N	5.64	128.16	120.54
1	C	458	LEU	C-N-CA	5.64	128.16	120.54
8	N	413	MET	CA-C-N	5.64	128.43	120.42
8	N	413	MET	C-N-CA	5.64	128.43	120.42
9	Y	66	VAL	CA-C-N	5.64	128.19	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Y	66	VAL	C-N-CA	5.64	128.19	120.46
1	B	326	SER	N-CA-C	5.64	122.81	110.80
3	G	8	ARG	CA-C-N	5.64	132.31	121.54
3	G	8	ARG	C-N-CA	5.64	132.31	121.54
3	G	58	LYS	CA-C-N	5.63	132.30	121.54
3	G	58	LYS	C-N-CA	5.63	132.30	121.54
5	I	71	ALA	CA-C-N	5.63	127.83	120.28
5	I	71	ALA	C-N-CA	5.63	127.83	120.28
4	H	52	LEU	N-CA-C	-5.63	97.36	109.81
1	C	368	VAL	N-CA-C	5.63	118.67	109.78
1	B	294	MET	CA-C-N	5.62	126.87	119.84
1	B	294	MET	C-N-CA	5.62	126.87	119.84
2	E	212	GLY	N-CA-C	-5.62	99.86	113.18
4	H	68	LEU	CA-C-N	5.62	126.87	119.84
4	H	68	LEU	C-N-CA	5.62	126.87	119.84
1	C	234	LYS	CA-C-N	5.62	128.58	120.38
1	C	234	LYS	C-N-CA	5.62	128.58	120.38
2	D	323	HIS	CA-C-N	5.62	126.86	119.84
2	D	323	HIS	C-N-CA	5.62	126.86	119.84
9	O	75	ILE	CA-C-N	5.62	128.08	120.44
9	O	75	ILE	C-N-CA	5.62	128.08	120.44
1	C	410	ASP	CA-C-N	5.61	127.80	120.28
1	C	410	ASP	C-N-CA	5.61	127.80	120.28
5	K	22	LEU	CA-C-N	5.61	132.07	121.97
5	K	22	LEU	C-N-CA	5.61	132.07	121.97
2	F	201	LEU	N-CA-C	-5.61	104.00	111.24
7	M	245	SER	N-CA-C	-5.61	99.16	108.75
8	N	153	VAL	CA-C-N	5.61	127.79	120.28
8	N	153	VAL	C-N-CA	5.61	127.79	120.28
1	C	85	ASP	N-CA-C	-5.60	101.24	109.81
2	E	120	ASN	N-CA-C	-5.60	101.53	110.10
9	S	37	ILE	CA-C-N	5.60	126.19	119.98
9	S	37	ILE	C-N-CA	5.60	126.19	119.98
9	Z	26	ALA	CA-C-N	5.60	127.72	120.44
9	Z	26	ALA	C-N-CA	5.60	127.72	120.44
2	F	398	ILE	CA-C-N	5.60	128.13	120.46
2	F	398	ILE	C-N-CA	5.60	128.13	120.46
8	N	148	LYS	N-CA-C	-5.59	105.08	111.07
9	R	10	LEU	CA-C-N	5.59	127.71	120.44
9	R	10	LEU	C-N-CA	5.59	127.71	120.44
6	L	181	LYS	CA-C-N	5.59	128.35	120.42
6	L	181	LYS	C-N-CA	5.59	128.35	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	TYR	N-CA-C	5.59	117.56	109.07
2	D	49	GLU	N-CA-C	-5.59	100.84	108.38
2	F	226	ASP	CA-C-N	5.59	126.82	119.84
2	F	226	ASP	C-N-CA	5.59	126.82	119.84
8	N	480	ALA	CA-C-N	5.58	127.76	120.28
8	N	480	ALA	C-N-CA	5.58	127.76	120.28
8	N	548	ILE	CA-C-N	5.58	126.82	119.84
8	N	548	ILE	C-N-CA	5.58	126.82	119.84
6	J	117	GLY	N-CA-C	-5.58	104.06	112.60
8	N	41	SER	N-CA-C	-5.57	106.44	113.18
2	E	279	GLY	N-CA-C	-5.57	97.84	111.04
3	G	18	LEU	N-CA-C	-5.57	104.43	111.11
2	F	191	PHE	N-CA-C	-5.57	100.32	109.40
3	G	72	GLY	N-CA-C	-5.56	100.99	112.34
6	L	119	LYS	N-CA-C	-5.56	108.28	114.62
8	N	429	GLY	CA-C-N	5.56	127.73	120.28
8	N	429	GLY	C-N-CA	5.56	127.73	120.28
2	D	438	ILE	CA-C-N	5.56	128.00	120.38
2	D	438	ILE	C-N-CA	5.56	128.00	120.38
2	D	414	PHE	N-CA-C	-5.56	106.63	113.41
8	N	546	LEU	N-CA-C	-5.55	106.36	113.02
2	F	169	ARG	N-CA-C	-5.55	106.64	113.41
9	S	48	ASP	CA-C-N	5.55	128.75	120.31
9	S	48	ASP	C-N-CA	5.55	128.75	120.31
8	N	30	VAL	CA-C-N	5.55	130.02	122.19
8	N	30	VAL	C-N-CA	5.55	130.02	122.19
2	D	260	MET	CA-C-N	5.55	127.71	120.28
2	D	260	MET	C-N-CA	5.55	127.71	120.28
9	Q	11	ASP	CA-C-N	5.55	127.71	120.28
9	Q	11	ASP	C-N-CA	5.55	127.71	120.28
7	M	283	VAL	CA-C-N	5.54	126.24	120.03
7	M	283	VAL	C-N-CA	5.54	126.24	120.03
6	J	64	GLY	N-CA-C	5.54	119.37	112.73
6	J	152	VAL	N-CA-C	-5.53	100.26	108.45
7	M	246	GLY	N-CA-C	-5.53	108.10	115.40
1	C	165	GLU	N-CA-C	5.53	118.25	110.23
8	N	37	PRO	N-CA-C	5.52	121.02	113.84
9	Y	57	ILE	N-CA-C	-5.52	104.99	110.62
2	E	83	GLY	N-CA-C	-5.52	100.10	113.18
2	F	197	THR	CA-C-N	5.52	132.08	121.54
2	F	197	THR	C-N-CA	5.52	132.08	121.54
1	B	33	GLU	N-CA-C	-5.52	106.43	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	92	ARG	N-CA-C	-5.52	98.20	108.02
2	F	453	ARG	N-CA-C	-5.52	106.34	112.57
8	N	203	ARG	N-CA-C	-5.52	100.93	108.38
2	F	114	ILE	CA-C-N	5.51	128.12	120.29
2	F	114	ILE	C-N-CA	5.51	128.12	120.29
1	B	452	ASP	N-CA-C	-5.51	105.29	112.23
6	L	29	ALA	CA-C-N	5.51	127.50	120.56
6	L	29	ALA	C-N-CA	5.51	127.50	120.56
6	L	92	GLU	N-CA-C	-5.50	106.57	113.28
1	C	532	ARG	N-CA-C	-5.50	106.34	113.16
8	N	52	GLU	CA-C-N	5.50	127.65	120.28
8	N	52	GLU	C-N-CA	5.50	127.65	120.28
2	D	435	SER	CA-C-N	5.50	132.04	121.54
2	D	435	SER	C-N-CA	5.50	132.04	121.54
2	F	87	GLU	CA-C-O	5.50	126.31	120.10
1	B	113	ARG	N-CA-C	-5.49	106.43	113.02
8	N	528	MET	N-CA-C	-5.49	105.31	112.23
2	E	122	VAL	N-CA-C	-5.49	107.39	112.83
2	F	173	VAL	N-CA-C	-5.49	100.42	108.11
1	A	319	SER	N-CA-C	-5.49	98.82	108.20
2	D	190	VAL	N-CA-C	-5.49	100.22	108.12
7	M	141	ALA	CA-C-N	5.49	125.70	120.43
7	M	141	ALA	C-N-CA	5.49	125.70	120.43
8	N	401	GLN	CA-C-N	5.49	127.47	120.56
8	N	401	GLN	C-N-CA	5.49	127.47	120.56
1	B	542	LEU	CA-C-N	5.48	125.31	119.28
1	B	542	LEU	C-N-CA	5.48	125.31	119.28
9	X	58	PHE	N-CA-C	5.48	116.94	111.07
1	A	265	VAL	CA-C-N	5.48	127.56	120.44
1	A	265	VAL	C-N-CA	5.48	127.56	120.44
8	N	648	VAL	N-CA-C	5.48	115.68	110.53
1	C	341	LEU	CA-C-N	5.48	127.62	120.28
1	C	341	LEU	C-N-CA	5.48	127.62	120.28
2	F	308	VAL	N-CA-C	-5.47	100.72	108.65
2	F	317	PRO	N-CA-C	-5.47	101.19	112.47
8	N	409	ILE	CA-C-N	5.47	127.61	120.28
8	N	409	ILE	C-N-CA	5.47	127.61	120.28
8	N	78	ARG	CA-C-N	5.47	126.67	119.84
8	N	78	ARG	C-N-CA	5.47	126.67	119.84
2	D	131	ILE	N-CA-C	-5.46	99.93	108.95
1	C	492	GLU	N-CA-C	-5.46	106.98	113.97
5	K	103	ALA	CA-C-O	-5.46	115.28	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	THR	N-CA-C	5.46	117.01	109.15
2	D	314	LEU	N-CA-C	-5.46	101.11	109.41
4	H	42	TYR	N-CA-C	-5.46	100.81	109.76
1	B	575	LYS	CA-C-N	5.46	127.85	120.65
1	B	575	LYS	C-N-CA	5.46	127.85	120.65
6	J	101	PRO	CA-C-N	5.45	127.53	120.44
6	J	101	PRO	C-N-CA	5.45	127.53	120.44
8	N	133	ASP	CA-C-N	5.45	127.59	120.28
8	N	133	ASP	C-N-CA	5.45	127.59	120.28
2	F	96	ILE	CA-C-N	5.45	132.50	121.93
2	F	96	ILE	C-N-CA	5.45	132.50	121.93
9	O	7	SER	N-CA-C	-5.45	105.42	111.36
8	N	234	VAL	CA-C-N	5.44	127.57	120.28
8	N	234	VAL	C-N-CA	5.44	127.57	120.28
2	F	276	GLU	N-CA-C	5.44	120.02	113.17
1	A	563	PHE	CA-C-N	5.44	128.01	120.29
1	A	563	PHE	C-N-CA	5.44	128.01	120.29
9	P	10	LEU	CA-C-N	5.43	127.56	120.28
9	P	10	LEU	C-N-CA	5.43	127.56	120.28
2	E	326	PRO	N-CA-C	-5.43	101.28	112.47
7	M	104	ALA	N-CA-C	5.43	118.11	111.82
1	B	12	PRO	N-CA-C	-5.42	101.30	112.47
8	N	456	THR	CA-C-N	5.42	127.86	120.54
8	N	456	THR	C-N-CA	5.42	127.86	120.54
1	A	476	LEU	CA-C-N	5.42	131.89	121.54
1	A	476	LEU	C-N-CA	5.42	131.89	121.54
3	G	37	ALA	N-CA-C	-5.42	105.27	111.07
1	C	40	ILE	N-CA-C	-5.42	98.07	109.34
1	C	35	LEU	N-CA-C	-5.41	101.72	110.32
1	B	55	THR	N-CA-C	-5.41	100.85	109.07
2	D	278	PRO	N-CA-C	-5.41	103.35	111.57
1	C	112	ASP	N-CA-C	-5.41	99.87	109.06
1	A	72	ALA	N-CA-C	-5.41	98.75	108.48
9	W	62	PRO	CA-C-N	5.40	129.25	120.60
9	W	62	PRO	C-N-CA	5.40	129.25	120.60
7	M	106	GLY	N-CA-C	-5.40	108.18	115.36
9	P	28	LEU	CA-C-N	5.39	125.93	120.00
9	P	28	LEU	C-N-CA	5.39	125.93	120.00
3	G	85	PRO	CA-C-N	5.39	129.79	122.19
3	G	85	PRO	C-N-CA	5.39	129.79	122.19
6	L	159	GLY	N-CA-C	-5.39	108.26	115.32
8	N	361	MET	N-CA-C	-5.39	105.49	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	78	GLY	CA-C-N	5.39	127.50	120.28
9	S	78	GLY	C-N-CA	5.39	127.50	120.28
1	C	177	ASP	N-CA-C	-5.39	107.26	112.97
1	B	499	ALA	CA-C-N	5.38	127.49	120.28
1	B	499	ALA	C-N-CA	5.38	127.49	120.28
9	S	78	GLY	N-CA-C	-5.38	100.42	113.18
9	X	59	LEU	N-CA-C	5.38	117.90	111.71
2	E	118	PRO	CA-C-N	5.38	131.82	121.54
2	E	118	PRO	C-N-CA	5.38	131.82	121.54
9	R	56	LEU	N-CA-C	-5.38	105.33	111.14
3	G	103	ARG	N-CA-C	-5.38	101.26	109.65
2	F	229	ILE	CA-C-N	5.38	127.75	120.38
2	F	229	ILE	C-N-CA	5.38	127.75	120.38
8	N	586	ALA	CA-C-N	5.38	131.81	121.54
8	N	586	ALA	C-N-CA	5.38	131.81	121.54
2	D	10	GLY	N-CA-C	-5.37	100.44	113.18
2	D	157	GLY	N-CA-C	-5.37	106.81	115.08
9	P	61	LEU	N-CA-C	5.37	120.05	112.75
8	N	404	GLY	N-CA-C	5.37	119.17	112.73
2	F	108	PRO	N-CA-C	-5.37	101.41	112.47
2	F	382	LEU	N-CA-C	5.37	117.55	111.11
6	L	73	THR	CA-C-N	5.37	127.47	120.28
6	L	73	THR	C-N-CA	5.37	127.47	120.28
1	B	573	ALA	N-CA-C	-5.36	106.51	112.57
8	N	402	VAL	CA-C-N	5.36	127.80	120.46
8	N	402	VAL	C-N-CA	5.36	127.80	120.46
9	S	66	VAL	CA-C-N	5.36	127.81	120.46
9	S	66	VAL	C-N-CA	5.36	127.81	120.46
9	U	56	LEU	N-CA-C	-5.36	105.52	111.36
7	M	102	ALA	CA-C-N	5.36	127.46	120.28
7	M	102	ALA	C-N-CA	5.36	127.46	120.28
8	N	213	LEU	CA-C-N	5.36	127.41	120.44
8	N	213	LEU	C-N-CA	5.36	127.41	120.44
1	C	72	ALA	N-CA-C	-5.36	101.27	109.41
2	E	329	THR	CA-C-N	5.36	131.91	121.41
2	E	329	THR	C-N-CA	5.36	131.91	121.41
2	F	48	ILE	N-CA-C	-5.36	100.70	108.36
5	I	22	LEU	CA-C-N	5.36	131.61	121.97
5	I	22	LEU	C-N-CA	5.36	131.61	121.97
7	M	131	GLN	N-CA-C	5.36	116.92	111.14
9	X	55	ALA	CA-C-N	5.36	127.89	120.29
9	X	55	ALA	C-N-CA	5.36	127.89	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	41	ARG	N-CA-C	-5.35	99.96	109.06
2	D	246	ALA	N-CA-C	-5.35	104.87	111.40
9	P	53	GLY	CA-C-N	5.35	127.45	120.28
9	P	53	GLY	C-N-CA	5.35	127.45	120.28
1	A	193	ARG	N-CA-C	-5.35	102.24	110.32
8	N	504	GLY	CA-C-N	5.35	127.45	120.28
8	N	504	GLY	C-N-CA	5.35	127.45	120.28
7	M	91	ASN	CA-C-N	5.35	127.98	120.28
7	M	91	ASN	C-N-CA	5.35	127.98	120.28
2	E	450	GLU	N-CA-C	-5.35	105.03	112.03
2	F	233	LEU	N-CA-C	-5.34	105.57	112.68
6	J	135	ALA	N-CA-C	-5.34	105.12	111.69
1	C	128	GLU	N-CA-C	-5.34	100.59	109.46
2	D	277	ILE	N-CA-C	-5.34	97.35	108.88
6	J	162	GLN	CA-C-N	5.34	131.58	121.97
6	J	162	GLN	C-N-CA	5.34	131.58	121.97
3	G	69	ALA	N-CA-C	-5.34	99.74	109.56
1	C	525	GLU	N-CA-C	-5.33	107.14	113.97
3	G	179	ILE	CA-C-N	5.33	131.72	121.54
3	G	179	ILE	C-N-CA	5.33	131.72	121.54
9	P	35	ALA	N-CA-C	5.33	116.77	111.07
1	B	480	GLU	CA-C-N	5.33	130.90	120.99
1	B	480	GLU	C-N-CA	5.33	130.90	120.99
2	D	182	GLU	CA-C-N	5.33	127.42	120.28
2	D	182	GLU	C-N-CA	5.33	127.42	120.28
2	F	391	ASP	CA-C-N	5.32	127.36	120.70
2	F	391	ASP	C-N-CA	5.32	127.36	120.70
8	N	287	LYS	N-CA-C	5.32	120.72	113.16
9	V	10	LEU	N-CA-C	5.32	117.83	111.71
8	N	613	THR	CA-C-N	5.32	128.40	120.31
8	N	613	THR	C-N-CA	5.32	128.40	120.31
9	X	61	LEU	N-CA-C	5.32	120.71	113.16
7	M	281	LEU	N-CA-C	-5.32	105.57	111.36
9	P	79	ARG	CA-C-N	5.31	131.26	121.70
9	P	79	ARG	C-N-CA	5.31	131.26	121.70
8	N	515	TYR	N-CA-C	-5.31	107.46	114.31
9	V	21	LEU	CA-C-N	5.31	127.34	120.44
9	V	21	LEU	C-N-CA	5.31	127.34	120.44
2	D	179	GLY	N-CA-C	-5.30	106.26	113.37
9	T	65	LEU	CA-C-N	5.30	127.73	120.46
9	T	65	LEU	C-N-CA	5.30	127.73	120.46
9	R	15	ILE	N-CA-C	5.30	116.08	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Z	51	ASN	CA-C-N	5.30	128.12	120.38
9	Z	51	ASN	C-N-CA	5.30	128.12	120.38
8	N	47	PRO	CA-C-N	5.30	127.81	120.29
8	N	47	PRO	C-N-CA	5.30	127.81	120.29
1	A	108	VAL	N-CA-C	-5.30	98.32	109.34
1	B	379	THR	CA-C-N	5.30	130.30	122.94
1	B	379	THR	C-N-CA	5.30	130.30	122.94
2	E	235	PRO	CA-C-N	5.30	128.11	120.38
2	E	235	PRO	C-N-CA	5.30	128.11	120.38
7	M	175	ASP	CA-C-N	5.29	128.00	120.53
7	M	175	ASP	C-N-CA	5.29	128.00	120.53
9	S	61	LEU	N-CA-C	5.29	120.68	113.16
1	B	274	ASP	N-CA-C	-5.29	101.72	109.50
9	P	19	MET	N-CA-C	5.29	117.05	111.28
9	U	9	GLY	CA-C-N	5.29	128.35	120.31
9	U	9	GLY	C-N-CA	5.29	128.35	120.31
2	D	252	HIS	CA-C-N	5.29	127.59	120.50
2	D	252	HIS	C-N-CA	5.29	127.59	120.50
7	M	161	LEU	N-CA-C	5.29	117.45	111.11
1	A	170	GLU	N-CA-C	5.29	117.09	109.48
1	C	229	PRO	CA-C-N	5.28	131.63	121.54
1	C	229	PRO	C-N-CA	5.28	131.63	121.54
1	B	301	ALA	CA-C-N	5.28	131.62	121.54
1	B	301	ALA	C-N-CA	5.28	131.62	121.54
1	B	259	GLY	CA-C-N	5.28	128.33	120.31
1	B	259	GLY	C-N-CA	5.28	128.33	120.31
7	M	209	GLY	N-CA-C	-5.27	108.35	115.21
1	B	323	MET	CA-C-N	5.27	129.42	122.30
1	B	323	MET	C-N-CA	5.27	129.42	122.30
2	D	152	ILE	N-CA-C	-5.27	99.37	106.85
6	J	22	GLU	CA-C-N	5.27	127.34	120.28
6	J	22	GLU	C-N-CA	5.27	127.34	120.28
1	B	248	ASP	N-CA-C	-5.26	105.60	112.23
4	H	90	MET	CA-C-N	5.26	128.31	120.31
4	H	90	MET	C-N-CA	5.26	128.31	120.31
8	N	405	LYS	N-CA-C	5.26	117.09	111.36
8	N	440	THR	CA-C-N	5.26	126.41	119.84
8	N	440	THR	C-N-CA	5.26	126.41	119.84
1	C	20	LEU	N-CA-C	-5.25	100.93	108.60
2	F	200	GLU	N-CA-C	5.25	118.47	111.75
9	W	58	PHE	N-CA-C	5.25	116.69	111.07
4	H	7	PRO	CA-C-N	5.25	127.84	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	7	PRO	C-N-CA	5.25	127.84	120.28
2	F	447	PRO	CA-C-N	5.25	127.31	120.28
2	F	447	PRO	C-N-CA	5.25	127.31	120.28
7	M	217	PHE	N-CA-C	-5.25	106.83	114.12
2	F	375	HIS	CA-C-N	5.25	127.57	120.38
2	F	375	HIS	C-N-CA	5.25	127.57	120.38
9	O	57	ILE	CA-C-N	5.25	127.31	120.28
9	O	57	ILE	C-N-CA	5.25	127.31	120.28
2	E	36	LYS	N-CA-C	-5.24	100.15	109.06
1	B	355	ALA	CA-C-N	5.24	128.68	120.82
1	B	355	ALA	C-N-CA	5.24	128.68	120.82
2	E	40	GLY	CA-C-N	5.24	128.53	120.82
2	E	40	GLY	C-N-CA	5.24	128.53	120.82
8	N	619	GLN	CA-C-N	5.24	125.29	119.32
8	N	619	GLN	C-N-CA	5.24	125.29	119.32
1	C	274	ASP	N-CA-C	-5.23	98.33	108.59
4	H	9	THR	N-CA-C	-5.23	107.06	113.50
1	C	461	GLU	CA-C-N	5.23	129.51	121.19
1	C	461	GLU	C-N-CA	5.23	129.51	121.19
9	X	61	LEU	CA-C-N	5.23	125.03	119.28
9	X	61	LEU	C-N-CA	5.23	125.03	119.28
8	N	141	ILE	N-CA-C	-5.23	97.58	108.88
1	C	576	ALA	N-CA-C	-5.23	105.58	111.28
9	T	8	GLY	N-CA-C	-5.23	103.67	112.77
9	Y	7	SER	CA-C-N	5.23	125.31	120.34
9	Y	7	SER	C-N-CA	5.23	125.31	120.34
1	C	379	THR	CA-C-N	5.22	130.27	123.06
1	C	379	THR	C-N-CA	5.22	130.27	123.06
9	V	65	LEU	N-CA-C	5.22	116.66	111.07
2	D	272	ALA	N-CA-C	-5.22	106.86	113.43
2	F	175	PRO	N-CA-C	-5.22	107.39	114.80
9	P	78	GLY	CA-C-N	5.22	131.50	121.54
9	P	78	GLY	C-N-CA	5.22	131.50	121.54
3	G	118	GLY	N-CA-C	-5.21	100.82	113.18
1	A	54	ASP	N-CA-C	5.21	118.12	110.30
1	C	133	MET	N-CA-C	-5.21	101.51	108.86
1	C	120	THR	N-CA-C	-5.21	98.30	109.81
9	R	23	VAL	CA-C-N	5.21	125.62	119.94
9	R	23	VAL	C-N-CA	5.21	125.62	119.94
2	D	67	ASP	CA-C-N	5.21	131.49	121.54
2	D	67	ASP	C-N-CA	5.21	131.49	121.54
6	L	121	LEU	N-CA-C	-5.21	100.81	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	110	LYS	N-CA-C	-5.21	99.71	110.80
8	N	417	THR	CA-C-N	5.21	127.59	120.46
8	N	417	THR	C-N-CA	5.21	127.59	120.46
1	B	91	LEU	CA-C-N	5.20	127.52	120.65
1	B	91	LEU	C-N-CA	5.20	127.52	120.65
6	J	59	ARG	CA-C-N	5.20	127.68	120.29
6	J	59	ARG	C-N-CA	5.20	127.68	120.29
9	X	68	PHE	CA-C-N	5.20	125.75	119.98
9	X	68	PHE	C-N-CA	5.20	125.75	119.98
1	B	142	GLY	N-CA-C	-5.20	108.51	115.32
9	U	64	THR	CA-C-N	5.19	127.23	120.28
9	U	64	THR	C-N-CA	5.19	127.23	120.28
2	F	329	THR	CA-C-N	5.19	131.57	121.41
2	F	329	THR	C-N-CA	5.19	131.57	121.41
2	D	135	ILE	CA-C-N	5.18	127.54	120.54
2	D	135	ILE	C-N-CA	5.18	127.54	120.54
1	B	216	PHE	N-CA-C	-5.17	98.37	109.81
2	E	88	MET	N-CA-C	-5.17	100.65	108.67
6	J	125	PRO	N-CA-C	-5.17	103.15	111.38
1	C	155	GLY	N-CA-C	-5.17	100.92	113.18
1	A	76	GLY	CA-C-N	5.17	125.17	119.90
1	A	76	GLY	C-N-CA	5.17	125.17	119.90
9	O	73	ALA	N-CA-C	5.17	116.60	111.07
8	N	36	ARG	CA-C-N	5.16	124.83	119.56
8	N	36	ARG	C-N-CA	5.16	124.83	119.56
9	R	66	VAL	CA-C-N	5.16	127.53	120.46
9	R	66	VAL	C-N-CA	5.16	127.53	120.46
5	I	24	LYS	CA-C-N	5.16	127.97	120.79
5	I	24	LYS	C-N-CA	5.16	127.97	120.79
1	C	147	ILE	N-CA-C	-5.16	100.33	108.23
9	R	26	ALA	CA-C-N	5.16	127.19	120.28
9	R	26	ALA	C-N-CA	5.16	127.19	120.28
9	T	54	THR	CA-C-N	5.16	127.20	120.28
9	T	54	THR	C-N-CA	5.16	127.20	120.28
2	D	39	THR	N-CA-C	-5.16	107.15	112.93
7	M	91	ASN	CA-C-O	5.16	125.89	120.42
2	F	386	TYR	CA-C-N	5.16	129.39	121.19
2	F	386	TYR	C-N-CA	5.16	129.39	121.19
8	N	386	ASN	CA-C-N	5.15	126.53	120.09
8	N	386	ASN	C-N-CA	5.15	126.53	120.09
1	C	303	ILE	CA-C-N	5.15	131.38	121.54
1	C	303	ILE	C-N-CA	5.15	131.38	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	384	LYS	CA-C-N	5.15	127.18	120.28
8	N	384	LYS	C-N-CA	5.15	127.18	120.28
1	A	393	GLU	CA-C-N	5.15	124.65	119.19
1	A	393	GLU	C-N-CA	5.15	124.65	119.19
2	D	302	GLU	N-CA-C	-5.15	101.01	109.40
6	L	109	LEU	CA-C-N	5.15	127.43	120.38
6	L	109	LEU	C-N-CA	5.15	127.43	120.38
8	N	592	LEU	N-CA-C	5.15	116.70	111.14
3	G	142	ASN	N-CA-C	-5.14	107.67	114.04
8	N	561	HIS	CA-C-N	5.14	127.04	120.56
8	N	561	HIS	C-N-CA	5.14	127.04	120.56
9	U	10	LEU	CA-C-N	5.14	127.12	120.44
9	U	10	LEU	C-N-CA	5.14	127.12	120.44
9	W	57	ILE	N-CA-C	5.14	115.91	110.72
1	B	499	ALA	N-CA-C	-5.13	105.37	111.69
3	G	188	ARG	N-CA-C	-5.13	105.33	111.03
2	F	441	ALA	N-CA-C	-5.13	105.77	111.36
1	B	252	TYR	N-CA-C	-5.13	100.95	109.46
2	E	260	MET	CA-C-N	5.13	131.34	121.54
2	E	260	MET	C-N-CA	5.13	131.34	121.54
1	A	203	THR	CA-C-N	5.13	125.11	120.03
1	A	203	THR	C-N-CA	5.13	125.11	120.03
1	B	400	LEU	O-C-N	5.12	129.06	123.01
9	Y	10	LEU	CA-C-N	5.12	127.10	120.44
9	Y	10	LEU	C-N-CA	5.12	127.10	120.44
4	H	98	ILE	N-CA-C	5.12	119.99	109.34
8	N	69	LEU	CA-C-N	5.12	127.14	120.28
8	N	69	LEU	C-N-CA	5.12	127.14	120.28
6	L	122	VAL	N-CA-C	-5.12	100.91	108.23
2	D	152	ILE	CA-C-N	5.12	128.12	120.95
2	D	152	ILE	C-N-CA	5.12	128.12	120.95
1	C	71	LEU	N-CA-C	5.12	117.65	110.23
1	C	485	GLU	CA-C-N	5.12	127.00	120.56
1	C	485	GLU	C-N-CA	5.12	127.00	120.56
8	N	256	ALA	CA-C-N	5.12	127.14	120.28
8	N	256	ALA	C-N-CA	5.12	127.14	120.28
2	E	81	ARG	N-CA-C	-5.11	100.37	108.14
7	M	92	ASP	CA-C-N	5.11	127.13	120.28
7	M	92	ASP	C-N-CA	5.11	127.13	120.28
8	N	604	LEU	N-CA-C	5.11	116.85	111.28
9	R	76	LEU	N-CA-C	5.11	116.66	111.14
8	N	622	ARG	CA-C-N	5.11	127.08	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	622	ARG	C-N-CA	5.11	127.08	120.44
9	V	64	THR	N-CA-C	5.10	117.58	111.71
1	A	176	GLU	N-CA-C	-5.10	107.01	113.18
1	C	352	PRO	CA-C-N	5.10	129.76	122.21
1	C	352	PRO	C-N-CA	5.10	129.76	122.21
1	C	575	LYS	N-CA-C	-5.10	107.06	113.28
9	Z	68	PHE	CA-C-N	5.10	125.64	119.98
9	Z	68	PHE	C-N-CA	5.10	125.64	119.98
1	A	571	GLN	N-CA-C	-5.09	107.02	113.18
2	E	454	ILE	N-CA-C	-5.09	98.75	109.34
7	M	95	ASN	CA-C-N	5.09	127.10	120.28
7	M	95	ASN	C-N-CA	5.09	127.10	120.28
5	I	81	THR	CA-C-N	5.09	127.52	120.29
5	I	81	THR	C-N-CA	5.09	127.52	120.29
9	W	46	ALA	N-CA-C	-5.09	105.62	111.07
1	B	26	ASP	CA-C-N	5.09	128.18	120.75
1	B	26	ASP	C-N-CA	5.09	128.18	120.75
2	D	431	SER	CA-C-N	5.09	127.70	120.53
2	D	431	SER	C-N-CA	5.09	127.70	120.53
6	L	98	PRO	N-CA-C	-5.09	106.10	114.75
9	P	5	ALA	CA-C-N	5.09	131.26	121.54
9	P	5	ALA	C-N-CA	5.09	131.26	121.54
1	A	428	TYR	N-CA-C	-5.08	101.53	108.24
2	D	197	THR	CA-C-N	5.08	132.46	121.64
2	D	197	THR	C-N-CA	5.08	132.46	121.64
9	V	61	LEU	N-CA-C	5.08	120.37	113.16
1	A	187	TRP	CA-C-N	5.08	126.19	119.84
1	A	187	TRP	C-N-CA	5.08	126.19	119.84
2	D	346	LYS	N-CA-C	-5.08	106.60	112.89
2	E	54	TYR	N-CA-C	-5.08	101.58	109.14
1	A	523	TYR	CA-C-N	5.07	127.79	120.38
1	A	523	TYR	C-N-CA	5.07	127.79	120.38
1	B	64	VAL	N-CA-C	-5.07	98.79	109.34
2	E	56	VAL	N-CA-C	-5.07	100.81	108.12
2	E	449	GLY	N-CA-C	-5.07	107.66	115.73
2	D	415	ALA	CA-C-N	5.07	131.22	121.54
2	D	415	ALA	C-N-CA	5.07	131.22	121.54
1	C	270	PRO	N-CA-C	-5.07	107.14	114.18
5	K	118	VAL	CA-C-N	5.07	127.05	120.26
5	K	118	VAL	C-N-CA	5.07	127.05	120.26
9	W	54	THR	CA-C-N	5.07	127.07	120.28
9	W	54	THR	C-N-CA	5.07	127.07	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	GLU	N-CA-C	-5.07	107.49	113.97
2	E	269	GLU	CA-C-N	5.07	127.14	120.60
2	E	269	GLU	C-N-CA	5.07	127.14	120.60
2	D	451	LEU	N-CA-C	-5.06	100.01	110.80
4	H	54	ASP	CA-C-O	-5.06	113.22	120.16
6	J	23	ALA	CA-C-N	5.06	127.02	120.44
6	J	23	ALA	C-N-CA	5.06	127.02	120.44
6	J	8	LEU	CA-C-N	5.06	127.33	120.65
6	J	8	LEU	C-N-CA	5.06	127.33	120.65
8	N	453	ARG	N-CA-C	-5.06	105.84	111.36
1	A	130	ARG	CA-C-N	5.06	124.77	119.92
1	A	130	ARG	C-N-CA	5.06	124.77	119.92
6	J	181	LYS	CA-C-N	5.06	127.60	120.42
6	J	181	LYS	C-N-CA	5.06	127.60	120.42
1	A	294	MET	CA-C-N	5.05	125.05	119.90
1	A	294	MET	C-N-CA	5.05	125.05	119.90
1	C	512	ALA	CA-C-N	5.05	127.36	120.54
1	C	512	ALA	C-N-CA	5.05	127.36	120.54
1	C	11	GLY	CA-C-N	5.05	124.83	119.28
1	C	11	GLY	C-N-CA	5.05	124.83	119.28
8	N	572	GLY	CA-C-N	5.05	127.59	120.42
8	N	572	GLY	C-N-CA	5.05	127.59	120.42
9	Y	40	ALA	N-CA-C	5.05	116.78	111.28
8	N	157	LEU	CA-C-N	5.05	127.00	120.44
8	N	157	LEU	C-N-CA	5.05	127.00	120.44
9	P	14	LEU	N-CA-C	5.05	116.86	111.36
7	M	134	ALA	CA-C-N	5.04	125.58	119.98
7	M	134	ALA	C-N-CA	5.04	125.58	119.98
8	N	420	TRP	CA-C-N	5.04	126.45	120.14
8	N	420	TRP	C-N-CA	5.04	126.45	120.14
2	D	188	ALA	N-CA-C	-5.04	101.07	108.99
4	H	58	ALA	CA-C-N	5.04	127.37	120.46
4	H	58	ALA	C-N-CA	5.04	127.37	120.46
2	F	410	ARG	N-CA-C	-5.04	106.82	113.12
9	U	8	GLY	CA-C-N	5.04	124.89	120.10
9	U	8	GLY	C-N-CA	5.04	124.89	120.10
9	X	54	THR	CA-C-N	5.04	127.03	120.28
9	X	54	THR	C-N-CA	5.04	127.03	120.28
1	B	371	LEU	N-CA-C	-5.03	107.09	113.18
1	B	474	ASP	N-CA-C	-5.03	100.08	110.80
2	E	175	PRO	CA-C-N	5.03	128.37	120.82
2	E	175	PRO	C-N-CA	5.03	128.37	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	68	SER	N-CA-C	5.03	116.45	111.07
2	F	390	VAL	CA-C-N	5.03	128.36	120.82
2	F	390	VAL	C-N-CA	5.03	128.36	120.82
8	N	645	PHE	CA-C-N	5.03	127.32	120.54
8	N	645	PHE	C-N-CA	5.03	127.32	120.54
1	A	137	THR	CA-C-N	5.02	127.22	122.85
1	A	137	THR	C-N-CA	5.02	127.22	122.85
2	F	286	TYR	N-CA-C	-5.02	105.81	111.28
2	E	52	GLU	N-CA-C	-5.02	100.11	110.80
9	O	66	VAL	CA-C-N	5.02	127.34	120.46
9	O	66	VAL	C-N-CA	5.02	127.34	120.46
3	G	86	LEU	N-CA-C	-5.02	104.97	111.74
6	J	65	GLU	CA-C-N	5.02	127.94	120.31
6	J	65	GLU	C-N-CA	5.02	127.94	120.31
2	D	449	GLY	N-CA-C	-5.02	107.73	114.25
2	E	327	ASP	CA-C-N	5.01	131.11	121.54
2	E	327	ASP	C-N-CA	5.01	131.11	121.54
8	N	502	LEU	CA-C-N	5.01	126.41	120.14
8	N	502	LEU	C-N-CA	5.01	126.41	120.14
2	D	362	MET	CA-C-N	5.01	126.96	120.44
2	D	362	MET	C-N-CA	5.01	126.96	120.44
2	F	213	ALA	N-CA-C	-5.01	107.00	113.01
8	N	80	PHE	CA-C-N	5.01	126.11	119.84
8	N	80	PHE	C-N-CA	5.01	126.11	119.84
9	X	45	ILE	CA-C-N	5.01	126.95	120.44
9	X	45	ILE	C-N-CA	5.01	126.95	120.44
4	H	30	GLN	CA-C-N	5.01	131.10	121.54
4	H	30	GLN	C-N-CA	5.01	131.10	121.54
4	H	49	GLU	N-CA-C	-5.01	107.12	113.18
2	F	172	THR	N-CA-C	-5.00	101.68	109.14
9	T	45	ILE	CA-C-N	5.00	126.94	120.44
9	T	45	ILE	C-N-CA	5.00	126.94	120.44
5	K	47	ARG	N-CA-C	5.00	117.46	111.71

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	VAL	Mainchain
1	A	49	VAL	Mainchain
1	B	358	LEU	Peptide,Mainchain
1	B	379	THR	Mainchain

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Mol	Chain	Res	Type	Group
1	C	346	ALA	Mainchain
2	F	160	ALA	Mainchain
2	F	204	PHE	Mainchain
7	M	183	LEU	Peptide
7	M	3	ASP	Peptide
7	M	5	PHE	Mainchain
9	P	60	LEU	Mainchain
9	U	48	ASP	Mainchain
9	Y	41	GLY	Peptide,Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2307	0	654	4	0
1	B	2307	0	654	7	0
1	C	2307	0	654	6	0
2	D	1835	0	512	2	0
2	E	1835	0	512	2	0
2	F	1835	0	512	4	0
3	G	839	0	230	1	0
4	H	399	0	119	2	0
5	I	399	0	100	0	0
5	K	399	0	100	0	0
6	J	738	0	192	1	0
6	L	738	0	192	2	0
7	M	1279	0	357	0	0
8	N	2526	0	709	1	0
9	O	303	0	102	0	0
9	P	303	0	102	1	0
9	Q	303	0	102	0	0
9	R	303	0	102	0	0
9	S	303	0	102	0	0
9	T	303	0	102	0	0
9	U	303	0	102	0	0
9	V	303	0	102	0	0
9	W	303	0	102	0	0
9	X	303	0	102	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Y	303	0	102	1	0
9	Z	303	0	102	0	0
10	A	27	0	12	0	0
10	B	27	0	12	1	0
All	All	23433	0	6745	33	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (33) 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:352:PRO:C	1:A:354:LEU:H	2.08	0.61
1:B:6:ILE:H	1:B:62:GLU:H	1.51	0.58
6:L:151:GLY:HA2	6:L:167:LEU:H	1.69	0.57
1:C:24:MET:H	2:F:66:LEU:N	2.10	0.50
1:A:489:ILE:C	1:A:491:ARG:H	2.20	0.50
1:B:236:VAL:H	10:B:600:ADP:PA	2.35	0.49
9:X:11:ASP:H	9:Y:8:GLY:H	1.61	0.49
2:F:259:ASP:C	2:F:261:THR:H	2.21	0.48
8:N:526:GLY:C	8:N:528:MET:H	2.22	0.48
9:P:78:GLY:C	9:P:80:LEU:H	2.22	0.48
1:C:339:SER:C	1:C:341:LEU:H	2.22	0.48
1:C:493:ASP:C	1:C:495:LEU:H	2.23	0.46
2:E:214:LEU:C	2:E:216:ARG:H	2.24	0.46
3:G:8:ARG:C	3:G:10:ASN:H	2.23	0.46
1:C:345:PRO:C	1:C:347:GLU:H	2.22	0.46
1:C:151:PRO:C	1:C:153:VAL:H	2.24	0.45
1:C:345:PRO:C	1:C:347:GLU:N	2.76	0.44
6:J:51:ALA:C	6:J:53:TYR:H	2.26	0.43
2:F:51:SER:C	2:F:53:GLU:H	2.27	0.43
1:B:133:MET:H	1:B:149:VAL:H	1.66	0.43
1:A:414:ALA:C	1:A:417:ARG:H	2.26	0.42
4:H:5:ALA:H	4:H:22:GLY:HA2	1.85	0.42
2:D:321:ARG:C	2:D:323:HIS:H	2.28	0.42
2:E:452:LYS:C	2:E:454:ILE:H	2.28	0.42
2:D:227:PRO:C	2:D:229:ILE:H	2.28	0.41
6:L:151:GLY:CA	6:L:167:LEU:H	2.32	0.41
1:B:262:MET:C	1:B:264:ASP:H	2.28	0.41
1:A:557:GLU:C	1:A:559:PHE:H	2.28	0.41
1:B:281:LEU:C	1:B:283:HIS:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ASN:C	1:B:427:SER:H	2.29	0.41
1:B:6:ILE:H	1:B:62:GLU:N	2.18	0.40
4:H:5:ALA:H	4:H:22:GLY:CA	2.34	0.40
2:F:122:VAL:C	2:F:124:ARG:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/578 (100%)	462 (80%)	75 (13%)	38 (7%)	1	12
1	B	575/578 (100%)	448 (78%)	86 (15%)	41 (7%)	1	11
1	C	575/578 (100%)	417 (72%)	102 (18%)	56 (10%)	0	7
2	D	457/478 (96%)	355 (78%)	75 (16%)	27 (6%)	1	13
2	E	457/478 (96%)	334 (73%)	84 (18%)	39 (8%)	0	9
2	F	457/478 (96%)	334 (73%)	79 (17%)	44 (10%)	0	7
3	G	208/223 (93%)	149 (72%)	39 (19%)	20 (10%)	0	7
4	H	98/104 (94%)	62 (63%)	24 (24%)	12 (12%)	0	4
5	I	98/120 (82%)	91 (93%)	5 (5%)	2 (2%)	6	31
5	K	98/120 (82%)	94 (96%)	2 (2%)	2 (2%)	6	31
6	J	181/188 (96%)	155 (86%)	19 (10%)	7 (4%)	2	19
6	L	181/188 (96%)	155 (86%)	22 (12%)	4 (2%)	5	29
7	M	318/323 (98%)	299 (94%)	12 (4%)	7 (2%)	5	29
8	N	628/652 (96%)	550 (88%)	49 (8%)	29 (5%)	2	17
9	O	74/99 (75%)	70 (95%)	4 (5%)	0	100	100
9	P	74/99 (75%)	71 (96%)	2 (3%)	1 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Q	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	9	40
9	R	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	S	74/99 (75%)	73 (99%)	1 (1%)	0	100	100
9	T	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	U	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	V	74/99 (75%)	74 (100%)	0	0	100	100
9	W	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	9	40
9	X	74/99 (75%)	73 (99%)	1 (1%)	0	100	100
9	Y	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	Z	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	9	40
All	All	5794/6274 (92%)	4770 (82%)	692 (12%)	332 (6%)	2	14

All (332) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	THR
1	A	210	ARG
1	A	227	PRO
1	A	229	PRO
1	A	233	GLY
1	A	354	LEU
1	A	375	GLU
1	A	390	ASP
1	A	477	GLN
1	B	14	VAL
1	B	70	PRO
1	B	234	LYS
1	B	326	SER
1	B	392	SER
1	B	471	VAL
1	B	480	GLU
1	C	30	VAL
1	C	134	VAL
1	C	159	GLU
1	C	210	ARG
1	C	227	PRO
1	C	246	ASN
1	C	303	ILE

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Mol	Chain	Res	Type
1	C	304	TYR
1	C	305	VAL
1	C	370	THR
1	C	466	GLU
1	C	472	GLY
2	D	15	SER
2	D	94	ASN
2	D	110	LYS
2	D	128	GLU
2	D	139	ASP
2	D	276	GLU
2	D	327	ASP
2	D	356	PRO
2	D	375	HIS
2	D	403	ALA
2	E	24	ALA
2	E	84	VAL
2	E	119	LEU
2	E	175	PRO
2	E	216	ARG
2	E	250	ASP
2	E	278	PRO
2	E	286	TYR
2	E	354	PRO
2	F	96	ILE
2	F	351	PRO
2	F	357	SER
2	F	419	GLU
3	G	4	VAL
3	G	64	LEU
3	G	70	PHE
3	G	96	VAL
3	G	99	SER
4	H	79	GLU
5	I	23	ILE
6	J	163	VAL
6	J	180	SER
5	K	23	ILE
6	L	180	SER
7	M	4	ASP
8	N	38	GLU
8	N	173	ALA

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Mol	Chain	Res	Type
8	N	273	ARG
8	N	348	THR
8	N	544	ILE
8	N	642	TYR
9	P	6	ALA
1	A	31	GLY
1	A	108	VAL
1	A	154	ARG
1	A	202	ASN
1	A	222	GLY
1	A	255	CYS
1	A	326	SER
1	A	377	ALA
1	A	384	VAL
1	A	429	SER
1	A	444	ALA
1	A	463	GLY
1	A	512	ALA
1	B	64	VAL
1	B	140	GLU
1	B	153	VAL
1	B	202	ASN
1	B	282	MET
1	B	416	ARG
1	B	432	THR
1	C	53	GLU
1	C	77	PRO
1	C	233	GLY
1	C	259	GLY
1	C	290	ASN
1	C	292	SER
1	C	340	ARG
1	C	365	ALA
1	C	386	PRO
1	C	397	GLN
1	C	443	VAL
1	C	510	LYS
2	D	23	ASN
2	D	69	ALA
2	D	140	VAL
2	D	389	GLY
2	D	402	ASP

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Mol	Chain	Res	Type
2	D	436	LEU
2	E	49	GLU
2	E	77	GLU
2	E	156	SER
2	E	164	ALA
2	E	210	ARG
2	E	293	THR
2	E	330	GLY
2	E	371	THR
2	E	452	LYS
2	F	12	THR
2	F	17	PRO
2	F	26	ASP
2	F	61	GLU
2	F	137	THR
2	F	147	GLY
2	F	188	ALA
2	F	189	VAL
2	F	215	SER
2	F	216	ARG
2	F	225	ASP
2	F	239	LEU
2	F	274	ARG
2	F	278	PRO
2	F	280	ARG
2	F	298	ALA
2	F	332	ILE
2	F	340	SER
2	F	356	PRO
3	G	85	PRO
3	G	89	VAL
3	G	134	ALA
3	G	174	ALA
3	G	180	GLN
4	H	18	LEU
4	H	48	ASP
4	H	74	ILE
4	H	80	ALA
6	J	179	SER
6	L	143	GLN
7	M	76	VAL
7	M	280	PRO

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Mol	Chain	Res	Type
8	N	5	MET
8	N	277	ALA
8	N	434	HIS
8	N	586	ALA
1	A	90	PRO
1	A	152	ASP
1	A	280	PRO
1	B	12	PRO
1	B	13	ALA
1	B	63	PRO
1	B	66	SER
1	B	139	PRO
1	B	233	GLY
1	B	295	PRO
1	B	302	SER
1	B	347	GLU
1	B	348	GLU
1	B	478	ASP
1	B	551	ALA
1	C	142	GLY
1	C	163	ALA
1	C	170	GLU
1	C	199	LEU
1	C	255	CYS
1	C	256	GLY
1	C	291	THR
1	C	302	SER
1	C	347	GLU
1	C	359	ALA
1	C	418	HIS
1	C	475	ALA
1	C	535	SER
2	D	146	ARG
2	E	78	ASP
2	E	95	GLY
2	E	105	PRO
2	E	116	GLY
2	E	128	GLU
2	E	159	PRO
2	E	215	SER
2	E	237	MET
2	E	259	ASP

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Mol	Chain	Res	Type
2	E	317	PRO
2	E	326	PRO
2	E	401	GLU
2	F	128	GLU
2	F	227	PRO
2	F	358	LEU
2	F	398	ILE
3	G	110	ASP
3	G	117	VAL
3	G	168	VAL
4	H	5	ALA
4	H	15	LEU
6	J	127	ASP
6	L	144	ALA
8	N	162	GLU
8	N	271	SER
8	N	340	PRO
8	N	341	LYS
8	N	441	PRO
9	Q	77	ASN
1	A	3	GLN
1	A	475	ALA
1	B	71	LEU
1	B	214	VAL
1	B	257	GLU
1	B	280	PRO
1	C	195	VAL
1	C	230	PHE
1	C	432	THR
2	D	27	LEU
2	D	280	ARG
2	D	383	TYR
2	E	99	PRO
2	E	336	GLN
2	E	351	PRO
2	E	362	MET
2	E	404	LEU
2	F	10	GLY
2	F	54	TYR
2	F	166	GLN
2	F	235	PRO
2	F	309	THR

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Mol	Chain	Res	Type
2	F	435	SER
2	F	444	SER
3	G	108	PHE
4	H	25	SER
4	H	54	ASP
5	I	104	MET
6	J	157	ALA
6	J	162	GLN
5	K	104	MET
8	N	36	ARG
8	N	74	ALA
8	N	270	ALA
8	N	278	LEU
8	N	388	PRO
8	N	436	GLY
8	N	640	ARG
9	W	79	ARG
1	A	36	VAL
1	A	403	VAL
1	A	473	PRO
1	A	542	LEU
1	B	204	PRO
1	B	278	GLY
1	B	304	TYR
1	B	484	ILE
1	C	25	TYR
1	C	179	THR
1	C	229	PRO
1	C	296	VAL
1	C	324	ALA
1	C	478	ASP
2	D	99	PRO
2	D	143	THR
2	D	351	PRO
2	D	358	LEU
2	D	390	VAL
2	E	168	ALA
2	E	425	GLN
2	F	6	LYS
2	F	136	SER
2	F	256	ILE
2	F	270	ILE

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Mol	Chain	Res	Type
2	F	317	PRO
3	G	116	PRO
3	G	119	THR
3	G	123	THR
4	H	55	PRO
6	J	52	GLN
6	L	52	GLN
7	M	77	THR
8	N	136	PRO
8	N	294	LEU
8	N	437	VAL
9	Z	6	ALA
1	B	428	TYR
1	C	395	VAL
1	C	413	LEU
1	C	471	VAL
1	C	500	TYR
1	C	509	MET
2	D	316	MET
2	F	139	ASP
2	F	412	LEU
3	G	84	PRO
7	M	212	LEU
8	N	446	LEU
1	A	443	VAL
1	A	514	GLY
2	D	355	LEU
2	F	284	PRO
4	H	53	PRO
7	M	185	GLN
7	M	277	VAL
8	N	79	PRO
8	N	390	VAL
1	B	275	PRO
1	B	443	VAL
2	E	117	LEU
2	F	185	GLU
3	G	154	ILE
1	A	5	VAL
1	A	345	PRO
1	A	490	ILE
1	B	222	GLY

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Mol	Chain	Res	Type
1	C	172	VAL
1	C	394	PRO
1	C	468	VAL
3	G	179	ILE
1	A	40	ILE
1	A	447	TYR
1	B	172	VAL
1	C	40	ILE
1	C	236	VAL
2	E	106	ILE
2	F	326	PRO
8	N	131	GLY
1	B	366	GLY
1	B	560	PRO
4	H	98	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	ADP	A	600	-	28,29,29	1.29	2 (7%)	43,45,45	0.95	1 (2%)
10	ADP	B	600	-	28,29,29	0.78	0	43,45,45	1.12	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	A	600	-	-	5/16/32/32	0/3/3/3
10	ADP	B	600	-	-	6/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	600	ADP	PA-O3A	-5.32	1.53	1.59
10	A	600	ADP	PA-O2A	-2.04	1.45	1.55

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	600	ADP	N6-C6-N1	3.20	125.51	118.38
10	A	600	ADP	N6-C6-N1	2.64	124.25	118.38
10	B	600	ADP	C4'-O4'-C1'	-2.27	104.44	109.47

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	600	ADP	C5'-O5'-PA-O3A
10	B	600	ADP	C5'-O5'-PA-O2A
10	B	600	ADP	C5'-O5'-PA-O3A
10	A	600	ADP	C3'-C4'-C5'-O5'
10	B	600	ADP	C3'-C4'-C5'-O5'
10	A	600	ADP	O4'-C4'-C5'-O5'
10	A	600	ADP	C4'-C5'-O5'-PA

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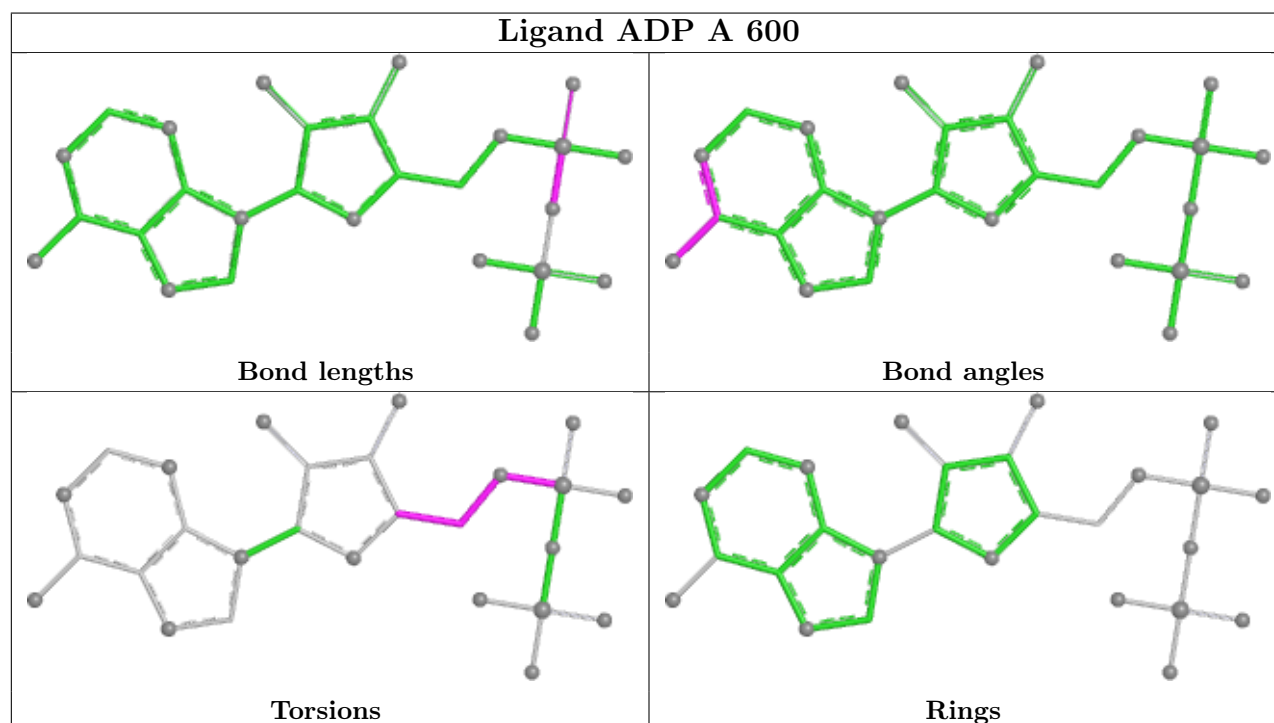
Mol	Chain	Res	Type	Atoms
10	B	600	ADP	O4'-C4'-C5'-O5'
10	B	600	ADP	PB-O3A-PA-O5'
10	A	600	ADP	C5'-O5'-PA-O1A
10	B	600	ADP	C4'-C5'-O5'-PA

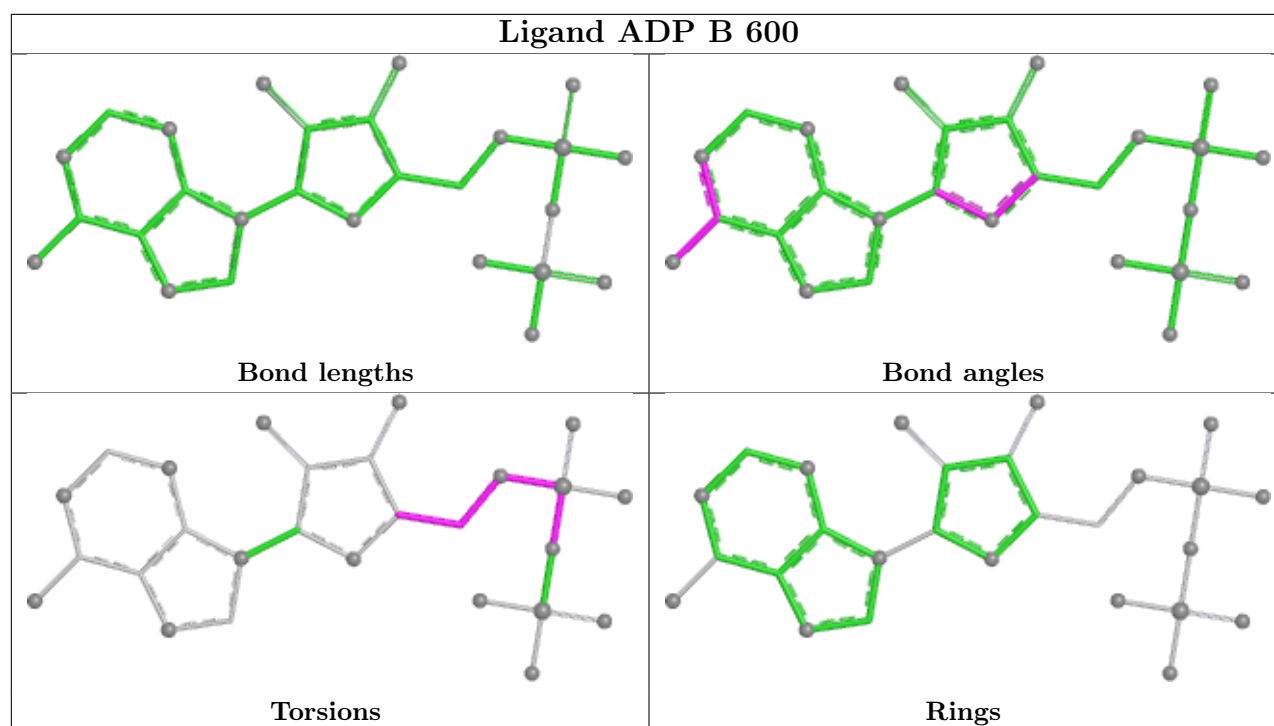
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	600	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

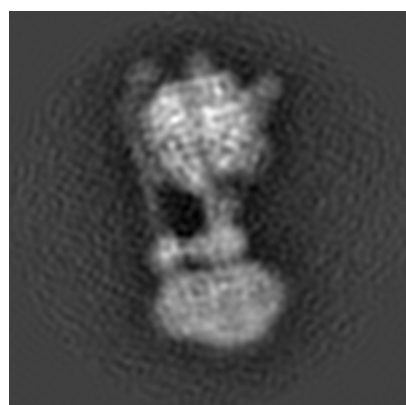
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6813. These allow visual inspection of the internal detail of the map and identification of artifacts.

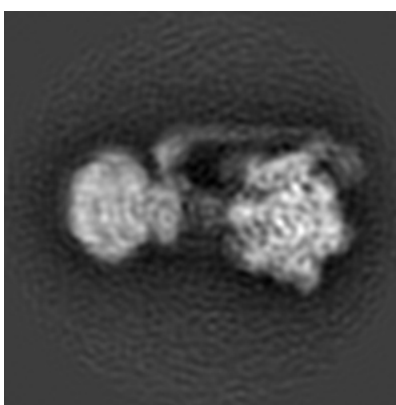
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

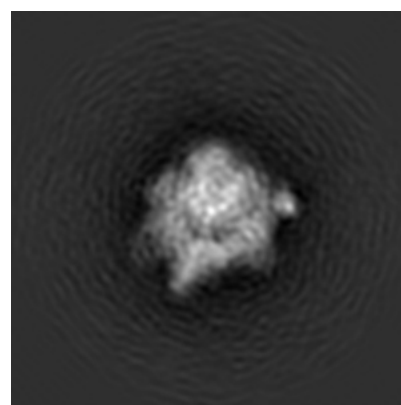
6.1.1 Primary map



X



Y



Z

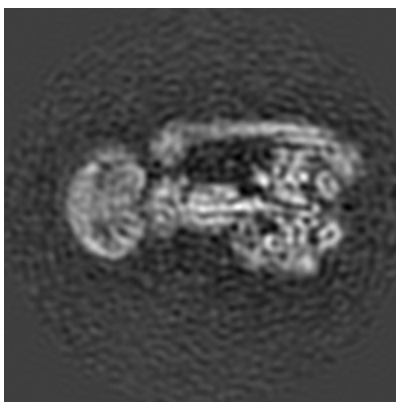
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

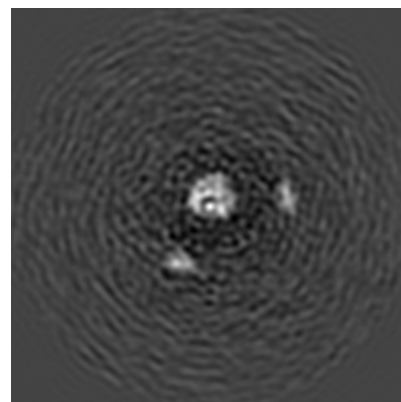
6.2.1 Primary map



X Index: 118



Y Index: 118



Z Index: 118

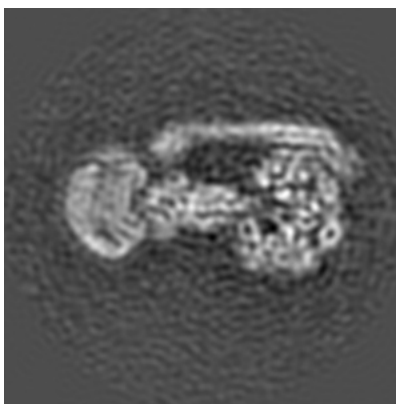
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

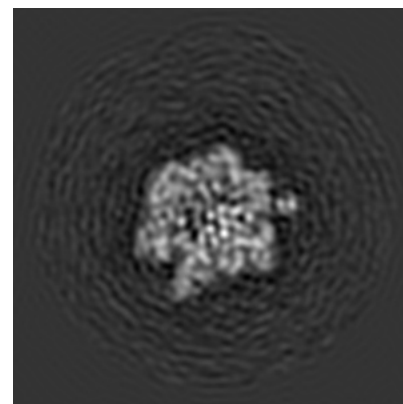
6.3.1 Primary map



X Index: 117



Y Index: 120

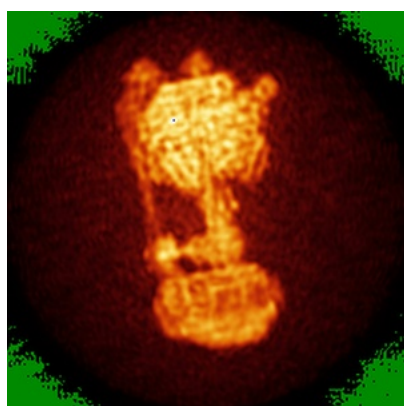


Z Index: 171

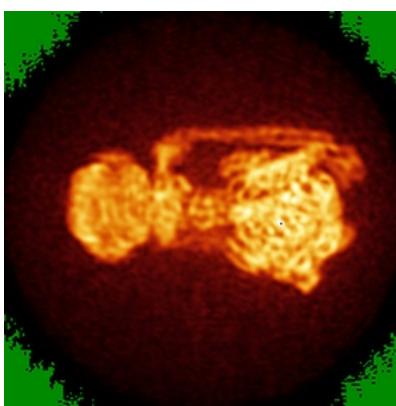
The images above show the largest variance slices of the map in three orthogonal directions.

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

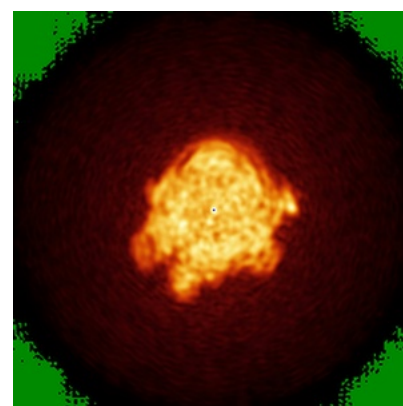
6.4.1 Primary map



X



Y

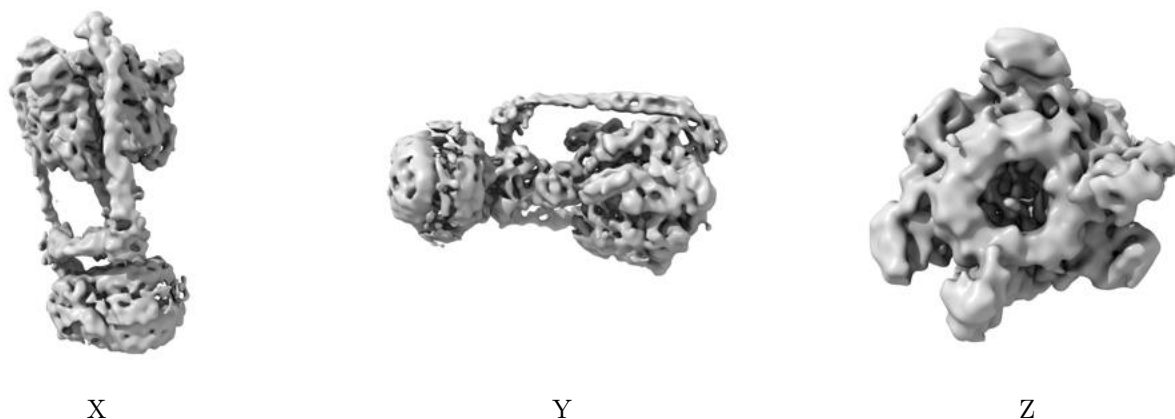


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

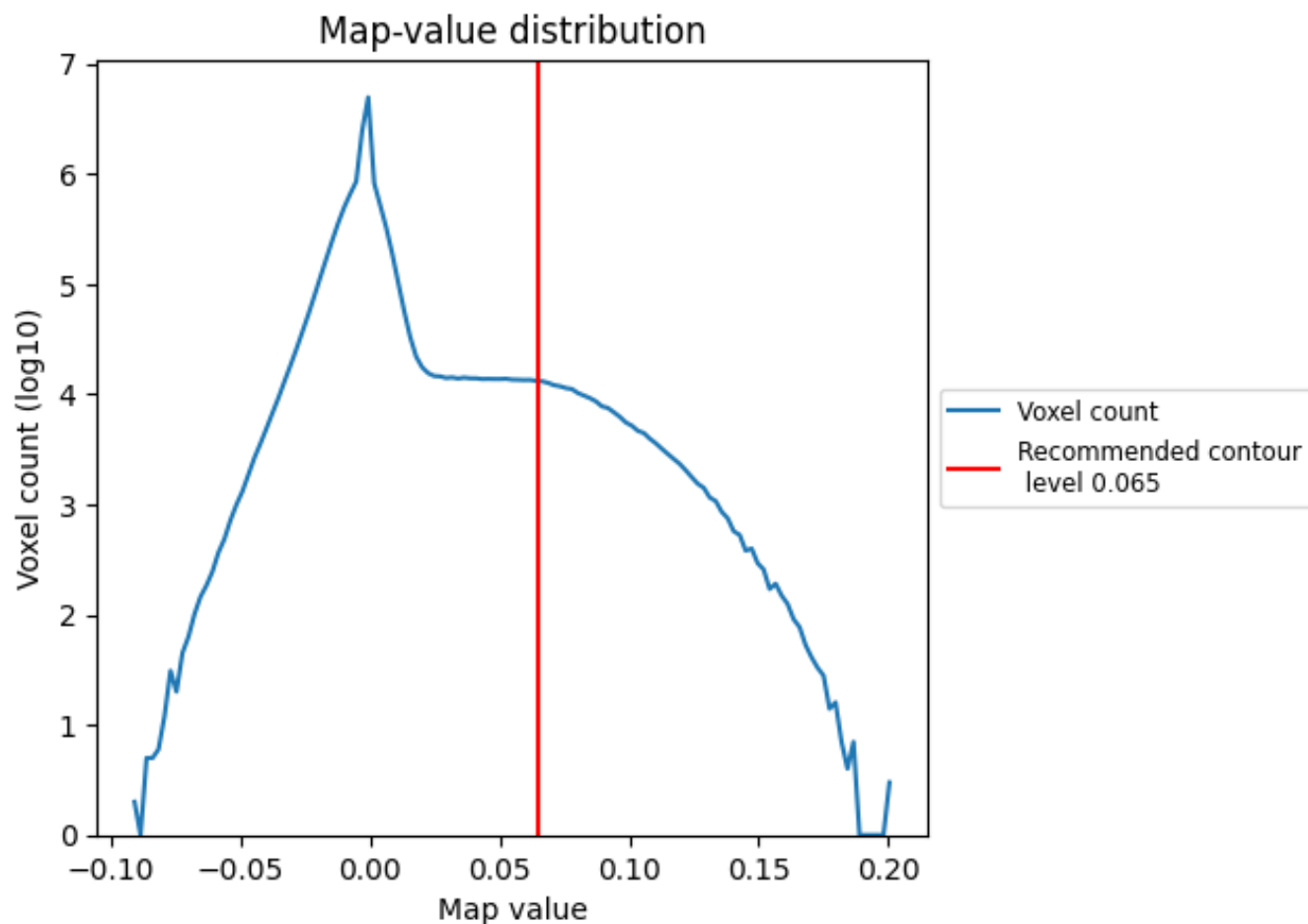
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

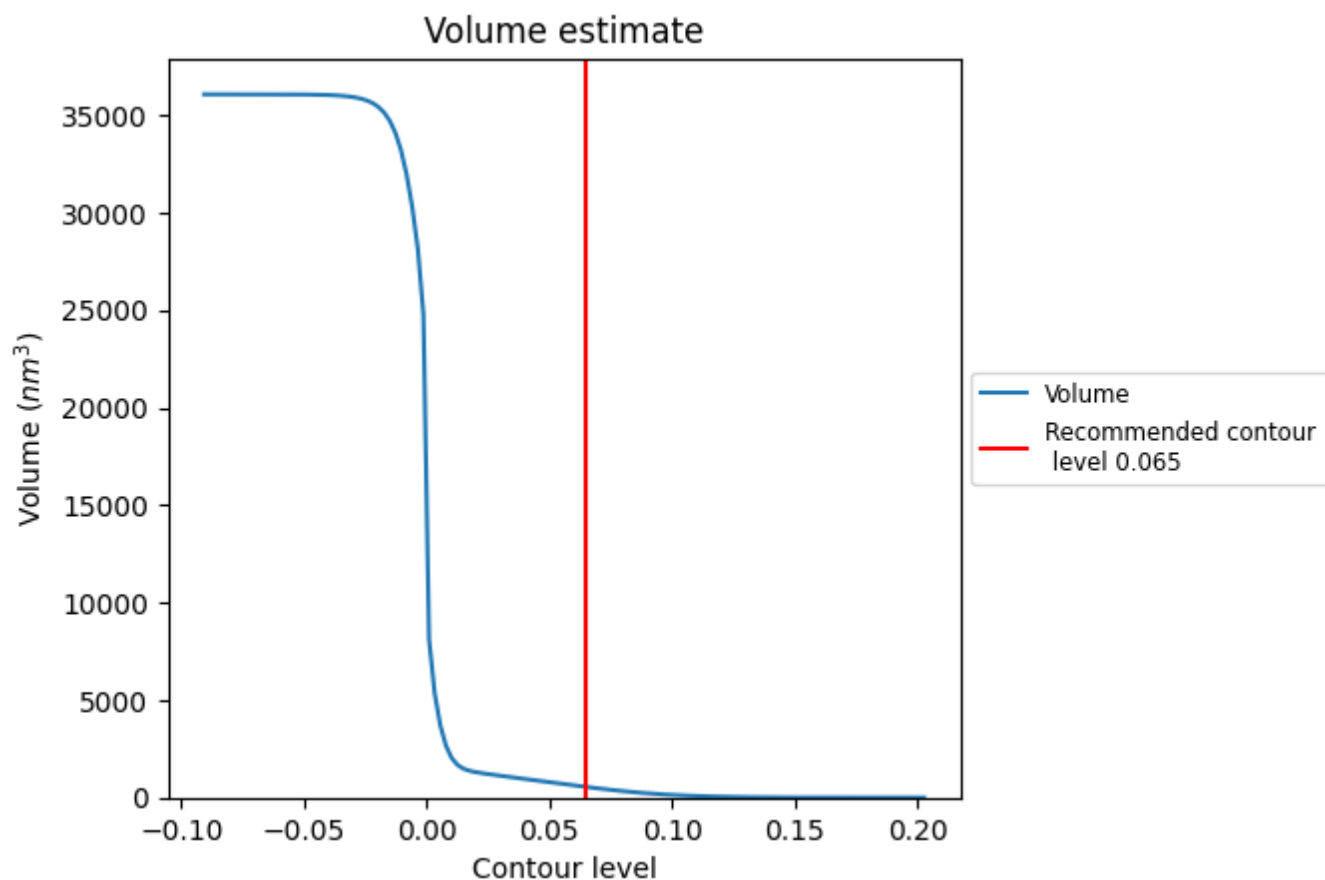
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

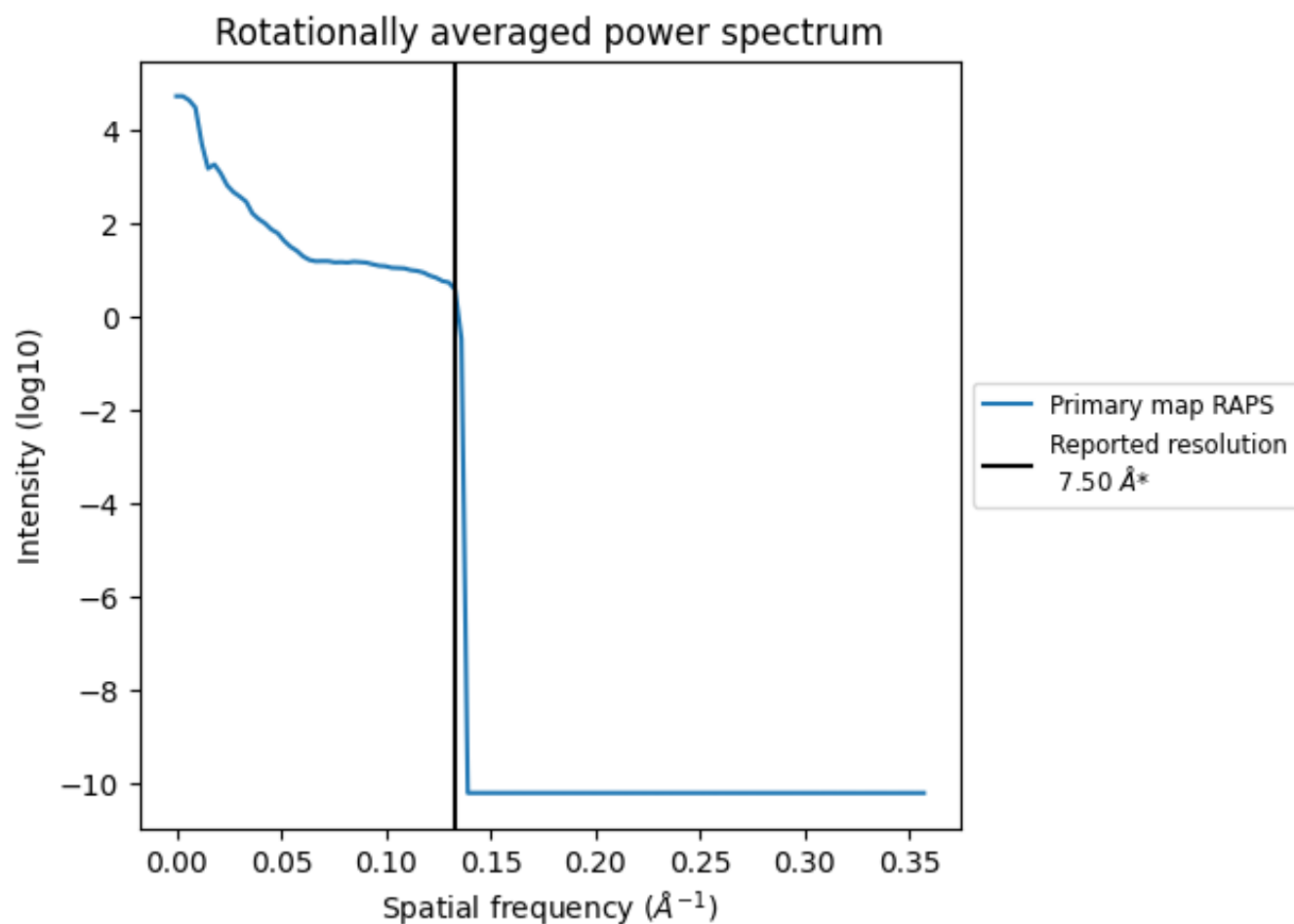
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 545 nm³; this corresponds to an approximate mass of 493 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 ⓘ

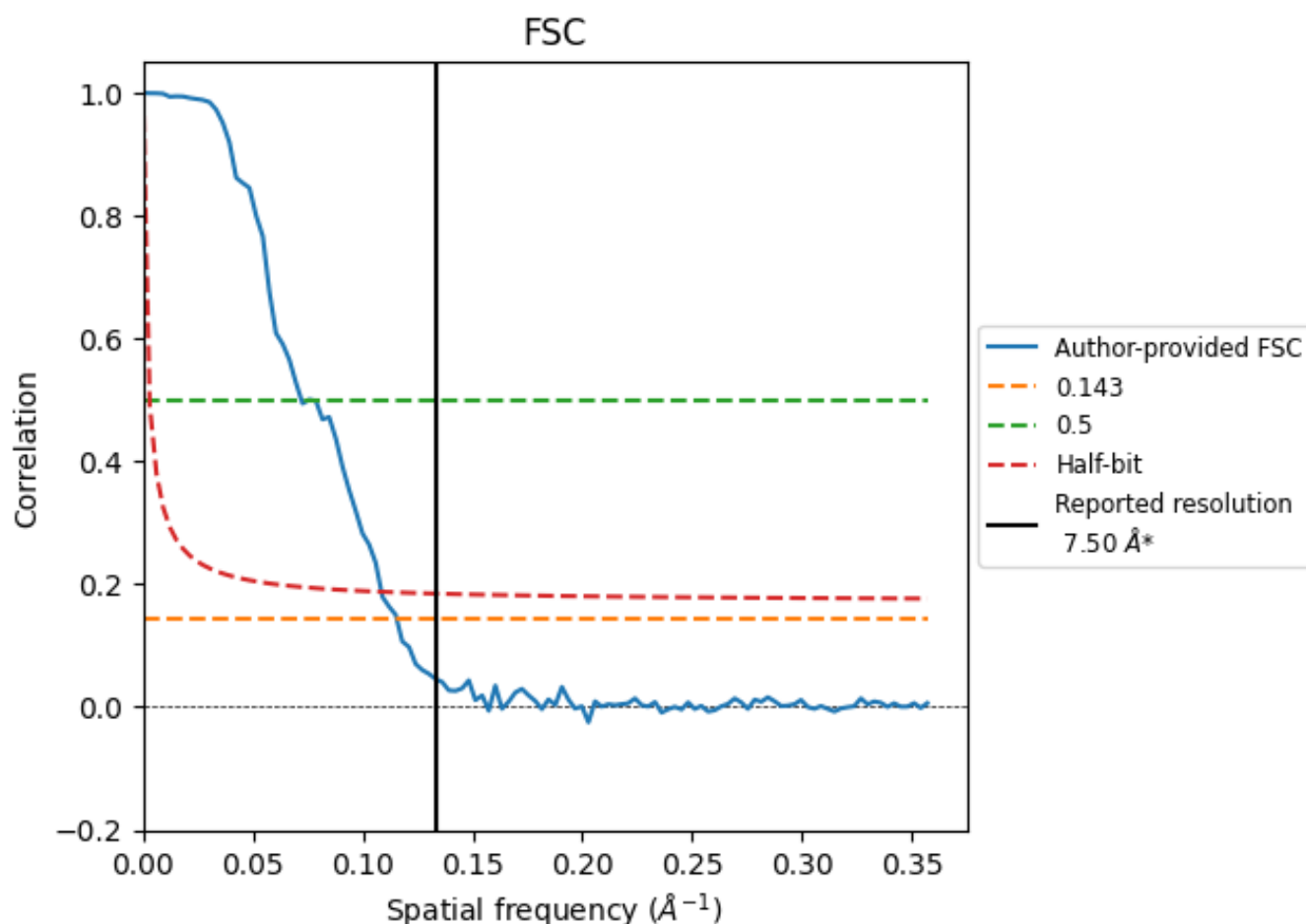


*Reported resolution corresponds to spatial frequency of 0.133 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.133 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.50	-	-
Author-provided FSC curve	8.66	13.87	9.22
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.66 differs from the reported value 7.5 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6813 and PDB model 5Y60. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

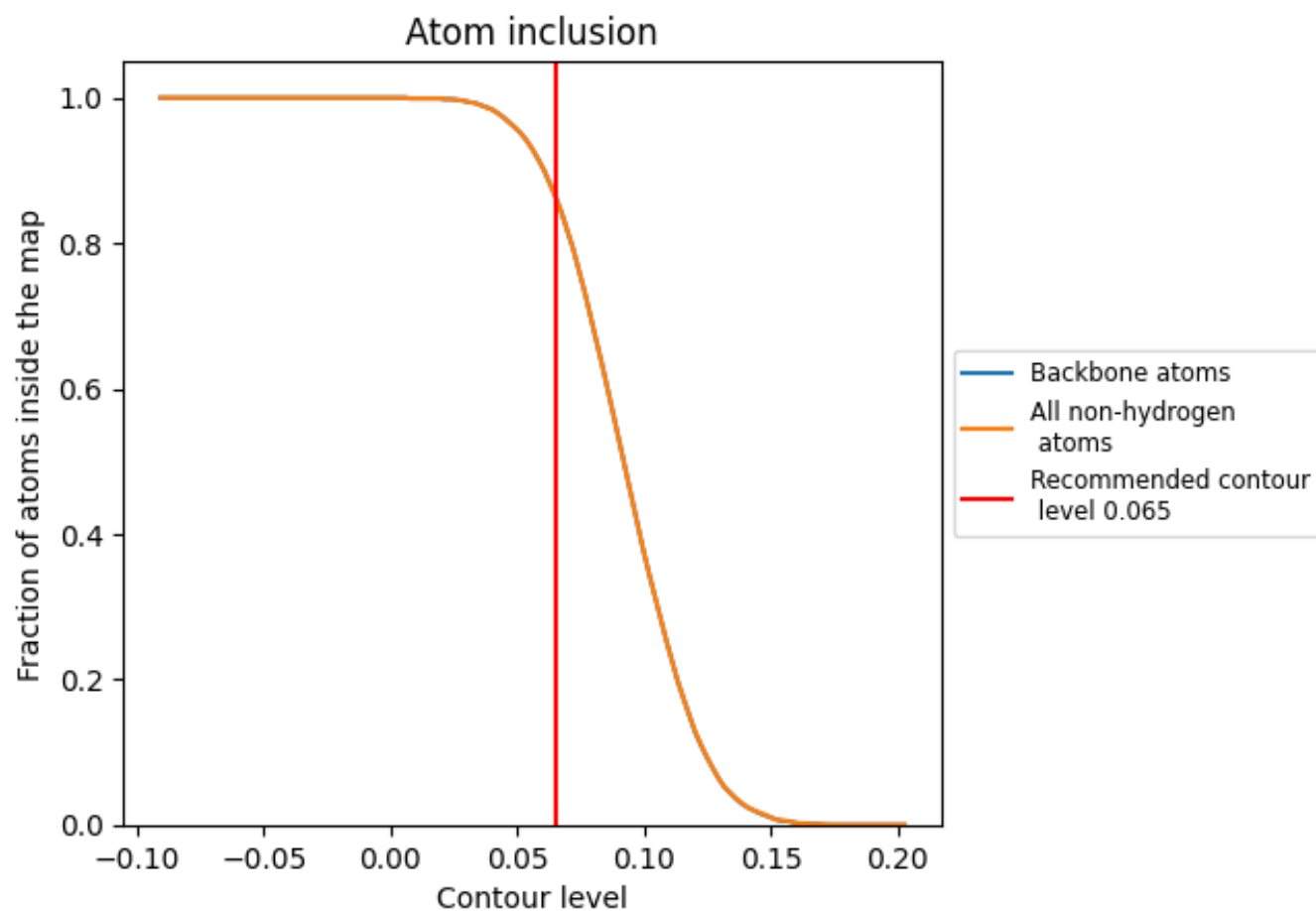


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8640	 0.2320
A	 0.9550	 0.2700
B	 0.9590	 0.2770
C	 0.9560	 0.2780
D	 0.9410	 0.2640
E	 0.9500	 0.2710
F	 0.9660	 0.2860
G	 0.9280	 0.2860
H	 0.8950	 0.2500
I	 0.9270	 0.2490
J	 0.8850	 0.2280
K	 0.9050	 0.2530
L	 0.8860	 0.2340
M	 0.8300	 0.2270
N	 0.7960	 0.1880
O	 0.5050	 0.0790
P	 0.5840	 0.1160
Q	 0.6930	 0.1400
R	 0.5810	 0.1280
S	 0.6800	 0.1360
T	 0.6470	 0.1220
U	 0.5350	 0.0720
V	 0.6010	 0.0510
W	 0.5180	 0.0450
X	 0.5710	 0.1120
Y	 0.4980	 0.0960
Z	 0.4850	 0.1330

