



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 10:45 PM UTC

PDB ID : 5Y5X / pdb_00005y5x
EMDB ID : EMD-6810
Title : V/A-type ATPase/synthase from *Thermus thermophilus*, rotational state 1
Authors : Nakanishi, A.; Kishikawa, J.; Tamakoshi, M.; Mitsuoka, K.; Yokoyama, K.
Deposited on : 2017-08-10
Resolution : 5.00 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

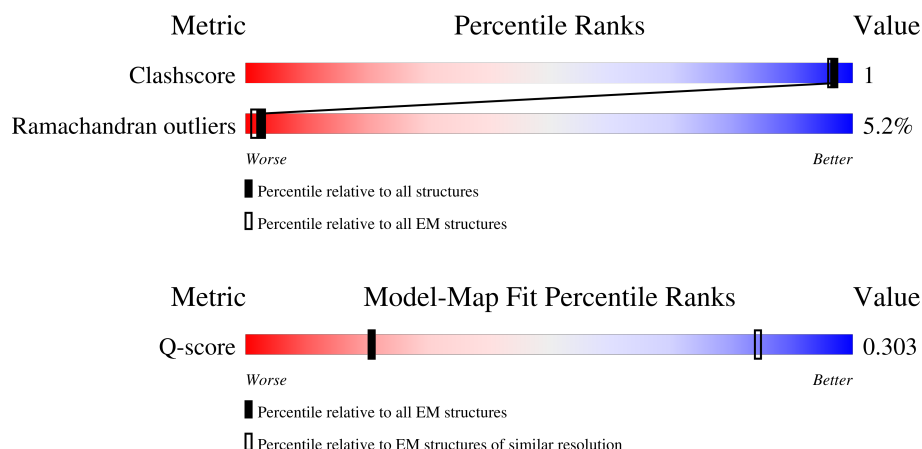
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 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.



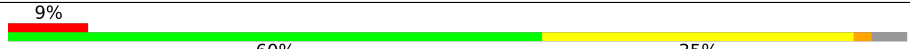
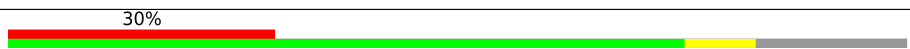
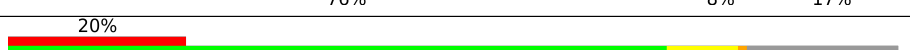
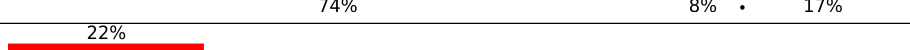
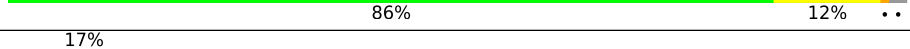
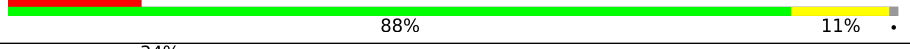
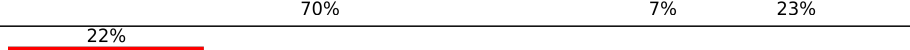
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	1057 (4.50 - 5.50)

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	 72% 27%
1	B	578	 73% 25%
1	C	578	 70% 28%
2	D	478	 65% 30%
2	E	478	 62% 32%

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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.

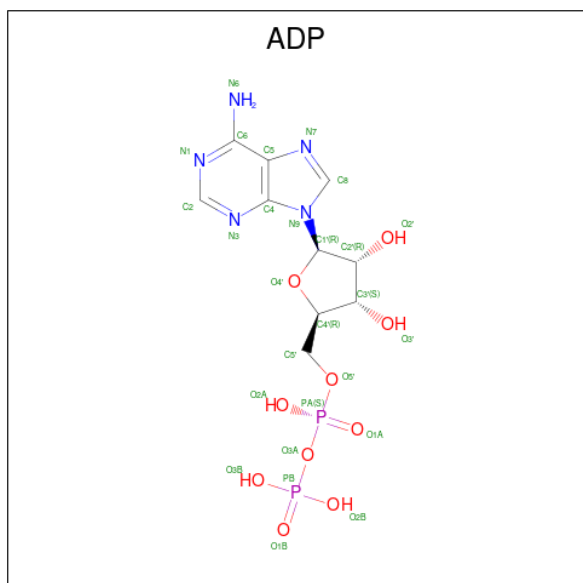
Mol	Chain	Residues	Atoms				AltConf	Trace
9	O	76	Total	C	N	O	0	0
			303	152	76	75		
9	P	76	Total	C	N	O	0	0
			303	152	76	75		

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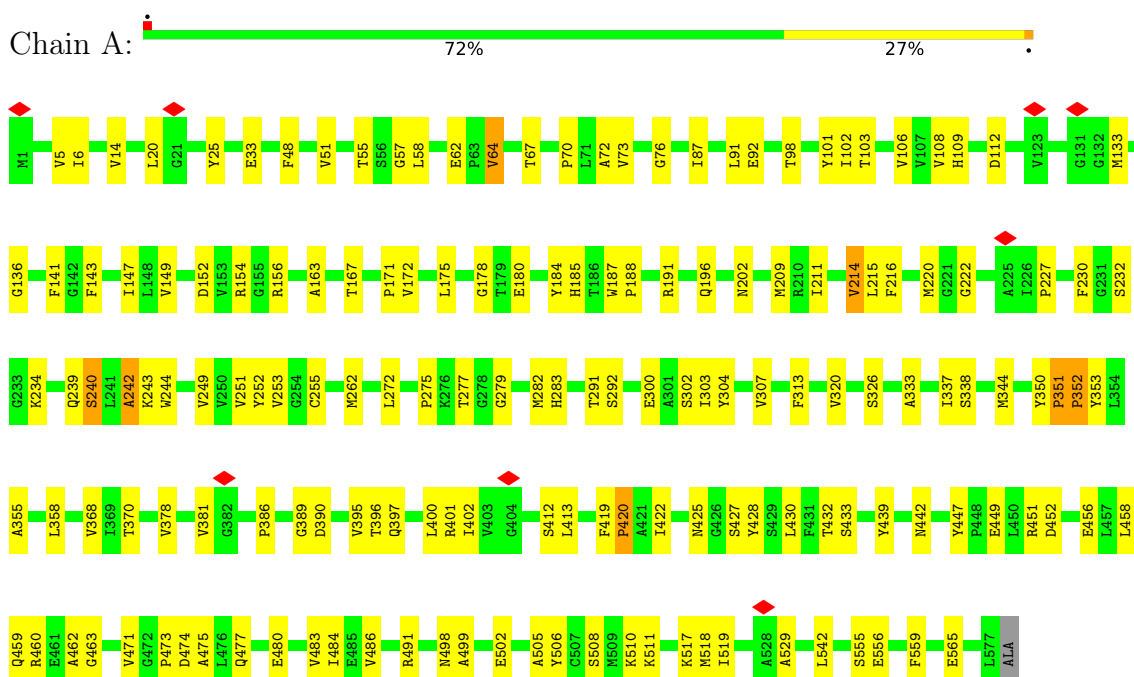
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	C	1	27	10	5	10	2	0

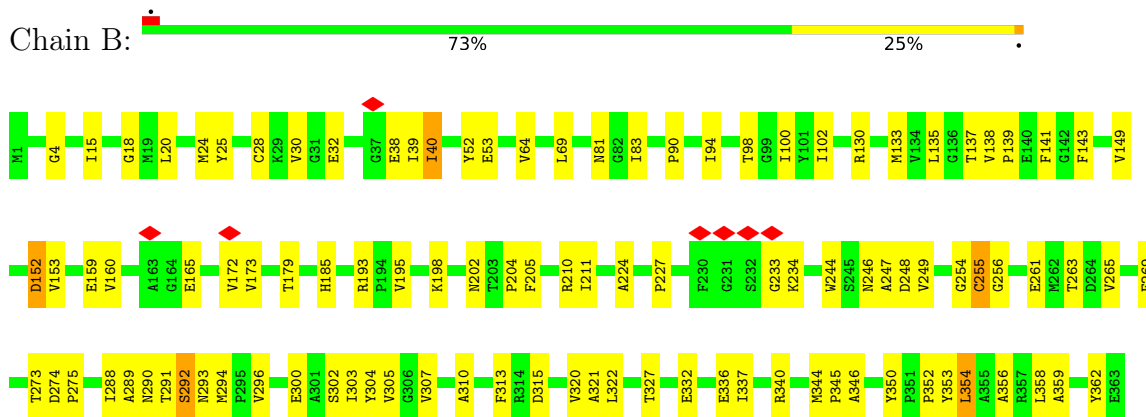
3 Residue-property plots

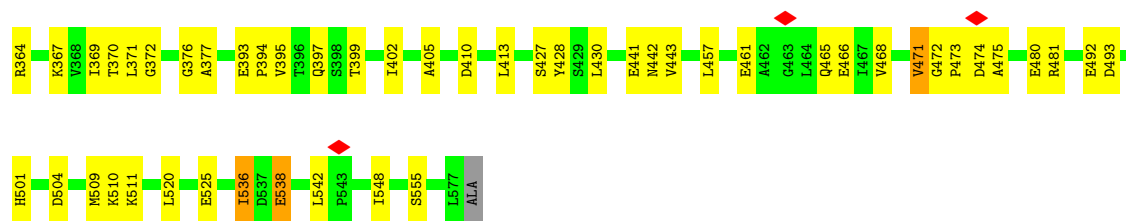
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

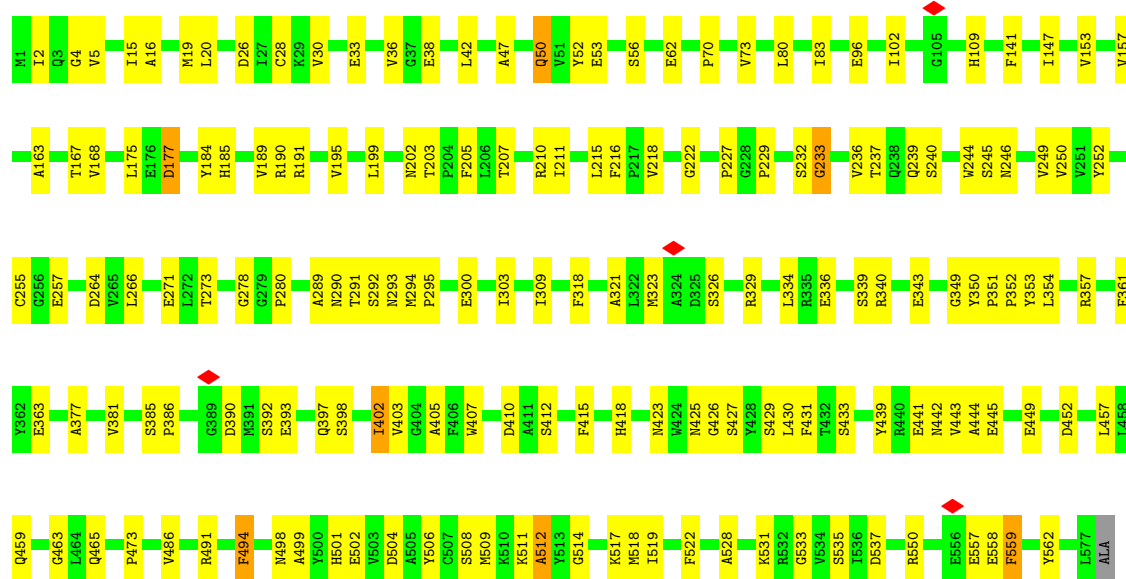


• Molecule 1: V-type ATP synthase alpha chain

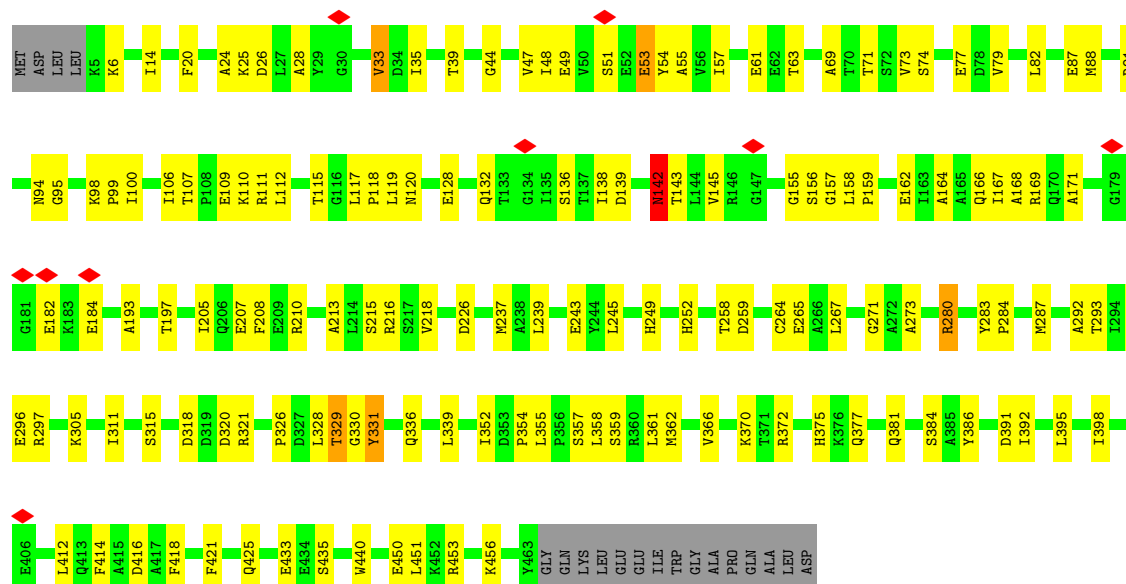




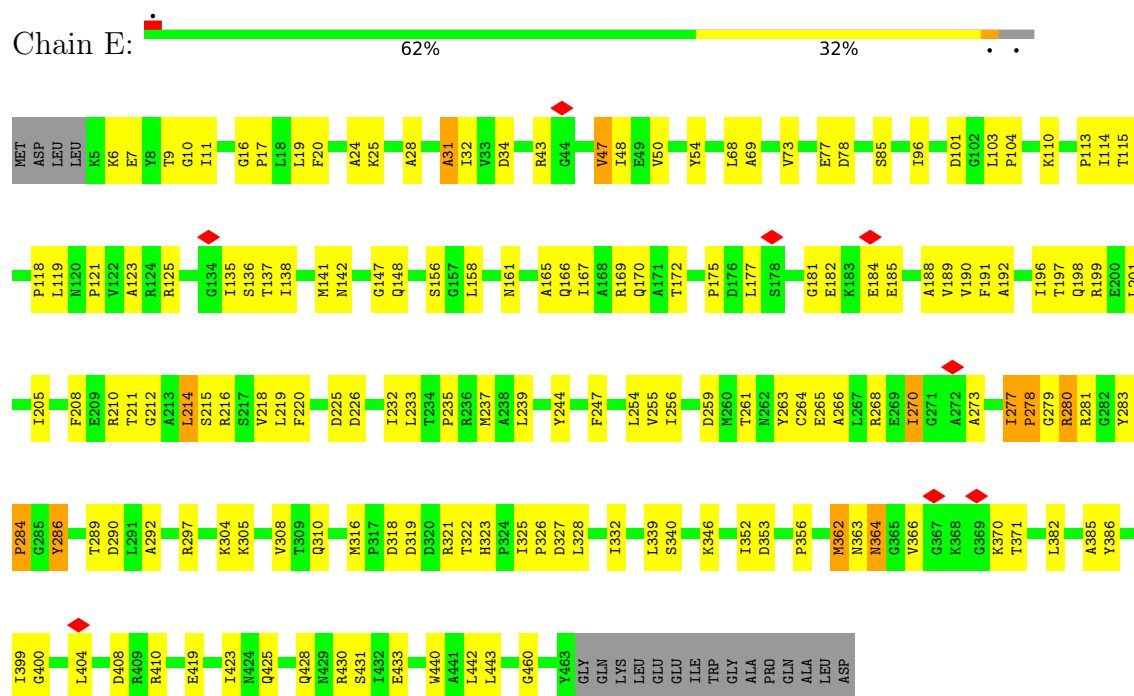
• Molecule 1: V-type ATP synthase alpha chain



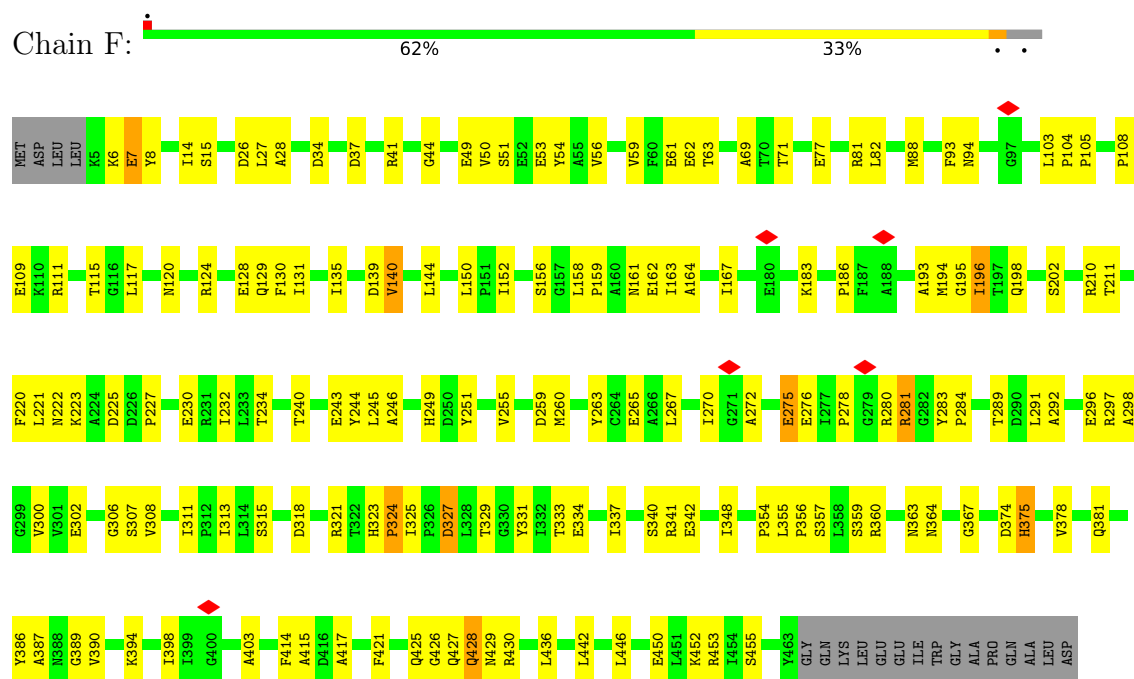
• Molecule 2: V-type ATP synthase beta chain



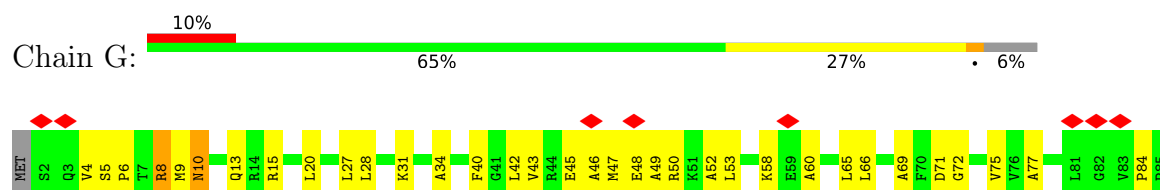
- Molecule 2: V-type ATP synthase beta chain

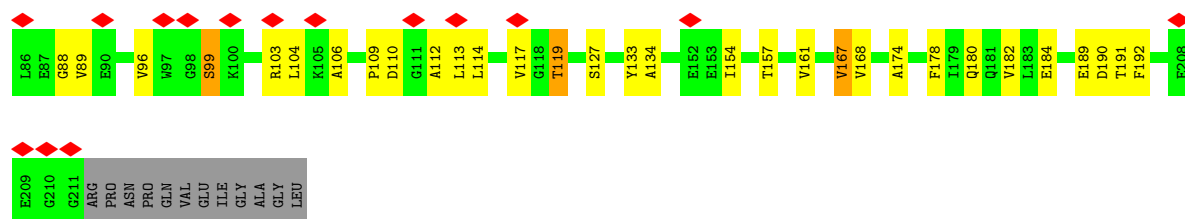


- Molecule 2: V-type ATP synthase beta chain



- Molecule 3: V-type ATP synthase subunit D

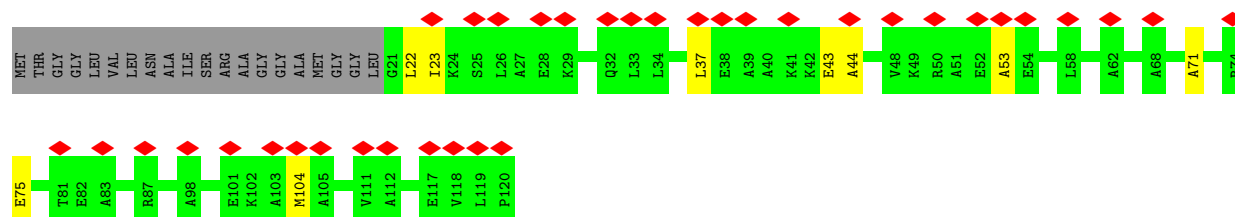
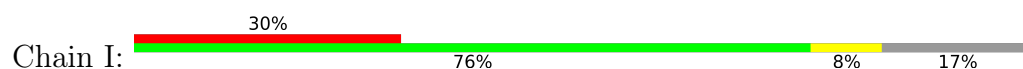




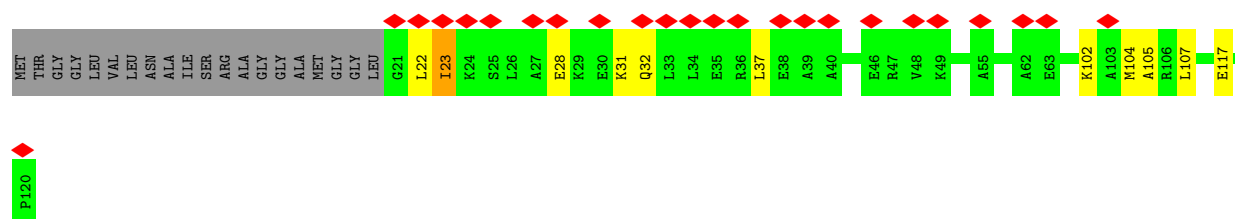
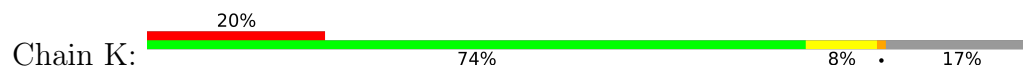
• Molecule 4: V-type ATP synthase subunit F



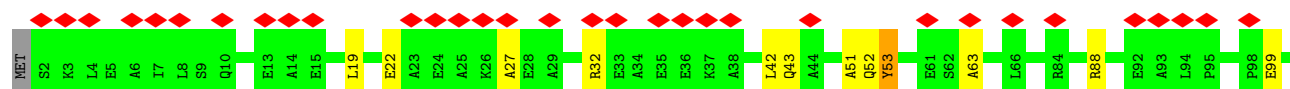
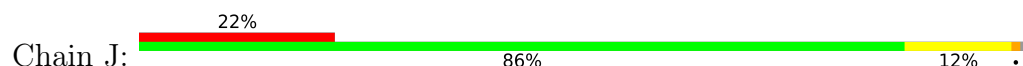
• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

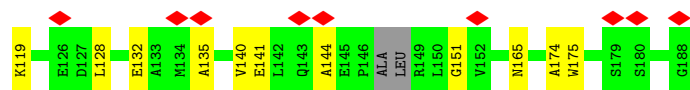


• Molecule 5: V-type ATP synthase, subunit (VAPC-THERM)

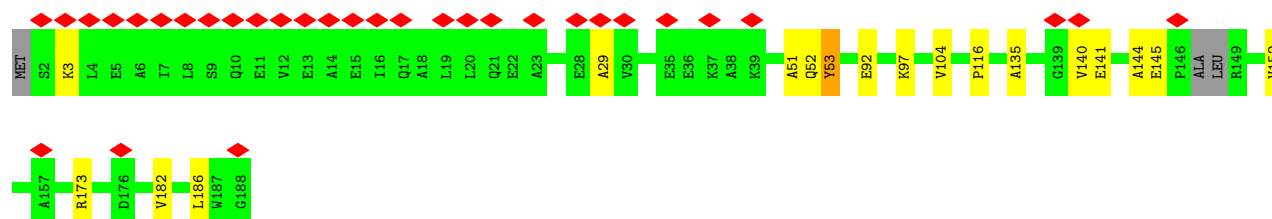
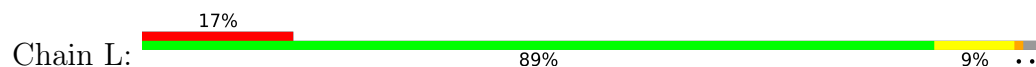


• Molecule 6: V-type ATP synthase subunit E

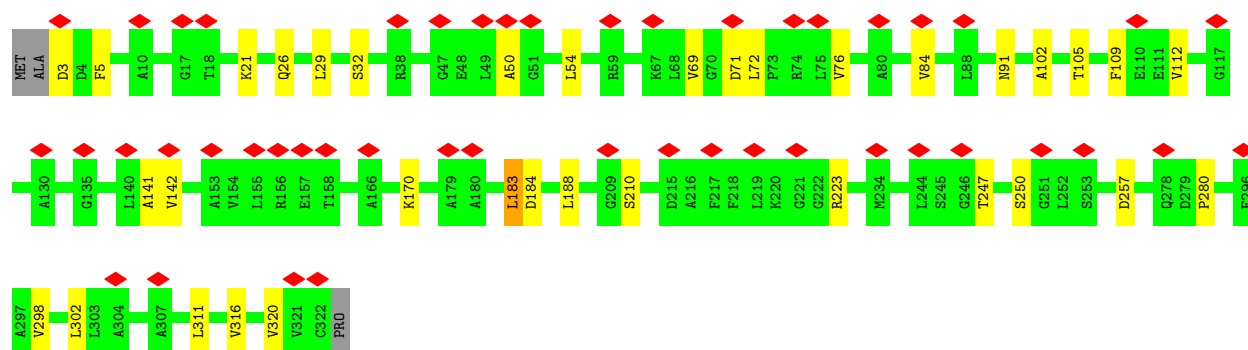
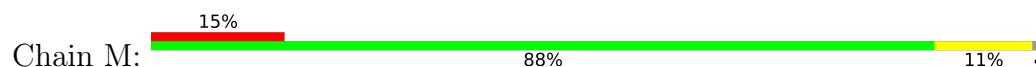




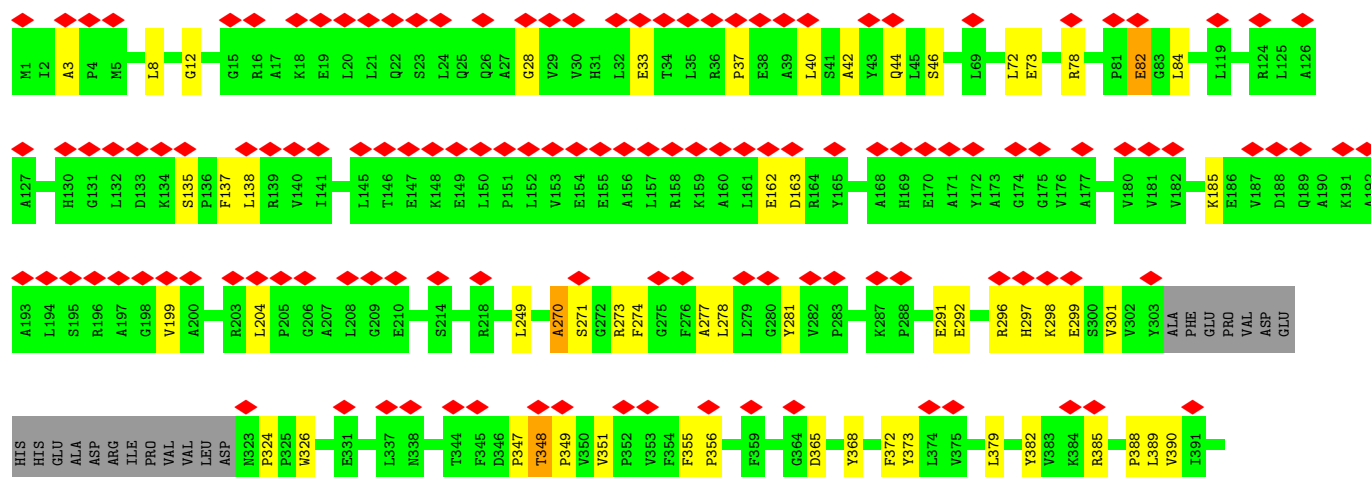
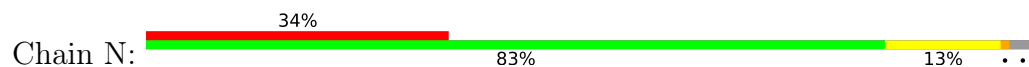
- Molecule 6: V-type ATP synthase subunit E

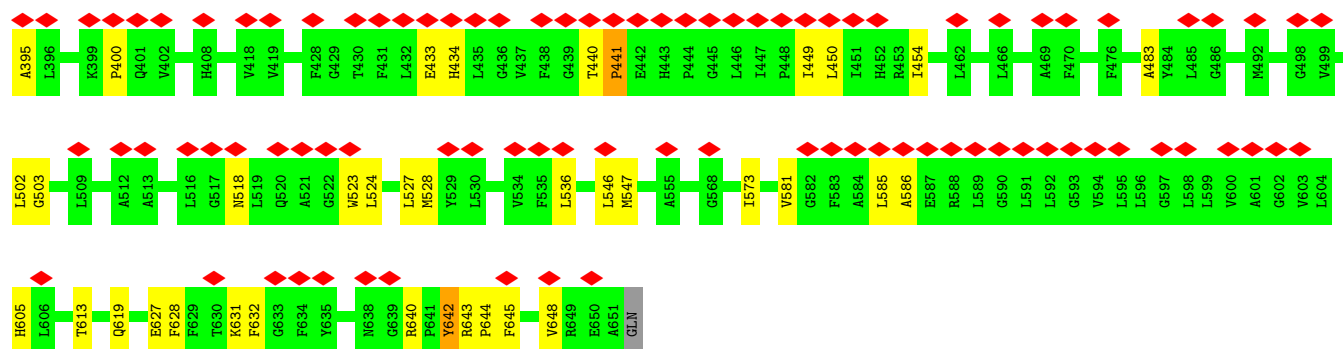


- Molecule 7: V-type ATP synthase subunit C

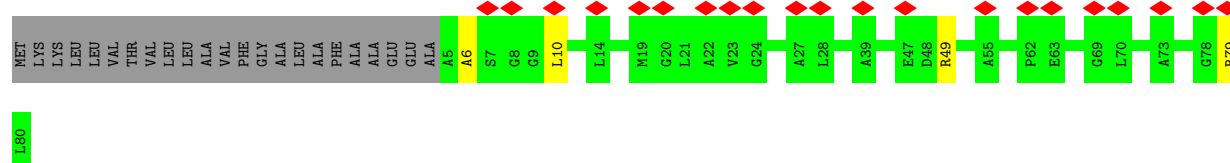


- Molecule 8: V-type ATP synthase subunit I

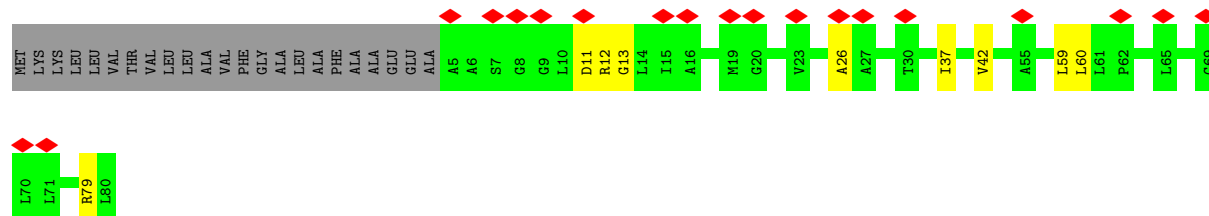




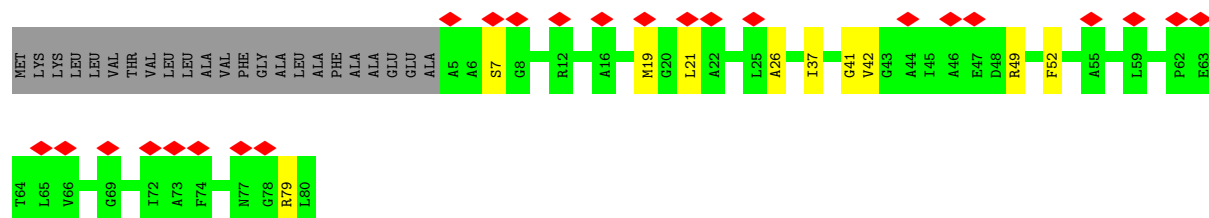
• Molecule 9: V-type ATP synthase, subunit K



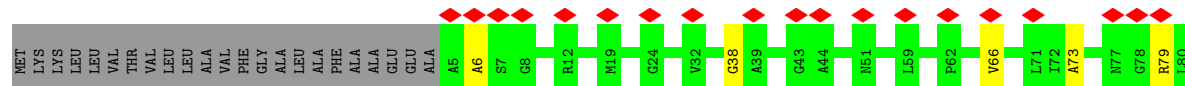
• Molecule 9: V-type ATP synthase, subunit K



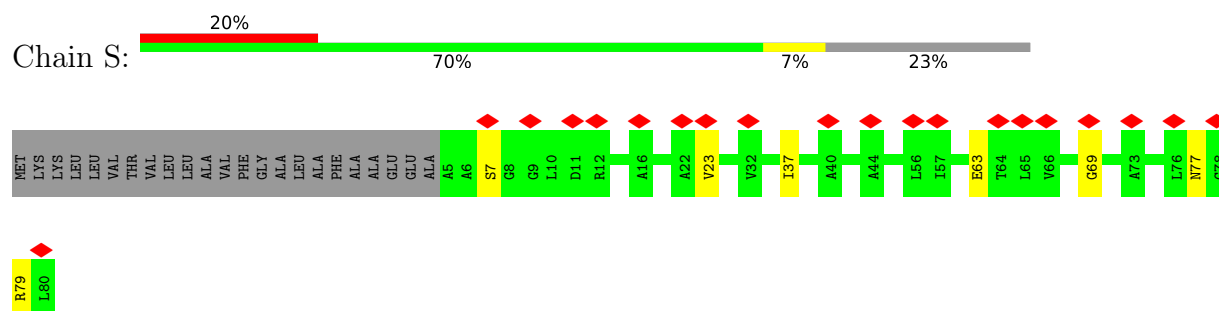
• Molecule 9: V-type ATP synthase, subunit K



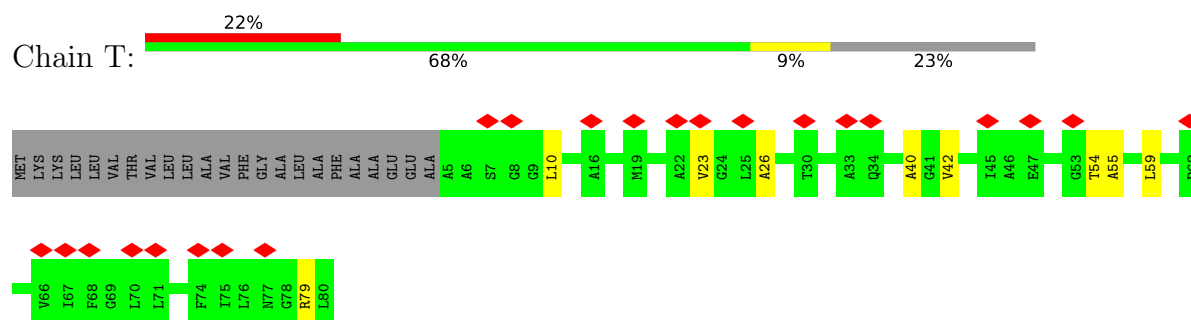
• Molecule 9: V-type ATP synthase, subunit K



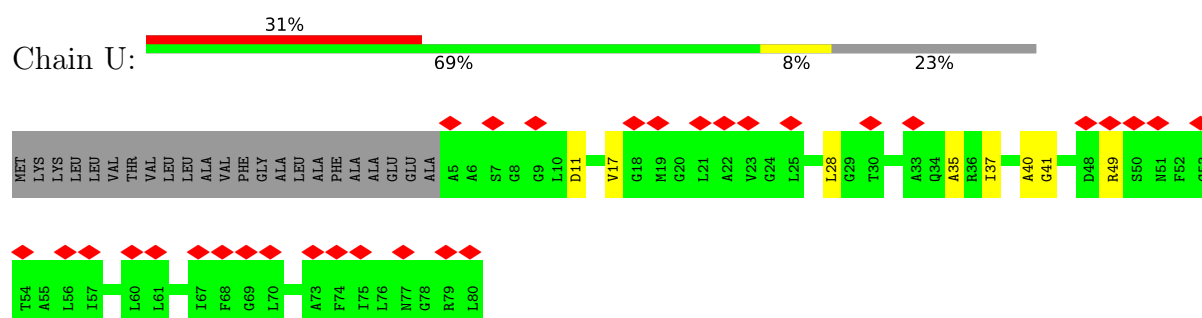
- Molecule 9: V-type ATP synthase, subunit K



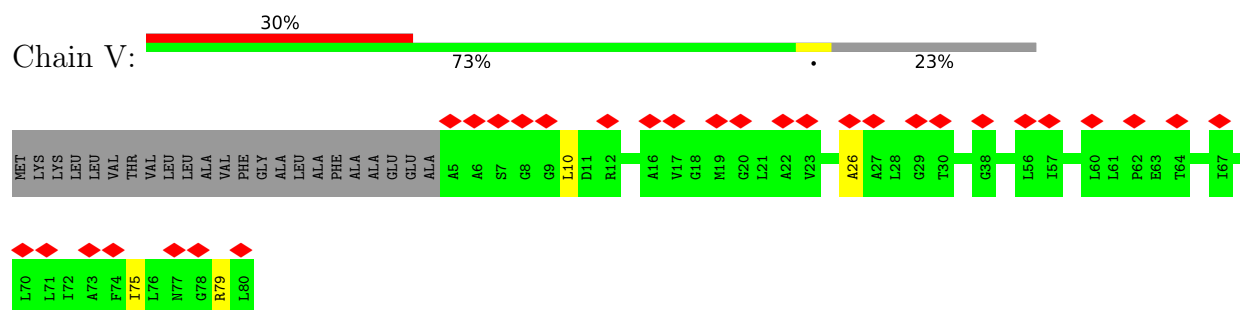
- Molecule 9: V-type ATP synthase, subunit K



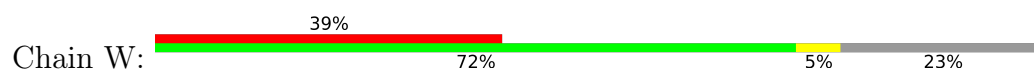
- Molecule 9: V-type ATP synthase, subunit K

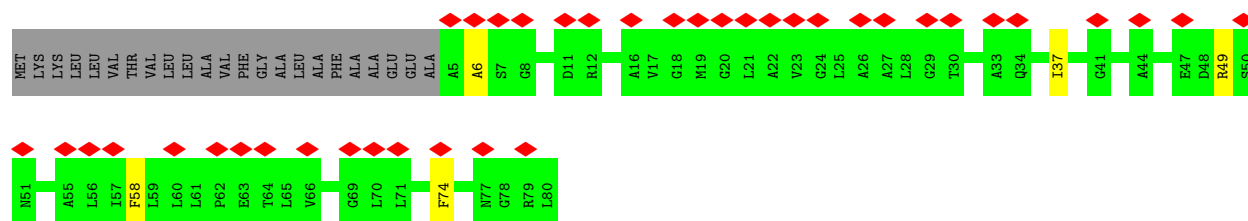


- Molecule 9: V-type ATP synthase, subunit K

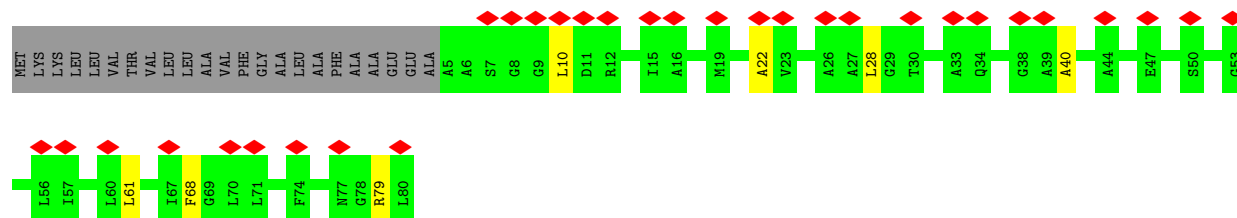


- Molecule 9: V-type ATP synthase, subunit K

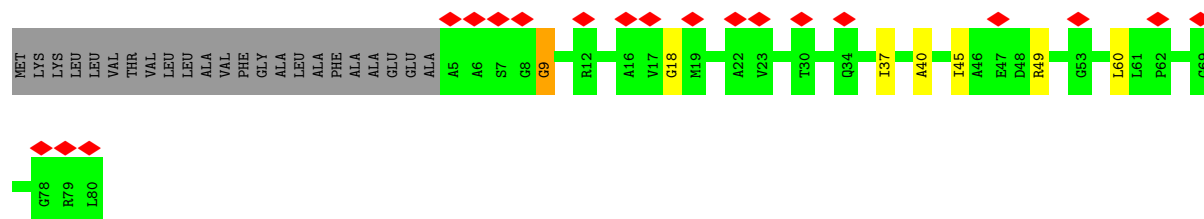




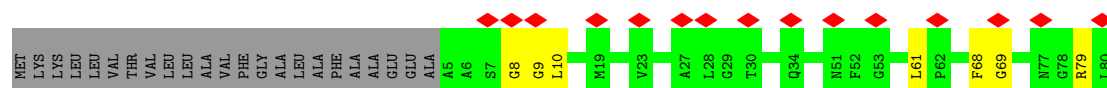
- Molecule 9: V-type ATP synthase, subunit K



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



- 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	117938	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	0.544	Depositor
Minimum map value	-0.340	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.098	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	2.47	92/2306 (4.0%)	2.05	82/2881 (2.8%)
1	B	2.34	68/2306 (2.9%)	2.08	78/2881 (2.7%)
1	C	2.47	96/2306 (4.2%)	2.13	87/2881 (3.0%)
2	D	2.41	65/1834 (3.5%)	2.16	78/2291 (3.4%)
2	E	2.47	88/1834 (4.8%)	2.12	81/2291 (3.5%)
2	F	2.57	87/1834 (4.7%)	2.12	79/2291 (3.4%)
3	G	2.18	24/838 (2.9%)	2.25	41/1046 (3.9%)
4	H	2.13	12/398 (3.0%)	2.42	31/496 (6.2%)
5	I	1.65	0/398	2.18	12/496 (2.4%)
5	K	1.62	0/398	2.18	16/496 (3.2%)
6	J	1.69	1/736 (0.1%)	2.05	24/917 (2.6%)
6	L	1.81	3/736 (0.4%)	1.93	12/917 (1.3%)
7	M	1.79	4/1278 (0.3%)	1.98	40/1596 (2.5%)
8	N	1.66	3/2524 (0.1%)	2.19	95/3152 (3.0%)
9	O	1.59	0/302	2.18	4/376 (1.1%)
9	P	1.54	0/302	2.15	12/376 (3.2%)
9	Q	1.48	0/302	2.51	14/376 (3.7%)
9	R	1.54	1/302 (0.3%)	2.14	5/376 (1.3%)
9	S	1.61	0/302	2.12	9/376 (2.4%)
9	T	1.46	0/302	2.19	16/376 (4.3%)
9	U	1.43	0/302	2.36	13/376 (3.5%)
9	V	1.51	0/302	2.11	7/376 (1.9%)
9	W	1.50	0/302	2.15	7/376 (1.9%)
9	X	1.50	0/302	2.23	11/376 (2.9%)
9	Y	1.60	0/302	2.17	12/376 (3.2%)
9	Z	1.64	0/302	2.25	10/376 (2.7%)
All	All	2.14	544/23350 (2.3%)	2.13	876/29144 (3.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
2	D	0	2
2	E	0	1
2	F	0	1
7	M	0	2
8	N	0	2
All	All	0	10

All (544) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	53	GLU	CA-C	-10.22	1.45	1.52
4	H	85	ASP	CA-C	-9.67	1.44	1.53
1	A	358	LEU	CA-C	-9.38	1.43	1.53
1	A	350	TYR	CA-C	-9.17	1.42	1.52
1	B	493	ASP	CA-C	-9.06	1.44	1.52
2	D	320	ASP	CA-C	-9.03	1.42	1.52
1	C	559	PHE	N-CA	-8.90	1.39	1.46
2	E	321	ARG	CA-C	-8.76	1.44	1.53
1	C	449	GLU	CA-C	-8.72	1.45	1.52
1	C	28	CYS	CA-C	-8.66	1.42	1.53
1	A	386	PRO	CA-C	-8.59	1.44	1.52
1	A	6	ILE	CA-C	-8.37	1.43	1.52
2	E	201	LEU	CA-C	-8.36	1.42	1.52
1	B	358	LEU	CA-C	-8.35	1.42	1.52
2	F	430	ARG	CA-C	-8.23	1.42	1.52
2	E	286	TYR	N-CA	-8.22	1.38	1.46
1	C	249	VAL	CA-C	-8.14	1.44	1.53
1	B	354	LEU	CA-C	-8.09	1.42	1.52
1	B	461	GLU	CA-C	-7.98	1.44	1.52
2	F	292	ALA	CA-C	-7.93	1.44	1.53
2	E	77	GLU	CA-C	-7.58	1.43	1.52
2	F	53	GLU	CA-C	-7.57	1.43	1.52
1	C	218	VAL	CA-C	-7.52	1.44	1.52
2	F	109	GLU	CA-C	-7.52	1.44	1.52
1	A	243	LYS	CA-C	-7.39	1.46	1.52
1	B	4	GLY	CA-C	-7.39	1.44	1.52
1	A	249	VAL	CA-C	-7.37	1.43	1.52
4	H	48	ASP	CA-C	-7.37	1.43	1.52
1	A	425	ASN	N-CA	-7.36	1.37	1.46
3	G	31	LYS	CA-C	-7.36	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	352	PRO	CA-C	-7.34	1.45	1.52
2	D	284	PRO	CA-C	-7.32	1.44	1.52
1	C	522	PHE	CA-C	-7.31	1.43	1.52
1	C	415	PHE	CA-C	-7.30	1.43	1.52
2	E	316	MET	CA-C	-7.27	1.45	1.53
1	C	418	HIS	CA-C	-7.21	1.44	1.52
2	D	54	TYR	CA-C	-7.20	1.43	1.52
2	E	135	ILE	CA-C	-7.19	1.43	1.52
2	D	398	ILE	CA-C	-7.17	1.45	1.52
2	F	267	LEU	CA-C	-7.16	1.43	1.52
2	F	194	MET	CA-C	-7.12	1.44	1.53
2	F	340	SER	CA-C	-7.09	1.44	1.52
1	A	272	LEU	CA-C	-7.01	1.44	1.52
2	F	51	SER	CA-C	-6.92	1.44	1.52
2	F	284	PRO	CA-C	-6.92	1.45	1.52
2	E	113	PRO	CA-C	-6.92	1.43	1.52
2	F	394	LYS	CA-C	-6.91	1.46	1.53
1	C	350	TYR	CA-C	-6.90	1.44	1.52
1	C	336	GLU	CA-C	-6.89	1.44	1.52
2	F	221	LEU	CA-C	-6.86	1.44	1.52
2	D	381	GLN	CA-C	-6.84	1.45	1.53
1	A	209	MET	CA-C	-6.82	1.44	1.52
1	B	320	VAL	CA-C	-6.82	1.44	1.53
2	D	421	PHE	CA-C	-6.80	1.45	1.52
2	F	318	ASP	CA-C	-6.80	1.46	1.52
1	B	457	LEU	CA-C	-6.79	1.44	1.52
1	A	353	TYR	CA-C	-6.79	1.45	1.52
2	D	162	GLU	CA-C	-6.78	1.44	1.52
7	M	298	VAL	CA-C	-6.77	1.44	1.52
1	C	363	GLU	CA-C	-6.77	1.44	1.52
2	D	425	GLN	CA-C	-6.77	1.44	1.52
2	D	245	LEU	CA-C	-6.76	1.45	1.53
1	C	323	MET	CA-C	-6.75	1.45	1.53
2	F	291	LEU	CA-C	-6.73	1.44	1.52
1	A	396	THR	CA-C	-6.72	1.44	1.52
1	B	538	GLU	CA-C	-6.71	1.45	1.52
1	C	50	GLN	CA-C	-6.70	1.46	1.53
2	F	162	GLU	CA-C	-6.67	1.44	1.52
2	E	32	ILE	CA-C	-6.67	1.44	1.52
1	C	211	ILE	CA-C	-6.66	1.45	1.52
2	F	26	ASP	CA-C	-6.66	1.46	1.53
2	E	156	SER	CA-C	-6.66	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	LEU	CA-C	-6.65	1.45	1.52
2	F	381	GLN	CA-C	-6.65	1.44	1.52
1	A	368	VAL	CA-C	-6.63	1.44	1.52
1	A	422	ILE	CA-C	-6.62	1.44	1.52
6	L	53	TYR	CA-C	-6.62	1.46	1.52
2	F	220	PHE	CA-C	-6.62	1.44	1.52
1	C	352	PRO	N-CA	-6.61	1.40	1.47
2	F	82	LEU	CA-C	-6.61	1.44	1.52
2	F	374	ASP	CA-C	-6.59	1.43	1.53
2	F	308	VAL	CA-C	-6.57	1.45	1.52
1	A	449	GLU	CA-C	-6.57	1.43	1.52
2	D	292	ALA	CA-C	-6.55	1.44	1.52
2	E	286	TYR	CA-C	-6.55	1.45	1.53
1	C	300	GLU	CA-C	-6.54	1.45	1.53
1	B	327	THR	CA-C	-6.53	1.44	1.52
2	F	272	ALA	CA-C	-6.51	1.44	1.52
1	C	430	LEU	CA-C	-6.50	1.46	1.53
4	H	44	LEU	CA-C	-6.50	1.44	1.52
1	A	101	TYR	CA-C	-6.50	1.44	1.52
1	C	501	HIS	CA-C	-6.49	1.44	1.52
1	C	498	ASN	CA-C	-6.49	1.44	1.52
1	B	332	GLU	CA-C	-6.49	1.43	1.52
1	A	141	PHE	CA-C	-6.48	1.47	1.53
8	N	379	LEU	CA-C	-6.48	1.47	1.52
2	E	323	HIS	CA-C	-6.48	1.46	1.53
1	B	402	ILE	CA-C	-6.48	1.45	1.52
1	B	265	VAL	CA-C	-6.47	1.45	1.52
1	C	36	VAL	CA-C	-6.46	1.45	1.53
3	G	9	MET	CA-C	-6.46	1.44	1.52
2	E	382	LEU	CA-C	-6.44	1.44	1.52
1	B	211	ILE	CA-C	-6.43	1.44	1.52
1	C	442	ASN	CA-C	-6.43	1.47	1.52
2	F	265	GLU	CA-C	-6.43	1.44	1.52
2	F	120	ASN	CA-C	-6.41	1.47	1.52
1	A	149	VAL	CA-C	-6.41	1.47	1.53
1	A	92	GLU	CA-C	-6.36	1.44	1.52
1	A	242	ALA	CA-C	-6.35	1.44	1.52
2	E	325	ILE	CA-C	-6.35	1.46	1.52
1	B	536	ILE	CA-C	-6.33	1.44	1.52
1	B	173	VAL	CA-C	-6.32	1.45	1.53
2	F	281	ARG	CA-C	-6.32	1.44	1.52
1	C	397	GLN	CA-C	-6.30	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	104	LEU	CA-C	-6.30	1.44	1.52
2	E	323	HIS	C-N	-6.29	1.26	1.34
1	A	351	PRO	CA-C	-6.29	1.46	1.52
2	F	452	LYS	CA-C	-6.29	1.44	1.53
2	D	267	LEU	CA-C	-6.28	1.44	1.52
1	A	338	SER	CA-C	-6.28	1.44	1.52
1	A	307	VAL	N-CA	-6.27	1.38	1.46
1	C	403	VAL	CA-C	-6.26	1.44	1.52
1	B	39	ILE	CA-C	-6.25	1.45	1.52
2	E	263	TYR	CA-C	-6.25	1.45	1.52
2	D	391	ASP	CA-C	-6.24	1.45	1.52
1	C	519	ILE	CA-C	-6.23	1.44	1.52
3	G	161	VAL	CA-C	-6.23	1.44	1.52
1	A	463	GLY	CA-C	-6.22	1.44	1.52
1	C	215	LEU	CA-C	-6.21	1.45	1.53
2	F	50	VAL	CA-C	-6.21	1.43	1.53
1	C	340	ARG	N-CA	-6.21	1.39	1.46
1	B	288	ILE	CA-C	-6.20	1.45	1.52
1	C	511	LYS	CA-C	-6.20	1.44	1.52
1	A	447	TYR	N-CA	-6.20	1.40	1.46
8	N	281	TYR	CA-C	-6.20	1.45	1.52
2	F	327	ASP	CA-C	-6.19	1.44	1.52
1	C	329	ARG	CA-C	-6.19	1.45	1.52
1	A	395	VAL	CA-C	-6.19	1.43	1.52
1	A	397	GLN	CA-C	-6.19	1.44	1.52
2	D	418	PHE	CA-C	-6.19	1.44	1.52
2	E	161	ASN	CA-C	-6.18	1.45	1.52
1	C	245	SER	CA-C	-6.17	1.45	1.52
2	D	119	LEU	CA-C	-6.16	1.45	1.52
2	D	14	ILE	CA-C	-6.14	1.44	1.52
1	C	4	GLY	CA-C	-6.13	1.45	1.51
2	F	425	GLN	CA-C	-6.13	1.45	1.52
2	D	280	ARG	CA-C	-6.13	1.44	1.52
2	D	412	LEU	CA-C	-6.13	1.45	1.53
3	G	27	LEU	CA-C	-6.12	1.44	1.52
1	C	257	GLU	CA-C	-6.11	1.45	1.52
3	G	192	PHE	CA-C	-6.11	1.44	1.52
2	E	292	ALA	CA-C	-6.10	1.44	1.52
2	E	220	PHE	CA-C	-6.09	1.44	1.52
2	E	430	ARG	CA-C	-6.09	1.45	1.52
2	E	158	LEU	CA-C	-6.08	1.46	1.52
2	D	381	GLN	N-CA	-6.08	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	511	LYS	CA-C	-6.08	1.45	1.52
2	E	196	ILE	CA-C	-6.07	1.46	1.52
1	A	5	VAL	CA-C	-6.07	1.47	1.52
1	C	343	GLU	CA-C	-6.04	1.45	1.52
2	D	435	SER	N-CA	-6.04	1.38	1.46
3	G	10	ASN	N-CA	-6.04	1.38	1.46
1	C	264	ASP	CA-C	-6.03	1.45	1.52
1	C	229	PRO	CA-C	-6.02	1.43	1.52
1	B	441	GLU	CA-C	-6.02	1.45	1.52
2	E	366	VAL	CA-C	-6.01	1.45	1.52
3	G	58	LYS	CA-C	-6.01	1.44	1.52
1	A	216	PHE	CA-C	-6.01	1.45	1.52
1	A	214	VAL	CA-C	-6.00	1.45	1.52
1	C	252	TYR	CA-C	-6.00	1.45	1.52
2	F	124	ARG	CA-C	-6.00	1.45	1.52
2	F	341	ARG	CA-C	-6.00	1.44	1.52
2	E	254	LEU	CA-C	-6.00	1.45	1.52
1	C	16	ALA	CA-C	-6.00	1.45	1.52
1	B	362	TYR	CA-C	-5.99	1.44	1.52
2	D	283	TYR	CA-C	-5.98	1.45	1.52
2	D	384	SER	CA-C	-5.98	1.44	1.52
2	E	25	LYS	CA-C	-5.98	1.47	1.52
2	F	363	ASN	CA-C	-5.96	1.45	1.52
1	B	255	CYS	CA-C	-5.96	1.44	1.52
4	H	78	LYS	CA-C	-5.96	1.45	1.52
1	C	386	PRO	CA-C	-5.96	1.48	1.52
1	C	412	SER	CA-C	-5.95	1.45	1.52
1	B	300	GLU	CA-C	-5.95	1.44	1.52
1	A	419	PHE	CA-C	-5.94	1.44	1.52
1	A	243	LYS	N-CA	-5.93	1.42	1.47
1	C	240	SER	N-CA	-5.93	1.39	1.46
2	E	326	PRO	CA-C	-5.93	1.44	1.52
2	D	145	VAL	CA-C	-5.93	1.45	1.52
2	F	129	GLN	CA-C	-5.93	1.45	1.52
1	B	143	PHE	CA-C	-5.92	1.45	1.52
2	D	318	ASP	CA-C	-5.92	1.46	1.53
2	F	270	ILE	CA-C	-5.92	1.45	1.52
2	D	386	TYR	CA-C	-5.91	1.45	1.52
1	A	252	TYR	CA-C	-5.91	1.45	1.52
1	A	506	TYR	CA-C	-5.91	1.45	1.52
1	B	405	ALA	CA-C	-5.91	1.45	1.52
1	B	313	PHE	CA-C	-5.90	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	140	VAL	CA-C	-5.90	1.45	1.52
2	F	54	TYR	CA-C	-5.90	1.45	1.52
1	C	512	ALA	CA-C	-5.89	1.44	1.52
1	C	506	TYR	CA-C	-5.89	1.45	1.52
2	F	94	ASN	CA-C	-5.89	1.45	1.53
2	D	25	LYS	CA-C	-5.88	1.44	1.52
1	C	80	LEU	CA-C	-5.87	1.45	1.52
1	B	336	GLU	CA-C	-5.87	1.45	1.52
2	F	117	LEU	CA-C	-5.87	1.46	1.52
2	D	33	VAL	CA-C	-5.87	1.45	1.52
1	C	30	VAL	CA-C	-5.86	1.45	1.52
3	G	167	VAL	CA-C	-5.86	1.45	1.52
1	B	20	LEU	CA-C	-5.86	1.45	1.52
1	C	236	VAL	CA-C	-5.86	1.45	1.52
2	E	281	ARG	CA-C	-5.86	1.45	1.52
7	M	69	VAL	CA-C	-5.86	1.45	1.52
2	D	24	ALA	CA-C	-5.86	1.45	1.52
1	C	244	TRP	CA-C	-5.85	1.45	1.52
1	C	205	PHE	CA-C	-5.84	1.45	1.52
2	E	310	GLN	CA-C	-5.84	1.45	1.52
1	A	253	VAL	CA-C	-5.83	1.45	1.52
1	C	232	SER	CA-C	-5.83	1.45	1.52
2	F	167	ILE	CA-C	-5.83	1.44	1.52
2	E	289	THR	CA-C	-5.82	1.44	1.52
1	B	38	GLU	CA-C	-5.80	1.45	1.52
3	G	65	LEU	N-CA	-5.80	1.39	1.46
2	D	265	GLU	CA-C	-5.80	1.45	1.52
2	D	207	GLU	CA-C	-5.80	1.45	1.52
3	G	191	THR	CA-C	-5.80	1.45	1.52
2	E	34	ASP	CA-C	-5.80	1.45	1.52
1	A	230	PHE	CA-C	-5.79	1.45	1.53
2	D	357	SER	CA-C	-5.79	1.46	1.52
1	B	224	ALA	CA-C	-5.79	1.45	1.53
2	D	115	THR	CA-C	-5.79	1.45	1.52
2	F	289	THR	CA-C	-5.79	1.45	1.52
1	A	239	GLN	CA-C	-5.78	1.45	1.52
1	A	413	LEU	N-CA	-5.78	1.39	1.46
2	F	313	ILE	CA-C	-5.77	1.45	1.52
2	E	247	PHE	CA-C	-5.76	1.45	1.52
1	C	491	ARG	CA-C	-5.76	1.45	1.52
1	B	185	HIS	CA-C	-5.74	1.45	1.52
2	E	261	THR	CA-C	-5.74	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	246	ALA	CA-C	-5.74	1.45	1.52
1	B	427	SER	CA-C	-5.73	1.45	1.52
1	C	339	SER	CA-C	-5.72	1.45	1.52
2	F	195	GLY	CA-C	-5.72	1.43	1.51
1	A	255	CYS	CA-C	-5.71	1.46	1.52
1	C	216	PHE	CA-C	-5.71	1.46	1.52
1	A	232	SER	N-CA	-5.71	1.41	1.46
2	F	357	SER	CA-C	-5.70	1.45	1.52
2	D	120	ASN	CA-C	-5.69	1.47	1.53
1	B	64	VAL	CA-C	-5.69	1.45	1.52
3	G	42	LEU	CA-C	-5.69	1.45	1.52
2	F	386	TYR	CA-C	-5.68	1.45	1.52
1	A	147	ILE	CA-C	-5.68	1.45	1.52
4	H	16	ALA	CA-C	-5.68	1.45	1.52
1	C	102	ILE	CA-C	-5.68	1.45	1.52
2	E	440	TRP	CA-C	-5.67	1.44	1.52
1	C	19	MET	CA-C	-5.67	1.45	1.52
7	M	302	LEU	CA-C	-5.67	1.45	1.52
2	F	378	VAL	CA-C	-5.67	1.46	1.52
2	F	278	PRO	CA-C	-5.66	1.45	1.52
2	D	94	ASN	CA-C	-5.66	1.46	1.52
3	G	157	THR	CA-C	-5.66	1.45	1.52
2	E	232	ILE	CA-C	-5.65	1.45	1.53
2	E	316	MET	C-N	-5.64	1.28	1.34
1	C	255	CYS	CA-C	-5.64	1.45	1.52
2	E	47	VAL	CA-C	-5.64	1.45	1.52
2	D	329	THR	CA-C	-5.63	1.45	1.52
1	B	501	HIS	CA-C	-5.63	1.45	1.52
3	G	20	LEU	CA-C	-5.62	1.45	1.52
2	E	48	ILE	CA-C	-5.61	1.45	1.52
6	J	165	ASN	CA-C	-5.61	1.48	1.53
2	E	339	LEU	CA-C	-5.61	1.45	1.52
1	A	355	ALA	CA-C	-5.61	1.45	1.52
1	A	425	ASN	CA-C	-5.61	1.46	1.52
2	D	71	THR	CA-C	-5.61	1.48	1.53
2	E	235	PRO	CA-C	-5.60	1.44	1.52
2	F	156	SER	CA-C	-5.60	1.45	1.52
2	F	150	LEU	CA-C	-5.60	1.48	1.52
2	F	398	ILE	N-CA	-5.60	1.41	1.46
2	D	377	GLN	CA-C	-5.59	1.44	1.52
4	H	45	VAL	CA-C	-5.59	1.45	1.52
1	A	251	VAL	CA-C	-5.59	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	ILE	CA-C	-5.59	1.45	1.52
3	G	178	PHE	CA-C	-5.58	1.45	1.52
2	F	398	ILE	CA-C	-5.58	1.47	1.52
1	C	295	PRO	CA-C	-5.58	1.45	1.52
1	C	452	ASP	CA-C	-5.58	1.45	1.52
2	D	361	LEU	CA-C	-5.58	1.46	1.52
2	F	331	TYR	CA-C	-5.58	1.45	1.52
2	E	28	ALA	CA-C	-5.57	1.45	1.52
2	F	117	LEU	N-CA	-5.57	1.41	1.45
9	R	38	GLY	CA-C	-5.57	1.45	1.52
4	H	12	GLY	CA-C	-5.56	1.46	1.52
2	F	342	GLU	N-CA	-5.56	1.39	1.46
2	E	233	LEU	CA-C	-5.55	1.46	1.52
2	E	11	ILE	CA-C	-5.55	1.46	1.52
1	A	55	THR	CA-C	-5.54	1.45	1.52
1	C	203	THR	CA-C	-5.54	1.48	1.52
1	B	468	VAL	N-CA	-5.54	1.40	1.46
1	B	249	VAL	CA-C	-5.54	1.45	1.52
2	E	277	ILE	CA-C	-5.53	1.47	1.52
1	C	350	TYR	C-N	-5.53	1.26	1.33
1	C	334	LEU	CA-C	-5.52	1.45	1.52
2	F	329	THR	CA-C	-5.52	1.45	1.52
3	G	15	ARG	CA-C	-5.52	1.45	1.52
1	A	51	VAL	CA-C	-5.51	1.45	1.52
1	B	442	ASN	CA-C	-5.51	1.45	1.53
1	B	337	ILE	CA-C	-5.51	1.46	1.52
2	E	31	ALA	CA-C	-5.51	1.45	1.52
1	A	483	VAL	CA-C	-5.50	1.46	1.52
1	B	307	VAL	CA-C	-5.50	1.46	1.52
2	E	283	TYR	CA-C	-5.50	1.47	1.52
1	B	94	ILE	N-CA	-5.50	1.39	1.46
1	C	303	ILE	CA-C	-5.49	1.46	1.52
1	A	136	GLY	CA-C	-5.49	1.46	1.51
2	E	237	MET	CA-C	-5.49	1.46	1.52
2	F	240	THR	CA-C	-5.49	1.45	1.52
2	F	111	ARG	CA-C	-5.49	1.45	1.52
1	B	39	ILE	N-CA	-5.48	1.39	1.46
1	A	519	ILE	N-CA	-5.47	1.40	1.46
1	C	321	ALA	CA-C	-5.47	1.46	1.52
2	D	82	LEU	CA-C	-5.47	1.45	1.52
2	D	311	ILE	CA-C	-5.47	1.47	1.52
1	B	291	THR	CA-C	-5.46	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	318	ASP	CA-C	-5.46	1.45	1.52
2	D	87	GLU	CA-C	-5.46	1.46	1.53
2	E	284	PRO	CA-C	-5.46	1.46	1.52
2	E	290	ASP	CA-C	-5.46	1.45	1.52
2	E	308	VAL	CA-C	-5.45	1.46	1.52
2	E	25	LYS	N-CA	-5.45	1.42	1.47
2	F	221	LEU	N-CA	-5.44	1.39	1.46
2	F	387	ALA	CA-C	-5.44	1.46	1.52
2	F	196	ILE	CA-C	-5.44	1.45	1.52
3	G	182	VAL	CA-C	-5.43	1.45	1.52
2	F	354	PRO	CA-C	-5.43	1.44	1.52
2	D	28	ALA	CA-C	-5.43	1.46	1.52
2	F	249	HIS	CA-C	-5.42	1.45	1.52
1	B	289	ALA	CA-C	-5.42	1.46	1.52
1	C	157	VAL	CA-C	-5.42	1.46	1.52
1	A	292	SER	CA-C	-5.42	1.45	1.52
1	C	53	GLU	CA-C	-5.41	1.46	1.52
2	E	9	THR	CA-C	-5.40	1.46	1.52
1	B	261	GLU	CA-C	-5.39	1.45	1.52
1	B	244	TRP	CA-C	-5.39	1.46	1.52
2	F	59	VAL	CA-C	-5.39	1.46	1.52
1	C	309	ILE	CA-C	-5.38	1.45	1.52
6	L	186	LEU	CA-C	-5.38	1.45	1.52
8	N	249	LEU	CA-C	-5.38	1.45	1.52
2	E	273	ALA	CA-C	-5.38	1.45	1.53
2	F	260	MET	CA-C	-5.37	1.45	1.52
1	A	508	SER	CA-C	-5.37	1.46	1.52
2	E	385	ALA	CA-C	-5.36	1.46	1.52
1	A	378	VAL	CA-C	-5.36	1.45	1.52
2	D	143	THR	CA-C	-5.36	1.46	1.52
2	E	270	ILE	CA-C	-5.36	1.46	1.52
2	E	125	ARG	CA-C	-5.36	1.45	1.52
3	G	191	THR	N-CA	-5.36	1.40	1.46
1	C	393	GLU	CA-C	-5.35	1.46	1.52
2	D	239	LEU	CA-C	-5.35	1.46	1.52
2	E	280	ARG	CA-C	-5.34	1.45	1.52
2	F	311	ILE	CA-C	-5.34	1.47	1.52
1	C	237	THR	CA-C	-5.34	1.45	1.52
2	F	421	PHE	CA-C	-5.34	1.45	1.52
1	A	20	LEU	CA-C	-5.34	1.46	1.52
2	E	431	SER	CA-C	-5.34	1.46	1.52
1	A	386	PRO	C-N	-5.33	1.27	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	LYS	N-CA	-5.33	1.39	1.46
2	F	337	ILE	CA-C	-5.33	1.46	1.52
1	B	153	VAL	CA-C	-5.32	1.46	1.52
2	D	352	ILE	N-CA	-5.32	1.39	1.46
1	C	271	GLU	CA-C	-5.32	1.45	1.52
4	H	18	LEU	CA-C	-5.32	1.45	1.52
1	B	430	LEU	CA-C	-5.32	1.45	1.52
2	D	433	GLU	CA-C	-5.32	1.45	1.52
3	G	50	ARG	CA-C	-5.32	1.46	1.52
2	F	163	ILE	N-CA	-5.32	1.40	1.46
2	E	197	THR	CA-C	-5.31	1.45	1.53
1	C	246	ASN	CA-C	-5.30	1.46	1.53
1	C	273	THR	CA-C	-5.30	1.46	1.52
6	L	182	VAL	CA-C	-5.30	1.46	1.52
1	A	102	ILE	CA-C	-5.30	1.47	1.53
1	A	133	MET	CA-C	-5.30	1.46	1.52
1	A	427	SER	CA-C	-5.30	1.46	1.52
2	F	8	TYR	CA-C	-5.29	1.45	1.52
2	E	327	ASP	N-CA	-5.29	1.40	1.46
2	E	141	MET	CA-C	-5.29	1.46	1.52
4	H	77	LEU	CA-C	-5.29	1.45	1.52
1	A	439	TYR	CA-C	-5.28	1.46	1.52
1	B	141	PHE	CA-C	-5.28	1.46	1.53
1	C	457	LEU	N-CA	-5.28	1.40	1.46
1	B	346	ALA	N-CA	-5.27	1.40	1.46
2	F	315	SER	CA-C	-5.27	1.46	1.52
1	C	184	TYR	CA-C	-5.27	1.46	1.52
1	B	350	TYR	CA-C	-5.27	1.47	1.53
1	B	367	LYS	CA-C	-5.27	1.47	1.53
2	F	108	PRO	CA-C	-5.26	1.47	1.53
2	E	188	ALA	CA-C	-5.26	1.46	1.52
1	C	83	ILE	CA-C	-5.25	1.46	1.52
2	D	296	GLU	CA-C	-5.25	1.46	1.52
2	F	244	TYR	CA-C	-5.25	1.45	1.52
2	E	265	GLU	CA-C	-5.25	1.45	1.52
1	C	62	GLU	CA-C	-5.25	1.46	1.53
1	A	344	MET	CA-C	-5.25	1.46	1.52
1	B	322	LEU	CA-C	-5.25	1.45	1.52
2	E	226	ASP	CA-C	-5.24	1.46	1.52
2	E	346	LYS	CA-C	-5.24	1.45	1.52
2	E	255	VAL	CA-C	-5.24	1.46	1.52
2	E	290	ASP	N-CA	-5.24	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	399	THR	CA-C	-5.24	1.46	1.52
2	D	166	GLN	CA-C	-5.24	1.46	1.52
1	A	458	LEU	CA-C	-5.23	1.45	1.52
1	A	171	PRO	CA-C	-5.23	1.47	1.52
1	B	83	ILE	CA-C	-5.23	1.46	1.52
3	G	184	GLU	CA-C	-5.23	1.46	1.52
1	C	402	ILE	CA-C	-5.23	1.46	1.52
2	E	268	ARG	CA-C	-5.23	1.46	1.52
1	A	191	ARG	CA-C	-5.22	1.46	1.52
3	G	47	MET	CA-C	-5.22	1.45	1.52
1	C	190	ARG	CA-C	-5.22	1.46	1.53
1	C	195	VAL	CA-C	-5.22	1.46	1.52
2	D	355	LEU	N-CA	-5.22	1.41	1.46
1	A	184	TYR	CA-C	-5.22	1.46	1.52
1	C	405	ALA	CA-C	-5.22	1.46	1.53
1	B	274	ASP	CA-C	-5.21	1.47	1.53
1	C	535	SER	CA-C	-5.21	1.46	1.52
1	B	165	GLU	CA-C	-5.21	1.46	1.52
2	E	11	ILE	N-CA	-5.21	1.40	1.46
1	A	491	ARG	CA-C	-5.20	1.45	1.52
2	E	244	TYR	CA-C	-5.19	1.46	1.52
1	A	167	THR	CA-C	-5.19	1.46	1.53
1	A	451	ARG	CA-C	-5.19	1.45	1.52
1	B	102	ILE	CA-C	-5.19	1.46	1.52
2	D	47	VAL	CA-C	-5.19	1.46	1.52
2	F	255	VAL	CA-C	-5.18	1.46	1.52
1	C	250	VAL	N-CA	-5.18	1.40	1.46
2	E	167	ILE	CA-C	-5.18	1.45	1.52
2	F	131	ILE	CA-C	-5.17	1.46	1.52
1	C	361	PHE	CA-C	-5.17	1.46	1.52
1	C	216	PHE	N-CA	-5.17	1.40	1.46
1	C	357	ARG	CA-C	-5.17	1.45	1.52
2	E	24	ALA	CA-C	-5.17	1.46	1.52
2	F	161	ASN	CA-C	-5.17	1.45	1.52
1	B	428	TYR	CA-C	-5.17	1.46	1.52
1	B	149	VAL	CA-C	-5.16	1.48	1.52
2	F	130	PHE	CA-C	-5.16	1.46	1.52
2	F	71	THR	CA-C	-5.16	1.46	1.52
1	B	160	VAL	CA-C	-5.16	1.46	1.52
2	E	169	ARG	CA-C	-5.16	1.45	1.52
2	E	266	ALA	CA-C	-5.16	1.46	1.52
1	A	565	GLU	CA-C	-5.15	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	PHE	CA-C	-5.15	1.46	1.53
1	A	211	ILE	CA-C	-5.15	1.46	1.52
2	D	414	PHE	CA-C	-5.15	1.46	1.52
1	A	460	ARG	CA-C	-5.14	1.45	1.52
2	D	295	TYR	CA-C	-5.14	1.45	1.52
2	F	144	LEU	CA-C	-5.14	1.46	1.52
1	A	73	VAL	N-CA	-5.14	1.40	1.46
1	B	457	LEU	N-CA	-5.14	1.40	1.46
2	E	256	ILE	CA-C	-5.13	1.46	1.52
2	E	264	CYS	CA-C	-5.13	1.46	1.52
3	G	190	ASP	CA-C	-5.13	1.46	1.52
1	C	290	ASN	CA-C	-5.12	1.46	1.52
2	F	302	GLU	CA-C	-5.12	1.46	1.52
1	A	103	THR	CA-C	-5.12	1.46	1.52
1	B	30	VAL	CA-C	-5.12	1.46	1.52
1	A	428	TYR	CA-C	-5.12	1.46	1.52
1	C	506	TYR	N-CA	-5.11	1.39	1.45
1	C	96	GLU	CA-C	-5.11	1.46	1.52
2	E	192	ALA	CA-C	-5.11	1.46	1.52
1	C	42	LEU	CA-C	-5.11	1.46	1.52
2	D	156	SER	CA-C	-5.11	1.46	1.52
2	D	416	ASP	CA-C	-5.11	1.46	1.52
2	F	115	THR	CA-C	-5.10	1.45	1.52
1	C	96	GLU	N-CA	-5.10	1.40	1.46
1	A	109	HIS	CA-C	-5.10	1.46	1.52
1	A	283	HIS	CA-C	-5.10	1.46	1.52
7	M	188	LEU	CA-C	-5.10	1.46	1.52
2	D	167	ILE	CA-C	-5.10	1.46	1.52
2	D	366	VAL	CA-C	-5.09	1.47	1.52
2	F	56	VAL	CA-C	-5.09	1.46	1.52
3	G	13	GLN	CA-C	-5.09	1.46	1.52
2	E	165	ALA	CA-C	-5.09	1.46	1.52
2	E	175	PRO	CA-C	-5.09	1.47	1.52
2	D	359	SER	CA-C	-5.08	1.46	1.52
2	E	364	ASN	N-CA	-5.08	1.39	1.46
2	D	218	VAL	CA-C	-5.08	1.46	1.52
1	A	98	THR	CA-C	-5.08	1.49	1.52
1	C	502	GLU	N-CA	-5.08	1.40	1.46
4	H	96	LYS	CA-C	-5.08	1.46	1.52
1	B	369	ILE	CA-C	-5.08	1.46	1.52
1	B	100	ILE	CA-C	-5.08	1.46	1.52
4	H	4	ILE	CA-C	-5.08	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	352	ILE	N-CA	-5.08	1.39	1.46
2	E	114	ILE	CA-C	-5.07	1.46	1.52
1	C	292	SER	CA-C	-5.07	1.46	1.52
1	A	419	PHE	N-CA	-5.07	1.40	1.46
2	D	120	ASN	C-N	-5.06	1.27	1.34
3	G	34	ALA	CA-C	-5.06	1.46	1.52
1	C	377	ALA	CA-C	-5.06	1.46	1.52
1	A	352	PRO	CA-C	-5.06	1.45	1.52
1	A	456	GLU	N-CA	-5.06	1.40	1.46
1	C	509	MET	CA-C	-5.06	1.45	1.52
1	A	106	VAL	CA-C	-5.06	1.46	1.52
1	A	313	PHE	CA-C	-5.06	1.45	1.52
2	E	353	ASP	C-N	-5.06	1.27	1.34
1	B	292	SER	CA-C	-5.05	1.46	1.52
2	E	423	ILE	CA-C	-5.05	1.47	1.52
2	E	278	PRO	CA-C	-5.05	1.45	1.52
2	F	34	ASP	CA-C	-5.04	1.46	1.52
1	C	294	MET	CA-C	-5.04	1.46	1.52
1	C	508	SER	CA-C	-5.04	1.46	1.52
1	B	53	GLU	CA-C	-5.04	1.46	1.53
1	B	269	PHE	N-CA	-5.04	1.42	1.46
1	C	518	MET	CA-C	-5.04	1.46	1.52
2	D	372	ARG	CA-C	-5.04	1.46	1.52
1	C	20	LEU	CA-C	-5.03	1.46	1.52
2	D	315	SER	CA-C	-5.03	1.46	1.52
1	B	32	GLU	CA-C	-5.03	1.46	1.52
2	F	105	PRO	CA-C	-5.03	1.46	1.52
2	D	24	ALA	N-CA	-5.03	1.40	1.46
2	F	93	PHE	CA-C	-5.03	1.46	1.52
1	A	300	GLU	CA-C	-5.03	1.46	1.52
2	E	442	LEU	N-CA	-5.03	1.40	1.46
2	F	375	HIS	CA-C	-5.03	1.46	1.52
2	F	334	GLU	CA-C	-5.02	1.46	1.52
2	D	26	ASP	CA-C	-5.02	1.45	1.52
2	D	252	HIS	CA-C	-5.02	1.46	1.52
1	C	26	ASP	CA-C	-5.02	1.46	1.52
2	F	28	ALA	CA-C	-5.02	1.46	1.52
1	B	352	PRO	CA-C	-5.01	1.44	1.52
2	E	138	ILE	CA-C	-5.01	1.46	1.52
1	A	396	THR	N-CA	-5.01	1.40	1.46
2	E	50	VAL	CA-C	-5.01	1.46	1.52
4	H	47	VAL	CA-C	-5.01	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	326	SER	CA-C	-5.01	1.47	1.53
1	A	180	GLU	CA-C	-5.01	1.46	1.52
1	A	518	MET	CA-C	-5.01	1.46	1.52
2	F	202	SER	CA-C	-5.01	1.46	1.52
2	E	219	LEU	CA-C	-5.01	1.47	1.53
1	A	220	MET	CA-C	-5.00	1.46	1.52
1	B	321	ALA	CA-C	-5.00	1.48	1.53
1	A	64	VAL	CA-C	-5.00	1.46	1.52
1	A	368	VAL	N-CA	-5.00	1.40	1.46
2	D	358	LEU	CA-C	-5.00	1.46	1.52

All (876) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	VAL	N-CA-C	-13.28	98.30	109.19
3	G	46	ALA	N-CA-C	12.20	125.91	111.02
6	L	53	TYR	N-CA-C	-11.81	96.30	112.12
8	N	3	ALA	N-CA-C	-11.59	97.76	108.07
3	G	71	ASP	N-CA-C	-11.46	98.10	112.88
1	B	410	ASP	CA-C-N	11.04	135.08	120.28
1	B	410	ASP	C-N-CA	11.04	135.08	120.28
8	N	547	MET	CA-C-N	10.65	126.95	120.24
8	N	547	MET	C-N-CA	10.65	126.95	120.24
3	G	31	LYS	N-CA-C	-10.55	99.32	111.03
8	N	632	PHE	N-CA-C	-10.50	98.02	110.41
1	A	462	ALA	CA-C-N	10.49	131.78	120.03
1	A	462	ALA	C-N-CA	10.49	131.78	120.03
9	Q	79	ARG	N-CA-C	-10.44	101.60	114.75
2	E	319	ASP	N-CA-C	-10.35	98.02	110.44
2	D	213	ALA	N-CA-C	-10.08	103.13	114.62
1	C	381	VAL	CA-C-N	9.91	131.95	121.45
1	C	381	VAL	C-N-CA	9.91	131.95	121.45
1	C	185	HIS	CA-C-N	9.90	137.10	121.66
1	C	185	HIS	C-N-CA	9.90	137.10	121.66
2	E	19	LEU	CA-C-N	9.43	134.54	121.05
2	E	19	LEU	C-N-CA	9.43	134.54	121.05
7	M	280	PRO	CA-C-N	9.43	132.91	120.28
7	M	280	PRO	C-N-CA	9.43	132.91	120.28
8	N	546	LEU	N-CA-C	-9.26	102.56	114.04
2	F	450	GLU	N-CA-C	-9.24	103.11	114.75
1	C	352	PRO	N-CA-C	-9.23	103.94	114.92
1	B	172	VAL	N-CA-C	-9.18	103.78	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	412	LEU	N-CA-C	-9.01	97.78	111.56
3	G	40	PHE	N-CA-C	8.92	121.01	111.28
1	C	168	VAL	CA-C-N	8.76	132.36	120.54
1	C	168	VAL	C-N-CA	8.76	132.36	120.54
1	B	376	GLY	CA-C-N	8.62	133.65	121.24
1	B	376	GLY	C-N-CA	8.62	133.65	121.24
1	C	528	ALA	N-CA-C	-8.58	102.74	113.55
5	K	107	LEU	CA-C-N	8.56	133.66	120.82
5	K	107	LEU	C-N-CA	8.56	133.66	120.82
2	D	162	GLU	N-CA-C	-8.55	101.53	111.03
2	D	155	GLY	N-CA-C	-8.55	100.24	112.55
2	D	370	LYS	N-CA-C	-8.55	104.88	114.62
2	D	139	ASP	N-CA-C	-8.53	104.01	114.75
9	Q	42	VAL	CA-C-N	8.53	129.44	119.98
9	Q	42	VAL	C-N-CA	8.53	129.44	119.98
2	F	245	LEU	N-CA-C	-8.49	102.70	113.23
2	F	292	ALA	N-CA-C	-8.46	100.03	111.96
5	K	28	GLU	N-CA-C	-8.42	102.94	113.55
8	N	326	TRP	N-CA-C	-8.40	102.62	113.12
1	B	263	THR	N-CA-C	-8.38	103.65	114.04
1	A	389	GLY	N-CA-C	-8.38	103.76	115.32
1	B	538	GLU	N-CA-C	-8.37	102.00	112.72
2	E	25	LYS	N-CA-C	-8.36	101.51	113.21
2	F	222	ASN	N-CA-C	-8.34	95.31	109.24
9	Q	37	ILE	CA-C-N	8.34	129.24	119.98
9	Q	37	ILE	C-N-CA	8.34	129.24	119.98
2	D	331	TYR	N-CA-C	-8.34	102.92	113.43
2	D	53	GLU	N-CA-C	-8.33	98.36	111.02
9	U	40	ALA	CA-C-N	8.30	129.20	119.98
9	U	40	ALA	C-N-CA	8.30	129.20	119.98
7	M	76	VAL	N-CA-C	-8.28	95.99	107.75
8	N	528	MET	CA-C-N	8.26	131.70	120.38
8	N	528	MET	C-N-CA	8.26	131.70	120.38
1	B	461	GLU	N-CA-C	-8.25	101.95	112.93
9	R	79	ARG	N-CA-C	-8.22	105.25	114.62
2	D	109	GLU	N-CA-C	-8.17	103.10	113.23
2	F	109	GLU	N-CA-C	-8.17	102.27	112.72
1	B	32	GLU	N-CA-C	-8.16	105.32	114.62
1	A	425	ASN	N-CA-C	-8.04	93.70	108.02
2	F	61	GLU	N-CA-C	-8.02	98.40	109.95
7	M	29	LEU	N-CA-C	8.00	120.91	111.71
2	D	73	VAL	CA-C-N	7.97	133.03	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	73	VAL	C-N-CA	7.97	133.03	122.42
8	N	292	GLU	N-CA-C	7.90	119.52	111.07
2	D	142	ASN	N-CA-C	-7.89	94.00	110.80
8	N	356	PRO	CA-C-N	7.88	130.84	120.28
8	N	356	PRO	C-N-CA	7.88	130.84	120.28
1	C	52	TYR	N-CA-C	-7.88	100.31	112.99
2	F	398	ILE	N-CA-C	-7.87	105.40	111.62
9	W	49	ARG	CA-C-N	7.84	130.79	120.28
9	W	49	ARG	C-N-CA	7.84	130.79	120.28
2	F	104	PRO	N-CA-C	7.84	120.26	110.70
1	B	344	MET	N-CA-C	-7.83	99.86	110.36
3	G	66	LEU	N-CA-C	-7.82	103.73	113.28
9	X	10	LEU	N-CA-C	7.78	119.76	111.28
1	B	233	GLY	CA-C-N	7.74	131.43	120.28
1	B	233	GLY	C-N-CA	7.74	131.43	120.28
8	N	73	GLU	CA-C-N	7.71	132.39	120.75
8	N	73	GLU	C-N-CA	7.71	132.39	120.75
2	F	403	ALA	N-CA-C	-7.67	102.98	114.64
1	C	425	ASN	N-CA-C	-7.65	102.16	112.26
1	A	351	PRO	N-CA-C	-7.61	101.42	110.70
6	L	97	LYS	N-CA-C	-7.61	100.49	110.07
1	A	185	HIS	CA-C-N	7.58	131.63	120.87
1	A	185	HIS	C-N-CA	7.58	131.63	120.87
1	B	52	TYR	N-CA-C	7.58	119.18	111.07
4	H	47	VAL	N-CA-C	-7.57	97.75	108.80
1	B	102	ILE	N-CA-C	-7.56	97.59	108.48
1	A	517	LYS	N-CA-C	-7.55	104.04	113.55
2	E	226	ASP	N-CA-C	-7.54	99.50	108.25
2	D	273	ALA	N-CA-C	-7.52	102.93	112.93
1	B	346	ALA	N-CA-C	-7.48	97.68	108.60
2	D	339	LEU	N-CA-C	-7.44	96.81	109.24
2	F	297	ARG	N-CA-C	7.43	120.25	111.71
1	C	465	GLN	CA-C-N	7.38	131.05	120.79
1	C	465	GLN	C-N-CA	7.38	131.05	120.79
6	J	63	ALA	CA-C-N	7.36	128.27	120.03
6	J	63	ALA	C-N-CA	7.36	128.27	120.03
2	D	453	ARG	N-CA-C	-7.35	103.40	112.88
5	I	22	LEU	CA-C-N	7.35	135.20	121.97
5	I	22	LEU	C-N-CA	7.35	135.20	121.97
1	B	525	GLU	N-CA-C	-7.33	104.59	113.97
1	C	73	VAL	N-CA-C	7.32	118.82	108.36
1	C	506	TYR	N-CA-C	-7.32	97.50	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207	THR	N-CA-C	-7.31	103.96	113.17
1	C	246	ASN	N-CA-C	-7.31	98.50	109.83
8	N	440	THR	CA-C-N	7.30	128.96	119.84
8	N	440	THR	C-N-CA	7.30	128.96	119.84
1	C	494	PHE	CA-C-N	7.29	130.39	120.54
1	C	494	PHE	C-N-CA	7.29	130.39	120.54
1	C	486	VAL	CA-C-N	7.27	128.17	120.03
1	C	486	VAL	C-N-CA	7.27	128.17	120.03
1	C	433	SER	N-CA-C	-7.26	103.73	112.59
1	A	442	ASN	N-CA-C	7.25	118.87	110.97
8	N	138	LEU	N-CA-C	-7.23	98.45	109.95
1	C	499	ALA	N-CA-C	-7.23	99.72	110.06
2	E	68	LEU	N-CA-C	-7.22	98.35	108.54
1	C	102	ILE	N-CA-C	-7.22	97.63	108.17
7	M	280	PRO	N-CA-C	-7.21	102.50	114.75
2	D	451	LEU	N-CA-C	-7.20	97.00	108.73
8	N	524	LEU	N-CA-C	-7.20	102.62	111.40
2	D	158	LEU	N-CA-C	-7.17	101.88	110.13
2	E	210	ARG	N-CA-C	-7.17	104.15	113.12
5	K	22	LEU	CA-C-N	7.16	134.86	121.97
5	K	22	LEU	C-N-CA	7.16	134.86	121.97
2	E	286	TYR	N-CA-C	-7.14	101.49	112.99
2	D	258	THR	CA-C-N	7.14	135.18	121.54
2	D	258	THR	C-N-CA	7.14	135.18	121.54
9	W	58	PHE	N-CA-C	7.14	118.71	111.07
1	C	266	LEU	N-CA-C	7.13	118.74	110.97
2	E	110	LYS	CA-C-N	7.11	131.90	122.30
2	E	110	LYS	C-N-CA	7.11	131.90	122.30
2	F	158	LEU	N-CA-C	-7.11	99.97	108.14
8	N	385	ARG	N-CA-C	-7.10	104.77	113.50
2	E	185	GLU	N-CA-C	-7.10	100.85	109.72
8	N	33	GLU	CA-C-N	7.09	134.47	121.70
8	N	33	GLU	C-N-CA	7.09	134.47	121.70
1	C	318	PHE	N-CA-C	7.09	121.13	110.14
1	A	156	ARG	CA-C-N	7.07	131.30	120.13
1	A	156	ARG	C-N-CA	7.07	131.30	120.13
1	A	477	GLN	N-CA-C	-7.07	95.75	110.80
2	E	189	VAL	N-CA-C	-7.06	98.32	108.42
1	A	154	ARG	N-CA-C	-7.05	95.78	108.48
9	T	42	VAL	N-CA-C	7.05	117.81	110.62
8	N	372	PHE	CA-C-N	7.05	129.73	120.28
8	N	372	PHE	C-N-CA	7.05	129.73	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Z	10	LEU	CA-C-N	7.05	129.60	120.44
9	Z	10	LEU	C-N-CA	7.05	129.60	120.44
1	B	254	GLY	N-CA-C	-7.04	100.63	111.12
8	N	365	ASP	CA-C-N	7.04	130.11	120.46
8	N	365	ASP	C-N-CA	7.04	130.11	120.46
8	N	299	GLU	N-CA-C	-7.03	97.50	109.24
1	A	57	GLY	N-CA-C	-7.02	96.53	113.18
2	E	410	ARG	N-CA-C	-7.02	104.35	113.12
2	E	364	ASN	N-CA-C	-7.01	97.69	108.76
1	C	153	VAL	N-CA-C	-7.01	97.94	108.17
1	A	420	PRO	N-CA-C	-7.00	93.90	112.10
2	E	184	GLU	N-CA-C	-6.99	106.65	114.62
6	J	22	GLU	CA-C-N	6.99	129.64	120.28
6	J	22	GLU	C-N-CA	6.99	129.64	120.28
8	N	528	MET	N-CA-C	-6.98	103.43	112.23
2	D	88	MET	N-CA-C	-6.98	104.80	113.38
1	A	381	VAL	CA-C-N	6.96	128.93	120.92
1	A	381	VAL	C-N-CA	6.96	128.93	120.92
2	D	98	LYS	CA-C-N	6.96	128.54	119.84
2	D	98	LYS	C-N-CA	6.96	128.54	119.84
8	N	643	ARG	CA-C-O	-6.94	113.51	120.66
3	G	103	ARG	N-CA-C	-6.94	98.83	109.65
8	N	82	GLU	N-CA-C	-6.93	96.05	110.80
1	A	430	LEU	N-CA-C	-6.92	103.86	112.72
2	D	39	THR	N-CA-C	-6.91	104.04	113.30
1	B	393	GLU	N-CA-C	-6.91	101.36	109.93
2	F	81	ARG	N-CA-C	-6.91	98.85	109.14
2	D	79	VAL	N-CA-C	-6.90	98.37	108.23
1	C	398	SER	N-CA-C	-6.89	104.68	113.23
3	G	77	ALA	CA-C-N	6.89	134.91	121.41
3	G	77	ALA	C-N-CA	6.89	134.91	121.41
9	S	79	ARG	N-CA-C	-6.88	104.41	114.39
1	C	271	GLU	N-CA-C	-6.88	105.17	113.97
2	E	371	THR	N-CA-C	-6.86	99.12	108.38
9	P	12	ARG	N-CA-C	6.85	118.75	111.28
1	A	239	GLN	CA-C-N	6.83	129.43	120.28
1	A	239	GLN	C-N-CA	6.83	129.43	120.28
1	B	256	GLY	N-CA-C	-6.80	105.70	115.64
1	C	350	TYR	N-CA-C	-6.80	102.02	108.07
2	D	287	MET	N-CA-C	6.80	118.48	111.14
2	E	104	PRO	N-CA-C	6.79	118.99	110.70
3	G	10	ASN	N-CA-C	-6.79	103.94	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	48	GLU	N-CA-C	6.78	119.29	111.02
8	N	270	ALA	CA-C-N	6.77	134.47	121.54
8	N	270	ALA	C-N-CA	6.77	134.47	121.54
9	Z	9	GLY	CA-C-N	6.75	130.00	120.28
9	Z	9	GLY	C-N-CA	6.75	130.00	120.28
1	A	370	THR	CA-C-N	6.74	129.99	120.28
1	A	370	THR	C-N-CA	6.74	129.99	120.28
4	H	9	THR	N-CA-C	-6.74	105.10	113.38
1	A	419	PHE	N-CA-C	-6.73	99.43	108.11
4	H	27	GLU	N-CA-C	-6.72	102.58	113.19
3	G	45	GLU	N-CA-C	6.71	119.43	111.71
2	D	264	CYS	N-CA-C	-6.66	104.80	113.12
6	L	145	GLU	N-CA-C	-6.66	99.52	108.11
8	N	503	GLY	CA-C-N	6.65	127.36	119.98
8	N	503	GLY	C-N-CA	6.65	127.36	119.98
9	P	59	LEU	CA-C-N	6.64	129.18	120.28
9	P	59	LEU	C-N-CA	6.64	129.18	120.28
2	F	152	ILE	CA-C-N	6.64	130.25	120.95
2	F	152	ILE	C-N-CA	6.64	130.25	120.95
2	E	147	GLY	CA-C-N	6.62	134.19	121.54
2	E	147	GLY	C-N-CA	6.62	134.19	121.54
4	H	93	LEU	N-CA-C	6.62	119.32	111.71
9	U	41	GLY	N-CA-C	6.61	120.66	112.73
3	G	106	ALA	N-CA-C	-6.60	100.18	110.42
5	I	75	GLU	N-CA-C	-6.60	103.70	111.03
2	D	418	PHE	N-CA-C	-6.59	103.30	112.45
4	H	54	ASP	N-CA-C	6.56	122.48	113.16
2	F	183	LYS	N-CA-C	-6.56	105.02	113.16
1	B	548	ILE	N-CA-C	-6.56	103.85	111.00
1	B	371	LEU	N-CA-C	-6.55	105.59	112.93
8	N	28	GLY	CA-C-N	6.55	130.32	120.75
8	N	28	GLY	C-N-CA	6.55	130.32	120.75
1	B	234	LYS	CA-C-N	6.55	131.17	120.63
1	B	234	LYS	C-N-CA	6.55	131.17	120.63
1	A	511	LYS	N-CA-C	-6.54	103.42	111.40
6	L	173	ARG	N-CA-C	-6.54	102.80	111.24
4	H	43	ALA	N-CA-C	-6.54	104.54	113.30
1	A	58	LEU	N-CA-C	-6.51	100.24	108.45
3	G	60	ALA	CA-C-N	6.51	131.53	121.19
3	G	60	ALA	C-N-CA	6.51	131.53	121.19
1	A	499	ALA	N-CA-C	-6.50	102.71	111.87
9	V	79	ARG	N-CA-C	-6.50	103.78	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	26	GLN	CA-C-N	6.49	128.98	120.28
7	M	26	GLN	C-N-CA	6.49	128.98	120.28
8	N	613	THR	N-CA-C	-6.49	105.36	113.28
9	R	66	VAL	CA-C-N	6.48	129.34	120.46
9	R	66	VAL	C-N-CA	6.48	129.34	120.46
1	A	555	SER	CA-C-N	6.48	133.91	121.54
1	A	555	SER	C-N-CA	6.48	133.91	121.54
3	G	189	GLU	CA-C-N	6.46	129.78	120.79
3	G	189	GLU	C-N-CA	6.46	129.78	120.79
2	E	408	ASP	N-CA-C	-6.46	105.29	113.43
7	M	32	SER	N-CA-C	-6.45	100.41	109.69
8	N	536	LEU	N-CA-C	6.45	117.97	111.07
1	C	177	ASP	N-CA-C	-6.44	103.42	113.02
9	T	55	ALA	CA-C-N	6.44	129.20	120.44
9	T	55	ALA	C-N-CA	6.44	129.20	120.44
9	Y	45	ILE	CA-C-N	6.43	128.80	120.44
9	Y	45	ILE	C-N-CA	6.43	128.80	120.44
1	B	90	PRO	CA-C-N	6.41	130.95	120.63
1	B	90	PRO	C-N-CA	6.41	130.95	120.63
2	E	177	LEU	N-CA-C	-6.40	104.51	112.90
1	C	423	ASN	N-CA-C	-6.39	99.48	109.25
8	N	324	PRO	CA-C-N	6.38	126.87	119.47
8	N	324	PRO	C-N-CA	6.38	126.87	119.47
1	C	533	GLY	CA-C-N	6.38	129.21	120.35
1	C	533	GLY	C-N-CA	6.38	129.21	120.35
8	N	37	PRO	N-CA-C	6.38	121.87	114.03
2	F	27	LEU	N-CA-C	-6.37	100.26	110.14
1	B	520	LEU	N-CA-C	-6.37	103.03	111.24
1	B	18	GLY	N-CA-C	-6.36	105.91	115.32
1	B	354	LEU	N-CA-C	-6.36	97.26	110.80
9	S	63	GLU	CA-C-N	6.35	129.43	120.28
9	S	63	GLU	C-N-CA	6.35	129.43	120.28
2	F	195	GLY	N-CA-C	-6.35	98.13	113.18
9	Q	19	MET	CA-C-N	6.34	126.98	120.00
9	Q	19	MET	C-N-CA	6.34	126.98	120.00
2	D	197	THR	CA-C-N	6.34	128.78	120.28
2	D	197	THR	C-N-CA	6.34	128.78	120.28
6	J	53	TYR	N-CA-C	-6.34	103.62	112.12
2	D	398	ILE	N-CA-C	-6.33	106.80	112.12
8	N	605	HIS	CA-C-N	6.32	128.66	120.44
8	N	605	HIS	C-N-CA	6.32	128.66	120.44
1	A	62	GLU	N-CA-C	-6.32	100.44	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	O	79	ARG	N-CA-C	-6.31	107.42	114.62
2	F	240	THR	N-CA-C	-6.31	105.74	113.50
2	F	455	SER	CA-C-N	6.30	129.01	120.38
2	F	455	SER	C-N-CA	6.30	129.01	120.38
2	D	392	ILE	N-CA-C	-6.30	103.22	111.09
2	E	346	LYS	N-CA-C	-6.29	106.14	113.88
8	N	527	LEU	N-CA-C	-6.29	105.28	114.39
9	Y	60	LEU	N-CA-C	6.28	118.12	111.28
1	A	102	ILE	N-CA-C	-6.28	98.50	107.98
1	A	91	LEU	CA-C-N	6.27	128.60	120.44
1	A	91	LEU	C-N-CA	6.27	128.60	120.44
2	D	24	ALA	N-CA-C	-6.27	99.44	108.60
9	X	68	PHE	CA-C-N	6.26	126.92	119.98
9	X	68	PHE	C-N-CA	6.26	126.92	119.98
2	D	193	ALA	N-CA-C	-6.25	100.08	109.96
2	F	321	ARG	N-CA-C	-6.25	105.61	113.18
2	F	232	ILE	N-CA-C	-6.25	106.62	113.43
6	J	151	GLY	N-CA-C	-6.25	102.06	110.56
2	F	234	THR	N-CA-C	6.25	121.37	113.25
8	N	368	TYR	CA-C-N	6.25	128.65	120.28
8	N	368	TYR	C-N-CA	6.25	128.65	120.28
1	A	48	PHE	CA-C-N	6.25	128.94	120.63
1	A	48	PHE	C-N-CA	6.25	128.94	120.63
1	A	400	LEU	N-CA-C	-6.24	99.84	109.76
2	F	429	ASN	N-CA-C	-6.24	98.08	108.75
4	H	96	LYS	N-CA-C	-6.23	99.83	109.24
2	E	201	LEU	N-CA-C	-6.23	103.20	111.24
1	A	33	GLU	N-CA-C	-6.23	105.17	112.89
2	D	138	ILE	N-CA-C	-6.21	106.38	111.91
8	N	502	LEU	CA-C-N	6.21	126.83	120.00
8	N	502	LEU	C-N-CA	6.21	126.83	120.00
6	L	92	GLU	N-CA-C	-6.20	105.54	113.23
4	H	86	VAL	CA-C-N	6.20	131.06	120.71
4	H	86	VAL	C-N-CA	6.20	131.06	120.71
1	C	410	ASP	CA-C-N	6.20	128.49	120.44
1	C	410	ASP	C-N-CA	6.20	128.49	120.44
2	F	374	ASP	N-CA-C	-6.19	94.60	107.67
8	N	373	TYR	CA-C-N	6.19	128.58	120.28
8	N	373	TYR	C-N-CA	6.19	128.58	120.28
1	C	309	ILE	N-CA-C	-6.18	104.26	111.00
2	E	136	SER	CA-C-N	6.18	133.35	121.54
2	E	136	SER	C-N-CA	6.18	133.35	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	HIS	N-CA-C	-6.18	98.19	108.75
7	M	316	VAL	CA-C-N	6.17	128.55	120.28
7	M	316	VAL	C-N-CA	6.17	128.55	120.28
8	N	627	GLU	N-CA-C	-6.17	105.40	113.12
9	P	13	GLY	N-CA-C	6.17	120.14	112.73
2	E	443	LEU	N-CA-C	6.17	118.00	111.28
2	D	456	LYS	CA-C-N	6.17	128.46	120.44
2	D	456	LYS	C-N-CA	6.17	128.46	120.44
6	J	128	LEU	N-CA-C	6.17	121.91	113.77
2	D	74	SER	N-CA-C	6.16	118.33	108.41
2	E	281	ARG	N-CA-C	-6.16	97.68	110.80
1	B	492	GLU	N-CA-C	-6.14	106.11	113.97
1	C	280	PRO	N-CA-C	-6.14	99.83	112.47
9	T	79	ARG	N-CA-C	-6.14	105.08	114.16
1	C	2	ILE	N-CA-C	-6.13	99.66	108.42
7	M	109	PHE	CA-C-N	6.13	129.10	120.28
7	M	109	PHE	C-N-CA	6.13	129.10	120.28
1	C	407	TRP	CA-C-N	6.12	129.99	120.75
1	C	407	TRP	C-N-CA	6.12	129.99	120.75
2	E	208	PHE	CA-C-N	6.10	133.20	121.54
2	E	208	PHE	C-N-CA	6.10	133.20	121.54
9	Y	40	ALA	CA-C-N	6.10	126.75	119.98
9	Y	40	ALA	C-N-CA	6.10	126.75	119.98
2	F	193	ALA	N-CA-C	-6.10	97.81	110.80
7	M	141	ALA	CA-C-N	6.10	126.28	120.43
7	M	141	ALA	C-N-CA	6.10	126.28	120.43
1	A	459	GLN	N-CA-C	-6.09	106.00	113.50
1	C	418	HIS	N-CA-C	-6.09	98.15	108.26
2	F	117	LEU	N-CA-C	-6.09	98.50	109.09
8	N	84	LEU	CA-C-N	6.09	128.44	120.28
8	N	84	LEU	C-N-CA	6.09	128.44	120.28
5	K	37	LEU	CA-C-N	6.08	129.25	120.79
5	K	37	LEU	C-N-CA	6.08	129.25	120.79
9	S	69	GLY	CA-C-N	6.08	128.43	120.28
9	S	69	GLY	C-N-CA	6.08	128.43	120.28
2	F	77	GLU	CA-C-N	6.07	128.41	120.28
2	F	77	GLU	C-N-CA	6.07	128.41	120.28
2	F	275	GLU	CA-C-N	6.06	133.12	121.54
2	F	275	GLU	C-N-CA	6.06	133.12	121.54
2	D	132	GLN	N-CA-C	-6.06	101.80	110.59
8	N	137	PHE	N-CA-C	-6.06	105.43	114.64
1	A	390	ASP	N-CA-C	-6.05	99.79	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	305	LYS	CA-C-N	6.05	125.85	120.10
2	D	305	LYS	C-N-CA	6.05	125.85	120.10
6	J	132	GLU	N-CA-C	-6.05	106.53	114.04
3	G	72	GLY	N-CA-C	-6.05	100.00	112.34
2	D	450	GLU	N-CA-C	-6.04	106.07	113.50
1	C	473	PRO	CA-C-N	6.04	128.65	120.44
1	C	473	PRO	C-N-CA	6.04	128.65	120.44
2	F	49	GLU	CA-C-N	6.04	128.74	120.35
2	F	49	GLU	C-N-CA	6.04	128.74	120.35
9	X	40	ALA	CA-C-N	6.04	126.68	119.98
9	X	40	ALA	C-N-CA	6.04	126.68	119.98
1	A	178	GLY	N-CA-C	-6.04	106.11	116.01
6	J	43	GLN	N-CA-C	6.03	117.86	111.28
3	G	99	SER	N-CA-C	-6.03	97.96	110.80
9	O	10	LEU	CA-C-N	6.03	128.28	120.44
9	O	10	LEU	C-N-CA	6.03	128.28	120.44
1	C	353	TYR	N-CA-C	-6.03	104.63	111.14
1	C	459	GLN	N-CA-C	-6.02	104.41	110.97
8	N	450	LEU	N-CA-C	-6.02	107.75	114.62
2	F	220	PHE	N-CA-C	-6.01	99.60	109.40
8	N	351	VAL	CA-C-O	-6.01	114.66	118.69
7	M	210	SER	N-CA-C	-6.00	104.94	112.93
1	A	529	ALA	N-CA-C	-6.00	104.37	111.03
4	H	89	TYR	N-CA-C	-5.99	104.66	111.07
9	O	49	ARG	N-CA-C	-5.99	104.87	111.82
1	C	531	LYS	N-CA-C	-5.99	105.90	112.72
9	X	79	ARG	N-CA-C	-5.98	105.30	114.16
2	D	321	ARG	CA-C-N	5.97	128.88	120.28
2	D	321	ARG	C-N-CA	5.97	128.88	120.28
6	J	135	ALA	CA-C-N	5.97	128.56	120.44
6	J	135	ALA	C-N-CA	5.97	128.56	120.44
2	F	244	TYR	N-CA-C	-5.97	105.08	112.90
1	C	300	GLU	N-CA-C	-5.97	102.43	111.56
1	A	187	TRP	CA-C-N	5.97	127.30	119.84
1	A	187	TRP	C-N-CA	5.97	127.30	119.84
7	M	72	LEU	N-CA-C	5.94	121.60	113.16
9	P	11	ASP	N-CA-C	5.94	117.42	111.07
9	T	59	LEU	CA-C-N	5.94	128.24	120.28
9	T	59	LEU	C-N-CA	5.94	128.24	120.28
2	F	442	LEU	N-CA-C	-5.93	105.87	113.23
8	N	433	GLU	CA-C-N	5.93	132.87	121.54
8	N	433	GLU	C-N-CA	5.93	132.87	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	10	LEU	CA-C-N	5.93	128.15	120.44
9	V	10	LEU	C-N-CA	5.93	128.15	120.44
7	M	142	VAL	O-C-N	-5.92	116.63	120.42
2	D	55	ALA	N-CA-C	-5.92	101.17	109.69
2	E	273	ALA	N-CA-C	-5.92	101.43	109.54
7	M	320	VAL	N-CA-C	-5.92	106.97	112.83
2	E	255	VAL	N-CA-C	-5.92	99.90	108.36
2	F	135	ILE	CA-C-N	5.92	128.53	120.54
2	F	135	ILE	C-N-CA	5.92	128.53	120.54
9	W	74	PHE	N-CA-C	-5.92	104.74	111.07
2	F	427	GLN	CA-C-N	5.91	132.84	121.54
2	F	427	GLN	C-N-CA	5.91	132.84	121.54
1	B	133	MET	CA-C-N	5.90	128.64	120.49
1	B	133	MET	C-N-CA	5.90	128.64	120.49
2	E	433	GLU	CA-C-N	5.90	128.47	120.38
2	E	433	GLU	C-N-CA	5.90	128.47	120.38
1	B	293	ASN	N-CA-C	-5.90	104.28	112.30
2	D	271	GLY	CA-C-N	5.90	130.13	120.63
2	D	271	GLY	C-N-CA	5.90	130.13	120.63
9	Z	68	PHE	CA-C-N	5.88	126.51	119.98
9	Z	68	PHE	C-N-CA	5.88	126.51	119.98
1	A	475	ALA	N-CA-C	-5.88	105.96	113.02
3	G	75	VAL	N-CA-C	5.88	116.62	110.62
6	L	135	ALA	N-CA-C	-5.88	105.20	112.90
9	Y	37	ILE	CA-C-N	5.87	126.50	119.98
9	Y	37	ILE	C-N-CA	5.87	126.50	119.98
4	H	5	ALA	CA-C-N	5.87	129.58	120.60
4	H	5	ALA	C-N-CA	5.87	129.58	120.60
2	F	367	GLY	N-CA-C	-5.87	107.14	115.30
1	B	310	ALA	N-CA-C	5.87	118.15	111.11
2	D	352	ILE	N-CA-C	-5.87	99.09	107.77
3	G	96	VAL	N-CA-C	-5.87	100.61	108.35
2	E	115	THR	N-CA-C	-5.86	103.93	113.19
2	F	62	GLU	N-CA-C	-5.86	102.27	110.35
1	B	137	THR	CA-C-N	5.85	129.93	121.68
1	B	137	THR	C-N-CA	5.85	129.93	121.68
1	B	555	SER	CA-C-N	5.84	132.70	121.54
1	B	555	SER	C-N-CA	5.84	132.70	121.54
2	D	115	THR	N-CA-C	-5.84	99.21	108.73
2	D	57	ILE	N-CA-C	-5.83	99.87	108.85
8	N	400	PRO	CA-C-N	5.83	128.10	120.28
8	N	400	PRO	C-N-CA	5.83	128.10	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	304	LYS	N-CA-C	-5.83	100.51	108.38
1	A	67	THR	N-CA-C	-5.82	106.31	113.41
2	E	328	LEU	N-CA-C	5.81	118.39	111.71
1	A	542	LEU	N-CA-C	-5.81	102.73	109.93
7	M	311	LEU	CA-C-O	-5.81	115.31	120.19
2	E	244	TYR	N-CA-C	-5.80	104.65	110.97
1	B	473	PRO	CA-C-O	-5.80	115.18	121.27
5	K	23	ILE	CA-C-N	5.79	129.51	120.82
5	K	23	ILE	C-N-CA	5.79	129.51	120.82
2	E	85	SER	N-CA-C	-5.79	101.62	109.95
5	I	71	ALA	CA-C-N	5.79	128.03	120.28
5	I	71	ALA	C-N-CA	5.79	128.03	120.28
2	F	414	PHE	N-CA-C	-5.78	106.36	113.41
2	E	318	ASP	N-CA-C	-5.78	98.50	110.80
4	H	41	GLY	N-CA-C	-5.78	107.75	115.32
7	M	5	PHE	N-CA-C	-5.78	105.89	113.17
1	C	290	ASN	CA-C-N	5.77	132.57	121.54
1	C	290	ASN	C-N-CA	5.77	132.57	121.54
3	G	119	THR	O-C-N	-5.77	114.68	121.32
2	E	460	GLY	N-CA-C	-5.77	105.57	115.61
7	M	170	LYS	CA-C-N	5.76	128.00	120.28
7	M	170	LYS	C-N-CA	5.76	128.00	120.28
9	V	26	ALA	CA-C-N	5.76	128.00	120.28
9	V	26	ALA	C-N-CA	5.76	128.00	120.28
4	H	58	ALA	CA-C-N	5.76	128.35	120.46
4	H	58	ALA	C-N-CA	5.76	128.35	120.46
8	N	40	LEU	N-CA-C	-5.76	105.15	113.21
1	C	559	PHE	CA-C-O	-5.75	113.27	118.79
1	C	351	PRO	N-CA-C	-5.75	103.69	110.70
2	D	395	LEU	N-CA-C	-5.73	106.24	113.18
1	B	130	ARG	N-CA-C	-5.73	100.70	109.41
1	A	240	SER	N-CA-C	-5.73	105.03	111.28
6	J	32	ARG	CA-C-N	5.73	127.95	120.28
6	J	32	ARG	C-N-CA	5.73	127.95	120.28
1	C	562	TYR	N-CA-C	-5.72	106.46	113.50
2	F	63	THR	N-CA-C	-5.72	100.56	109.72
3	G	28	LEU	N-CA-C	5.72	119.78	112.34
9	W	37	ILE	CA-C-N	5.72	126.33	119.98
9	W	37	ILE	C-N-CA	5.72	126.33	119.98
2	D	208	PHE	CA-C-N	5.72	130.28	120.72
2	D	208	PHE	C-N-CA	5.72	130.28	120.72
3	G	133	TYR	N-CA-C	-5.72	98.61	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	278	GLY	N-CA-C	-5.71	107.76	115.36
9	U	17	VAL	N-CA-C	5.71	115.84	110.30
7	M	250	SER	N-CA-C	5.71	118.27	111.71
2	E	9	THR	N-CA-C	-5.70	99.60	108.90
2	E	142	ASN	CA-C-O	5.69	126.55	120.46
7	M	311	LEU	CA-C-N	5.68	126.94	119.84
7	M	311	LEU	C-N-CA	5.68	126.94	119.84
9	P	26	ALA	CA-C-N	5.68	127.89	120.28
9	P	26	ALA	C-N-CA	5.68	127.89	120.28
1	C	15	ILE	N-CA-C	-5.67	100.14	108.99
3	G	52	ALA	N-CA-C	5.67	117.14	111.07
2	E	370	LYS	N-CA-C	-5.67	107.01	114.04
2	E	103	LEU	CA-C-N	5.67	126.22	120.38
2	E	103	LEU	C-N-CA	5.67	126.22	120.38
2	E	175	PRO	N-CA-C	-5.66	108.19	114.92
6	L	152	VAL	N-CA-C	-5.65	100.08	108.45
2	D	283	TYR	CA-C-N	5.65	125.65	119.89
2	D	283	TYR	C-N-CA	5.65	125.65	119.89
9	Y	18	GLY	CA-C-N	5.65	127.85	120.28
9	Y	18	GLY	C-N-CA	5.65	127.85	120.28
2	E	123	ALA	N-CA-C	-5.64	104.15	111.71
1	B	288	ILE	N-CA-C	-5.64	100.00	108.12
3	G	72	GLY	CA-C-N	5.64	126.89	119.84
3	G	72	GLY	C-N-CA	5.64	126.89	119.84
8	N	204	LEU	N-CA-C	-5.64	101.63	110.14
1	C	33	GLU	N-CA-C	-5.63	105.28	111.82
1	C	233	GLY	N-CA-C	5.63	126.53	113.18
1	C	239	GLN	N-CA-C	-5.63	105.22	111.36
8	N	483	ALA	N-CA-C	-5.63	105.28	111.82
8	N	44	GLN	CA-C-N	5.62	128.68	120.71
8	N	44	GLN	C-N-CA	5.62	128.68	120.71
8	N	348	THR	CA-C-N	5.62	126.86	119.84
8	N	348	THR	C-N-CA	5.62	126.86	119.84
1	C	517	LYS	N-CA-C	-5.61	106.57	113.41
9	U	37	ILE	CA-C-N	5.61	126.20	119.98
9	U	37	ILE	C-N-CA	5.61	126.20	119.98
9	X	22	ALA	CA-C-N	5.60	128.38	120.42
9	X	22	ALA	C-N-CA	5.60	128.38	120.42
3	G	190	ASP	CA-C-N	5.59	127.71	120.44
3	G	190	ASP	C-N-CA	5.59	127.71	120.44
1	B	69	LEU	O-C-N	-5.58	117.94	121.85
2	F	296	GLU	N-CA-C	5.58	119.19	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	147	ILE	CA-C-N	5.58	128.77	120.95
1	C	147	ILE	C-N-CA	5.58	128.77	120.95
6	J	19	LEU	CA-C-N	5.58	127.76	120.28
6	J	19	LEU	C-N-CA	5.58	127.76	120.28
2	D	100	ILE	N-CA-C	-5.58	105.97	111.77
8	N	619	GLN	CA-C-N	5.58	125.04	119.24
8	N	619	GLN	C-N-CA	5.58	125.04	119.24
9	Q	41	GLY	N-CA-C	5.58	119.42	112.73
1	B	40	ILE	N-CA-C	-5.57	97.75	109.34
3	G	49	ALA	CA-C-N	5.57	128.54	120.79
3	G	49	ALA	C-N-CA	5.57	128.54	120.79
2	F	164	ALA	N-CA-C	5.57	118.07	111.33
8	N	628	PHE	N-CA-C	5.57	117.43	111.36
5	K	117	GLU	N-CA-C	5.57	117.15	111.14
6	J	27	ALA	CA-C-N	5.56	127.74	120.28
6	J	27	ALA	C-N-CA	5.56	127.74	120.28
2	D	48	ILE	CA-C-N	5.56	132.16	121.54
2	D	48	ILE	C-N-CA	5.56	132.16	121.54
7	M	105	THR	N-CA-C	-5.56	106.08	112.92
1	C	504	ASP	CA-C-N	5.56	128.50	120.38
1	C	504	ASP	C-N-CA	5.56	128.50	120.38
2	D	375	HIS	N-CA-C	5.56	117.34	111.28
4	H	87	GLU	CA-C-N	5.56	127.13	120.13
4	H	87	GLU	C-N-CA	5.56	127.13	120.13
7	M	112	VAL	N-CA-C	-5.54	99.75	108.23
6	J	175	TRP	CA-C-N	5.54	128.26	120.28
6	J	175	TRP	C-N-CA	5.54	128.26	120.28
6	J	174	ALA	N-CA-C	5.54	117.40	111.36
2	F	300	VAL	CA-C-N	5.54	128.19	122.27
2	F	300	VAL	C-N-CA	5.54	128.19	122.27
4	H	55	PRO	CA-C-N	5.54	132.14	121.18
4	H	55	PRO	C-N-CA	5.54	132.14	121.18
2	D	375	HIS	CA-C-N	5.53	129.98	121.19
2	D	375	HIS	C-N-CA	5.53	129.98	121.19
1	A	307	VAL	N-CA-C	-5.53	105.14	110.72
9	Q	21	LEU	CA-C-N	5.52	127.68	120.28
9	Q	21	LEU	C-N-CA	5.52	127.68	120.28
1	B	135	LEU	CA-C-N	-5.52	113.03	121.09
1	B	135	LEU	C-N-CA	-5.52	113.03	121.09
9	P	79	ARG	N-CA-C	-5.52	106.13	112.92
9	Q	52	PHE	N-CA-C	5.51	117.29	111.28
9	S	37	ILE	CA-C-N	5.51	126.10	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	37	ILE	C-N-CA	5.51	126.10	119.98
1	A	255	CYS	N-CA-C	-5.51	101.19	109.95
5	I	44	ALA	N-CA-C	5.51	116.98	110.97
5	I	37	LEU	CA-C-N	5.51	128.45	120.79
5	I	37	LEU	C-N-CA	5.51	128.45	120.79
9	Z	9	GLY	N-CA-C	5.51	117.66	112.04
2	F	313	ILE	N-CA-C	-5.51	101.08	108.35
1	B	337	ILE	N-CA-C	-5.50	105.14	110.42
1	C	189	VAL	N-CA-C	5.50	116.23	110.62
8	N	645	PHE	CA-C-N	5.49	127.95	120.54
8	N	645	PHE	C-N-CA	5.49	127.95	120.54
9	S	23	VAL	CA-C-N	5.49	125.92	119.94
9	S	23	VAL	C-N-CA	5.49	125.92	119.94
1	A	14	VAL	N-CA-C	-5.48	101.84	108.53
8	N	573	ILE	N-CA-C	-5.48	105.18	110.72
4	H	39	ARG	N-CA-C	-5.48	105.64	112.93
1	A	76	GLY	CA-C-N	5.47	125.45	120.03
1	A	76	GLY	C-N-CA	5.47	125.45	120.03
2	F	198	GLN	N-CA-C	-5.47	104.84	112.45
1	B	353	TYR	N-CA-C	-5.47	102.18	110.28
8	N	441	PRO	N-CA-C	5.47	123.74	112.47
2	E	305	LYS	N-CA-C	-5.47	106.54	113.43
2	F	446	LEU	N-CA-C	-5.47	101.69	109.62
2	E	211	THR	N-CA-C	-5.47	106.19	112.92
9	T	40	ALA	CA-C-N	5.47	126.05	119.98
9	T	40	ALA	C-N-CA	5.47	126.05	119.98
4	H	23	ALA	N-CA-C	-5.46	101.00	108.38
1	C	558	GLU	N-CA-C	-5.46	106.93	113.21
1	C	167	THR	N-CA-C	-5.46	101.96	110.42
9	W	49	ARG	N-CA-C	-5.46	105.49	111.82
1	B	542	LEU	CA-C-N	5.45	125.16	119.82
1	B	542	LEU	C-N-CA	5.45	125.16	119.82
2	F	210	ARG	N-CA-C	-5.45	106.80	113.50
1	C	386	PRO	CA-C-N	5.44	125.09	119.05
1	C	386	PRO	C-N-CA	5.44	125.09	119.05
1	B	290	ASN	N-CA-C	-5.44	100.17	108.76
1	A	337	ILE	CA-C-N	5.44	127.88	120.54
1	A	337	ILE	C-N-CA	5.44	127.88	120.54
2	E	218	VAL	N-CA-C	-5.43	100.48	108.85
1	C	329	ARG	CA-C-N	5.43	128.97	120.82
1	C	329	ARG	C-N-CA	5.43	128.97	120.82
7	M	91	ASN	N-CA-C	5.43	117.28	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	PRO	CA-C-N	5.43	131.74	121.97
1	B	394	PRO	C-N-CA	5.43	131.74	121.97
2	F	230	GLU	CA-C-N	5.43	129.78	120.72
2	F	230	GLU	C-N-CA	5.43	129.78	120.72
2	F	227	PRO	CA-C-N	5.42	128.30	120.38
2	F	227	PRO	C-N-CA	5.42	128.30	120.38
6	J	42	LEU	CA-C-N	5.42	127.55	120.28
6	J	42	LEU	C-N-CA	5.42	127.55	120.28
1	A	498	ASN	N-CA-C	-5.42	101.74	110.14
3	G	8	ARG	CA-C-N	5.42	131.89	121.54
3	G	8	ARG	C-N-CA	5.42	131.89	121.54
4	H	7	PRO	CA-C-N	5.41	127.53	120.28
4	H	7	PRO	C-N-CA	5.41	127.53	120.28
7	M	257	ASP	CA-C-N	5.41	127.53	120.28
7	M	257	ASP	C-N-CA	5.41	127.53	120.28
8	N	527	LEU	CA-C-N	5.41	129.88	120.68
8	N	527	LEU	C-N-CA	5.41	129.88	120.68
1	A	333	ALA	N-CA-C	-5.41	105.04	111.69
2	D	157	GLY	N-CA-C	-5.41	108.17	115.36
9	Z	61	LEU	N-CA-C	5.41	120.84	113.16
2	E	20	PHE	N-CA-C	5.40	118.18	110.24
1	B	273	THR	N-CA-C	-5.40	99.64	108.76
8	N	137	PHE	CA-C-N	5.40	131.56	122.87
8	N	137	PHE	C-N-CA	5.40	131.56	122.87
9	U	28	LEU	CA-C-N	5.40	125.97	119.98
9	U	28	LEU	C-N-CA	5.40	125.97	119.98
3	G	72	GLY	CA-C-O	-5.39	113.81	121.52
1	C	429	SER	N-CA-C	-5.39	101.22	109.41
6	L	3	LYS	CA-C-N	5.39	127.44	120.44
6	L	3	LYS	C-N-CA	5.39	127.44	120.44
1	A	147	ILE	N-CA-C	-5.38	100.37	108.12
5	K	102	LYS	CA-C-N	5.38	127.95	120.63
5	K	102	LYS	C-N-CA	5.38	127.95	120.63
1	B	480	GLU	CA-C-N	5.38	127.44	120.44
1	B	480	GLU	C-N-CA	5.38	127.44	120.44
9	P	37	ILE	CA-C-N	5.38	125.95	119.98
9	P	37	ILE	C-N-CA	5.38	125.95	119.98
1	B	205	PHE	N-CA-C	-5.37	98.81	108.48
2	F	211	THR	N-CA-C	-5.37	105.08	111.69
9	P	42	VAL	N-CA-C	5.37	116.10	110.62
2	E	254	LEU	N-CA-C	-5.37	100.42	109.07
3	G	127	SER	CA-C-N	5.37	128.01	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	127	SER	C-N-CA	5.37	128.01	120.28
2	F	323	HIS	CA-C-N	5.37	126.55	119.84
2	F	323	HIS	C-N-CA	5.37	126.55	119.84
1	C	385	SER	CA-C-N	5.36	123.52	119.66
1	C	385	SER	C-N-CA	5.36	123.52	119.66
2	E	386	TYR	N-CA-C	-5.36	105.33	111.07
1	C	537	ASP	CA-C-N	5.36	127.46	120.28
1	C	537	ASP	C-N-CA	5.36	127.46	120.28
1	A	262	MET	CA-C-N	5.36	127.72	120.38
1	A	262	MET	C-N-CA	5.36	127.72	120.38
2	F	378	VAL	N-CA-C	-5.36	105.38	110.42
2	F	14	ILE	N-CA-C	-5.35	100.53	108.45
7	M	102	ALA	CA-C-N	5.35	127.45	120.28
7	M	102	ALA	C-N-CA	5.35	127.45	120.28
2	E	11	ILE	N-CA-C	-5.34	100.63	108.54
4	H	68	LEU	CA-C-N	5.34	126.52	119.84
4	H	68	LEU	C-N-CA	5.34	126.52	119.84
2	F	283	TYR	N-CA-C	-5.34	103.41	108.22
2	F	348	ILE	N-CA-C	-5.33	100.39	108.17
2	E	118	PRO	CA-C-N	5.33	131.72	121.54
2	E	118	PRO	C-N-CA	5.33	131.72	121.54
8	N	389	LEU	N-CA-C	-5.33	101.54	109.11
2	F	7	GLU	N-CA-C	-5.33	99.45	110.80
8	N	281	TYR	N-CA-C	-5.33	100.72	109.40
8	N	78	ARG	CA-C-N	5.32	125.33	119.90
8	N	78	ARG	C-N-CA	5.32	125.33	119.90
1	A	475	ALA	CA-C-N	5.32	128.79	120.75
1	A	475	ALA	C-N-CA	5.32	128.79	120.75
8	N	648	VAL	N-CA-C	5.32	115.53	110.53
5	I	53	ALA	CA-C-N	5.31	127.93	120.28
5	I	53	ALA	C-N-CA	5.31	127.93	120.28
2	F	111	ARG	N-CA-C	-5.31	102.19	110.42
7	M	21	LYS	N-CA-C	-5.31	102.61	110.46
1	B	336	GLU	N-CA-C	5.30	117.47	111.11
9	Y	49	ARG	N-CA-C	-5.30	105.58	111.36
9	T	26	ALA	CA-C-N	5.30	127.38	120.28
9	T	26	ALA	C-N-CA	5.30	127.38	120.28
1	A	320	VAL	N-CA-C	5.30	116.24	109.30
1	C	550	ARG	N-CA-C	-5.30	106.40	112.92
1	C	47	ALA	N-CA-C	5.29	117.35	108.73
9	U	35	ALA	N-CA-C	5.28	116.72	111.07
1	C	205	PHE	N-CA-C	-5.28	99.68	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	161	ASN	CA-C-N	5.28	127.61	120.38
2	E	161	ASN	C-N-CA	5.28	127.61	120.38
7	M	183	LEU	CA-C-N	5.28	131.62	121.54
7	M	183	LEU	C-N-CA	5.28	131.62	121.54
2	E	78	ASP	N-CA-C	-5.28	104.44	112.04
8	N	291	GLU	CA-C-N	5.27	127.30	120.44
8	N	291	GLU	C-N-CA	5.27	127.30	120.44
1	B	152	ASP	N-CA-C	-5.27	99.57	110.80
2	E	198	GLN	CA-C-N	5.27	127.29	120.44
2	E	198	GLN	C-N-CA	5.27	127.29	120.44
9	X	28	LEU	CA-C-N	5.27	125.83	119.98
9	X	28	LEU	C-N-CA	5.27	125.83	119.98
9	Y	9	GLY	CA-C-N	5.27	127.86	120.28
9	Y	9	GLY	C-N-CA	5.27	127.86	120.28
6	L	116	PRO	N-CA-C	-5.27	106.86	114.18
1	C	426	GLY	CA-C-N	5.26	131.59	121.54
1	C	426	GLY	C-N-CA	5.26	131.59	121.54
2	E	16	GLY	CA-C-N	-5.26	113.26	119.84
2	E	16	GLY	C-N-CA	-5.26	113.26	119.84
8	N	46	SER	CA-C-N	5.26	125.32	119.32
8	N	46	SER	C-N-CA	5.26	125.32	119.32
9	T	10	LEU	CA-C-N	5.26	127.28	120.44
9	T	10	LEU	C-N-CA	5.26	127.28	120.44
9	X	61	LEU	CA-C-O	-5.26	113.24	118.34
1	B	64	VAL	N-CA-C	-5.25	100.76	108.85
8	N	301	VAL	N-CA-C	-5.25	98.42	109.34
1	A	412	SER	CA-C-N	5.25	127.58	120.65
1	A	412	SER	C-N-CA	5.25	127.58	120.65
9	U	49	ARG	CA-C-N	5.25	127.31	120.28
9	U	49	ARG	C-N-CA	5.25	127.31	120.28
2	E	43	ARG	N-CA-C	-5.25	101.50	108.74
2	F	120	ASN	N-CA-C	-5.24	98.33	108.45
2	F	223	LYS	N-CA-C	-5.24	101.34	109.72
1	B	24	MET	N-CA-C	5.23	117.23	108.23
1	A	279	GLY	N-CA-C	-5.23	105.90	112.23
4	H	85	ASP	N-CA-C	-5.23	100.42	110.56
1	B	465	GLN	CA-C-N	5.23	131.53	121.54
1	B	465	GLN	C-N-CA	5.23	131.53	121.54
3	G	182	VAL	N-CA-C	-5.22	105.31	111.00
4	H	88	GLY	CA-C-N	5.21	127.21	120.44
4	H	88	GLY	C-N-CA	5.21	127.21	120.44
3	G	43	VAL	N-CA-C	-5.21	105.64	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	112	LEU	CA-C-N	5.20	125.49	119.92
2	D	112	LEU	C-N-CA	5.20	125.49	119.92
1	B	193	ARG	CA-C-N	5.20	125.49	119.92
1	B	193	ARG	C-N-CA	5.20	125.49	119.92
2	D	169	ARG	N-CA-C	5.20	116.95	111.28
9	V	75	ILE	CA-C-N	5.19	127.19	120.44
9	V	75	ILE	C-N-CA	5.19	127.19	120.44
1	A	559	PHE	CA-C-N	5.19	126.33	119.84
1	A	559	PHE	C-N-CA	5.19	126.33	119.84
2	E	172	THR	CA-C-N	5.19	129.94	123.14
2	E	172	THR	C-N-CA	5.19	129.94	123.14
1	B	173	VAL	CA-C-N	5.19	127.92	122.11
1	B	173	VAL	C-N-CA	5.19	127.92	122.11
2	E	199	ARG	N-CA-C	-5.19	105.52	111.07
2	E	205	ILE	N-CA-C	5.18	115.62	110.23
9	Q	26	ALA	CA-C-N	5.18	127.22	120.28
9	Q	26	ALA	C-N-CA	5.18	127.22	120.28
5	K	31	LYS	N-CA-C	-5.18	105.79	112.68
1	A	559	PHE	CA-C-O	-5.17	113.07	120.16
2	F	359	SER	CA-C-N	5.17	131.42	121.54
2	F	359	SER	C-N-CA	5.17	131.42	121.54
7	M	84	VAL	CA-C-N	5.17	127.21	120.28
7	M	84	VAL	C-N-CA	5.17	127.21	120.28
1	A	87	ILE	CA-C-N	5.17	129.70	122.36
1	A	87	ILE	C-N-CA	5.17	129.70	122.36
5	K	32	GLN	CA-C-N	5.17	127.16	120.44
5	K	32	GLN	C-N-CA	5.17	127.16	120.44
8	N	349	PRO	CA-C-N	5.17	127.82	120.53
8	N	349	PRO	C-N-CA	5.17	127.82	120.53
1	A	277	THR	N-CA-C	-5.17	108.73	114.62
4	H	4	ILE	N-CA-C	-5.16	100.33	108.90
2	E	73	VAL	CA-C-N	5.16	130.01	121.86
2	E	73	VAL	C-N-CA	5.16	130.01	121.86
2	F	325	ILE	CA-C-N	5.16	126.29	119.84
2	F	325	ILE	C-N-CA	5.16	126.29	119.84
9	U	11	ASP	CA-C-N	5.16	127.20	120.28
9	U	11	ASP	C-N-CA	5.16	127.20	120.28
1	C	501	HIS	CA-C-N	5.16	127.70	120.28
1	C	501	HIS	C-N-CA	5.16	127.70	120.28
2	F	140	VAL	N-CA-C	-5.15	98.62	109.34
1	C	336	GLU	N-CA-C	-5.15	105.83	112.68
9	P	60	LEU	N-CA-C	5.15	116.89	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	12	GLY	CA-C-N	5.15	126.27	119.84
8	N	12	GLY	C-N-CA	5.15	126.27	119.84
2	D	328	LEU	CA-C-N	5.14	127.94	120.79
2	D	328	LEU	C-N-CA	5.14	127.94	120.79
8	N	355	PHE	CA-C-N	5.14	124.32	118.97
8	N	355	PHE	C-N-CA	5.14	124.32	118.97
9	R	73	ALA	CA-C-N	5.14	127.13	120.44
9	R	73	ALA	C-N-CA	5.14	127.13	120.44
8	N	199	VAL	N-CA-C	-5.14	104.45	110.05
1	C	4	GLY	N-CA-C	-5.14	103.28	110.88
5	I	43	GLU	CA-C-N	5.14	127.43	120.65
5	I	43	GLU	C-N-CA	5.14	127.43	120.65
1	C	109	HIS	N-CA-C	-5.13	103.91	110.53
1	A	433	SER	N-CA-C	-5.13	107.53	112.97
2	E	399	ILE	N-CA-C	5.12	115.34	110.42
1	A	175	LEU	CA-C-N	5.12	128.09	120.31
1	A	175	LEU	C-N-CA	5.12	128.09	120.31
2	D	20	PHE	N-CA-C	-5.12	101.93	110.17
1	B	471	VAL	CA-C-N	5.12	129.90	121.87
1	B	471	VAL	C-N-CA	5.12	129.90	121.87
2	D	243	GLU	N-CA-C	5.12	117.25	111.11
2	E	440	TRP	N-CA-C	-5.11	106.20	112.90
1	B	536	ILE	CA-C-N	5.11	131.30	121.54
1	B	536	ILE	C-N-CA	5.11	131.30	121.54
2	D	440	TRP	CA-C-N	5.10	128.47	120.82
2	D	440	TRP	C-N-CA	5.10	128.47	120.82
9	T	54	THR	CA-C-N	5.10	127.12	120.28
9	T	54	THR	C-N-CA	5.10	127.12	120.28
9	Z	69	GLY	CA-C-N	5.10	127.12	120.28
9	Z	69	GLY	C-N-CA	5.10	127.12	120.28
2	F	417	ALA	CA-C-N	5.10	129.30	121.19
2	F	417	ALA	C-N-CA	5.10	129.30	121.19
1	A	452	ASP	N-CA-C	-5.10	105.81	112.23
2	F	103	LEU	CA-C-N	5.10	125.63	120.38
2	F	103	LEU	C-N-CA	5.10	125.63	120.38
9	T	23	VAL	CA-C-N	5.10	125.50	119.94
9	T	23	VAL	C-N-CA	5.10	125.50	119.94
2	E	404	LEU	CA-C-N	5.10	128.34	121.05
2	E	404	LEU	C-N-CA	5.10	128.34	121.05
3	G	20	LEU	N-CA-C	-5.10	105.37	111.03
5	K	105	ALA	N-CA-C	5.09	117.23	111.02
2	D	136	SER	CA-C-N	5.08	127.80	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	136	SER	C-N-CA	5.08	127.80	120.38
2	D	111	ARG	N-CA-C	-5.08	99.70	108.69
2	F	243	GLU	N-CA-C	5.07	118.94	112.34
1	B	198	LYS	N-CA-C	-5.07	106.51	113.30
1	A	542	LEU	CA-C-N	5.07	124.86	119.28
1	A	542	LEU	C-N-CA	5.07	124.86	119.28
2	D	110	LYS	N-CA-C	-5.07	101.20	108.60
2	E	165	ALA	N-CA-C	-5.07	105.41	111.03
7	M	54	LEU	CA-C-N	5.07	124.73	119.56
7	M	54	LEU	C-N-CA	5.07	124.73	119.56
8	N	33	GLU	O-C-N	-5.06	117.04	123.17
7	M	71	ASP	N-CA-C	5.06	116.88	111.36
8	N	8	LEU	N-CA-C	-5.06	101.15	109.40
1	A	279	GLY	CA-C-O	-5.06	117.17	122.38
1	A	112	ASP	N-CA-C	-5.06	103.25	110.59
3	G	53	LEU	CA-C-N	5.06	127.47	120.29
3	G	53	LEU	C-N-CA	5.06	127.47	120.29
4	H	77	LEU	N-CA-C	-5.06	100.02	110.80
2	E	363	ASN	N-CA-C	-5.06	105.84	112.72
1	C	191	ARG	N-CA-C	-5.05	101.22	108.60
1	A	215	LEU	CA-C-N	-5.05	117.29	122.85
1	A	215	LEU	C-N-CA	-5.05	117.29	122.85
2	E	279	GLY	N-CA-C	-5.05	101.22	113.18
2	F	324	PRO	N-CA-C	5.04	122.86	112.47
2	D	82	LEU	CA-C-N	5.04	127.62	121.06
2	D	82	LEU	C-N-CA	5.04	127.62	121.06
6	L	29	ALA	CA-C-N	5.04	126.91	120.56
6	L	29	ALA	C-N-CA	5.04	126.91	120.56
1	B	15	ILE	N-CA-C	-5.04	100.99	108.45
1	B	377	ALA	N-CA-C	5.04	117.00	109.59
2	D	107	THR	N-CA-C	-5.04	101.78	109.64
2	E	181	GLY	CA-C-N	5.03	131.16	121.54
2	E	181	GLY	C-N-CA	5.03	131.16	121.54
1	A	413	LEU	N-CA-C	-5.03	105.49	110.97
2	F	394	LYS	N-CA-C	-5.03	104.87	111.96
3	G	113	LEU	N-CA-C	5.03	118.26	111.17
4	H	51	LEU	N-CA-C	-5.03	100.09	110.80
2	D	171	ALA	N-CA-C	5.03	116.77	110.24
2	E	214	LEU	N-CA-C	-5.02	98.89	108.17
1	A	508	SER	N-CA-C	-5.02	102.37	110.14
9	Q	49	ARG	N-CA-C	-5.02	106.00	111.82
1	B	481	ARG	CA-C-N	5.01	131.12	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	ARG	C-N-CA	5.01	131.12	121.54
2	E	400	GLY	N-CA-C	-5.01	101.30	113.18
1	B	364	ARG	N-CA-C	-5.01	102.68	109.54
6	J	88	ARG	CA-C-N	5.01	127.24	120.38
6	J	88	ARG	C-N-CA	5.01	127.24	120.38
1	B	511	LYS	N-CA-C	-5.00	103.90	111.56
1	C	318	PHE	CA-C-N	5.00	129.08	122.42
1	C	318	PHE	C-N-CA	5.00	129.08	122.42

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	204	PRO	Mainchain
1	C	199	LEU	Mainchain
2	D	142	ASN	Mainchain
2	D	6	LYS	Peptide
2	E	6	LYS	Peptide
2	F	6	LYS	Peptide
7	M	183	LEU	Peptide
7	M	3	ASP	Peptide
8	N	642	TYR	Mainchain,Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2307	0	654	1	0
1	B	2307	0	654	2	0
1	C	2307	0	654	4	0
2	D	1835	0	512	6	0
2	E	1835	0	512	4	0
2	F	1835	0	512	2	0
3	G	839	0	230	1	0
4	H	399	0	119	0	0
5	I	399	0	100	0	0
5	K	399	0	100	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	738	0	192	1	0
6	L	738	0	192	1	0
7	M	1279	0	357	0	0
8	N	2526	0	709	0	0
9	O	303	0	102	0	0
9	P	303	0	102	0	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	0	0
9	Y	303	0	102	0	0
9	Z	303	0	102	0	0
10	A	27	0	12	0	0
10	C	27	0	12	0	0
All	All	23433	0	6745	22	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 (22) 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)
2:D:35:ILE:H	2:D:44:GLY:H	1.54	0.56
2:F:251:TYR:H	2:F:306:GLY:HA2	1.72	0.54
3:G:8:ARG:C	3:G:10:ASN:H	2.16	0.53
2:F:426:GLY:C	2:F:428:GLN:H	2.17	0.52
1:C:557:GLU:C	1:C:559:PHE:H	2.19	0.51
1:C:38:GLU:H	1:C:50:GLN:H	1.60	0.49
1:B:536:ILE:C	1:B:538:GLU:H	2.22	0.48
1:C:175:LEU:C	1:C:177:ASP:H	2.22	0.48
2:E:362:MET:C	2:E:364:ASN:H	2.22	0.46
2:E:212:GLY:C	2:E:214:LEU:H	2.25	0.45
2:E:31:ALA:H	2:E:47:VAL:H	1.65	0.44
2:D:51:SER:C	2:D:53:GLU:H	2.25	0.44
2:D:33:VAL:O	2:D:44:GLY:HA2	2.17	0.43
2:D:35:ILE:H	2:D:44:GLY:N	2.15	0.43
6:J:51:ALA:C	6:J:53:TYR:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:51:ALA:C	6:L:53:TYR:H	2.28	0.41
2:D:182:GLU:C	2:D:184:GLU:H	2.28	0.41
2:D:329:THR:C	2:D:331:TYR:H	2.28	0.41
1:A:240:SER:C	1:A:242:ALA:H	2.29	0.41
1:B:370:THR:C	1:B:372:GLY:H	2.27	0.41
2:E:284:PRO:C	2:E:286:TYR:H	2.28	0.41
1:C:439:TYR:C	1:C:441:GLU:H	2.28	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/578 (100%)	452 (79%)	87 (15%)	36 (6%)	1	12
1	B	575/578 (100%)	431 (75%)	101 (18%)	43 (8%)	1	9
1	C	575/578 (100%)	451 (78%)	96 (17%)	28 (5%)	1	15
2	D	457/478 (96%)	342 (75%)	83 (18%)	32 (7%)	1	10
2	E	457/478 (96%)	332 (73%)	91 (20%)	34 (7%)	1	10
2	F	457/478 (96%)	347 (76%)	74 (16%)	36 (8%)	1	9
3	G	208/223 (93%)	151 (73%)	37 (18%)	20 (10%)	0	7
4	H	98/104 (94%)	74 (76%)	14 (14%)	10 (10%)	0	6
5	I	98/120 (82%)	93 (95%)	3 (3%)	2 (2%)	6	30
5	K	98/120 (82%)	96 (98%)	0	2 (2%)	6	30
6	J	181/188 (96%)	157 (87%)	18 (10%)	6 (3%)	3	20
6	L	181/188 (96%)	162 (90%)	14 (8%)	5 (3%)	4	24
7	M	318/323 (98%)	296 (93%)	18 (6%)	4 (1%)	9	40
8	N	628/652 (96%)	555 (88%)	38 (6%)	35 (6%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	O	74/99 (75%)	71 (96%)	2 (3%)	1 (1%)	9	38
9	P	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	Q	74/99 (75%)	71 (96%)	2 (3%)	1 (1%)	9	38
9	R	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	9	38
9	S	74/99 (75%)	70 (95%)	2 (3%)	2 (3%)	4	24
9	T	74/99 (75%)	71 (96%)	3 (4%)	0	100	100
9	U	74/99 (75%)	71 (96%)	3 (4%)	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	38
9	X	74/99 (75%)	72 (97%)	2 (3%)	0	100	100
9	Y	74/99 (75%)	72 (97%)	1 (1%)	1 (1%)	9	38
9	Z	74/99 (75%)	70 (95%)	2 (3%)	2 (3%)	4	24
All	All	5794/6274 (92%)	4797 (83%)	695 (12%)	302 (5%)	3	14

All (302) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	PRO
1	A	227	PRO
1	A	401	ARG
1	A	471	VAL
1	A	480	GLU
1	B	152	ASP
1	B	159	GLU
1	B	202	ASN
1	B	227	PRO
1	B	303	ILE
1	B	304	TYR
1	B	305	VAL
1	B	356	ALA
1	B	466	GLU
1	C	70	PRO
1	C	202	ASN
1	C	227	PRO
1	C	233	GLY
1	C	291	THR
1	C	293	ASN
1	C	392	SER

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Mol	Chain	Res	Type
1	C	427	SER
1	C	444	ALA
2	D	49	GLU
2	D	63	THR
2	D	215	SER
2	D	216	ARG
2	D	354	PRO
2	E	7	GLU
2	E	17	PRO
2	E	137	THR
2	E	148	GLN
2	E	215	SER
2	E	216	ARG
2	E	278	PRO
2	E	280	ARG
2	E	297	ARG
2	E	362	MET
2	E	419	GLU
2	F	88	MET
2	F	139	ASP
2	F	225	ASP
2	F	259	ASP
2	F	276	GLU
2	F	280	ARG
2	F	298	ALA
2	F	324	PRO
2	F	327	ASP
2	F	355	LEU
2	F	356	PRO
2	F	360	ARG
2	F	364	ASN
2	F	428	GLN
3	G	112	ALA
3	G	117	VAL
3	G	134	ALA
4	H	81	PHE
5	I	23	ILE
6	J	99	GLU
6	J	144	ALA
5	K	23	ILE
7	M	184	ASP
8	N	135	SER

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Mol	Chain	Res	Type
8	N	162	GLU
8	N	163	ASP
8	N	185	LYS
8	N	298	LYS
8	N	434	HIS
8	N	441	PRO
9	Q	7	SER
9	R	6	ALA
1	A	64	VAL
1	A	72	ALA
1	A	108	VAL
1	A	163	ALA
1	A	188	PRO
1	A	402	ILE
1	A	474	ASP
1	A	505	ALA
1	B	25	TYR
1	B	28	CYS
1	B	179	THR
1	B	210	ARG
1	B	292	SER
1	B	302	SER
1	B	340	ARG
1	B	397	GLN
1	B	443	VAL
1	B	471	VAL
1	B	472	GLY
1	B	474	ASP
1	C	210	ARG
1	C	222	GLY
1	C	289	ALA
1	C	326	SER
1	C	390	ASP
1	C	445	GLU
1	C	512	ALA
2	D	61	GLU
2	D	91	ARG
2	D	95	GLY
2	D	106	ILE
2	D	210	ARG
2	D	259	ASP
2	D	293	THR

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Mol	Chain	Res	Type
2	D	297	ARG
2	D	330	GLY
2	E	69	ALA
2	E	96	ILE
2	E	119	LEU
2	E	182	GLU
2	E	239	LEU
2	E	259	ASP
2	E	332	ILE
2	E	340	SER
2	E	428	GLN
2	F	7	GLU
2	F	15	SER
2	F	41	ARG
2	F	140	VAL
2	F	281	ARG
2	F	333	THR
2	F	389	GLY
2	F	390	VAL
3	G	4	VAL
3	G	84	PRO
3	G	89	VAL
3	G	99	SER
3	G	119	THR
3	G	168	VAL
3	G	180	GLN
4	H	15	LEU
4	H	69	PRO
4	H	79	GLU
4	H	80	ALA
6	J	119	LYS
6	L	141	GLU
6	L	144	ALA
7	M	50	ALA
8	N	72	LEU
8	N	82	GLU
8	N	277	ALA
8	N	390	VAL
8	N	395	ALA
8	N	454	ILE
9	S	7	SER
9	W	6	ALA

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Mol	Chain	Res	Type
9	Y	9	GLY
1	A	152	ASP
1	A	196	GLN
1	A	202	ASN
1	A	302	SER
1	A	304	TYR
1	A	352	PRO
1	A	432	THR
1	A	556	GLU
1	B	195	VAL
1	B	294	MET
1	B	315	ASP
1	B	354	LEU
1	B	475	ALA
1	B	510	LYS
1	C	56	SER
1	C	354	LEU
1	C	431	PHE
1	C	463	GLY
2	D	69	ALA
2	D	77	GLU
2	D	117	LEU
2	D	159	PRO
2	D	164	ALA
2	D	168	ALA
2	D	249	HIS
2	D	280	ARG
2	D	326	PRO
2	E	10	GLY
2	E	54	TYR
2	E	101	ASP
2	E	121	PRO
2	E	170	GLN
2	F	69	ALA
2	F	275	GLU
2	F	307	SER
2	F	375	HIS
2	F	436	LEU
3	G	6	PRO
3	G	69	ALA
3	G	88	GLY
3	G	114	LEU

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Mol	Chain	Res	Type
3	G	174	ALA
4	H	77	LEU
6	J	141	GLU
5	K	104	MET
8	N	270	ALA
8	N	347	PRO
8	N	518	ASN
8	N	523	TRP
8	N	585	LEU
9	O	6	ALA
9	S	77	ASN
9	Z	79	ARG
1	A	244	TRP
1	A	282	MET
1	A	291	THR
1	A	502	GLU
1	B	247	ALA
1	B	248	ASP
1	B	359	ALA
1	B	395	VAL
1	B	504	ASP
1	C	141	PHE
1	C	494	PHE
2	D	128	GLU
2	D	237	MET
2	D	336	GLN
2	D	362	MET
2	E	166	GLN
2	E	322	THR
2	E	425	GLN
2	F	415	ALA
2	F	453	ARG
4	H	5	ALA
4	H	53	PRO
6	J	52	GLN
6	J	140	VAL
6	L	140	VAL
7	M	223	ARG
8	N	42	ALA
8	N	296	ARG
8	N	297	HIS
8	N	382	TYR

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Mol	Chain	Res	Type
8	N	449	ILE
1	A	275	PRO
1	A	351	PRO
1	A	473	PRO
1	B	81	ASN
1	B	246	ASN
1	B	255	CYS
1	B	345	PRO
1	B	413	LEU
2	D	99	PRO
2	D	142	ASN
2	D	226	ASP
2	E	191	PHE
2	E	225	ASP
2	E	277	ILE
2	F	128	GLU
2	F	186	PRO
2	F	263	TYR
3	G	5	SER
3	G	110	ASP
4	H	33	LEU
4	H	57	ARG
5	I	104	MET
6	L	52	GLN
8	N	274	PHE
8	N	278	LEU
8	N	388	PRO
8	N	586	ALA
8	N	631	LYS
8	N	644	PRO
1	A	25	TYR
1	A	222	GLY
1	A	484	ILE
1	A	510	LYS
1	B	98	THR
1	B	509	MET
1	C	163	ALA
1	C	349	GLY
1	C	443	VAL
2	E	190	VAL
2	F	37	ASP
2	F	196	ILE

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Mol	Chain	Res	Type
8	N	271	SER
8	N	273	ARG
8	N	642	TYR
1	A	214	VAL
1	B	296	VAL
1	C	514	GLY
2	E	270	ILE
3	G	154	ILE
8	N	581	VAL
9	Z	8	GLY
1	A	172	VAL
1	B	40	ILE
1	B	275	PRO
2	F	44	GLY
3	G	167	VAL
1	A	486	VAL
1	C	5	VAL
2	D	118	PRO
2	E	356	PRO
2	F	159	PRO
8	N	348	THR
8	N	640	ARG
1	B	139	PRO
6	L	104	VAL
7	M	247	THR
1	C	402	ILE
2	D	205	ILE
3	G	109	PRO
1	A	420	PRO

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1.21	2 (7%)	43,45,45	1.11	3 (6%)
10	ADP	C	600	-	28,29,29	1.18	2 (7%)	43,45,45	1.22	4 (9%)

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	-	-	9/16/32/32	0/3/3/3
10	ADP	C	600	-	-	9/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	600	ADP	C5-N7	-2.89	1.33	1.39
10	A	600	ADP	C5-N7	-2.58	1.34	1.39
10	C	600	ADP	PA-O3A	2.32	1.62	1.59
10	A	600	ADP	PA-O3A	-2.31	1.57	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	600	ADP	N6-C6-N1	4.03	127.35	118.38
10	C	600	ADP	O4'-C4'-C3'	-3.11	98.98	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	600	ADP	N6-C6-N1	2.85	124.73	118.38
10	C	600	ADP	C3'-C2'-C1'	-2.64	96.47	101.46
10	A	600	ADP	C6-C5-C4	2.60	120.72	117.18
10	A	600	ADP	C5-C6-N6	-2.41	117.31	123.29
10	C	600	ADP	O4'-C4'-C5'	2.17	116.28	109.33

There are no chirality outliers.

All (18) torsion outliers are listed below:

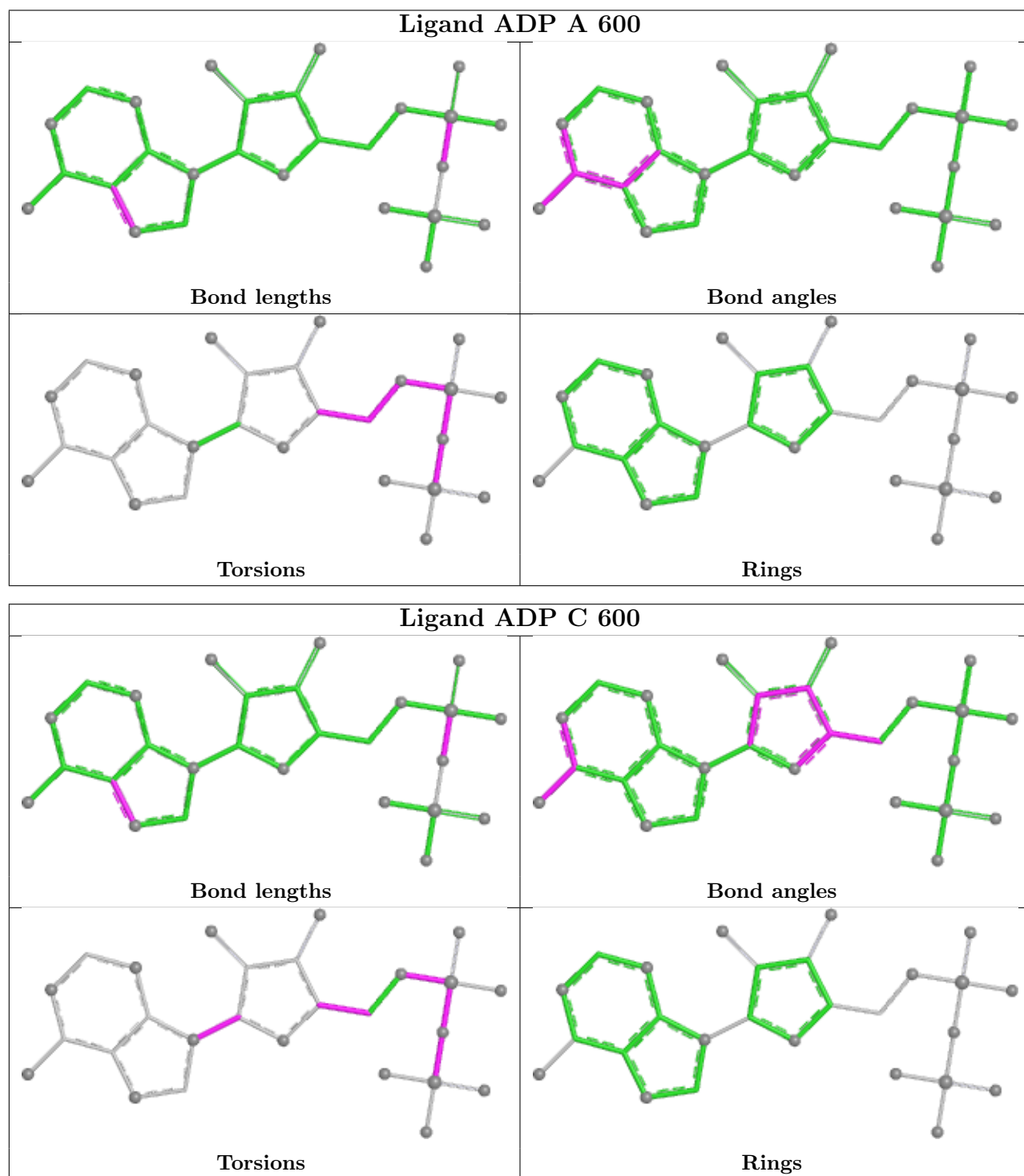
Mol	Chain	Res	Type	Atoms
10	A	600	ADP	PA-O3A-PB-O2B
10	A	600	ADP	PA-O3A-PB-O3B
10	A	600	ADP	C5'-O5'-PA-O1A
10	A	600	ADP	C5'-O5'-PA-O3A
10	C	600	ADP	C5'-O5'-PA-O2A
10	C	600	ADP	C5'-O5'-PA-O3A
10	C	600	ADP	C2'-C1'-N9-C8
10	C	600	ADP	PB-O3A-PA-O1A
10	A	600	ADP	O4'-C4'-C5'-O5'
10	C	600	ADP	PA-O3A-PB-O3B
10	A	600	ADP	PB-O3A-PA-O1A
10	A	600	ADP	C5'-O5'-PA-O2A
10	C	600	ADP	C5'-O5'-PA-O1A
10	C	600	ADP	C2'-C1'-N9-C4
10	A	600	ADP	C3'-C4'-C5'-O5'
10	C	600	ADP	O4'-C4'-C5'-O5'
10	A	600	ADP	C4'-C5'-O5'-PA
10	C	600	ADP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

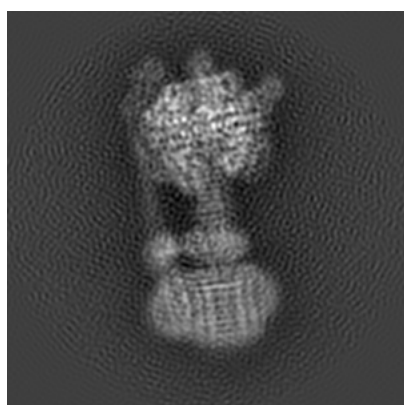
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6810. These allow visual inspection of the internal detail of the map and identification of artifacts.

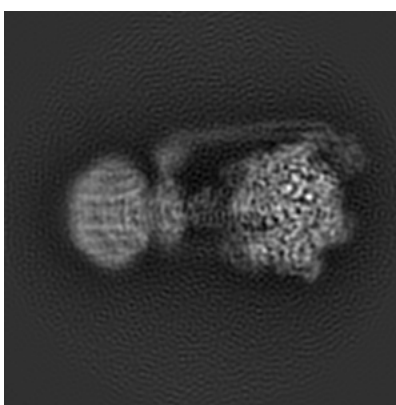
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

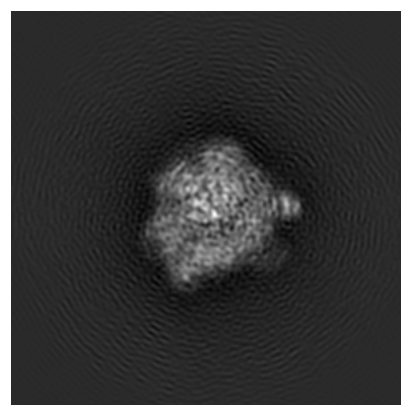
6.1.1 Primary map



X



Y



Z

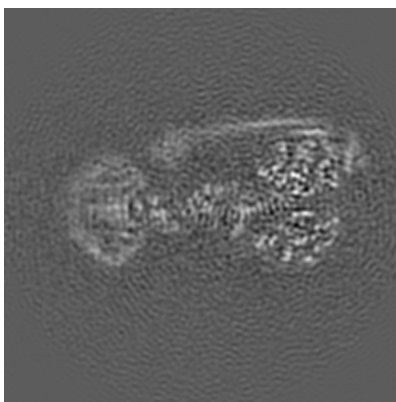
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

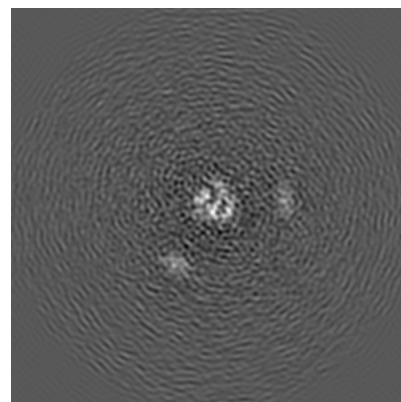
6.2.1 Primary map



X Index: 118



Y Index: 118

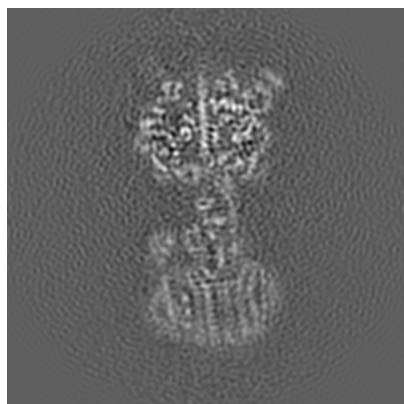


Z Index: 118

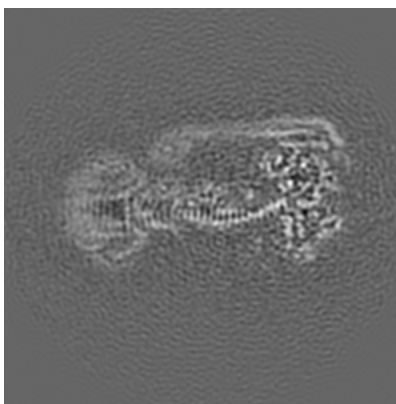
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

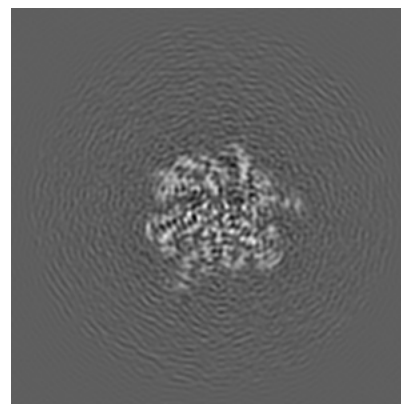
6.3.1 Primary map



X Index: 119



Y Index: 122

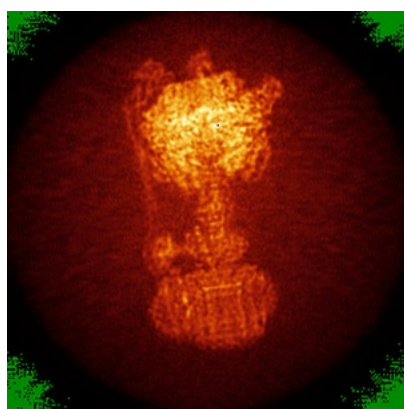


Z Index: 171

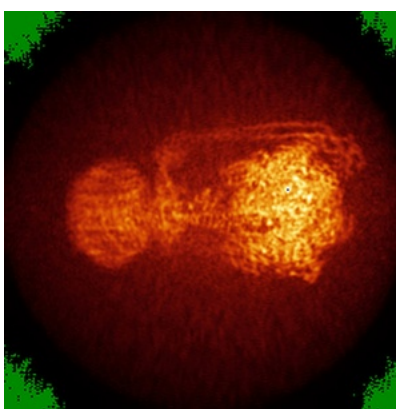
The images above show the largest variance slices of the map in three orthogonal directions.

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

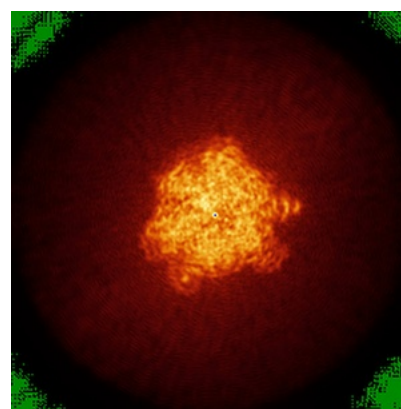
6.4.1 Primary map



X



Y

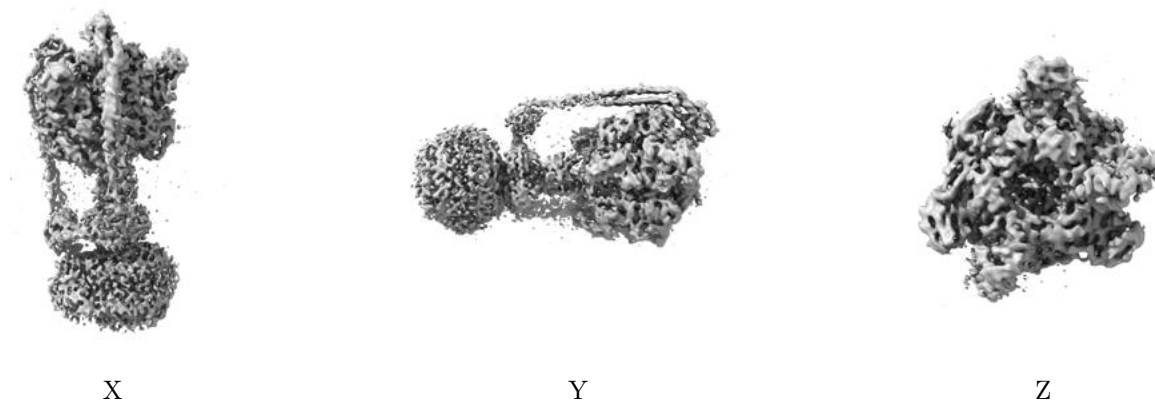


Z

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 0.098. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

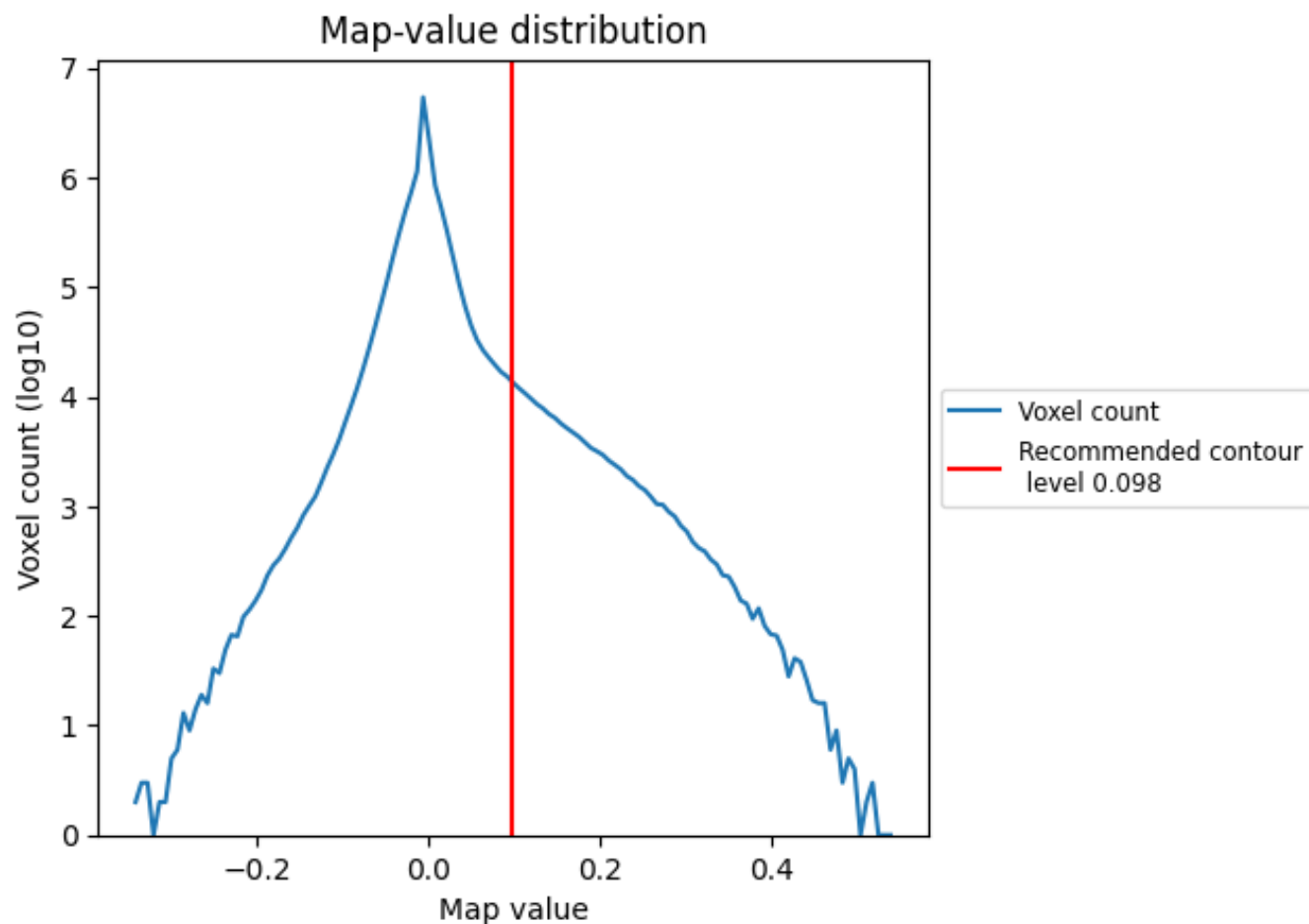
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

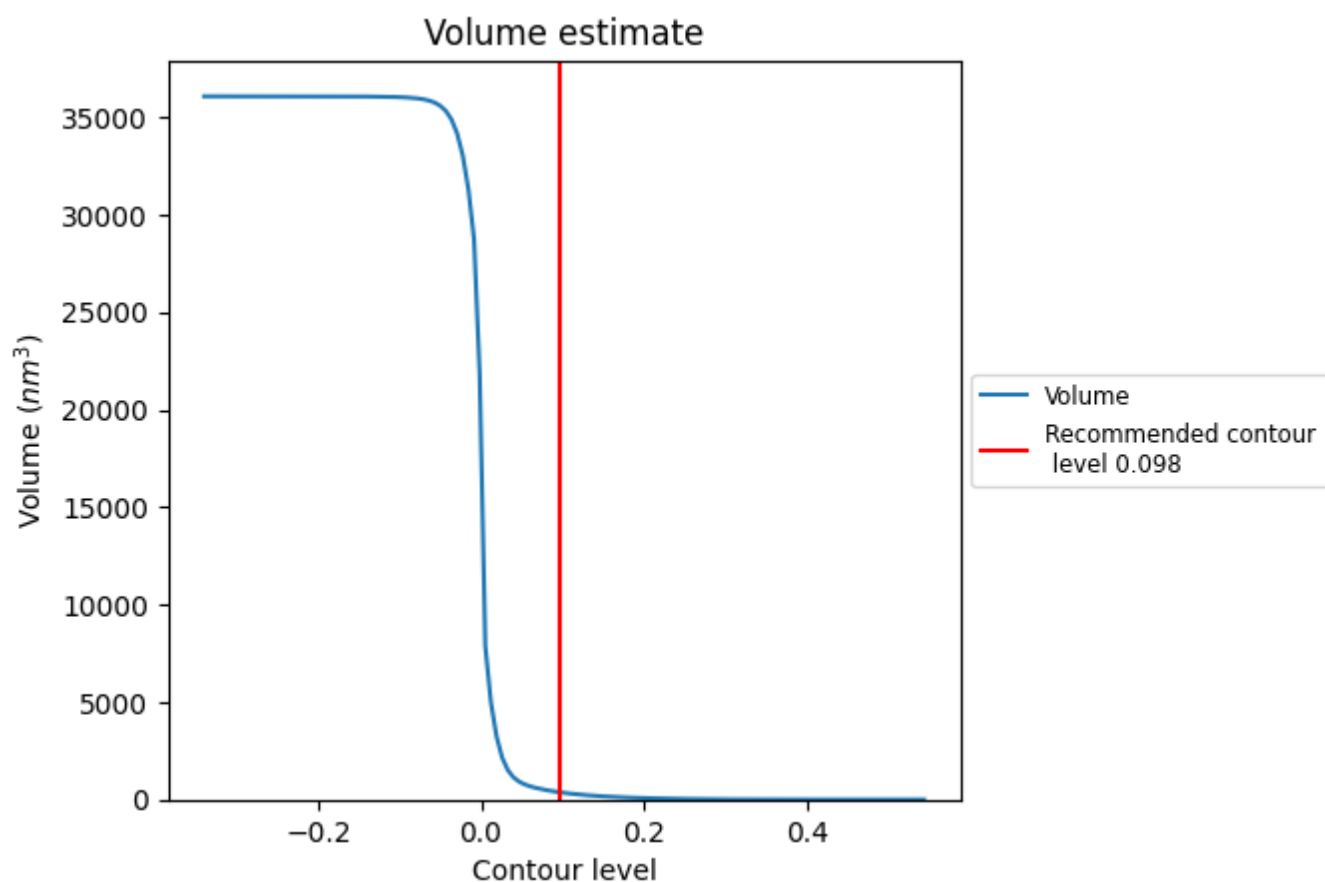
This section contains the results of statistical analysis of the map.

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.

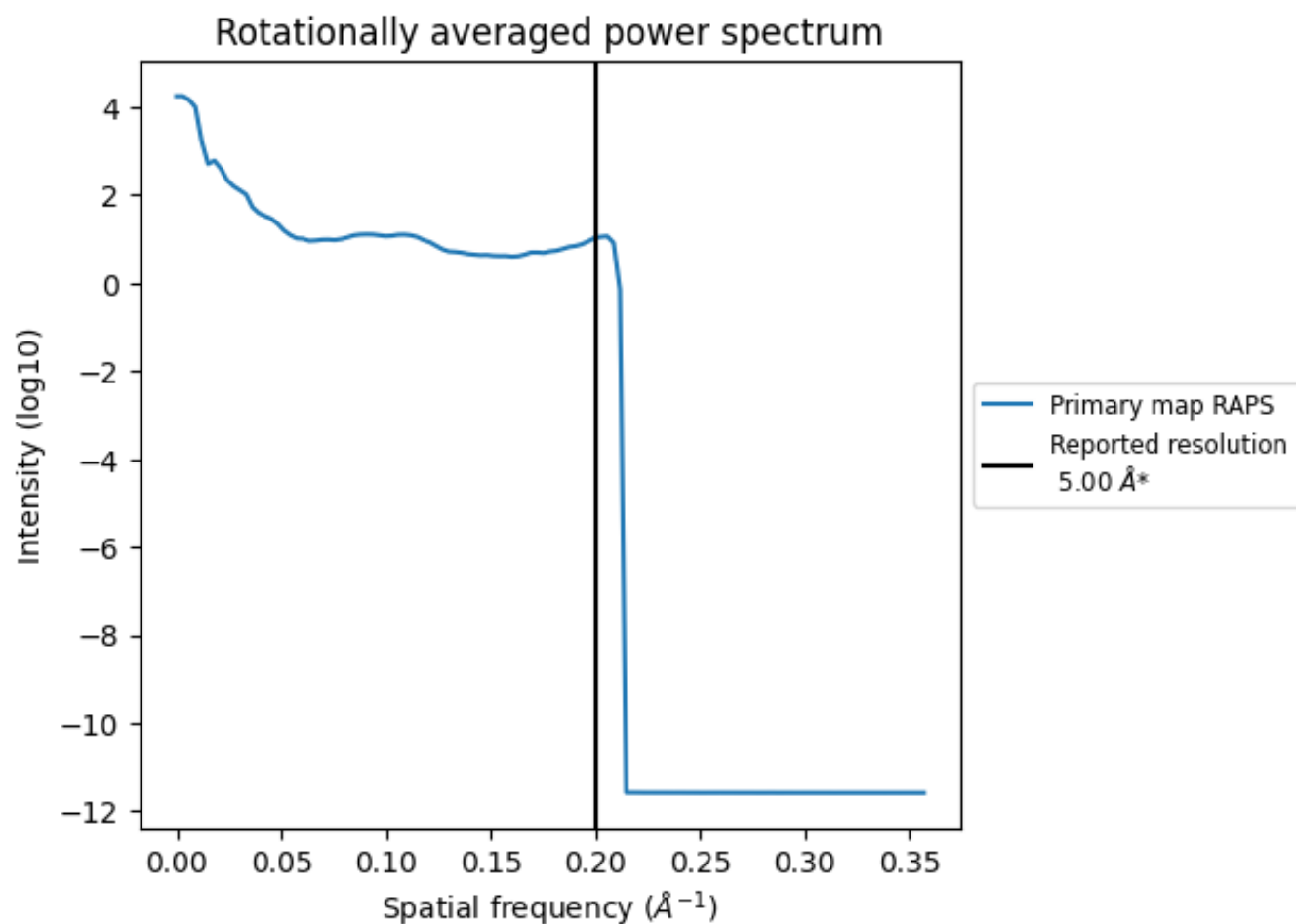
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 367 nm³; this corresponds to an approximate mass of 331 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 ⓘ

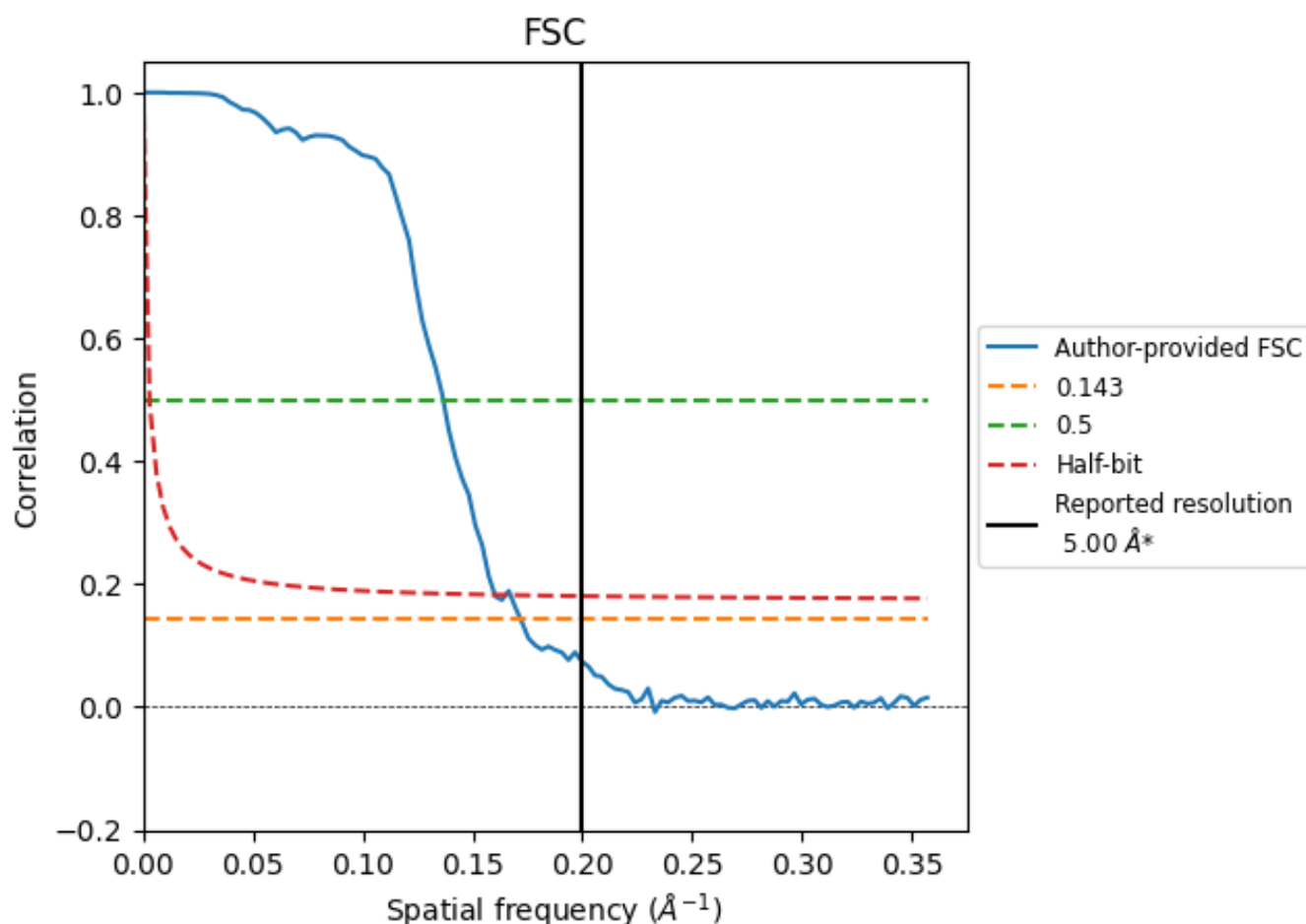


*Reported resolution corresponds to spatial frequency of 0.200 Å⁻¹

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 0.200 Å⁻¹

8.2 Resolution estimates [i](#)

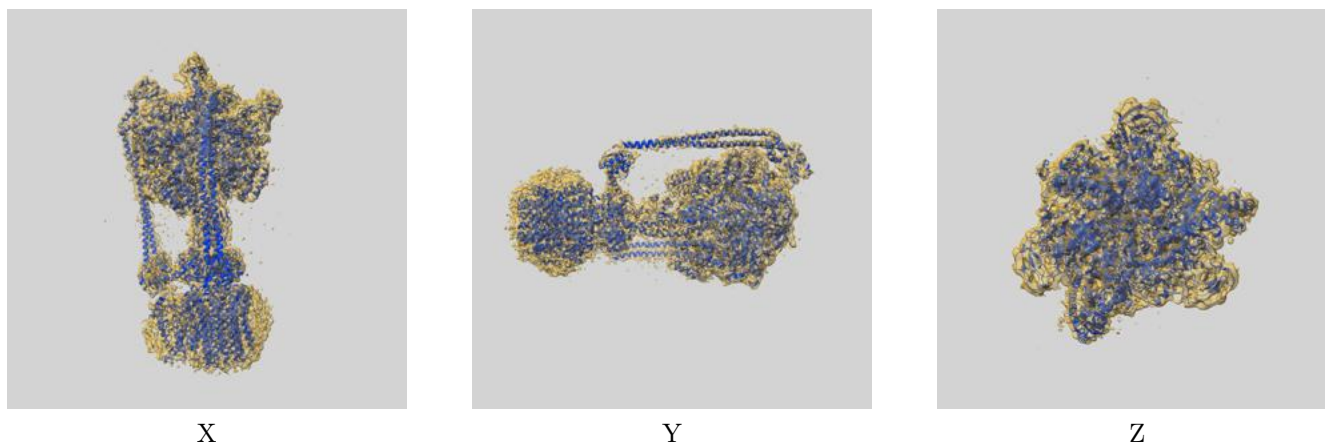
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	5.82	7.32	6.24
Unmasked-calculated*	-	-	-

*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 5.82 differs from the reported value 5.0 by more than 10 %

9 Map-model fit [i](#)

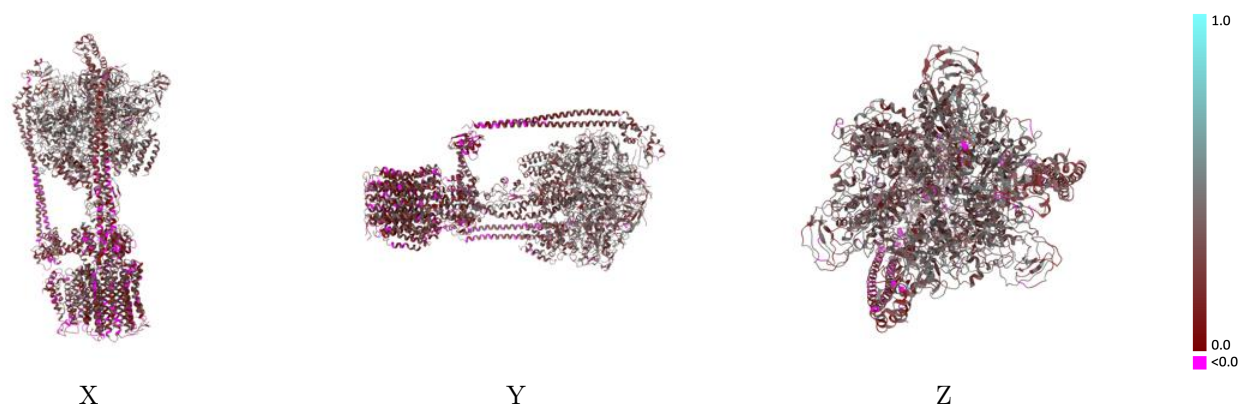
This section contains information regarding the fit between EMDB map EMD-6810 and PDB model 5Y5X. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



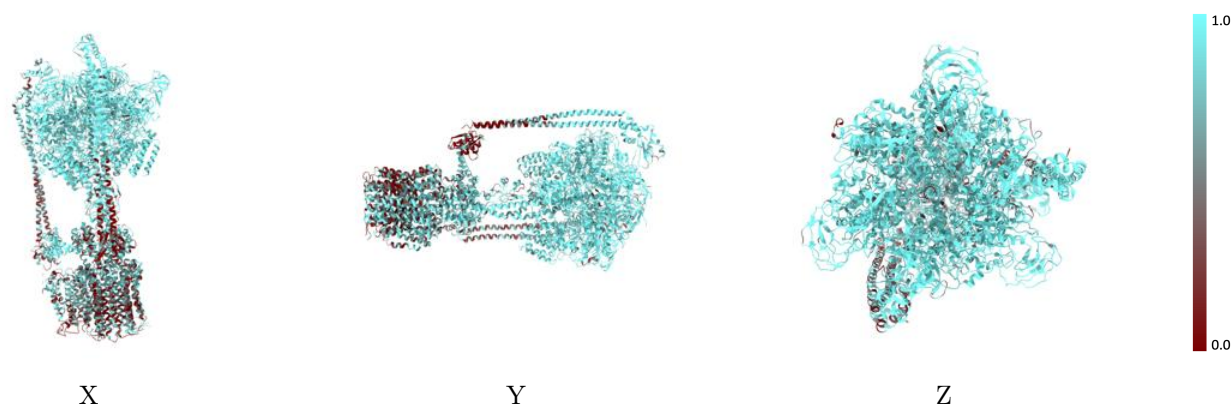
The images above show the 3D surface view of the map at the recommended contour level 0.098 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



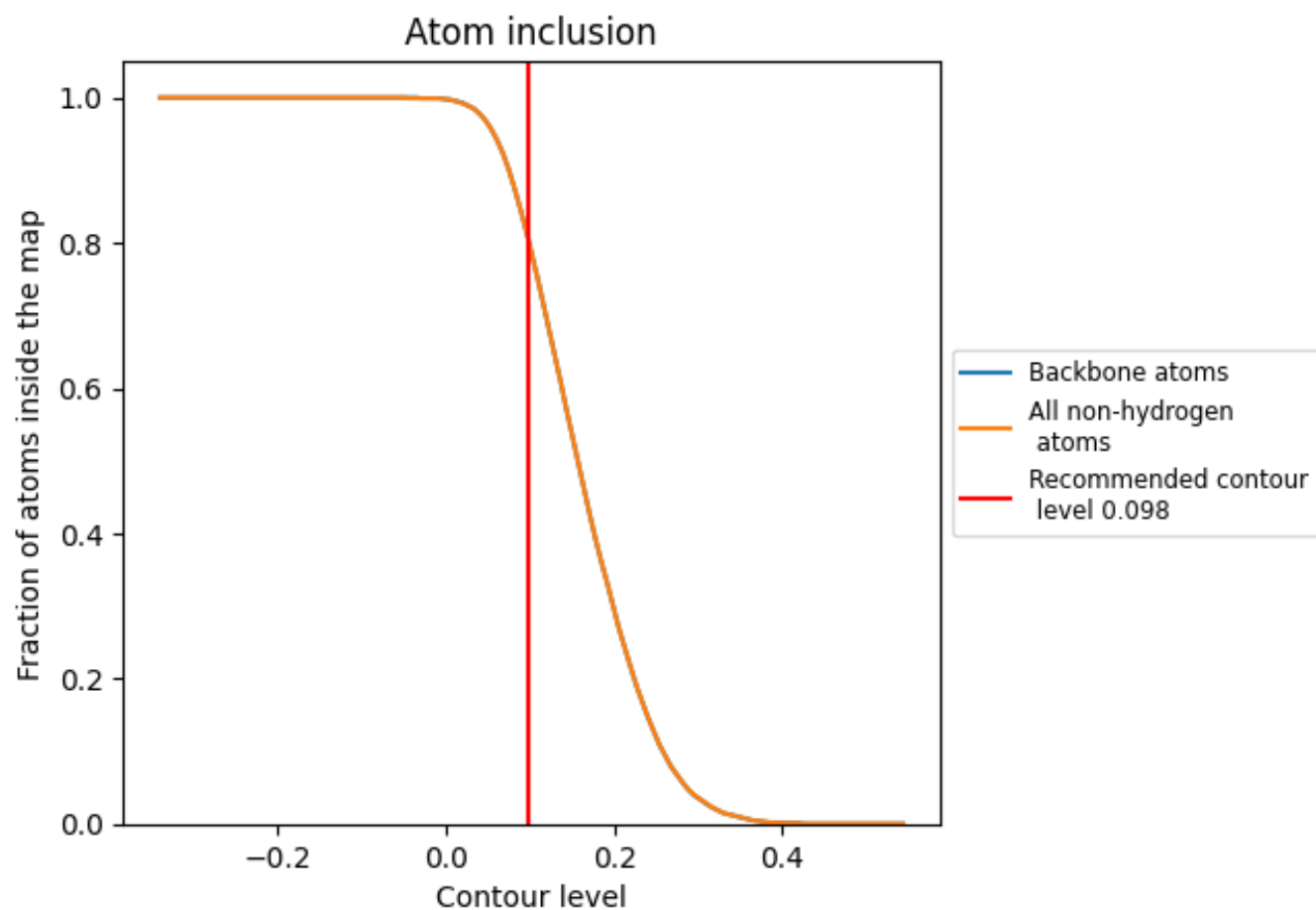
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.098).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.098) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8060	 0.3030
A	 0.9530	 0.3780
B	 0.9410	 0.3630
C	 0.9430	 0.3750
D	 0.9380	 0.3670
E	 0.9530	 0.3850
F	 0.9440	 0.3860
G	 0.8440	 0.3050
H	 0.8250	 0.3170
I	 0.5460	 0.1610
J	 0.7030	 0.2360
K	 0.6870	 0.1820
L	 0.7560	 0.2390
M	 0.7460	 0.2590
N	 0.5610	 0.1760
O	 0.6040	 0.2300
P	 0.6400	 0.2310
Q	 0.5410	 0.2010
R	 0.6340	 0.2440
S	 0.6770	 0.2260
T	 0.5680	 0.1940
U	 0.4880	 0.1870
V	 0.5510	 0.1990
W	 0.4260	 0.2090
X	 0.4750	 0.1880
Y	 0.6470	 0.2270
Z	 0.6860	 0.2400

