



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:31 PM UTC

PDB ID : 6HE4 / pdb_00006he4
EMDB ID : EMD-0209
Title : AAA-ATPase ring of PAN-proteasomes
Authors : Majumder, P.; Rudack, T.; Beck, F.; Baumeister, W.
Deposited on : 2018-08-20
Resolution : 4.85 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:

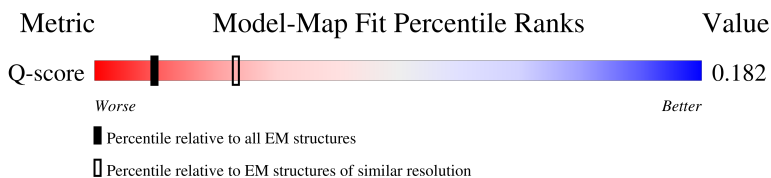
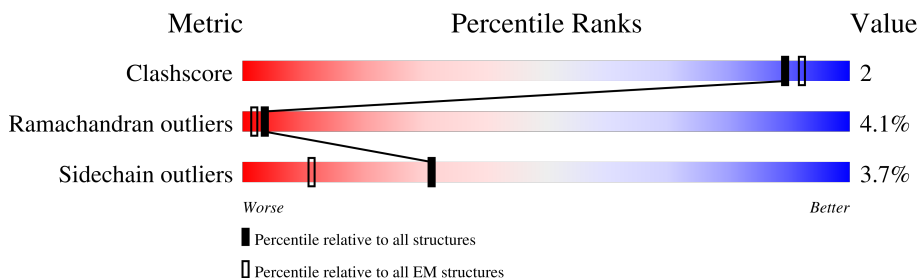
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.85 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1289 (4.35 - 5.35)

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	H	267	28% 35% 54% 9% .
1	I	267	33% 40% 50% 8% .
1	J	267	28% 43% 46% 10% .
1	K	267	28% 41% 52% 6% .

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Mol	Chain	Length	Quality of chain
1	L	267	28% 39% 52% 8%
1	M	267	37% 43% 49% 7%

2 Entry composition [i](#)

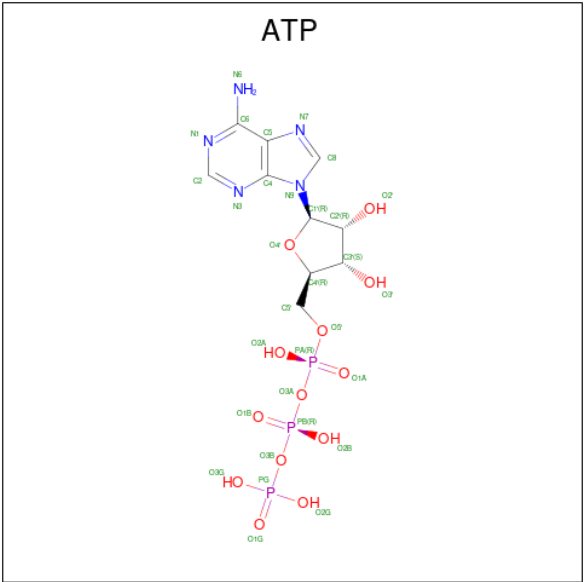
There are 4 unique types of molecules in this entry. The entry contains 12684 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Proteasome-activating nucleotidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	267	Total	C	N	O	S	0	0
			2088	1332	356	393	7		
1	I	267	Total	C	N	O	S	0	0
			2088	1332	356	393	7		
1	K	267	Total	C	N	O	S	0	0
			2088	1332	356	393	7		
1	L	267	Total	C	N	O	S	0	0
			2088	1332	356	393	7		
1	M	267	Total	C	N	O	S	0	0
			2088	1332	356	393	7		
1	J	267	Total	C	N	O	S	0	0
			2088	1332	356	393	7		

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



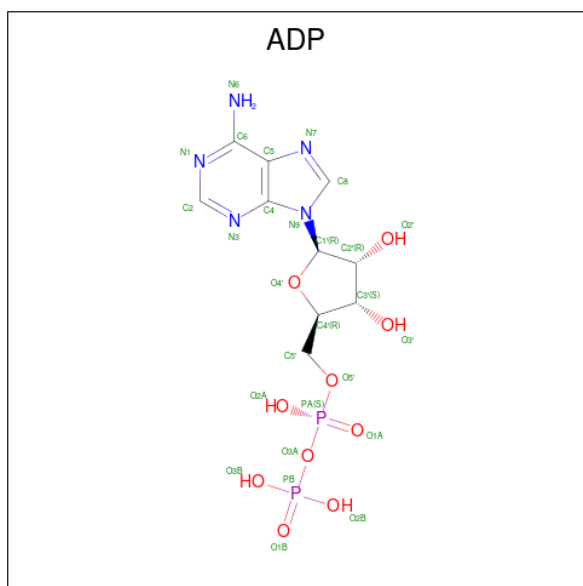
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Mol	Chain	Residues	Atoms					AltConf
2	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	H	1	Total	Mg	0
			1	1	
3	I	1	Total	Mg	0
			1	1	
3	K	1	Total	Mg	0
			1	1	
3	L	1	Total	Mg	0
			1	1	
3	J	1	Total	Mg	0
			1	1	

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

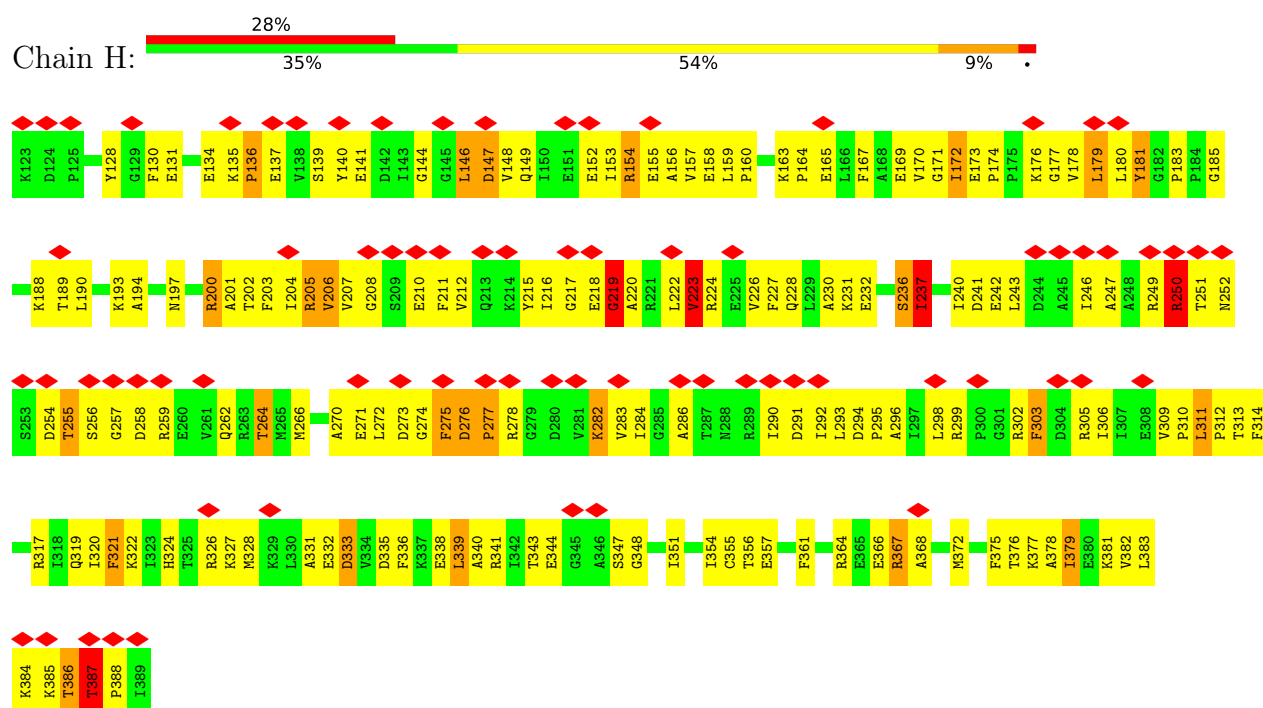


Mol	Chain	Residues	Atoms					AltConf
4	L	1	Total	C	N	O	P	0
			27	10	5	10	2	

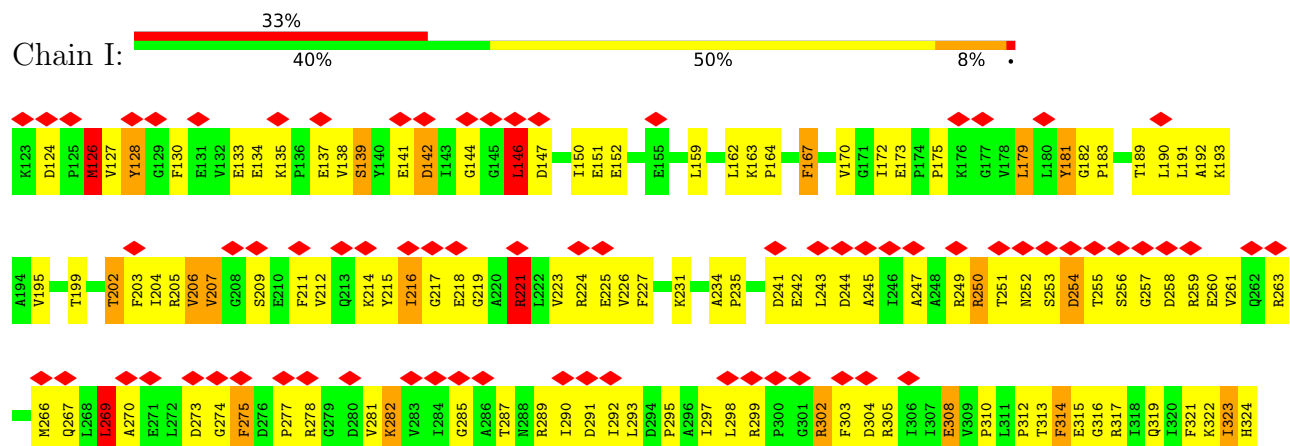
3 Residue-property plots

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: Proteasome-activating nucleotidase

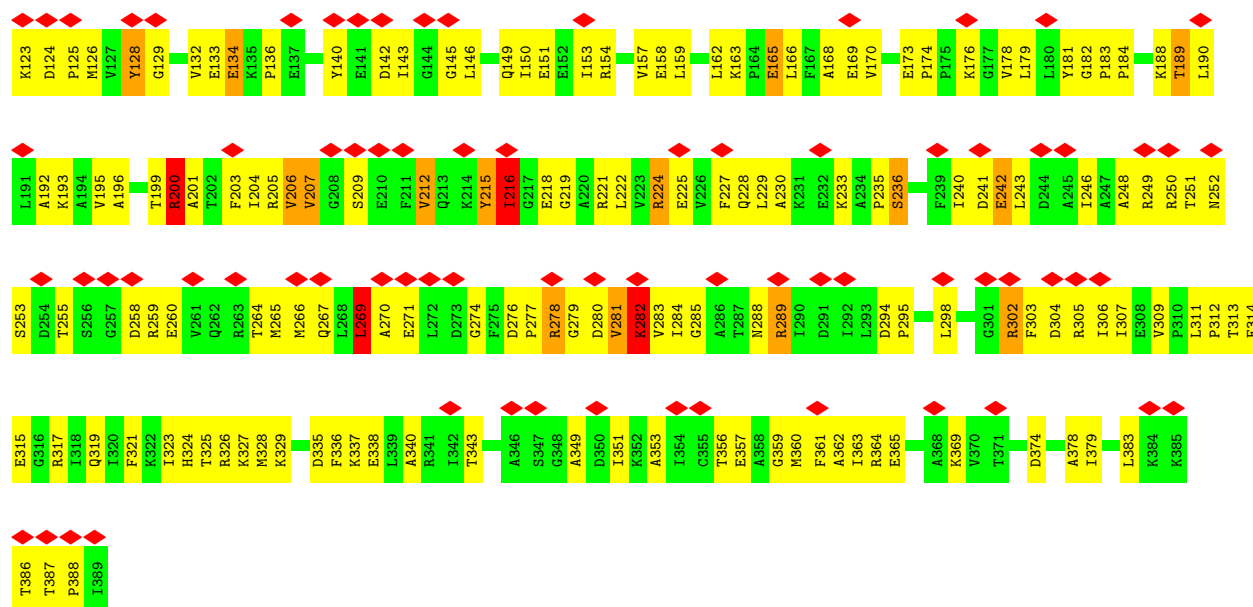
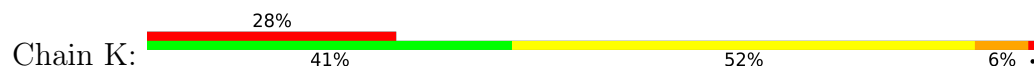


• Molecule 1: Proteasome-activating nucleotidase

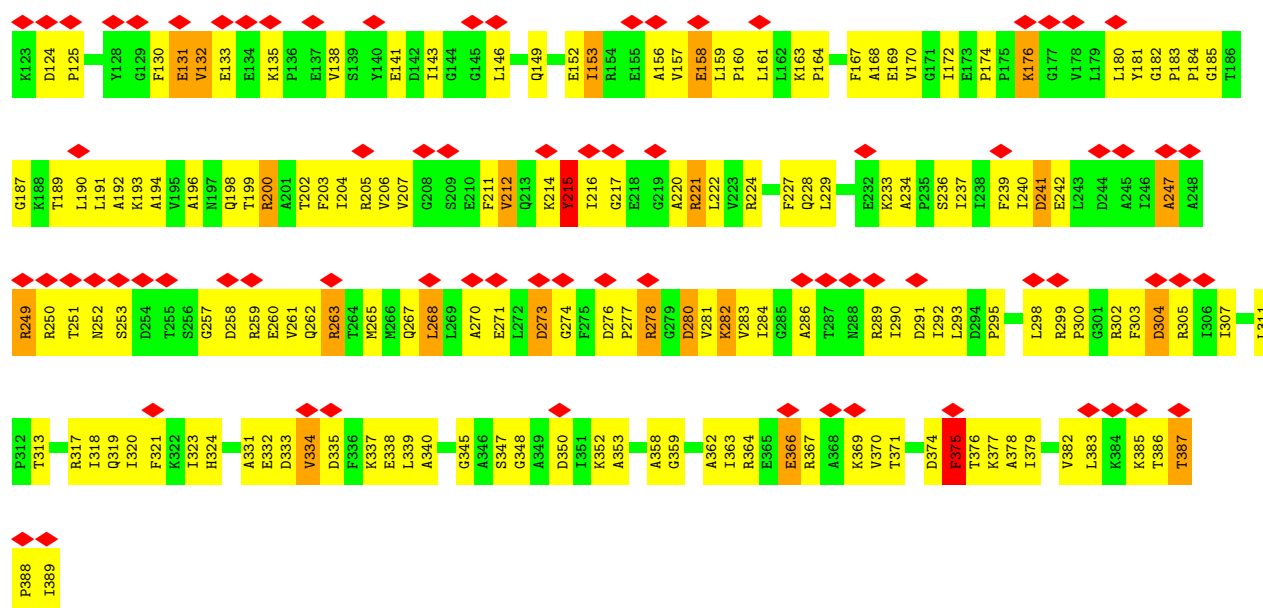




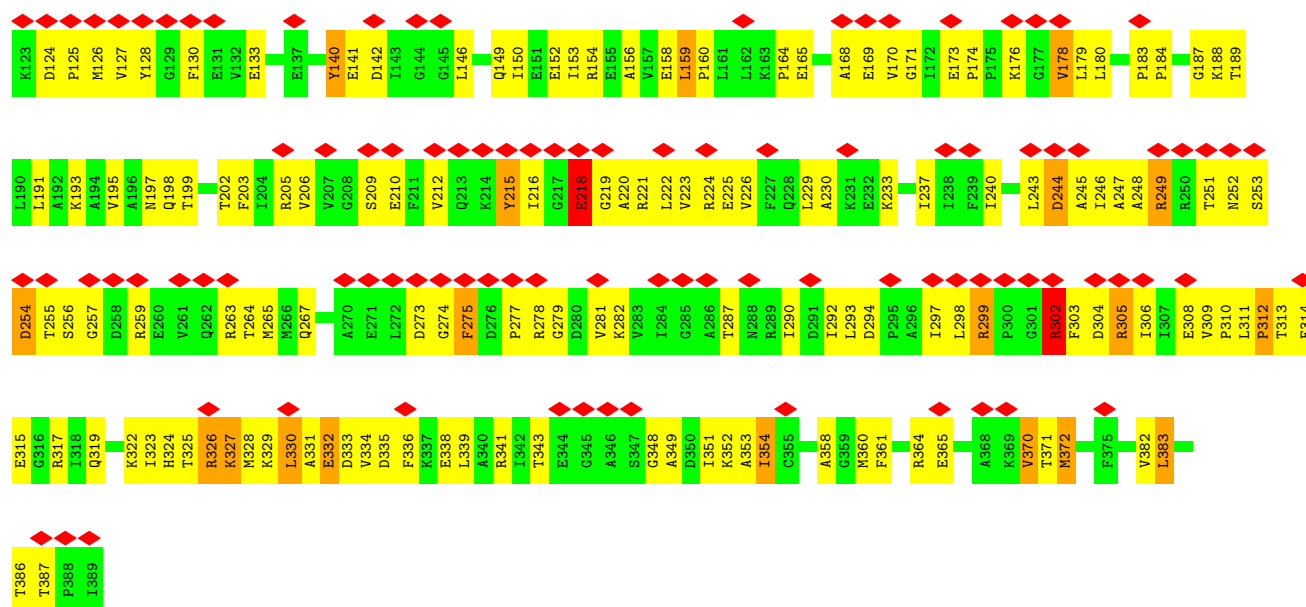
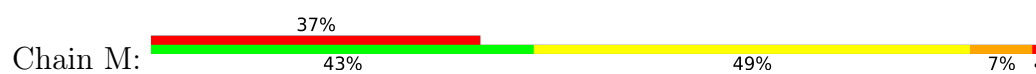
• Molecule 1: Proteasome-activating nucleotidase



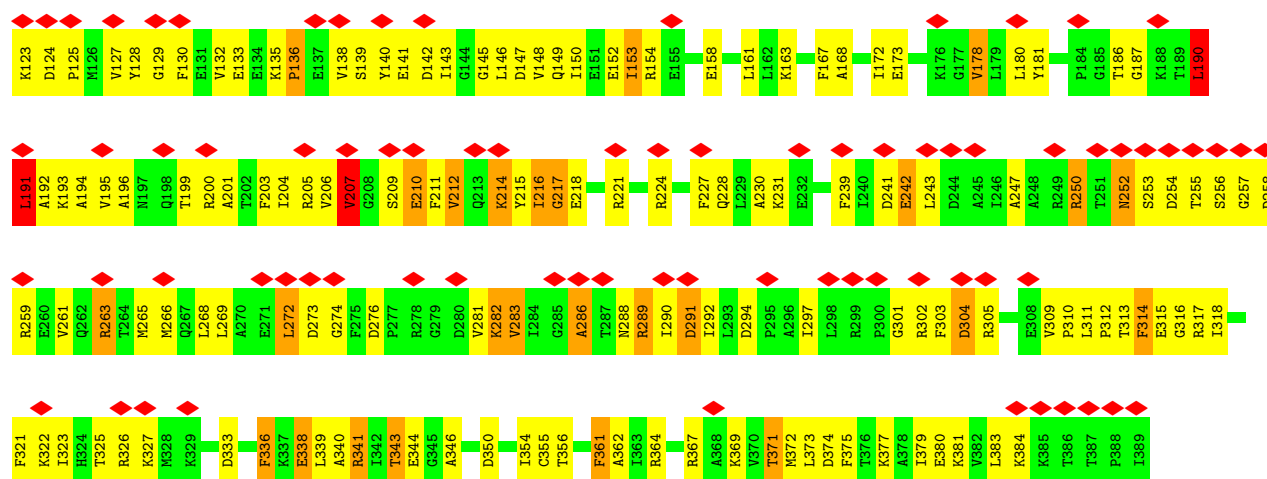
• Molecule 1: Proteasome-activating nucleotidase



• Molecule 1: Proteasome-activating nucleotidase



• Molecule 1: Proteasome-activating nucleotidase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	82207	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.106	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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, ATP, MG

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	H	2.32	91/2120 (4.3%)	2.59	176/2859 (6.2%)
1	I	2.27	83/2120 (3.9%)	2.52	151/2859 (5.3%)
1	J	2.30	83/2120 (3.9%)	2.53	156/2859 (5.5%)
1	K	2.30	83/2120 (3.9%)	2.54	176/2859 (6.2%)
1	L	2.28	84/2120 (4.0%)	2.54	160/2859 (5.6%)
1	M	2.24	75/2120 (3.5%)	2.49	159/2859 (5.6%)
All	All	2.29	499/12720 (3.9%)	2.53	978/17154 (5.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	20
1	I	0	12
1	J	0	10
1	K	0	12
1	L	0	11
1	M	0	9
All	All	0	74

All (499) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	206	VAL	CA-C	-12.09	1.38	1.52
1	L	353	ALA	N-CA	-11.82	1.31	1.46
1	I	163	LYS	CA-C	-10.58	1.39	1.52
1	H	181	TYR	CA-C	-10.53	1.39	1.52
1	L	174	PRO	CA-C	-10.52	1.45	1.52
1	I	162	LEU	C-N	10.38	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	135	LYS	CA-CB	9.81	1.59	1.52
1	K	306	ILE	CA-C	9.64	1.63	1.52
1	L	211	PHE	CA-C	-9.63	1.40	1.52
1	J	218	GLU	N-CA	-9.49	1.34	1.46
1	H	177	GLY	CA-C	-9.30	1.41	1.51
1	H	250	ARG	CD-NE	9.23	1.59	1.46
1	L	364	ARG	CD-NE	9.18	1.59	1.46
1	J	274	GLY	CA-C	-9.09	1.42	1.52
1	K	132	VAL	C-N	8.95	1.47	1.33
1	K	265	MET	CA-C	-8.82	1.41	1.52
1	I	203	PHE	CA-C	8.74	1.64	1.52
1	H	355	CYS	CA-C	-8.70	1.41	1.52
1	L	184	PRO	CA-CB	-8.60	1.42	1.53
1	M	308	GLU	CA-C	-8.46	1.42	1.52
1	H	327	LYS	CA-C	-8.34	1.42	1.52
1	K	183	PRO	CA-C	-8.32	1.47	1.51
1	J	302	ARG	CZ-NH2	8.28	1.44	1.33
1	L	293	LEU	CA-C	-8.27	1.42	1.52
1	L	259	ARG	NE-CZ	8.24	1.42	1.33
1	J	150	ILE	CA-C	-8.19	1.42	1.52
1	I	260	GLU	C-N	8.10	1.43	1.33
1	L	366	GLU	CA-C	-8.04	1.42	1.52
1	H	312	PRO	CA-C	-8.02	1.44	1.52
1	I	224	ARG	CZ-NH2	7.94	1.43	1.33
1	L	352	LYS	N-CA	7.91	1.55	1.46
1	K	224	ARG	CA-C	7.91	1.63	1.52
1	M	309	VAL	CA-C	-7.86	1.46	1.53
1	K	337	LYS	CA-CB	7.80	1.65	1.53
1	J	239	PHE	CA-C	-7.70	1.43	1.52
1	I	195	VAL	N-CA	7.70	1.56	1.46
1	H	188	LYS	CA-C	-7.68	1.44	1.52
1	J	172	ILE	CA-CB	-7.67	1.45	1.54
1	H	284	ILE	CA-C	-7.65	1.43	1.52
1	M	202	THR	CA-CB	-7.65	1.43	1.53
1	H	266	MET	CA-CB	7.65	1.65	1.53
1	M	252	ASN	CA-C	-7.61	1.42	1.52
1	I	368	ALA	C-N	7.60	1.44	1.33
1	M	237	ILE	CA-C	-7.59	1.42	1.52
1	L	352	LYS	CA-C	-7.56	1.43	1.52
1	L	221	ARG	NE-CZ	7.46	1.41	1.33
1	K	184	PRO	CA-C	-7.46	1.42	1.52
1	H	364	ARG	CD-NE	7.44	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	206	VAL	N-CA	-7.43	1.38	1.46
1	M	141	GLU	CA-C	-7.42	1.42	1.52
1	M	224	ARG	N-CA	-7.42	1.37	1.46
1	J	317	ARG	NE-CZ	7.41	1.41	1.33
1	L	305	ARG	CD-NE	7.41	1.56	1.46
1	J	362	ALA	C-N	7.38	1.42	1.34
1	I	175	PRO	CA-C	-7.38	1.43	1.52
1	L	159	LEU	CA-C	-7.23	1.43	1.52
1	L	305	ARG	NE-CZ	7.22	1.41	1.33
1	M	292	ILE	CA-CB	7.21	1.62	1.54
1	M	259	ARG	NE-CZ	7.20	1.41	1.33
1	K	206	VAL	CA-C	-7.19	1.46	1.52
1	H	278	ARG	NE-CZ	7.18	1.41	1.33
1	K	250	ARG	CD-NE	7.17	1.56	1.46
1	M	133	GLU	CA-C	-7.17	1.44	1.52
1	J	344	GLU	C-N	7.14	1.41	1.33
1	K	203	PHE	C-N	7.14	1.42	1.33
1	J	263	ARG	CA-C	-7.11	1.43	1.52
1	K	305	ARG	CD-NE	7.07	1.56	1.46
1	J	303	PHE	N-CA	-7.06	1.37	1.46
1	H	322	LYS	CA-C	-7.05	1.43	1.52
1	H	277	PRO	N-CA	-7.04	1.38	1.47
1	L	240	ILE	CA-C	-7.04	1.45	1.52
1	L	363	ILE	C-N	7.03	1.43	1.33
1	M	224	ARG	CZ-NH2	7.03	1.42	1.33
1	H	291	ASP	CA-C	-7.02	1.43	1.52
1	J	317	ARG	CD-NE	6.99	1.56	1.46
1	K	224	ARG	CD-NE	6.98	1.56	1.46
1	H	317	ARG	CA-C	-6.97	1.44	1.52
1	K	149	GLN	C-N	6.97	1.42	1.33
1	H	299	ARG	CZ-NH1	6.93	1.42	1.32
1	K	357	GLU	N-CA	-6.92	1.37	1.46
1	L	298	LEU	CA-C	6.91	1.61	1.52
1	J	283	VAL	C-N	6.91	1.42	1.33
1	H	148	VAL	CA-C	-6.90	1.43	1.53
1	I	263	ARG	NE-CZ	6.90	1.40	1.33
1	M	354	ILE	CA-CB	6.87	1.63	1.54
1	L	280	ASP	CA-CB	6.86	1.65	1.53
1	L	152	GLU	CA-C	-6.86	1.44	1.52
1	M	314	PHE	CA-C	-6.85	1.44	1.52
1	M	164	PRO	N-CA	-6.82	1.39	1.47
1	H	305	ARG	NE-CZ	6.81	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	302	ARG	CD-NE	6.81	1.55	1.46
1	H	271	GLU	C-N	6.79	1.42	1.33
1	J	313	THR	CA-CB	-6.79	1.43	1.53
1	L	383	LEU	N-CA	6.77	1.55	1.46
1	I	182	GLY	CA-C	-6.76	1.42	1.51
1	J	333	ASP	C-N	6.75	1.41	1.33
1	L	307	ILE	CA-CB	-6.75	1.46	1.54
1	J	204	ILE	CA-C	-6.74	1.44	1.52
1	K	288	ASN	N-CA	-6.73	1.37	1.46
1	M	154	ARG	NE-CZ	6.72	1.40	1.33
1	H	321	PHE	N-CA	-6.71	1.38	1.46
1	L	206	VAL	CA-CB	-6.70	1.46	1.54
1	H	252	ASN	CA-CB	6.69	1.63	1.53
1	K	176	LYS	C-N	6.68	1.41	1.33
1	I	142	ASP	CA-C	6.68	1.60	1.52
1	M	248	ALA	CA-C	-6.67	1.44	1.52
1	J	294	ASP	C-N	6.65	1.42	1.34
1	H	146	LEU	CA-C	-6.65	1.44	1.52
1	I	317	ARG	NE-CZ	6.64	1.40	1.33
1	L	168	ALA	CA-C	-6.64	1.44	1.52
1	H	335	ASP	CA-C	-6.64	1.44	1.52
1	L	192	ALA	C-N	6.64	1.42	1.33
1	I	269	LEU	CA-C	-6.63	1.43	1.52
1	J	218	GLU	C-N	6.63	1.42	1.33
1	I	382	VAL	N-CA	-6.60	1.38	1.46
1	H	178	VAL	C-N	6.59	1.42	1.33
1	J	371	THR	CA-C	-6.58	1.44	1.53
1	M	341	ARG	CD-NE	6.57	1.55	1.46
1	L	303	PHE	N-CA	-6.56	1.37	1.46
1	K	154	ARG	CD-NE	6.55	1.55	1.46
1	K	183	PRO	C-O	-6.55	1.19	1.25
1	M	330	LEU	CA-C	-6.54	1.44	1.52
1	L	271	GLU	C-O	-6.54	1.15	1.24
1	J	326	ARG	CZ-NH2	6.54	1.42	1.33
1	H	146	LEU	N-CA	-6.53	1.37	1.46
1	K	289	ARG	NE-CZ	6.52	1.40	1.33
1	K	133	GLU	CA-C	-6.51	1.44	1.52
1	H	341	ARG	NE-CZ	6.51	1.40	1.33
1	J	338	GLU	CA-CB	6.49	1.63	1.53
1	J	286	ALA	CA-C	-6.48	1.44	1.52
1	I	334	VAL	CA-C	-6.48	1.44	1.52
1	M	221	ARG	N-CA	-6.46	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	178	VAL	C-N	6.46	1.42	1.33
1	H	354	ILE	CA-CB	-6.45	1.46	1.54
1	H	341	ARG	CZ-NH2	6.45	1.41	1.33
1	K	374	ASP	CA-CB	6.44	1.63	1.53
1	K	134	GLU	CA-C	-6.43	1.44	1.52
1	I	340	ALA	CA-C	-6.42	1.44	1.52
1	I	326	ARG	NE-CZ	6.41	1.40	1.33
1	L	236	SER	C-N	-6.41	1.25	1.33
1	H	202	THR	C-N	6.41	1.42	1.33
1	J	304	ASP	CA-CB	6.40	1.64	1.53
1	M	229	LEU	CA-C	-6.39	1.44	1.52
1	M	382	VAL	CA-C	-6.39	1.44	1.52
1	K	327	LYS	CA-C	-6.38	1.44	1.52
1	L	274	GLY	CA-C	-6.38	1.45	1.52
1	L	205	ARG	CA-CB	6.37	1.62	1.53
1	J	289	ARG	CA-C	-6.37	1.44	1.52
1	I	159	LEU	C-N	6.33	1.42	1.34
1	L	138	VAL	N-CA	-6.33	1.39	1.46
1	J	200	ARG	NE-CZ	6.32	1.40	1.33
1	I	378	ALA	C-N	6.31	1.41	1.33
1	J	259	ARG	CZ-NH2	6.29	1.41	1.33
1	K	315	GLU	N-CA	-6.29	1.38	1.46
1	H	332	GLU	CA-C	-6.28	1.45	1.52
1	K	324	HIS	ND1-CE1	6.28	1.38	1.32
1	J	327	LYS	CA-CB	6.28	1.63	1.53
1	I	287	THR	CA-C	-6.28	1.44	1.52
1	J	355	CYS	C-N	6.28	1.41	1.33
1	H	278	ARG	CZ-NH2	6.28	1.41	1.33
1	I	361	PHE	CA-C	-6.28	1.44	1.52
1	H	147	ASP	C-N	6.27	1.41	1.33
1	H	379	ILE	CA-C	-6.27	1.44	1.52
1	I	278	ARG	NE-CZ	6.26	1.40	1.33
1	J	123	LYS	C-N	6.26	1.40	1.33
1	J	255	THR	CA-C	-6.26	1.44	1.52
1	H	264	THR	C-N	6.25	1.42	1.33
1	M	297	ILE	C-N	6.25	1.42	1.33
1	K	125	PRO	C-N	6.25	1.42	1.33
1	H	294	ASP	CA-C	-6.22	1.45	1.53
1	M	327	LYS	N-CA	-6.22	1.39	1.46
1	K	236	SER	N-CA	-6.22	1.38	1.46
1	J	216	ILE	CB-CG1	6.21	1.65	1.53
1	I	316	GLY	CA-C	-6.20	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	222	LEU	CA-CB	6.20	1.62	1.53
1	H	212	VAL	N-CA	-6.20	1.38	1.46
1	K	154	ARG	CA-C	-6.19	1.45	1.52
1	H	157	VAL	CA-C	-6.19	1.44	1.52
1	J	191	LEU	C-N	6.18	1.41	1.33
1	I	254	ASP	C-N	6.18	1.42	1.33
1	L	263	ARG	N-CA	6.18	1.53	1.46
1	H	270	ALA	C-N	6.18	1.41	1.33
1	M	124	ASP	C-N	6.18	1.41	1.33
1	I	191	LEU	C-N	6.17	1.42	1.33
1	M	361	PHE	CA-CB	6.17	1.62	1.53
1	K	264	THR	CA-C	6.17	1.60	1.52
1	L	304	ASP	C-N	6.16	1.42	1.33
1	H	333	ASP	N-CA	-6.15	1.38	1.46
1	H	174	PRO	C-N	6.15	1.41	1.33
1	H	249	ARG	NE-CZ	6.15	1.39	1.33
1	L	271	GLU	CA-CB	6.14	1.63	1.53
1	I	312	PRO	N-CA	6.12	1.54	1.47
1	J	369	LYS	N-CA	-6.11	1.37	1.45
1	H	273	ASP	CA-C	-6.10	1.44	1.52
1	I	250	ARG	CD-NE	6.10	1.54	1.46
1	H	224	ARG	NE-CZ	6.10	1.39	1.33
1	I	152	GLU	CA-C	-6.10	1.45	1.52
1	K	193	LYS	CA-C	-6.10	1.44	1.52
1	L	257	GLY	N-CA	6.09	1.54	1.45
1	J	266	MET	N-CA	-6.09	1.38	1.46
1	K	125	PRO	N-CD	-6.09	1.39	1.47
1	K	302	ARG	N-CA	-6.07	1.38	1.46
1	I	234	ALA	CA-C	6.07	1.60	1.52
1	K	143	ILE	N-CA	-6.06	1.39	1.46
1	K	307	ILE	CA-CB	-6.04	1.46	1.53
1	M	278	ARG	NE-CZ	6.04	1.39	1.33
1	H	326	ARG	NE-CZ	6.04	1.39	1.33
1	K	269	LEU	CA-CB	6.03	1.63	1.53
1	J	205	ARG	CD-NE	6.03	1.54	1.46
1	L	180	LEU	CA-CB	6.02	1.62	1.53
1	J	152	GLU	C-N	6.01	1.41	1.33
1	J	317	ARG	CA-C	-6.01	1.45	1.52
1	K	386	THR	CA-C	-6.01	1.45	1.52
1	H	201	ALA	C-N	6.00	1.42	1.33
1	M	154	ARG	CZ-NH2	6.00	1.41	1.33
1	I	375	PHE	CA-C	-6.00	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	354	ILE	CA-CB	5.98	1.61	1.54
1	M	310	PRO	N-CA	-5.98	1.41	1.46
1	L	241	ASP	CA-CB	5.97	1.62	1.53
1	L	276	ASP	CA-CB	5.97	1.62	1.53
1	I	331	ALA	N-CA	-5.97	1.38	1.46
1	I	349	ALA	CA-C	-5.95	1.45	1.52
1	I	302	ARG	C-O	-5.95	1.16	1.24
1	H	312	PRO	C-N	5.95	1.41	1.33
1	L	228	GLN	N-CA	-5.95	1.39	1.46
1	L	313	THR	N-CA	-5.94	1.38	1.45
1	H	348	GLY	C-N	5.93	1.42	1.34
1	L	124	ASP	CA-CB	5.92	1.62	1.53
1	L	214	LYS	CA-CB	5.91	1.62	1.53
1	K	336	PHE	CA-C	-5.90	1.44	1.52
1	K	305	ARG	NE-CZ	5.90	1.39	1.33
1	K	317	ARG	CA-C	-5.90	1.44	1.52
1	H	305	ARG	CA-CB	5.89	1.62	1.53
1	J	230	ALA	CA-CB	5.89	1.62	1.53
1	M	206	VAL	CA-CB	-5.87	1.46	1.54
1	J	380	GLU	C-N	5.86	1.41	1.33
1	I	366	GLU	N-CA	-5.86	1.38	1.46
1	M	223	VAL	CA-C	-5.86	1.45	1.52
1	L	205	ARG	CD-NE	5.85	1.54	1.46
1	M	205	ARG	CD-NE	5.85	1.54	1.46
1	H	355	CYS	C-N	5.84	1.42	1.34
1	M	249	ARG	CZ-NH1	5.84	1.41	1.32
1	J	199	THR	CA-C	-5.84	1.45	1.52
1	I	363	ILE	C-N	5.84	1.41	1.34
1	K	307	ILE	CA-C	-5.83	1.45	1.52
1	K	383	LEU	CA-CB	5.82	1.62	1.53
1	I	367	ARG	CZ-NH2	5.82	1.41	1.33
1	K	369	LYS	CA-C	-5.81	1.45	1.52
1	J	224	ARG	CA-C	-5.81	1.45	1.52
1	J	341	ARG	NE-CZ	5.80	1.39	1.33
1	K	365	GLU	C-N	5.79	1.42	1.33
1	M	274	GLY	C-N	5.78	1.41	1.33
1	J	383	LEU	C-O	-5.78	1.16	1.24
1	K	140	TYR	CZ-OH	5.78	1.50	1.38
1	M	299	ARG	CZ-NH2	5.78	1.41	1.33
1	H	205	ARG	CA-C	-5.77	1.45	1.52
1	K	205	ARG	CA-C	-5.76	1.45	1.52
1	L	221	ARG	N-CA	-5.76	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	173	GLU	CA-C	-5.76	1.46	1.52
1	H	179	LEU	C-O	5.75	1.31	1.24
1	H	128	TYR	N-CA	-5.75	1.39	1.46
1	H	324	HIS	C-N	5.75	1.41	1.33
1	K	178	VAL	CA-CB	-5.74	1.47	1.54
1	K	363	ILE	N-CA	-5.74	1.39	1.46
1	K	357	GLU	CA-C	-5.74	1.45	1.52
1	K	360	MET	N-CA	5.74	1.53	1.46
1	I	356	THR	N-CA	5.73	1.53	1.46
1	H	283	VAL	CA-CB	5.72	1.61	1.54
1	K	228	GLN	CA-C	-5.71	1.44	1.52
1	L	181	TYR	CA-C	-5.71	1.45	1.52
1	I	298	LEU	C-O	-5.70	1.17	1.24
1	L	236	SER	CA-C	-5.70	1.45	1.52
1	K	281	VAL	C-N	5.68	1.41	1.33
1	L	289	ARG	NE-CZ	5.68	1.39	1.33
1	K	162	LEU	CA-C	-5.68	1.45	1.52
1	I	363	ILE	C-O	-5.67	1.17	1.24
1	L	302	ARG	NE-CZ	5.67	1.39	1.33
1	L	203	PHE	C-N	5.66	1.40	1.33
1	K	285	GLY	N-CA	-5.66	1.38	1.45
1	J	187	GLY	CA-C	-5.66	1.44	1.51
1	I	329	LYS	CA-C	-5.66	1.45	1.52
1	J	257	GLY	C-N	5.65	1.41	1.33
1	M	335	ASP	CA-CB	5.65	1.61	1.53
1	M	189	THR	CA-C	-5.64	1.45	1.52
1	J	180	LEU	C-O	-5.63	1.17	1.24
1	H	160	PRO	CA-C	-5.62	1.42	1.52
1	M	267	GLN	N-CA	-5.60	1.38	1.46
1	K	317	ARG	NE-CZ	5.60	1.39	1.33
1	J	129	GLY	CA-C	-5.59	1.44	1.51
1	J	148	VAL	CA-CB	-5.59	1.47	1.54
1	H	347	SER	CA-C	-5.58	1.45	1.52
1	H	172	ILE	CA-C	-5.58	1.47	1.53
1	H	275	PHE	CA-C	5.57	1.59	1.52
1	J	375	PHE	CA-CB	5.57	1.61	1.53
1	I	350	ASP	N-CA	5.56	1.53	1.46
1	L	206	VAL	N-CA	-5.56	1.39	1.46
1	L	212	VAL	C-O	-5.56	1.17	1.24
1	M	152	GLU	CA-C	-5.55	1.45	1.52
1	M	195	VAL	C-N	5.55	1.41	1.33
1	L	338	GLU	N-CA	-5.55	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	299	ARG	NE-CZ	5.55	1.39	1.33
1	M	317	ARG	NE-CZ	5.55	1.39	1.33
1	M	130	PHE	CA-C	-5.55	1.45	1.52
1	I	332	GLU	CA-C	5.55	1.60	1.52
1	J	288	ASN	CA-C	-5.54	1.44	1.52
1	I	282	LYS	C-N	5.53	1.40	1.33
1	L	206	VAL	C-N	5.53	1.39	1.33
1	I	313	THR	C-N	5.52	1.41	1.33
1	I	219	GLY	C-N	5.52	1.40	1.33
1	J	350	ASP	CA-C	-5.52	1.45	1.52
1	I	218	GLU	N-CA	-5.52	1.39	1.46
1	K	235	PRO	CA-C	-5.52	1.41	1.52
1	I	127	VAL	N-CA	-5.51	1.39	1.46
1	H	344	GLU	C-O	-5.51	1.17	1.23
1	K	379	ILE	N-CA	-5.51	1.39	1.46
1	H	367	ARG	NE-CZ	5.50	1.39	1.33
1	I	285	GLY	N-CA	-5.50	1.39	1.44
1	I	130	PHE	CA-C	-5.50	1.45	1.52
1	L	202	THR	CA-C	5.50	1.59	1.52
1	K	312	PRO	C-N	5.49	1.42	1.33
1	J	250	ARG	CZ-NH1	5.49	1.40	1.32
1	K	168	ALA	CA-C	-5.48	1.45	1.52
1	L	156	ALA	CA-C	-5.48	1.45	1.52
1	J	384	LYS	CA-C	-5.48	1.45	1.52
1	I	244	ASP	CA-CB	5.48	1.62	1.53
1	K	284	ILE	CA-C	-5.48	1.46	1.52
1	H	309	VAL	CA-C	-5.47	1.47	1.52
1	H	139	SER	N-CA	5.47	1.53	1.45
1	H	351	ILE	CA-C	-5.47	1.45	1.52
1	L	347	SER	C-N	5.47	1.40	1.33
1	J	135	LYS	N-CA	-5.46	1.38	1.46
1	H	210	GLU	CA-C	-5.46	1.45	1.52
1	I	259	ARG	CA-C	-5.46	1.45	1.52
1	K	360	MET	C-N	5.46	1.41	1.33
1	I	204	ILE	CA-C	-5.45	1.46	1.52
1	L	262	GLN	N-CA	-5.45	1.39	1.46
1	K	374	ASP	N-CA	5.45	1.52	1.46
1	I	167	PHE	CA-C	-5.44	1.45	1.52
1	K	169	GLU	C-N	5.44	1.40	1.33
1	H	160	PRO	C-O	-5.44	1.17	1.24
1	K	241	ASP	CA-C	-5.43	1.46	1.52
1	H	284	ILE	N-CA	-5.43	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	281	VAL	CA-C	-5.43	1.46	1.52
1	I	267	GLN	CA-CB	5.43	1.61	1.53
1	J	168	ALA	C-N	5.42	1.41	1.33
1	L	138	VAL	C-N	5.42	1.41	1.33
1	M	323	ILE	CA-CB	-5.42	1.47	1.54
1	J	252	ASN	CA-CB	5.42	1.61	1.53
1	I	216	ILE	N-CA	-5.41	1.39	1.46
1	I	223	VAL	CA-CB	5.41	1.61	1.54
1	J	346	ALA	CA-CB	5.41	1.62	1.53
1	K	294	ASP	CA-CB	5.41	1.61	1.53
1	M	259	ARG	CZ-NH2	5.40	1.40	1.33
1	J	259	ARG	N-CA	-5.39	1.39	1.46
1	I	308	GLU	CA-C	-5.38	1.46	1.52
1	K	351	ILE	CB-CG1	5.38	1.64	1.53
1	I	221	ARG	NE-CZ	5.38	1.39	1.33
1	L	258	ASP	CA-CB	5.38	1.61	1.53
1	M	126	MET	CA-CB	5.37	1.61	1.53
1	L	278	ARG	CD-NE	5.37	1.53	1.46
1	M	184	PRO	N-CA	-5.37	1.40	1.47
1	K	289	ARG	C-N	5.36	1.39	1.34
1	M	221	ARG	NE-CZ	5.36	1.39	1.33
1	K	205	ARG	CZ-NH2	5.35	1.40	1.33
1	H	224	ARG	CZ-NH2	5.35	1.40	1.33
1	H	298	LEU	CA-CB	5.35	1.62	1.53
1	L	190	LEU	CA-C	-5.35	1.45	1.52
1	K	204	ILE	CB-CG1	5.35	1.64	1.53
1	L	369	LYS	N-CA	5.34	1.52	1.46
1	H	170	VAL	CA-C	5.34	1.59	1.52
1	I	350	ASP	C-N	5.34	1.40	1.33
1	M	339	LEU	CB-CG	5.33	1.64	1.53
1	M	314	PHE	C-N	5.33	1.41	1.34
1	I	226	VAL	C-O	5.33	1.30	1.24
1	I	193	LYS	CA-CB	5.32	1.62	1.53
1	M	326	ARG	C-N	-5.32	1.26	1.33
1	I	133	GLU	C-N	5.32	1.41	1.33
1	I	377	LYS	N-CA	-5.32	1.40	1.46
1	M	140	TYR	C-N	5.32	1.41	1.33
1	H	205	ARG	NE-CZ	5.31	1.38	1.33
1	I	364	ARG	NE-CZ	5.31	1.38	1.33
1	L	276	ASP	C-N	5.31	1.40	1.33
1	M	297	ILE	CA-CB	-5.31	1.47	1.54
1	M	173	GLU	C-N	5.31	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	289	ARG	C-N	5.30	1.40	1.33
1	J	221	ARG	CZ-NH2	5.30	1.40	1.33
1	J	201	ALA	CA-C	-5.30	1.45	1.53
1	H	339	LEU	N-CA	-5.29	1.40	1.46
1	H	367	ARG	CD-NE	5.29	1.53	1.46
1	H	155	GLU	CA-C	5.29	1.59	1.52
1	K	212	VAL	N-CA	-5.29	1.39	1.46
1	K	258	ASP	C-O	5.28	1.28	1.23
1	L	252	ASN	C-N	5.28	1.41	1.33
1	J	269	LEU	N-CA	-5.28	1.40	1.46
1	I	170	VAL	C-N	5.28	1.40	1.33
1	J	291	ASP	C-N	5.28	1.40	1.33
1	I	384	LYS	CA-CB	5.27	1.61	1.53
1	M	156	ALA	N-CA	-5.27	1.40	1.46
1	L	362	ALA	CA-C	-5.27	1.46	1.52
1	L	376	THR	C-O	-5.27	1.18	1.24
1	M	152	GLU	CG-CD	5.27	1.65	1.52
1	J	259	ARG	CD-NE	5.27	1.53	1.46
1	J	149	GLN	CA-CB	5.26	1.61	1.53
1	L	317	ARG	N-CA	-5.26	1.40	1.46
1	I	214	LYS	C-N	5.26	1.40	1.33
1	I	305	ARG	NE-CZ	5.26	1.38	1.33
1	K	326	ARG	NE-CZ	5.26	1.38	1.33
1	K	329	LYS	CA-C	-5.26	1.46	1.52
1	K	216	ILE	CB-CG1	5.26	1.64	1.53
1	I	259	ARG	NE-CZ	5.25	1.38	1.33
1	H	275	PHE	C-N	5.25	1.38	1.33
1	M	339	LEU	CA-C	5.25	1.59	1.52
1	H	278	ARG	CD-NE	5.25	1.53	1.46
1	M	165	GLU	CA-C	-5.25	1.45	1.52
1	M	168	ALA	CA-C	5.25	1.58	1.52
1	H	326	ARG	CD-NE	5.24	1.53	1.46
1	L	332	GLU	CA-C	-5.24	1.45	1.52
1	I	376	THR	C-O	-5.24	1.18	1.24
1	M	237	ILE	CB-CG1	5.24	1.64	1.53
1	H	331	ALA	N-CA	-5.23	1.39	1.46
1	I	181	TYR	N-CA	-5.23	1.39	1.45
1	J	364	ARG	CD-NE	5.22	1.53	1.46
1	L	350	ASP	CA-CB	5.22	1.61	1.53
1	M	319	GLN	CD-NE2	5.22	1.44	1.33
1	M	332	GLU	N-CA	-5.22	1.39	1.46
1	K	154	ARG	NE-CZ	5.22	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	235	PRO	CA-C	-5.21	1.42	1.52
1	K	157	VAL	C-N	5.21	1.40	1.33
1	H	134	GLU	CA-CB	5.21	1.61	1.53
1	K	295	PRO	N-CA	-5.21	1.40	1.47
1	M	218	GLU	CA-C	-5.21	1.45	1.52
1	H	341	ARG	N-CA	-5.20	1.40	1.46
1	M	188	LYS	N-CA	-5.20	1.39	1.46
1	M	309	VAL	N-CA	-5.20	1.42	1.46
1	J	139	SER	CA-C	-5.20	1.46	1.52
1	H	171	GLY	C-O	-5.19	1.17	1.23
1	L	196	ALA	C-N	5.19	1.40	1.33
1	K	259	ARG	NE-CZ	5.19	1.38	1.33
1	K	179	LEU	CA-CB	5.19	1.60	1.53
1	J	297	ILE	N-CA	5.18	1.52	1.46
1	L	157	VAL	CA-CB	5.18	1.60	1.55
1	J	302	ARG	NE-CZ	5.17	1.38	1.33
1	J	292	ILE	CB-CG1	5.16	1.63	1.53
1	M	225	GLU	CA-C	-5.16	1.46	1.52
1	J	356	THR	N-CA	5.16	1.52	1.46
1	I	179	LEU	CB-CG	5.16	1.63	1.53
1	L	250	ARG	C-N	5.16	1.40	1.33
1	J	310	PRO	CA-C	-5.16	1.45	1.52
1	H	383	LEU	CA-C	-5.16	1.46	1.52
1	H	322	LYS	C-N	5.15	1.40	1.33
1	K	249	ARG	CD-NE	5.15	1.53	1.46
1	K	153	ILE	CA-C	-5.15	1.46	1.52
1	J	243	LEU	CA-C	-5.15	1.45	1.52
1	M	267	GLN	CA-C	-5.14	1.45	1.52
1	J	323	ILE	CB-CG1	5.14	1.63	1.53
1	L	133	GLU	CA-CB	5.13	1.59	1.52
1	J	200	ARG	CZ-NH1	5.13	1.40	1.32
1	L	333	ASP	C-N	5.13	1.40	1.33
1	L	207	VAL	CA-C	-5.12	1.47	1.52
1	J	196	ALA	C-N	5.12	1.41	1.34
1	L	233	LYS	N-CA	-5.12	1.40	1.46
1	L	237	ILE	CA-CB	-5.12	1.48	1.54
1	M	240	ILE	N-CA	-5.11	1.41	1.46
1	M	304	ASP	CA-CB	5.11	1.61	1.53
1	L	187	GLY	CA-C	-5.10	1.44	1.51
1	I	150	ILE	CA-CB	-5.10	1.48	1.54
1	J	163	LYS	CA-CB	5.10	1.60	1.53
1	L	233	LYS	C-N	5.10	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	322	LYS	C-N	5.08	1.40	1.33
1	H	276	ASP	C-O	-5.08	1.20	1.24
1	K	182	GLY	N-CA	-5.08	1.37	1.44
1	I	342	ILE	C-O	5.08	1.30	1.24
1	J	268	LEU	C-N	5.07	1.40	1.33
1	H	309	VAL	CA-CB	-5.07	1.47	1.54
1	K	340	ALA	N-CA	-5.07	1.39	1.46
1	H	347	SER	CA-CB	5.07	1.62	1.53
1	L	299	ARG	NE-CZ	5.07	1.38	1.33
1	K	307	ILE	C-N	5.07	1.40	1.33
1	L	371	THR	CA-C	-5.06	1.46	1.52
1	J	377	LYS	CA-C	-5.06	1.46	1.52
1	I	329	LYS	C-N	5.05	1.40	1.33
1	H	302	ARG	C-O	-5.05	1.17	1.24
1	I	329	LYS	N-CA	-5.05	1.39	1.46
1	H	153	ILE	N-CA	-5.05	1.40	1.46
1	M	249	ARG	CD-NE	5.04	1.53	1.46
1	J	289	ARG	NE-CZ	5.04	1.38	1.33
1	L	169	GLU	C-N	5.04	1.40	1.34
1	J	125	PRO	CA-CB	5.04	1.60	1.53
1	M	278	ARG	CD-NE	5.04	1.53	1.46
1	H	159	LEU	CA-CB	5.03	1.60	1.53
1	I	152	GLU	C-N	5.03	1.40	1.33
1	M	263	ARG	CZ-NH1	5.03	1.39	1.32
1	M	343	THR	CA-CB	5.03	1.59	1.52
1	L	267	GLN	C-N	5.02	1.40	1.33
1	I	367	ARG	CA-C	5.02	1.58	1.52
1	M	220	ALA	N-CA	-5.01	1.39	1.46
1	J	154	ARG	NE-CZ	5.01	1.38	1.33
1	L	293	LEU	CB-CG	5.00	1.63	1.53
1	H	293	LEU	CA-C	-5.00	1.46	1.52

All (978) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	305	ARG	CA-C-O	15.45	137.02	120.33
1	K	189	THR	CA-C-N	13.24	138.02	120.28
1	K	189	THR	C-N-CA	13.24	138.02	120.28
1	J	211	PHE	CA-CB-CG	-12.62	101.18	113.80
1	H	241	ASP	N-CA-C	-12.33	100.57	114.62
1	M	197	ASN	CA-CB-CG	12.01	124.61	112.60
1	K	325	THR	CA-C-N	11.49	135.67	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	325	THR	C-N-CA	11.49	135.67	120.28
1	K	227	PHE	CA-CB-CG	-11.39	102.41	113.80
1	I	261	VAL	N-CA-C	-11.24	101.00	111.45
1	M	146	LEU	N-CA-C	-11.17	96.75	111.71
1	K	271	GLU	N-CA-C	-10.71	101.26	114.75
1	H	164	PRO	CA-C-N	10.66	134.94	120.44
1	H	164	PRO	C-N-CA	10.66	134.94	120.44
1	H	188	LYS	N-CA-C	-10.22	99.64	112.72
1	L	281	VAL	CA-C-N	10.09	139.86	121.70
1	L	281	VAL	C-N-CA	10.09	139.86	121.70
1	H	311	LEU	CA-C-N	-9.68	110.10	120.66
1	H	311	LEU	C-N-CA	-9.68	110.10	120.66
1	K	170	VAL	N-CA-C	-9.33	101.77	110.82
1	K	302	ARG	N-CA-CB	9.31	126.22	110.49
1	I	135	LYS	CA-C-O	-9.24	113.36	120.48
1	J	147	ASP	CA-CB-CG	-9.23	103.37	112.60
1	K	173	GLU	CA-C-O	-9.21	110.83	120.23
1	M	255	THR	CA-C-N	9.21	132.41	120.44
1	M	255	THR	C-N-CA	9.21	132.41	120.44
1	L	215	TYR	N-CA-C	-9.20	99.40	110.44
1	I	207	VAL	N-CA-C	-9.19	94.75	108.17
1	M	372	MET	CA-C-N	9.09	132.25	120.44
1	M	372	MET	C-N-CA	9.09	132.25	120.44
1	K	276	ASP	CA-CB-CG	-9.03	103.57	112.60
1	K	224	ARG	NE-CZ-NH1	-9.02	112.48	121.50
1	I	384	LYS	CA-C-N	9.02	132.36	120.28
1	I	384	LYS	C-N-CA	9.02	132.36	120.28
1	J	210	GLU	N-CA-C	-9.00	102.30	113.28
1	K	267	GLN	CA-C-O	8.97	129.93	120.42
1	J	257	GLY	O-C-N	-8.93	112.85	122.67
1	L	375	PHE	CA-CB-CG	-8.80	105.00	113.80
1	I	299	ARG	CA-C-N	8.65	128.59	119.85
1	I	299	ARG	C-N-CA	8.65	128.59	119.85
1	I	372	MET	CA-C-O	8.59	129.92	119.79
1	I	357	GLU	CA-C-N	8.55	131.55	120.44
1	I	357	GLU	C-N-CA	8.55	131.55	120.44
1	H	165	GLU	N-CA-C	-8.51	101.95	111.14
1	L	268	LEU	CA-C-N	8.39	131.53	120.28
1	L	268	LEU	C-N-CA	8.39	131.53	120.28
1	H	247	ALA	O-C-N	-8.39	113.21	121.85
1	J	372	MET	CG-SD-CE	-8.39	82.45	100.90
1	H	381	LYS	CA-C-N	8.38	131.12	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	381	LYS	C-N-CA	8.38	131.12	120.56
1	K	280	ASP	N-CA-C	-8.36	100.54	110.41
1	K	356	THR	CA-C-N	8.36	132.16	120.29
1	K	356	THR	C-N-CA	8.36	132.16	120.29
1	I	182	GLY	CA-C-N	8.35	128.98	120.38
1	I	182	GLY	C-N-CA	8.35	128.98	120.38
1	K	207	VAL	N-CA-C	-8.33	96.13	108.45
1	I	139	SER	N-CA-C	-8.32	96.59	108.07
1	L	159	LEU	CA-C-O	-8.22	110.37	118.34
1	L	311	LEU	CA-C-N	8.17	128.24	119.90
1	L	311	LEU	C-N-CA	8.17	128.24	119.90
1	L	291	ASP	N-CA-C	-8.15	102.90	113.17
1	H	154	ARG	CA-C-N	8.13	131.18	120.28
1	H	154	ARG	C-N-CA	8.13	131.18	120.28
1	I	297	ILE	CA-C-O	-8.12	112.24	120.85
1	J	212	VAL	CA-C-N	8.12	131.16	120.28
1	J	212	VAL	C-N-CA	8.12	131.16	120.28
1	I	364	ARG	CA-C-O	-8.11	110.94	120.10
1	M	335	ASP	CA-C-N	8.09	132.61	120.31
1	M	335	ASP	C-N-CA	8.09	132.61	120.31
1	M	256	SER	N-CA-C	8.07	119.70	111.07
1	I	134	GLU	CA-C-N	8.06	131.53	122.83
1	I	134	GLU	C-N-CA	8.06	131.53	122.83
1	H	159	LEU	CA-C-N	8.02	127.66	119.56
1	H	159	LEU	C-N-CA	8.02	127.66	119.56
1	M	170	VAL	N-CA-C	-8.02	104.92	111.81
1	J	309	VAL	CA-C-O	-8.00	115.44	120.88
1	L	125	PRO	CA-C-N	7.98	130.98	120.28
1	L	125	PRO	C-N-CA	7.98	130.98	120.28
1	L	124	ASP	CA-C-N	7.97	127.69	119.56
1	L	124	ASP	C-N-CA	7.97	127.69	119.56
1	M	353	ALA	CA-C-N	7.95	131.71	120.42
1	M	353	ALA	C-N-CA	7.95	131.71	120.42
1	L	281	VAL	N-CA-C	-7.94	96.58	108.17
1	M	159	LEU	CA-C-N	7.93	127.49	119.24
1	M	159	LEU	C-N-CA	7.93	127.49	119.24
1	J	304	ASP	N-CA-CB	7.93	123.89	110.49
1	L	348	GLY	CA-C-N	7.92	131.68	120.28
1	L	348	GLY	C-N-CA	7.92	131.68	120.28
1	M	253	SER	N-CA-C	-7.89	103.46	113.72
1	J	254	ASP	CA-CB-CG	7.88	120.48	112.60
1	K	227	PHE	N-CA-C	7.88	119.95	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	158	GLU	N-CA-C	7.85	119.83	111.28
1	H	148	VAL	N-CA-C	-7.84	101.30	112.35
1	H	368	ALA	N-CA-C	-7.84	103.79	112.72
1	J	336	PHE	CA-CB-CG	-7.84	105.96	113.80
1	J	282	LYS	N-CA-CB	7.80	123.77	110.50
1	K	362	ALA	CA-C-N	7.79	130.53	120.56
1	K	362	ALA	C-N-CA	7.79	130.53	120.56
1	L	212	VAL	N-CA-CB	7.78	124.06	111.23
1	J	381	LYS	CA-C-N	7.77	130.35	120.56
1	J	381	LYS	C-N-CA	7.77	130.35	120.56
1	I	367	ARG	NE-CZ-NH2	-7.76	112.21	119.20
1	I	151	GLU	N-CA-CB	7.74	122.28	110.28
1	H	236	SER	O-C-N	-7.74	115.14	123.26
1	H	317	ARG	CA-C-N	7.73	131.05	120.46
1	H	317	ARG	C-N-CA	7.73	131.05	120.46
1	H	379	ILE	N-CA-C	-7.73	102.91	110.72
1	K	242	GLU	N-CA-CB	7.71	123.52	110.49
1	K	304	ASP	CB-CA-C	-7.70	96.38	110.63
1	M	215	TYR	N-CA-C	-7.69	94.43	110.80
1	I	206	VAL	N-CA-C	-7.68	97.58	108.80
1	I	142	ASP	CA-CB-CG	-7.67	104.93	112.60
1	I	328	MET	CA-C-N	7.66	131.62	120.82
1	I	328	MET	C-N-CA	7.66	131.62	120.82
1	J	341	ARG	NE-CZ-NH2	-7.63	112.33	119.20
1	H	146	LEU	CA-C-N	7.63	135.43	121.70
1	H	146	LEU	C-N-CA	7.63	135.43	121.70
1	I	281	VAL	CA-C-N	7.62	135.41	121.70
1	I	281	VAL	C-N-CA	7.62	135.41	121.70
1	M	210	GLU	N-CA-C	-7.61	104.02	113.38
1	M	360	MET	CA-C-N	7.60	130.46	120.28
1	M	360	MET	C-N-CA	7.60	130.46	120.28
1	I	133	GLU	CA-C-O	7.58	128.69	120.58
1	I	297	ILE	O-C-N	7.58	129.64	121.83
1	K	182	GLY	CA-C-N	7.58	125.19	119.66
1	K	182	GLY	C-N-CA	7.58	125.19	119.66
1	I	273	ASP	CA-C-N	7.56	128.32	120.00
1	I	273	ASP	C-N-CA	7.56	128.32	120.00
1	L	194	ALA	CB-CA-C	-7.56	99.01	110.88
1	I	142	ASP	N-CA-C	-7.55	102.98	114.16
1	J	239	PHE	CA-CB-CG	7.53	121.33	113.80
1	H	223	VAL	N-CA-C	7.53	118.30	110.62
1	H	203	PHE	CA-C-N	7.48	132.27	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	203	PHE	C-N-CA	7.48	132.27	121.80
1	L	386	THR	N-CA-C	-7.46	102.76	112.68
1	L	292	ILE	N-CA-C	-7.45	105.75	112.90
1	L	324	HIS	ND1-CE1-NE2	7.43	115.83	108.40
1	K	269	LEU	N-CA-C	7.42	126.61	110.80
1	J	138	VAL	N-CA-CB	7.39	119.02	110.82
1	M	303	PHE	CA-CB-CG	-7.38	106.42	113.80
1	M	245	ALA	N-CA-C	-7.34	101.59	113.19
1	H	361	PHE	CA-CB-CG	-7.34	106.46	113.80
1	K	315	GLU	CA-C-N	7.33	128.25	120.03
1	K	315	GLU	C-N-CA	7.33	128.25	120.03
1	K	126	MET	N-CA-C	-7.33	104.07	113.16
1	M	282	LYS	N-CA-C	-7.33	98.36	110.17
1	L	251	THR	CA-C-N	7.33	131.28	120.87
1	L	251	THR	C-N-CA	7.33	131.28	120.87
1	L	299	ARG	CA-C-O	-7.32	112.82	120.87
1	J	216	ILE	O-C-N	-7.30	115.69	123.14
1	J	252	ASN	O-C-N	-7.30	114.71	122.96
1	M	197	ASN	CA-C-N	7.29	130.65	120.29
1	M	197	ASN	C-N-CA	7.29	130.65	120.29
1	M	218	GLU	N-CA-C	-7.29	105.00	114.04
1	H	379	ILE	CA-C-N	7.28	129.91	120.44
1	H	379	ILE	C-N-CA	7.28	129.91	120.44
1	J	318	ILE	CA-C-N	7.28	130.04	120.28
1	J	318	ILE	C-N-CA	7.28	130.04	120.28
1	K	196	ALA	O-C-N	7.28	129.84	122.12
1	H	131	GLU	O-C-N	-7.27	114.96	123.25
1	I	218	GLU	CA-C-O	-7.27	112.71	120.42
1	K	146	LEU	CA-C-N	7.27	130.02	120.28
1	K	146	LEU	C-N-CA	7.27	130.02	120.28
1	K	206	VAL	N-CA-C	-7.26	99.68	108.53
1	J	291	ASP	N-CA-C	-7.21	103.80	112.59
1	K	319	GLN	CA-C-N	7.20	129.63	120.56
1	K	319	GLN	C-N-CA	7.20	129.63	120.56
1	M	220	ALA	CA-C-N	7.20	130.51	120.29
1	M	220	ALA	C-N-CA	7.20	130.51	120.29
1	J	154	ARG	CA-C-N	7.17	129.90	120.28
1	J	154	ARG	C-N-CA	7.17	129.90	120.28
1	J	142	ASP	N-CA-C	-7.17	101.84	110.44
1	L	366	GLU	N-CA-CB	7.15	122.58	110.49
1	L	174	PRO	CA-C-N	7.13	128.75	119.84
1	L	174	PRO	C-N-CA	7.13	128.75	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	367	ARG	N-CA-C	-7.12	98.12	109.59
1	J	303	PHE	CA-CB-CG	-7.12	106.68	113.80
1	I	324	HIS	CA-C-N	7.11	129.81	120.28
1	I	324	HIS	C-N-CA	7.11	129.81	120.28
1	K	302	ARG	N-CA-C	-7.11	95.65	110.80
1	L	378	ALA	CA-C-N	7.11	129.51	120.56
1	L	378	ALA	C-N-CA	7.11	129.51	120.56
1	M	203	PHE	N-CA-CB	7.10	121.73	110.23
1	L	382	VAL	CA-C-O	-7.09	113.18	121.05
1	J	322	LYS	CB-CA-C	-7.09	99.76	110.88
1	K	195	VAL	CA-C-N	7.08	129.77	120.28
1	K	195	VAL	C-N-CA	7.08	129.77	120.28
1	H	341	ARG	CA-C-N	7.08	130.47	120.42
1	H	341	ARG	C-N-CA	7.08	130.47	120.42
1	L	204	ILE	O-C-N	-7.07	115.42	122.99
1	J	146	LEU	N-CA-CB	7.07	122.53	110.50
1	H	355	CYS	N-CA-C	7.07	118.63	111.07
1	K	207	VAL	N-CA-CB	7.05	123.01	111.45
1	M	309	VAL	CB-CA-C	7.02	119.32	111.04
1	K	253	SER	N-CA-C	-6.98	97.59	109.24
1	H	194	ALA	CA-C-N	6.97	130.02	120.46
1	H	194	ALA	C-N-CA	6.97	130.02	120.46
1	I	314	PHE	CA-C-N	6.97	130.19	120.29
1	I	314	PHE	C-N-CA	6.97	130.19	120.29
1	H	250	ARG	NE-CZ-NH1	6.94	128.44	121.50
1	J	340	ALA	N-CA-CB	6.94	120.33	110.12
1	H	219	GLY	N-CA-C	-6.94	96.73	113.18
1	M	317	ARG	NH1-CZ-NH2	6.94	128.32	119.30
1	K	359	GLY	O-C-N	6.93	129.58	122.24
1	M	251	THR	O-C-N	6.93	131.38	123.27
1	J	217	GLY	N-CA-C	-6.93	106.15	115.36
1	I	361	PHE	N-CA-CB	6.92	120.30	110.12
1	L	163	LYS	CA-C-N	6.92	126.73	119.05
1	L	163	LYS	C-N-CA	6.92	126.73	119.05
1	L	282	LYS	N-CA-CB	6.92	122.26	110.50
1	M	358	ALA	CA-C-N	6.90	128.99	120.22
1	M	358	ALA	C-N-CA	6.90	128.99	120.22
1	L	320	ILE	CA-C-N	6.90	129.41	120.44
1	L	320	ILE	C-N-CA	6.90	129.41	120.44
1	K	205	ARG	NE-CZ-NH2	-6.89	113.00	119.20
1	H	226	VAL	N-CA-CB	6.88	119.90	110.54
1	J	194	ALA	N-CA-C	-6.87	103.87	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	316	GLY	CA-C-N	6.87	129.48	120.28
1	J	316	GLY	C-N-CA	6.87	129.48	120.28
1	H	338	GLU	CB-CG-CD	-6.87	100.93	112.60
1	M	387	THR	N-CA-C	-6.86	101.43	110.07
1	I	251	THR	O-C-N	-6.84	113.49	122.59
1	L	337	LYS	CA-C-N	6.81	129.41	120.28
1	L	337	LYS	C-N-CA	6.81	129.41	120.28
1	H	275	PHE	CA-CB-CG	6.81	120.61	113.80
1	L	205	ARG	NE-CZ-NH1	-6.81	114.69	121.50
1	H	185	GLY	N-CA-C	-6.80	106.07	114.92
1	H	236	SER	N-CA-C	-6.80	98.67	108.60
1	H	176	LYS	N-CA-CB	6.80	120.22	110.16
1	M	174	PRO	N-CA-C	6.79	118.98	110.70
1	J	217	GLY	CA-C-N	6.79	129.93	120.29
1	J	217	GLY	C-N-CA	6.79	129.93	120.29
1	K	134	GLU	CA-C-O	-6.79	110.81	120.51
1	L	273	ASP	CA-C-N	6.77	127.32	119.94
1	L	273	ASP	C-N-CA	6.77	127.32	119.94
1	J	195	VAL	CA-C-N	6.75	129.33	120.28
1	J	195	VAL	C-N-CA	6.75	129.33	120.28
1	H	224	ARG	CA-C-N	6.75	129.32	120.28
1	H	224	ARG	C-N-CA	6.75	129.32	120.28
1	L	382	VAL	N-CA-C	-6.75	104.19	110.53
1	M	372	MET	N-CA-C	-6.75	105.18	113.41
1	I	252	ASN	OD1-CG-ND2	6.74	129.34	122.60
1	I	183	PRO	N-CA-C	6.74	118.92	110.70
1	K	125	PRO	N-CA-C	-6.74	106.06	114.68
1	M	230	ALA	N-CA-C	6.74	118.70	111.36
1	K	218	GLU	N-CA-C	-6.73	104.01	111.82
1	J	281	VAL	CA-C-N	6.72	133.80	121.70
1	J	281	VAL	C-N-CA	6.72	133.80	121.70
1	M	203	PHE	N-CA-C	-6.72	98.67	109.96
1	K	303	PHE	N-CA-CB	6.72	121.84	110.49
1	L	334	VAL	CA-C-O	-6.70	112.40	120.78
1	I	173	GLU	N-CA-C	-6.70	99.19	109.64
1	L	160	PRO	CA-C-N	6.69	129.79	120.29
1	L	160	PRO	C-N-CA	6.69	129.79	120.29
1	M	256	SER	CA-C-N	6.69	127.40	119.98
1	M	256	SER	C-N-CA	6.69	127.40	119.98
1	J	163	LYS	CA-C-N	6.67	126.27	119.19
1	J	163	LYS	C-N-CA	6.67	126.27	119.19
1	K	353	ALA	CA-C-N	6.66	128.95	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	353	ALA	C-N-CA	6.66	128.95	120.56
1	K	199	THR	N-CA-C	-6.66	104.87	114.12
1	J	124	ASP	CA-C-O	-6.66	113.48	121.00
1	K	173	GLU	CB-CA-C	-6.65	99.48	109.26
1	L	333	ASP	CA-C-N	6.65	133.94	121.97
1	L	333	ASP	C-N-CA	6.65	133.94	121.97
1	J	309	VAL	CA-C-N	6.65	128.15	119.84
1	J	309	VAL	C-N-CA	6.65	128.15	119.84
1	J	228	GLN	N-CA-CB	6.64	119.99	110.16
1	J	317	ARG	CA-C-O	6.64	127.59	120.55
1	L	283	VAL	CA-C-N	6.63	133.64	121.70
1	L	283	VAL	C-N-CA	6.63	133.64	121.70
1	J	228	GLN	CA-C-N	6.62	129.16	120.28
1	J	228	GLN	C-N-CA	6.62	129.16	120.28
1	K	215	TYR	CB-CA-C	-6.62	99.86	111.05
1	M	156	ALA	CA-C-O	-6.62	113.88	120.70
1	H	305	ARG	O-C-N	-6.61	114.40	123.12
1	K	240	ILE	CA-C-N	-6.61	113.60	122.72
1	K	240	ILE	C-N-CA	-6.61	113.60	122.72
1	J	309	VAL	N-CA-CB	6.60	118.16	111.36
1	H	205	ARG	N-CA-C	-6.60	97.77	108.52
1	H	324	HIS	CG-CD2-NE2	6.60	113.80	107.20
1	I	205	ARG	N-CA-C	-6.59	97.78	108.52
1	M	169	GLU	CB-CA-C	-6.59	99.64	110.85
1	I	256	SER	N-CA-C	6.59	119.06	111.02
1	K	313	THR	CA-C-N	6.58	128.99	120.44
1	K	313	THR	C-N-CA	6.58	128.99	120.44
1	J	149	GLN	N-CA-CB	6.58	119.79	110.12
1	H	379	ILE	O-C-N	-6.57	115.07	121.83
1	L	345	GLY	N-CA-C	-6.57	105.24	116.01
1	M	277	PRO	N-CA-C	-6.56	105.41	114.27
1	I	144	GLY	N-CA-C	-6.55	97.65	113.18
1	J	178	VAL	N-CA-CB	6.55	120.15	111.64
1	M	322	LYS	CA-C-N	6.55	129.43	120.46
1	M	322	LYS	C-N-CA	6.55	129.43	120.46
1	M	206	VAL	N-CA-C	-6.54	98.19	107.75
1	J	263	ARG	CA-C-N	6.54	130.26	120.31
1	J	263	ARG	C-N-CA	6.54	130.26	120.31
1	I	367	ARG	NE-CZ-NH1	6.53	128.03	121.50
1	J	322	LYS	N-CA-CB	6.53	119.48	110.01
1	J	224	ARG	NE-CZ-NH2	6.52	125.07	119.20
1	H	252	ASN	CA-C-N	6.52	133.43	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	252	ASN	C-N-CA	6.52	133.43	121.70
1	I	377	LYS	CA-C-N	6.50	128.99	120.28
1	I	377	LYS	C-N-CA	6.50	128.99	120.28
1	J	380	GLU	CA-C-O	-6.49	113.67	120.55
1	L	227	PHE	N-CA-C	6.46	118.33	111.28
1	H	194	ALA	N-CA-C	6.46	118.32	111.28
1	L	290	ILE	CA-C-O	6.45	125.08	118.96
1	H	376	THR	CA-C-O	6.45	127.38	120.55
1	K	387	THR	CA-C-N	6.44	127.89	119.84
1	K	387	THR	C-N-CA	6.44	127.89	119.84
1	I	321	PHE	CA-C-N	6.44	128.91	120.28
1	I	321	PHE	C-N-CA	6.44	128.91	120.28
1	K	143	ILE	N-CA-C	-6.43	98.47	108.44
1	L	167	PHE	N-CA-C	-6.43	103.51	112.45
1	K	169	GLU	N-CA-CB	6.43	119.67	110.16
1	J	127	VAL	CA-C-N	6.42	133.81	121.54
1	J	127	VAL	C-N-CA	6.42	133.81	121.54
1	M	259	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	K	173	GLU	CA-C-N	6.41	126.98	120.38
1	K	173	GLU	C-N-CA	6.41	126.98	120.38
1	M	274	GLY	O-C-N	6.41	129.03	122.24
1	I	289	ARG	CA-C-N	6.41	128.76	120.56
1	I	289	ARG	C-N-CA	6.41	128.76	120.56
1	L	358	ALA	CA-C-N	6.39	127.03	120.00
1	L	358	ALA	C-N-CA	6.39	127.03	120.00
1	J	194	ALA	CA-C-N	6.38	129.21	120.46
1	J	194	ALA	C-N-CA	6.38	129.21	120.46
1	K	225	GLU	CA-C-N	6.37	128.59	120.56
1	K	225	GLU	C-N-CA	6.37	128.59	120.56
1	M	333	ASP	CA-CB-CG	-6.37	106.23	112.60
1	H	272	LEU	CA-C-N	6.36	128.80	120.28
1	H	272	LEU	C-N-CA	6.36	128.80	120.28
1	L	160	PRO	N-CD-CG	6.36	112.73	103.20
1	H	231	LYS	O-C-N	6.35	128.85	122.12
1	K	269	LEU	CB-CA-C	-6.35	97.79	110.42
1	I	333	ASP	N-CA-C	-6.34	105.30	113.16
1	J	161	LEU	CB-CA-C	-6.34	100.88	110.90
1	M	226	VAL	CA-CB-CG2	6.33	121.16	110.40
1	H	343	THR	N-CA-CB	6.33	120.12	110.70
1	K	219	GLY	CA-C-N	6.32	129.04	120.44
1	K	219	GLY	C-N-CA	6.32	129.04	120.44
1	I	249	ARG	NE-CZ-NH1	-6.32	115.18	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	336	PHE	CA-C-N	6.32	129.26	120.29
1	M	336	PHE	C-N-CA	6.32	129.26	120.29
1	L	270	ALA	N-CA-CB	6.31	119.17	110.01
1	K	225	GLU	O-C-N	-6.31	115.57	122.07
1	L	234	ALA	CA-C-O	-6.31	113.61	120.17
1	L	229	LEU	CA-C-N	6.31	129.36	120.28
1	L	229	LEU	C-N-CA	6.31	129.36	120.28
1	H	236	SER	CA-C-N	6.30	133.04	121.70
1	H	236	SER	C-N-CA	6.30	133.04	121.70
1	J	214	LYS	CG-CD-CE	6.30	125.79	111.30
1	H	144	GLY	CA-C-N	6.30	125.97	119.92
1	H	144	GLY	C-N-CA	6.30	125.97	119.92
1	L	262	GLN	N-CA-CB	6.29	119.37	110.12
1	K	221	ARG	CA-C-N	6.29	128.70	120.28
1	K	221	ARG	C-N-CA	6.29	128.70	120.28
1	K	321	PHE	N-CA-CB	6.28	119.29	109.94
1	M	302	ARG	N-CA-C	-6.27	97.44	110.80
1	H	179	LEU	N-CA-C	-6.27	99.50	109.59
1	K	295	PRO	N-CA-CB	6.27	109.29	103.46
1	H	190	LEU	CA-C-N	6.26	129.82	120.31
1	H	190	LEU	C-N-CA	6.26	129.82	120.31
1	H	236	SER	CA-C-O	-6.26	114.75	121.38
1	L	164	PRO	O-C-N	6.25	129.73	122.23
1	J	288	ASN	OD1-CG-ND2	6.25	128.85	122.60
1	H	335	ASP	CA-C-N	6.25	129.80	120.31
1	H	335	ASP	C-N-CA	6.25	129.80	120.31
1	M	317	ARG	NE-CZ-NH2	-6.24	113.58	119.20
1	L	339	LEU	CA-C-N	6.24	128.64	120.28
1	L	339	LEU	C-N-CA	6.24	128.64	120.28
1	I	375	PHE	CA-C-O	-6.24	113.81	120.42
1	L	217	GLY	O-C-N	-6.24	114.51	122.43
1	H	310	PRO	O-C-N	6.23	130.51	123.04
1	H	204	ILE	CB-CA-C	6.22	118.36	111.08
1	I	368	ALA	N-CA-C	-6.22	105.33	113.17
1	K	145	GLY	CA-C-N	6.22	133.86	122.54
1	K	145	GLY	C-N-CA	6.22	133.86	122.54
1	L	261	VAL	CA-C-N	6.22	128.61	120.28
1	L	261	VAL	C-N-CA	6.22	128.61	120.28
1	K	351	ILE	N-CA-C	6.21	116.96	110.62
1	I	349	ALA	CA-C-O	-6.21	113.97	120.55
1	M	299	ARG	CA-C-N	6.21	126.22	119.89
1	M	299	ARG	C-N-CA	6.21	126.22	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	283	VAL	CA-C-N	6.20	131.05	122.93
1	K	283	VAL	C-N-CA	6.20	131.05	122.93
1	I	231	LYS	N-CA-C	-6.20	104.63	111.82
1	M	293	LEU	CA-C-N	6.20	129.29	120.49
1	M	293	LEU	C-N-CA	6.20	129.29	120.49
1	K	336	PHE	CA-CB-CG	-6.19	107.61	113.80
1	I	341	ARG	NE-CZ-NH2	-6.18	113.63	119.20
1	H	257	GLY	CA-C-N	6.18	128.84	120.44
1	H	257	GLY	C-N-CA	6.18	128.84	120.44
1	K	364	ARG	N-CA-CB	6.18	119.20	110.12
1	I	247	ALA	N-CA-CB	6.18	120.93	110.49
1	J	145	GLY	CA-C-N	6.18	132.82	121.70
1	J	145	GLY	C-N-CA	6.18	132.82	121.70
1	J	187	GLY	N-CA-C	-6.18	98.54	113.18
1	M	365	GLU	CA-C-O	6.17	126.90	119.43
1	M	305	ARG	NE-CZ-NH2	6.16	124.74	119.20
1	K	294	ASP	O-C-N	-6.15	114.96	121.30
1	H	139	SER	N-CA-CB	-6.15	101.83	111.05
1	L	158	GLU	CA-C-N	6.15	127.78	120.09
1	L	158	GLU	C-N-CA	6.15	127.78	120.09
1	M	383	LEU	CA-C-O	-6.14	113.91	120.42
1	L	371	THR	CA-C-N	6.13	128.78	120.38
1	L	371	THR	C-N-CA	6.13	128.78	120.38
1	I	190	LEU	CA-C-N	6.13	128.50	120.28
1	I	190	LEU	C-N-CA	6.13	128.50	120.28
1	I	266	MET	CA-C-N	6.13	128.50	120.28
1	I	266	MET	C-N-CA	6.13	128.50	120.28
1	I	199	THR	N-CA-CB	6.13	118.90	110.01
1	L	367	ARG	NE-CZ-NH1	6.13	127.63	121.50
1	M	324	HIS	CA-CB-CG	-6.13	107.67	113.80
1	I	291	ASP	N-CA-C	-6.13	98.09	108.26
1	M	128	TYR	N-CA-C	-6.13	100.03	109.52
1	H	366	GLU	N-CA-CB	6.12	120.84	110.49
1	M	198	GLN	CB-CA-C	-6.12	100.44	110.85
1	M	338	GLU	N-CA-C	-6.12	104.16	111.69
1	I	323	ILE	N-CA-C	-6.12	104.54	110.72
1	M	224	ARG	CA-C-N	6.11	128.79	120.54
1	M	224	ARG	C-N-CA	6.11	128.79	120.54
1	J	124	ASP	CA-C-N	6.11	127.48	119.84
1	J	124	ASP	C-N-CA	6.11	127.48	119.84
1	H	242	GLU	N-CA-C	-6.11	98.31	108.75
1	H	386	THR	N-CA-C	-6.11	100.14	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	197	ASN	OD1-CG-ND2	6.10	128.70	122.60
1	H	303	PHE	CA-CB-CG	-6.10	107.70	113.80
1	I	218	GLU	CA-C-N	6.09	126.87	119.99
1	I	218	GLU	C-N-CA	6.09	126.87	119.99
1	M	312	PRO	N-CA-CB	-6.08	97.90	103.25
1	L	170	VAL	O-C-N	6.08	128.28	122.20
1	L	331	ALA	N-CA-C	-6.08	102.94	110.41
1	K	328	MET	CA-C-O	6.08	129.00	121.89
1	I	362	ALA	O-C-N	6.07	128.56	122.12
1	J	290	ILE	CA-C-O	6.07	125.92	119.91
1	L	157	VAL	CA-C-O	-6.07	114.90	120.73
1	J	290	ILE	CA-C-N	6.07	132.32	122.67
1	J	290	ILE	C-N-CA	6.07	132.32	122.67
1	M	331	ALA	O-C-N	-6.07	116.17	123.27
1	K	294	ASP	CA-C-N	6.06	125.76	119.64
1	K	294	ASP	C-N-CA	6.06	125.76	119.64
1	J	224	ARG	N-CA-CB	6.06	119.12	110.16
1	K	361	PHE	CB-CG-CD1	6.05	130.99	120.70
1	J	173	GLU	CA-C-O	6.05	123.80	119.32
1	K	203	PHE	N-CA-C	-6.04	97.86	108.20
1	J	340	ALA	N-CA-C	6.04	117.86	111.28
1	L	283	VAL	O-C-N	-6.03	116.81	123.20
1	J	209	SER	N-CA-C	-6.03	97.95	110.80
1	I	372	MET	CA-C-N	6.03	129.47	120.31
1	I	372	MET	C-N-CA	6.03	129.47	120.31
1	I	128	TYR	O-C-N	6.02	128.27	122.07
1	L	168	ALA	CA-C-N	6.02	128.35	120.28
1	L	168	ALA	C-N-CA	6.02	128.35	120.28
1	L	359	GLY	O-C-N	6.02	128.03	122.19
1	J	239	PHE	N-CA-CB	6.02	120.23	110.42
1	I	152	GLU	N-CA-CB	6.01	119.06	110.16
1	H	230	ALA	CA-C-O	-6.01	114.51	120.82
1	K	150	ILE	N-CA-CB	6.01	117.58	110.55
1	I	263	ARG	CA-C-N	6.00	128.81	120.29
1	I	263	ARG	C-N-CA	6.00	128.81	120.29
1	K	264	THR	CA-C-N	5.99	128.23	120.44
1	K	264	THR	C-N-CA	5.99	128.23	120.44
1	L	280	ASP	N-CA-C	-5.99	98.05	110.80
1	M	244	ASP	CA-CB-CG	5.99	118.59	112.60
1	H	243	LEU	N-CA-C	-5.99	104.63	112.41
1	H	376	THR	N-CA-CB	5.99	118.92	110.12
1	L	167	PHE	CA-CB-CG	-5.99	107.81	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	195	VAL	CA-C-N	5.98	128.30	120.28
1	M	195	VAL	C-N-CA	5.98	128.30	120.28
1	H	252	ASN	CA-CB-CG	-5.97	106.63	112.60
1	I	221	ARG	CA-C-N	5.97	128.78	120.29
1	I	221	ARG	C-N-CA	5.97	128.78	120.29
1	M	178	VAL	N-CA-C	-5.97	99.56	108.46
1	I	287	THR	CA-CB-OG1	5.97	118.56	109.60
1	H	208	GLY	CA-C-N	5.96	131.58	121.14
1	H	208	GLY	C-N-CA	5.96	131.58	121.14
1	M	248	ALA	CA-C-N	5.96	131.82	120.97
1	M	248	ALA	C-N-CA	5.96	131.82	120.97
1	M	142	ASP	CA-C-O	5.96	126.32	119.35
1	K	337	LYS	CA-C-N	5.96	128.75	120.29
1	K	337	LYS	C-N-CA	5.96	128.75	120.29
1	L	319	GLN	CA-C-N	5.96	128.88	120.42
1	L	319	GLN	C-N-CA	5.96	128.88	120.42
1	L	324	HIS	CE1-NE2-CD2	-5.96	103.04	109.00
1	J	212	VAL	CA-C-O	5.96	128.22	120.78
1	I	354	ILE	CA-C-N	5.95	128.18	120.44
1	I	354	ILE	C-N-CA	5.95	128.18	120.44
1	M	158	GLU	CA-C-O	-5.95	114.53	121.07
1	I	253	SER	O-C-N	-5.95	115.70	123.02
1	I	242	GLU	CB-CA-C	-5.94	101.65	110.62
1	M	273	ASP	CA-C-N	5.94	127.57	120.14
1	M	273	ASP	C-N-CA	5.94	127.57	120.14
1	K	192	ALA	N-CA-C	5.92	117.82	111.36
1	J	190	LEU	CA-C-N	5.92	132.85	121.54
1	J	190	LEU	C-N-CA	5.92	132.85	121.54
1	K	357	GLU	N-CA-CB	5.92	118.92	110.16
1	K	306	ILE	N-CA-C	-5.91	97.89	106.88
1	H	189	THR	N-CA-C	-5.91	105.56	112.89
1	J	253	SER	CA-C-N	5.91	132.34	121.70
1	J	253	SER	C-N-CA	5.91	132.34	121.70
1	H	357	GLU	CA-C-N	5.90	128.67	120.29
1	H	357	GLU	C-N-CA	5.90	128.67	120.29
1	H	314	PHE	CB-CG-CD2	-5.89	110.68	120.70
1	K	326	ARG	N-CA-C	-5.89	104.86	111.28
1	L	249	ARG	N-CA-C	-5.89	99.80	109.40
1	J	384	LYS	CA-C-O	5.88	126.79	120.55
1	K	387	THR	CB-CA-C	-5.88	101.93	109.92
1	H	387	THR	CA-C-O	-5.87	112.11	120.16
1	M	329	LYS	CA-C-N	5.87	132.76	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	329	LYS	C-N-CA	5.87	132.76	121.54
1	K	343	THR	N-CA-CB	5.87	118.66	110.56
1	M	315	GLU	CA-C-N	5.87	126.46	119.94
1	M	315	GLU	C-N-CA	5.87	126.46	119.94
1	M	336	PHE	CA-CB-CG	-5.87	107.93	113.80
1	I	281	VAL	O-C-N	-5.87	117.02	123.18
1	M	205	ARG	NH1-CZ-NH2	-5.87	111.67	119.30
1	I	204	ILE	O-C-N	-5.86	116.26	122.83
1	J	192	ALA	N-CA-C	5.86	117.34	111.07
1	M	312	PRO	N-CA-C	5.86	120.41	111.15
1	L	253	SER	O-C-N	5.86	130.38	122.59
1	M	187	GLY	CA-C-N	5.86	129.22	120.31
1	M	187	GLY	C-N-CA	5.86	129.22	120.31
1	M	305	ARG	N-CA-CB	5.86	121.11	111.62
1	H	211	PHE	N-CA-C	-5.85	104.26	111.40
1	K	206	VAL	O-C-N	-5.85	116.55	122.75
1	H	384	LYS	N-CA-C	5.85	117.65	111.28
1	H	255	THR	N-CA-CB	5.85	120.37	110.49
1	K	216	ILE	CA-C-O	5.85	128.09	120.78
1	J	350	ASP	CB-CA-C	-5.84	101.71	110.88
1	J	136	PRO	CA-C-N	5.84	132.21	121.70
1	J	136	PRO	C-N-CA	5.84	132.21	121.70
1	J	321	PHE	CA-C-N	5.84	128.03	120.44
1	J	321	PHE	C-N-CA	5.84	128.03	120.44
1	I	254	ASP	N-CA-C	-5.84	103.97	113.19
1	K	163	LYS	O-C-N	-5.84	114.61	121.32
1	M	158	GLU	O-C-N	5.83	128.32	122.08
1	K	142	ASP	N-CA-C	-5.83	105.47	112.59
1	L	167	PHE	CA-C-N	5.83	128.10	120.28
1	L	167	PHE	C-N-CA	5.83	128.10	120.28
1	L	182	GLY	CA-C-N	5.83	126.38	120.38
1	L	182	GLY	C-N-CA	5.83	126.38	120.38
1	M	325	THR	CA-C-N	5.82	129.56	120.82
1	M	325	THR	C-N-CA	5.82	129.56	120.82
1	J	154	ARG	N-CA-CB	5.82	118.68	110.12
1	I	379	ILE	N-CA-CB	5.82	118.45	110.54
1	L	304	ASP	CA-CB-CG	5.82	118.42	112.60
1	L	200	ARG	CB-CA-C	5.81	121.98	110.42
1	J	312	PRO	N-CD-CG	5.81	111.92	103.20
1	H	149	GLN	OE1-CD-NE2	5.80	128.40	122.60
1	K	365	GLU	CA-C-N	5.80	130.40	122.34
1	K	365	GLU	C-N-CA	5.80	130.40	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	306	ILE	N-CA-C	-5.80	99.42	108.81
1	J	261	VAL	CA-C-O	-5.79	114.71	120.85
1	M	349	ALA	N-CA-C	-5.79	105.04	111.36
1	L	224	ARG	CA-C-N	5.79	128.51	120.29
1	L	224	ARG	C-N-CA	5.79	128.51	120.29
1	H	348	GLY	O-C-N	5.78	128.58	122.28
1	K	124	ASP	O-C-N	5.78	126.53	121.39
1	K	278	ARG	CA-C-N	5.78	130.01	120.25
1	K	278	ARG	C-N-CA	5.78	130.01	120.25
1	H	382	VAL	CA-C-N	5.78	128.02	120.28
1	H	382	VAL	C-N-CA	5.78	128.02	120.28
1	H	274	GLY	N-CA-C	-5.77	106.65	115.66
1	K	248	ALA	CA-C-O	-5.77	113.44	120.54
1	K	133	GLU	CA-C-N	5.77	132.57	121.54
1	K	133	GLU	C-N-CA	5.77	132.57	121.54
1	M	386	THR	N-CA-C	-5.76	105.92	113.12
1	K	134	GLU	O-C-N	5.76	130.25	122.59
1	L	374	ASP	CA-CB-CG	-5.76	106.84	112.60
1	I	321	PHE	N-CA-CB	5.76	118.58	110.12
1	I	182	GLY	N-CA-C	-5.75	100.60	112.34
1	M	297	ILE	CA-C-O	5.75	125.60	119.91
1	L	192	ALA	N-CA-C	5.75	117.54	111.28
1	I	146	LEU	CA-C-N	5.75	132.04	121.70
1	I	146	LEU	C-N-CA	5.75	132.04	121.70
1	H	173	GLU	CA-C-O	-5.74	112.30	119.54
1	L	172	ILE	CA-CB-CG2	-5.74	100.74	110.50
1	J	152	GLU	CB-CG-CD	5.74	122.35	112.60
1	H	228	GLN	CA-C-N	5.74	127.97	120.28
1	H	228	GLN	C-N-CA	5.74	127.97	120.28
1	I	258	ASP	N-CA-C	-5.73	105.11	111.36
1	M	259	ARG	CD-NE-CZ	-5.73	116.38	124.40
1	M	222	LEU	CA-C-N	5.71	128.29	120.46
1	M	222	LEU	C-N-CA	5.71	128.29	120.46
1	J	242	GLU	CA-C-N	5.71	128.99	120.31
1	J	242	GLU	C-N-CA	5.71	128.99	120.31
1	L	302	ARG	O-C-N	5.71	128.45	122.23
1	K	158	GLU	N-CA-C	5.71	117.18	111.07
1	L	375	PHE	N-CA-CB	5.71	118.24	109.91
1	M	180	LEU	CA-C-O	-5.70	114.47	120.80
1	M	298	LEU	CA-C-N	5.70	129.53	121.61
1	M	298	LEU	C-N-CA	5.70	129.53	121.61
1	J	314	PHE	O-C-N	5.70	127.94	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	311	LEU	CA-C-N	5.70	125.71	119.90
1	J	311	LEU	C-N-CA	5.70	125.71	119.90
1	I	179	LEU	CA-C-O	-5.70	114.17	120.38
1	L	250	ARG	N-CA-C	-5.70	104.99	111.14
1	L	277	PRO	CA-C-N	5.69	127.84	120.44
1	L	277	PRO	C-N-CA	5.69	127.84	120.44
1	I	285	GLY	N-CA-C	5.69	121.57	112.58
1	K	335	ASP	N-CA-C	-5.69	99.14	108.41
1	I	141	GLU	N-CA-C	-5.69	105.02	112.41
1	K	266	MET	N-CA-CB	5.69	118.98	110.22
1	K	134	GLU	N-CA-CB	5.69	120.10	110.49
1	M	383	LEU	O-C-N	5.68	128.63	122.15
1	L	189	THR	CB-CA-C	-5.68	101.36	110.79
1	J	290	ILE	N-CA-C	-5.68	106.77	112.17
1	I	126	MET	CA-C-N	5.68	129.94	121.77
1	I	126	MET	C-N-CA	5.68	129.94	121.77
1	L	364	ARG	NH1-CZ-NH2	5.68	126.68	119.30
1	L	300	PRO	O-C-N	5.67	129.98	122.89
1	H	220	ALA	CA-C-N	5.65	128.13	120.38
1	H	220	ALA	C-N-CA	5.65	128.13	120.38
1	J	355	CYS	O-C-N	5.65	128.11	122.12
1	L	131	GLU	CA-C-N	5.65	132.13	121.97
1	L	131	GLU	C-N-CA	5.65	132.13	121.97
1	J	212	VAL	O-C-N	-5.64	115.52	122.57
1	M	205	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	K	311	LEU	N-CA-CB	5.64	118.34	110.11
1	K	233	LYS	CA-C-N	5.63	129.21	120.60
1	K	233	LYS	C-N-CA	5.63	129.21	120.60
1	I	243	LEU	CA-C-N	5.63	130.12	120.72
1	I	243	LEU	C-N-CA	5.63	130.12	120.72
1	L	161	LEU	N-CA-C	-5.63	105.23	111.36
1	L	374	ASP	CA-C-N	5.61	128.06	120.65
1	L	374	ASP	C-N-CA	5.61	128.06	120.65
1	H	292	ILE	N-CA-C	-5.61	107.28	112.83
1	H	324	HIS	CE1-NE2-CD2	-5.61	103.39	109.00
1	I	192	ALA	CA-C-O	5.61	126.50	120.55
1	K	228	GLN	CA-CB-CG	5.60	125.31	114.10
1	H	314	PHE	CA-C-O	5.60	126.68	120.63
1	L	317	ARG	CB-CA-C	-5.59	102.10	110.88
1	J	199	THR	O-C-N	5.59	128.13	122.09
1	I	381	LYS	CB-CG-CD	5.58	124.15	111.30
1	K	230	ALA	CA-C-N	5.58	128.03	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	230	ALA	C-N-CA	5.58	128.03	120.44
1	L	369	LYS	N-CA-C	-5.58	99.20	108.75
1	I	172	ILE	CA-CB-CG2	-5.58	101.02	110.50
1	L	157	VAL	O-C-N	5.57	126.94	121.98
1	L	376	THR	N-CA-CB	5.57	118.30	110.12
1	H	167	PHE	CA-CB-CG	-5.56	108.24	113.80
1	M	203	PHE	CA-CB-CG	5.56	119.36	113.80
1	H	179	LEU	N-CA-CB	5.56	119.64	110.69
1	M	264	THR	CA-C-N	5.56	128.18	120.29
1	M	264	THR	C-N-CA	5.56	128.18	120.29
1	L	364	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	L	378	ALA	O-C-N	-5.55	116.23	122.12
1	H	372	MET	N-CA-C	5.55	117.41	111.36
1	H	243	LEU	CA-C-N	5.55	128.04	120.54
1	H	243	LEU	C-N-CA	5.55	128.04	120.54
1	H	152	GLU	CA-C-N	5.55	128.30	120.42
1	H	152	GLU	C-N-CA	5.55	128.30	120.42
1	K	378	ALA	CA-C-N	5.54	128.29	120.42
1	K	378	ALA	C-N-CA	5.54	128.29	120.42
1	L	340	ALA	N-CA-C	5.54	117.32	111.28
1	H	319	GLN	N-CA-C	5.54	117.40	111.36
1	K	264	THR	N-CA-C	-5.54	107.07	113.88
1	M	226	VAL	CA-CB-CG1	-5.53	100.99	110.40
1	H	237	ILE	N-CA-CB	5.53	120.91	111.50
1	H	386	THR	O-C-N	5.53	128.91	122.99
1	L	125	PRO	CB-CA-C	5.53	119.70	111.85
1	H	386	THR	CA-C-O	-5.53	115.40	121.31
1	J	154	ARG	O-C-N	-5.53	116.26	122.12
1	L	387	THR	O-C-N	-5.53	116.47	121.66
1	H	262	GLN	CA-C-N	5.52	127.62	120.44
1	H	262	GLN	C-N-CA	5.52	127.62	120.44
1	I	243	LEU	CA-C-O	5.51	126.33	120.10
1	J	266	MET	O-C-N	5.51	129.05	122.27
1	H	312	PRO	CB-CA-C	5.51	118.16	110.17
1	I	245	ALA	CA-C-N	5.51	130.30	122.09
1	I	245	ALA	C-N-CA	5.51	130.30	122.09
1	I	378	ALA	N-CA-C	5.51	117.28	111.28
1	K	125	PRO	CA-C-O	5.50	123.58	118.29
1	K	224	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	H	183	PRO	CA-C-N	5.50	125.42	119.76
1	H	183	PRO	C-N-CA	5.50	125.42	119.76
1	M	309	VAL	N-CA-C	-5.50	102.11	107.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	315	GLU	CA-C-N	5.50	126.04	120.00
1	I	315	GLU	C-N-CA	5.50	126.04	120.00
1	L	224	ARG	CD-NE-CZ	5.50	132.09	124.40
1	H	156	ALA	N-CA-C	5.49	117.35	111.36
1	I	151	GLU	O-C-N	5.49	129.02	122.27
1	I	321	PHE	N-CA-C	-5.49	105.30	111.28
1	K	176	LYS	CA-CB-CG	-5.49	103.13	114.10
1	M	229	LEU	N-CA-CB	5.49	118.18	110.12
1	H	286	ALA	N-CA-C	-5.48	100.60	108.60
1	I	340	ALA	CB-CA-C	-5.47	101.55	110.85
1	L	153	ILE	CA-C-N	5.47	127.61	120.28
1	L	153	ILE	C-N-CA	5.47	127.61	120.28
1	I	314	PHE	O-C-N	-5.47	116.32	122.12
1	K	314	PHE	CA-C-N	5.47	128.05	120.29
1	K	314	PHE	C-N-CA	5.47	128.05	120.29
1	J	343	THR	CA-CB-OG1	5.47	117.80	109.60
1	M	164	PRO	N-CA-C	-5.46	107.52	114.35
1	L	132	VAL	CA-C-N	5.46	133.20	122.61
1	L	132	VAL	C-N-CA	5.46	133.20	122.61
1	H	232	GLU	N-CA-CB	5.46	118.51	110.33
1	J	338	GLU	N-CA-CB	5.46	118.24	110.16
1	I	164	PRO	CA-C-N	5.45	127.58	120.28
1	I	164	PRO	C-N-CA	5.45	127.58	120.28
1	L	300	PRO	CA-C-O	-5.45	113.89	121.90
1	J	241	ASP	N-CA-CB	5.45	118.75	109.87
1	I	215	TYR	CA-C-O	5.44	127.55	121.40
1	J	256	SER	CA-C-O	5.44	125.66	119.18
1	H	313	THR	N-CA-CB	5.44	118.03	110.26
1	H	356	THR	N-CA-CB	5.43	118.70	110.28
1	I	217	GLY	N-CA-C	-5.43	108.23	114.69
1	K	174	PRO	N-CA-C	-5.43	104.07	110.70
1	L	141	GLU	CA-C-O	5.43	125.59	119.18
1	J	141	GLU	N-CA-C	-5.43	104.92	113.02
1	K	279	GLY	CA-C-N	-5.43	113.22	121.53
1	K	279	GLY	C-N-CA	-5.43	113.22	121.53
1	H	328	MET	N-CA-C	5.42	118.10	110.23
1	I	282	LYS	N-CA-CB	5.42	119.72	110.50
1	K	129	GLY	N-CA-C	-5.42	106.28	115.34
1	K	338	GLU	N-CA-C	-5.42	105.46	111.36
1	J	310	PRO	N-CA-C	-5.42	101.31	112.47
1	M	199	THR	CA-C-N	5.41	129.82	122.19
1	M	199	THR	C-N-CA	5.41	129.82	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	290	ILE	N-CA-C	-5.41	105.45	110.53
1	K	361	PHE	O-C-N	5.41	128.31	122.15
1	L	386	THR	N-CA-CB	5.41	119.41	110.33
1	I	209	SER	CA-C-O	-5.41	113.75	119.97
1	K	362	ALA	N-CA-CB	5.41	118.07	110.12
1	J	133	GLU	N-CA-C	-5.41	100.52	108.79
1	I	124	ASP	CA-C-N	5.40	125.48	119.32
1	I	124	ASP	C-N-CA	5.40	125.48	119.32
1	L	164	PRO	CA-C-O	-5.40	111.43	119.86
1	L	374	ASP	CB-CA-C	-5.40	101.67	110.85
1	H	180	LEU	CB-CA-C	5.39	119.05	109.72
1	H	271	GLU	CA-C-O	-5.38	115.17	120.82
1	K	166	LEU	CA-C-O	5.38	126.13	120.42
1	K	267	GLN	CG-CD-NE2	-5.38	108.33	116.40
1	K	274	GLY	N-CA-C	-5.38	100.43	113.18
1	K	379	ILE	N-CA-C	-5.38	105.29	110.72
1	L	286	ALA	CA-C-O	-5.37	115.17	121.46
1	J	227	PHE	N-CA-C	5.37	117.21	111.36
1	H	170	VAL	CA-C-O	-5.37	115.09	121.05
1	M	348	GLY	N-CA-C	5.37	120.27	113.24
1	L	323	ILE	O-C-N	5.36	127.17	121.91
1	J	371	THR	CA-C-N	5.36	129.75	120.58
1	J	371	THR	C-N-CA	5.36	129.75	120.58
1	H	140	TYR	CA-C-N	5.36	127.40	120.44
1	H	140	TYR	C-N-CA	5.36	127.40	120.44
1	M	209	SER	N-CA-C	-5.36	106.74	113.28
1	M	191	LEU	O-C-N	5.36	127.80	122.12
1	M	216	ILE	N-CA-CB	5.36	120.07	111.23
1	M	324	HIS	ND1-CE1-NE2	5.36	113.76	108.40
1	I	135	LYS	CA-C-N	5.35	126.53	119.84
1	I	135	LYS	C-N-CA	5.35	126.53	119.84
1	J	193	LYS	N-CA-C	5.35	118.02	111.82
1	K	230	ALA	N-CA-CB	5.34	117.97	110.12
1	M	257	GLY	CA-C-N	5.34	127.87	120.29
1	M	257	GLY	C-N-CA	5.34	127.87	120.29
1	J	191	LEU	CA-C-O	5.34	128.15	120.51
1	H	207	VAL	N-CA-C	-5.34	100.79	108.53
1	K	337	LYS	N-CA-CB	5.34	118.06	110.16
1	H	276	ASP	O-C-N	5.33	127.66	121.47
1	J	153	ILE	CA-C-O	-5.33	115.20	120.85
1	K	221	ARG	CA-C-O	5.33	126.89	120.92
1	I	305	ARG	N-CA-CB	5.33	119.10	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	189	THR	N-CA-C	-5.33	106.63	113.23
1	M	171	GLY	N-CA-C	-5.33	107.92	115.43
1	J	152	GLU	O-C-N	-5.33	116.47	122.12
1	I	206	VAL	CB-CA-C	5.32	118.70	110.82
1	H	298	LEU	CA-C-O	5.32	124.99	119.14
1	M	215	TYR	CA-C-N	5.32	131.54	121.97
1	M	215	TYR	C-N-CA	5.32	131.54	121.97
1	M	126	MET	N-CA-CB	5.32	118.92	110.84
1	J	373	LEU	N-CA-C	5.32	117.08	111.28
1	L	250	ARG	CA-C-O	-5.31	115.23	120.70
1	M	370	VAL	N-CA-CB	5.31	118.15	111.46
1	J	336	PHE	CA-C-N	5.31	127.83	120.29
1	J	336	PHE	C-N-CA	5.31	127.83	120.29
1	K	309	VAL	N-CA-CB	5.31	118.64	111.21
1	M	233	LYS	N-CA-C	-5.31	104.59	111.71
1	J	257	GLY	CA-C-N	5.31	131.26	121.70
1	J	257	GLY	C-N-CA	5.31	131.26	121.70
1	J	136	PRO	N-CA-C	5.30	123.40	112.47
1	I	202	THR	N-CA-CB	5.30	119.45	110.49
1	M	358	ALA	N-CA-C	5.30	117.14	111.36
1	H	159	LEU	CA-C-O	-5.30	113.54	118.73
1	K	151	GLU	CA-C-O	-5.30	114.80	120.42
1	K	229	LEU	CA-C-N	5.30	127.38	120.28
1	K	229	LEU	C-N-CA	5.30	127.38	120.28
1	L	367	ARG	NE-CZ-NH2	-5.30	114.43	119.20
1	J	294	ASP	N-CA-C	-5.29	103.27	110.36
1	K	128	TYR	CA-CB-CG	-5.29	104.38	113.90
1	M	354	ILE	CA-C-N	5.29	127.80	120.29
1	M	354	ILE	C-N-CA	5.29	127.80	120.29
1	I	322	LYS	N-CA-CB	5.29	117.89	110.12
1	H	231	LYS	N-CA-C	5.28	117.04	111.28
1	K	123	LYS	CB-CA-C	-5.28	100.06	110.10
1	K	357	GLU	O-C-N	-5.28	116.13	122.15
1	M	168	ALA	CA-C-O	5.28	125.93	119.64
1	J	339	LEU	CA-C-N	5.28	127.36	120.28
1	J	339	LEU	C-N-CA	5.28	127.36	120.28
1	J	258	ASP	CA-C-N	5.28	128.34	120.31
1	J	258	ASP	C-N-CA	5.28	128.34	120.31
1	J	361	PHE	CA-C-N	5.28	127.36	120.28
1	J	361	PHE	C-N-CA	5.28	127.36	120.28
1	M	221	ARG	CD-NE-CZ	-5.28	117.01	124.40
1	H	247	ALA	CA-C-O	5.28	124.33	118.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	312	PRO	CA-C-O	-5.27	115.33	122.08
1	L	176	LYS	N-CA-CB	5.27	117.72	110.07
1	I	304	ASP	N-CA-CB	5.27	118.99	110.40
1	J	150	ILE	CA-C-O	-5.27	115.27	120.85
1	I	241	ASP	CA-CB-CG	5.26	117.86	112.60
1	M	127	VAL	N-CA-C	5.26	118.10	109.78
1	L	299	ARG	CD-NE-CZ	-5.26	117.03	124.40
1	H	200	ARG	CD-NE-CZ	-5.26	117.04	124.40
1	K	136	PRO	N-CA-CB	5.26	109.33	102.86
1	K	218	GLU	CA-C-O	-5.26	113.93	119.97
1	J	199	THR	CA-C-O	-5.26	115.29	120.70
1	M	313	THR	CA-C-N	5.25	127.27	120.44
1	M	313	THR	C-N-CA	5.25	127.27	120.44
1	K	326	ARG	CA-C-N	5.25	127.75	120.29
1	K	326	ARG	C-N-CA	5.25	127.75	120.29
1	H	319	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	L	247	ALA	N-CA-C	-5.24	101.33	109.72
1	L	377	LYS	CA-C-N	5.24	127.31	120.28
1	L	377	LYS	C-N-CA	5.24	127.31	120.28
1	H	258	ASP	CA-CB-CG	-5.24	107.36	112.60
1	J	230	ALA	CA-C-N	5.24	127.30	120.28
1	J	230	ALA	C-N-CA	5.24	127.30	120.28
1	H	295	PRO	O-C-N	5.24	129.03	123.01
1	K	260	GLU	O-C-N	5.24	129.63	122.46
1	H	333	ASP	CA-CB-CG	5.23	117.83	112.60
1	L	146	LEU	O-C-N	5.23	129.20	122.19
1	M	279	GLY	CA-C-N	-5.23	115.73	123.05
1	M	279	GLY	C-N-CA	-5.23	115.73	123.05
1	M	193	LYS	N-CA-CB	5.23	117.90	110.16
1	H	375	PHE	CA-C-N	5.22	127.27	120.28
1	H	375	PHE	C-N-CA	5.22	127.27	120.28
1	L	198	GLN	N-CA-C	5.22	117.88	111.82
1	I	364	ARG	CD-NE-CZ	-5.22	117.10	124.40
1	I	159	LEU	O-C-N	-5.21	115.84	120.48
1	M	174	PRO	CA-C-N	5.21	125.22	119.90
1	M	174	PRO	C-N-CA	5.21	125.22	119.90
1	H	282	LYS	CA-C-O	-5.21	114.93	120.92
1	J	221	ARG	CA-C-N	5.21	127.26	120.28
1	J	221	ARG	C-N-CA	5.21	127.26	120.28
1	H	320	ILE	CA-C-N	5.21	127.21	120.44
1	H	320	ILE	C-N-CA	5.21	127.21	120.44
1	L	281	VAL	O-C-N	-5.20	117.45	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	376	THR	CA-C-O	-5.20	115.03	120.55
1	J	315	GLU	CA-C-O	5.20	125.95	119.97
1	K	222	LEU	CA-C-N	5.20	127.11	120.56
1	K	222	LEU	C-N-CA	5.20	127.11	120.56
1	M	252	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	H	340	ALA	N-CA-C	5.19	116.94	111.28
1	I	362	ALA	CA-C-O	-5.19	115.05	120.55
1	M	351	ILE	CA-C-N	5.19	127.19	120.44
1	M	351	ILE	C-N-CA	5.19	127.19	120.44
1	I	254	ASP	O-C-N	-5.19	115.03	122.04
1	L	184	PRO	CA-C-N	5.19	130.86	122.09
1	L	184	PRO	C-N-CA	5.19	130.86	122.09
1	K	190	LEU	CA-C-O	-5.19	115.05	120.55
1	L	260	GLU	CB-CG-CD	-5.18	103.79	112.60
1	I	128	TYR	CA-C-O	5.17	126.25	120.82
1	M	247	ALA	N-CA-C	-5.17	98.97	108.02
1	K	165	GLU	N-CA-C	5.17	118.85	112.54
1	K	260	GLU	N-CA-C	-5.17	106.82	113.23
1	H	378	ALA	N-CA-CB	5.17	117.81	110.16
1	M	352	LYS	CA-C-N	5.17	127.72	120.28
1	M	352	LYS	C-N-CA	5.17	127.72	120.28
1	J	158	GLU	N-CA-C	5.16	117.80	111.82
1	J	180	LEU	CB-CA-C	-5.16	101.24	109.75
1	I	189	THR	CA-C-N	5.16	127.61	120.29
1	I	189	THR	C-N-CA	5.16	127.61	120.29
1	M	265	MET	O-C-N	-5.16	116.27	122.15
1	H	282	LYS	CA-C-N	5.15	129.58	123.19
1	H	282	LYS	C-N-CA	5.15	129.58	123.19
1	I	234	ALA	O-C-N	-5.15	116.83	121.31
1	K	209	SER	N-CA-C	-5.15	106.94	113.18
1	I	353	ALA	N-CA-C	5.15	116.89	111.28
1	K	349	ALA	CA-C-N	5.14	127.17	120.28
1	K	349	ALA	C-N-CA	5.14	127.17	120.28
1	J	276	ASP	N-CA-C	-5.14	100.56	109.15
1	K	153	ILE	CA-CB-CG2	-5.14	101.76	110.50
1	J	196	ALA	N-CA-C	5.14	116.88	111.28
1	K	243	LEU	N-CA-CB	5.13	118.09	110.49
1	K	360	MET	CA-C-N	5.13	127.58	120.29
1	K	360	MET	C-N-CA	5.13	127.58	120.29
1	L	318	ILE	CA-C-O	-5.13	115.73	121.17
1	J	243	LEU	N-CA-CB	5.13	118.24	110.28
1	K	267	GLN	CA-C-N	5.13	127.15	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	267	GLN	C-N-CA	5.13	127.15	120.28
1	K	309	VAL	N-CA-C	-5.13	97.80	108.88
1	H	169	GLU	CA-C-N	5.13	127.12	120.56
1	H	169	GLU	C-N-CA	5.13	127.12	120.56
1	I	323	ILE	CA-CB-CG2	5.13	119.21	110.50
1	M	183	PRO	N-CA-C	5.12	116.94	110.70
1	J	325	THR	CA-C-N	5.11	127.09	120.44
1	J	325	THR	C-N-CA	5.11	127.09	120.44
1	L	237	ILE	O-C-N	-5.11	117.81	123.18
1	I	275	PHE	O-C-N	5.11	129.38	122.59
1	H	141	GLU	CB-CA-C	-5.10	102.87	110.88
1	L	149	GLN	N-CA-C	-5.10	105.80	111.36
1	K	188	LYS	N-CA-C	5.10	116.84	111.28
1	M	203	PHE	CB-CA-C	-5.09	101.13	109.53
1	J	141	GLU	CB-CA-C	-5.09	101.88	110.44
1	M	159	LEU	CA-C-O	-5.09	113.40	118.34
1	L	379	ILE	N-CA-C	-5.09	105.53	110.42
1	J	173	GLU	O-C-N	-5.09	116.67	121.35
1	J	258	ASP	N-CA-CB	5.09	119.15	110.50
1	M	256	SER	CA-C-O	-5.09	115.48	120.82
1	H	146	LEU	N-CA-C	-5.08	107.03	113.43
1	I	319	GLN	OE1-CD-NE2	5.08	127.68	122.60
1	L	193	LYS	CB-CA-C	-5.08	102.36	110.79
1	M	294	ASP	CA-CB-CG	5.08	117.68	112.60
1	I	337	LYS	O-C-N	5.08	127.57	122.09
1	H	333	ASP	CA-C-N	5.08	127.96	120.91
1	H	333	ASP	C-N-CA	5.08	127.96	120.91
1	J	199	THR	CA-C-N	5.08	129.82	122.36
1	J	199	THR	C-N-CA	5.08	129.82	122.36
1	I	299	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	I	321	PHE	CB-CA-C	-5.07	102.37	110.79
1	L	220	ALA	CA-C-N	5.07	128.43	120.82
1	L	220	ALA	C-N-CA	5.07	128.43	120.82
1	K	124	ASP	N-CA-C	-5.07	101.29	109.40
1	H	336	PHE	CA-C-N	5.07	127.48	120.29
1	H	336	PHE	C-N-CA	5.07	127.48	120.29
1	M	311	LEU	CA-C-O	-5.07	114.73	119.80
1	H	327	LYS	CA-C-O	5.06	125.79	120.42
1	M	254	ASP	N-CA-CB	5.06	119.05	110.49
1	H	176	LYS	CA-C-O	5.06	125.78	120.42
1	H	338	GLU	CA-C-N	5.06	127.06	120.28
1	H	338	GLU	C-N-CA	5.06	127.06	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	354	ILE	N-CA-C	-5.06	105.61	110.72
1	J	367	ARG	CA-CB-CG	5.06	124.22	114.10
1	H	216	ILE	N-CA-CB	5.05	118.38	111.41
1	K	150	ILE	CA-CB-CG2	5.05	119.09	110.50
1	J	380	GLU	O-C-N	5.05	127.47	122.12
1	H	243	LEU	CA-C-O	5.05	126.06	119.95
1	I	159	LEU	N-CA-CB	5.05	117.82	110.30
1	I	314	PHE	CA-CB-CG	-5.05	108.75	113.80
1	M	188	LYS	N-CA-C	-5.05	105.96	111.82
1	J	317	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	L	259	ARG	CA-C-N	5.05	127.46	120.29
1	L	259	ARG	C-N-CA	5.05	127.46	120.29
1	H	266	MET	N-CA-C	5.05	116.78	111.28
1	K	323	ILE	N-CA-C	5.05	115.77	110.62
1	J	130	PHE	CB-CG-CD2	-5.05	112.12	120.70
1	L	124	ASP	CB-CA-C	-5.04	102.70	110.62
1	L	185	GLY	CA-C-O	5.04	124.39	119.04
1	H	376	THR	CA-C-N	5.04	127.03	120.28
1	H	376	THR	C-N-CA	5.04	127.03	120.28
1	K	157	VAL	CA-C-N	5.04	126.99	120.44
1	K	157	VAL	C-N-CA	5.04	126.99	120.44
1	J	130	PHE	O-C-N	5.04	127.46	122.12
1	L	282	LYS	CA-C-N	5.04	129.80	123.10
1	L	282	LYS	C-N-CA	5.04	129.80	123.10
1	M	150	ILE	N-CA-C	-5.04	105.80	110.53
1	H	306	ILE	N-CA-CB	5.03	118.18	111.64
1	K	251	THR	CA-CB-OG1	5.03	117.15	109.60
1	M	349	ALA	N-CA-CB	5.03	117.60	110.16
1	I	138	VAL	N-CA-C	-5.02	101.08	108.11
1	I	245	ALA	N-CA-C	5.02	116.75	111.28
1	I	312	PRO	N-CA-CB	-5.02	98.67	103.39
1	K	184	PRO	O-C-N	-5.02	116.88	123.06
1	H	197	ASN	CA-C-O	-5.01	113.21	119.38
1	H	312	PRO	N-CA-C	-5.01	103.39	111.77
1	I	274	GLY	O-C-N	-5.01	117.33	122.19
1	J	201	ALA	CA-C-O	-5.01	114.96	121.73
1	H	172	ILE	CA-CB-CG2	-5.01	101.98	110.50
1	M	149	GLN	N-CA-C	-5.01	106.01	111.82
1	K	200	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	K	288	ASN	N-CA-C	-5.01	107.34	113.50
1	L	379	ILE	CA-CB-CG1	-5.01	101.88	110.40
1	H	328	MET	N-CA-CB	5.01	117.39	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	225	GLU	CA-C-O	-5.01	115.11	120.42
1	J	205	ARG	CD-NE-CZ	-5.01	117.39	124.40
1	H	256	SER	N-CA-C	-5.00	106.03	112.68
1	I	203	PHE	N-CA-CB	5.00	118.63	110.37
1	M	125	PRO	CB-CA-C	-5.00	103.48	110.63

There are no chirality outliers.

All (74) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	137	GLU	Peptide
1	H	154	ARG	Sidechain
1	H	200	ARG	Sidechain
1	H	215	TYR	Sidechain,Peptide
1	H	217	GLY	Peptide
1	H	218	GLU	Peptide
1	H	219	GLY	Mainchain
1	H	227	PHE	Sidechain
1	H	236	SER	Peptide
1	H	240	ILE	Peptide
1	H	250	ARG	Sidechain
1	H	254	ASP	Peptide
1	H	259	ARG	Sidechain
1	H	276	ASP	Peptide
1	H	303	PHE	Sidechain
1	H	311	LEU	Peptide
1	H	321	PHE	Sidechain
1	H	367	ARG	Sidechain
1	H	387	THR	Peptide
1	I	128	TYR	Sidechain
1	I	137	GLU	Peptide
1	I	167	PHE	Sidechain
1	I	181	TYR	Peptide
1	I	211	PHE	Sidechain
1	I	221	ARG	Sidechain
1	I	254	ASP	Peptide
1	I	269	LEU	Peptide
1	I	302	ARG	Sidechain
1	I	303	PHE	Peptide
1	I	314	PHE	Sidechain
1	I	387	THR	Peptide
1	J	140	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	J	167	PHE	Sidechain
1	J	181	TYR	Sidechain
1	J	186	THR	Peptide
1	J	207	VAL	Peptide
1	J	215	TYR	Peptide
1	J	305	ARG	Sidechain
1	J	314	PHE	Sidechain
1	J	336	PHE	Sidechain
1	J	361	PHE	Sidechain
1	K	128	TYR	Sidechain
1	K	181	TYR	Sidechain
1	K	201	ALA	Peptide
1	K	215	TYR	Sidechain,Mainchain,Peptide
1	K	224	ARG	Sidechain
1	K	269	LEU	Mainchain,Peptide
1	K	277	PRO	Peptide
1	K	289	ARG	Sidechain
1	K	302	ARG	Sidechain
1	L	130	PHE	Sidechain
1	L	131	GLU	Peptide
1	L	200	ARG	Sidechain
1	L	215	TYR	Peptide
1	L	221	ARG	Sidechain
1	L	249	ARG	Sidechain
1	L	263	ARG	Sidechain
1	L	278	ARG	Sidechain
1	L	375	PHE	Sidechain
1	L	385	LYS	Peptide
1	L	387	THR	Peptide
1	M	140	TYR	Sidechain
1	M	218	GLU	Peptide
1	M	249	ARG	Sidechain
1	M	254	ASP	Peptide
1	M	275	PHE	Sidechain
1	M	302	ARG	Sidechain
1	M	326	ARG	Sidechain
1	M	364	ARG	Sidechain
1	M	371	THR	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	H	2088	0	2159	13	0
1	I	2088	0	2159	8	0
1	J	2088	0	2159	11	0
1	K	2088	0	2159	3	0
1	L	2088	0	2159	8	0
1	M	2088	0	2159	8	0
2	H	31	0	12	0	0
2	I	31	0	12	0	0
2	J	31	0	12	0	0
2	K	31	0	12	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	L	27	0	12	0	0
All	All	12684	0	13014	47	0

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

All (47) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:LEU:H	1:H:147:ASP:HA	1.61	0.64
1:H:339:LEU:HD22	1:H:379:ILE:CD1	2.30	0.61
1:I:323:ILE:HD13	1:I:326:ARG:HH21	1.72	0.55
1:I:257:GLY:HA3	1:J:216:ILE:HG21	1.90	0.53
1:L:176:LYS:H	1:L:304:ASP:HB2	1.73	0.53
1:K:236:SER:O	1:K:281:VAL:HG12	2.10	0.52
1:M:354:ILE:HD11	1:M:383:LEU:HB2	1.91	0.52
1:J:272:LEU:HG	1:J:283:VAL:HG21	1.92	0.52
1:I:361:PHE:HA	1:I:364:ARG:HE	1.75	0.51
1:H:219:GLY:H	1:H:222:LEU:H	1.58	0.51
1:H:339:LEU:HD22	1:H:379:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:339:LEU:HD22	1:H:379:ILE:HD11	1.92	0.51
1:H:193:LYS:HG2	1:I:275:PHE:CE1	2.46	0.51
1:M:179:LEU:HD13	1:M:243:LEU:HD12	1.93	0.50
1:H:251:THR:HG23	1:L:215:TYR:CE2	2.46	0.49
1:L:370:VAL:HG12	1:L:375:PHE:CZ	2.48	0.49
1:H:237:ILE:HD13	1:H:282:LYS:HB2	1.95	0.48
1:L:389:ILE:HD12	1:L:389:ILE:H	1.79	0.48
1:J:242:GLU:H	1:J:286:ALA:HB3	1.78	0.48
1:H:386:THR:HG22	1:H:387:THR:H	1.79	0.47
1:H:181:TYR:CZ	1:H:290:ILE:HG22	2.50	0.47
1:K:206:VAL:HG22	1:K:207:VAL:H	1.81	0.46
1:H:130:PHE:CZ	1:H:206:VAL:HG23	2.51	0.46
1:L:158:GLU:HG3	1:L:199:THR:HG22	1.98	0.46
1:J:289:ARG:HE	1:J:291:ASP:HB2	1.81	0.46
1:L:153:ILE:HD12	1:L:191:LEU:HD22	1.98	0.45
1:M:178:VAL:HG23	1:M:305:ARG:HG3	1.98	0.45
1:M:334:VAL:HA	1:M:372:MET:HB2	1.98	0.45
1:L:239:PHE:CE2	1:L:241:ASP:HB2	2.52	0.45
1:K:281:VAL:HA	1:K:282:LYS:HB2	1.98	0.45
1:M:159:LEU:HB3	1:M:160:PRO:HD3	1.98	0.45
1:J:153:ILE:HD11	1:J:191:LEU:HD23	1.98	0.44
1:I:139:SER:H	1:I:142:ASP:HB2	1.83	0.43
1:I:206:VAL:HG22	1:I:207:VAL:H	1.84	0.43
1:M:287:THR:HG21	1:M:290:ILE:HG23	2.00	0.43
1:L:247:ALA:HA	1:L:265:MET:HE2	2.01	0.42
1:J:206:VAL:HG22	1:J:207:VAL:H	1.84	0.42
1:J:343:THR:HG22	1:J:379:ILE:HG23	2.01	0.42
1:J:132:VAL:HG13	1:J:203:PHE:H	1.85	0.42
1:H:172:ILE:HG23	1:M:328:MET:HE1	2.02	0.41
1:M:299:ARG:HE	1:M:302:ARG:CZ	2.34	0.41
1:I:146:LEU:H	1:I:147:ASP:CG	2.29	0.41
1:I:308:GLU:O	1:I:310:PRO:HD3	2.21	0.41
1:J:338:GLU:HA	1:J:341:ARG:HE	1.86	0.41
1:J:217:GLY:HA2	1:J:263:ARG:HH22	1.86	0.41
1:H:223:VAL:HG21	1:H:264:THR:HG22	2.03	0.40
1:J:371:THR:O	1:J:374:ASP:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	265/267 (99%)	240 (91%)	14 (5%)	11 (4%)	2	17
1	I	265/267 (99%)	234 (88%)	18 (7%)	13 (5%)	1	16
1	J	265/267 (99%)	227 (86%)	26 (10%)	12 (4%)	2	16
1	K	265/267 (99%)	240 (91%)	15 (6%)	10 (4%)	2	19
1	L	265/267 (99%)	239 (90%)	12 (4%)	14 (5%)	1	15
1	M	265/267 (99%)	243 (92%)	17 (6%)	5 (2%)	6	31
All	All	1590/1602 (99%)	1423 (90%)	102 (6%)	65 (4%)	4	17

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	163	LYS
1	H	237	ILE
1	H	246	ILE
1	H	255	THR
1	I	255	THR
1	I	270	ALA
1	I	292	ILE
1	I	331	ALA
1	K	134	GLU
1	K	216	ILE
1	K	269	LEU
1	L	212	VAL
1	L	216	ILE
1	L	282	LYS
1	L	388	PRO
1	M	212	VAL
1	M	244	ASP
1	J	128	TYR
1	J	190	LEU
1	J	191	LEU

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Mol	Chain	Res	Type
1	H	388	PRO
1	I	126	MET
1	I	212	VAL
1	I	221	ARG
1	I	269	LEU
1	K	212	VAL
1	K	270	ALA
1	K	278	ARG
1	L	132	VAL
1	L	273	ASP
1	L	280	ASP
1	L	335	ASP
1	M	246	ILE
1	M	330	LEU
1	J	304	ASP
1	H	296	ALA
1	H	333	ASP
1	I	146	LEU
1	I	282	LYS
1	K	388	PRO
1	L	242	GLU
1	L	366	GLU
1	J	214	LYS
1	J	273	ASP
1	J	282	LYS
1	J	301	GLY
1	H	135	LYS
1	I	202	THR
1	I	277	PRO
1	I	330	LEU
1	K	282	LYS
1	L	135	LYS
1	L	334	VAL
1	J	247	ALA
1	K	200	ARG
1	L	284	ILE
1	J	212	VAL
1	H	219	GLY
1	M	219	GLY
1	J	143	ILE
1	H	136	PRO
1	L	183	PRO

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Mol	Chain	Res	Type
1	J	136	PRO
1	K	246	ILE
1	H	277	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	223/223 (100%)	215 (96%)	8 (4%)	31	52
1	I	223/223 (100%)	214 (96%)	9 (4%)	28	49
1	J	223/223 (100%)	214 (96%)	9 (4%)	28	49
1	K	223/223 (100%)	213 (96%)	10 (4%)	24	46
1	L	223/223 (100%)	219 (98%)	4 (2%)	51	67
1	M	223/223 (100%)	214 (96%)	9 (4%)	28	49
All	All	1338/1338 (100%)	1289 (96%)	49 (4%)	31	51

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	136	PRO
1	H	179	LEU
1	H	205	ARG
1	H	223	VAL
1	H	250	ARG
1	H	275	PHE
1	H	377	LYS
1	H	385	LYS
1	I	126	MET
1	I	179	LEU
1	I	216	ILE
1	I	227	PHE
1	I	250	ARG
1	I	293	LEU
1	I	295	PRO

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Mol	Chain	Res	Type
1	I	386	THR
1	I	389	ILE
1	K	159	LEU
1	K	165	GLU
1	K	189	THR
1	K	200	ARG
1	K	216	ILE
1	K	242	GLU
1	K	252	ASN
1	K	255	THR
1	K	282	LYS
1	K	298	LEU
1	L	143	ILE
1	L	268	LEU
1	L	295	PRO
1	L	321	PHE
1	M	153	ILE
1	M	176	LYS
1	M	215	TYR
1	M	218	GLU
1	M	275	PHE
1	M	312	PRO
1	M	327	LYS
1	M	332	GLU
1	M	370	VAL
1	J	178	VAL
1	J	190	LEU
1	J	207	VAL
1	J	210	GLU
1	J	231	LYS
1	J	250	ARG
1	J	252	ASN
1	J	265	MET
1	J	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	149	GLN
1	H	197	ASN
1	H	267	GLN
1	H	324	HIS

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Mol	Chain	Res	Type
1	I	288	ASN
1	I	319	GLN
1	K	267	GLN
1	L	267	GLN
1	J	149	GLN
1	J	213	GLN
1	J	267	GLN
1	J	324	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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$
2	ATP	H	401	3	32,33,33	4.10	8 (25%)	48,52,52	1.34	5 (10%)
4	ADP	L	401	3	28,29,29	1.73	1 (3%)	43,45,45	1.38	7 (16%)
2	ATP	K	401	3	32,33,33	4.10	4 (12%)	48,52,52	1.49	9 (18%)
2	ATP	J	401	3	32,33,33	4.86	7 (21%)	48,52,52	1.27	6 (12%)
2	ATP	I	401	3	32,33,33	4.11	5 (15%)	48,52,52	1.36	8 (16%)

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
2	ATP	H	401	3	-	6/22/38/38	0/3/3/3
4	ADP	L	401	3	-	5/16/32/32	0/3/3/3
2	ATP	K	401	3	-	4/22/38/38	0/3/3/3
2	ATP	J	401	3	-	7/22/38/38	0/3/3/3
2	ATP	I	401	3	-	1/22/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	401	ATP	PB-O3B	19.11	1.80	1.59
2	J	401	ATP	PB-O3A	18.11	1.79	1.59
2	J	401	ATP	PB-O3B	17.15	1.78	1.59
2	K	401	ATP	PB-O3A	16.10	1.76	1.59
2	H	401	ATP	PB-O3B	14.78	1.75	1.59
2	K	401	ATP	PB-O3B	12.20	1.72	1.59
2	I	401	ATP	PB-O3A	11.60	1.72	1.59
2	H	401	ATP	PB-O3A	11.57	1.72	1.59
2	H	401	ATP	PA-O3A	11.30	1.71	1.59
2	J	401	ATP	PA-O3A	9.49	1.69	1.59
2	K	401	ATP	PA-O3A	9.47	1.69	1.59
4	L	401	ADP	PA-O3A	7.59	1.67	1.59
2	K	401	ATP	C4-N3	-3.60	1.27	1.34
2	H	401	ATP	C8-N9	3.24	1.43	1.37
2	H	401	ATP	C5-N7	-3.07	1.33	1.39
2	H	401	ATP	C2-N3	-2.85	1.28	1.33
2	I	401	ATP	C5-N7	-2.53	1.34	1.39
2	J	401	ATP	C2'-C3'	-2.49	1.46	1.53
2	I	401	ATP	C2-N3	2.49	1.38	1.33
2	J	401	ATP	C2-N3	-2.45	1.29	1.33
2	I	401	ATP	PG-O2G	-2.34	1.46	1.54
2	H	401	ATP	O4'-C1'	2.30	1.47	1.42
2	H	401	ATP	O4'-C4'	2.27	1.50	1.45
2	J	401	ATP	PG-O1G	2.26	1.57	1.50
2	J	401	ATP	C5-C4	-2.13	1.35	1.39

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	ATP	C4-N9-C8	-5.51	99.95	105.74
2	J	401	ATP	N6-C6-N1	3.77	126.78	118.38
2	K	401	ATP	N6-C6-N1	3.61	126.41	118.38
2	K	401	ATP	C6-C5-C4	3.33	121.72	117.18
2	I	401	ATP	N6-C6-N1	2.98	125.00	118.38
4	L	401	ADP	N6-C6-N1	2.91	124.86	118.38
2	J	401	ATP	C6-C5-C4	2.82	121.03	117.18
2	J	401	ATP	C5-C6-N6	-2.78	116.41	123.29
2	I	401	ATP	O3G-PG-O2G	2.74	118.06	107.80
2	I	401	ATP	C6-C5-C4	2.71	120.88	117.18
2	K	401	ATP	C5-C6-N1	-2.69	110.68	117.51
2	J	401	ATP	C5'-C4'-C3'	2.64	124.72	115.21
2	H	401	ATP	C5-C4-N9	2.61	108.65	105.81
4	L	401	ADP	C4-N9-C8	-2.59	103.02	105.74
4	L	401	ADP	C6-C5-C4	2.56	120.67	117.18
2	K	401	ATP	C4-C5-N7	-2.47	107.76	110.58
2	J	401	ATP	C5-C4-N3	-2.46	123.33	126.72
2	K	401	ATP	C5-N7-C8	2.43	107.27	103.45
2	I	401	ATP	C4-C5-N7	-2.43	107.80	110.58
2	H	401	ATP	N6-C6-N1	2.42	123.77	118.38
2	I	401	ATP	O2B-PB-O3A	-2.39	100.82	107.27
2	K	401	ATP	C2-N1-C6	2.29	122.49	118.73
2	I	401	ATP	C5-C4-N9	2.26	108.27	105.81
4	L	401	ADP	C4-C5-N7	-2.23	108.04	110.58
2	K	401	ATP	O4'-C1'-C2'	2.21	111.35	106.62
4	L	401	ADP	C1'-N9-C8	2.18	131.92	127.09
4	L	401	ADP	C5-C4-N3	-2.16	123.75	126.72
2	I	401	ATP	O2G-PG-O3B	-2.16	97.41	104.64
2	J	401	ATP	O3'-C3'-C4'	-2.15	104.91	111.08
2	K	401	ATP	O5'-C5'-C4'	2.14	116.29	108.99
2	H	401	ATP	C4-N9-C1'	2.12	131.59	126.63
2	I	401	ATP	O2G-PG-O1G	2.12	119.08	110.83
2	H	401	ATP	O2B-PB-O1B	2.09	122.17	112.44
4	L	401	ADP	O2B-PB-O3A	2.07	111.59	104.64
2	K	401	ATP	O3'-C3'-C2'	2.05	118.40	111.82

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	401	ATP	PB-O3A-PA-O5'
2	H	401	ATP	C5'-O5'-PA-O1A
2	H	401	ATP	C5'-O5'-PA-O3A

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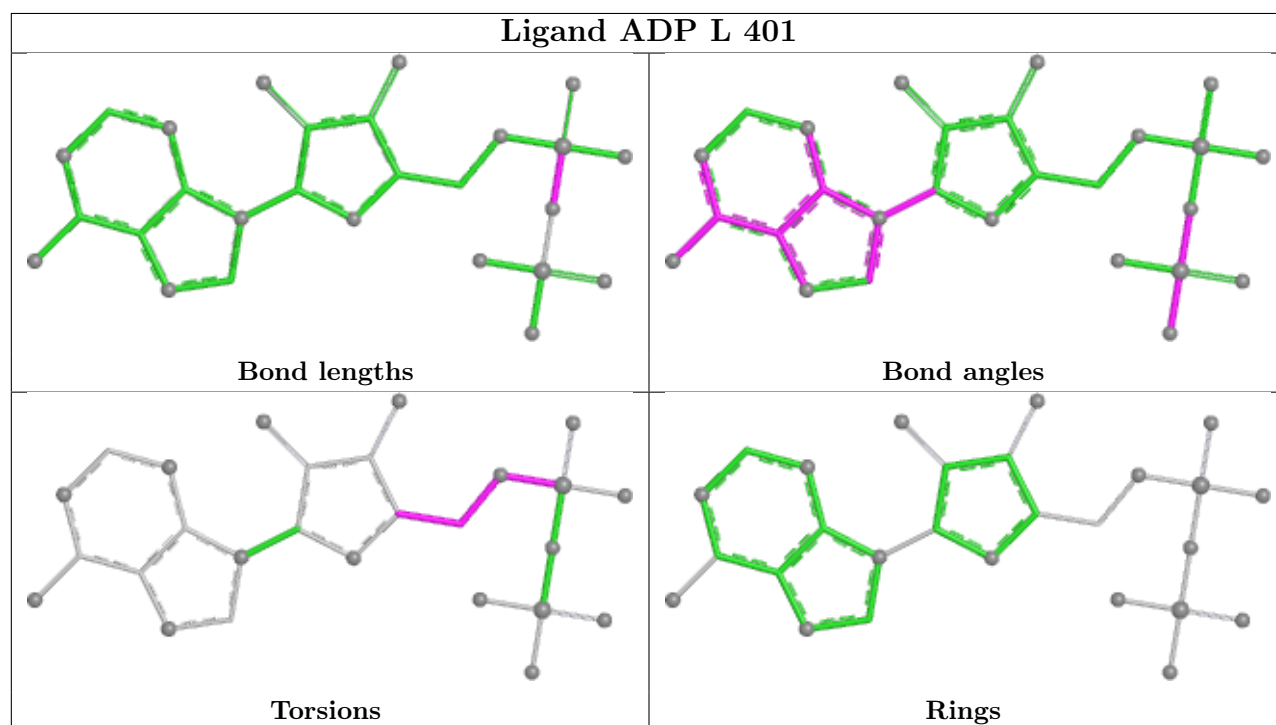
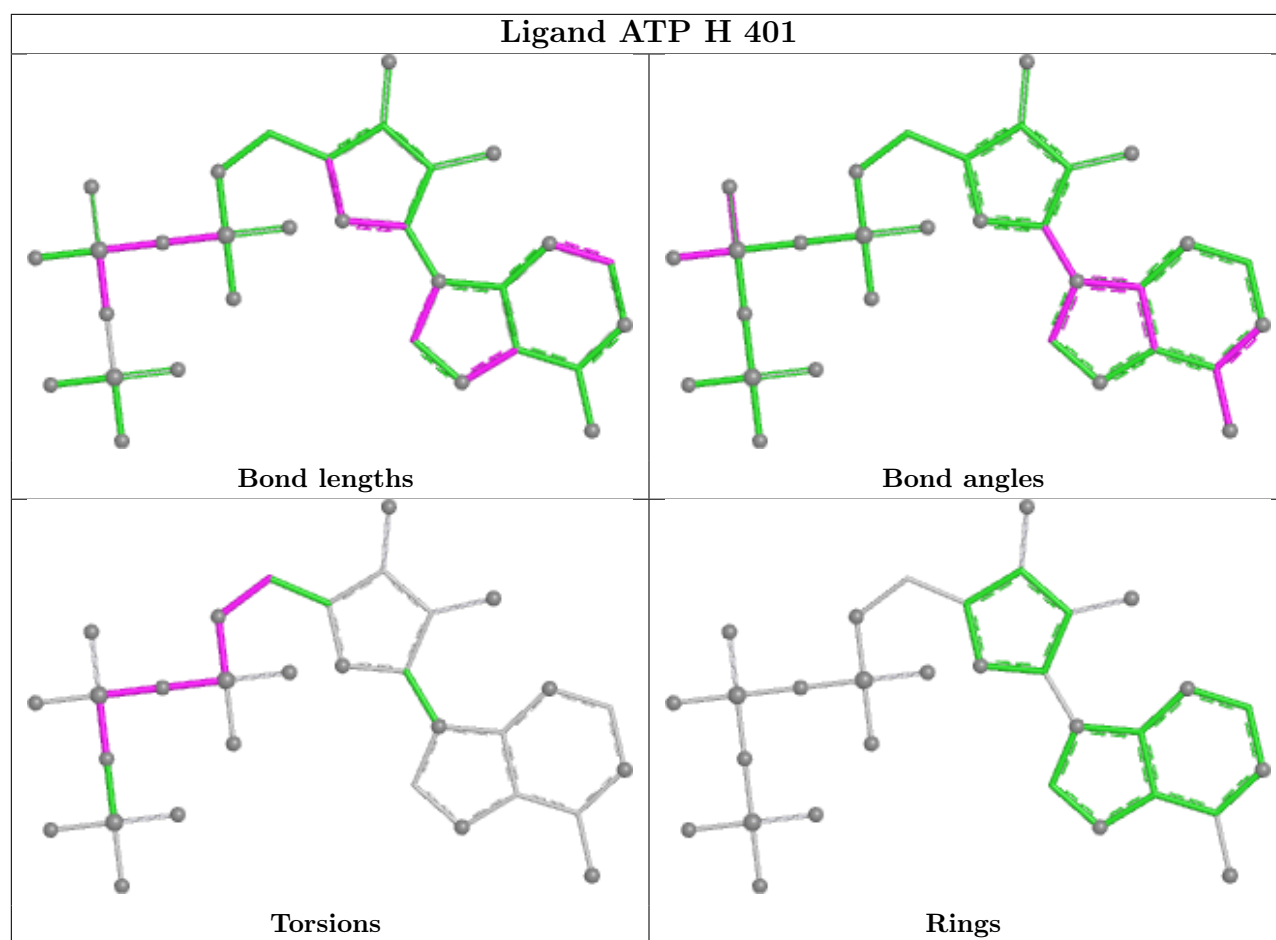
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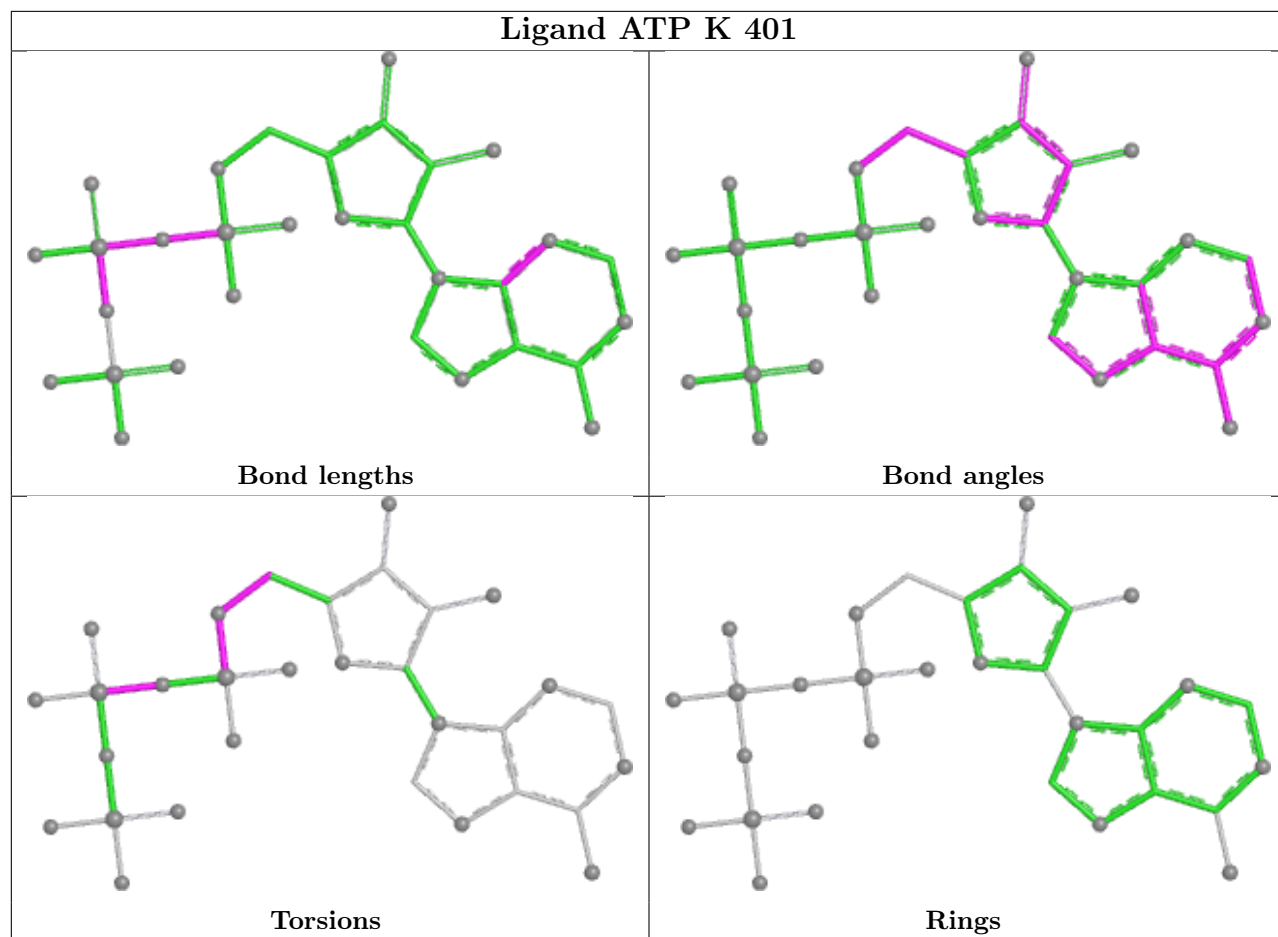
Mol	Chain	Res	Type	Atoms
2	H	401	ATP	C4'-C5'-O5'-PA
2	K	401	ATP	C5'-O5'-PA-O1A
2	J	401	ATP	C5'-O5'-PA-O3A
4	L	401	ADP	C5'-O5'-PA-O1A
4	L	401	ADP	C5'-O5'-PA-O2A
4	L	401	ADP	C5'-O5'-PA-O3A
2	J	401	ATP	C3'-C4'-C5'-O5'
2	J	401	ATP	O4'-C4'-C5'-O5'
2	K	401	ATP	PA-O3A-PB-O2B
2	J	401	ATP	C5'-O5'-PA-O1A
2	K	401	ATP	C4'-C5'-O5'-PA
2	J	401	ATP	C4'-C5'-O5'-PA
2	K	401	ATP	PA-O3A-PB-O1B
2	J	401	ATP	PG-O3B-PB-O2B
2	J	401	ATP	PA-O3A-PB-O2B
4	L	401	ADP	C4'-C5'-O5'-PA
4	L	401	ADP	C3'-C4'-C5'-O5'
2	H	401	ATP	PG-O3B-PB-O1B
2	H	401	ATP	PA-O3A-PB-O1B
2	I	401	ATP	PG-O3B-PB-O1B

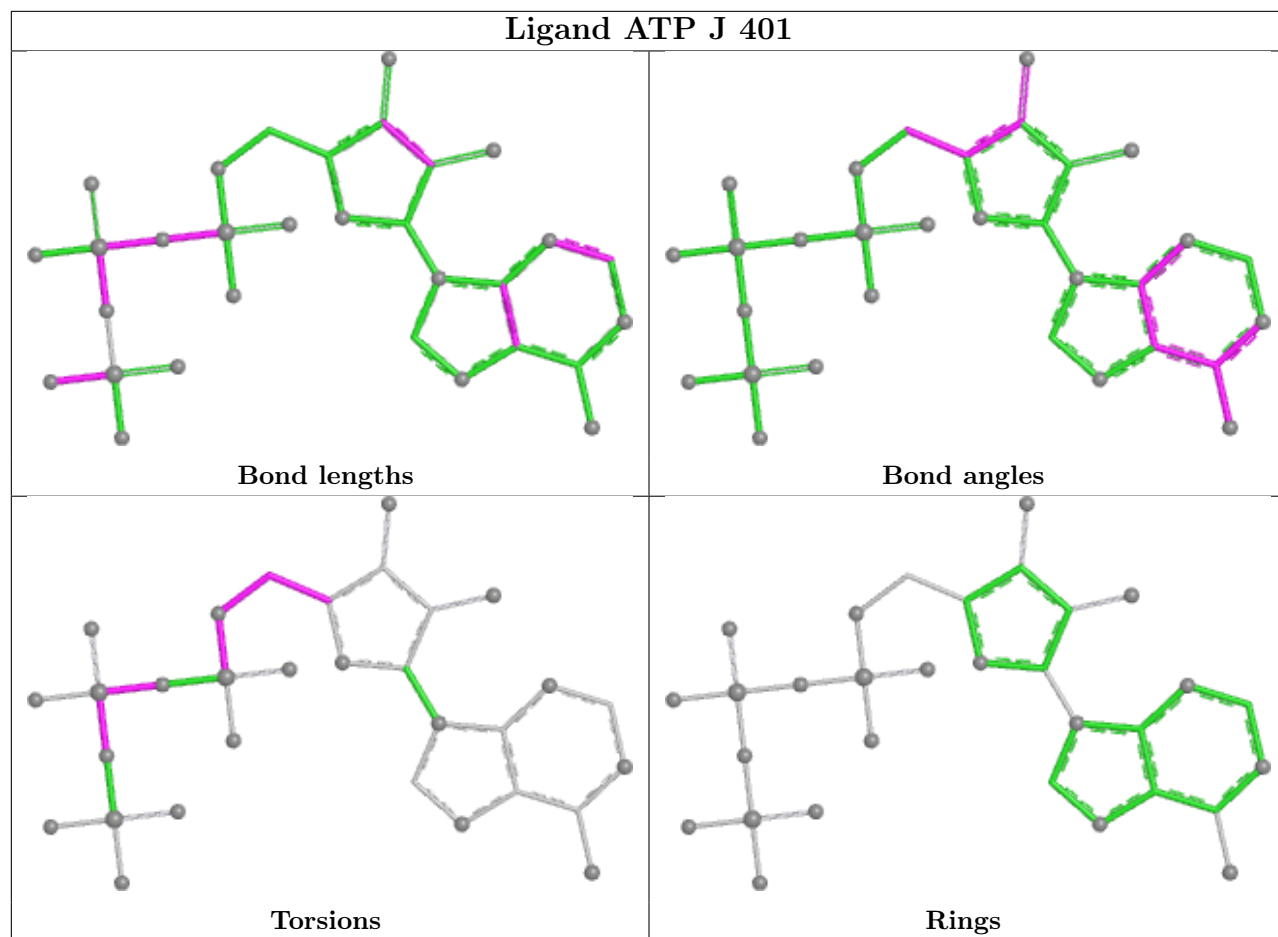
There are no ring outliers.

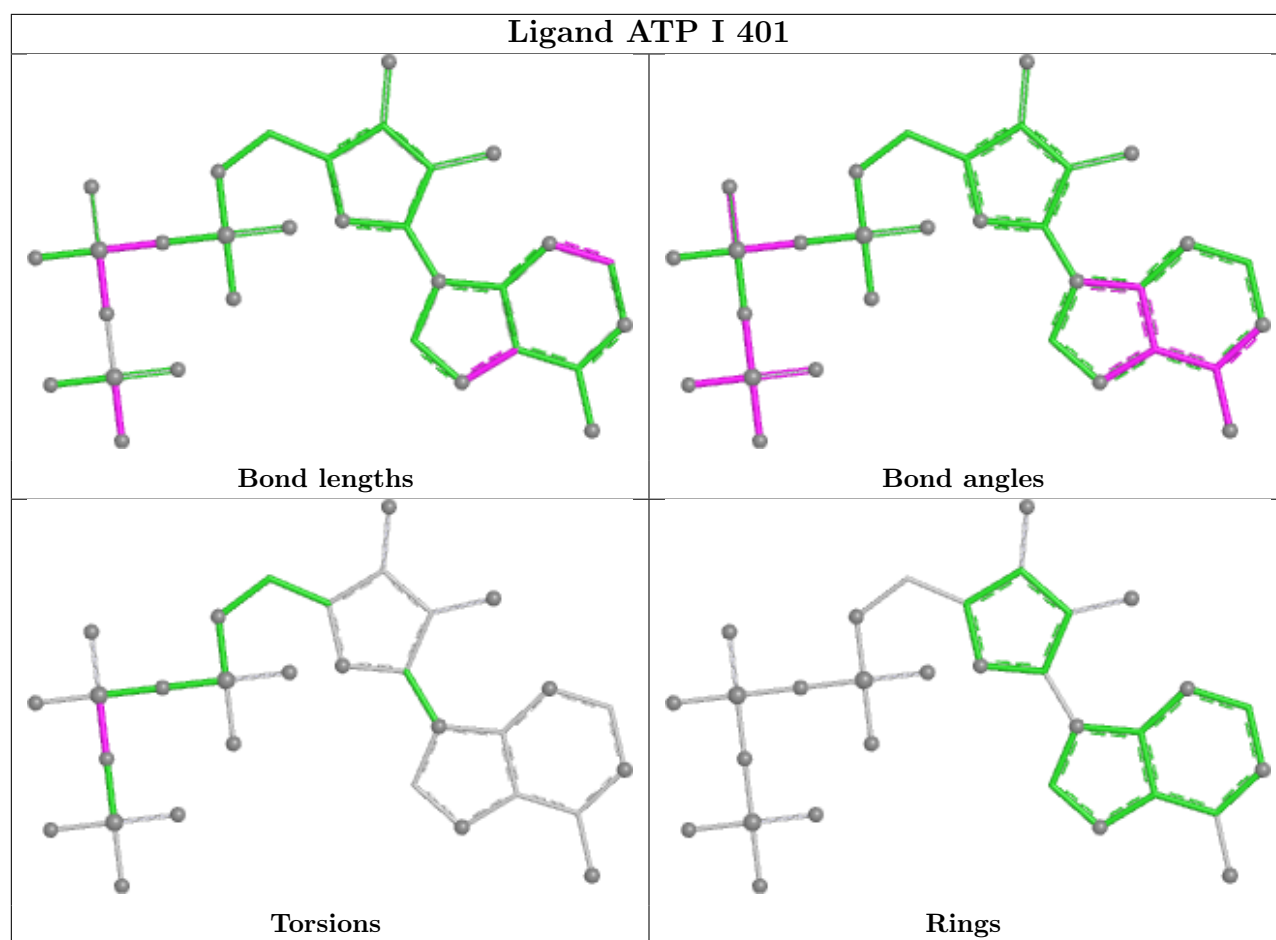
No monomer is involved in short contacts.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

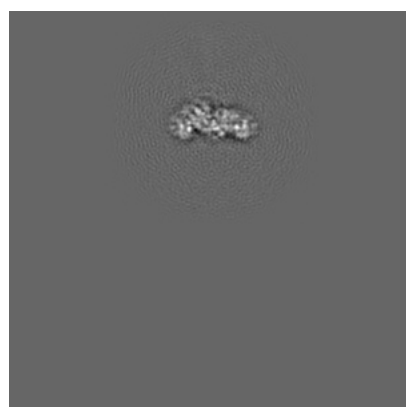
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0209. These allow visual inspection of the internal detail of the map and identification of artifacts.

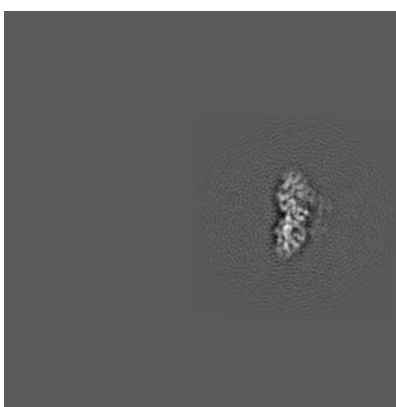
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

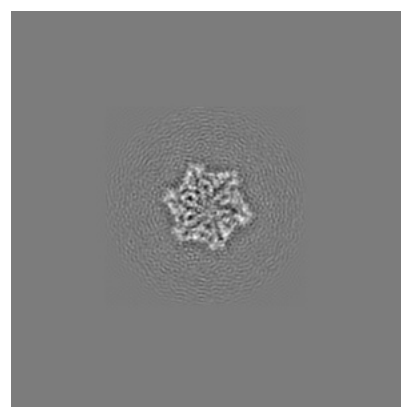
6.1.1 Primary map



X



Y

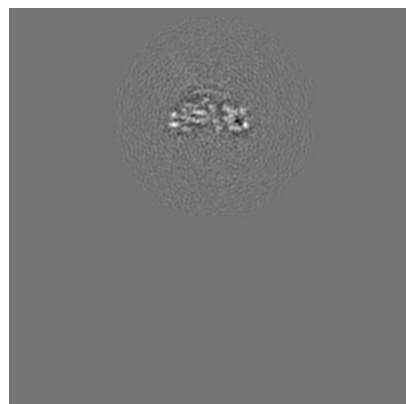


Z

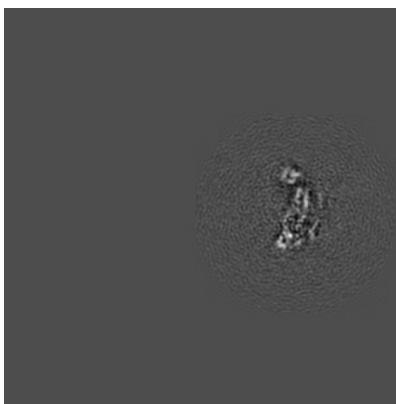
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

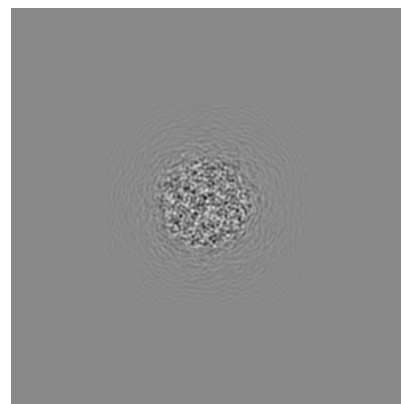
6.2.1 Primary map



X Index: 192



Y Index: 192

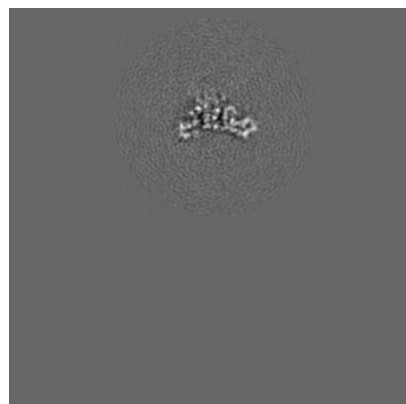


Z Index: 192

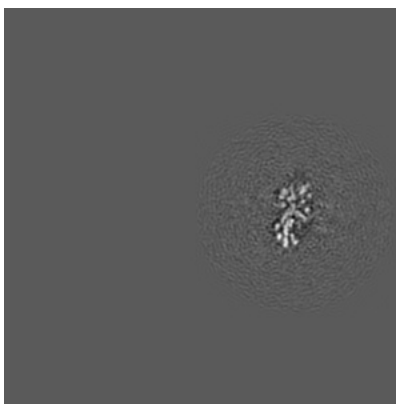
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

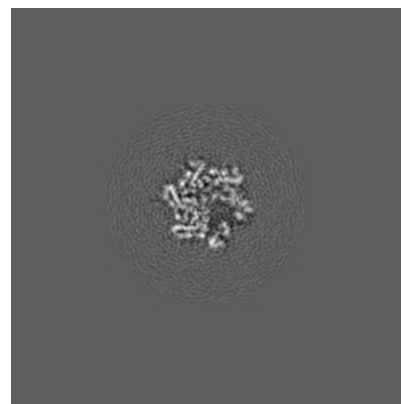
6.3.1 Primary map



X Index: 172



Y Index: 172

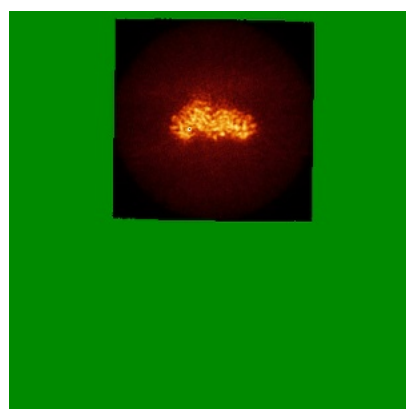


Z Index: 271

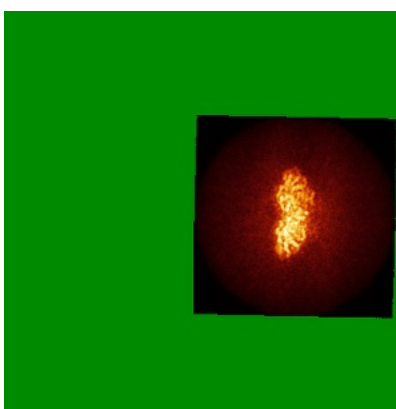
The images above show the largest variance slices of the map in three orthogonal directions.

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

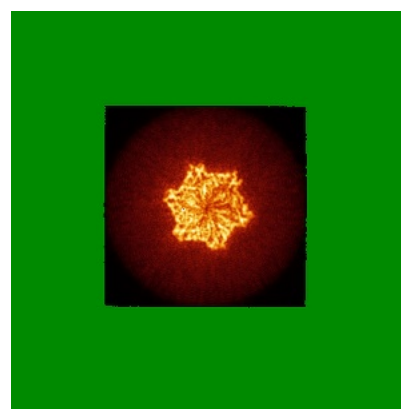
6.4.1 Primary map



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

This section was not generated.

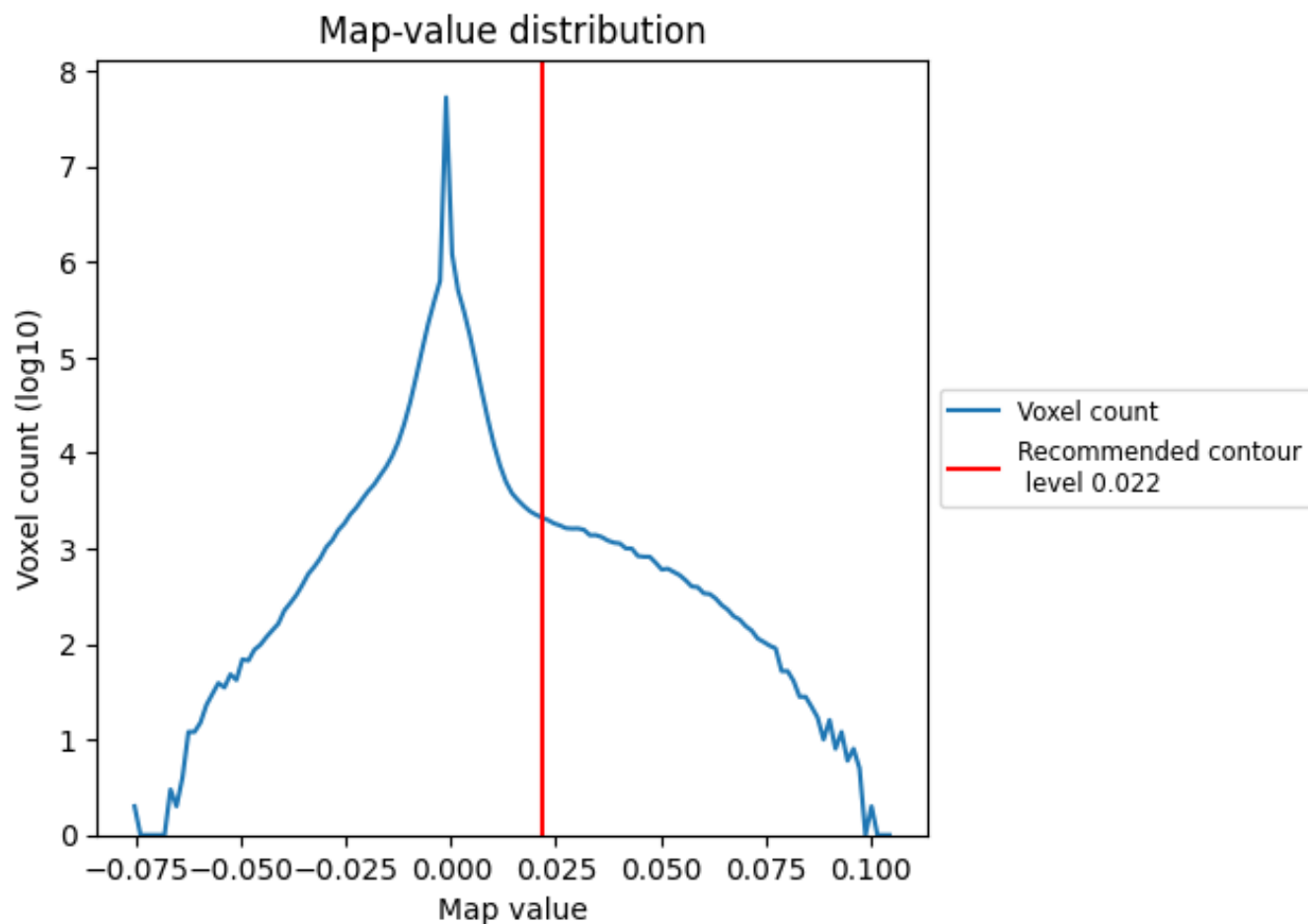
6.6 Mask visualisation

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

7 Map analysis [i](#)

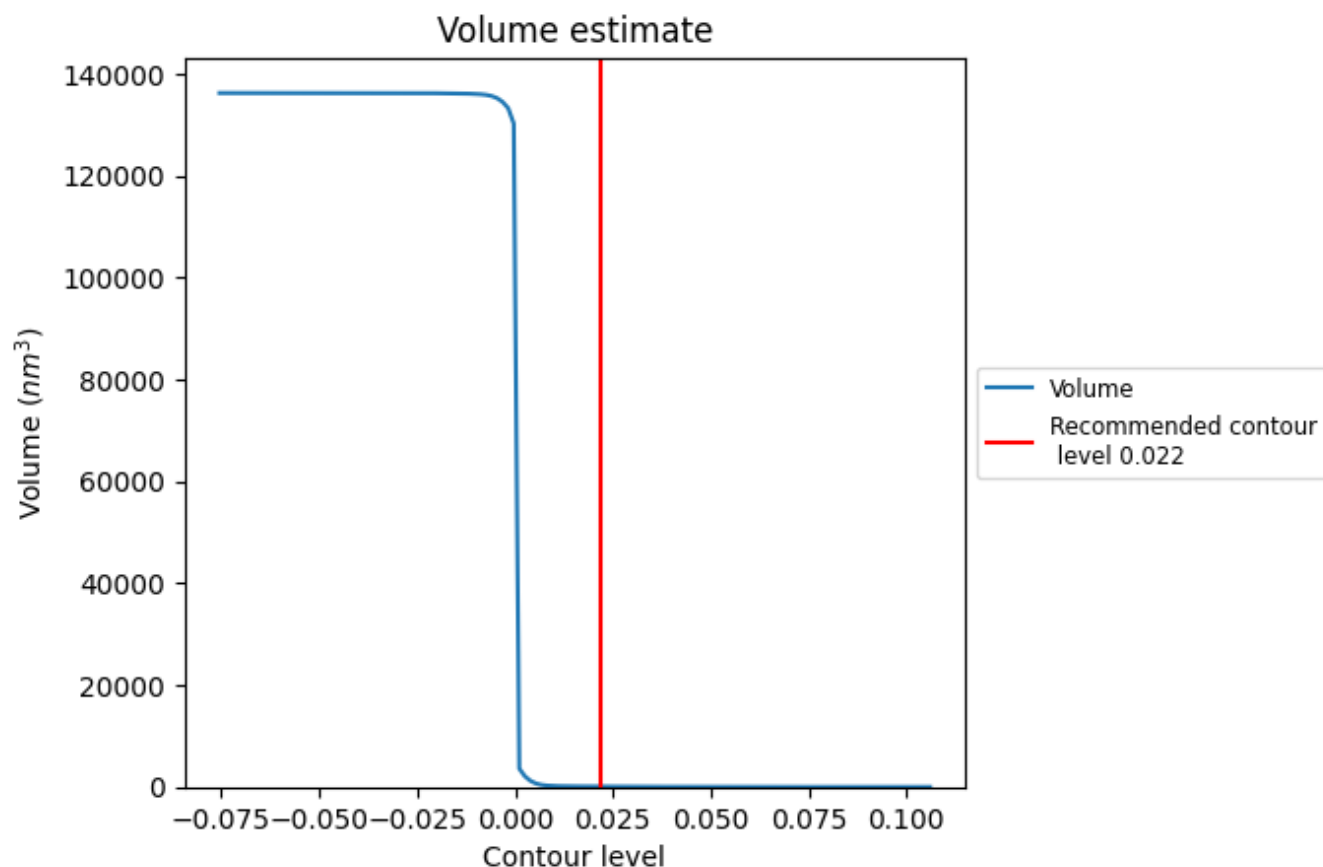
This section contains the results of statistical analysis of the map.

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.

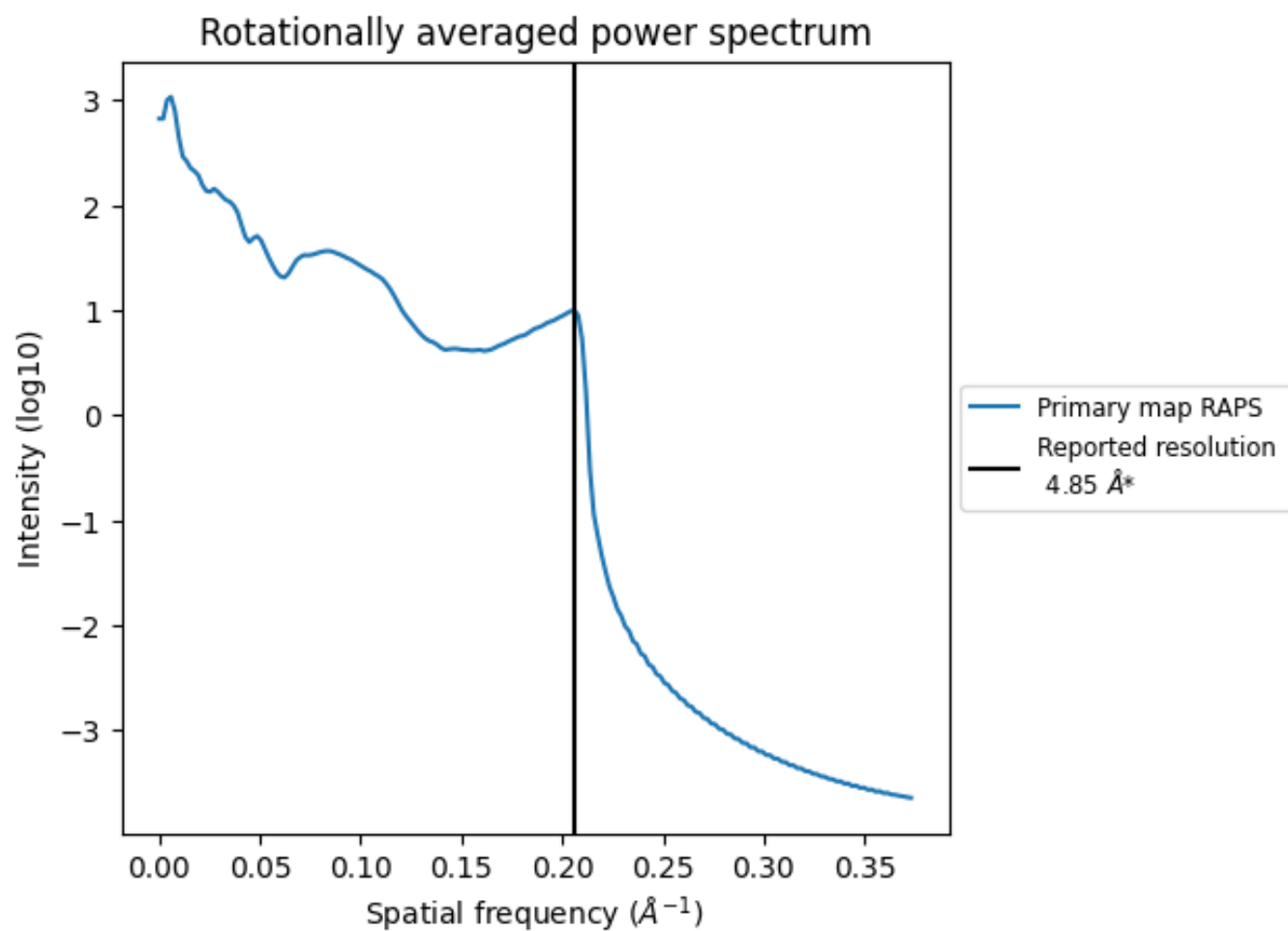
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79 nm^3 ; this corresponds to an approximate mass of 71 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 0.206 Å⁻¹

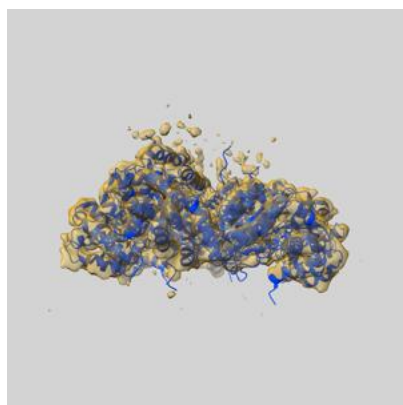
8 Fourier-Shell correlation ⓘ

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

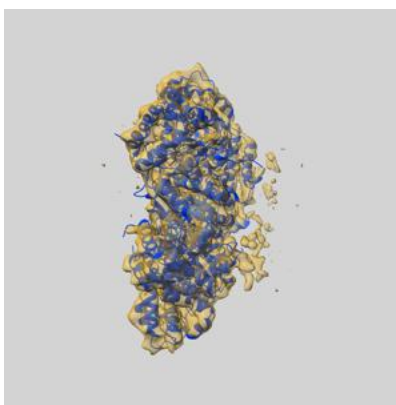
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0209 and PDB model 6HE4. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

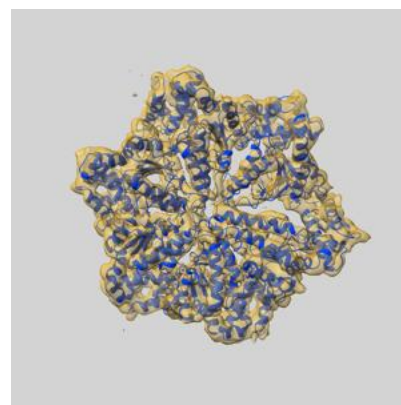
9.1 Map-model overlay [i](#)



X



Y



Z

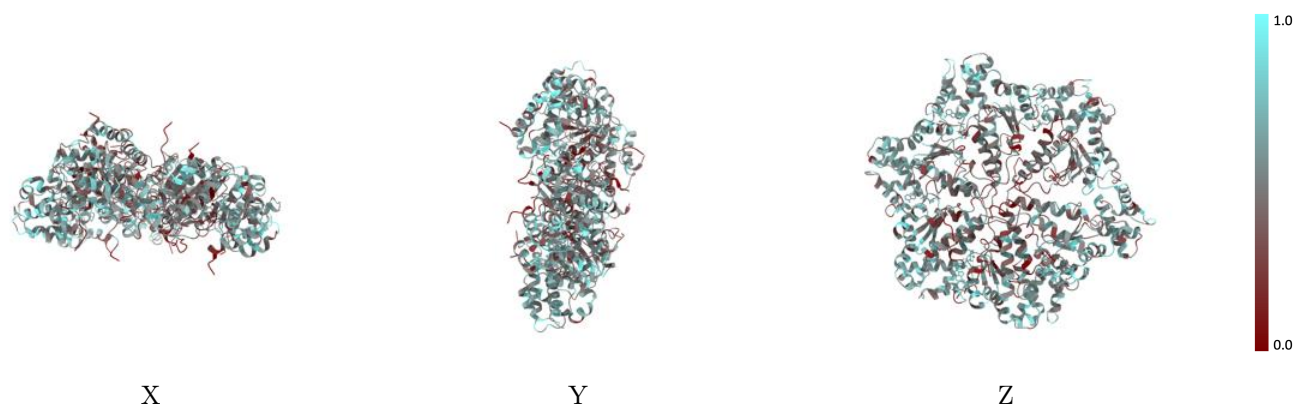
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



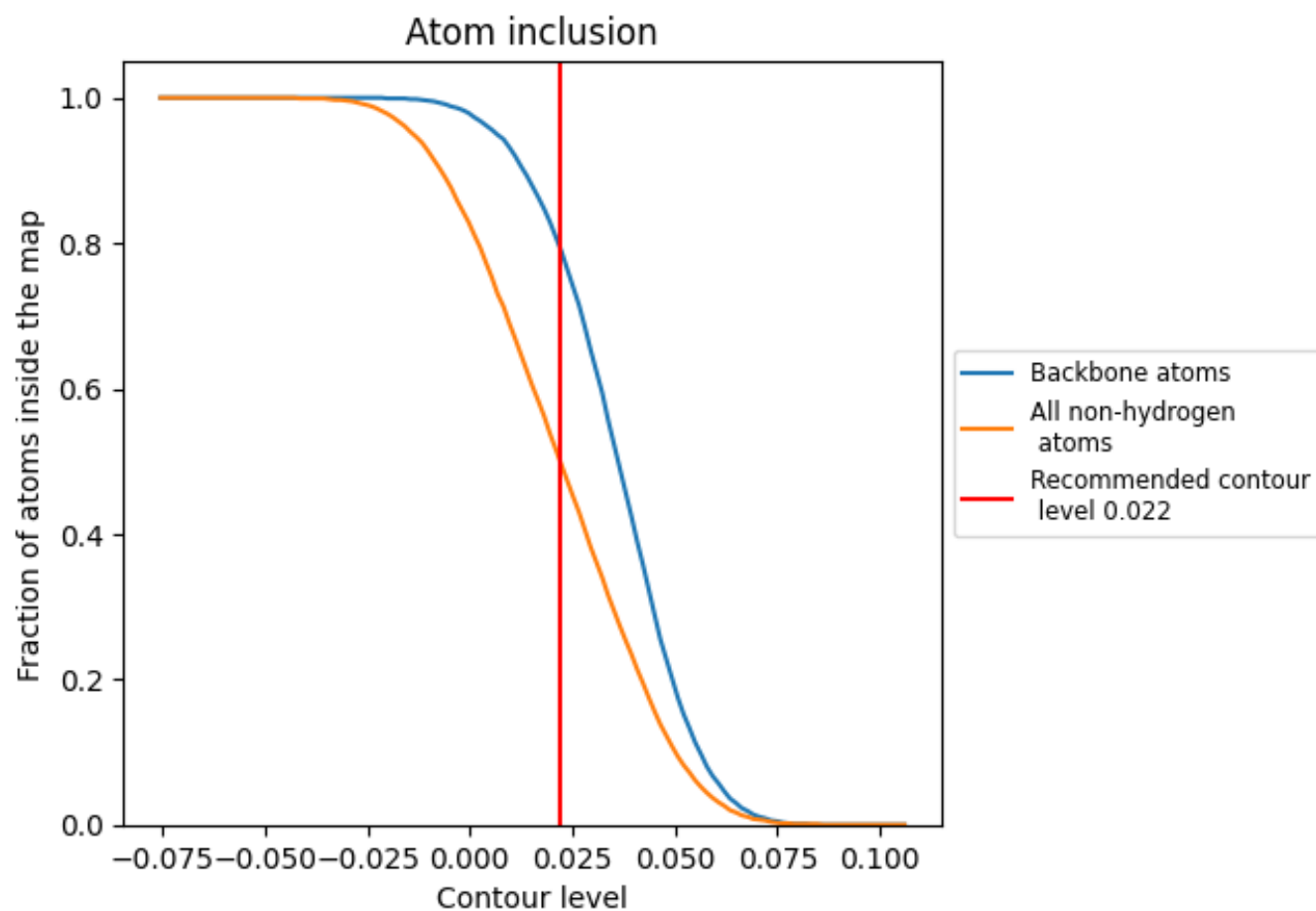
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 50% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5000	0.1820
H	0.5080	0.1880
I	0.4990	0.1760
J	0.5040	0.1780
K	0.5140	0.1880
L	0.5120	0.1960
M	0.4630	0.1670

1.0

0.0

<0.0