



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:53 PM UTC

PDB ID : 9DXK / pdb\_00009dxk  
EMDB ID : EMD-47290  
Title : attPmm bound serine integrase complex in the tetrameric state  
Authors : Shin, H.; Rice, P.A.; Olorunniji, F.J.  
Deposited on : 2024-10-11  
Resolution : 4.81 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](mailto: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>.

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

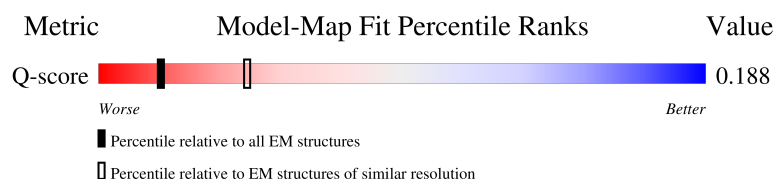
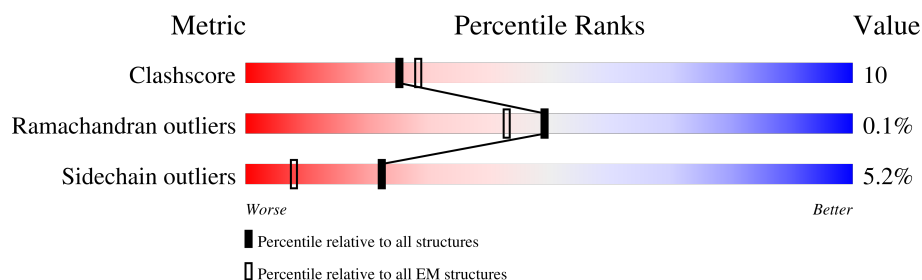
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.81 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	1324 ( 4.31 - 5.30 )

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  $\geq 3$ , 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	545	
1	C	545	
1	I	545	
1	K	545	

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Mol	Chain	Length	Quality of chain
2	E	34	
2	G	34	
2	M	34	
2	O	34	
3	F	33	
3	H	33	
3	N	33	
3	P	33	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 42020 atoms, of which 20174 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 Resolvase homolog YokA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	535	Total	C	H	N	O	S	0	0
			8782	2741	4428	753	841	19		
1	C	535	Total	C	H	N	O	S	0	0
			8782	2741	4428	753	841	19		
1	I	535	Total	C	H	N	O	S	0	0
			8782	2741	4428	753	841	19		
1	K	535	Total	C	H	N	O	S	0	0
			8782	2741	4428	753	841	19		

- Molecule 2 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	28	Total	C	H	N	O	P	0	0
			895	277	321	98	171	28		
2	G	26	Total	C	H	N	O	P	0	0
			831	257	297	94	157	26		
2	M	28	Total	C	H	N	O	P	0	0
			895	277	321	98	171	28		
2	O	28	Total	C	H	N	O	P	0	0
			895	277	321	98	171	28		

- Molecule 3 is a DNA chain called DNA (33-MER).

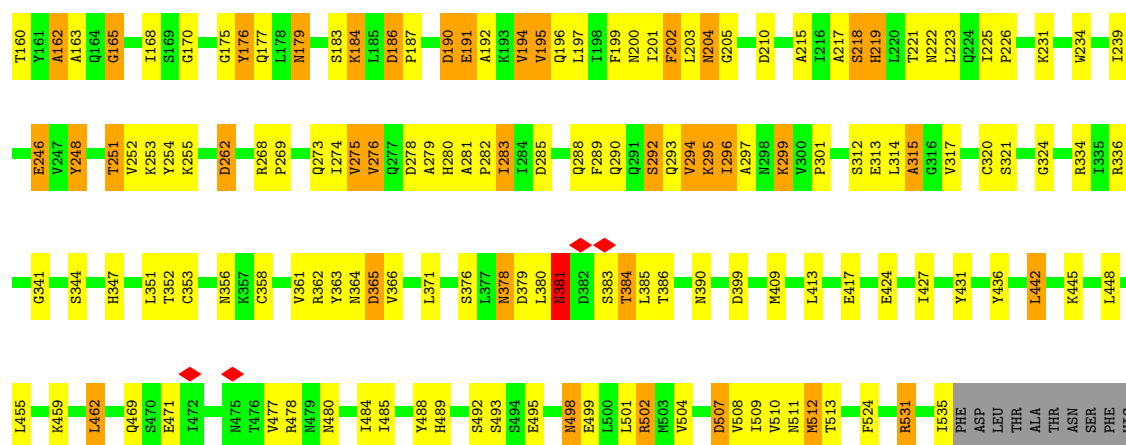
Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	27	Total	C	H	N	O	P	0	0
			859	266	306	100	160	27		
3	H	25	Total	C	H	N	O	P	0	0
			795	246	284	90	150	25		
3	N	27	Total	C	H	N	O	P	0	0
			859	266	306	100	160	27		
3	P	27	Total	C	H	N	O	P	0	0
			859	266	306	100	160	27		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by

depositor).

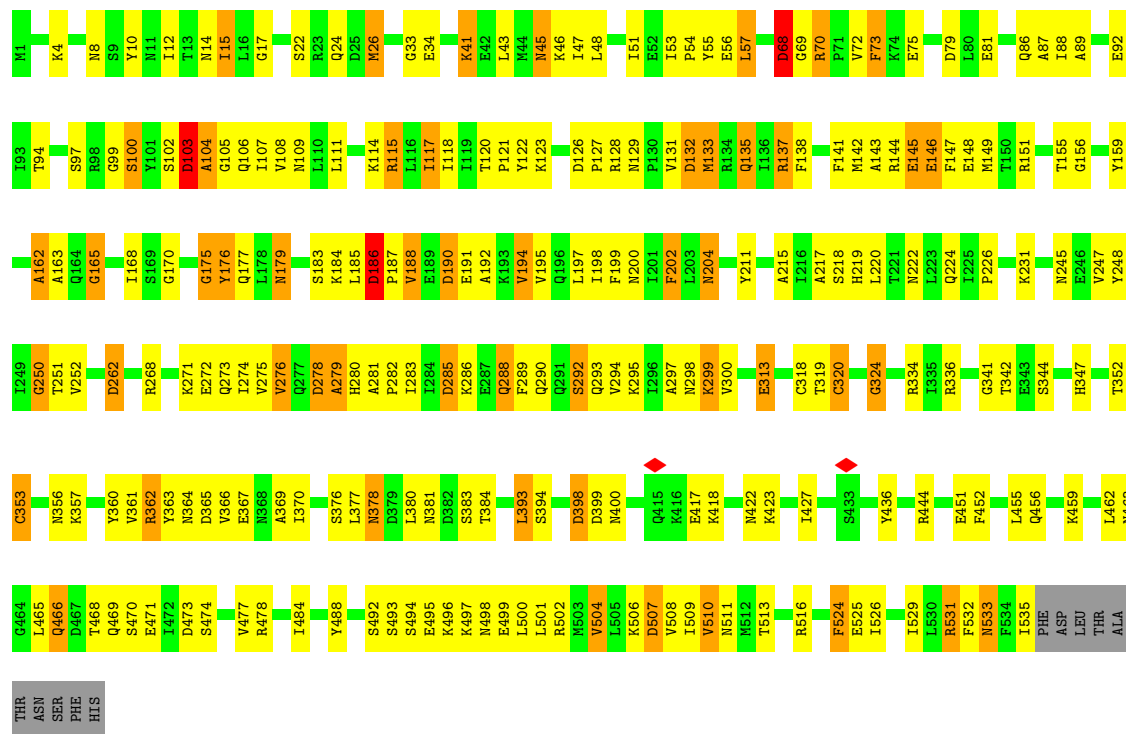
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	C	1	Total 1	Zn 1	0
4	I	1	Total 1	Zn 1	0
4	K	1	Total 1	Zn 1	0





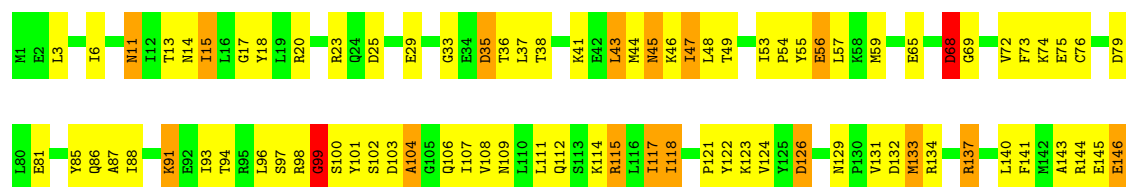
• Molecule 1: Resolvase homolog Yoka

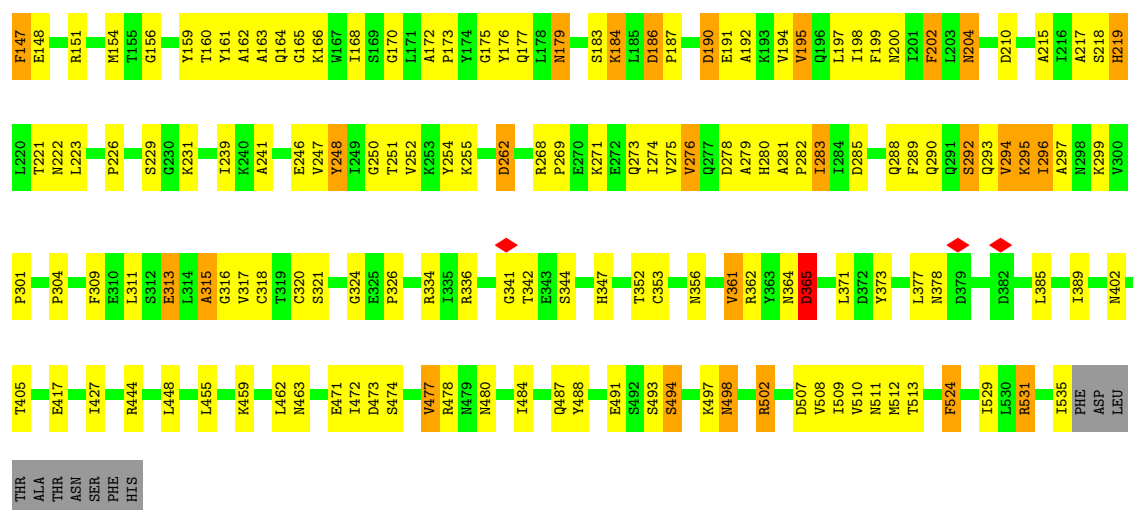
Chain I: 54% 34% 9% ..



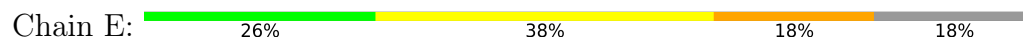
• Molecule 1: Resolvase homolog Yoka

Chain K: 55% 35% 8% ..





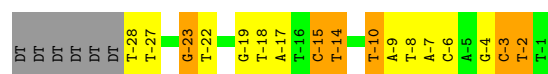
• Molecule 2: DNA (34-MER)



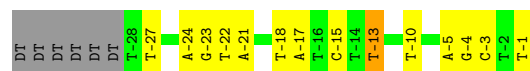
• Molecule 2: DNA (34-MER)



• Molecule 2: DNA (34-MER)



• Molecule 2: DNA (34-MER)



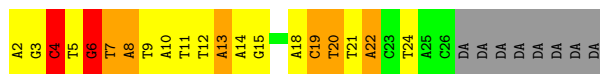
• Molecule 3: DNA (33-MER)





## ● Molecule 3: DNA (33-MER)

Chain H: 



## ● Molecule 3: DNA (33-MER)

Chain N: 



## ● Molecule 3: DNA (33-MER)

Chain P: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92812	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.481	Depositor
Minimum map value	-0.176	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.04	Depositor
Map size ( $\text{\AA}$ )	340.80002, 340.80002, 340.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.065, 1.065, 1.065	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.94	50/4420 (1.1%)	1.95	205/5937 (3.5%)
1	C	1.90	46/4420 (1.0%)	1.92	209/5937 (3.5%)
1	I	1.97	50/4420 (1.1%)	1.99	212/5937 (3.6%)
1	K	1.91	52/4420 (1.2%)	1.93	203/5937 (3.4%)
2	E	0.67	0/642	1.42	2/989 (0.2%)
2	G	0.69	0/598	1.39	3/921 (0.3%)
2	M	0.68	0/642	1.37	1/989 (0.1%)
2	O	0.67	0/642	1.42	3/989 (0.3%)
3	F	0.71	0/620	1.49	2/954 (0.2%)
3	H	0.71	0/572	1.60	6/880 (0.7%)
3	N	0.72	0/620	1.42	2/954 (0.2%)
3	P	0.70	0/620	1.45	6/954 (0.6%)
All	All	1.74	198/22636 (0.9%)	1.84	854/31378 (2.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	5
1	K	0	3
2	E	0	11
2	G	0	12
2	M	0	11
2	O	0	9
3	F	0	13
3	H	0	11
3	N	0	10
3	P	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	95

All (198) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	HIS	CE1-NE2	-8.86	1.23	1.32
1	A	280	HIS	CE1-NE2	-8.85	1.23	1.32
1	C	219	HIS	CE1-NE2	-8.84	1.23	1.32
1	K	280	HIS	CE1-NE2	-8.84	1.23	1.32
1	C	280	HIS	CE1-NE2	-8.82	1.23	1.32
1	I	280	HIS	CE1-NE2	-8.79	1.23	1.32
1	A	347	HIS	ND1-CE1	-8.79	1.23	1.32
1	I	347	HIS	ND1-CE1	-8.75	1.23	1.32
1	K	219	HIS	CE1-NE2	-8.72	1.23	1.32
1	I	219	HIS	CE1-NE2	-8.71	1.23	1.32
1	C	347	HIS	ND1-CE1	-8.64	1.24	1.32
1	K	347	HIS	ND1-CE1	-8.64	1.24	1.32
1	C	134	ARG	CZ-NH2	-8.22	1.22	1.33
1	K	280	HIS	CD2-NE2	-8.21	1.28	1.37
1	C	280	HIS	CD2-NE2	-8.21	1.28	1.37
1	C	137	ARG	CZ-NH2	-8.20	1.22	1.33
1	K	134	ARG	CZ-NH2	-8.15	1.22	1.33
1	A	137	ARG	CZ-NH2	-8.12	1.23	1.33
1	K	219	HIS	CD2-NE2	-8.10	1.28	1.37
1	I	137	ARG	CZ-NH2	-8.10	1.23	1.33
1	C	144	ARG	CZ-NH2	-8.09	1.23	1.33
1	A	362	ARG	CZ-NH2	-8.09	1.23	1.33
1	A	280	HIS	CD2-NE2	-8.09	1.28	1.37
1	A	219	HIS	CD2-NE2	-8.07	1.28	1.37
1	C	115	ARG	CZ-NH2	-8.06	1.23	1.33
1	A	502	ARG	CZ-NH2	-8.06	1.23	1.33
1	I	144	ARG	CZ-NH2	-8.05	1.23	1.33
1	A	115	ARG	CZ-NH2	-8.04	1.23	1.33
1	C	219	HIS	CD2-NE2	-8.04	1.29	1.37
1	I	219	HIS	CD2-NE2	-8.03	1.29	1.37
1	A	144	ARG	CZ-NH2	-8.02	1.23	1.33
1	C	502	ARG	CZ-NH2	-8.01	1.23	1.33
1	A	531	ARG	CZ-NH2	-8.00	1.23	1.33
1	I	115	ARG	CZ-NH2	-7.99	1.23	1.33
1	K	137	ARG	CZ-NH2	-7.98	1.23	1.33
1	C	531	ARG	CZ-NH2	-7.97	1.23	1.33
1	I	502	ARG	CZ-NH2	-7.97	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	115	ARG	CZ-NH2	-7.96	1.23	1.33
1	K	502	ARG	CZ-NH2	-7.96	1.23	1.33
1	I	362	ARG	CZ-NH2	-7.96	1.23	1.33
1	K	144	ARG	CZ-NH2	-7.95	1.23	1.33
1	A	128	ARG	CZ-NH2	-7.95	1.23	1.33
1	I	531	ARG	CZ-NH2	-7.94	1.23	1.33
1	C	362	ARG	CZ-NH2	-7.93	1.23	1.33
1	I	280	HIS	CD2-NE2	-7.92	1.29	1.37
1	K	531	ARG	CZ-NH2	-7.91	1.23	1.33
1	I	128	ARG	CZ-NH2	-7.90	1.23	1.33
1	K	362	ARG	CZ-NH2	-7.87	1.23	1.33
1	A	522	ALA	CA-CB	-7.56	1.42	1.53
1	K	23	ARG	CZ-NH2	-7.20	1.24	1.33
1	A	89	ALA	CA-CB	-7.14	1.42	1.53
1	A	162	ALA	CA-CB	-7.07	1.42	1.53
1	A	192	ALA	CA-CB	-6.90	1.42	1.53
1	A	297	ALA	CA-CB	-6.90	1.42	1.53
1	A	215	ALA	CA-CB	-6.89	1.42	1.53
1	A	143	ALA	CA-CB	-6.81	1.42	1.53
1	I	104	ALA	CA-CB	-6.81	1.42	1.53
1	C	162	ALA	CA-CB	-6.79	1.42	1.53
1	K	241	ALA	CA-CB	-6.79	1.42	1.53
1	I	100	SER	CA-CB	-6.79	1.46	1.54
1	C	143	ALA	CA-CB	-6.78	1.42	1.53
1	C	215	ALA	CA-CB	-6.78	1.42	1.53
1	K	217	ALA	CA-CB	-6.78	1.42	1.53
1	C	192	ALA	CA-CB	-6.78	1.42	1.53
1	K	143	ALA	CA-CB	-6.77	1.42	1.53
1	K	172	ALA	CA-CB	-6.75	1.42	1.53
1	C	163	ALA	CA-CB	-6.74	1.42	1.53
1	C	297	ALA	CA-CB	-6.74	1.43	1.53
1	K	215	ALA	CA-CB	-6.73	1.43	1.53
1	K	162	ALA	CA-CB	-6.71	1.43	1.53
1	I	143	ALA	CA-CB	-6.69	1.43	1.53
1	K	297	ALA	CA-CB	-6.69	1.43	1.53
1	K	192	ALA	CA-CB	-6.68	1.43	1.53
1	I	215	ALA	CA-CB	-6.67	1.43	1.53
1	I	297	ALA	CA-CB	-6.65	1.43	1.53
1	I	162	ALA	CA-CB	-6.65	1.43	1.53
1	C	137	ARG	CZ-NH1	-6.63	1.23	1.32
1	K	163	ALA	CA-CB	-6.63	1.42	1.53
1	K	134	ARG	CZ-NH1	-6.61	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	134	ARG	CZ-NH1	-6.61	1.23	1.32
1	I	192	ALA	CA-CB	-6.58	1.43	1.53
1	A	502	ARG	CZ-NH1	-6.55	1.23	1.32
1	A	531	ARG	CZ-NH1	-6.55	1.23	1.32
1	C	115	ARG	CZ-NH1	-6.53	1.23	1.32
1	C	144	ARG	CZ-NH1	-6.52	1.23	1.32
1	K	87	ALA	CA-CB	-6.51	1.43	1.53
1	K	137	ARG	CZ-NH1	-6.51	1.23	1.32
1	A	115	ARG	CZ-NH1	-6.49	1.23	1.32
1	A	104	ALA	CA-CB	-6.48	1.42	1.53
1	A	137	ARG	CZ-NH1	-6.47	1.23	1.32
1	C	87	ALA	CA-CB	-6.47	1.43	1.53
1	A	362	ARG	CZ-NH1	-6.47	1.23	1.32
1	A	128	ARG	CZ-NH1	-6.46	1.23	1.32
1	C	531	ARG	CZ-NH1	-6.45	1.23	1.32
1	K	362	ARG	CZ-NH1	-6.45	1.23	1.32
1	I	156	GLY	N-CA	-6.45	1.37	1.45
1	C	362	ARG	CZ-NH1	-6.44	1.23	1.32
1	A	87	ALA	CA-CB	-6.44	1.42	1.53
1	A	144	ARG	CZ-NH1	-6.44	1.23	1.32
1	I	137	ARG	CZ-NH1	-6.44	1.23	1.32
1	I	128	ARG	CZ-NH1	-6.43	1.23	1.32
1	I	502	ARG	CZ-NH1	-6.43	1.23	1.32
1	I	362	ARG	CZ-NH1	-6.42	1.23	1.32
1	I	144	ARG	CZ-NH1	-6.42	1.23	1.32
1	C	502	ARG	CZ-NH1	-6.42	1.23	1.32
1	I	115	ARG	CZ-NH1	-6.41	1.23	1.32
1	I	531	ARG	CZ-NH1	-6.41	1.23	1.32
1	C	104	ALA	CA-CB	-6.40	1.42	1.53
1	K	115	ARG	CZ-NH1	-6.40	1.23	1.32
1	K	144	ARG	CZ-NH1	-6.39	1.23	1.32
1	K	502	ARG	CZ-NH1	-6.35	1.23	1.32
1	C	279	ALA	CA-CB	-6.34	1.42	1.53
1	K	104	ALA	CA-CB	-6.33	1.42	1.53
1	K	531	ARG	CZ-NH1	-6.33	1.23	1.32
1	A	156	GLY	N-CA	-6.31	1.37	1.45
1	A	163	ALA	CA-CB	-6.30	1.42	1.53
1	C	156	GLY	N-CA	-6.27	1.37	1.45
1	A	279	ALA	CA-CB	-6.24	1.42	1.53
1	K	279	ALA	CA-CB	-6.21	1.43	1.53
1	K	156	GLY	N-CA	-6.18	1.37	1.45
1	I	163	ALA	CA-CB	-6.16	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	315	ALA	CA-CB	-6.14	1.43	1.53
1	I	89	ALA	CA-CB	-6.11	1.43	1.53
1	K	315	ALA	CA-CB	-6.09	1.43	1.53
1	A	175	GLY	N-CA	-5.75	1.38	1.45
1	I	279	ALA	CA-CB	-5.63	1.43	1.53
1	C	17	GLY	N-CA	-5.62	1.37	1.45
1	I	17	GLY	N-CA	-5.61	1.37	1.45
1	C	362	ARG	CD-NE	-5.60	1.38	1.46
1	K	69	GLY	N-CA	-5.60	1.37	1.45
1	C	33	GLY	N-CA	-5.59	1.37	1.45
1	K	165	GLY	N-CA	-5.58	1.37	1.45
1	I	531	ARG	CD-NE	-5.58	1.38	1.46
1	C	165	GLY	N-CA	-5.58	1.37	1.45
1	A	502	ARG	CD-NE	-5.57	1.38	1.46
1	C	144	ARG	CD-NE	-5.55	1.38	1.46
1	K	33	GLY	N-CA	-5.55	1.37	1.45
1	A	165	GLY	N-CA	-5.54	1.37	1.45
1	I	122	TYR	CA-CB	-5.53	1.46	1.54
1	I	165	GLY	N-CA	-5.52	1.37	1.45
1	K	531	ARG	CD-NE	-5.52	1.38	1.46
1	I	69	GLY	N-CA	-5.51	1.37	1.45
1	I	87	ALA	CA-CB	-5.50	1.43	1.53
1	C	531	ARG	CD-NE	-5.50	1.38	1.46
1	A	531	ARG	CD-NE	-5.49	1.38	1.46
1	K	144	ARG	CD-NE	-5.47	1.38	1.46
1	A	316	GLY	N-CA	-5.45	1.37	1.45
1	C	115	ARG	CD-NE	-5.45	1.38	1.46
1	C	69	GLY	N-CA	-5.44	1.37	1.45
1	K	326	PRO	CA-CB	-5.43	1.46	1.53
1	A	362	ARG	CD-NE	-5.43	1.38	1.46
1	K	362	ARG	CD-NE	-5.42	1.38	1.46
1	K	115	ARG	CD-NE	-5.41	1.38	1.46
1	I	362	ARG	CD-NE	-5.40	1.38	1.46
1	C	137	ARG	CD-NE	-5.40	1.38	1.46
1	I	137	ARG	CD-NE	-5.38	1.38	1.46
1	C	134	ARG	CD-NE	-5.36	1.38	1.46
1	I	280	HIS	CA-CB	-5.36	1.46	1.53
1	A	137	ARG	CD-NE	-5.35	1.38	1.46
1	A	115	ARG	CD-NE	-5.34	1.38	1.46
1	I	115	ARG	CD-NE	-5.34	1.38	1.46
1	A	282	PRO	CA-CB	-5.33	1.46	1.53
1	I	144	ARG	CD-NE	-5.33	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	GLY	N-CA	-5.31	1.37	1.45
1	K	137	ARG	CD-NE	-5.31	1.38	1.46
1	K	502	ARG	CD-NE	-5.26	1.38	1.46
1	I	502	ARG	CD-NE	-5.25	1.38	1.46
1	C	502	ARG	CD-NE	-5.24	1.39	1.46
1	I	179	ASN	CA-CB	-5.22	1.46	1.52
1	K	134	ARG	CD-NE	-5.22	1.39	1.46
1	K	17	GLY	N-CA	-5.21	1.37	1.45
1	I	282	PRO	CA-CB	-5.21	1.46	1.53
1	A	179	ASN	CA-CB	-5.19	1.46	1.52
1	A	226	PRO	CA-CB	-5.19	1.46	1.53
1	I	175	GLY	N-CA	-5.19	1.38	1.45
1	K	99	GLY	N-CA	-5.17	1.37	1.45
1	C	175	GLY	N-CA	-5.17	1.37	1.45
1	I	187	PRO	CA-CB	-5.15	1.47	1.53
1	A	269	PRO	CA-CB	-5.15	1.46	1.53
1	K	316	GLY	N-CA	-5.14	1.38	1.45
1	I	281	ALA	CA-CB	-5.13	1.42	1.53
1	C	269	PRO	CA-CB	-5.12	1.46	1.53
1	C	301	PRO	CA-CB	-5.12	1.47	1.53
1	I	128	ARG	CD-NE	-5.12	1.39	1.46
1	A	281	ALA	CA-CB	-5.11	1.42	1.53
1	A	128	ARG	CD-NE	-5.11	1.39	1.46
1	A	187	PRO	CA-CB	-5.10	1.46	1.53
1	C	226	PRO	CA-CB	-5.10	1.46	1.53
1	K	301	PRO	CA-CB	-5.09	1.47	1.53
1	C	341	GLY	N-CA	-5.09	1.37	1.45
1	I	226	PRO	CA-CB	-5.08	1.47	1.53
1	K	269	PRO	CA-CB	-5.07	1.46	1.53
1	K	226	PRO	CA-CB	-5.05	1.47	1.53
1	A	144	ARG	CD-NE	-5.02	1.39	1.46
1	I	107	ILE	N-CA	-5.02	1.41	1.46
1	A	521	PRO	CA-CB	-5.01	1.47	1.53
1	A	93	ILE	N-CA	-5.00	1.41	1.46
1	K	187	PRO	CA-CB	-5.00	1.47	1.53

All (854) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	-24	DA	C4'-C3'-O3'	9.27	123.91	110.00
1	I	73	PHE	CA-CB-CG	8.30	122.10	113.80
1	I	507	ASP	CA-C-N	8.15	130.71	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	507	ASP	C-N-CA	8.15	130.71	122.96
1	A	73	PHE	CA-CB-CG	8.01	121.81	113.80
1	C	199	PHE	CA-CB-CG	7.08	120.88	113.80
1	K	199	PHE	CA-CB-CG	7.06	120.86	113.80
1	K	282	PRO	CA-C-N	7.04	129.80	121.84
1	K	282	PRO	C-N-CA	7.04	129.80	121.84
1	C	141	PHE	CA-CB-CG	7.03	120.83	113.80
1	K	141	PHE	CA-CB-CG	7.03	120.83	113.80
1	A	141	PHE	CA-CB-CG	6.97	120.78	113.80
1	C	73	PHE	CA-CB-CG	6.97	120.77	113.80
1	A	309	PHE	CA-C-N	6.87	130.63	120.87
1	A	309	PHE	C-N-CA	6.87	130.63	120.87
1	K	73	PHE	CA-CB-CG	6.84	120.64	113.80
1	I	45	ASN	CA-CB-CG	6.78	119.38	112.60
1	I	199	PHE	CA-CB-CG	6.78	120.58	113.80
1	I	268	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	K	268	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	A	312	SER	CA-C-N	6.72	130.90	120.82
1	A	312	SER	C-N-CA	6.72	130.90	120.82
1	A	45	ASN	CA-CB-CG	6.71	119.31	112.60
1	C	45	ASN	CA-CB-CG	6.69	119.29	112.60
1	K	278	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	199	PHE	CA-CB-CG	6.69	120.49	113.80
1	C	282	PRO	CA-C-N	6.66	129.78	121.85
1	C	282	PRO	C-N-CA	6.66	129.78	121.85
1	K	364	ASN	CA-CB-CG	6.66	119.26	112.60
1	K	309	PHE	CA-C-N	6.64	130.92	121.42
1	K	309	PHE	C-N-CA	6.64	130.92	121.42
1	K	347	HIS	CA-CB-CG	6.64	120.44	113.80
1	I	398	ASP	CA-CB-CG	6.64	119.24	112.60
1	K	509	ILE	CA-C-N	6.60	130.62	122.37
1	K	509	ILE	C-N-CA	6.60	130.62	122.37
1	I	14	ASN	CA-C-N	6.59	131.36	123.19
1	I	14	ASN	C-N-CA	6.59	131.36	123.19
1	K	45	ASN	CA-CB-CG	6.58	119.18	112.60
1	C	347	HIS	CA-CB-CG	6.58	120.38	113.80
1	K	103	ASP	CA-CB-CG	6.57	119.17	112.60
1	C	273	GLN	CA-C-N	6.55	131.31	123.19
1	C	273	GLN	C-N-CA	6.55	131.31	123.19
1	A	365	ASP	CA-CB-CG	6.55	119.15	112.60
1	K	231	LYS	CA-C-N	6.54	132.56	122.42
1	K	231	LYS	C-N-CA	6.54	132.56	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	526	ILE	CA-C-N	6.52	131.04	123.15
1	I	526	ILE	C-N-CA	6.52	131.04	123.15
1	C	179	ASN	CA-CB-CG	6.49	119.09	112.60
1	I	298	ASN	CA-CB-CG	6.49	119.09	112.60
1	K	356	ASN	CA-CB-CG	6.46	119.06	112.60
1	I	507	ASP	CA-CB-CG	6.45	119.05	112.60
1	I	300	VAL	N-CA-CB	6.43	116.06	110.08
1	A	103	ASP	CA-CB-CG	6.42	119.02	112.60
1	C	118	ILE	CA-C-N	6.41	131.14	123.19
1	C	118	ILE	C-N-CA	6.41	131.14	123.19
1	A	118	ILE	CA-C-N	6.40	131.13	123.19
1	A	118	ILE	C-N-CA	6.40	131.13	123.19
1	K	186	ASP	CA-CB-CG	6.39	119.00	112.60
1	C	186	ASP	CA-CB-CG	6.39	118.99	112.60
1	C	117	ILE	CA-C-N	6.39	131.43	123.12
1	C	117	ILE	C-N-CA	6.39	131.43	123.12
1	K	35	ASP	CA-CB-CG	6.39	118.99	112.60
1	K	262	ASP	CA-CB-CG	6.38	118.98	112.60
1	I	356	ASN	CA-CB-CG	6.37	118.97	112.60
1	K	118	ILE	CA-C-N	6.37	131.09	123.19
1	K	118	ILE	C-N-CA	6.37	131.09	123.19
1	K	179	ASN	CA-CB-CG	6.37	118.97	112.60
1	K	187	PRO	CA-C-N	6.36	130.45	122.43
1	K	187	PRO	C-N-CA	6.36	130.45	122.43
1	C	356	ASN	CA-CB-CG	6.35	118.95	112.60
1	K	117	ILE	CA-C-N	6.34	131.02	122.90
1	K	117	ILE	C-N-CA	6.34	131.02	122.90
1	A	33	GLY	CA-C-N	6.31	129.67	120.71
1	A	33	GLY	C-N-CA	6.31	129.67	120.71
1	A	117	ILE	CA-C-N	6.31	130.88	122.93
1	A	117	ILE	C-N-CA	6.31	130.88	122.93
1	A	347	HIS	CA-CB-CG	6.29	120.09	113.80
1	I	251	THR	CA-C-N	6.29	131.38	123.14
1	I	251	THR	C-N-CA	6.29	131.38	123.14
1	I	118	ILE	CA-C-N	6.28	131.20	123.10
1	I	118	ILE	C-N-CA	6.28	131.20	123.10
1	A	507	ASP	CA-CB-CG	6.27	118.87	112.60
1	I	141	PHE	CA-CB-CG	6.27	120.07	113.80
3	H	4	DC	C5'-C4'-C3'	-6.26	105.50	114.90
1	I	347	HIS	CA-CB-CG	6.26	120.06	113.80
2	G	-3	DC	C5'-C4'-O4'	6.26	118.78	109.40
1	I	289	PHE	CA-CB-CG	6.24	120.04	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	365	ASP	CA-CB-CG	6.24	118.84	112.60
1	C	289	PHE	CA-CB-CG	6.24	120.04	113.80
1	A	144	ARG	CD-NE-CZ	6.24	133.13	124.40
1	I	190	ASP	CA-CB-CG	6.23	118.83	112.60
1	C	278	ASP	CA-CB-CG	6.23	118.83	112.60
1	C	14	ASN	CA-C-N	6.22	131.29	123.14
1	C	14	ASN	C-N-CA	6.22	131.29	123.14
1	K	334	ARG	CA-C-N	6.22	131.08	122.93
1	K	334	ARG	C-N-CA	6.22	131.08	122.93
1	A	273	GLN	CA-C-N	6.22	131.20	123.12
1	A	273	GLN	C-N-CA	6.22	131.20	123.12
1	I	498	ASN	CA-CB-CG	6.21	118.81	112.60
1	A	498	ASN	CA-CB-CG	6.20	118.80	112.60
1	C	507	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	298	ASN	CA-CB-CG	6.19	118.79	112.60
1	I	509	ILE	CA-C-N	6.19	130.87	123.19
1	I	509	ILE	C-N-CA	6.19	130.87	123.19
1	K	268	ARG	NE-CZ-NH1	-6.18	115.32	121.50
1	I	194	VAL	CA-C-N	6.17	128.33	120.56
1	I	194	VAL	C-N-CA	6.17	128.33	120.56
1	I	273	GLN	CA-C-N	6.16	131.00	122.93
1	I	273	GLN	C-N-CA	6.16	131.00	122.93
1	I	179	ASN	CA-CB-CG	6.16	118.76	112.60
1	K	248	TYR	CA-C-N	6.13	129.86	122.26
1	K	248	TYR	C-N-CA	6.13	129.86	122.26
1	C	365	ASP	CA-CB-CG	6.11	118.71	112.60
1	C	187	PRO	CA-C-N	6.09	130.10	122.43
1	C	187	PRO	C-N-CA	6.09	130.10	122.43
1	C	364	ASN	CA-CB-CG	6.09	118.69	112.60
1	A	14	ASN	CA-C-N	6.08	131.19	123.10
1	A	14	ASN	C-N-CA	6.08	131.19	123.10
1	K	344	SER	CA-C-N	6.08	130.68	122.90
1	K	344	SER	C-N-CA	6.08	130.68	122.90
3	N	2	DA	O5'-C5'-C4'	6.07	119.91	110.80
1	A	115	ARG	CD-NE-CZ	6.07	132.89	124.40
1	C	103	ASP	CA-CB-CG	6.07	118.67	112.60
1	I	115	ARG	CD-NE-CZ	6.07	132.90	124.40
1	C	248	TYR	CA-C-N	6.06	129.78	122.26
1	C	248	TYR	C-N-CA	6.06	129.78	122.26
1	C	251	THR	CA-C-N	6.06	131.16	123.10
1	C	251	THR	C-N-CA	6.06	131.16	123.10
1	I	511	ASN	CA-CB-CG	6.05	118.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	202	PHE	CA-CB-CG	6.05	119.85	113.80
1	K	336	ARG	CA-C-N	6.04	130.46	122.42
1	K	336	ARG	C-N-CA	6.04	130.46	122.42
1	K	289	PHE	CA-CB-CG	6.04	119.84	113.80
1	A	342	THR	CA-C-N	6.02	130.43	122.30
1	A	342	THR	C-N-CA	6.02	130.43	122.30
1	C	509	ILE	CA-C-N	6.02	130.60	122.90
1	C	509	ILE	C-N-CA	6.02	130.60	122.90
1	I	342	THR	CA-C-N	6.01	130.42	122.42
1	I	342	THR	C-N-CA	6.01	130.42	122.42
1	A	179	ASN	CA-CB-CG	6.00	118.60	112.60
1	A	128	ARG	CD-NE-CZ	5.99	132.78	124.40
1	A	79	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	202	PHE	CA-CB-CG	5.99	119.78	113.80
1	I	128	ARG	CD-NE-CZ	5.98	132.77	124.40
1	A	511	ASN	CA-CB-CG	5.97	118.58	112.60
1	K	134	ARG	CD-NE-CZ	5.97	132.76	124.40
1	A	190	ASP	CA-CB-CG	5.95	118.55	112.60
1	K	115	ARG	CD-NE-CZ	5.95	132.73	124.40
1	C	115	ARG	CD-NE-CZ	5.94	132.72	124.40
1	A	187	PRO	CA-C-N	5.93	130.70	122.93
1	A	187	PRO	C-N-CA	5.93	130.70	122.93
1	K	342	THR	CA-C-N	5.92	130.29	122.30
1	K	342	THR	C-N-CA	5.92	130.29	122.30
1	C	134	ARG	CD-NE-CZ	5.92	132.69	124.40
1	K	33	GLY	CA-C-N	5.92	130.64	122.77
1	K	33	GLY	C-N-CA	5.92	130.64	122.77
3	H	19	DC	C4'-C3'-O3'	5.92	118.88	110.00
1	A	222	ASN	CA-CB-CG	5.91	118.51	112.60
1	A	300	VAL	N-CA-CB	5.91	115.58	110.08
1	C	511	ASN	CA-CB-CG	5.91	118.51	112.60
1	K	87	ALA	CA-C-N	5.91	130.72	123.10
1	K	87	ALA	C-N-CA	5.91	130.72	123.10
1	A	347	HIS	N-CA-CB	5.91	118.80	110.24
1	C	507	ASP	CA-C-N	5.91	130.73	123.17
1	C	507	ASP	C-N-CA	5.91	130.73	123.17
1	I	117	ILE	CA-C-N	5.91	130.80	123.12
1	I	117	ILE	C-N-CA	5.91	130.80	123.12
1	C	194	VAL	CA-C-N	5.90	127.99	120.56
1	C	194	VAL	C-N-CA	5.90	127.99	120.56
1	K	498	ASN	CA-CB-CG	5.90	118.50	112.60
1	I	364	ASN	CA-CB-CG	5.88	118.48	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	87	ALA	CA-C-N	5.88	130.76	123.12
1	I	87	ALA	C-N-CA	5.88	130.76	123.12
1	I	141	PHE	CA-C-N	5.88	128.41	120.65
1	I	141	PHE	C-N-CA	5.88	128.41	120.65
1	K	14	ASN	CA-C-N	5.87	131.16	122.99
1	K	14	ASN	C-N-CA	5.87	131.16	122.99
1	K	511	ASN	CA-CB-CG	5.87	118.47	112.60
1	K	194	VAL	CA-C-N	5.87	127.95	120.56
1	K	194	VAL	C-N-CA	5.87	127.95	120.56
1	K	222	ASN	CA-CB-CG	5.86	118.46	112.60
1	I	222	ASN	CA-CB-CG	5.86	118.46	112.60
1	C	222	ASN	CA-CB-CG	5.85	118.45	112.60
1	I	144	ARG	CD-NE-CZ	5.85	132.59	124.40
1	K	365	ASP	CA-CB-CG	5.85	118.45	112.60
1	C	87	ALA	CA-C-N	5.85	130.64	123.10
1	C	87	ALA	C-N-CA	5.85	130.64	123.10
1	A	179	ASN	N-CA-CB	5.84	118.72	110.24
1	I	187	PRO	CA-C-N	5.84	130.38	122.90
1	I	187	PRO	C-N-CA	5.84	130.38	122.90
1	K	273	GLN	CA-C-N	5.84	131.11	122.99
1	K	273	GLN	C-N-CA	5.84	131.11	122.99
1	C	190	ASP	CA-CB-CG	5.84	118.44	112.60
1	C	512	MET	CA-C-N	5.83	128.57	120.29
1	C	512	MET	C-N-CA	5.83	128.57	120.29
1	C	46	LYS	CA-C-N	5.83	127.90	120.56
1	C	46	LYS	C-N-CA	5.83	127.90	120.56
1	A	194	VAL	CA-C-N	5.82	127.89	120.56
1	A	194	VAL	C-N-CA	5.82	127.89	120.56
1	A	148	GLU	CA-C-N	5.81	128.32	120.65
1	A	148	GLU	C-N-CA	5.81	128.32	120.65
1	A	250	GLY	CA-C-N	5.80	129.72	121.42
1	A	250	GLY	C-N-CA	5.80	129.72	121.42
2	O	-23	DG	O4'-C1'-C2'	-5.80	97.69	106.40
1	I	344	SER	CA-C-N	5.80	130.66	123.12
1	I	344	SER	C-N-CA	5.80	130.66	123.12
1	C	106	GLN	CA-C-N	5.78	127.85	120.56
1	C	106	GLN	C-N-CA	5.78	127.85	120.56
1	K	251	THR	CA-C-N	5.78	130.87	123.13
1	K	251	THR	C-N-CA	5.78	130.87	123.13
1	I	504	VAL	CA-C-N	5.78	130.35	122.84
1	I	504	VAL	C-N-CA	5.78	130.35	122.84
1	A	509	ILE	CA-C-N	5.77	131.17	122.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	ILE	C-N-CA	5.77	131.17	122.91
1	C	79	ASP	CA-C-N	5.77	127.94	120.44
1	C	79	ASP	C-N-CA	5.77	127.94	120.44
1	C	524	PHE	CA-C-N	5.77	132.10	121.94
1	C	524	PHE	C-N-CA	5.77	132.10	121.94
1	A	364	ASN	CA-CB-CG	5.77	118.37	112.60
1	A	87	ALA	CA-C-N	5.76	130.34	123.19
1	A	87	ALA	C-N-CA	5.76	130.34	123.19
1	A	295	LYS	CA-C-N	5.76	127.91	120.70
1	A	295	LYS	C-N-CA	5.76	127.91	120.70
1	K	190	ASP	CA-CB-CG	5.76	118.36	112.60
1	I	352	THR	CA-C-N	5.75	130.56	122.05
1	I	352	THR	C-N-CA	5.75	130.56	122.05
1	C	510	VAL	CA-C-N	5.75	131.09	123.05
1	C	510	VAL	C-N-CA	5.75	131.09	123.05
1	I	353	CYS	N-CA-CB	5.75	117.54	110.53
2	O	-17	DA	C4'-C3'-O3'	5.74	118.61	110.00
1	A	251	THR	CA-C-N	5.74	130.97	122.99
1	A	251	THR	C-N-CA	5.74	130.97	122.99
1	K	79	ASP	CA-C-N	5.74	127.90	120.44
1	K	79	ASP	C-N-CA	5.74	127.90	120.44
1	A	297	ALA	CA-C-N	5.74	129.03	120.31
1	A	297	ALA	C-N-CA	5.74	129.03	120.31
1	A	510	VAL	CA-C-N	5.73	130.85	122.77
1	A	510	VAL	C-N-CA	5.73	130.85	122.77
1	K	46	LYS	CA-C-N	5.73	127.78	120.56
1	K	46	LYS	C-N-CA	5.73	127.78	120.56
1	C	336	ARG	CA-C-N	5.72	130.03	122.42
1	C	336	ARG	C-N-CA	5.72	130.03	122.42
1	K	106	GLN	CA-C-N	5.72	127.77	120.56
1	K	106	GLN	C-N-CA	5.72	127.77	120.56
1	K	352	THR	CA-C-N	5.72	130.74	122.16
1	K	352	THR	C-N-CA	5.72	130.74	122.16
3	H	19	DC	C5'-C4'-O4'	5.72	117.98	109.40
1	K	361	VAL	CA-C-N	5.72	129.68	121.50
1	K	361	VAL	C-N-CA	5.72	129.68	121.50
1	I	219	HIS	N-CA-CB	5.71	118.30	110.01
1	I	510	VAL	CA-C-N	5.71	131.06	123.00
1	I	510	VAL	C-N-CA	5.71	131.06	123.00
1	A	184	LYS	CA-C-N	5.71	128.94	120.95
1	A	184	LYS	C-N-CA	5.71	128.94	120.95
1	C	276	VAL	CA-C-N	5.71	128.97	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	VAL	C-N-CA	5.71	128.97	120.87
1	A	88	ILE	CA-C-N	5.70	130.86	123.00
1	A	88	ILE	C-N-CA	5.70	130.86	123.00
1	K	184	LYS	CA-C-N	5.70	128.96	120.87
1	K	184	LYS	C-N-CA	5.70	128.96	120.87
1	C	498	ASN	CA-CB-CG	5.70	118.30	112.60
1	K	512	MET	CA-C-N	5.70	128.38	120.29
1	K	512	MET	C-N-CA	5.70	128.38	120.29
1	I	276	VAL	CA-C-N	5.69	129.56	121.42
1	I	276	VAL	C-N-CA	5.69	129.56	121.42
1	I	524	PHE	CA-C-N	5.69	131.95	122.73
1	I	524	PHE	C-N-CA	5.69	131.95	122.73
1	K	524	PHE	CA-C-N	5.69	131.95	121.94
1	K	524	PHE	C-N-CA	5.69	131.95	121.94
1	I	533	ASN	CA-CB-CG	5.69	118.29	112.60
1	I	184	LYS	CA-C-N	5.68	128.84	120.82
1	I	184	LYS	C-N-CA	5.68	128.84	120.82
1	I	121	PRO	CA-C-N	5.68	131.42	122.11
1	I	121	PRO	C-N-CA	5.68	131.42	122.11
1	I	179	ASN	N-CA-CB	5.68	118.47	110.24
1	I	274	ILE	CA-C-N	5.67	130.64	123.10
1	I	274	ILE	C-N-CA	5.67	130.64	123.10
3	P	19	DC	C4'-C3'-O3'	5.67	118.50	110.00
1	A	141	PHE	CA-C-N	5.67	127.81	120.44
1	A	141	PHE	C-N-CA	5.67	127.81	120.44
1	C	362	ARG	CA-C-N	5.66	128.13	120.65
1	C	362	ARG	C-N-CA	5.66	128.13	120.65
3	P	14	DA	C2'-C3'-O3'	5.66	120.00	111.50
1	A	41	LYS	CA-CB-CG	5.65	125.39	114.10
1	K	271	LYS	CA-C-N	5.64	128.12	120.44
1	K	271	LYS	C-N-CA	5.64	128.12	120.44
1	I	299	LYS	N-CA-CB	5.64	118.32	109.69
1	A	299	LYS	N-CA-CB	5.64	118.32	109.69
1	A	275	VAL	CA-C-N	5.64	130.69	123.13
1	A	275	VAL	C-N-CA	5.64	130.69	123.13
1	A	271	LYS	CA-C-N	5.64	128.29	120.29
1	A	271	LYS	C-N-CA	5.64	128.29	120.29
1	I	185	LEU	CA-C-N	5.63	131.57	121.76
1	I	185	LEU	C-N-CA	5.63	131.57	121.76
3	H	6	DG	C2'-C3'-O3'	5.63	119.95	111.50
1	A	219	HIS	N-CA-CB	5.63	118.17	110.01
1	A	289	PHE	N-CA-CB	5.62	118.16	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	510	VAL	CA-C-N	5.62	130.92	123.05
1	K	510	VAL	C-N-CA	5.62	130.92	123.05
3	P	16	DA	C2'-C3'-O3'	5.62	119.93	111.50
1	C	219	HIS	CA-CB-CG	5.62	119.42	113.80
1	C	352	THR	CA-C-N	5.62	130.59	122.16
1	C	352	THR	C-N-CA	5.62	130.59	122.16
1	C	268	ARG	CD-NE-CZ	5.62	132.26	124.40
1	K	72	VAL	N-CA-CB	5.61	116.74	110.51
1	A	344	SER	CA-C-N	5.61	130.08	122.90
1	A	344	SER	C-N-CA	5.61	130.08	122.90
1	I	197	LEU	CA-C-N	5.61	127.63	120.56
1	I	197	LEU	C-N-CA	5.61	127.63	120.56
1	I	347	HIS	N-CA-CB	5.61	118.65	110.58
3	H	20	DT	C4'-C3'-O3'	5.61	118.41	110.00
1	K	498	ASN	CA-C-N	5.60	127.72	120.44
1	K	498	ASN	C-N-CA	5.60	127.72	120.44
1	A	174	TYR	CA-C-N	5.59	129.34	123.08
1	A	174	TYR	C-N-CA	5.59	129.34	123.08
1	C	312	SER	CA-C-N	5.58	127.76	120.28
1	C	312	SER	C-N-CA	5.58	127.76	120.28
1	C	72	VAL	N-CA-CB	5.58	116.70	110.51
1	C	344	SER	CA-C-N	5.58	130.23	122.93
1	C	344	SER	C-N-CA	5.58	130.23	122.93
1	K	276	VAL	CA-C-N	5.58	128.63	120.71
1	K	276	VAL	C-N-CA	5.58	128.63	120.71
1	I	148	GLU	CA-C-N	5.57	127.69	120.44
1	I	148	GLU	C-N-CA	5.57	127.69	120.44
1	K	283	ILE	CA-C-N	5.57	130.75	123.06
1	K	283	ILE	C-N-CA	5.57	130.75	123.06
1	C	294	VAL	CA-C-N	5.56	127.67	120.44
1	C	294	VAL	C-N-CA	5.56	127.67	120.44
1	I	369	ALA	CA-C-N	5.56	127.56	120.56
1	I	369	ALA	C-N-CA	5.56	127.56	120.56
1	A	185	LEU	CA-C-N	5.55	131.42	121.76
1	A	185	LEU	C-N-CA	5.55	131.42	121.76
1	C	295	LYS	CA-C-N	5.55	127.64	120.70
1	C	295	LYS	C-N-CA	5.55	127.64	120.70
1	C	231	LYS	CA-C-N	5.55	132.23	122.79
1	C	231	LYS	C-N-CA	5.55	132.23	122.79
1	I	271	LYS	CA-C-N	5.55	127.72	120.28
1	I	271	LYS	C-N-CA	5.55	127.72	120.28
1	A	276	VAL	CA-C-N	5.55	129.35	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	VAL	C-N-CA	5.55	129.35	121.42
2	E	-17	DA	C4'-C3'-O3'	5.55	118.32	110.00
1	K	268	ARG	CD-NE-CZ	5.54	132.16	124.40
1	A	508	VAL	CA-C-N	5.53	129.40	122.48
1	A	508	VAL	C-N-CA	5.53	129.40	122.48
1	A	283	ILE	CA-C-N	5.53	130.69	123.06
1	A	283	ILE	C-N-CA	5.53	130.69	123.06
1	C	347	HIS	N-CA-CB	5.53	118.26	110.24
1	C	219	HIS	CA-C-N	5.52	127.62	120.44
1	C	219	HIS	C-N-CA	5.52	127.62	120.44
1	K	202	PHE	N-CA-CB	5.52	117.97	109.91
1	A	68	ASP	CA-CB-CG	5.51	118.11	112.60
1	K	43	LEU	CA-C-N	5.51	127.60	120.44
1	K	43	LEU	C-N-CA	5.51	127.60	120.44
1	A	248	TYR	CA-C-N	5.51	129.09	122.26
1	A	248	TYR	C-N-CA	5.51	129.09	122.26
1	I	289	PHE	N-CA-CB	5.50	117.99	110.01
1	C	202	PHE	N-CA-CB	5.50	117.94	109.91
1	K	56	GLU	CA-C-N	5.50	130.75	123.05
1	K	56	GLU	C-N-CA	5.50	130.75	123.05
1	K	341	GLY	CA-C-N	5.50	129.29	121.42
1	K	341	GLY	C-N-CA	5.50	129.29	121.42
1	K	197	LEU	CA-C-N	5.50	127.49	120.56
1	K	197	LEU	C-N-CA	5.50	127.49	120.56
1	K	219	HIS	CA-CB-CG	5.50	119.30	113.80
1	K	192	ALA	CA-C-N	5.50	127.59	120.44
1	K	192	ALA	C-N-CA	5.50	127.59	120.44
3	P	4	DC	C4'-C3'-O3'	-5.50	101.76	110.00
1	A	497	LYS	CA-C-N	5.49	127.58	120.44
1	A	497	LYS	C-N-CA	5.49	127.58	120.44
1	C	192	ALA	CA-C-N	5.49	127.58	120.44
1	C	192	ALA	C-N-CA	5.49	127.58	120.44
1	A	215	ALA	CA-C-N	5.49	127.48	120.56
1	A	215	ALA	C-N-CA	5.49	127.48	120.56
1	A	334	ARG	CA-C-N	5.49	130.40	123.10
1	A	334	ARG	C-N-CA	5.49	130.40	123.10
1	K	219	HIS	CA-C-N	5.48	127.63	120.28
1	K	219	HIS	C-N-CA	5.48	127.63	120.28
1	A	56	GLU	CA-C-N	5.48	130.72	123.00
1	A	56	GLU	C-N-CA	5.48	130.72	123.00
1	C	33	GLY	CA-C-N	5.48	130.72	123.05
1	C	33	GLY	C-N-CA	5.48	130.72	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	16	DA	C5'-C4'-O4'	5.48	117.61	109.40
1	I	70	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	I	202	PHE	N-CA-CB	5.47	117.90	109.91
1	C	197	LEU	CA-C-N	5.47	127.45	120.56
1	C	197	LEU	C-N-CA	5.47	127.45	120.56
1	K	239	ILE	N-CA-CB	5.47	116.36	110.62
1	C	365	ASP	CA-C-N	5.46	127.45	120.56
1	C	365	ASP	C-N-CA	5.46	127.45	120.56
2	G	-17	DA	C4'-C3'-O3'	5.46	118.20	110.00
1	I	324	GLY	CA-C-N	5.46	127.99	120.67
1	I	324	GLY	C-N-CA	5.46	127.99	120.67
1	C	283	ILE	CA-C-N	5.45	130.59	123.06
1	C	283	ILE	C-N-CA	5.45	130.59	123.06
1	A	352	THR	CA-C-N	5.45	130.33	122.16
1	A	352	THR	C-N-CA	5.45	130.33	122.16
1	C	140	LEU	CA-C-N	5.45	127.89	120.54
1	C	140	LEU	C-N-CA	5.45	127.89	120.54
1	A	79	ASP	CA-C-N	5.44	127.52	120.44
1	A	79	ASP	C-N-CA	5.44	127.52	120.44
1	C	91	LYS	CA-CB-CG	5.44	124.98	114.10
1	I	513	THR	CA-C-N	5.44	130.66	122.99
1	I	513	THR	C-N-CA	5.44	130.66	122.99
1	A	40	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	C	151	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	K	320	CYS	N-CA-CB	5.44	118.04	109.83
1	I	506	LYS	N-CA-CB	5.44	117.95	110.07
1	C	502	ARG	CD-NE-CZ	5.43	132.00	124.40
1	C	320	CYS	N-CA-CB	5.43	117.94	109.85
1	C	3	LEU	N-CA-C	-5.43	105.96	113.18
1	C	43	LEU	CA-C-N	5.42	127.49	120.44
1	C	43	LEU	C-N-CA	5.42	127.49	120.44
1	C	184	LYS	CA-C-N	5.42	128.93	120.75
1	C	184	LYS	C-N-CA	5.42	128.93	120.75
1	K	47	ILE	CA-C-N	5.42	127.54	120.28
1	K	47	ILE	C-N-CA	5.42	127.54	120.28
1	I	41	LYS	CA-CB-CG	5.42	124.94	114.10
1	A	347	HIS	CE1-NE2-CD2	-5.42	103.58	109.00
1	C	47	ILE	CA-C-N	5.41	127.53	120.28
1	C	47	ILE	C-N-CA	5.41	127.53	120.28
1	K	218	SER	CA-C-N	5.41	127.84	120.54
1	K	218	SER	C-N-CA	5.41	127.84	120.54
1	I	41	LYS	CA-C-N	5.41	127.47	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	41	LYS	C-N-CA	5.41	127.47	120.44
1	K	493	SER	CA-C-N	5.40	127.46	120.44
1	K	493	SER	C-N-CA	5.40	127.46	120.44
1	K	347	HIS	CE1-NE2-CD2	-5.40	103.60	109.00
1	I	248	TYR	CA-C-N	5.40	131.09	122.56
1	I	248	TYR	C-N-CA	5.40	131.09	122.56
1	K	76	CYS	CA-C-N	5.39	127.45	120.44
1	K	76	CYS	C-N-CA	5.39	127.45	120.44
1	I	492	SER	CA-C-N	5.39	128.42	120.82
1	I	492	SER	C-N-CA	5.39	128.42	120.82
1	K	221	THR	CA-C-N	5.39	127.45	120.44
1	K	221	THR	C-N-CA	5.39	127.45	120.44
1	C	45	ASN	CA-C-N	5.39	127.82	120.54
1	C	45	ASN	C-N-CA	5.39	127.82	120.54
1	I	497	LYS	CA-C-N	5.39	127.44	120.44
1	I	497	LYS	C-N-CA	5.39	127.44	120.44
1	C	68	ASP	CA-CB-CG	5.39	117.99	112.60
1	I	106	GLN	CA-C-N	5.39	127.55	120.60
1	I	106	GLN	C-N-CA	5.39	127.55	120.60
1	I	494	SER	CA-C-N	5.39	127.44	120.44
1	I	494	SER	C-N-CA	5.39	127.44	120.44
1	C	493	SER	CA-C-N	5.38	127.49	120.28
1	C	493	SER	C-N-CA	5.38	127.49	120.28
1	K	75	GLU	CA-C-N	5.38	127.44	120.44
1	K	75	GLU	C-N-CA	5.38	127.44	120.44
1	C	218	SER	CA-C-N	5.38	127.80	120.54
1	C	218	SER	C-N-CA	5.38	127.80	120.54
1	C	347	HIS	CE1-NE2-CD2	-5.38	103.62	109.00
1	I	46	LYS	CA-C-N	5.38	127.42	120.70
1	I	46	LYS	C-N-CA	5.38	127.42	120.70
2	M	-8	DT	O3'-P-O5'	5.38	112.06	104.00
1	A	92	GLU	CA-C-N	5.37	127.81	120.77
1	A	92	GLU	C-N-CA	5.37	127.81	120.77
1	K	241	ALA	CA-C-N	5.37	127.42	120.70
1	K	241	ALA	C-N-CA	5.37	127.42	120.70
1	I	341	GLY	CA-C-N	5.37	129.10	121.42
1	I	341	GLY	C-N-CA	5.37	129.10	121.42
1	C	15	ILE	CA-C-N	5.37	129.82	122.84
1	C	15	ILE	C-N-CA	5.37	129.82	122.84
1	I	34	GLU	CB-CG-CD	5.37	121.72	112.60
1	I	525	GLU	CA-C-N	5.37	129.85	123.19
1	I	525	GLU	C-N-CA	5.37	129.85	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	274	ILE	CA-C-N	5.37	130.44	122.71
1	K	274	ILE	C-N-CA	5.37	130.44	122.71
1	I	347	HIS	CE1-NE2-CD2	-5.37	103.63	109.00
1	K	365	ASP	CA-C-N	5.36	127.31	120.56
1	K	365	ASP	C-N-CA	5.36	127.31	120.56
1	I	215	ALA	CA-C-N	5.36	127.31	120.56
1	I	215	ALA	C-N-CA	5.36	127.31	120.56
1	K	202	PHE	CA-CB-CG	5.36	119.16	113.80
1	K	294	VAL	CA-C-N	5.36	127.40	120.44
1	K	294	VAL	C-N-CA	5.36	127.40	120.44
1	K	362	ARG	CA-C-N	5.36	127.72	120.65
1	K	362	ARG	C-N-CA	5.36	127.72	120.65
1	A	507	ASP	CA-C-N	5.36	130.50	123.11
1	A	507	ASP	C-N-CA	5.36	130.50	123.11
1	K	502	ARG	CD-NE-CZ	5.35	131.90	124.40
1	I	56	GLU	CA-C-N	5.35	130.54	123.05
1	I	56	GLU	C-N-CA	5.35	130.54	123.05
1	C	202	PHE	CA-CB-CG	5.34	119.14	113.80
1	K	512	MET	N-CA-CB	5.34	117.99	110.24
1	I	68	ASP	CA-CB-CG	5.34	117.94	112.60
1	I	115	ARG	CB-CG-CD	5.34	123.57	111.30
1	A	72	VAL	N-CA-CB	5.33	116.43	110.51
1	A	202	PHE	N-CA-CB	5.33	117.89	109.94
1	A	72	VAL	CA-C-N	5.33	127.73	120.54
1	A	72	VAL	C-N-CA	5.33	127.73	120.54
1	C	75	GLU	CA-C-N	5.33	127.37	120.44
1	C	75	GLU	C-N-CA	5.33	127.37	120.44
1	K	295	LYS	CA-C-N	5.33	127.75	120.77
1	K	295	LYS	C-N-CA	5.33	127.75	120.77
1	K	347	HIS	N-CA-CB	5.33	118.25	110.58
1	C	76	CYS	CA-C-N	5.32	127.36	120.44
1	C	76	CYS	C-N-CA	5.32	127.36	120.44
1	A	217	ALA	CA-C-N	5.32	127.36	120.44
1	A	217	ALA	C-N-CA	5.32	127.36	120.44
1	K	250	GLY	CA-C-N	5.32	128.40	120.95
1	K	250	GLY	C-N-CA	5.32	128.40	120.95
1	K	210	ASP	CA-C-N	5.31	130.49	123.00
1	K	210	ASP	C-N-CA	5.31	130.49	123.00
1	C	274	ILE	CA-C-N	5.31	130.36	122.71
1	C	274	ILE	C-N-CA	5.31	130.36	122.71
1	A	106	GLN	CA-C-N	5.31	127.45	120.60
1	A	106	GLN	C-N-CA	5.31	127.45	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	497	LYS	CA-CB-CG	5.31	124.72	114.10
1	I	285	ASP	CA-CB-CG	5.31	117.91	112.60
1	I	365	ASP	CA-C-N	5.31	127.25	120.56
1	I	365	ASP	C-N-CA	5.31	127.25	120.56
3	H	6	DG	C5'-C4'-C3'	-5.31	106.94	114.90
1	I	176	TYR	CA-C-N	5.30	131.24	121.85
1	I	176	TYR	C-N-CA	5.30	131.24	121.85
1	I	192	ALA	CA-C-N	5.30	127.33	120.44
1	I	192	ALA	C-N-CA	5.30	127.33	120.44
1	I	250	GLY	CA-C-N	5.30	129.94	122.09
1	I	250	GLY	C-N-CA	5.30	129.94	122.09
1	I	144	ARG	CG-CD-NE	5.30	123.66	112.00
1	A	310	GLU	CA-CB-CG	5.30	124.69	114.10
1	A	61	ILE	N-CA-CB	5.29	116.17	110.62
1	A	289	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	492	SER	CA-C-N	5.29	128.28	120.82
1	A	492	SER	C-N-CA	5.29	128.28	120.82
1	C	56	GLU	CA-C-N	5.29	130.62	123.11
1	C	56	GLU	C-N-CA	5.29	130.62	123.11
1	K	15	ILE	CA-C-N	5.29	129.71	122.84
1	K	15	ILE	C-N-CA	5.29	129.71	122.84
1	K	217	ALA	CA-C-N	5.28	127.31	120.44
1	K	217	ALA	C-N-CA	5.28	127.31	120.44
1	K	321	SER	CA-C-N	5.28	127.31	120.44
1	K	321	SER	C-N-CA	5.28	127.31	120.44
1	I	502	ARG	CA-C-N	5.28	127.31	120.44
1	I	502	ARG	C-N-CA	5.28	127.31	120.44
1	I	211	TYR	CA-C-N	5.28	130.16	121.39
1	I	211	TYR	C-N-CA	5.28	130.16	121.39
1	K	45	ASN	CA-C-N	5.28	127.67	120.54
1	K	45	ASN	C-N-CA	5.28	127.67	120.54
1	I	509	ILE	N-CA-CB	5.28	117.11	111.46
1	I	88	ILE	CA-C-N	5.28	130.58	122.93
1	I	88	ILE	C-N-CA	5.28	130.58	122.93
1	K	68	ASP	CA-CB-CG	5.27	117.87	112.60
1	I	43	LEU	CA-C-N	5.27	127.29	120.44
1	I	43	LEU	C-N-CA	5.27	127.29	120.44
1	C	321	SER	CA-C-N	5.26	127.33	120.28
1	C	321	SER	C-N-CA	5.26	127.33	120.28
1	A	41	LYS	CA-C-N	5.26	127.28	120.44
1	A	41	LYS	C-N-CA	5.26	127.28	120.44
1	A	115	ARG	CB-CG-CD	5.26	123.40	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ALA	CA-C-N	5.26	127.33	120.28
1	A	192	ALA	C-N-CA	5.26	127.33	120.28
1	A	347	HIS	ND1-CG-CD2	-5.25	100.84	106.10
1	C	121	PRO	CA-C-N	5.25	130.91	121.66
1	C	121	PRO	C-N-CA	5.25	130.91	121.66
1	A	341	GLY	CA-C-N	5.25	128.93	121.42
1	A	341	GLY	C-N-CA	5.25	128.93	121.42
1	C	57	LEU	CA-C-N	5.25	130.41	123.00
1	C	57	LEU	C-N-CA	5.25	130.41	123.00
1	I	94	THR	CB-CA-C	-5.25	100.92	110.63
1	A	137	ARG	CA-CB-CG	5.25	124.60	114.10
1	I	135	GLN	CA-C-N	5.25	127.17	120.56
1	I	135	GLN	C-N-CA	5.25	127.17	120.56
1	I	347	HIS	ND1-CG-CD2	-5.25	100.85	106.10
3	F	3	DG	C4'-C3'-O3'	5.25	117.87	110.00
1	A	268	ARG	CA-C-N	5.25	125.16	119.76
1	A	268	ARG	C-N-CA	5.25	125.16	119.76
3	N	15	DG	C4'-C3'-O3'	5.25	117.87	110.00
1	A	20	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	A	363	TYR	CA-C-N	5.24	127.31	120.28
1	A	363	TYR	C-N-CA	5.24	127.31	120.28
1	I	272	GLU	CA-C-N	5.24	128.16	120.71
1	I	272	GLU	C-N-CA	5.24	128.16	120.71
1	K	141	PHE	CA-C-N	5.24	127.26	120.44
1	K	141	PHE	C-N-CA	5.24	127.26	120.44
1	A	501	LEU	CA-C-N	5.24	127.30	120.28
1	A	501	LEU	C-N-CA	5.24	127.30	120.28
1	K	494	SER	CA-C-N	5.24	127.25	120.44
1	K	494	SER	C-N-CA	5.24	127.25	120.44
1	K	91	LYS	CA-CB-CG	5.24	124.57	114.10
1	K	121	PRO	CA-C-N	5.24	130.98	121.92
1	K	121	PRO	C-N-CA	5.24	130.98	121.92
1	A	274	ILE	CA-C-N	5.23	130.41	122.98
1	A	274	ILE	C-N-CA	5.23	130.41	122.98
1	C	495	GLU	CA-C-N	5.23	127.24	120.44
1	C	495	GLU	C-N-CA	5.23	127.24	120.44
1	A	347	HIS	CG-CD2-NE2	5.23	112.43	107.20
1	I	336	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	499	GLU	N-CA-CB	5.23	117.59	110.01
1	K	347	HIS	ND1-CG-CD2	-5.23	100.87	106.10
1	A	336	ARG	NE-CZ-NH2	5.23	123.90	119.20
1	A	198	ILE	CA-C-N	5.22	127.23	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ILE	C-N-CA	5.22	127.23	120.44
1	I	103	ASP	CA-CB-CG	5.22	117.83	112.60
1	A	197	LEU	CA-C-N	5.22	127.34	120.60
1	A	197	LEU	C-N-CA	5.22	127.34	120.60
1	I	275	VAL	CA-C-N	5.22	130.21	123.11
1	I	275	VAL	C-N-CA	5.22	130.21	123.11
1	A	271	LYS	CB-CG-CD	5.22	123.30	111.30
1	I	499	GLU	CA-C-N	5.22	127.22	120.44
1	I	499	GLU	C-N-CA	5.22	127.22	120.44
1	I	33	GLY	CA-C-N	5.22	129.92	122.72
1	I	33	GLY	C-N-CA	5.22	129.92	122.72
1	A	358	CYS	CA-C-N	5.21	129.33	121.40
1	A	358	CYS	C-N-CA	5.21	129.33	121.40
1	I	75	GLU	CA-C-N	5.21	127.22	120.44
1	I	75	GLU	C-N-CA	5.21	127.22	120.44
3	F	16	DA	C5'-C4'-O4'	5.21	117.22	109.40
1	I	493	SER	N-CA-CB	5.21	117.67	109.69
1	K	347	HIS	CG-CD2-NE2	5.21	112.41	107.20
1	C	97	SER	N-CA-C	5.21	116.44	108.52
1	C	195	VAL	CA-C-N	5.20	127.20	120.44
1	C	195	VAL	C-N-CA	5.20	127.20	120.44
1	C	362	ARG	N-CA-CB	5.20	118.02	109.95
1	C	210	ASP	CA-C-N	5.20	130.33	123.00
1	C	210	ASP	C-N-CA	5.20	130.33	123.00
1	I	493	SER	CA-C-N	5.20	127.20	120.44
1	I	493	SER	C-N-CA	5.20	127.20	120.44
1	I	496	LYS	CA-C-N	5.20	127.20	120.44
1	I	496	LYS	C-N-CA	5.20	127.20	120.44
1	C	221	THR	CA-C-N	5.20	127.20	120.44
1	C	221	THR	C-N-CA	5.20	127.20	120.44
1	I	347	HIS	CG-CD2-NE2	5.20	112.40	107.20
1	C	239	ILE	N-CA-CB	5.20	116.08	110.62
1	C	130	PRO	CA-C-N	5.19	127.10	120.56
1	C	130	PRO	C-N-CA	5.19	127.10	120.56
1	C	334	ARG	CA-C-N	5.19	128.97	122.43
1	C	334	ARG	C-N-CA	5.19	128.97	122.43
1	K	74	LYS	CB-CG-CD	5.19	123.24	111.30
1	K	296	ILE	CA-C-N	5.19	127.19	120.44
1	K	296	ILE	C-N-CA	5.19	127.19	120.44
1	C	46	LYS	CA-CB-CG	5.19	124.48	114.10
1	A	239	ILE	N-CA-CB	5.19	116.07	110.62
1	A	495	GLU	CA-C-N	5.19	127.18	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	GLU	C-N-CA	5.19	127.18	120.44
1	C	347	HIS	CG-CD2-NE2	5.19	112.39	107.20
1	I	73	PHE	CA-C-N	5.19	127.18	120.44
1	I	73	PHE	C-N-CA	5.19	127.18	120.44
1	I	497	LYS	CB-CG-CD	5.19	123.23	111.30
1	C	347	HIS	ND1-CG-CD2	-5.19	100.91	106.10
1	K	292	SER	CA-C-N	5.18	127.18	120.44
1	K	292	SER	C-N-CA	5.18	127.18	120.44
1	C	324	GLY	CA-C-N	5.18	127.61	120.67
1	C	324	GLY	C-N-CA	5.18	127.61	120.67
1	I	367	GLU	N-CA-CB	5.18	117.52	110.01
1	I	188	VAL	CA-C-N	5.18	127.48	120.65
1	I	188	VAL	C-N-CA	5.18	127.48	120.65
1	K	318	CYS	CA-C-N	5.17	131.11	122.73
1	K	318	CYS	C-N-CA	5.17	131.11	122.73
1	C	66	SER	CA-C-N	5.17	127.82	120.53
1	C	66	SER	C-N-CA	5.17	127.82	120.53
1	C	88	ILE	CA-C-N	5.17	130.69	122.94
1	C	88	ILE	C-N-CA	5.17	130.69	122.94
1	C	498	ASN	N-CA-CB	5.17	117.50	110.01
1	I	217	ALA	CA-C-N	5.17	127.16	120.44
1	I	217	ALA	C-N-CA	5.17	127.16	120.44
1	C	351	LEU	CA-C-N	5.17	130.42	122.93
1	C	351	LEU	C-N-CA	5.17	130.42	122.93
1	K	497	LYS	CA-C-N	5.17	127.15	120.44
1	K	497	LYS	C-N-CA	5.17	127.15	120.44
1	A	255	LYS	N-CA-CB	-5.16	104.88	112.78
1	I	500	LEU	CA-C-N	5.16	127.15	120.44
1	I	500	LEU	C-N-CA	5.16	127.15	120.44
1	A	231	LYS	CA-C-N	5.16	131.02	121.52
1	A	231	LYS	C-N-CA	5.16	131.02	121.52
1	A	361	VAL	CA-C-N	5.16	129.20	121.72
1	A	361	VAL	C-N-CA	5.16	129.20	121.72
1	C	512	MET	N-CA-CB	5.16	118.20	109.94
1	I	15	ILE	CA-C-N	5.16	129.55	122.84
1	I	15	ILE	C-N-CA	5.16	129.55	122.84
1	K	57	LEU	CA-C-N	5.15	130.27	123.00
1	K	57	LEU	C-N-CA	5.15	130.27	123.00
1	C	292	SER	CA-C-N	5.15	127.14	120.44
1	C	292	SER	C-N-CA	5.15	127.14	120.44
1	K	324	GLY	CA-C-N	5.15	127.81	120.49
1	K	324	GLY	C-N-CA	5.15	127.81	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	198	ILE	CA-C-N	5.15	127.13	120.44
1	I	198	ILE	C-N-CA	5.15	127.13	120.44
1	I	334	ARG	CA-C-N	5.15	129.95	123.10
1	I	334	ARG	C-N-CA	5.15	129.95	123.10
1	A	15	ILE	CA-C-N	5.14	129.61	122.77
1	A	15	ILE	C-N-CA	5.14	129.61	122.77
1	I	72	VAL	CA-C-N	5.14	127.48	120.54
1	I	72	VAL	C-N-CA	5.14	127.48	120.54
1	K	159	TYR	CA-C-N	5.14	127.12	120.44
1	K	159	TYR	C-N-CA	5.14	127.12	120.44
1	K	313	GLU	CA-C-N	5.14	130.73	122.86
1	K	313	GLU	C-N-CA	5.14	130.73	122.86
1	C	288	GLN	CA-C-N	5.14	127.12	120.44
1	C	288	GLN	C-N-CA	5.14	127.12	120.44
1	A	493	SER	N-CA-CB	5.14	117.55	109.69
1	C	190	ASP	CA-C-N	5.14	127.12	120.44
1	C	190	ASP	C-N-CA	5.14	127.12	120.44
1	C	320	CYS	CA-C-N	5.14	127.12	120.44
1	C	320	CYS	C-N-CA	5.14	127.12	120.44
1	A	221	THR	CA-C-N	5.14	127.12	120.44
1	A	221	THR	C-N-CA	5.14	127.12	120.44
1	A	320	CYS	N-CA-CB	5.13	117.61	109.71
1	A	90	VAL	CA-C-N	5.13	127.47	120.54
1	A	90	VAL	C-N-CA	5.13	127.47	120.54
1	I	362	ARG	CA-C-N	5.13	127.92	120.79
1	I	362	ARG	C-N-CA	5.13	127.92	120.79
1	K	20	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	C	196	GLN	CA-C-N	5.12	127.10	120.44
1	C	196	GLN	C-N-CA	5.12	127.10	120.44
1	C	492	SER	CA-C-N	5.12	128.59	121.02
1	C	492	SER	C-N-CA	5.12	128.59	121.02
1	I	79	ASP	CA-C-N	5.12	127.09	120.44
1	I	79	ASP	C-N-CA	5.12	127.09	120.44
1	I	286	LYS	CB-CG-CD	5.12	123.07	111.30
1	I	184	LYS	CB-CG-CD	5.11	123.06	111.30
1	A	278	ASP	CA-CB-CG	5.11	117.71	112.60
1	I	498	ASN	CA-C-N	5.11	127.44	120.54
1	I	498	ASN	C-N-CA	5.11	127.44	120.54
1	C	148	GLU	CA-C-N	5.11	127.08	120.44
1	C	148	GLU	C-N-CA	5.11	127.08	120.44
1	C	246	GLU	CA-CB-CG	5.11	124.32	114.10
1	K	145	GLU	CA-C-N	5.11	127.12	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	145	GLU	C-N-CA	5.11	127.12	120.28
1	A	176	TYR	CA-C-N	5.10	130.60	122.74
1	A	176	TYR	C-N-CA	5.10	130.60	122.74
1	C	74	LYS	CA-C-N	5.10	127.08	120.44
1	C	74	LYS	C-N-CA	5.10	127.08	120.44
1	I	363	TYR	CA-C-N	5.10	127.12	120.28
1	I	363	TYR	C-N-CA	5.10	127.12	120.28
1	A	488	TYR	N-CA-CB	5.10	117.54	109.94
1	C	296	ILE	CA-C-N	5.10	127.07	120.44
1	C	296	ILE	C-N-CA	5.10	127.07	120.44
1	A	320	CYS	CA-C-N	5.10	127.07	120.44
1	A	320	CYS	C-N-CA	5.10	127.07	120.44
1	C	138	PHE	CA-C-N	5.10	127.07	120.44
1	C	138	PHE	C-N-CA	5.10	127.07	120.44
1	K	288	GLN	CA-C-N	5.10	127.07	120.44
1	K	288	GLN	C-N-CA	5.10	127.07	120.44
1	A	190	ASP	CA-C-N	5.09	127.11	120.28
1	A	190	ASP	C-N-CA	5.09	127.11	120.28
1	A	324	GLY	CA-C-N	5.09	127.58	120.65
1	A	324	GLY	C-N-CA	5.09	127.58	120.65
1	C	493	SER	N-CA-CB	5.09	117.56	109.51
1	C	93	ILE	N-CA-CB	5.09	116.16	110.51
1	C	295	LYS	CG-CD-CE	5.09	123.01	111.30
1	K	299	LYS	CB-CG-CD	5.09	123.01	111.30
1	K	353	CYS	N-CA-CB	5.09	117.44	110.57
3	P	22	DA	C5'-C4'-C3'	-5.09	107.26	114.90
1	K	513	THR	CA-C-N	5.09	130.57	122.74
1	K	513	THR	C-N-CA	5.09	130.57	122.74
1	I	313	GLU	CA-C-N	5.08	130.76	122.67
1	I	313	GLU	C-N-CA	5.08	130.76	122.67
1	A	75	GLU	CA-C-N	5.08	127.05	120.44
1	A	75	GLU	C-N-CA	5.08	127.05	120.44
1	C	74	LYS	CB-CG-CD	5.08	122.99	111.30
1	A	495	GLU	CA-CB-CG	5.08	124.26	114.10
1	C	353	CYS	N-CA-CB	5.08	117.43	110.57
1	K	137	ARG	CA-CB-CG	5.08	124.26	114.10
1	A	322	LYS	CA-C-N	5.08	129.75	121.98
1	A	322	LYS	C-N-CA	5.08	129.75	121.98
1	I	186	ASP	CA-CB-CG	5.08	117.68	112.60
1	I	320	CYS	N-CA-CB	5.08	117.42	109.85
1	A	367	GLU	N-CA-CB	5.08	117.37	110.01
1	I	319	THR	CA-C-N	5.08	128.06	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	319	THR	C-N-CA	5.08	128.06	120.95
1	K	362	ARG	CA-CB-CG	5.08	124.25	114.10
1	I	231	LYS	CA-C-N	5.08	132.45	121.64
1	I	231	LYS	C-N-CA	5.08	132.45	121.64
1	K	320	CYS	CA-C-N	5.08	127.34	120.44
1	K	320	CYS	C-N-CA	5.08	127.34	120.44
1	A	498	ASN	N-CA-CB	5.07	117.36	110.01
1	C	498	ASN	CA-C-N	5.07	127.03	120.44
1	C	498	ASN	C-N-CA	5.07	127.03	120.44
2	G	-1	DT	C6-C5-C7	-5.07	116.39	124.00
1	C	217	ALA	CA-C-N	5.07	127.03	120.44
1	C	217	ALA	C-N-CA	5.07	127.03	120.44
1	C	513	THR	CA-C-N	5.07	130.55	122.74
1	C	513	THR	C-N-CA	5.07	130.55	122.74
1	A	494	SER	CA-C-N	5.07	127.34	120.65
1	A	494	SER	C-N-CA	5.07	127.34	120.65
2	E	-24	DA	C2'-C3'-O3'	-5.07	103.90	111.50
1	A	362	ARG	CA-C-N	5.07	127.83	120.79
1	A	362	ARG	C-N-CA	5.07	127.83	120.79
1	K	295	LYS	CG-CD-CE	5.07	122.95	111.30
1	A	38	THR	CA-C-N	5.06	127.33	120.65
1	A	38	THR	C-N-CA	5.06	127.33	120.65
1	C	295	LYS	CA-CB-CG	5.06	124.23	114.10
1	K	161	TYR	CA-C-N	5.06	127.02	120.44
1	K	161	TYR	C-N-CA	5.06	127.02	120.44
1	I	488	TYR	N-CA-CB	5.06	117.35	110.01
1	K	289	PHE	N-CA-CB	5.06	117.35	110.01
1	K	194	VAL	N-CA-CB	5.06	116.13	110.51
1	A	143	ALA	CA-C-N	5.06	127.37	120.54
1	A	143	ALA	C-N-CA	5.06	127.37	120.54
1	C	197	LEU	N-CA-CB	5.06	117.34	110.01
1	C	176	TYR	CA-C-N	5.06	130.13	123.00
1	C	176	TYR	C-N-CA	5.06	130.13	123.00
1	A	365	ASP	CA-C-N	5.05	126.93	120.56
1	A	365	ASP	C-N-CA	5.05	126.93	120.56
1	K	88	ILE	CA-C-N	5.05	130.92	122.73
1	K	88	ILE	C-N-CA	5.05	130.92	122.73
1	I	516	ARG	NE-CZ-NH1	-5.05	116.45	121.50
1	A	186	ASP	CA-CB-CG	5.05	117.65	112.60
1	K	165	GLY	CA-C-N	5.05	128.64	121.42
1	K	165	GLY	C-N-CA	5.05	128.64	121.42
1	C	91	LYS	CG-CD-CE	5.05	122.91	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	288	GLN	CA-CB-CG	5.05	124.19	114.10
1	K	364	ASN	CA-C-N	5.05	127.00	120.44
1	K	364	ASN	C-N-CA	5.05	127.00	120.44
1	I	72	VAL	N-CA-CB	5.04	116.11	110.51
1	I	495	GLU	CA-C-N	5.04	127.00	120.44
1	I	495	GLU	C-N-CA	5.04	127.00	120.44
1	K	195	VAL	CA-C-N	5.04	127.00	120.44
1	K	195	VAL	C-N-CA	5.04	127.00	120.44
1	I	57	LEU	CA-C-N	5.04	130.50	122.74
1	I	57	LEU	C-N-CA	5.04	130.50	122.74
1	I	318	CYS	CA-C-N	5.04	131.03	122.37
1	I	318	CYS	C-N-CA	5.04	131.03	122.37
1	I	47	ILE	CA-C-N	5.04	126.98	120.44
1	I	47	ILE	C-N-CA	5.04	126.98	120.44
1	C	78	LYS	CA-CB-CG	5.03	124.17	114.10
1	C	137	ARG	CA-CB-CG	5.03	124.16	114.10
1	C	191	GLU	CA-C-N	5.03	126.98	120.44
1	C	191	GLU	C-N-CA	5.03	126.98	120.44
1	I	501	LEU	CA-C-N	5.03	127.02	120.28
1	I	501	LEU	C-N-CA	5.03	127.02	120.28
1	K	198	ILE	CA-C-N	5.03	126.98	120.44
1	K	198	ILE	C-N-CA	5.03	126.98	120.44
1	A	496	LYS	CA-C-N	5.03	126.97	120.44
1	A	496	LYS	C-N-CA	5.03	126.97	120.44
1	C	366	VAL	N-CA-CB	5.03	116.43	110.55
1	C	179	ASN	N-CA-CB	5.02	118.98	110.49
1	K	275	VAL	CA-C-N	5.02	131.01	121.97
1	K	275	VAL	C-N-CA	5.02	131.01	121.97
1	A	353	CYS	N-CA-CB	5.02	117.35	110.57
1	C	165	GLY	CA-C-N	5.02	128.60	121.42
1	C	165	GLY	C-N-CA	5.02	128.60	121.42
1	A	107	ILE	N-CA-CB	5.02	116.08	110.51
1	C	313	GLU	CA-C-N	5.02	130.97	122.79
1	C	313	GLU	C-N-CA	5.02	130.97	122.79
1	C	499	GLU	N-CA-CB	5.02	117.28	110.01
1	I	370	ILE	N-CA-CB	5.01	116.42	110.55
1	A	506	LYS	N-CA-CB	5.01	117.58	110.16
1	C	299	LYS	CB-CG-CD	5.01	122.82	111.30
1	A	41	LYS	CG-CD-CE	5.01	122.82	111.30
1	A	493	SER	CA-C-N	5.01	126.99	120.28
1	A	493	SER	C-N-CA	5.01	126.99	120.28
1	A	291	GLN	CA-C-N	5.01	126.95	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	GLN	C-N-CA	5.01	126.95	120.44
1	C	362	ARG	CB-CG-CD	5.01	122.82	111.30
1	K	246	GLU	CA-CB-CG	5.01	124.11	114.10
1	A	295	LYS	CG-CD-CE	5.00	122.81	111.30
1	K	295	LYS	CA-CB-CG	5.00	124.11	114.10
1	A	137	ARG	CA-C-N	5.00	127.23	120.38
1	A	137	ARG	C-N-CA	5.00	127.23	120.38
1	C	275	VAL	CA-C-N	5.00	130.97	121.97
1	C	275	VAL	C-N-CA	5.00	130.97	121.97
1	I	292	SER	CA-C-N	5.00	126.94	120.44
1	I	292	SER	C-N-CA	5.00	126.94	120.44

There are no chirality outliers.

All (95) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ARG	Sidechain
1	C	151	ARG	Sidechain
1	C	18	TYR	Sidechain
1	C	20	ARG	Sidechain
1	C	381	ASN	Peptide
1	C	98	ARG	Peptide
2	E	-10	DT	Sidechain
2	E	-13	DT	Sidechain
2	E	-15	DC	Sidechain
2	E	-18	DT	Sidechain
2	E	-19	DG	Sidechain
2	E	-2	DT	Sidechain
2	E	-21	DA	Sidechain
2	E	-22	DT	Sidechain
2	E	-3	DC	Sidechain
2	E	-5	DA	Sidechain
2	E	-7	DA	Sidechain
3	F	11	DT	Sidechain
3	F	12	DT	Sidechain
3	F	14	DA	Sidechain
3	F	15	DG	Sidechain
3	F	17	DT	Sidechain
3	F	19	DC	Sidechain
3	F	20	DT	Sidechain
3	F	21	DT	Sidechain
3	F	24	DT	Sidechain

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Mol	Chain	Res	Type	Group
3	F	25	DA	Sidechain
3	F	26	DC	Sidechain
3	F	3	DG	Sidechain
3	F	7	DT	Sidechain
2	G	-1	DT	Sidechain
2	G	-13	DT	Sidechain
2	G	-14	DT	Sidechain
2	G	-15	DC	Sidechain
2	G	-18	DT	Sidechain
2	G	-19	DG	Sidechain
2	G	-21	DA	Sidechain
2	G	-22	DT	Sidechain
2	G	-3	DC	Sidechain
2	G	-5	DA	Sidechain
2	G	-8	DT	Sidechain
2	G	-9	DA	Sidechain
3	H	11	DT	Sidechain
3	H	12	DT	Sidechain
3	H	13	DA	Sidechain
3	H	14	DA	Sidechain
3	H	15	DG	Sidechain
3	H	22	DA	Sidechain
3	H	24	DT	Sidechain
3	H	4	DC	Sidechain
3	H	6	DG	Sidechain
3	H	7	DT	Sidechain
3	H	8	DA	Sidechain
1	K	18	TYR	Sidechain
1	K	98	ARG	Sidechain,Peptide
2	M	-10	DT	Sidechain
2	M	-14	DT	Sidechain
2	M	-15	DC	Sidechain
2	M	-18	DT	Sidechain
2	M	-19	DG	Sidechain
2	M	-2	DT	Sidechain
2	M	-22	DT	Sidechain
2	M	-23	DG	Sidechain
2	M	-27	DT	Sidechain
2	M	-28	DT	Sidechain
2	M	-3	DC	Sidechain
3	N	12	DT	Sidechain
3	N	15	DG	Sidechain

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Mol	Chain	Res	Type	Group
3	N	17	DT	Sidechain
3	N	18	DA	Sidechain
3	N	2	DA	Sidechain
3	N	25	DA	Sidechain
3	N	26	DC	Sidechain
3	N	4	DC	Sidechain
3	N	6	DG	Sidechain
3	N	9	DT	Sidechain
2	O	-10	DT	Sidechain
2	O	-13	DT	Sidechain
2	O	-15	DC	Sidechain
2	O	-18	DT	Sidechain
2	O	-21	DA	Sidechain
2	O	-22	DT	Sidechain
2	O	-27	DT	Sidechain
2	O	-3	DC	Sidechain
2	O	-5	DA	Sidechain
3	P	12	DT	Sidechain
3	P	14	DA	Sidechain
3	P	15	DG	Sidechain
3	P	18	DA	Sidechain
3	P	20	DT	Sidechain
3	P	21	DT	Sidechain
3	P	27	DA	Sidechain
3	P	28	DA	Sidechain
3	P	4	DC	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4354	4428	4424	106	0
1	C	4354	4428	4424	99	0
1	I	4354	4428	4424	104	0
1	K	4354	4428	4424	92	0
2	E	574	321	319	11	0
2	G	534	297	295	17	0
2	M	574	321	319	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	574	321	321	4	0
3	F	553	306	305	6	0
3	H	511	284	285	15	0
3	N	553	306	305	3	0
3	P	553	306	307	3	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
All	All	21846	20174	20152	437	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 10.

All (437) 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:C:56:GLU:OE1	1:C:85:TYR:OH	1.89	0.90
1:C:81:GLU:O	1:C:114:LYS:NZ	2.05	0.90
1:A:56:GLU:OE1	1:A:85:TYR:OH	1.90	0.89
1:I:470:SER:OG	1:I:532:PHE:O	1.91	0.89
1:K:81:GLU:O	1:K:114:LYS:NZ	2.07	0.86
1:C:126:ASP:N	1:C:132:ASP:OD2	2.09	0.85
1:K:56:GLU:OE1	1:K:85:TYR:OH	1.94	0.84
1:K:126:ASP:N	1:K:132:ASP:OD2	2.11	0.83
1:K:459:LYS:O	1:K:463:ASN:ND2	2.11	0.83
1:C:200:ASN:OD1	1:C:204:ASN:ND2	2.11	0.83
1:C:383:SER:O	1:C:386:THR:OG1	1.96	0.82
1:K:35:ASP:OD2	1:K:38:THR:OG1	1.97	0.81
1:A:200:ASN:OD1	1:A:204:ASN:ND2	2.14	0.81
1:I:200:ASN:OD1	1:I:204:ASN:ND2	2.15	0.80
1:A:381:ASN:OD1	1:A:384:THR:OG1	1.99	0.79
1:K:200:ASN:OD1	1:K:204:ASN:ND2	2.15	0.79
1:C:202:PHE:O	1:C:295:LYS:NZ	2.19	0.76
1:I:381:ASN:OD1	1:I:383:SER:OG	2.03	0.74
1:A:381:ASN:O	1:A:384:THR:N	2.21	0.74
1:I:100:SER:OG	1:I:103:ASP:OD1	2.05	0.73
1:K:292:SER:OG	1:K:293:GLN:NE2	2.22	0.73
1:C:376:SER:O	1:C:380:LEU:N	2.22	0.72
1:I:468:THR:HG21	1:I:473:ASP:HB2	1.71	0.72
1:A:92:GLU:OE1	1:A:94:THR:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:111:LEU:O	1:I:115:ARG:N	2.21	0.71
1:I:162:ALA:O	1:I:165:GLY:N	2.22	0.71
1:A:378:ASN:ND2	1:A:482:ASN:OD1	2.25	0.69
1:C:3:LEU:O	1:C:7:VAL:HG23	1.92	0.69
1:I:129:ASN:OD1	1:I:131:VAL:N	2.26	0.69
1:K:385:LEU:HD21	1:K:473:ASP:N	2.07	0.69
1:I:145:GLU:OE2	1:K:137:ARG:NE	2.25	0.69
1:C:11:ASN:N	1:C:11:ASN:OD1	2.27	0.68
1:A:118:ILE:O	1:A:124:VAL:HG13	1.93	0.67
1:I:179:ASN:O	1:I:183:SER:N	2.28	0.67
1:C:390:ASN:OD1	1:C:469:GLN:NE2	2.26	0.67
1:I:179:ASN:N	1:I:186:ASP:OD1	2.27	0.66
1:C:469:GLN:OE1	1:C:469:GLN:N	2.28	0.66
1:I:459:LYS:O	1:I:463:ASN:N	2.27	0.66
1:A:162:ALA:O	1:A:165:GLY:N	2.28	0.66
1:I:290:GLN:O	1:I:294:VAL:HG23	1.97	0.65
1:A:92:GLU:OE1	1:A:93:ILE:N	2.29	0.65
1:A:507:ASP:O	1:A:529:ILE:N	2.28	0.65
1:C:290:GLN:O	1:C:294:VAL:HG23	1.96	0.64
1:A:186:ASP:N	1:A:186:ASP:OD1	2.27	0.64
1:A:179:ASN:N	1:A:186:ASP:OD1	2.31	0.64
1:I:186:ASP:OD1	1:I:186:ASP:N	2.29	0.64
1:I:474:SER:O	1:I:477:VAL:HG22	1.97	0.64
1:A:94:THR:O	1:A:97:SER:N	2.31	0.64
1:C:86:GLN:OE1	1:C:86:GLN:N	2.30	0.64
2:G:-2:DT:C6	2:G:-1:DT:H72	2.32	0.64
1:I:423:LYS:NZ	1:I:451:GLU:OE1	2.30	0.63
1:I:466:GLN:OE1	1:I:466:GLN:N	2.30	0.63
1:C:48:LEU:HD13	1:C:55:TYR:CD2	2.32	0.63
1:K:290:GLN:O	1:K:294:VAL:HG23	1.99	0.63
1:A:179:ASN:O	1:A:183:SER:N	2.31	0.63
1:C:179:ASN:N	1:C:184:LYS:O	2.30	0.63
1:K:11:ASN:OD1	1:K:11:ASN:N	2.29	0.63
1:A:132:ASP:OD1	1:A:132:ASP:N	2.30	0.63
1:K:427:ILE:HD12	1:K:448:LEU:HD22	1.81	0.63
1:K:129:ASN:OD1	1:K:131:VAL:N	2.31	0.63
1:I:250:GLY:O	1:I:279:ALA:N	2.32	0.62
1:K:48:LEU:HD13	1:K:55:TYR:CE2	2.34	0.62
1:A:362:ARG:O	1:A:366:VAL:HG23	1.99	0.62
1:I:462:LEU:HD12	1:I:465:LEU:HD11	1.82	0.61
1:A:262:ASP:OD1	1:A:262:ASP:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:THR:OG1	1:A:324:GLY:O	2.19	0.61
1:I:484:ILE:HG21	1:I:504:VAL:HG21	1.83	0.61
1:K:371:LEU:HD21	1:K:488:TYR:CD1	2.35	0.61
1:C:380:LEU:O	1:C:381:ASN:C	2.43	0.61
1:I:103:ASP:OD1	1:I:103:ASP:N	2.33	0.61
1:C:139:GLU:OE1	1:C:140:LEU:N	2.34	0.60
1:A:427:ILE:HD11	1:A:444:ARG:NH1	2.16	0.60
1:K:48:LEU:HD13	1:K:55:TYR:CD2	2.36	0.60
1:A:3:LEU:O	1:A:7:VAL:HG23	2.01	0.60
1:A:48:LEU:HD13	1:A:55:TYR:CD1	2.36	0.59
1:A:19:LEU:HD12	1:A:59:MET:HG3	1.84	0.59
1:I:202:PHE:O	1:I:295:LYS:NZ	2.31	0.59
1:C:502:ARG:O	1:C:531:ARG:NE	2.34	0.59
1:I:104:ALA:O	1:I:108:VAL:HG23	2.03	0.59
1:I:48:LEU:HD13	1:I:55:TYR:CD1	2.38	0.59
1:A:532:PHE:HA	1:A:535:ILE:HD12	1.84	0.59
1:A:116:LEU:C	1:A:117:ILE:HD12	2.28	0.59
1:K:389:ILE:HD11	1:K:471:GLU:O	2.01	0.59
1:K:315:ALA:O	1:K:498:ASN:ND2	2.35	0.58
1:C:252:VAL:O	1:C:276:VAL:N	2.34	0.58
1:A:252:VAL:N	1:A:276:VAL:O	2.35	0.58
1:C:424:GLU:OE2	1:C:445:LYS:NZ	2.25	0.58
1:K:179:ASN:N	1:K:184:LYS:O	2.33	0.58
1:C:190:ASP:O	1:C:194:VAL:HG23	2.04	0.58
1:I:477:VAL:HG23	1:I:478:ARG:HD2	1.86	0.58
1:A:530:LEU:HB3	1:A:535:ILE:HD11	1.85	0.57
1:I:252:VAL:N	1:I:276:VAL:O	2.34	0.57
1:A:142:MET:HE1	1:I:142:MET:HE1	1.86	0.57
1:K:41:LYS:O	1:K:45:ASN:ND2	2.35	0.57
1:K:118:ILE:O	1:K:124:VAL:HG13	2.04	0.57
1:K:44:MET:O	1:K:48:LEU:HD12	2.04	0.57
1:K:252:VAL:O	1:K:276:VAL:N	2.34	0.57
1:A:380:LEU:O	1:A:381:ASN:C	2.46	0.57
1:C:129:ASN:OD1	1:C:131:VAL:N	2.36	0.57
1:C:117:ILE:HD12	1:C:117:ILE:N	2.20	0.57
1:C:118:ILE:O	1:C:124:VAL:HG13	2.06	0.56
1:A:68:ASP:OD1	1:A:68:ASP:N	2.38	0.56
1:A:290:GLN:O	1:A:294:VAL:HG23	2.05	0.56
1:C:41:LYS:O	1:C:45:ASN:ND2	2.37	0.56
1:A:417:GLU:OE1	1:A:459:LYS:NZ	2.28	0.56
1:I:68:ASP:OD1	1:I:68:ASP:N	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:117:ILE:N	1:K:117:ILE:HD12	2.20	0.56
1:C:48:LEU:HD13	1:C:55:TYR:CE2	2.41	0.56
1:C:381:ASN:O	1:C:384:THR:N	2.38	0.56
1:I:127:PRO:HB3	1:I:133:MET:HE1	1.88	0.56
1:I:190:ASP:O	1:I:194:VAL:HG23	2.06	0.56
1:I:262:ASP:OD1	1:I:262:ASP:N	2.33	0.56
1:I:507:ASP:O	1:I:529:ILE:N	2.37	0.55
1:A:477:VAL:HG13	1:A:535:ILE:HG23	1.86	0.55
1:I:376:SER:HA	1:I:380:LEU:HD12	1.86	0.55
1:I:41:LYS:O	1:I:45:ASN:ND2	2.40	0.55
1:I:398:ASP:OD1	1:I:532:PHE:N	2.40	0.55
1:K:176:TYR:OH	1:K:281:ALA:O	2.20	0.55
1:K:385:LEU:HD21	1:K:473:ASP:H	1.71	0.55
1:K:472:ILE:HG23	1:K:472:ILE:O	2.06	0.55
1:I:532:PHE:HA	1:I:535:ILE:HD12	1.89	0.55
1:K:313:GLU:OE1	1:K:313:GLU:N	2.37	0.55
1:K:179:ASN:O	1:K:183:SER:N	2.40	0.55
1:A:190:ASP:O	1:A:194:VAL:HG23	2.07	0.54
1:A:507:ASP:OD1	1:A:508:VAL:N	2.41	0.54
1:C:484:ILE:HG21	1:C:504:VAL:HG21	1.89	0.54
1:A:48:LEU:CD1	1:A:57:LEU:HD21	2.37	0.54
1:A:13:THR:HG1	1:A:86:GLN:CD	2.15	0.54
1:A:250:GLY:O	1:A:279:ALA:N	2.40	0.54
1:K:86:GLN:N	1:K:86:GLN:OE1	2.41	0.54
1:I:132:ASP:OD1	1:I:132:ASP:N	2.41	0.54
1:I:120:THR:HG1	1:I:123:LYS:C	2.11	0.54
1:K:101:TYR:O	1:K:102:SER:C	2.52	0.53
1:C:44:MET:O	1:C:48:LEU:HD12	2.08	0.53
1:I:377:LEU:HD23	1:I:384:THR:HG22	1.89	0.53
1:I:155:THR:HG22	1:I:159:TYR:CZ	2.42	0.53
1:K:68:ASP:OD1	1:K:68:ASP:N	2.41	0.53
1:C:431:TYR:HH	1:I:436:TYR:HH	1.55	0.53
1:A:41:LYS:O	1:A:45:ASN:ND2	2.40	0.53
1:A:11:ASN:N	1:A:11:ASN:OD1	2.42	0.53
1:C:219:HIS:CE1	1:C:223:LEU:HD11	2.43	0.53
1:A:53:ILE:HG23	1:A:54:PRO:HD2	1.91	0.53
1:A:170:GLY:HA2	2:E:-4:DG:H1'	1.90	0.53
1:A:466:GLN:O	1:A:469:GLN:NE2	2.39	0.53
1:C:413:LEU:HD22	1:C:455:LEU:HD12	1.91	0.53
1:C:204:ASN:OD1	1:C:204:ASN:N	2.42	0.52
1:K:101:TYR:O	1:K:104:ALA:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:TYR:O	1:C:283:ILE:N	2.41	0.52
2:M:-10:DT:H2''	2:M:-9:DA:C8	2.44	0.52
1:K:219:HIS:CE1	1:K:223:LEU:HD11	2.45	0.52
2:G:-3:DC:H2'	2:G:-2:DT:C6	2.45	0.52
1:I:295:LYS:O	1:I:299:LYS:N	2.42	0.52
1:I:469:GLN:NE2	1:I:470:SER:OG	2.42	0.52
1:C:177:GLN:O	1:C:186:ASP:N	2.42	0.52
2:G:-17:DA:C2	3:H:18:DA:C2	2.98	0.52
1:C:108:VAL:HG12	1:C:112:GLN:OE1	2.10	0.52
1:I:362:ARG:O	1:I:366:VAL:HG23	2.10	0.52
1:K:502:ARG:O	1:K:531:ARG:NE	2.35	0.52
1:A:389:ILE:HG23	1:A:396:TYR:CD1	2.44	0.51
1:K:53:ILE:HG23	1:K:54:PRO:HD2	1.92	0.51
1:C:101:TYR:O	1:C:102:SER:C	2.52	0.51
1:C:126:ASP:OD2	1:C:129:ASN:N	2.43	0.51
1:K:126:ASP:OD2	1:K:129:ASN:N	2.43	0.51
1:I:170:GLY:C	2:M:-4:DG:H4'	2.36	0.51
1:I:177:GLN:O	1:I:186:ASP:N	2.35	0.51
1:C:427:ILE:HG23	1:C:436:TYR:CE2	2.46	0.51
1:I:361:VAL:HG12	1:I:524:PHE:HB3	1.93	0.51
1:I:468:THR:HG23	1:I:471:GLU:HG3	1.93	0.51
1:C:68:ASP:OD1	1:C:68:ASP:N	2.41	0.51
1:A:149:MET:HE1	1:A:153:ARG:HE	1.75	0.51
1:I:278:ASP:N	1:I:278:ASP:OD1	2.41	0.51
2:G:-9:DA:C2	3:H:10:DA:C2	2.99	0.51
1:A:129:ASN:OD1	1:A:131:VAL:N	2.43	0.50
1:K:170:GLY:HA2	2:O:-4:DG:H1'	1.92	0.50
1:C:89:ALA:O	1:C:90:VAL:HG13	2.12	0.50
1:K:3:LEU:HA	1:K:6:ILE:HD12	1.94	0.50
1:I:120:THR:OG1	1:I:123:LYS:O	2.09	0.50
1:I:170:GLY:HA2	2:M:-4:DG:H1'	1.93	0.50
1:I:191:GLU:O	1:I:195:VAL:HG23	2.12	0.50
1:I:507:ASP:OD1	1:I:508:VAL:N	2.45	0.50
1:K:248:TYR:O	1:K:283:ILE:N	2.42	0.50
1:C:111:LEU:O	1:C:115:ARG:N	2.42	0.49
2:G:-21:DA:C2	3:H:22:DA:C2	3.00	0.49
1:C:507:ASP:OD1	1:C:508:VAL:N	2.44	0.49
1:A:413:LEU:HD13	1:A:459:LYS:HA	1.95	0.49
1:K:487:GLN:O	1:K:491:GLU:N	2.35	0.49
1:A:48:LEU:HD23	1:A:51:ILE:HD12	1.93	0.49
1:A:120:THR:OG1	1:A:123:LYS:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:81:GLU:O	1:I:114:LYS:NZ	2.34	0.49
2:G:-15:DC:H2'	2:G:-14:DT:C6	2.47	0.49
2:E:-17:DA:C2	3:F:18:DA:C2	3.00	0.49
1:C:379:ASP:OD2	1:C:478:ARG:NH1	2.42	0.49
1:I:48:LEU:CD1	1:I:57:LEU:HD21	2.42	0.49
2:G:-11:DA:C2	2:G:-10:DT:C2	3.00	0.49
1:C:147:PHE:CD1	1:C:147:PHE:C	2.90	0.49
1:C:262:ASP:OD1	1:C:262:ASP:N	2.41	0.49
1:C:371:LEU:HD21	1:C:488:TYR:CD1	2.47	0.49
1:K:507:ASP:O	1:K:529:ILE:N	2.45	0.49
1:K:204:ASN:OD1	1:K:204:ASN:N	2.44	0.49
1:C:191:GLU:O	1:C:195:VAL:HG23	2.13	0.49
1:K:427:ILE:HD11	1:K:444:ARG:NH1	2.28	0.49
3:H:20:DT:H2''	3:H:21:DT:O4'	2.13	0.49
1:C:4:LYS:O	1:C:7:VAL:N	2.46	0.48
1:K:173:PRO:HG2	1:K:247:VAL:HG11	1.93	0.48
1:I:48:LEU:HA	1:I:51:ILE:HD12	1.96	0.48
1:I:48:LEU:HD23	1:I:51:ILE:HD12	1.93	0.48
1:K:108:VAL:HG12	1:K:112:GLN:OE1	2.13	0.48
1:A:501:LEU:O	1:A:505:LEU:N	2.37	0.48
1:A:48:LEU:HA	1:A:51:ILE:HD12	1.95	0.48
1:K:317:VAL:HG22	1:K:502:ARG:HG3	1.94	0.48
1:C:378:ASN:OD1	1:C:478:ARG:NE	2.47	0.48
3:P:7:DT:H2''	3:P:8:DA:C8	2.49	0.48
1:C:254:TYR:CG	1:C:255:LYS:N	2.81	0.48
1:C:380:LEU:O	1:C:385:LEU:HB2	2.14	0.48
1:I:394:SER:O	1:I:400:ASN:ND2	2.41	0.48
1:K:91:LYS:O	1:K:122:TYR:OH	2.28	0.48
1:K:254:TYR:CE1	3:P:5:DT:H4'	2.48	0.48
1:A:472:ILE:HG22	1:A:472:ILE:O	2.14	0.48
1:I:100:SER:C	1:I:102:SER:H	2.20	0.48
2:E:-11:DA:C2	2:E:-10:DT:C2	3.02	0.48
2:E:-9:DA:C2	3:F:10:DA:C2	3.02	0.47
1:A:254:TYR:CG	1:A:255:LYS:N	2.81	0.47
1:K:202:PHE:O	1:K:295:LYS:NZ	2.41	0.47
1:C:477:VAL:HG21	1:C:535:ILE:HA	1.95	0.47
1:A:204:ASN:OD1	1:A:204:ASN:N	2.47	0.47
1:C:386:THR:HG22	1:C:471:GLU:HG2	1.96	0.47
1:I:117:ILE:N	1:I:117:ILE:HD12	2.29	0.47
1:K:385:LEU:HD21	1:K:473:ASP:CA	2.45	0.47
1:A:126:ASP:OD2	1:A:129:ASN:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:TYR:O	1:A:283:ILE:N	2.35	0.47
1:A:413:LEU:HD12	1:A:462:LEU:HD11	1.96	0.47
1:A:436:TYR:OH	1:A:444:ARG:NH2	2.48	0.47
1:C:100:SER:O	1:C:144:ARG:NH2	2.48	0.47
1:K:35:ASP:CG	1:K:38:THR:HG1	2.19	0.47
1:K:311:LEU:O	1:K:494:SER:OG	2.22	0.47
2:G:-5:DA:N1	3:H:6:DG:C2	2.83	0.47
1:A:168:ILE:CG2	2:E:-2:DT:H5'	2.45	0.47
1:C:179:ASN:O	1:C:183:SER:N	2.48	0.47
1:I:320:CYS:O	1:I:324:GLY:N	2.45	0.47
1:I:393:LEU:HD23	1:I:394:SER:N	2.30	0.47
1:A:117:ILE:HD12	1:A:117:ILE:N	2.29	0.47
1:C:315:ALA:O	1:C:498:ASN:ND2	2.47	0.47
1:K:146:GLU:OE1	1:K:147:PHE:N	2.48	0.47
2:G:-4:DG:C2	2:G:-3:DC:C2	3.02	0.47
1:A:471:GLU:CD	1:A:477:VAL:HG11	2.40	0.46
1:A:530:LEU:CB	1:A:535:ILE:HD11	2.44	0.46
1:K:99:GLY:O	1:K:100:SER:C	2.58	0.46
1:K:507:ASP:OD1	1:K:508:VAL:N	2.48	0.46
1:C:314:LEU:N	1:C:363:TYR:OH	2.42	0.46
1:A:177:GLN:O	1:A:186:ASP:N	2.38	0.46
1:C:203:LEU:HD21	1:C:292:SER:N	2.30	0.46
1:A:219:HIS:CE1	1:A:223:LEU:HD11	2.51	0.46
1:A:388:HIS:O	1:A:392:MET:N	2.49	0.46
1:C:176:TYR:CE2	1:C:283:ILE:HD12	2.51	0.46
1:K:177:GLN:O	1:K:186:ASP:N	2.46	0.46
1:A:93:ILE:O	1:A:96:LEU:HB2	2.15	0.46
2:M:-3:DC:H2'	2:M:-2:DT:C6	2.51	0.46
1:C:101:TYR:O	1:C:104:ALA:N	2.49	0.46
1:I:175:GLY:N	1:I:191:GLU:OE1	2.40	0.46
1:K:93:ILE:HG23	1:K:96:LEU:HD12	1.98	0.46
1:K:417:GLU:HB2	1:K:455:LEU:HD21	1.97	0.46
1:A:289:PHE:O	1:A:292:SER:OG	2.25	0.46
1:A:500:LEU:O	1:A:504:VAL:HG23	2.16	0.46
1:I:137:ARG:NH1	1:K:148:GLU:OE1	2.49	0.46
1:A:320:CYS:O	1:A:324:GLY:N	2.43	0.45
1:A:504:VAL:O	1:A:531:ARG:N	2.37	0.45
3:N:19:DC:H2'	3:N:20:DT:C6	2.51	0.45
1:I:12:ILE:HG23	1:I:86:GLN:HB2	1.99	0.45
1:I:102:SER:OG	1:I:103:ASP:OD1	2.34	0.45
1:I:427:ILE:HD11	1:I:444:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:18:DA:H2'	3:H:19:DC:O4'	2.16	0.45
3:N:2:DA:C6	3:N:3:DG:C6	3.04	0.45
1:A:81:GLU:O	1:A:114:LYS:NZ	2.42	0.45
1:A:319:THR:HG22	1:A:507:ASP:OD1	2.17	0.45
1:C:246:GLU:OE1	1:C:251:THR:HG21	2.16	0.45
1:C:292:SER:OG	1:C:293:GLN:NE2	2.50	0.45
1:K:147:PHE:CE1	1:K:151:ARG:HD3	2.52	0.45
1:C:99:GLY:O	1:C:100:SER:C	2.57	0.45
1:K:480:ASN:O	1:K:484:ILE:HD13	2.17	0.45
1:I:146:GLU:OE1	1:I:147:PHE:N	2.50	0.45
1:A:389:ILE:HG21	1:A:471:GLU:HB3	1.99	0.45
1:I:176:TYR:C	1:I:188:VAL:HG23	2.42	0.45
1:I:417:GLU:HB2	1:I:455:LEU:HD21	1.99	0.45
2:E:-3:DC:H2'	2:E:-2:DT:C6	2.52	0.45
1:I:245:ASN:OD1	1:I:247:VAL:HG23	2.17	0.44
3:P:19:DC:H3'	3:P:20:DT:H72	1.98	0.44
1:I:220:LEU:O	1:I:224:GLN:N	2.51	0.44
1:K:254:TYR:CG	1:K:255:LYS:N	2.86	0.44
1:I:70:ARG:HB3	1:I:73:PHE:HB2	2.00	0.44
3:H:20:DT:C2'	3:H:21:DT:O4'	2.66	0.44
1:C:86:GLN:N	1:C:86:GLN:CD	2.75	0.44
1:I:366:VAL:HG22	1:I:524:PHE:CE2	2.51	0.44
1:I:477:VAL:HB	1:I:535:ILE:HG23	1.98	0.44
1:K:45:ASN:O	1:K:49:THR:OG1	2.35	0.44
1:A:86:GLN:CD	1:A:86:GLN:N	2.76	0.44
1:I:204:ASN:OD1	1:I:204:ASN:N	2.49	0.44
1:K:15:ILE:O	1:K:55:TYR:HA	2.18	0.44
1:C:253:LYS:HG2	1:C:275:VAL:HG13	1.99	0.44
1:K:29:GLU:HG2	1:K:36:THR:H	1.82	0.44
1:K:37:LEU:C	1:K:37:LEU:HD23	2.42	0.44
1:I:176:TYR:CE1	1:I:283:ILE:HD12	2.53	0.44
1:I:26:MET:HE3	1:I:26:MET:HB2	1.97	0.44
2:E:-15:DC:H2'	2:E:-14:DT:C6	2.53	0.44
1:A:424:GLU:HB2	1:A:448:LEU:HD21	2.00	0.43
1:A:99:GLY:O	1:A:100:SER:C	2.60	0.43
1:C:93:ILE:HG23	1:C:96:LEU:HD12	1.99	0.43
1:I:4:LYS:O	1:I:8:ASN:N	2.40	0.43
1:I:135:GLN:CD	1:I:135:GLN:C	2.87	0.43
3:F:19:DC:H2'	3:F:20:DT:C6	2.53	0.43
2:G:-5:DA:C6	2:G:-4:DG:C6	3.05	0.43
1:A:476:THR:O	1:A:480:ASN:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:111:LEU:O	1:K:115:ARG:N	2.47	0.43
1:C:109:ASN:HA	1:C:112:GLN:OE1	2.18	0.43
1:I:53:ILE:HG23	1:I:54:PRO:HD2	2.00	0.43
1:A:176:TYR:OH	1:A:281:ALA:O	2.23	0.43
1:C:462:LEU:HD13	1:C:462:LEU:N	2.33	0.43
1:I:353:CYS:O	1:I:357:LYS:N	2.50	0.43
1:K:373:TYR:CE1	1:K:377:LEU:HD21	2.54	0.43
1:K:109:ASN:HA	1:K:112:GLN:OE1	2.19	0.43
1:A:360:TYR:CE1	2:E:-23:DG:H5'	2.54	0.43
1:C:317:VAL:HG22	1:C:502:ARG:CG	2.48	0.43
1:C:442:LEU:HD23	1:C:442:LEU:N	2.34	0.43
1:C:480:ASN:O	1:C:484:ILE:HD13	2.19	0.43
1:K:378:ASN:HA	1:K:478:ARG:HG3	2.01	0.43
1:K:361:VAL:HG11	1:K:524:PHE:HB3	2.01	0.43
1:C:292:SER:O	1:C:296:ILE:HG13	2.18	0.43
1:K:43:LEU:CD1	1:K:47:ILE:HD11	2.49	0.43
1:K:170:GLY:CA	2:O:-4:DG:H1'	2.49	0.43
1:A:252:VAL:O	1:A:276:VAL:N	2.38	0.43
1:K:292:SER:O	1:K:296:ILE:HG13	2.18	0.43
2:M:-7:DA:C5	2:M:-6:DC:C4	3.07	0.43
1:A:162:ALA:O	1:A:276:VAL:HG21	2.19	0.42
1:C:103:ASP:OD1	1:C:103:ASP:N	2.52	0.42
1:C:295:LYS:O	1:C:299:LYS:N	2.52	0.42
1:I:99:GLY:O	1:I:100:SER:CB	2.66	0.42
1:I:105:GLY:O	1:I:109:ASN:CG	2.62	0.42
1:I:376:SER:O	1:I:384:THR:HG21	2.19	0.42
1:K:123:LYS:CG	1:K:124:VAL:N	2.82	0.42
1:K:164:GLN:OE1	1:K:166:LYS:NZ	2.44	0.42
3:H:4:DC:H2'	3:H:5:DT:C6	2.54	0.42
2:M:-17:DA:C2	3:N:18:DA:C2	3.07	0.42
1:A:158:LYS:HE3	2:E:-2:DT:H1'	2.01	0.42
2:G:-13:DT:H2''	2:G:-12:DA:C8	2.55	0.42
2:M:-15:DC:H2'	2:M:-14:DT:C6	2.54	0.42
1:A:219:HIS:NE2	1:A:223:LEU:HD11	2.34	0.42
1:C:119:ILE:HA	1:C:124:VAL:HG22	2.01	0.42
2:G:-17:DA:C5	2:G:-16:DT:C4	3.07	0.42
1:A:48:LEU:HD12	1:A:57:LEU:HD21	2.02	0.42
1:I:99:GLY:O	1:I:100:SER:OG	2.37	0.42
1:C:427:ILE:HD12	1:C:448:LEU:HD22	2.02	0.42
1:I:418:LYS:O	1:I:422:ASN:ND2	2.53	0.42
1:A:108:VAL:HG12	1:A:112:GLN:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:129:ASN:OD1	1:I:129:ASN:C	2.63	0.42
1:I:504:VAL:O	1:I:531:ARG:N	2.34	0.42
1:K:176:TYR:CE2	1:K:283:ILE:HD12	2.54	0.42
1:A:109:ASN:HA	1:A:112:GLN:OE1	2.20	0.41
1:A:129:ASN:OD1	1:A:129:ASN:C	2.63	0.41
1:A:168:ILE:HG23	2:E:-2:DT:H5'	2.02	0.41
1:A:247:VAL:HA	1:A:251:THR:O	2.20	0.41
1:C:53:ILE:HG23	1:C:54:PRO:HD2	2.00	0.41
1:I:398:ASP:HB3	1:I:532:PHE:HD2	1.85	0.41
1:I:417:GLU:OE1	1:I:459:LYS:NZ	2.45	0.41
1:I:452:PHE:O	1:I:456:GLN:HG2	2.20	0.41
1:K:107:ILE:HG22	1:K:111:LEU:HD11	2.02	0.41
3:H:8:DA:C2	3:H:9:DT:C2	3.07	0.41
1:A:376:SER:O	1:A:380:LEU:HG	2.19	0.41
1:C:15:ILE:O	1:C:55:TYR:HA	2.20	0.41
1:C:15:ILE:O	1:C:56:GLU:N	2.52	0.41
1:C:170:GLY:C	2:G:-4:DG:H4'	2.45	0.41
1:K:154:MET:SD	2:O:-1:DT:C4	3.13	0.41
1:A:313:GLU:O	1:A:501:LEU:HD12	2.19	0.41
1:A:380:LEU:O	1:A:385:LEU:HB2	2.21	0.41
1:A:398:ASP:OD1	1:A:400:ASN:ND2	2.53	0.41
1:C:162:ALA:O	1:C:165:GLY:N	2.49	0.41
1:C:170:GLY:HA2	2:G:-4:DG:H4'	2.03	0.41
1:K:304:PRO:HB3	2:O:-13:DT:H1'	2.02	0.41
1:I:384:THR:HG22	1:I:384:THR:O	2.20	0.41
1:K:191:GLU:O	1:K:195:VAL:HG23	2.20	0.41
3:H:19:DC:H2'	3:H:20:DT:C6	2.54	0.41
1:A:175:GLY:N	1:A:191:GLU:OE1	2.46	0.41
1:A:385:LEU:O	1:A:389:ILE:HD13	2.19	0.41
1:C:485:ILE:HG22	1:C:489:HIS:CD2	2.56	0.41
3:H:2:DA:C2	3:H:3:DG:C2	3.08	0.41
1:A:381:ASN:O	1:A:383:SER:N	2.53	0.41
1:C:176:TYR:OH	1:C:281:ALA:O	2.25	0.41
1:I:378:ASN:OD1	1:I:378:ASN:C	2.62	0.41
1:K:175:GLY:HA2	1:K:191:GLU:HB2	2.02	0.41
1:A:13:THR:HG1	1:A:14:ASN:H	1.67	0.41
1:C:399:ASP:OD1	1:C:399:ASP:N	2.53	0.41
1:C:488:TYR:CE2	1:C:501:LEU:HD11	2.56	0.41
1:K:365:ASP:OD1	1:K:365:ASP:N	2.52	0.41
1:K:471:GLU:HB3	1:K:535:ILE:HG21	2.02	0.41
1:K:474:SER:O	1:K:477:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:-13:DT:H2''	2:E:-12:DA:C8	2.56	0.41
1:A:44:MET:HA	1:A:47:ILE:HD12	2.03	0.41
1:C:13:THR:OG1	1:C:14:ASN:N	2.53	0.41
1:C:23:ARG:HB2	3:H:2:DA:C8	2.55	0.41
1:C:170:GLY:CA	2:G:-4:DG:H4'	2.51	0.41
1:C:201:ILE:O	1:C:205:GLY:N	2.53	0.41
1:I:468:THR:HG23	1:I:471:GLU:CG	2.50	0.41
1:K:86:GLN:N	1:K:86:GLN:CD	2.78	0.41
3:F:18:DA:C2	3:F:19:DC:C2	3.09	0.41
3:H:7:DT:C4	3:H:8:DA:C6	3.09	0.41
1:C:6:ILE:O	1:C:10:TYR:CE2	2.73	0.41
1:C:219:HIS:NE2	1:C:223:LEU:HD11	2.35	0.41
1:I:102:SER:OG	1:I:103:ASP:N	2.53	0.41
1:K:317:VAL:HG23	1:K:498:ASN:ND2	2.35	0.41
3:F:6:DG:H2'	3:F:7:DT:H72	2.02	0.41
1:A:3:LEU:HA	1:A:6:ILE:HD12	2.02	0.40
1:A:108:VAL:HG12	1:A:112:GLN:OE1	2.21	0.40
1:C:133:MET:HA	1:C:133:MET:HE3	2.04	0.40
1:A:149:MET:SD	1:A:149:MET:C	3.04	0.40
1:A:254:TYR:CE1	3:F:5:DT:H4'	2.56	0.40
1:A:313:GLU:O	1:A:498:ASN:HA	2.20	0.40
1:C:225:ILE:O	1:C:234:TRP:NE1	2.54	0.40
1:I:313:GLU:OE1	1:I:313:GLU:N	2.44	0.40
1:I:320:CYS:O	1:I:324:GLY:CA	2.69	0.40
1:I:462:LEU:O	1:I:466:GLN:OE1	2.39	0.40
1:K:94:THR:O	1:K:97:SER:N	2.54	0.40
1:K:112:GLN:NE2	1:K:133:MET:SD	2.94	0.40
2:G:-12:DA:C2	3:H:13:DA:C2	3.09	0.40
1:A:13:THR:OG1	1:A:86:GLN:OE1	2.27	0.40
1:A:484:ILE:CG1	1:A:504:VAL:HG21	2.52	0.40
1:C:358:CYS:O	1:C:512:MET:HE2	2.22	0.40
1:C:379:ASP:O	1:C:380:LEU:C	2.64	0.40
1:C:417:GLU:HB2	1:C:455:LEU:HD21	2.03	0.40
1:I:361:VAL:HG11	1:I:510:VAL:HG11	2.03	0.40
1:A:378:ASN:HA	1:A:481:ILE:HG21	2.02	0.40
1:I:360:TYR:CE1	2:M:-23:DG:H5'	2.56	0.40
1:I:361:VAL:HG11	1:I:510:VAL:CG1	2.52	0.40
1:K:37:LEU:HD21	1:K:59:MET:SD	2.62	0.40
1:K:405:THR:HG22	1:K:463:ASN:CG	2.47	0.40
1:A:92:GLU:CD	1:A:93:ILE:N	2.79	0.40
1:C:417:GLU:OE1	1:C:459:LYS:NZ	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:179:ASN:OD1	1:I:179:ASN:C	2.64	0.40
1:I:292:SER:OG	1:I:293:GLN:NE2	2.55	0.40
2:G:-7:DA:C2	3:H:8:DA:C2	3.10	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	533/545 (98%)	498 (93%)	34 (6%)	1 (0%)	43	78
1	C	533/545 (98%)	503 (94%)	30 (6%)	0	100	100
1	I	533/545 (98%)	498 (93%)	35 (7%)	0	100	100
1	K	533/545 (98%)	504 (95%)	27 (5%)	2 (0%)	30	67
All	All	2132/2180 (98%)	2003 (94%)	126 (6%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	99	GLY
1	K	402	ASN
1	A	102	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	490/499 (98%)	463 (94%)	27 (6%)	19	42
1	C	490/499 (98%)	466 (95%)	24 (5%)	22	44
1	I	490/499 (98%)	460 (94%)	30 (6%)	17	39
1	K	490/499 (98%)	470 (96%)	20 (4%)	27	49
All	All	1960/1996 (98%)	1859 (95%)	101 (5%)	22	43

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	15	ILE
1	A	21	ARG
1	A	25	ASP
1	A	59	MET
1	A	68	ASP
1	A	92	GLU
1	A	97	SER
1	A	126	ASP
1	A	132	ASP
1	A	133	MET
1	A	135	GLN
1	A	138	PHE
1	A	140	LEU
1	A	148	GLU
1	A	149	MET
1	A	160	THR
1	A	168	ILE
1	A	186	ASP
1	A	204	ASN
1	A	257	ARG
1	A	262	ASP
1	A	278	ASP
1	A	288	GLN
1	A	302	LEU
1	A	381	ASN
1	A	484	ILE
1	C	11	ASN
1	C	13	THR
1	C	22	SER
1	C	68	ASP
1	C	103	ASP
1	C	126	ASP

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Mol	Chain	Res	Type
1	C	133	MET
1	C	138	PHE
1	C	139	GLU
1	C	147	PHE
1	C	160	THR
1	C	168	ILE
1	C	204	ASN
1	C	218	SER
1	C	262	ASP
1	C	285	ASP
1	C	361	VAL
1	C	365	ASP
1	C	378	ASN
1	C	381	ASN
1	C	384	THR
1	C	409	MET
1	C	442	LEU
1	C	462	LEU
1	I	10	TYR
1	I	15	ILE
1	I	22	SER
1	I	24	GLN
1	I	26	MET
1	I	68	ASP
1	I	92	GLU
1	I	97	SER
1	I	103	ASP
1	I	126	ASP
1	I	132	ASP
1	I	133	MET
1	I	138	PHE
1	I	145	GLU
1	I	146	GLU
1	I	149	MET
1	I	151	ARG
1	I	168	ILE
1	I	186	ASP
1	I	204	ASN
1	I	218	SER
1	I	262	ASP
1	I	278	ASP
1	I	285	ASP

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Mol	Chain	Res	Type
1	I	288	GLN
1	I	378	ASN
1	I	393	LEU
1	I	399	ASP
1	I	466	GLN
1	I	533	ASN
1	K	11	ASN
1	K	13	THR
1	K	25	ASP
1	K	65	GLU
1	K	68	ASP
1	K	126	ASP
1	K	133	MET
1	K	140	LEU
1	K	146	GLU
1	K	147	PHE
1	K	160	THR
1	K	168	ILE
1	K	190	ASP
1	K	204	ASN
1	K	229	SER
1	K	262	ASP
1	K	285	ASP
1	K	365	ASP
1	K	462	LEU
1	K	477	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	GLN
1	A	338	ASN
1	A	356	ASN
1	A	469	GLN
1	A	511	ASN
1	A	523	GLN
1	C	293	GLN
1	C	338	ASN
1	C	356	ASN
1	C	422	ASN
1	C	463	ASN
1	C	475	ASN

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Mol	Chain	Res	Type
1	C	489	HIS
1	C	523	GLN
1	I	293	GLN
1	I	356	ASN
1	I	364	ASN
1	I	523	GLN
1	K	293	GLN
1	K	338	ASN
1	K	356	ASN
1	K	498	ASN

### 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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



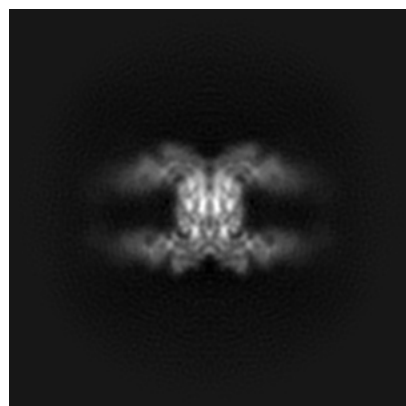
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47290. These allow visual inspection of the internal detail of the map and identification of artifacts.

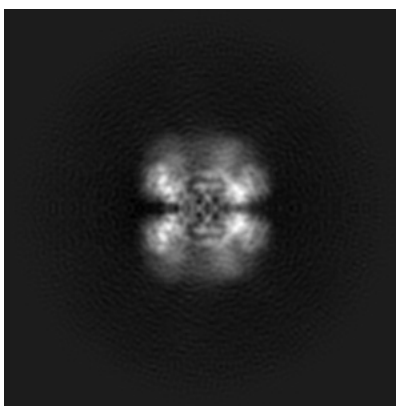
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

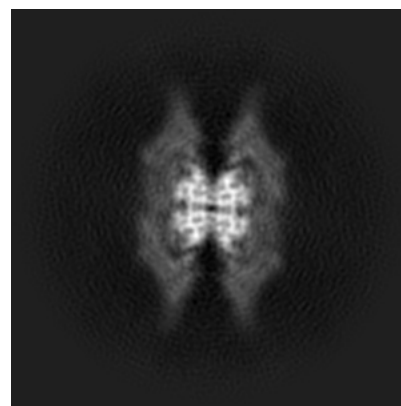
#### 6.1.1 Primary map



X

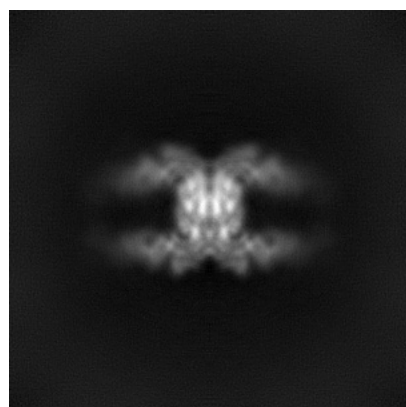


Y

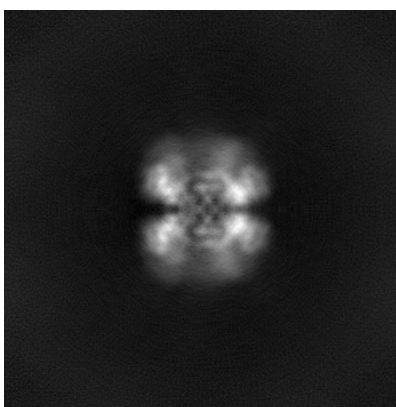


Z

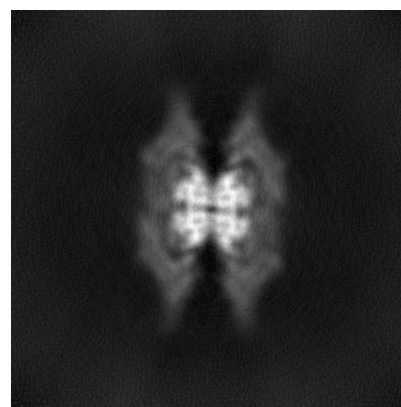
#### 6.1.2 Raw map



X



Y

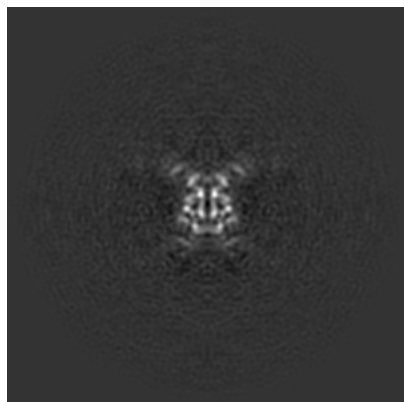


Z

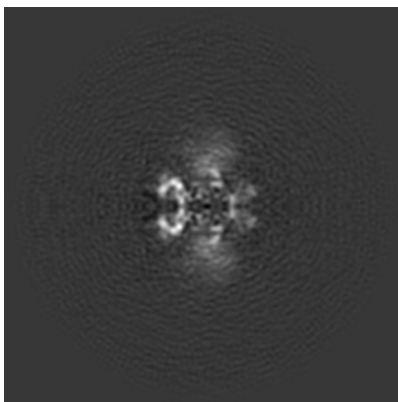
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

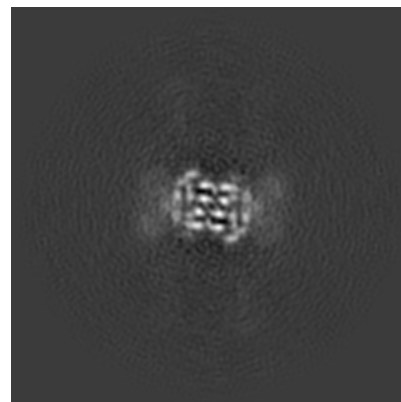
### 6.2.1 Primary map



X Index: 160

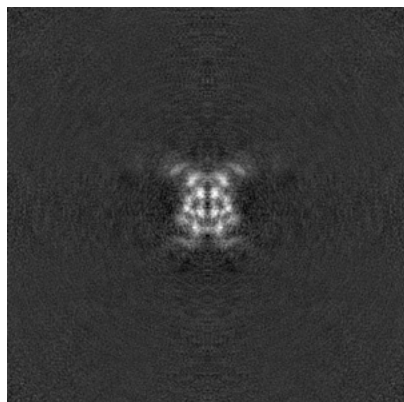


Y Index: 160

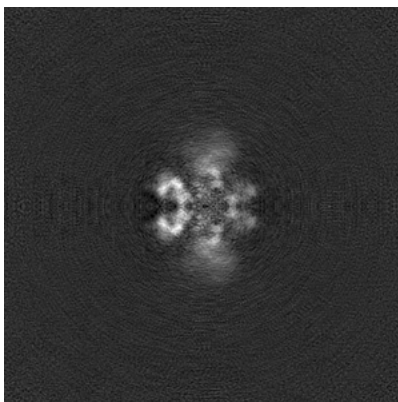


Z Index: 160

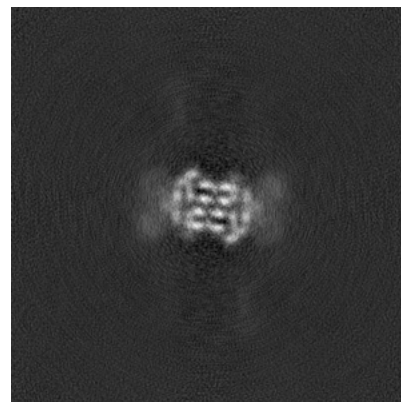
### 6.2.2 Raw map



X Index: 160



Y Index: 160

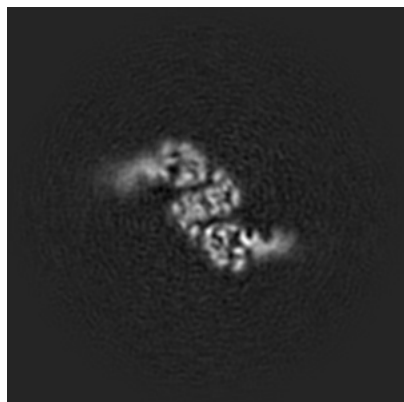


Z Index: 160

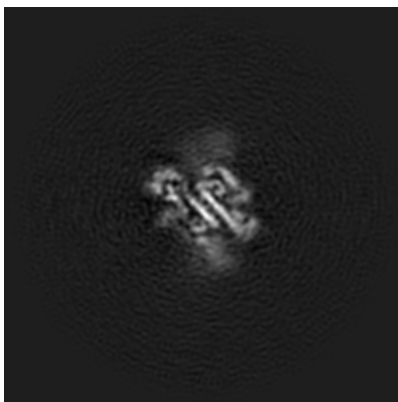
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

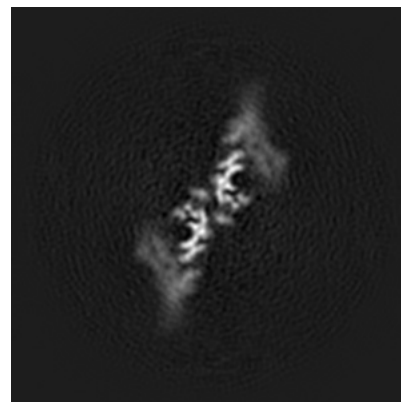
### 6.3.1 Primary map



X Index: 177

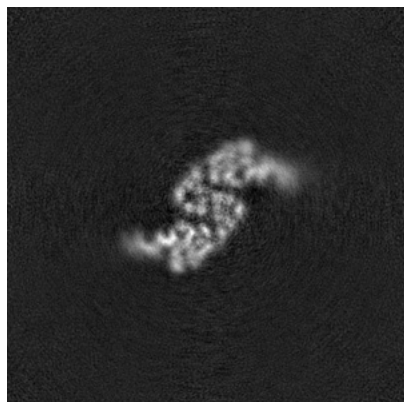


Y Index: 166

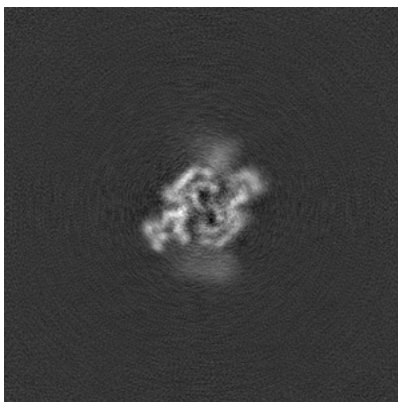


Z Index: 133

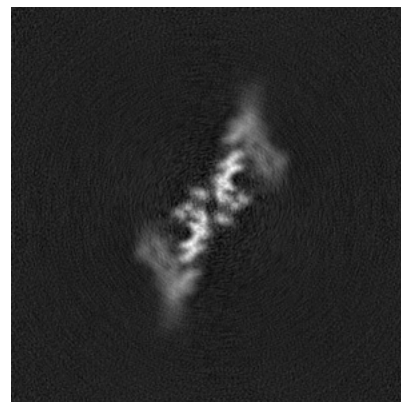
### 6.3.2 Raw map



X Index: 145



Y Index: 149

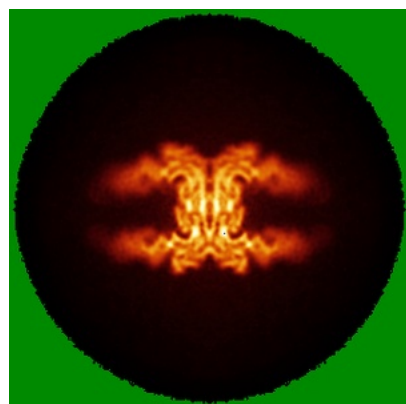


Z Index: 133

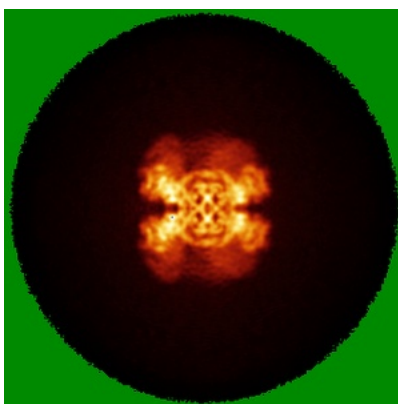
The images above show the largest variance slices of the map in three orthogonal directions.

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

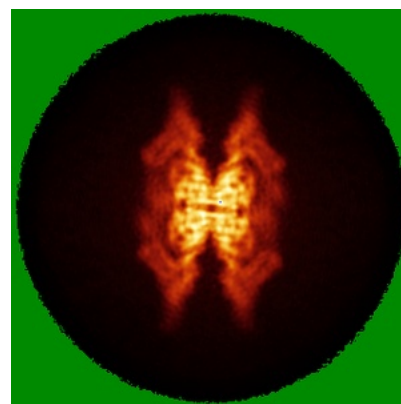
### 6.4.1 Primary map



X

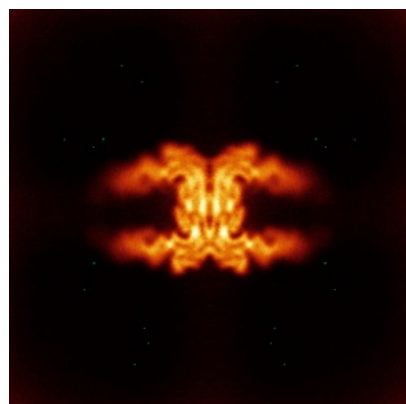


Y

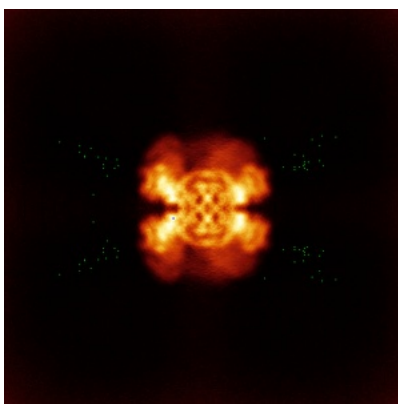


Z

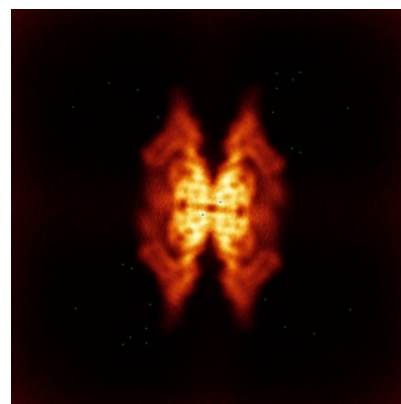
### 6.4.2 Raw map



X



Y

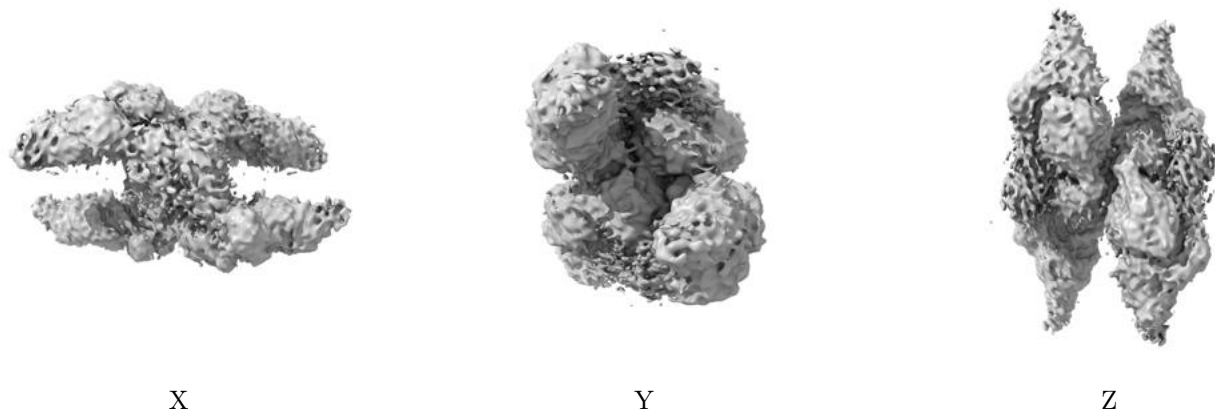


Z

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

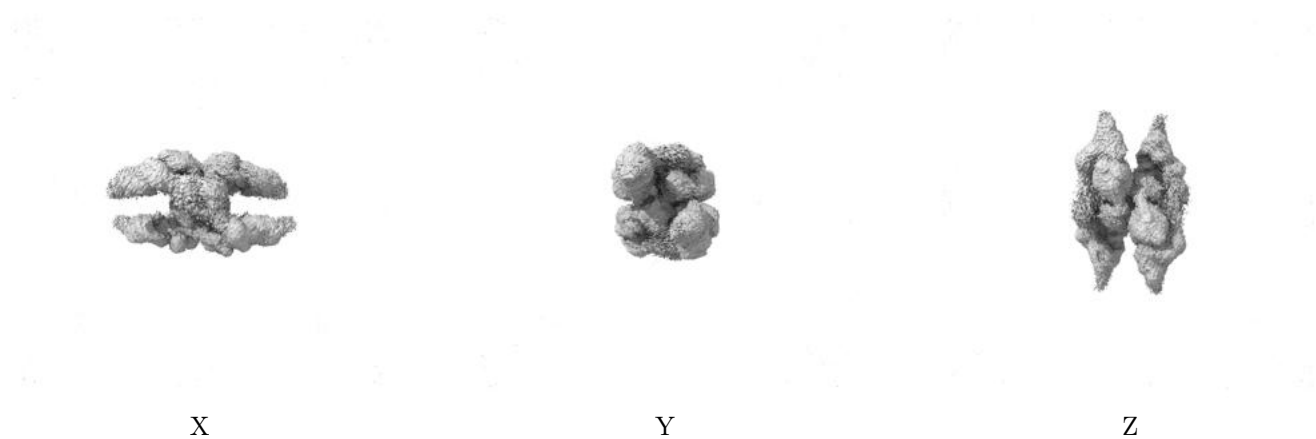
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

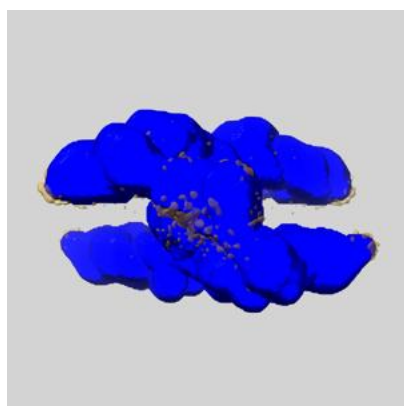
## 6.6 Mask visualisation [i](#)

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

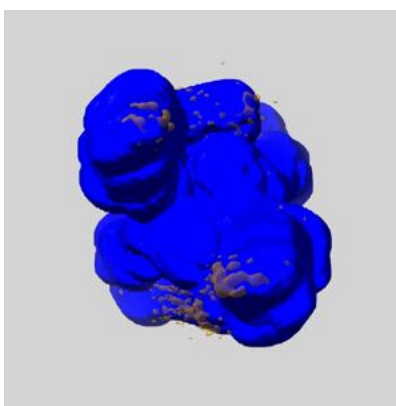
A mask typically either:

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

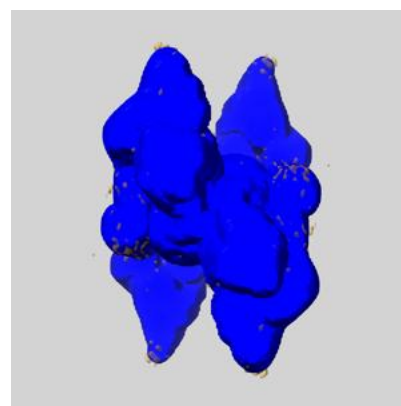
### 6.6.1 emd\_47290\_msk\_1.map [i](#)



X



Y

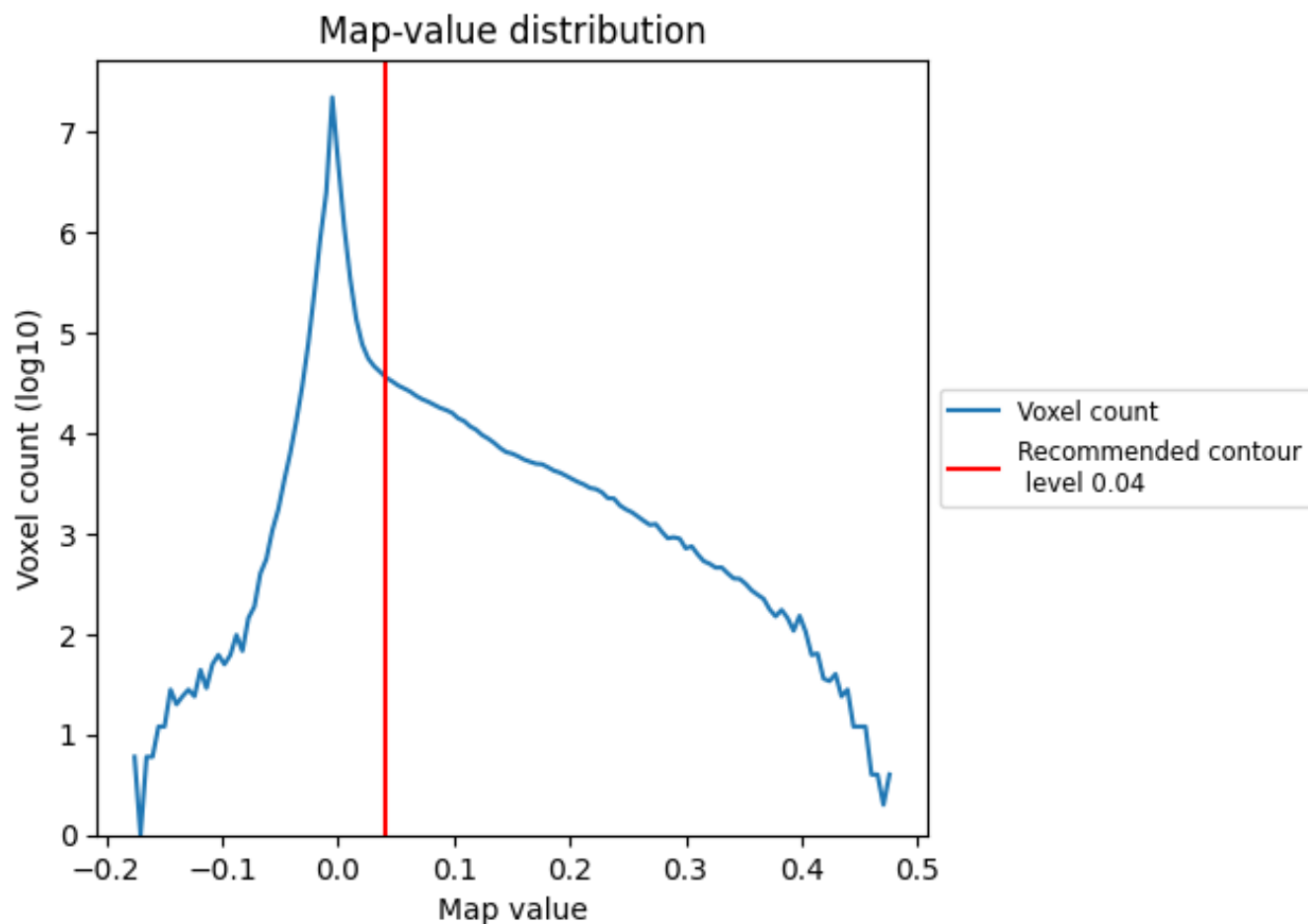


Z

## 7 Map analysis [i](#)

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

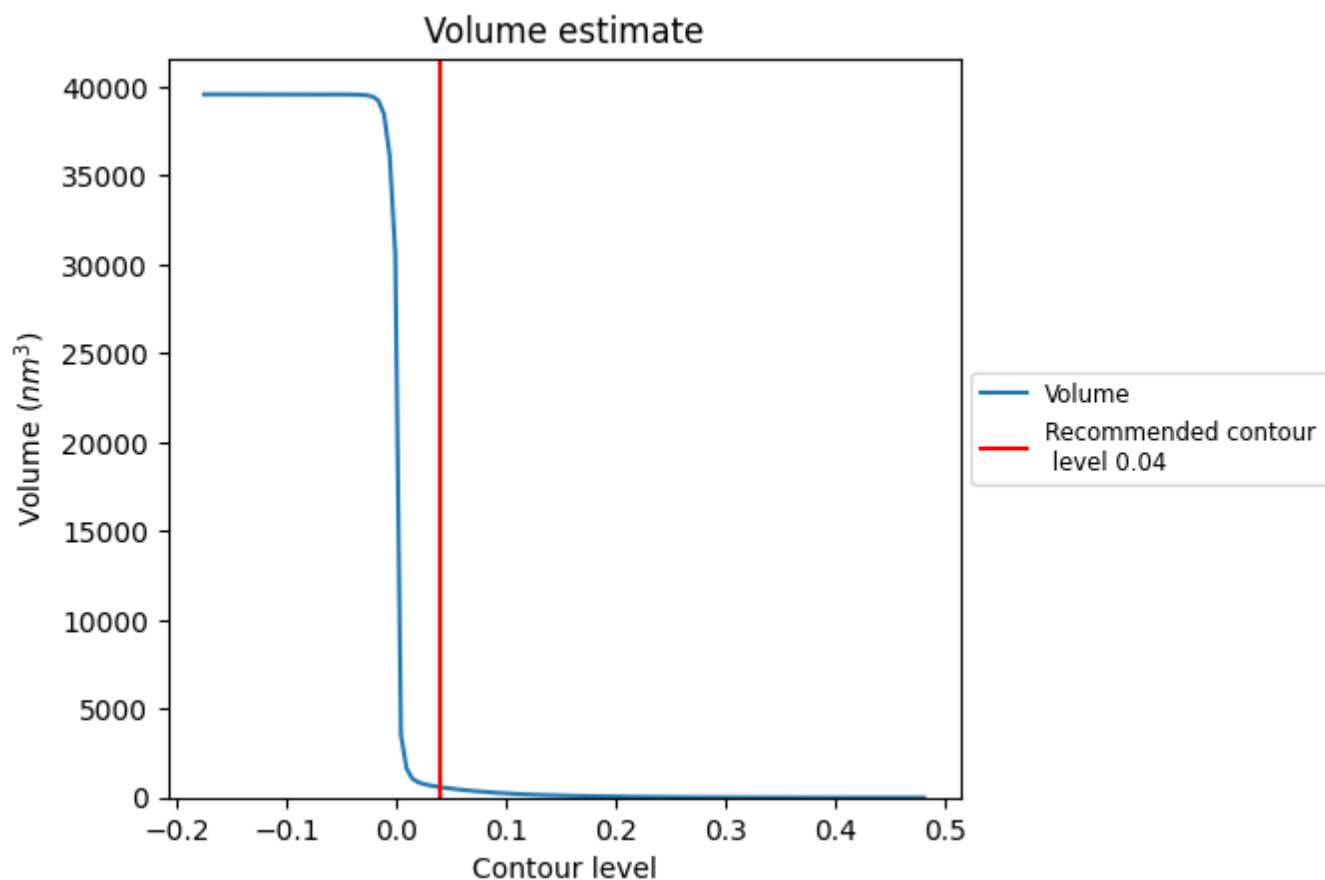
### 7.1 Map-value distribution [i](#)



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



## 7.2 Volume estimate [i](#)

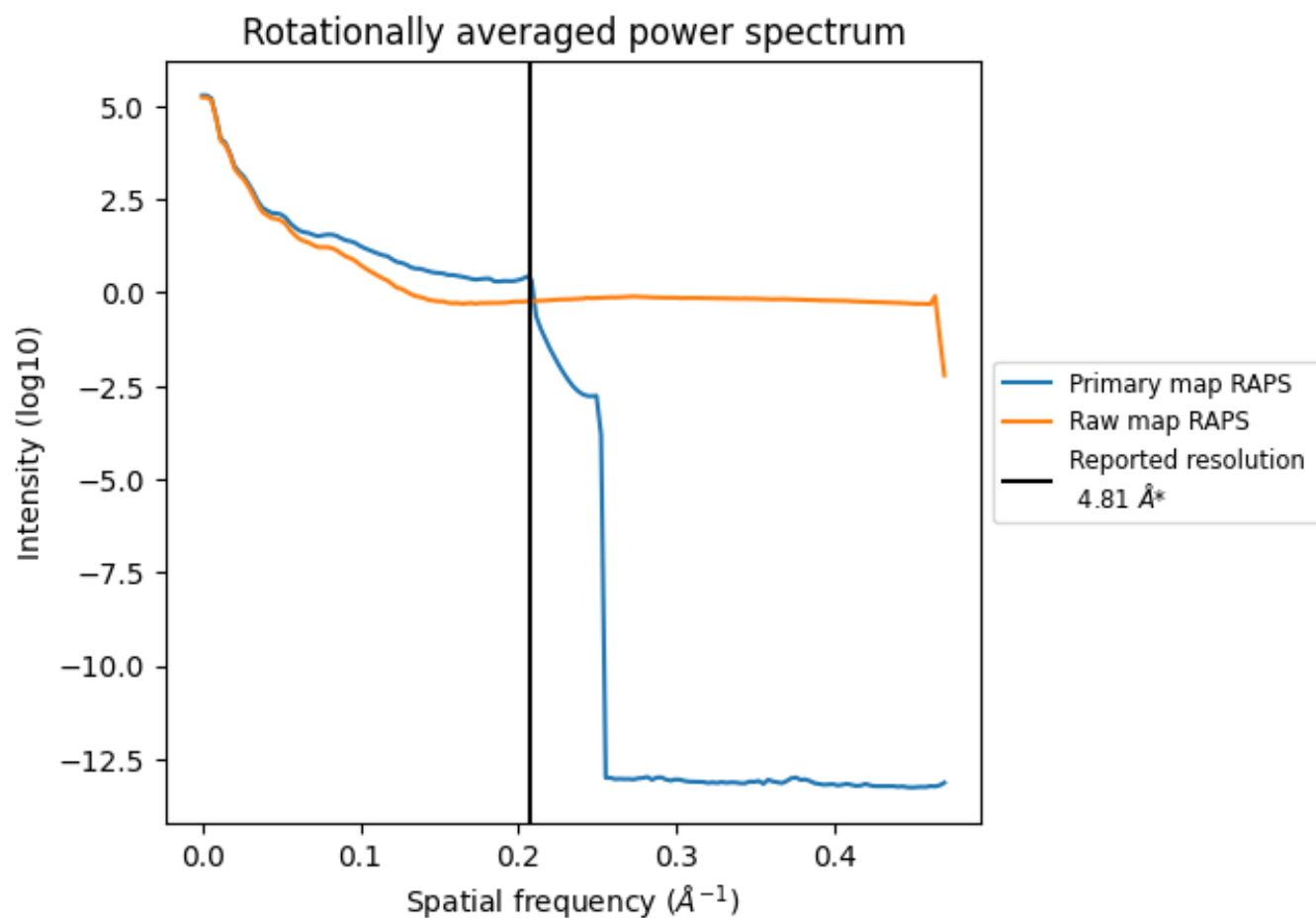


The volume at the recommended contour level is 582  $\text{nm}^3$ ; this corresponds to an approximate mass of 526 kDa.

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 ⓘ

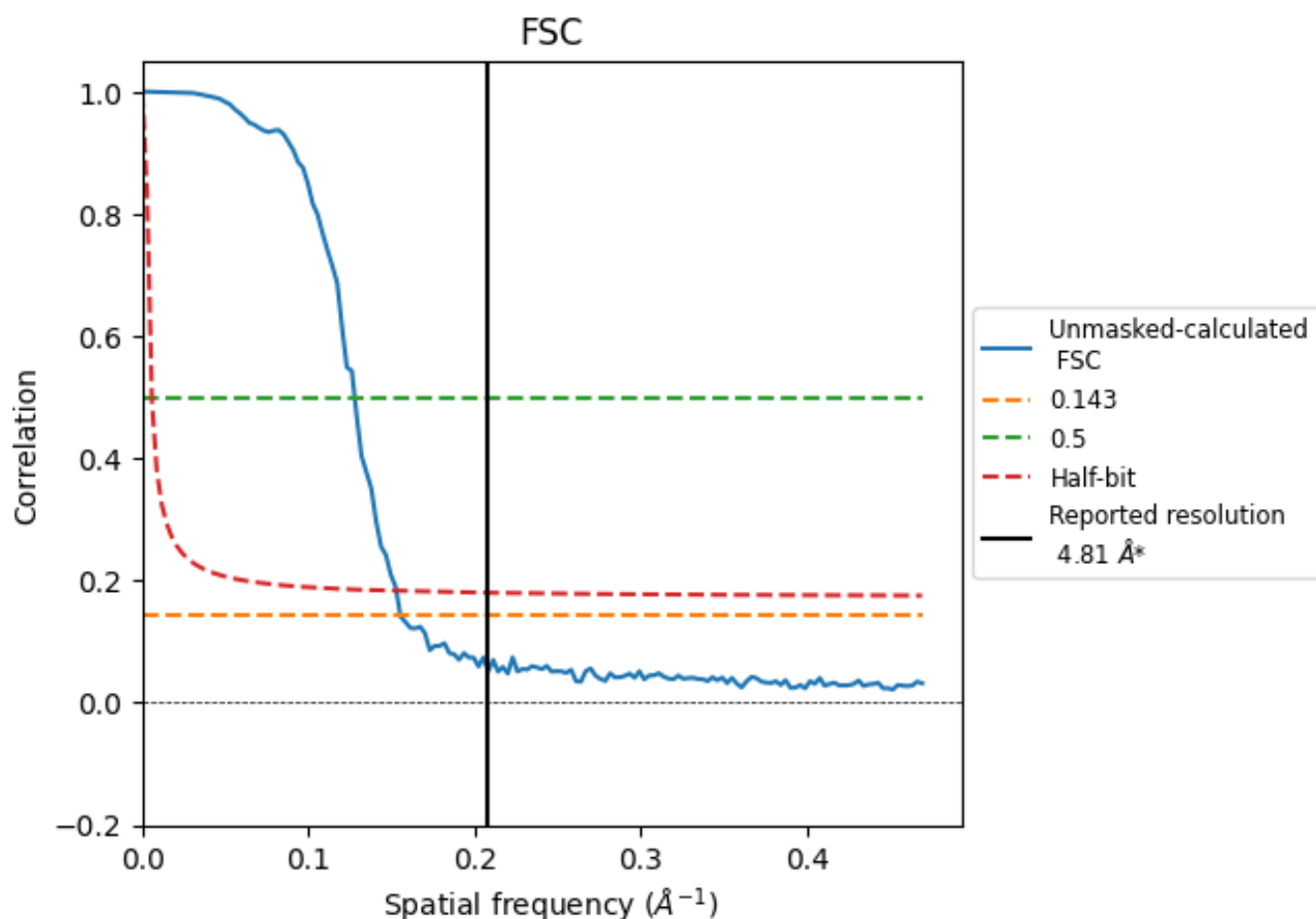


\*Reported resolution corresponds to spatial frequency of 0.208  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.208 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

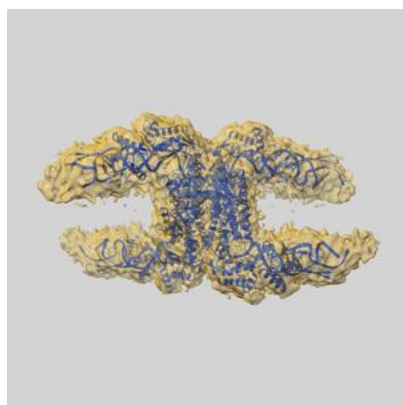
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.81	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.44	7.82	6.54

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.44 differs from the reported value 4.81 by more than 10 %

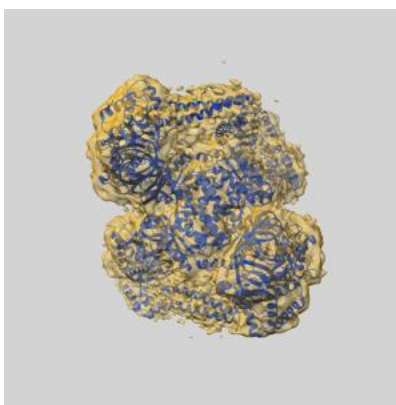
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47290 and PDB model 9DXK. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

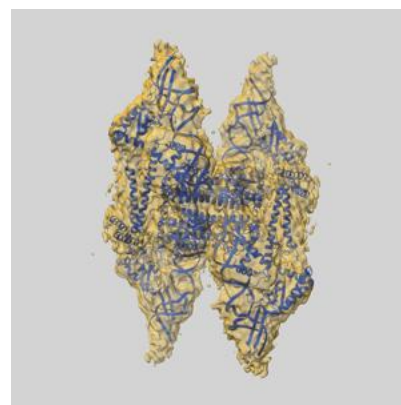
### 9.1 Map-model overlay [i](#)



X



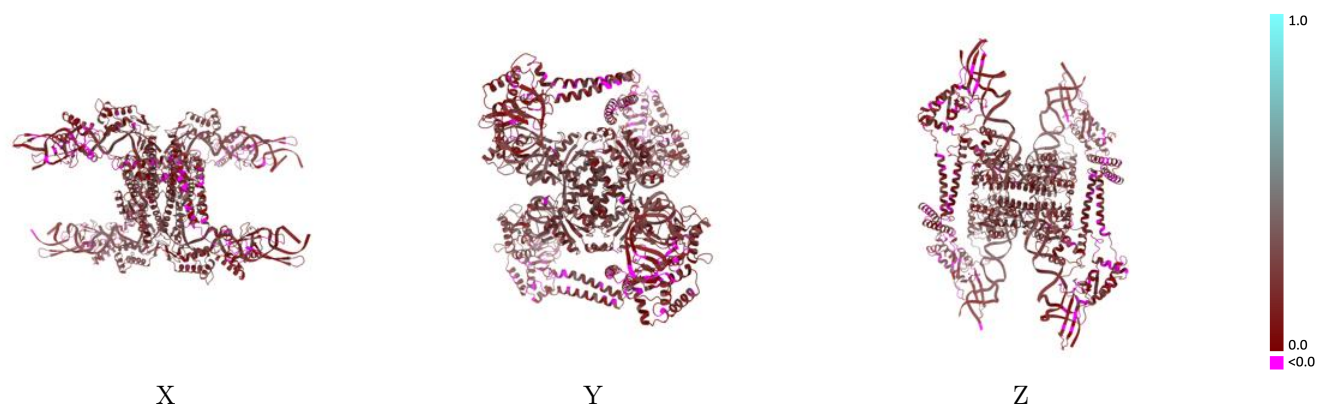
Y



Z

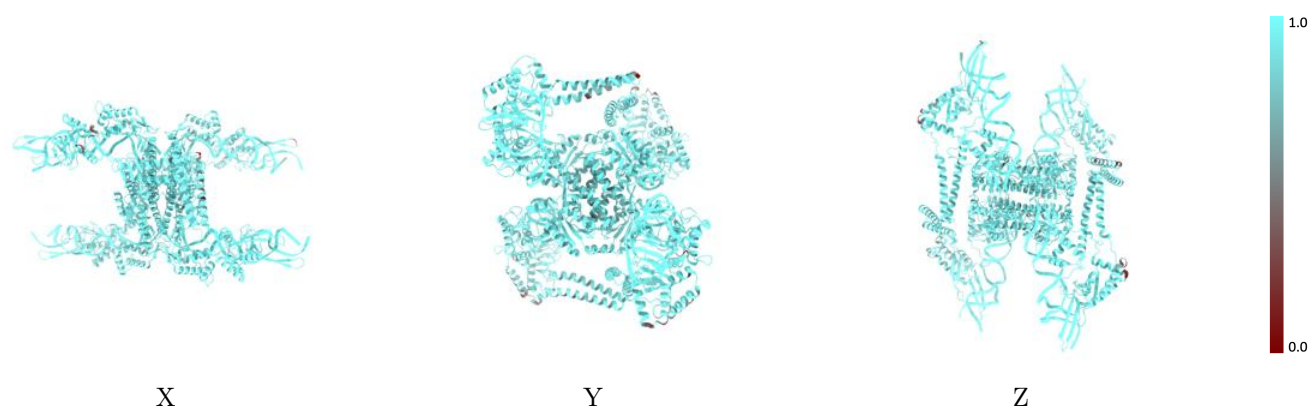
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



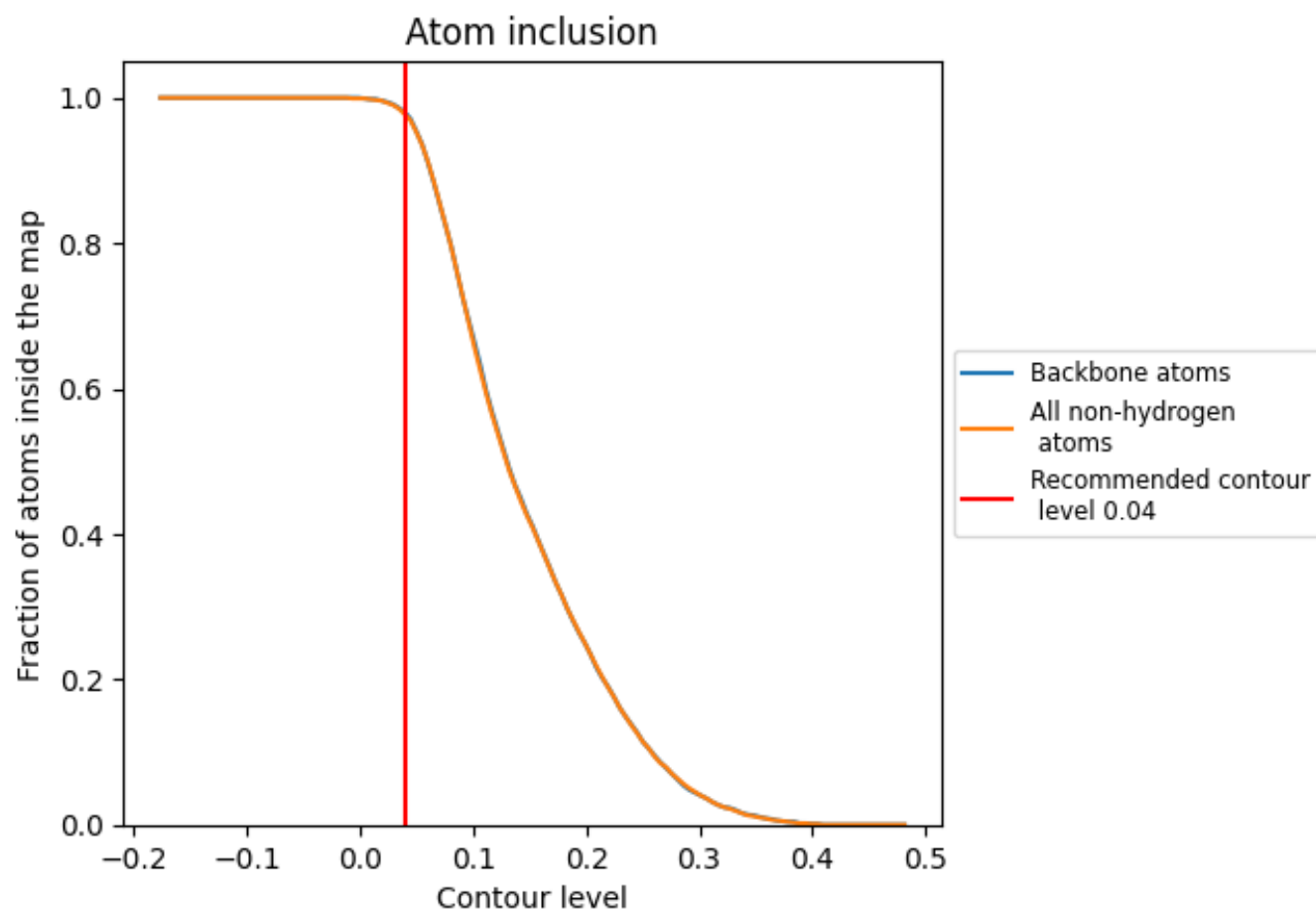
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9770	<div></div> 0.1880
A	<div></div> 0.9630	<div></div> 0.1810
C	<div></div> 0.9750	<div></div> 0.1720
E	<div></div> 1.0000	<div></div> 0.2450
F	<div></div> 0.9980	<div></div> 0.2440
G	<div></div> 1.0000	<div></div> 0.2210
H	<div></div> 1.0000	<div></div> 0.2170
I	<div></div> 0.9750	<div></div> 0.1890
K	<div></div> 0.9720	<div></div> 0.1650
M	<div></div> 0.9980	<div></div> 0.2530
N	<div></div> 1.0000	<div></div> 0.2460
O	<div></div> 1.0000	<div></div> 0.2110
P	<div></div> 0.9800	<div></div> 0.2110

