



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:02 PM UTC

PDB ID : 9DXF / pdb_00009dx
EMDB ID : EMD-47286
Title : attLmm bound serine integrase and RDF complex in the post-rotation state
Authors : Shin, H.; Rice, P.A.; Olorunniji, F.J.
Deposited on : 2024-10-11
Resolution : 4.16 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

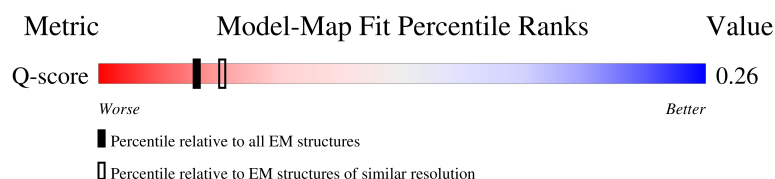
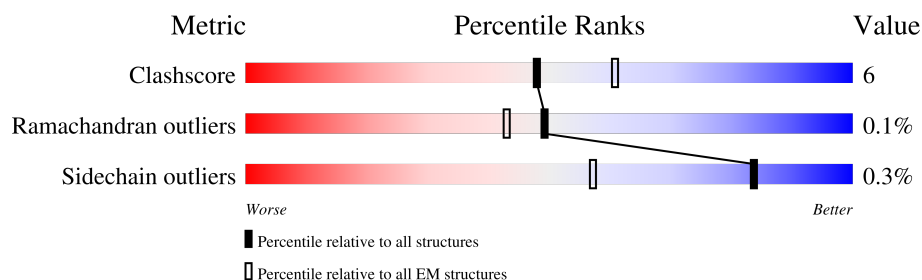
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.16 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	5480 (3.66 - 4.66)

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

Mol	Chain	Length	Quality of chain
1	A	620	<div> <div>7%</div> <div>62%</div> <div>23%</div> <div>14%</div> </div>
1	B	620	<div> <div>5%</div> <div>91%</div> </div>
1	C	620	<div> <div>14%</div> <div>66%</div> <div>19%</div> <div>14%</div> </div>
1	D	620	<div> <div>5%</div> <div>91%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	620	
1	J	620	
1	K	620	
1	L	620	
2	E	34	
2	M	34	
3	F	33	
3	N	33	
4	G	25	
4	O	25	
5	H	24	
5	P	24	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 46352 atoms, of which 22252 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,SPbeta prophage-derived uncharacterized protein YotN.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	534	Total	C	H	N	O	S	0	0
			8764	2736	4418	752	840	18		
1	B	56	Total	C	H	N	O		0	0
			955	306	474	81	94			
1	C	535	Total	C	H	N	O	S	0	0
			8783	2741	4429	753	841	19		
1	D	57	Total	C	H	N	O		0	0
			970	311	480	82	97			
1	I	535	Total	C	H	N	O	S	0	0
			8783	2741	4429	753	841	19		
1	J	56	Total	C	H	N	O		0	0
			955	306	474	81	94			
1	K	534	Total	C	H	N	O	S	0	0
			8764	2736	4418	752	840	18		
1	L	57	Total	C	H	N	O		0	0
			970	311	480	82	97			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	546	THR	-	linker	UNP O32006
A	547	SER	-	linker	UNP O32006
A	548	GLY	-	linker	UNP O32006
A	549	SER	-	linker	UNP O32006
A	550	GLY	-	linker	UNP O32006
A	551	GLY	-	linker	UNP O32006
A	552	SER	-	linker	UNP O32006
A	553	GLY	-	linker	UNP O32006
A	554	GLY	-	linker	UNP O32006
A	555	SER	-	linker	UNP O32006
A	556	GLY	-	linker	UNP O32006
A	557	GLY	-	linker	UNP O32006
A	558	SER	-	linker	UNP O32006

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Chain	Residue	Modelled	Actual	Comment	Reference
A	559	GLY	-	linker	UNP O32006
A	560	ARG	-	linker	UNP O32006
A	561	SER	-	linker	UNP O32006
A	562	GLY	-	linker	UNP O32006
A	563	THR	-	linker	UNP O32006
B	-16	THR	-	linker	UNP O32006
B	-15	SER	-	linker	UNP O32006
B	-14	GLY	-	linker	UNP O32006
B	-13	SER	-	linker	UNP O32006
B	-12	GLY	-	linker	UNP O32006
B	-11	GLY	-	linker	UNP O32006
B	-10	SER	-	linker	UNP O32006
B	-9	GLY	-	linker	UNP O32006
B	-8	GLY	-	linker	UNP O32006
B	-7	SER	-	linker	UNP O32006
B	-6	GLY	-	linker	UNP O32006
B	-5	GLY	-	linker	UNP O32006
B	-4	SER	-	linker	UNP O32006
B	-3	GLY	-	linker	UNP O32006
B	-2	ARG	-	linker	UNP O32006
B	-1	SER	-	linker	UNP O32006
B	0	GLY	-	linker	UNP O32006
B	1	THR	-	linker	UNP O32006
C	546	THR	-	linker	UNP O32006
C	547	SER	-	linker	UNP O32006
C	548	GLY	-	linker	UNP O32006
C	549	SER	-	linker	UNP O32006
C	550	GLY	-	linker	UNP O32006
C	551	GLY	-	linker	UNP O32006
C	552	SER	-	linker	UNP O32006
C	553	GLY	-	linker	UNP O32006
C	554	GLY	-	linker	UNP O32006
C	555	SER	-	linker	UNP O32006
C	556	GLY	-	linker	UNP O32006
C	557	GLY	-	linker	UNP O32006
C	558	SER	-	linker	UNP O32006
C	559	GLY	-	linker	UNP O32006
C	560	ARG	-	linker	UNP O32006
C	561	SER	-	linker	UNP O32006
C	562	GLY	-	linker	UNP O32006
C	563	THR	-	linker	UNP O32006
D	-16	THR	-	linker	UNP O32006

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	SER	-	linker	UNP O32006
D	-14	GLY	-	linker	UNP O32006
D	-13	SER	-	linker	UNP O32006
D	-12	GLY	-	linker	UNP O32006
D	-11	GLY	-	linker	UNP O32006
D	-10	SER	-	linker	UNP O32006
D	-9	GLY	-	linker	UNP O32006
D	-8	GLY	-	linker	UNP O32006
D	-7	SER	-	linker	UNP O32006
D	-6	GLY	-	linker	UNP O32006
D	-5	GLY	-	linker	UNP O32006
D	-4	SER	-	linker	UNP O32006
D	-3	GLY	-	linker	UNP O32006
D	-2	ARG	-	linker	UNP O32006
D	-1	SER	-	linker	UNP O32006
D	0	GLY	-	linker	UNP O32006
D	1	THR	-	linker	UNP O32006
I	546	THR	-	linker	UNP O32006
I	547	SER	-	linker	UNP O32006
I	548	GLY	-	linker	UNP O32006
I	549	SER	-	linker	UNP O32006
I	550	GLY	-	linker	UNP O32006
I	551	GLY	-	linker	UNP O32006
I	552	SER	-	linker	UNP O32006
I	553	GLY	-	linker	UNP O32006
I	554	GLY	-	linker	UNP O32006
I	555	SER	-	linker	UNP O32006
I	556	GLY	-	linker	UNP O32006
I	557	GLY	-	linker	UNP O32006
I	558	SER	-	linker	UNP O32006
I	559	GLY	-	linker	UNP O32006
I	560	ARG	-	linker	UNP O32006
I	561	SER	-	linker	UNP O32006
I	562	GLY	-	linker	UNP O32006
I	563	THR	-	linker	UNP O32006
J	-16	THR	-	linker	UNP O32006
J	-15	SER	-	linker	UNP O32006
J	-14	GLY	-	linker	UNP O32006
J	-13	SER	-	linker	UNP O32006
J	-12	GLY	-	linker	UNP O32006
J	-11	GLY	-	linker	UNP O32006
J	-10	SER	-	linker	UNP O32006

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-9	GLY	-	linker	UNP O32006
J	-8	GLY	-	linker	UNP O32006
J	-7	SER	-	linker	UNP O32006
J	-6	GLY	-	linker	UNP O32006
J	-5	GLY	-	linker	UNP O32006
J	-4	SER	-	linker	UNP O32006
J	-3	GLY	-	linker	UNP O32006
J	-2	ARG	-	linker	UNP O32006
J	-1	SER	-	linker	UNP O32006
J	0	GLY	-	linker	UNP O32006
J	1	THR	-	linker	UNP O32006
K	546	THR	-	linker	UNP O32006
K	547	SER	-	linker	UNP O32006
K	548	GLY	-	linker	UNP O32006
K	549	SER	-	linker	UNP O32006
K	550	GLY	-	linker	UNP O32006
K	551	GLY	-	linker	UNP O32006
K	552	SER	-	linker	UNP O32006
K	553	GLY	-	linker	UNP O32006
K	554	GLY	-	linker	UNP O32006
K	555	SER	-	linker	UNP O32006
K	556	GLY	-	linker	UNP O32006
K	557	GLY	-	linker	UNP O32006
K	558	SER	-	linker	UNP O32006
K	559	GLY	-	linker	UNP O32006
K	560	ARG	-	linker	UNP O32006
K	561	SER	-	linker	UNP O32006
K	562	GLY	-	linker	UNP O32006
K	563	THR	-	linker	UNP O32006
L	-16	THR	-	linker	UNP O32006
L	-15	SER	-	linker	UNP O32006
L	-14	GLY	-	linker	UNP O32006
L	-13	SER	-	linker	UNP O32006
L	-12	GLY	-	linker	UNP O32006
L	-11	GLY	-	linker	UNP O32006
L	-10	SER	-	linker	UNP O32006
L	-9	GLY	-	linker	UNP O32006
L	-8	GLY	-	linker	UNP O32006
L	-7	SER	-	linker	UNP O32006
L	-6	GLY	-	linker	UNP O32006
L	-5	GLY	-	linker	UNP O32006
L	-4	SER	-	linker	UNP O32006

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-3	GLY	-	linker	UNP O32006
L	-2	ARG	-	linker	UNP O32006
L	-1	SER	-	linker	UNP O32006
L	0	GLY	-	linker	UNP O32006
L	1	THR	-	linker	UNP O32006

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	34	Total	C	H	N	O	P	0	0
			1087	337	393	110	213	34		
2	M	34	Total	C	H	N	O	P	0	0
			1087	337	393	110	213	34		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	F	33	Total	C	H	N	O	P	0	0
			1052	326	373	130	190	33		
3	N	33	Total	C	H	N	O	P	0	0
			1052	326	373	130	190	33		

- Molecule 4 is a DNA chain called DNA (25-MER).

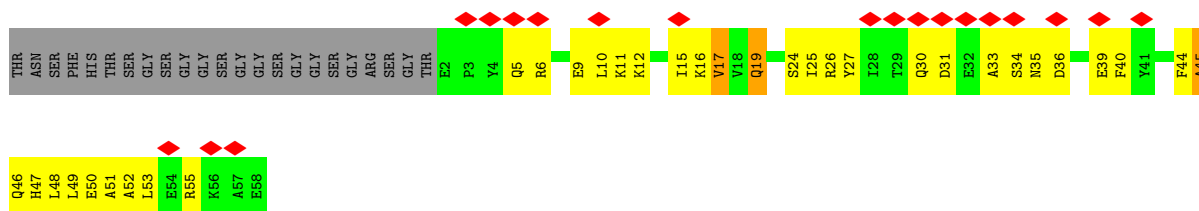
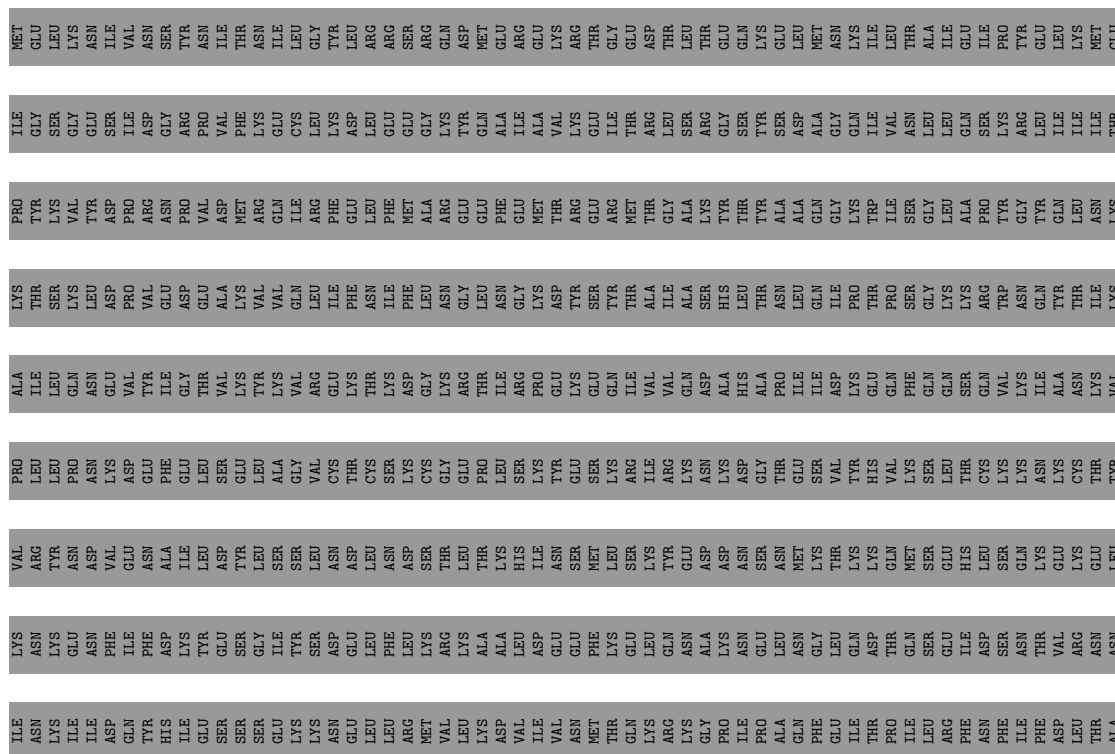
Mol	Chain	Residues	Atoms						AltConf	Trace
4	G	25	Total	C	H	N	O	P	0	0
			796	246	285	90	150	25		
4	O	25	Total	C	H	N	O	P	0	0
			796	246	285	90	150	25		

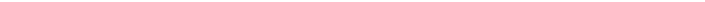
- Molecule 5 is a DNA chain called DNA (24-MER).

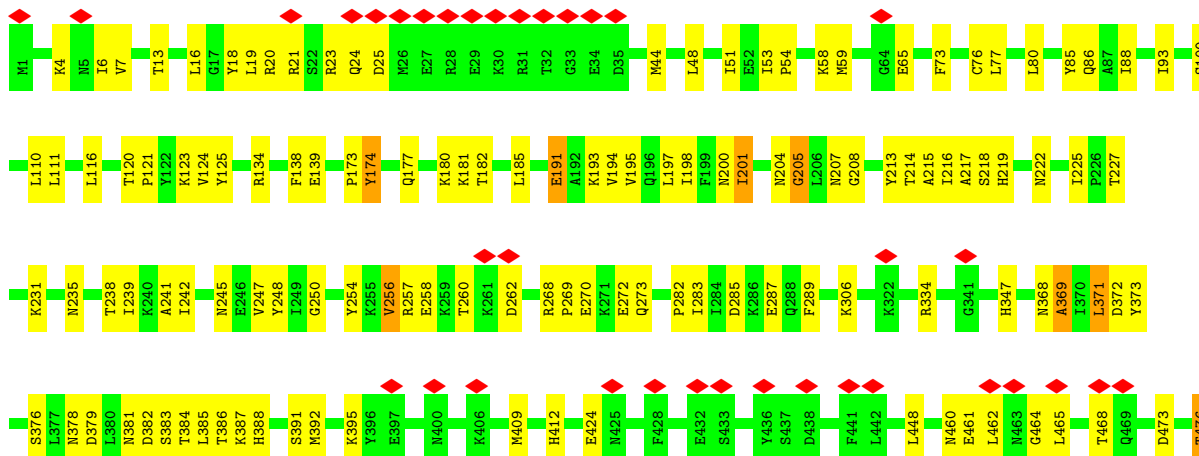
Mol	Chain	Residues	Atoms						AltConf	Trace
5	H	24	Total	C	H	N	O	P	0	0
			767	237	274	87	145	24		
5	P	24	Total	C	H	N	O	P	0	0
			767	237	274	87	145	24		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).


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



Chain I: 




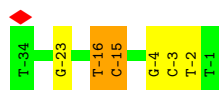


Chain E:  82% 15%



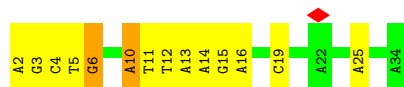
- Molecule 2: DNA (34-MER)

Chain M:  82% 12% 6%



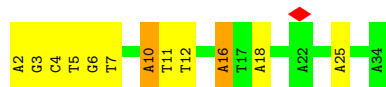
- Molecule 3: DNA (33-MER)

Chain F:  58% 36% 6%



- Molecule 3: DNA (33-MER)

Chain N:  64% 30% 6%



- Molecule 4: DNA (25-MER)

Chain G:  68% 32%



- Molecule 4: DNA (25-MER)

Chain O:  68% 28%




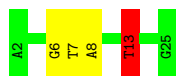
- Molecule 5: DNA (24-MER)

Chain H:  67% 33%



- Molecule 5: DNA (24-MER)

Chain P:  83% 12% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	210561	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	2.406	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0226	Depositor
Map size (\AA)	451.56003, 468.60004, 374.88	wwPDB
Map dimensions	424, 440, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\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	1.47	31/4412 (0.7%)	1.48	85/5927 (1.4%)
1	B	2.44	9/489 (1.8%)	2.55	29/654 (4.4%)
1	C	1.34	23/4420 (0.5%)	1.46	96/5937 (1.6%)
1	D	2.54	13/498 (2.6%)	2.67	57/667 (8.5%)
1	I	1.37	22/4420 (0.5%)	1.44	89/5937 (1.5%)
1	J	2.46	9/489 (1.8%)	2.63	37/654 (5.7%)
1	K	1.36	26/4412 (0.6%)	1.48	94/5927 (1.6%)
1	L	2.56	13/498 (2.6%)	2.69	64/667 (9.6%)
2	E	0.79	0/774	1.24	0/1193
2	M	0.84	0/774	1.23	1/1193 (0.1%)
3	F	1.36	3/764 (0.4%)	1.48	2/1176 (0.2%)
3	N	1.28	2/764 (0.3%)	1.42	2/1176 (0.2%)
4	G	0.84	0/572	1.24	0/880
4	O	0.83	0/572	1.24	0/880
5	H	1.30	0/552	1.45	1/850 (0.1%)
5	P	1.22	0/552	1.42	1/850 (0.1%)
All	All	1.45	151/24962 (0.6%)	1.56	558/34568 (1.6%)

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	C	0	1
1	I	0	3
1	K	0	2
2	E	0	3
2	M	0	3
3	F	0	2
3	N	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	G	0	4
4	O	0	3
5	H	0	3
5	P	0	1
All	All	0	27

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	HIS	CE1-NE2	-9.01	1.23	1.32
1	A	280	HIS	CE1-NE2	-8.97	1.23	1.32
1	B	47	HIS	CE1-NE2	-8.97	1.23	1.32
1	C	280	HIS	CE1-NE2	-8.94	1.23	1.32
1	I	219	HIS	CE1-NE2	-8.92	1.23	1.32
1	K	280	HIS	CE1-NE2	-8.91	1.23	1.32
1	C	489	HIS	CE1-NE2	-8.90	1.23	1.32
1	A	489	HIS	CE1-NE2	-8.89	1.23	1.32
1	I	388	HIS	CE1-NE2	-8.88	1.23	1.32
1	D	47	HIS	ND1-CE1	-8.85	1.23	1.32
1	K	219	HIS	CE1-NE2	-8.85	1.23	1.32
1	C	219	HIS	CE1-NE2	-8.83	1.23	1.32
1	K	489	HIS	CE1-NE2	-8.79	1.23	1.32
1	J	47	HIS	CE1-NE2	-8.78	1.23	1.32
1	I	489	HIS	CE1-NE2	-8.77	1.23	1.32
1	L	47	HIS	ND1-CE1	-8.77	1.23	1.32
1	A	388	HIS	ND1-CE1	-8.76	1.23	1.32
1	A	388	HIS	CE1-NE2	-8.75	1.23	1.32
1	C	489	HIS	ND1-CE1	-8.74	1.23	1.32
1	K	489	HIS	ND1-CE1	-8.74	1.23	1.32
1	I	388	HIS	ND1-CE1	-8.72	1.23	1.32
1	A	219	HIS	CD2-NE2	-8.40	1.28	1.37
1	I	219	HIS	CD2-NE2	-8.28	1.28	1.37
1	J	47	HIS	CD2-NE2	-8.28	1.28	1.37
1	A	280	HIS	CD2-NE2	-8.24	1.28	1.37
1	K	280	HIS	CD2-NE2	-8.22	1.28	1.37
1	C	280	HIS	CD2-NE2	-8.20	1.28	1.37
1	B	47	HIS	CD2-NE2	-8.18	1.28	1.37
1	C	219	HIS	CD2-NE2	-8.16	1.28	1.37
1	I	489	HIS	CD2-NE2	-8.12	1.28	1.37
1	K	219	HIS	CD2-NE2	-8.09	1.28	1.37
1	A	489	HIS	CD2-NE2	-8.08	1.28	1.37
1	L	55	ARG	CZ-NH2	-8.07	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	265	ARG	CZ-NH2	-8.06	1.23	1.33
1	A	257	ARG	CZ-NH2	-8.05	1.23	1.33
1	C	489	HIS	CD2-NE2	-8.05	1.28	1.37
1	K	489	HIS	CD2-NE2	-8.03	1.29	1.37
1	A	281	ALA	CA-CB	-8.01	1.42	1.53
1	A	388	HIS	CD2-NE2	-8.00	1.29	1.37
1	B	26	ARG	CZ-NH2	-7.99	1.23	1.33
1	C	257	ARG	CZ-NH2	-7.99	1.23	1.33
1	J	26	ARG	CZ-NH2	-7.99	1.23	1.33
1	I	388	HIS	CD2-NE2	-7.99	1.29	1.37
1	I	257	ARG	CZ-NH2	-7.97	1.23	1.33
1	A	516	ARG	CZ-NH2	-7.96	1.23	1.33
1	I	516	ARG	CZ-NH2	-7.95	1.23	1.33
1	K	257	ARG	CZ-NH2	-7.93	1.23	1.33
1	K	265	ARG	CZ-NH2	-7.92	1.23	1.33
1	D	55	ARG	CZ-NH2	-7.89	1.23	1.33
1	L	26	ARG	CZ-NH2	-7.82	1.23	1.33
1	D	26	ARG	CZ-NH2	-7.80	1.23	1.33
1	D	6	ARG	CZ-NH2	-7.72	1.23	1.33
1	L	6	ARG	CZ-NH2	-7.68	1.23	1.33
1	A	192	ALA	CA-CB	-7.08	1.42	1.53
1	L	52	ALA	CA-CB	-6.94	1.42	1.53
1	D	52	ALA	CA-CB	-6.75	1.42	1.53
1	A	215	ALA	CA-CB	-6.73	1.43	1.53
1	I	369	ALA	CA-CB	-6.70	1.43	1.53
1	I	215	ALA	CA-CB	-6.63	1.43	1.53
1	B	45	ALA	CA-CB	-6.57	1.43	1.53
1	I	217	ALA	CA-CB	-6.57	1.43	1.53
1	L	55	ARG	CZ-NH1	-6.56	1.23	1.32
1	B	51	ALA	CA-CB	-6.55	1.43	1.53
1	J	51	ALA	CA-CB	-6.55	1.43	1.53
1	J	33	ALA	CA-CB	-6.54	1.43	1.53
1	I	241	ALA	CA-CB	-6.54	1.43	1.53
1	J	45	ALA	CA-CB	-6.51	1.43	1.53
1	A	241	ALA	CA-CB	-6.50	1.43	1.53
1	B	33	ALA	CA-CB	-6.50	1.43	1.53
1	B	52	ALA	CA-CB	-6.49	1.43	1.53
1	J	52	ALA	CA-CB	-6.48	1.43	1.53
1	A	217	ALA	CA-CB	-6.42	1.43	1.53
1	I	516	ARG	CZ-NH1	-6.41	1.23	1.32
1	C	257	ARG	CZ-NH1	-6.39	1.23	1.32
1	A	516	ARG	CZ-NH1	-6.38	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	26	ARG	CZ-NH1	-6.38	1.23	1.32
1	K	265	ARG	CZ-NH1	-6.38	1.23	1.32
1	D	55	ARG	CZ-NH1	-6.37	1.23	1.32
1	K	257	ARG	CZ-NH1	-6.37	1.23	1.32
1	I	205	GLY	N-CA	-6.36	1.38	1.45
1	C	265	ARG	CZ-NH1	-6.34	1.23	1.32
1	B	26	ARG	CZ-NH1	-6.33	1.23	1.32
1	I	257	ARG	CZ-NH1	-6.33	1.23	1.32
1	A	257	ARG	CZ-NH1	-6.26	1.24	1.32
1	A	279	ALA	CA-CB	-6.24	1.43	1.53
1	L	26	ARG	CZ-NH1	-6.19	1.24	1.32
1	D	26	ARG	CZ-NH1	-6.15	1.24	1.32
1	L	6	ARG	CZ-NH1	-6.14	1.24	1.32
1	D	6	ARG	CZ-NH1	-6.13	1.24	1.32
1	K	172	ALA	CA-CB	-5.99	1.44	1.53
1	C	172	ALA	CA-CB	-5.84	1.44	1.53
1	K	283	ILE	N-CA	-5.79	1.41	1.46
1	K	192	ALA	CA-CB	-5.68	1.44	1.53
1	K	279	ALA	CA-CB	-5.66	1.44	1.53
1	K	215	ALA	CA-CB	-5.66	1.44	1.53
1	C	265	ARG	CD-NE	-5.61	1.38	1.46
1	K	217	ALA	CA-CB	-5.61	1.44	1.53
1	L	51	ALA	CA-CB	-5.61	1.44	1.53
1	C	205	GLY	N-CA	-5.55	1.37	1.45
1	A	250	GLY	N-CA	-5.49	1.37	1.45
1	K	241	ALA	CA-CB	-5.49	1.44	1.53
1	C	518	GLY	N-CA	-5.47	1.37	1.44
1	K	518	GLY	N-CA	-5.46	1.37	1.44
1	J	26	ARG	CD-NE	-5.46	1.38	1.46
1	K	265	ARG	CD-NE	-5.46	1.38	1.46
1	I	518	GLY	N-CA	-5.45	1.37	1.44
1	A	175	GLY	N-CA	-5.44	1.37	1.45
1	A	518	GLY	N-CA	-5.44	1.37	1.44
1	A	257	ARG	CD-NE	-5.43	1.38	1.46
1	K	257	ARG	CD-NE	-5.42	1.38	1.46
1	B	26	ARG	CD-NE	-5.42	1.38	1.46
1	A	173	PRO	CA-CB	-5.40	1.46	1.53
1	D	26	ARG	CD-NE	-5.40	1.38	1.46
1	I	257	ARG	CD-NE	-5.40	1.38	1.46
1	C	257	ARG	CD-NE	-5.39	1.38	1.46
1	C	279	ALA	CA-CB	-5.35	1.45	1.53
1	C	165	GLY	N-CA	-5.35	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	6	ARG	CD-NE	-5.34	1.38	1.46
1	L	26	ARG	CD-NE	-5.33	1.38	1.46
1	D	6	ARG	CD-NE	-5.33	1.38	1.46
1	I	208	GLY	N-CA	-5.29	1.37	1.45
1	C	217	ALA	CA-CB	-5.29	1.45	1.53
1	L	33	ALA	CA-CB	-5.28	1.44	1.53
1	K	165	GLY	N-CA	-5.26	1.37	1.45
1	A	358	CYS	CA-CB	-5.25	1.45	1.53
1	K	225	ILE	N-CA	-5.25	1.42	1.46
3	F	25	DA	C6-N6	-5.24	1.23	1.34
1	D	51	ALA	CA-CB	-5.23	1.45	1.53
1	L	55	ARG	CD-NE	-5.23	1.39	1.46
1	A	282	PRO	CA-CB	-5.22	1.47	1.54
1	K	175	GLY	N-CA	-5.20	1.37	1.45
1	C	162	ALA	CA-CB	-5.18	1.45	1.53
3	N	10	DA	C6-N6	-5.18	1.23	1.34
1	C	241	ALA	CA-CB	-5.17	1.45	1.53
1	K	173	PRO	CA-CB	-5.17	1.47	1.53
1	A	205	GLY	N-CA	-5.15	1.38	1.45
3	N	25	DA	C6-N6	-5.15	1.23	1.34
1	D	55	ARG	CD-NE	-5.14	1.39	1.46
3	F	10	DA	C6-N6	-5.14	1.23	1.34
1	I	521	PRO	CA-CB	-5.13	1.46	1.53
1	A	516	ARG	CD-NE	-5.13	1.39	1.46
1	A	208	GLY	N-CA	-5.12	1.38	1.45
1	I	516	ARG	CD-NE	-5.12	1.39	1.46
1	K	226	PRO	CA-CB	-5.11	1.46	1.53
3	F	6	DG	C2-N2	-5.07	1.24	1.34
1	D	33	ALA	CA-CB	-5.05	1.45	1.53
1	C	173	PRO	CA-CB	-5.05	1.46	1.53
1	I	282	PRO	CA-CB	-5.04	1.47	1.54
1	C	215	ALA	CA-CB	-5.03	1.45	1.53
1	A	519	PRO	CA-CB	-5.03	1.46	1.53
1	A	236	GLN	CA-CB	-5.02	1.47	1.53

All (558) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	24	SER	CA-C-N	9.27	130.36	121.65
1	J	24	SER	C-N-CA	9.27	130.36	121.65
1	B	24	SER	CA-C-N	8.86	129.98	121.65
1	B	24	SER	C-N-CA	8.86	129.98	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	512	MET	CA-C-N	8.41	131.37	120.44
1	K	512	MET	C-N-CA	8.41	131.37	120.44
1	C	224	GLN	CA-C-N	7.93	131.27	123.02
1	C	224	GLN	C-N-CA	7.93	131.27	123.02
1	C	512	MET	CA-C-N	7.80	130.95	120.65
1	C	512	MET	C-N-CA	7.80	130.95	120.65
5	H	13	DT	C4'-C3'-O3'	7.39	121.09	110.00
1	K	250	GLY	CA-C-N	7.39	131.20	120.71
1	K	250	GLY	C-N-CA	7.39	131.20	120.71
1	J	44	PHE	CA-CB-CG	7.25	121.06	113.80
1	I	245	ASN	CA-CB-CG	7.21	119.81	112.60
1	K	235	ASN	CA-C-N	7.13	129.72	120.44
1	K	235	ASN	C-N-CA	7.13	129.72	120.44
1	J	35	ASN	CA-CB-CG	7.13	119.73	112.60
1	A	245	ASN	CA-CB-CG	7.12	119.72	112.60
1	A	278	ASP	CA-CB-CG	7.09	119.69	112.60
1	B	35	ASN	CA-CB-CG	7.08	119.67	112.60
1	I	388	HIS	CA-CB-CG	6.98	120.78	113.80
1	J	4	TYR	CA-C-N	6.97	129.63	120.28
1	J	4	TYR	C-N-CA	6.97	129.63	120.28
1	I	368	ASN	CA-CB-CG	6.97	119.57	112.60
1	K	526	ILE	CA-C-N	6.96	130.69	122.89
1	K	526	ILE	C-N-CA	6.96	130.69	122.89
1	C	204	ASN	CA-CB-CG	6.95	119.55	112.60
1	L	22	ASN	CA-CB-CG	6.95	119.55	112.60
1	J	22	ASN	CA-CB-CG	6.92	119.52	112.60
1	B	31	ASP	CA-CB-CG	6.92	119.52	112.60
1	B	44	PHE	CA-CB-CG	6.92	120.72	113.80
1	C	167	TRP	CA-C-N	6.86	130.32	122.36
1	C	167	TRP	C-N-CA	6.86	130.32	122.36
1	K	222	ASN	CA-CB-CG	6.86	119.46	112.60
1	I	489	HIS	CA-CB-CG	6.80	120.60	113.80
1	A	486	ASP	CA-CB-CG	6.80	119.40	112.60
1	C	222	ASN	CA-CB-CG	6.79	119.39	112.60
1	A	204	ASN	CA-CB-CG	6.78	119.38	112.60
1	C	489	HIS	CA-CB-CG	6.78	120.58	113.80
1	K	489	HIS	CA-CB-CG	6.76	120.56	113.80
1	C	186	ASP	CA-CB-CG	6.76	119.36	112.60
1	K	186	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	388	HIS	CA-CB-CG	6.71	120.51	113.80
1	J	31	ASP	CA-CB-CG	6.71	119.31	112.60
1	I	486	ASP	CA-CB-CG	6.70	119.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	222	ASN	CA-CB-CG	6.68	119.28	112.60
1	C	498	ASN	CA-CB-CG	-6.65	105.95	112.60
1	C	533	ASN	CA-CB-CG	6.63	119.23	112.60
1	L	24	SER	CA-C-N	6.62	131.37	122.90
1	L	24	SER	C-N-CA	6.62	131.37	122.90
1	K	533	ASN	CA-CB-CG	6.59	119.19	112.60
1	B	22	ASN	CA-CB-CG	6.55	119.15	112.60
1	B	38	ASP	CA-CB-CG	6.54	119.14	112.60
1	C	250	GLY	CA-C-N	6.52	129.97	120.71
1	C	250	GLY	C-N-CA	6.52	129.97	120.71
1	C	534	PHE	CA-CB-CG	6.52	120.32	113.80
1	K	204	ASN	CA-CB-CG	6.52	119.12	112.60
1	C	179	ASN	CA-CB-CG	6.51	119.11	112.60
1	K	190	ASP	CA-CB-CG	6.51	119.11	112.60
1	L	36	ASP	CA-CB-CG	6.50	119.10	112.60
1	L	31	ASP	CA-CB-CG	6.50	119.10	112.60
1	D	31	ASP	CA-CB-CG	6.50	119.10	112.60
1	K	534	PHE	CA-CB-CG	6.49	120.29	113.80
1	D	36	ASP	CA-CB-CG	6.49	119.08	112.60
1	I	235	ASN	CA-CB-CG	6.48	119.08	112.60
1	L	44	PHE	CA-CB-CG	6.46	120.26	113.80
1	K	372	ASP	CA-CB-CG	6.45	119.05	112.60
1	C	190	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	489	HIS	CA-CB-CG	6.41	120.21	113.80
1	L	35	ASN	CA-CB-CG	6.41	119.00	112.60
1	L	47	HIS	CA-CB-CG	6.39	120.19	113.80
1	D	44	PHE	CA-CB-CG	6.39	120.19	113.80
1	C	251	THR	CA-C-N	6.38	131.59	123.10
1	C	251	THR	C-N-CA	6.38	131.59	123.10
1	D	24	SER	CA-C-N	6.37	131.05	122.90
1	D	24	SER	C-N-CA	6.37	131.05	122.90
1	K	251	THR	CA-C-N	6.36	131.56	123.10
1	K	251	THR	C-N-CA	6.36	131.56	123.10
1	D	35	ASN	CA-CB-CG	6.35	118.95	112.60
1	L	16	LYS	CA-C-N	6.35	131.03	122.90
1	L	16	LYS	C-N-CA	6.35	131.03	122.90
1	A	285	ASP	CA-CB-CG	6.34	118.94	112.60
1	D	47	HIS	CA-CB-CG	6.34	120.14	113.80
1	C	266	THR	CA-C-N	6.30	131.32	123.12
1	C	266	THR	C-N-CA	6.30	131.32	123.12
1	A	528	PRO	CA-C-N	6.30	131.67	123.11
1	A	528	PRO	C-N-CA	6.30	131.67	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	372	ASP	CA-CB-CG	6.29	118.89	112.60
1	I	285	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	219	HIS	CA-CB-CG	6.28	120.08	113.80
1	I	534	PHE	CA-CB-CG	6.26	120.06	113.80
1	J	16	LYS	CA-C-N	6.26	130.50	122.93
1	J	16	LYS	C-N-CA	6.26	130.50	122.93
1	K	528	PRO	CA-C-N	6.26	131.25	123.12
1	K	528	PRO	C-N-CA	6.26	131.25	123.12
1	K	187	PRO	CA-C-N	6.25	131.63	122.94
1	K	187	PRO	C-N-CA	6.25	131.63	122.94
1	J	47	HIS	CA-CB-CG	6.23	120.03	113.80
1	C	166	LYS	CA-C-N	6.21	130.68	122.30
1	C	166	LYS	C-N-CA	6.21	130.68	122.30
1	K	482	ASN	CA-CB-CG	6.20	118.80	112.60
1	B	47	HIS	CA-CB-CG	6.20	120.00	113.80
1	C	185	LEU	CA-C-N	6.19	130.86	122.56
1	C	185	LEU	C-N-CA	6.19	130.86	122.56
1	A	198	ILE	N-CA-CB	6.19	117.12	110.62
1	I	207	ASN	CA-CB-CG	6.19	118.79	112.60
1	I	528	PRO	CA-C-N	6.17	131.02	122.93
1	I	528	PRO	C-N-CA	6.17	131.02	122.93
1	K	185	LEU	CA-C-N	6.17	130.82	122.56
1	K	185	LEU	C-N-CA	6.17	130.82	122.56
1	A	372	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	482	ASN	CA-CB-CG	6.16	118.76	112.60
1	C	486	ASP	CA-CB-CG	6.16	118.76	112.60
1	D	16	LYS	CA-C-N	6.15	130.98	122.93
1	D	16	LYS	C-N-CA	6.15	130.98	122.93
1	I	198	ILE	N-CA-CB	6.15	117.07	110.62
1	K	486	ASP	CA-CB-CG	6.14	118.74	112.60
1	C	528	PRO	CA-C-N	6.14	131.10	123.12
1	C	528	PRO	C-N-CA	6.14	131.10	123.12
1	C	482	ASN	CA-CB-CG	6.13	118.73	112.60
1	A	534	PHE	CA-CB-CG	6.12	119.92	113.80
1	A	251	THR	CA-C-N	6.11	130.77	123.19
1	A	251	THR	C-N-CA	6.11	130.77	123.19
1	B	4	TYR	CA-C-N	6.11	128.75	120.38
1	B	4	TYR	C-N-CA	6.11	128.75	120.38
1	D	26	ARG	CA-C-N	6.10	130.88	122.77
1	D	26	ARG	C-N-CA	6.10	130.88	122.77
1	A	207	ASN	CA-CB-CG	6.10	118.70	112.60
1	I	516	ARG	CD-NE-CZ	6.08	132.92	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	GLU	CA-C-N	6.06	131.08	123.14
1	A	525	GLU	C-N-CA	6.06	131.08	123.14
1	J	38	ASP	CA-CB-CG	6.06	118.66	112.60
1	C	207	ASN	CA-CB-CG	6.06	118.66	112.60
1	A	239	ILE	N-CA-CB	6.05	117.22	110.51
1	K	208	GLY	CA-C-N	6.04	130.45	122.42
1	K	208	GLY	C-N-CA	6.04	130.45	122.42
1	C	532	PHE	CA-CB-CG	6.04	119.84	113.80
1	I	219	HIS	CA-CB-CG	6.03	119.83	113.80
1	C	216	ILE	N-CA-CB	6.03	117.20	110.51
1	K	532	PHE	CA-CB-CG	6.01	119.81	113.80
5	P	13	DT	C4'-C3'-O3'	6.00	119.01	110.00
1	K	219	HIS	CA-CB-CG	6.00	119.80	113.80
1	C	520	ILE	N-CA-CB	5.96	116.78	110.17
1	D	17	VAL	CA-C-N	5.95	130.85	123.12
1	D	17	VAL	C-N-CA	5.95	130.85	123.12
1	A	274	ILE	CA-C-N	5.95	130.93	123.14
1	A	274	ILE	C-N-CA	5.95	130.93	123.14
1	A	516	ARG	CD-NE-CZ	5.94	132.72	124.40
1	C	201	ILE	N-CA-CB	5.94	117.10	110.62
1	K	216	ILE	N-CA-CB	5.93	117.10	110.51
1	K	275	VAL	CA-C-N	5.90	131.19	122.99
1	K	275	VAL	C-N-CA	5.90	131.19	122.99
1	L	26	ARG	CA-C-N	5.88	130.59	122.77
1	L	26	ARG	C-N-CA	5.88	130.59	122.77
1	K	166	LYS	CA-C-N	5.88	130.59	122.77
1	K	166	LYS	C-N-CA	5.88	130.59	122.77
1	B	3	PRO	CA-N-CD	-5.88	103.77	112.00
1	K	201	ILE	N-CA-CB	5.85	117.39	110.55
1	K	520	ILE	N-CA-CB	5.84	116.66	110.17
1	A	257	ARG	CD-NE-CZ	5.84	132.57	124.40
1	I	257	ARG	CD-NE-CZ	5.84	132.58	124.40
1	I	482	ASN	CA-C-N	5.83	131.21	122.99
1	I	482	ASN	C-N-CA	5.83	131.21	122.99
1	I	513	THR	CA-C-N	5.82	131.19	123.05
1	I	513	THR	C-N-CA	5.82	131.19	123.05
1	L	55	ARG	CD-NE-CZ	5.81	132.54	124.40
1	K	525	GLU	CA-C-N	5.80	130.59	123.10
1	K	525	GLU	C-N-CA	5.80	130.59	123.10
1	K	239	ILE	N-CA-CB	5.80	117.34	110.55
1	C	273	GLN	CA-C-N	5.78	129.60	122.37
1	C	273	GLN	C-N-CA	5.78	129.60	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	17	VAL	CA-C-N	5.77	130.78	123.10
1	L	17	VAL	C-N-CA	5.77	130.78	123.10
2	M	-15	DC	C2'-C3'-O3'	5.76	120.15	111.50
1	K	205	GLY	CA-C-N	5.76	130.43	122.77
1	K	205	GLY	C-N-CA	5.76	130.43	122.77
1	J	40	PHE	CA-CB-CG	5.74	119.54	113.80
1	C	275	VAL	CA-C-N	5.73	130.96	122.99
1	C	275	VAL	C-N-CA	5.73	130.96	122.99
1	K	503	MET	CA-C-N	5.73	127.78	120.56
1	K	503	MET	C-N-CA	5.73	127.78	120.56
1	C	503	MET	CA-C-N	5.73	127.78	120.56
1	C	503	MET	C-N-CA	5.73	127.78	120.56
1	I	289	PHE	CA-CB-CG	5.72	119.52	113.80
1	K	198	ILE	N-CA-CB	5.72	116.62	110.62
1	D	55	ARG	CD-NE-CZ	5.71	132.40	124.40
1	A	532	PHE	CA-C-N	5.71	130.01	122.30
1	A	532	PHE	C-N-CA	5.71	130.01	122.30
1	J	3	PRO	CA-N-CD	-5.71	104.01	112.00
1	A	482	ASN	CA-C-N	5.71	131.05	123.00
1	A	482	ASN	C-N-CA	5.71	131.05	123.00
1	A	526	ILE	CA-C-N	5.71	131.16	123.46
1	A	526	ILE	C-N-CA	5.71	131.16	123.46
1	A	174	TYR	N-CA-CB	5.70	118.41	109.69
1	I	250	GLY	CA-C-N	5.67	130.82	123.00
1	I	250	GLY	C-N-CA	5.67	130.82	123.00
1	I	289	PHE	N-CA-CB	5.64	118.18	110.01
1	C	219	HIS	CA-CB-CG	5.63	119.43	113.80
1	I	214	THR	CA-C-N	5.63	127.76	120.44
1	I	214	THR	C-N-CA	5.63	127.76	120.44
1	C	184	LYS	CA-C-N	5.63	128.86	120.87
1	C	184	LYS	C-N-CA	5.63	128.86	120.87
1	D	40	PHE	CA-CB-CG	5.62	119.42	113.80
1	D	25	ILE	CA-C-N	5.61	130.74	123.00
1	D	25	ILE	C-N-CA	5.61	130.74	123.00
1	L	25	ILE	CA-C-N	5.61	130.74	123.00
1	L	25	ILE	C-N-CA	5.61	130.74	123.00
1	K	207	ASN	CA-CB-CG	5.60	118.20	112.60
1	K	174	TYR	N-CA-CB	5.60	118.15	109.48
1	L	40	PHE	CA-CB-CG	5.60	119.40	113.80
1	I	174	TYR	N-CA-CB	5.59	118.14	109.48
1	I	283	ILE	CA-C-N	5.57	130.75	123.06
1	I	283	ILE	C-N-CA	5.57	130.75	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	GLY	CA-C-N	5.57	130.18	122.77
1	C	205	GLY	C-N-CA	5.57	130.18	122.77
1	C	208	GLY	CA-C-N	5.54	130.81	123.05
1	C	208	GLY	C-N-CA	5.54	130.81	123.05
1	J	18	VAL	N-CA-CB	5.54	116.97	110.82
1	C	178	LEU	CA-C-N	5.54	129.79	122.42
1	C	178	LEU	C-N-CA	5.54	129.79	122.42
1	L	23	TYR	CA-C-N	5.52	130.78	123.05
1	L	23	TYR	C-N-CA	5.52	130.78	123.05
1	C	248	TYR	N-CA-C	5.51	118.47	111.69
1	A	464	GLY	CA-C-N	5.48	127.57	120.44
1	A	464	GLY	C-N-CA	5.48	127.57	120.44
1	C	177	GLN	CA-C-N	5.48	130.06	122.77
1	C	177	GLN	C-N-CA	5.48	130.06	122.77
1	C	483	LYS	CB-CG-CD	5.46	123.86	111.30
1	A	513	THR	CA-C-N	5.45	130.68	123.00
1	A	513	THR	C-N-CA	5.45	130.68	123.00
1	D	47	HIS	N-CA-CB	5.43	117.89	110.01
1	A	250	GLY	CA-C-N	5.43	130.65	122.99
1	A	250	GLY	C-N-CA	5.43	130.65	122.99
1	I	532	PHE	CA-C-N	5.43	129.59	121.72
1	I	532	PHE	C-N-CA	5.43	129.59	121.72
1	C	276	VAL	CA-C-N	5.43	130.21	122.72
1	C	276	VAL	C-N-CA	5.43	130.21	122.72
1	I	395	LYS	CA-C-N	5.42	127.49	120.44
1	I	395	LYS	C-N-CA	5.42	127.49	120.44
1	I	464	GLY	CA-C-N	5.42	127.48	120.44
1	I	464	GLY	C-N-CA	5.42	127.48	120.44
1	K	483	LYS	CB-CG-CD	5.42	123.76	111.30
1	I	193	LYS	CA-C-N	5.41	127.38	120.56
1	I	193	LYS	C-N-CA	5.41	127.38	120.56
1	J	44	PHE	CA-C-N	5.41	127.48	120.44
1	J	44	PHE	C-N-CA	5.41	127.48	120.44
1	C	529	ILE	CA-C-N	5.41	128.55	120.87
1	C	529	ILE	C-N-CA	5.41	128.55	120.87
1	I	461	GLU	CA-C-N	5.40	127.46	120.44
1	I	461	GLU	C-N-CA	5.40	127.46	120.44
1	J	29	THR	CA-C-N	5.40	130.04	122.05
1	J	29	THR	C-N-CA	5.40	130.04	122.05
1	A	461	GLU	CA-C-N	5.39	127.45	120.44
1	A	461	GLU	C-N-CA	5.39	127.45	120.44
1	K	529	ILE	CA-C-N	5.39	128.53	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	529	ILE	C-N-CA	5.39	128.53	120.87
1	L	47	HIS	CE1-NE2-CD2	-5.38	103.62	109.00
1	I	239	ILE	N-CA-CB	5.37	116.84	110.55
1	A	404	LYS	CA-C-N	5.37	127.42	120.44
1	A	404	LYS	C-N-CA	5.37	127.42	120.44
1	C	174	TYR	N-CA-CB	5.37	117.80	109.48
1	A	395	LYS	CA-C-N	5.36	127.41	120.44
1	A	395	LYS	C-N-CA	5.36	127.41	120.44
1	D	47	HIS	CE1-NE2-CD2	-5.35	103.65	109.00
1	L	47	HIS	ND1-CG-CD2	-5.34	100.76	106.10
1	C	197	LEU	N-CA-CB	5.34	117.75	110.01
1	K	241	ALA	CA-C-N	5.33	127.28	120.56
1	K	241	ALA	C-N-CA	5.33	127.28	120.56
1	K	183	SER	CA-C-N	5.33	131.18	122.81
1	K	183	SER	C-N-CA	5.33	131.18	122.81
1	L	47	HIS	N-CA-CB	5.31	117.71	110.01
1	A	487	GLN	N-CA-CB	5.30	117.91	110.12
1	I	385	LEU	N-CA-CB	5.30	117.69	110.01
1	A	197	LEU	N-CA-CB	5.29	117.69	110.01
1	I	484	ILE	N-CA-CB	5.29	116.39	110.51
1	K	489	HIS	CA-C-N	5.29	127.23	120.56
1	K	489	HIS	C-N-CA	5.29	127.23	120.56
1	B	29	THR	CA-C-N	5.29	129.88	122.05
1	B	29	THR	C-N-CA	5.29	129.88	122.05
1	C	274	ILE	N-CA-CB	5.29	117.03	111.00
1	A	476	THR	CA-C-N	5.29	129.48	121.65
1	A	476	THR	C-N-CA	5.29	129.48	121.65
1	D	9	GLU	CA-C-N	5.29	127.32	120.44
1	D	9	GLU	C-N-CA	5.29	127.32	120.44
1	A	237	TYR	CA-C-N	5.28	127.79	120.29
1	A	237	TYR	C-N-CA	5.28	127.79	120.29
1	C	489	HIS	CA-C-N	5.28	127.21	120.56
1	C	489	HIS	C-N-CA	5.28	127.21	120.56
1	L	48	LEU	CA-C-N	5.28	127.30	120.44
1	L	48	LEU	C-N-CA	5.28	127.30	120.44
1	I	201	ILE	N-CA-CB	5.28	116.72	110.55
1	L	47	HIS	CG-CD2-NE2	5.27	112.47	107.20
1	C	533	ASN	CA-C-N	5.26	130.83	122.62
1	C	533	ASN	C-N-CA	5.26	130.83	122.62
1	C	274	ILE	CA-C-N	5.26	130.26	122.94
1	C	274	ILE	C-N-CA	5.26	130.26	122.94
1	I	368	ASN	CA-C-N	5.26	127.28	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	368	ASN	C-N-CA	5.26	127.28	120.44
1	I	235	ASN	N-CA-CB	5.26	117.74	109.69
1	K	194	VAL	CA-C-N	5.26	127.19	120.56
1	K	194	VAL	C-N-CA	5.26	127.19	120.56
1	B	51	ALA	CA-C-N	5.26	127.27	120.44
1	B	51	ALA	C-N-CA	5.26	127.27	120.44
1	I	388	HIS	ND1-CG-CD2	-5.25	100.84	106.10
1	A	194	VAL	N-CA-CB	5.25	116.69	110.55
1	C	372	ASP	CA-C-N	5.25	127.26	120.44
1	C	372	ASP	C-N-CA	5.25	127.26	120.44
1	D	47	HIS	ND1-CG-CD2	-5.25	100.85	106.10
1	K	274	ILE	CA-C-N	5.25	130.24	122.94
1	K	274	ILE	C-N-CA	5.25	130.24	122.94
1	K	533	ASN	CA-C-N	5.25	130.81	122.62
1	K	533	ASN	C-N-CA	5.25	130.81	122.62
1	C	489	HIS	ND1-CG-CD2	-5.25	100.85	106.10
1	C	165	GLY	CA-C-N	5.24	130.81	122.94
1	C	165	GLY	C-N-CA	5.24	130.81	122.94
1	K	252	VAL	CA-C-N	5.24	130.38	122.99
1	K	252	VAL	C-N-CA	5.24	130.38	122.99
1	A	193	LYS	CA-C-N	5.24	127.17	120.56
1	A	193	LYS	C-N-CA	5.24	127.17	120.56
1	L	34	SER	N-CA-CB	5.24	117.67	109.97
1	D	40	PHE	N-CA-CB	5.24	117.61	110.01
1	D	34	SER	N-CA-CB	5.23	117.66	109.97
1	K	502	ARG	CA-C-N	5.23	127.24	120.44
1	K	502	ARG	C-N-CA	5.23	127.24	120.44
1	K	489	HIS	ND1-CG-CD2	-5.23	100.87	106.10
1	D	48	LEU	CA-C-N	5.22	127.23	120.44
1	D	48	LEU	C-N-CA	5.22	127.23	120.44
1	L	40	PHE	N-CA-CB	5.22	117.59	110.01
1	K	197	LEU	N-CA-CB	5.22	117.58	110.01
1	D	19	GLN	CA-C-N	5.22	130.41	122.11
1	D	19	GLN	C-N-CA	5.22	130.41	122.11
1	I	373	TYR	CA-C-N	5.22	127.70	120.29
1	I	373	TYR	C-N-CA	5.22	127.70	120.29
1	I	216	ILE	N-CA-CB	5.22	116.66	110.55
1	C	226	PRO	CA-C-N	5.21	127.89	120.49
1	C	226	PRO	C-N-CA	5.21	127.89	120.49
1	I	487	GLN	N-CA-CB	5.21	117.77	110.12
1	A	236	GLN	CA-C-N	5.20	130.41	122.24
1	A	236	GLN	C-N-CA	5.20	130.41	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	PHE	CA-CB-CG	5.20	119.00	113.80
1	D	5	GLN	CA-C-N	5.20	127.20	120.44
1	D	5	GLN	C-N-CA	5.20	127.20	120.44
1	J	48	LEU	CA-C-N	5.20	127.20	120.44
1	J	48	LEU	C-N-CA	5.20	127.20	120.44
1	I	489	HIS	CA-C-N	5.20	127.11	120.56
1	I	489	HIS	C-N-CA	5.20	127.11	120.56
1	K	282	PRO	CA-C-N	5.20	128.81	121.53
1	K	282	PRO	C-N-CA	5.20	128.81	121.53
1	C	237	TYR	N-CA-CB	5.19	117.54	110.01
1	L	5	GLN	CA-C-N	5.19	127.19	120.44
1	L	5	GLN	C-N-CA	5.19	127.19	120.44
1	A	219	HIS	N-CA-CB	5.18	117.47	109.91
1	C	189	GLU	CA-C-N	5.18	127.17	120.44
1	C	189	GLU	C-N-CA	5.18	127.17	120.44
1	I	387	LYS	N-CA-CB	5.18	117.52	110.01
1	D	47	HIS	CG-CD2-NE2	5.17	112.37	107.20
1	B	30	GLN	CA-C-N	5.17	128.17	120.31
1	B	30	GLN	C-N-CA	5.17	128.17	120.31
1	I	256	VAL	CA-C-N	5.17	129.86	122.72
1	I	256	VAL	C-N-CA	5.17	129.86	122.72
1	A	371	LEU	CA-C-N	5.17	127.16	120.44
1	A	371	LEU	C-N-CA	5.17	127.16	120.44
1	I	205	GLY	CA-C-O	-5.17	118.10	122.29
1	I	205	GLY	N-CA-C	5.17	119.19	112.68
1	K	195	VAL	N-CA-CB	5.17	116.60	110.55
1	K	516	ARG	CA-C-N	5.17	130.69	122.94
1	K	516	ARG	C-N-CA	5.17	130.69	122.94
1	B	6	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	D	11	LYS	CA-CB-CG	5.16	124.41	114.10
1	C	490	ILE	N-CA-CB	5.15	116.58	110.55
1	K	236	GLN	CA-C-N	5.15	129.39	120.58
1	K	236	GLN	C-N-CA	5.15	129.39	120.58
1	B	8	GLU	CA-C-N	5.15	127.14	120.44
1	B	8	GLU	C-N-CA	5.15	127.14	120.44
1	C	216	ILE	CA-C-N	5.15	127.14	120.44
1	C	216	ILE	C-N-CA	5.15	127.14	120.44
1	C	373	TYR	CA-C-N	5.15	127.18	120.28
1	C	373	TYR	C-N-CA	5.15	127.18	120.28
1	D	51	ALA	CA-C-N	5.15	127.14	120.44
1	D	51	ALA	C-N-CA	5.15	127.14	120.44
1	I	219	HIS	N-CA-CB	5.15	117.48	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	LEU	N-CA-CB	5.15	117.48	110.01
1	A	256	VAL	CA-C-N	5.15	129.82	122.72
1	A	256	VAL	C-N-CA	5.15	129.82	122.72
1	J	30	GLN	CA-C-N	5.14	128.13	120.31
1	J	30	GLN	C-N-CA	5.14	128.13	120.31
1	D	12	LYS	N-CA-CB	5.14	117.60	109.94
1	D	30	GLN	CA-C-N	5.14	127.12	120.44
1	D	30	GLN	C-N-CA	5.14	127.12	120.44
1	L	9	GLU	CA-C-N	5.14	127.12	120.44
1	L	9	GLU	C-N-CA	5.14	127.12	120.44
1	I	460	ASN	CA-C-N	5.13	127.11	120.44
1	I	460	ASN	C-N-CA	5.13	127.11	120.44
1	A	375	SER	CA-C-N	5.13	130.41	122.26
1	A	375	SER	C-N-CA	5.13	130.41	122.26
1	A	388	HIS	ND1-CG-CD2	-5.13	100.97	106.10
1	K	256	VAL	CA-C-N	5.13	130.37	122.93
1	K	256	VAL	C-N-CA	5.13	130.37	122.93
1	D	31	ASP	CA-C-N	5.13	127.66	120.28
1	D	31	ASP	C-N-CA	5.13	127.66	120.28
1	I	388	HIS	CA-C-N	5.12	127.02	120.56
1	I	388	HIS	C-N-CA	5.12	127.02	120.56
1	B	18	VAL	N-CA-CB	5.12	116.51	110.82
1	L	11	LYS	CA-CB-CG	5.12	124.35	114.10
1	L	8	GLU	CA-C-N	5.12	127.10	120.44
1	L	8	GLU	C-N-CA	5.12	127.10	120.44
1	I	372	ASP	N-CA-CB	5.12	117.43	110.01
1	D	53	LEU	CA-C-N	5.11	127.09	120.44
1	D	53	LEU	C-N-CA	5.11	127.09	120.44
1	L	51	ALA	CA-C-N	5.11	127.09	120.44
1	L	51	ALA	C-N-CA	5.11	127.09	120.44
1	D	46	GLN	N-CA-CB	5.11	117.42	110.01
1	L	39	GLU	CA-C-N	5.11	127.09	120.44
1	L	39	GLU	C-N-CA	5.11	127.09	120.44
1	I	371	LEU	CA-C-N	5.11	127.08	120.44
1	I	371	LEU	C-N-CA	5.11	127.08	120.44
1	L	46	GLN	N-CA-CB	5.11	117.42	110.01
1	B	40	PHE	N-CA-CB	5.11	117.72	110.06
1	B	48	LEU	CA-C-N	5.11	127.08	120.44
1	B	48	LEU	C-N-CA	5.11	127.08	120.44
1	L	50	GLU	CA-C-N	5.11	127.08	120.44
1	L	50	GLU	C-N-CA	5.11	127.08	120.44
1	K	193	LYS	CA-C-N	5.11	126.99	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	193	LYS	C-N-CA	5.11	126.99	120.56
1	K	244	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	I	476	THR	CA-C-N	5.10	129.60	121.34
1	I	476	THR	C-N-CA	5.10	129.60	121.34
1	L	31	ASP	CA-C-N	5.10	127.62	120.28
1	L	31	ASP	C-N-CA	5.10	127.62	120.28
1	D	39	GLU	CA-C-N	5.10	127.07	120.44
1	D	39	GLU	C-N-CA	5.10	127.07	120.44
1	A	384	THR	CA-C-N	5.09	127.06	120.44
1	A	384	THR	C-N-CA	5.09	127.06	120.44
1	B	50	GLU	CA-C-N	5.09	127.06	120.44
1	B	50	GLU	C-N-CA	5.09	127.06	120.44
1	C	375	SER	CA-C-N	5.09	127.06	120.44
1	C	375	SER	C-N-CA	5.09	127.06	120.44
1	C	533	ASN	N-CA-CB	5.09	117.48	109.69
1	J	17	VAL	CA-C-N	5.09	128.81	121.18
1	J	17	VAL	C-N-CA	5.09	128.81	121.18
1	J	50	GLU	CA-C-N	5.09	127.06	120.44
1	J	50	GLU	C-N-CA	5.09	127.06	120.44
1	A	460	ASN	CA-C-N	5.09	127.05	120.44
1	A	460	ASN	C-N-CA	5.09	127.05	120.44
1	J	8	GLU	CA-C-N	5.09	127.06	120.44
1	J	8	GLU	C-N-CA	5.09	127.06	120.44
1	A	392	MET	CA-C-N	5.09	127.10	120.28
1	A	392	MET	C-N-CA	5.09	127.10	120.28
1	L	20	LYS	CA-C-N	5.09	127.05	120.44
1	L	20	LYS	C-N-CA	5.09	127.05	120.44
3	N	12	DT	O5'-C5'-C4'	5.09	118.43	110.80
1	B	36	ASP	CA-C-N	5.08	127.35	120.38
1	B	36	ASP	C-N-CA	5.08	127.35	120.38
1	C	228	PRO	CA-C-N	5.08	127.05	120.44
1	C	228	PRO	C-N-CA	5.08	127.05	120.44
1	I	384	THR	CA-C-N	5.08	127.05	120.44
1	I	384	THR	C-N-CA	5.08	127.05	120.44
1	A	373	TYR	CA-C-N	5.08	127.60	120.28
1	A	373	TYR	C-N-CA	5.08	127.60	120.28
1	C	198	ILE	N-CA-CB	5.08	116.50	110.55
1	I	461	GLU	N-CA-CB	5.08	117.38	110.01
1	A	461	GLU	N-CA-CB	5.08	117.37	110.01
1	D	10	LEU	CA-C-N	5.08	127.40	120.54
1	D	10	LEU	C-N-CA	5.08	127.40	120.54
1	D	39	GLU	N-CA-CB	5.08	117.37	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	184	LYS	CA-C-N	5.08	128.08	120.87
1	K	184	LYS	C-N-CA	5.08	128.08	120.87
1	L	9	GLU	N-CA-CB	5.08	117.37	110.01
1	L	30	GLN	CA-C-N	5.08	127.04	120.44
1	L	30	GLN	C-N-CA	5.08	127.04	120.44
1	L	39	GLU	N-CA-CB	5.08	117.37	110.01
1	A	386	THR	CA-C-N	5.07	127.39	120.54
1	A	386	THR	C-N-CA	5.07	127.39	120.54
1	K	165	GLY	CA-C-N	5.07	130.55	122.94
1	K	165	GLY	C-N-CA	5.07	130.55	122.94
1	D	50	GLU	CA-C-N	5.07	127.03	120.44
1	D	50	GLU	C-N-CA	5.07	127.03	120.44
1	K	189	GLU	CA-C-N	5.07	127.34	120.65
1	K	189	GLU	C-N-CA	5.07	127.34	120.65
1	L	44	PHE	N-CA-CB	5.07	117.36	110.01
1	A	406	LYS	CB-CG-CD	5.07	122.96	111.30
1	L	52	ALA	CA-C-N	5.07	127.03	120.44
1	L	52	ALA	C-N-CA	5.07	127.03	120.44
1	C	486	ASP	CA-C-N	5.07	127.03	120.44
1	C	486	ASP	C-N-CA	5.07	127.03	120.44
1	D	44	PHE	N-CA-CB	5.07	117.35	110.01
1	L	49	LEU	N-CA-CB	5.07	117.35	110.01
1	C	487	GLN	N-CA-CB	5.06	117.35	110.01
1	D	49	LEU	N-CA-CB	5.06	117.35	110.01
1	I	484	ILE	CA-C-N	5.06	127.39	120.46
1	I	484	ILE	C-N-CA	5.06	127.39	120.46
1	K	486	ASP	CA-C-N	5.06	127.02	120.44
1	K	486	ASP	C-N-CA	5.06	127.02	120.44
1	A	516	ARG	N-CA-CB	5.05	117.73	109.69
1	J	50	GLU	N-CA-CB	5.05	117.34	110.01
1	K	375	SER	CA-C-N	5.05	127.01	120.44
1	K	375	SER	C-N-CA	5.05	127.01	120.44
1	I	462	LEU	N-CA-CB	5.05	117.34	110.01
1	J	23	TYR	CA-C-N	5.05	130.76	123.13
1	J	23	TYR	C-N-CA	5.05	130.76	123.13
1	L	49	LEU	CA-C-N	5.05	127.01	120.44
1	L	49	LEU	C-N-CA	5.05	127.01	120.44
1	I	516	ARG	N-CA-CB	5.05	117.71	109.69
1	L	42	LYS	CA-C-N	5.05	127.00	120.44
1	L	42	LYS	C-N-CA	5.05	127.00	120.44
1	K	219	HIS	N-CA-CB	5.04	117.49	109.82
1	A	166	LYS	CA-C-N	5.04	130.04	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	LYS	C-N-CA	5.04	130.04	122.47
1	C	273	GLN	CA-CB-CG	5.04	124.19	114.10
1	I	218	SER	CA-C-N	5.04	127.00	120.44
1	I	218	SER	C-N-CA	5.04	127.00	120.44
1	I	287	GLU	N-CA-CB	5.04	117.27	109.91
1	L	45	ALA	CA-C-N	5.04	127.00	120.44
1	L	45	ALA	C-N-CA	5.04	127.00	120.44
1	A	280	HIS	CA-C-N	5.04	127.82	120.51
1	A	280	HIS	C-N-CA	5.04	127.82	120.51
1	D	6	ARG	N-CA-CB	5.04	117.31	110.01
1	D	9	GLU	N-CA-CB	5.04	117.31	110.01
3	F	12	DT	O5'-C5'-C4'	5.04	118.36	110.80
1	L	53	LEU	CA-C-N	5.04	126.99	120.44
1	L	53	LEU	C-N-CA	5.04	126.99	120.44
1	C	500	LEU	N-CA-CB	5.03	117.25	109.91
1	I	392	MET	CA-C-N	5.03	127.02	120.28
1	I	392	MET	C-N-CA	5.03	127.02	120.28
1	C	532	PHE	CA-C-N	5.02	127.90	120.82
1	C	532	PHE	C-N-CA	5.02	127.90	120.82
1	J	47	HIS	N-CA-CB	5.02	117.29	110.01
1	J	51	ALA	CA-C-N	5.02	126.97	120.44
1	J	51	ALA	C-N-CA	5.02	126.97	120.44
1	K	487	GLN	N-CA-CB	5.02	117.29	110.01
1	A	321	SER	N-CA-C	5.02	116.83	111.36
1	D	45	ALA	CA-C-N	5.02	126.97	120.44
1	D	45	ALA	C-N-CA	5.02	126.97	120.44
1	I	194	VAL	N-CA-CB	5.02	116.42	110.55
1	I	287	GLU	CA-C-N	5.02	126.97	120.44
1	I	287	GLU	C-N-CA	5.02	126.97	120.44
1	I	383	SER	CA-C-N	5.02	126.97	120.44
1	I	383	SER	C-N-CA	5.02	126.97	120.44
1	J	49	LEU	CA-C-N	5.02	126.97	120.44
1	J	49	LEU	C-N-CA	5.02	126.97	120.44
1	A	372	ASP	N-CA-CB	5.02	117.29	110.01
1	I	391	SER	N-CA-CB	5.02	117.28	110.01
1	C	235	ASN	CA-C-N	5.01	126.96	120.44
1	C	235	ASN	C-N-CA	5.01	126.96	120.44
1	A	391	SER	CA-C-N	5.01	127.00	120.28
1	A	391	SER	C-N-CA	5.01	127.00	120.28
1	I	191	GLU	CA-C-N	5.01	126.95	120.44
1	I	191	GLU	C-N-CA	5.01	126.95	120.44
1	K	237	TYR	CA-C-N	5.01	127.41	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	237	TYR	C-N-CA	5.01	127.41	120.29
1	D	36	ASP	CA-C-N	5.01	127.49	120.28
1	D	36	ASP	C-N-CA	5.01	127.49	120.28
1	L	10	LEU	CA-C-N	5.01	127.30	120.54
1	L	10	LEU	C-N-CA	5.01	127.30	120.54
1	A	205	GLY	N-CA-C	5.01	118.54	112.48
3	F	19	DC	C2'-C3'-O3'	5.01	119.01	111.50
3	N	16	DA	C4'-C3'-O3'	5.00	117.50	110.00

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	176	TYR	Sidechain
2	E	-13	DT	Sidechain
2	E	-16	DT	Sidechain
2	E	-23	DG	Sidechain
3	F	15	DG	Sidechain
3	F	16	DA	Sidechain
4	G	-13	DA	Sidechain
4	G	-22	DG	Sidechain
4	G	-23	DT	Sidechain
4	G	-24	DA	Sidechain
5	H	10	DT	Sidechain
5	H	11	DG	Sidechain
5	H	16	DT	Sidechain
1	I	213	TYR	Sidechain
1	I	334	ARG	Sidechain
1	I	347	HIS	Sidechain
1	K	213	TYR	Sidechain
1	K	363	TYR	Sidechain
2	M	-15	DC	Sidechain
2	M	-16	DT	Sidechain
2	M	-23	DG	Sidechain
3	N	16	DA	Sidechain
3	N	18	DA	Sidechain
4	O	-22	DG	Sidechain
4	O	-23	DT	Sidechain
4	O	-24	DA	Sidechain
5	P	13	DT	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4346	4418	4412	68	0
1	B	481	474	474	9	0
1	C	4354	4429	4424	48	0
1	D	490	480	479	3	0
1	I	4354	4429	4424	73	0
1	J	481	474	474	8	0
1	K	4346	4418	4412	45	0
1	L	490	480	479	3	0
2	E	694	393	388	7	0
2	M	694	393	386	4	0
3	F	679	373	346	10	0
3	N	679	373	348	10	0
4	G	511	285	279	4	0
4	O	511	285	279	6	0
5	H	493	274	257	5	0
5	P	493	274	258	5	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	I	1	0	0	0	0
6	K	1	0	0	0	0
All	All	24100	22252	22119	272	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 6.

All (272) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:TYR:O	1:A:248:TYR:OH	1.82	0.97
1:A:80:LEU:HD11	1:A:88:ILE:HD11	1.42	0.97
1:A:120:THR:OG1	1:A:123:LYS:O	1.90	0.90
1:I:473:ASP:OD1	1:I:476:THR:OG1	1.90	0.90
1:I:174:TYR:O	1:I:248:TYR:OH	1.89	0.90
1:I:120:THR:OG1	1:I:123:LYS:O	1.92	0.86
1:I:80:LEU:HD11	1:I:88:ILE:HD11	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:GLN:OE1	1:C:166:LYS:NZ	2.10	0.84
1:K:164:GLN:OE1	1:K:166:LYS:NZ	2.12	0.80
1:C:477:VAL:HA	1:C:480:ASN:ND2	1.97	0.80
1:I:93:ILE:HD12	1:I:139:GLU:OE1	1.82	0.80
1:I:378:ASN:OD1	1:I:379:ASP:N	2.16	0.78
1:K:477:VAL:HA	1:K:480:ASN:ND2	2.00	0.77
1:A:473:ASP:OD1	1:A:476:THR:OG1	2.00	0.76
1:I:204:ASN:OD1	1:I:205:GLY:N	2.18	0.76
1:I:134:ARG:NH1	1:K:149:MET:SD	2.59	0.75
1:A:45:ASN:OD1	1:A:55:TYR:OH	2.05	0.72
1:K:227:THR:OG1	1:K:231:LYS:O	2.07	0.69
1:K:258:GLU:OE1	1:K:268:ARG:NH1	2.26	0.68
1:A:260:THR:OG1	1:A:262:ASP:OD1	2.07	0.68
1:I:93:ILE:HD11	1:I:125:TYR:CE1	2.28	0.68
1:A:19:LEU:HD21	1:A:44:MET:HG3	1.75	0.68
1:A:195:VAL:HG11	1:A:248:TYR:CE1	2.28	0.68
1:B:17:VAL:O	1:B:17:VAL:HG13	1.94	0.67
1:I:260:THR:OG1	1:I:262:ASP:OD1	2.07	0.66
1:I:13:THR:N	1:I:86:GLN:OE1	2.30	0.65
1:I:270:GLU:N	1:I:270:GLU:OE1	2.29	0.65
1:A:381:ASN:N	1:B:41:TYR:OH	2.27	0.64
1:C:477:VAL:HA	1:C:480:ASN:HD21	1.62	0.64
1:I:18:TYR:O	1:I:19:LEU:HD23	1.98	0.64
1:I:58:LYS:O	1:I:59:MET:HE2	1.98	0.64
1:A:80:LEU:HD11	1:A:88:ILE:CD1	2.24	0.64
1:A:18:TYR:O	1:A:19:LEU:HD23	1.98	0.64
1:I:53:ILE:HG22	1:I:54:PRO:HD2	1.80	0.64
1:K:224:GLN:N	1:K:224:GLN:OE1	2.31	0.63
1:C:255:LYS:N	5:H:6:DG:OP1	2.31	0.63
1:I:195:VAL:HG11	1:I:248:TYR:CE1	2.33	0.62
1:I:376:SER:OG	1:J:27:TYR:OH	2.18	0.61
1:K:256:VAL:HG23	1:K:273:GLN:OE1	1.99	0.61
1:I:80:LEU:HD11	1:I:88:ILE:CD1	2.30	0.61
1:K:477:VAL:HA	1:K:480:ASN:HD21	1.64	0.61
1:I:73:PHE:O	1:I:77:LEU:HD23	2.01	0.61
1:A:110:LEU:O	1:A:110:LEU:HD23	2.01	0.60
1:A:23:ARG:O	1:A:25:ASP:N	2.34	0.60
1:I:23:ARG:O	1:I:25:ASP:N	2.34	0.60
1:I:173:PRO:HG2	1:I:247:VAL:HG11	1.84	0.60
1:K:260:THR:OG1	1:K:262:ASP:OD1	2.13	0.59
1:I:200:ASN:OD1	1:I:201:ILE:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:381:ASN:N	1:J:41:TYR:OH	2.34	0.59
1:A:135:GLN:OE1	1:K:135:GLN:NE2	2.33	0.58
1:A:386:THR:O	1:A:390:ASN:OD1	2.20	0.58
1:I:529:ILE:HD13	1:J:28:ILE:HD11	1.84	0.58
1:K:98:ARG:O	1:K:98:ARG:HG3	2.04	0.58
3:N:6:DG:C8	3:N:7:DT:H72	2.38	0.58
1:A:98:ARG:NH2	3:F:2:DA:OP1	2.36	0.58
1:C:56:GLU:OE1	1:C:58:LYS:NZ	2.35	0.58
1:C:260:THR:OG1	1:C:262:ASP:OD1	2.15	0.57
1:C:7:VAL:CG2	1:C:12:ILE:HD13	2.35	0.57
1:K:111:LEU:HD13	1:K:118:ILE:HD11	1.86	0.57
1:C:111:LEU:HD13	1:C:118:ILE:HD11	1.87	0.57
1:A:16:LEU:HD21	1:A:76:CYS:HB3	1.87	0.56
1:I:227:THR:OG1	1:I:231:LYS:N	2.38	0.56
1:I:191:GLU:O	1:I:195:VAL:HG23	2.05	0.56
1:K:214:THR:HG21	4:O:-14:DT:H72	1.88	0.56
1:I:73:PHE:CZ	1:I:77:LEU:HD21	2.41	0.55
1:K:29:GLU:O	1:K:33:GLY:N	2.38	0.55
1:C:19:LEU:HD11	1:C:40:GLN:CD	2.32	0.55
1:A:272:GLU:O	1:A:272:GLU:OE2	2.25	0.55
1:A:191:GLU:O	1:A:195:VAL:HG23	2.07	0.54
1:A:227:THR:OG1	1:A:231:LYS:N	2.39	0.54
1:A:182:THR:HG22	1:A:182:THR:O	2.06	0.54
1:I:182:THR:HG22	1:I:182:THR:O	2.08	0.54
2:E:-3:DC:H2'	2:E:-2:DT:C5	2.43	0.53
1:A:65:GLU:OE2	1:A:100:SER:OG	2.27	0.53
1:C:53:ILE:HG22	1:C:54:PRO:HD2	1.91	0.53
1:K:190:ASP:O	1:K:194:VAL:HG23	2.09	0.53
1:C:4:LYS:HA	1:C:7:VAL:HG12	1.91	0.53
1:C:192:ALA:HA	1:C:283:ILE:HD11	1.91	0.52
1:C:167:TRP:HZ3	1:C:252:VAL:HG13	1.74	0.52
1:A:19:LEU:HD21	1:A:44:MET:CG	2.40	0.52
1:I:6:ILE:HG21	1:I:124:VAL:HG21	1.92	0.52
1:A:479:ASN:ND2	1:B:55:ARG:HH22	2.07	0.52
1:I:382:ASP:O	1:I:386:THR:HG23	2.10	0.52
1:I:258:GLU:OE1	1:K:128:ARG:NH1	2.42	0.52
1:K:169:SER:OG	1:K:170:GLY:N	2.42	0.52
2:M:-3:DC:H2'	2:M:-2:DT:C5	2.45	0.52
1:A:93:ILE:HD11	1:A:125:TYR:OH	2.10	0.52
1:A:110:LEU:HD23	1:A:110:LEU:C	2.35	0.52
1:I:256:VAL:HG13	1:I:273:GLN:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:LEU:HD21	1:I:76:CYS:HB3	1.91	0.51
3:N:5:DT:H2''	3:N:6:DG:C8	2.45	0.51
1:K:500:LEU:O	1:K:504:VAL:HG23	2.11	0.51
1:K:256:VAL:HG13	1:K:257:ARG:HG3	1.91	0.50
1:A:238:THR:HG22	1:A:242:ILE:HD12	1.93	0.50
1:A:93:ILE:HD11	1:A:125:TYR:CE2	2.47	0.50
1:K:152:GLU:OE1	1:K:152:GLU:HA	2.11	0.50
1:A:478:ARG:O	1:A:481:ILE:HD12	2.12	0.50
1:C:221:THR:HG23	1:C:232:LYS:O	2.11	0.50
1:D:17:VAL:HG12	1:D:19:GLN:OE1	2.12	0.50
1:I:65:GLU:OE2	1:I:100:SER:OG	2.30	0.50
1:A:473:ASP:OD1	1:A:476:THR:N	2.45	0.49
1:C:378:ASN:OD1	1:C:483:LYS:NZ	2.20	0.49
1:A:16:LEU:HD21	1:A:76:CYS:SG	2.53	0.49
3:F:5:DT:H2''	3:F:6:DG:C8	2.47	0.49
1:K:487:GLN:NE2	1:K:491:GLU:OE2	2.46	0.49
1:C:7:VAL:HG11	1:C:51:ILE:HG23	1.95	0.49
1:C:76:CYS:O	1:C:80:LEU:N	2.40	0.49
1:K:255:LYS:O	1:K:255:LYS:HG3	2.13	0.49
1:K:363:TYR:CD1	1:K:363:TYR:C	2.90	0.49
3:F:3:DG:H2'	3:F:4:DC:C6	2.47	0.49
1:A:465:LEU:O	1:A:468:THR:OG1	2.29	0.49
1:B:28:ILE:O	1:B:30:GLN:NE2	2.46	0.49
1:C:29:GLU:O	1:C:33:GLY:N	2.45	0.49
1:I:225:ILE:HD13	1:I:412:HIS:NE2	2.28	0.49
1:A:120:THR:HB	1:A:121:PRO:HD2	1.95	0.48
3:N:3:DG:H2'	3:N:4:DC:C6	2.48	0.48
1:A:73:PHE:CE2	1:A:77:LEU:HD11	2.48	0.48
1:C:7:VAL:HG21	1:C:12:ILE:HD13	1.95	0.48
1:J:28:ILE:O	1:J:30:GLN:NE2	2.46	0.48
1:K:167:TRP:HZ3	1:K:252:VAL:HG13	1.78	0.48
1:K:212:SER:O	1:K:216:ILE:HD12	2.13	0.48
1:I:16:LEU:HD21	1:I:76:CYS:SG	2.53	0.48
4:G:-6:DC:H2''	4:G:-5:DA:C8	2.49	0.48
1:I:258:GLU:OE1	1:I:268:ARG:NH1	2.47	0.48
1:J:49:LEU:O	1:J:53:LEU:HD23	2.14	0.47
1:A:249:ILE:O	1:A:249:ILE:HG13	2.14	0.47
1:A:258:GLU:OE1	1:A:268:ARG:NH1	2.47	0.47
1:C:500:LEU:O	1:C:504:VAL:HG23	2.15	0.47
5:H:7:DT:C2	5:H:8:DA:C8	3.02	0.47
1:A:135:GLN:HA	1:A:138:PHE:HD2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:19:LEU:HD21	1:I:44:MET:HG3	1.95	0.47
1:I:44:MET:HE3	1:I:44:MET:HA	1.96	0.47
1:B:49:LEU:O	1:B:53:LEU:HD23	2.14	0.47
1:K:167:TRP:CZ3	1:K:252:VAL:HG13	2.49	0.47
1:K:378:ASN:OD1	1:K:483:LYS:NZ	2.21	0.47
2:E:-4:DG:C2'	2:E:-3:DC:C6	2.97	0.47
5:H:6:DG:C5	5:H:7:DT:C4	3.02	0.47
1:A:93:ILE:HD11	1:A:125:TYR:CZ	2.49	0.47
1:I:478:ARG:O	1:I:478:ARG:HD3	2.14	0.47
1:I:478:ARG:O	1:I:481:ILE:HD12	2.15	0.47
1:A:199:PHE:CG	1:A:284:ILE:HD12	2.50	0.46
3:F:3:DG:H2''	3:F:4:DC:O5'	2.15	0.46
1:C:360:TYR:CE1	4:G:-19:DA:H3'	2.50	0.46
1:C:167:TRP:CZ3	1:C:252:VAL:HG13	2.50	0.46
1:C:93:ILE:CD1	1:C:118:ILE:HG21	2.45	0.46
1:I:16:LEU:HB2	1:I:85:TYR:CD2	2.50	0.46
1:D:15:ILE:N	1:D:27:TYR:O	2.40	0.46
1:I:86:GLN:O	1:I:86:GLN:HG2	2.16	0.46
1:A:16:LEU:HD21	1:A:76:CYS:CB	2.47	0.45
1:A:142:MET:HE3	1:K:138:PHE:CZ	2.51	0.45
1:A:225:ILE:HG23	1:A:226:PRO:HD2	1.97	0.45
4:G:-7:DA:H2''	4:G:-6:DC:C6	2.51	0.45
1:A:24:GLN:NE2	3:F:2:DA:OP1	2.47	0.45
1:K:7:VAL:HG11	1:K:51:ILE:HG23	1.97	0.45
1:A:16:LEU:HB2	1:A:85:TYR:CD2	2.51	0.45
1:K:372:ASP:OD2	1:L:20:LYS:NZ	2.40	0.45
1:C:190:ASP:O	1:C:194:VAL:HG23	2.17	0.45
1:I:465:LEU:O	1:I:468:THR:OG1	2.30	0.45
2:M:-4:DG:C2'	2:M:-3:DC:C6	3.00	0.45
1:C:255:LYS:O	1:C:255:LYS:HG2	2.17	0.45
3:N:3:DG:H2''	3:N:4:DC:O5'	2.17	0.45
1:K:360:TYR:CE1	4:O:-19:DA:H3'	2.52	0.45
1:A:20:ARG:HG2	1:A:21:ARG:N	2.32	0.44
1:C:142:MET:CG	1:I:138:PHE:CZ	3.00	0.44
2:E:-2:DT:H6	2:E:-2:DT:O5'	2.00	0.44
4:O:-6:DC:H2''	4:O:-5:DA:C8	2.51	0.44
1:I:53:ILE:HG22	1:I:54:PRO:CD	2.45	0.44
1:K:178:LEU:HD23	1:K:178:LEU:H	1.82	0.44
1:I:473:ASP:OD1	1:I:476:THR:N	2.51	0.44
3:N:4:DC:H2'	3:N:5:DT:H71	1.99	0.44
1:C:235:ASN:OD1	1:C:238:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:272:GLU:O	1:I:272:GLU:OE1	2.36	0.44
1:A:126:ASP:O	1:A:129:ASN:N	2.51	0.44
1:A:381:ASN:H	1:B:41:TYR:HH	1.62	0.44
1:A:134:ARG:NH1	1:C:149:MET:SD	2.91	0.44
1:I:134:ARG:HH11	1:K:149:MET:CE	2.30	0.44
1:K:93:ILE:CD1	1:K:118:ILE:HG21	2.48	0.44
5:H:6:DG:C2	5:H:7:DT:C2	3.06	0.44
1:I:19:LEU:HD21	1:I:44:MET:CG	2.48	0.44
1:I:58:LYS:C	1:I:59:MET:HE2	2.43	0.44
1:A:7:VAL:HG23	1:A:12:ILE:CD1	2.48	0.43
3:F:10:DA:H2'	3:F:11:DT:H71	2.00	0.43
2:E:-4:DG:H2''	2:E:-3:DC:H6	1.83	0.43
1:C:466:GLN:O	1:C:466:GLN:CD	2.61	0.43
5:P:7:DT:C2	5:P:8:DA:C8	3.06	0.43
1:A:155:THR:HG22	1:A:159:TYR:CE2	2.54	0.43
3:F:4:DC:H2'	3:F:5:DT:H71	2.00	0.43
1:I:19:LEU:HD12	1:I:59:MET:HE1	2.00	0.43
1:I:526:ILE:HG12	1:J:25:ILE:HD13	2.00	0.43
1:A:415:GLN:O	1:A:419:GLU:HG3	2.18	0.43
3:F:2:DA:C2	3:F:3:DG:C2	3.06	0.43
1:I:48:LEU:HA	1:I:51:ILE:HD12	2.01	0.43
1:A:180:LYS:O	1:A:181:LYS:C	2.62	0.43
1:K:466:GLN:CD	1:K:466:GLN:O	2.61	0.43
3:N:10:DA:H2'	3:N:11:DT:H71	2.01	0.43
1:A:86:GLN:O	1:A:86:GLN:CG	2.67	0.43
5:P:6:DG:C5	5:P:7:DT:C4	3.06	0.43
5:P:6:DG:C2	5:P:7:DT:C2	3.07	0.43
1:I:238:THR:HG22	1:I:242:ILE:HD12	2.01	0.42
1:I:180:LYS:O	1:I:181:LYS:C	2.61	0.42
1:C:197:LEU:HD11	1:C:201:ILE:HD11	2.00	0.42
1:C:392:MET:HE1	1:D:45:ALA:HB3	2.00	0.42
1:I:254:TYR:HE1	3:N:5:DT:H4'	1.84	0.42
1:I:424:GLU:HB2	1:I:448:LEU:HD21	2.01	0.42
3:N:5:DT:C2'	3:N:6:DG:C8	3.02	0.42
1:A:463:ASN:O	1:A:466:GLN:N	2.53	0.42
1:B:17:VAL:O	1:B:17:VAL:CG1	2.65	0.42
1:C:53:ILE:CG2	1:C:54:PRO:HD2	2.49	0.42
1:I:4:LYS:O	1:I:7:VAL:HG12	2.19	0.42
4:O:-7:DA:H2''	4:O:-6:DC:C6	2.54	0.42
1:I:197:LEU:HD11	1:I:409:MET:HE2	2.01	0.42
1:A:268:ARG:CG	1:A:269:PRO:HD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:-4:DG:H2''	2:E:-3:DC:O5'	2.20	0.42
1:K:192:ALA:HA	1:K:283:ILE:HD11	2.02	0.42
1:K:214:THR:HG21	4:O:-14:DT:C7	2.49	0.42
1:B:35:ASN:OD1	1:B:35:ASN:O	2.38	0.42
1:C:103:ASP:O	1:C:107:ILE:HG12	2.19	0.42
1:I:111:LEU:HD23	1:I:116:LEU:HB2	2.00	0.42
1:K:392:MET:HE1	1:L:45:ALA:HB3	2.01	0.42
1:A:126:ASP:O	1:A:128:ARG:N	2.53	0.42
1:A:302:LEU:HD22	2:E:-13:DT:H5''	2.02	0.42
1:C:16:LEU:HB2	1:C:85:TYR:CG	2.55	0.42
1:I:247:VAL:O	1:I:247:VAL:HG12	2.19	0.42
3:N:4:DC:H2''	3:N:5:DT:C6	2.55	0.42
1:C:171:LEU:HG	4:G:-5:DA:O4'	2.20	0.41
1:C:40:GLN:HE21	1:C:91:LYS:HB2	1.84	0.41
1:C:154:MET:HE1	5:H:2:DA:C2	2.56	0.41
1:I:371:LEU:HD22	1:I:485:ILE:CD1	2.50	0.41
2:M:-2:DT:H6	2:M:-2:DT:O5'	2.03	0.41
1:C:173:PRO:HB3	1:C:247:VAL:HG11	2.03	0.41
1:K:256:VAL:N	5:P:6:DG:OP1	2.53	0.41
1:K:303:LEU:HD11	5:P:13:DT:H2''	2.02	0.41
1:A:48:LEU:CD1	1:A:57:LEU:HD21	2.50	0.41
1:A:134:ARG:CG	1:C:145:GLU:OE2	2.69	0.41
1:C:227:THR:OG1	1:C:231:LYS:O	2.39	0.41
1:I:110:LEU:HD23	1:I:110:LEU:C	2.45	0.41
1:J:35:ASN:OD1	1:J:35:ASN:O	2.38	0.41
1:K:216:ILE:HD12	1:K:216:ILE:H	1.85	0.41
1:A:526:ILE:HD11	1:B:25:ILE:HG12	2.02	0.41
1:C:274:ILE:O	1:C:274:ILE:HG23	2.20	0.41
1:I:16:LEU:HD21	1:I:76:CYS:CB	2.50	0.41
1:I:120:THR:HB	1:I:121:PRO:HD2	2.02	0.41
3:N:2:DA:C2	3:N:3:DG:C2	3.09	0.41
1:K:339:LYS:HE3	4:O:-23:DT:OP1	2.20	0.41
1:A:239:ILE:HD13	1:A:239:ILE:HA	1.96	0.41
1:A:424:GLU:HB2	1:A:448:LEU:HD21	2.02	0.41
1:I:77:LEU:HD12	1:I:110:LEU:HD13	2.03	0.41
1:I:369:ALA:HA	1:J:23:TYR:CZ	2.55	0.41
1:K:51:ILE:HG22	1:K:53:ILE:H	1.84	0.41
1:K:254:TYR:O	1:K:255:LYS:HB3	2.21	0.41
1:A:236:GLN:CD	1:A:236:GLN:O	2.64	0.41
1:C:126:ASP:OD1	1:C:126:ASP:C	2.64	0.41
1:C:258:GLU:OE1	1:C:268:ARG:NE	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:13:DA:C6	3:F:14:DA:C6	3.08	0.41
1:I:268:ARG:CG	1:I:269:PRO:HD2	2.51	0.41
1:K:16:LEU:HB2	1:K:85:TYR:CG	2.56	0.41
1:L:15:ILE:N	1:L:27:TYR:O	2.45	0.41
1:A:6:ILE:HG21	1:A:124:VAL:HG21	2.03	0.41
1:A:478:ARG:O	1:A:480:ASN:N	2.53	0.41
1:C:417:GLU:HB2	1:C:455:LEU:HD21	2.03	0.41
3:F:5:DT:C2'	3:F:6:DG:C8	3.04	0.40
1:I:306:LYS:HE2	2:M:-16:DT:O2	2.21	0.40
1:A:352:THR:HG22	1:A:360:TYR:CD2	2.57	0.40
1:C:142:MET:HG2	1:I:138:PHE:CZ	2.56	0.40
1:I:20:ARG:HG2	1:I:21:ARG:N	2.36	0.40
1:A:202:PHE:CD2	1:A:243:LEU:HD13	2.56	0.40
1:C:300:VAL:HA	1:C:301:PRO:HD3	1.89	0.40
1:I:177:GLN:O	1:I:185:LEU:HD22	2.21	0.40
1:C:133:MET:HA	1:C:136:ILE:HG22	2.04	0.40
1:A:48:LEU:HD13	1:A:55:TYR:CD1	2.56	0.40
1:C:91:LYS:HD3	1:C:92:GLU:HG2	2.03	0.40
2:E:-4:DG:H2''	2:E:-3:DC:C6	2.56	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	532/620 (86%)	494 (93%)	37 (7%)	1 (0%)	43	76
1	B	54/620 (9%)	48 (89%)	6 (11%)	0	100	100
1	C	533/620 (86%)	496 (93%)	37 (7%)	0	100	100
1	D	55/620 (9%)	53 (96%)	2 (4%)	0	100	100
1	I	533/620 (86%)	503 (94%)	29 (5%)	1 (0%)	43	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	54/620 (9%)	49 (91%)	5 (9%)	0	100	100
1	K	532/620 (86%)	501 (94%)	31 (6%)	0	100	100
1	L	55/620 (9%)	53 (96%)	2 (4%)	0	100	100
All	All	2348/4960 (47%)	2197 (94%)	149 (6%)	2 (0%)	49	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	I	24	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	489/560 (87%)	489 (100%)	0	100	100
1	B	51/560 (9%)	51 (100%)	0	100	100
1	C	490/560 (88%)	488 (100%)	2 (0%)	84	82
1	D	52/560 (9%)	52 (100%)	0	100	100
1	I	490/560 (88%)	490 (100%)	0	100	100
1	J	51/560 (9%)	51 (100%)	0	100	100
1	K	489/560 (87%)	485 (99%)	4 (1%)	73	77
1	L	52/560 (9%)	52 (100%)	0	100	100
All	All	2164/4480 (48%)	2158 (100%)	6 (0%)	84	83

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	249	ILE
1	C	302	LEU
1	K	249	ILE
1	K	302	LEU

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Mol	Chain	Res	Type
1	K	363	TYR
1	K	493	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	177	GLN
1	A	291	GLN
1	A	456	GLN
1	A	479	ASN
1	A	482	ASN
1	C	207	ASN
1	C	219	HIS
1	C	280	HIS
1	C	338	ASN
1	C	347	HIS
1	C	356	ASN
1	C	498	ASN
1	I	109	ASN
1	I	293	GLN
1	I	364	ASN
1	I	390	ASN
1	J	35	ASN
1	K	40	GLN
1	K	338	ASN
1	K	482	ASN
1	K	523	GLN
1	L	22	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47286. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

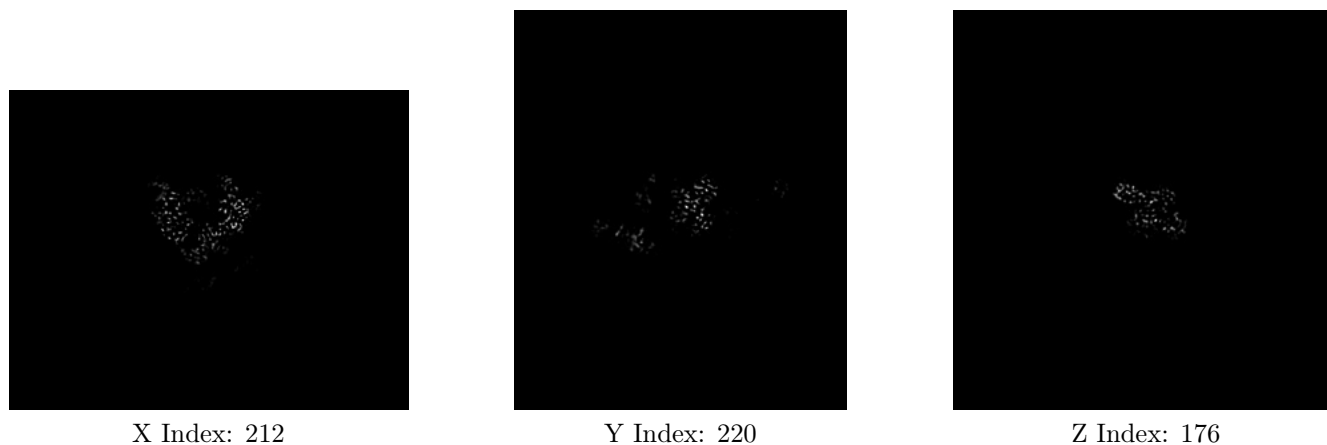
6.1.1 Primary map



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

6.2 Central slices [i](#)

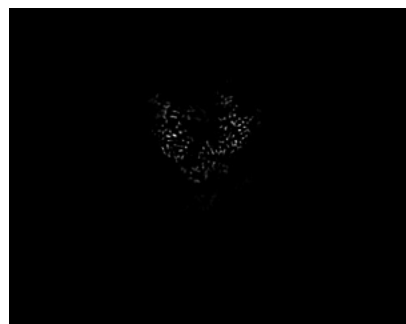
6.2.1 Primary map



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

6.3 Largest variance slices [i](#)

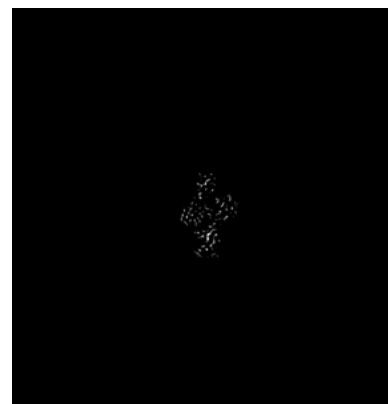
6.3.1 Primary map



X Index: 213



Y Index: 238

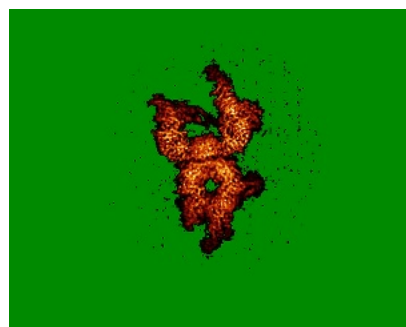


Z Index: 200

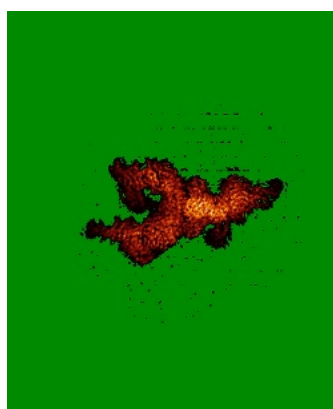
The images above show the largest variance slices of the map in three orthogonal directions.

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

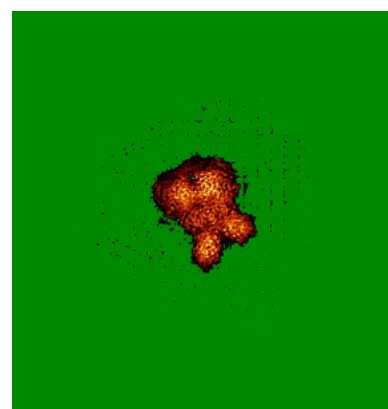
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0226. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

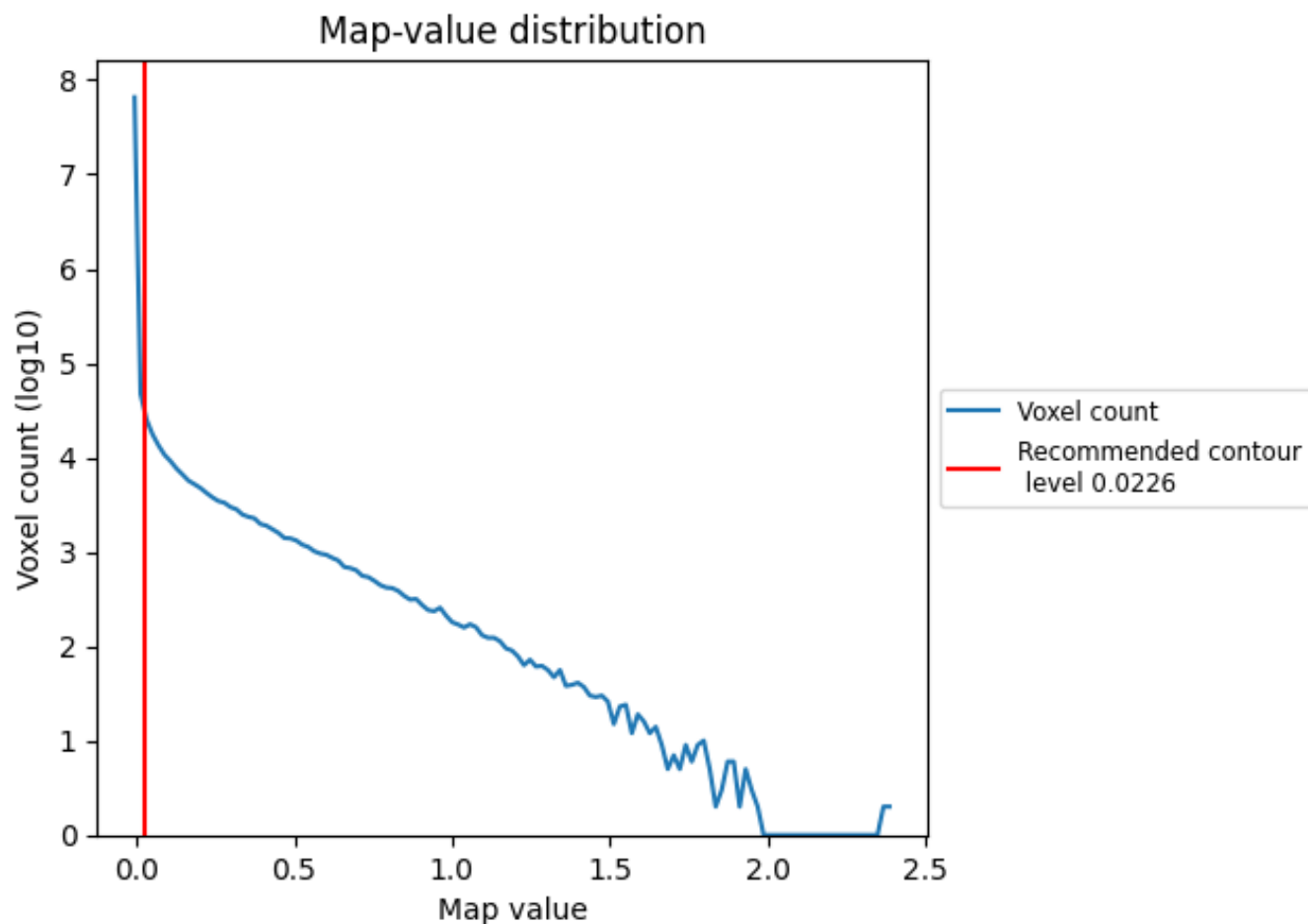
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

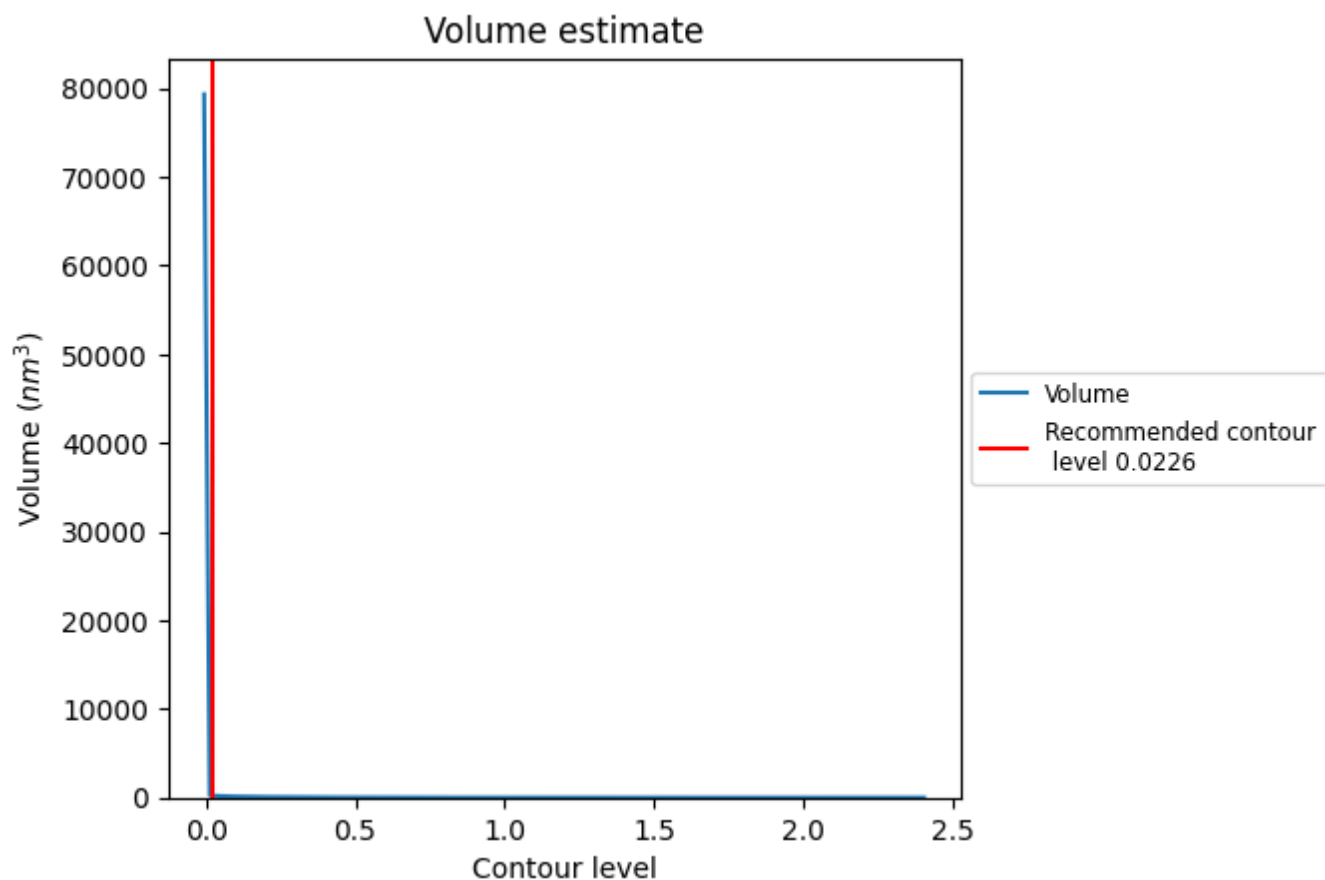
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 223 nm³; this corresponds to an approximate mass of 201 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

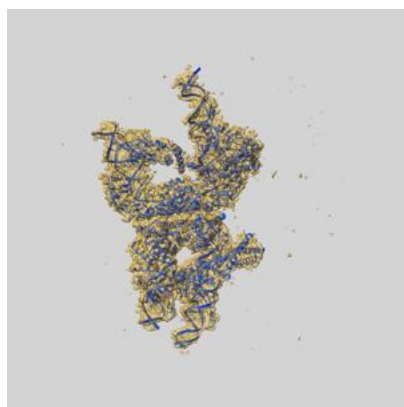
8 Fourier-Shell correlation

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

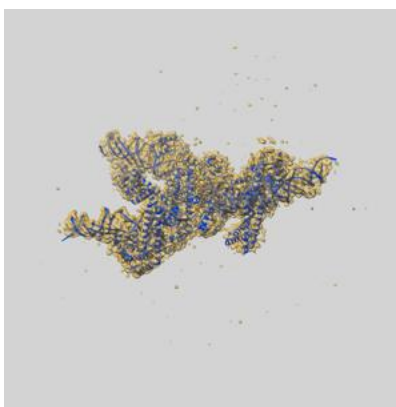
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47286 and PDB model 9DXF. Per-residue inclusion information can be found in section 3 on page 10.

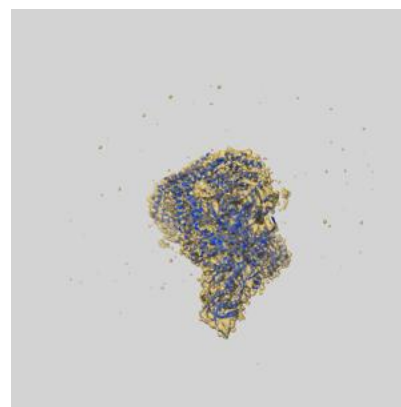
9.1 Map-model overlay [i](#)



X



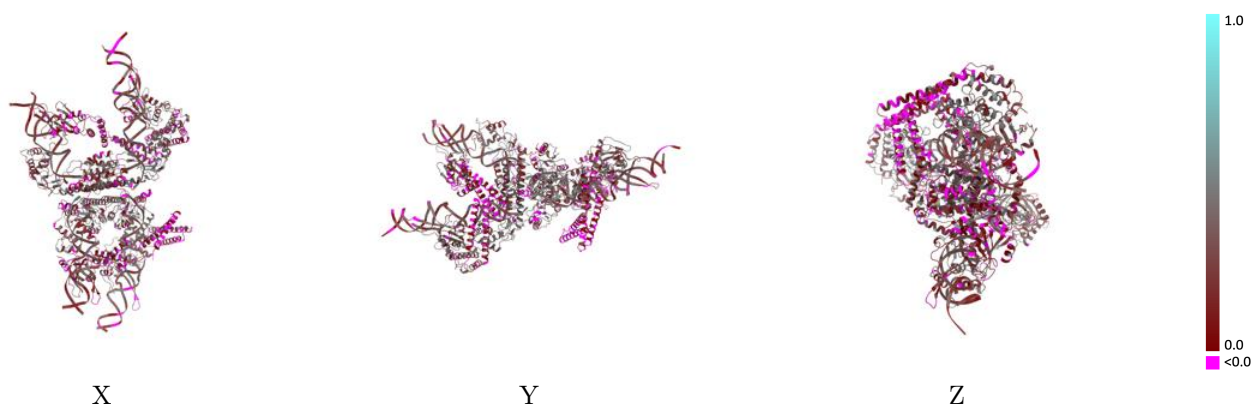
Y



Z

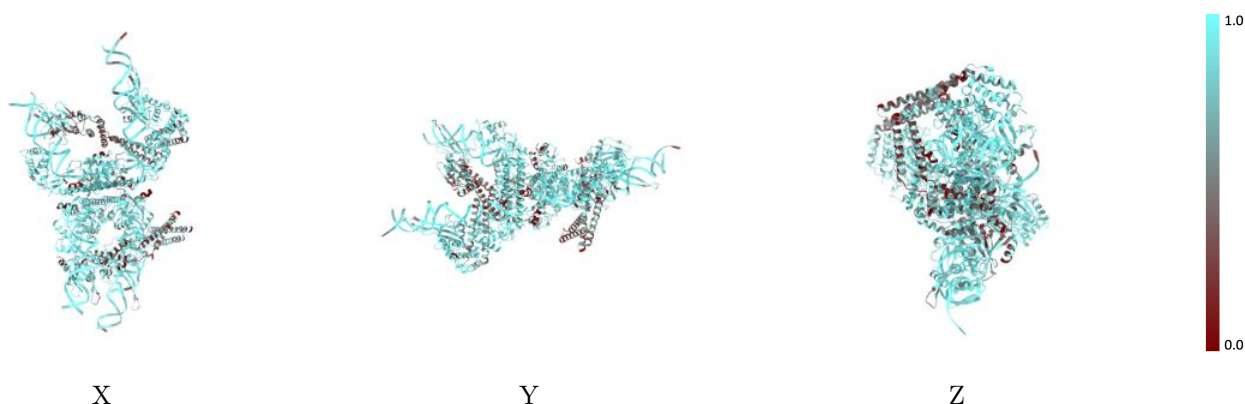
The images above show the 3D surface view of the map at the recommended contour level 0.0226 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



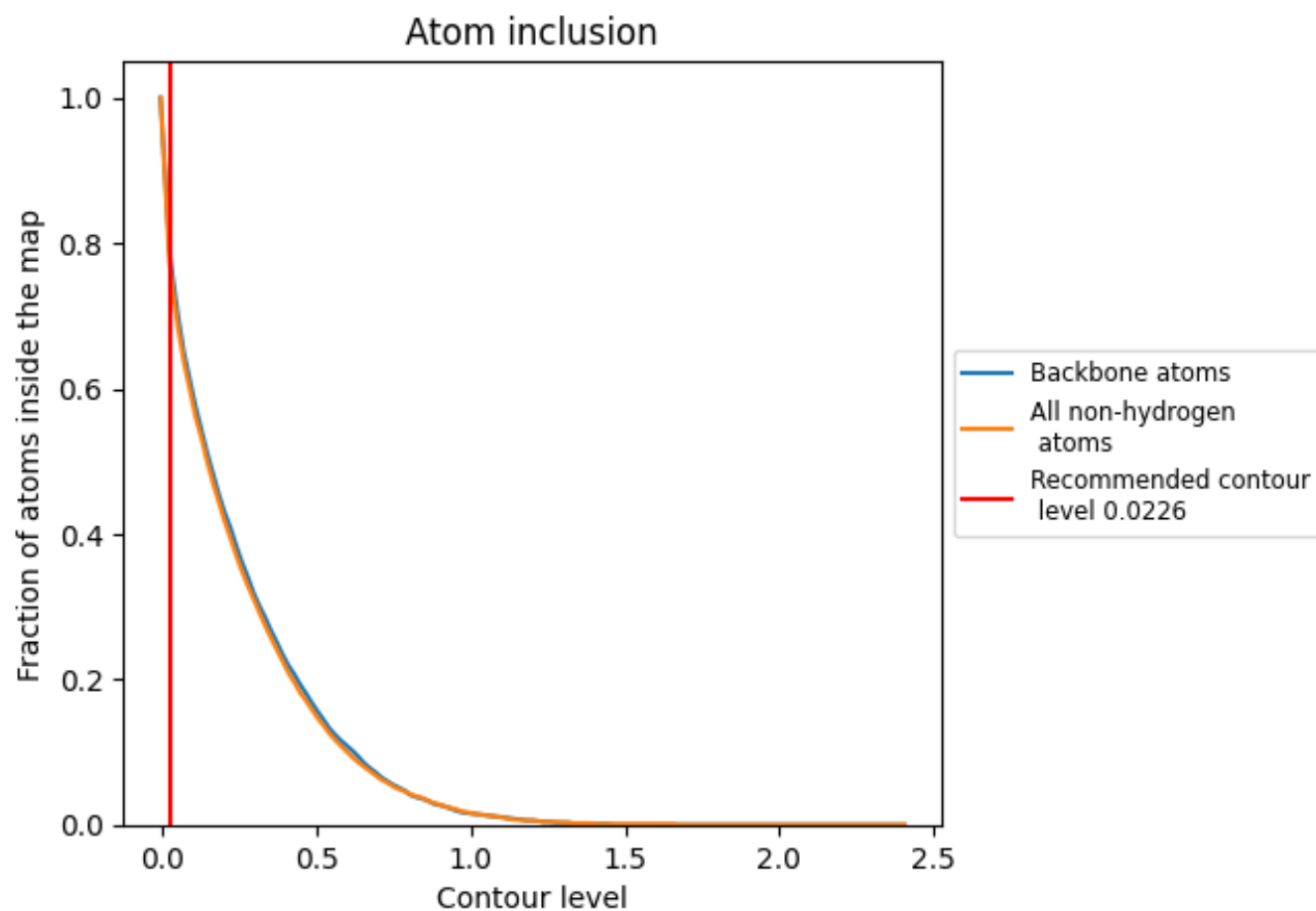
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0226).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 77% 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 (0.0226) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7740	 0.2600
A	 0.7990	 0.2910
B	 0.7640	 0.3020
C	 0.6960	 0.2170
D	 0.5200	 0.1340
E	 0.8750	 0.2700
F	 0.8870	 0.2990
G	 0.9330	 0.3040
H	 0.9070	 0.2840
I	 0.8280	 0.2920
J	 0.7810	 0.3020
K	 0.7230	 0.2240
L	 0.5070	 0.1350
M	 0.8950	 0.2750
N	 0.9150	 0.3070
O	 0.9590	 0.3030
P	 0.9370	 0.2910

