



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 07:59 AM UTC

PDB ID : 9DXJ / pdb_00009dxj
EMDB ID : EMD-47289
Title : attPmm and attBmm bound serine integrase complex in the post-rotation state
Authors : Shin, H.; Rice, P.A.; Olorunniji, F.J.
Deposited on : 2024-10-11
Resolution : 4.69 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

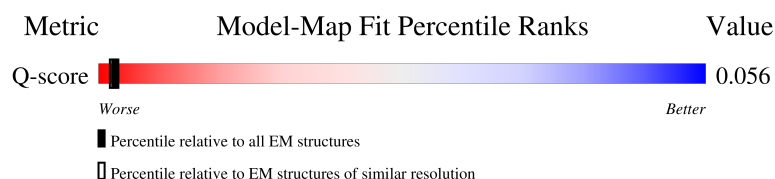
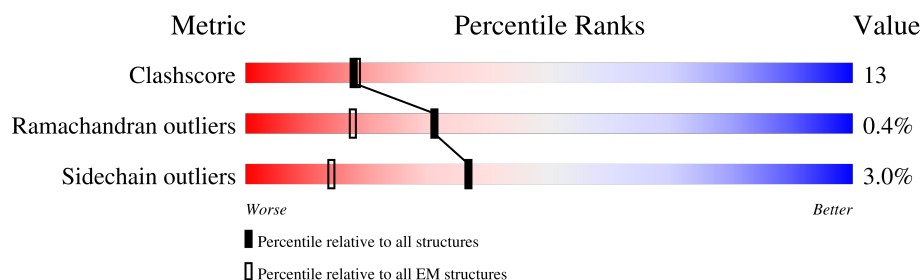
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.69 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	1970 (4.19 - 5.19)

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	545	<div> <div>8%</div> <div>72%</div> <div>24%</div> <div>..</div> </div>
1	C	545	<div> <div>8%</div> <div>65%</div> <div>28%</div> <div>..</div> </div>
1	I	545	<div> <div>6%</div> <div>71%</div> <div>25%</div> <div>..</div> </div>
1	K	545	<div> <div>7%</div> <div>66%</div> <div>28%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	34	 15% 18% 82%
2	M	34	 15% 24% 76%
3	F	33	 21% 27% 73%
3	N	33	 15% 27% 73%
4	G	25	 32% 68%
4	O	25	 28% 68%
5	H	24	 21% 79%
5	P	24	 21% 79%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 42532 atoms, of which 20350 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
			8781	2744	4425	753	841	18		
1	C	535	Total	C	H	N	O	S	0	0
			8781	2744	4425	753	841	18		
1	I	535	Total	C	H	N	O	S	0	0
			8781	2744	4425	753	841	18		
1	K	535	Total	C	H	N	O	S	0	0
			8781	2744	4425	753	841	18		

- 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).

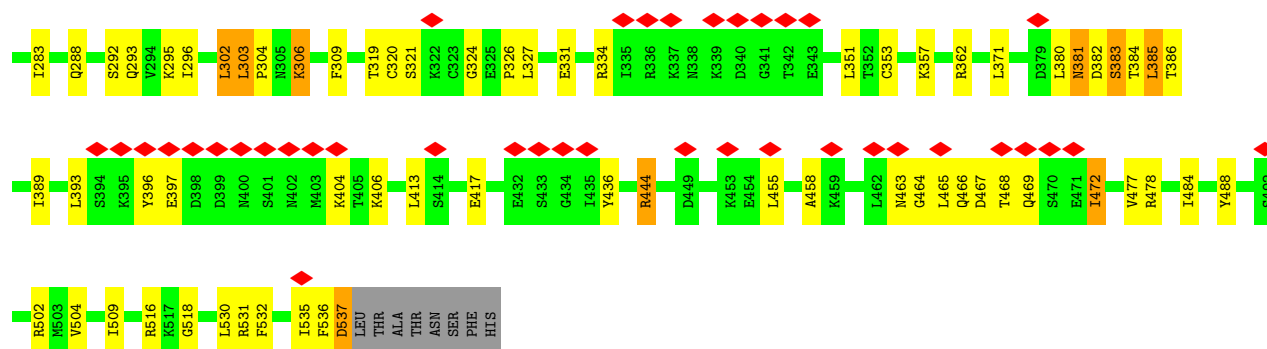
Mol	Chain	Residues	Atoms						AltConf	Trace
4	G	25	Total	C	H	N	O	P	0	0
			796	246	285	90	150	25		
4	O	25	Total	C	H	N	O	P	0	0
			796	246	285	90	150	25		

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

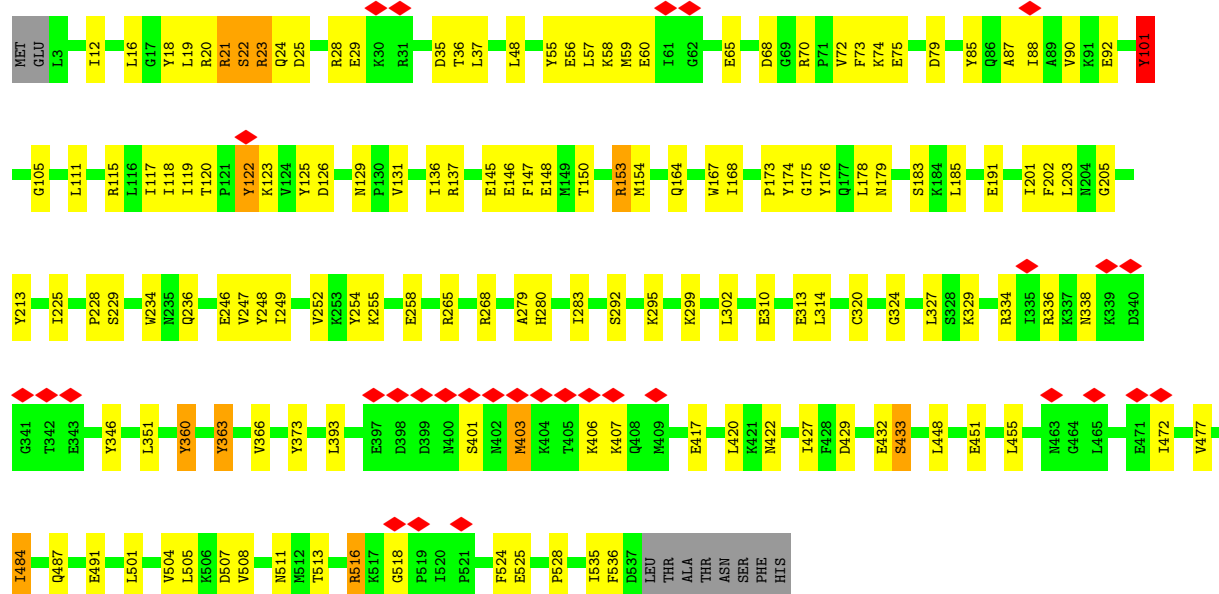
Mol	Chain	Residues	Atoms						AltConf	Trace
5	H	24	Total	C	H	N	O	P	0	0
			767	237	274	87	145	24		
5	P	24	Total	C	H	N	O	P	0	0
			767	237	274	87	145	24		

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

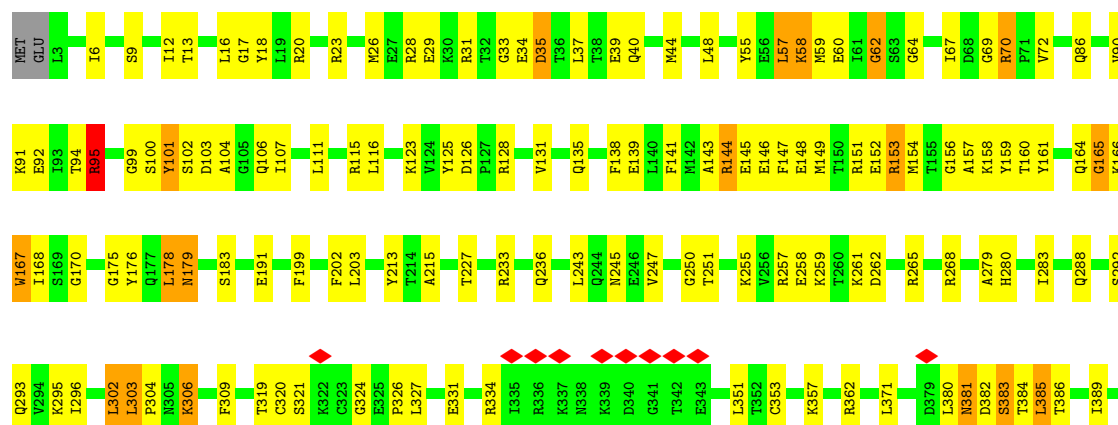
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	0
			1	1	
6	C	1	Total	Zn	0
			1	1	
6	I	1	Total	Zn	0
			1	1	
6	K	1	Total	Zn	0
			1	1	



• Molecule 1: Resolvase homolog Yoka

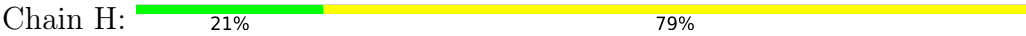


• Molecule 1: Resolvase homolog Yoka

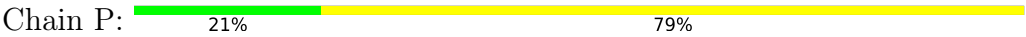




● Molecule 5: DNA (24-MER)



● Molecule 5: DNA (24-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44115	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	1.642	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.006	Depositor
Map size (\AA)	485.64, 472.86002, 453.69003	wwPDB
Map dimensions	456, 444, 426	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.065, 1.065, 1.065	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.45	9/4423 (0.2%)	0.62	10/5942 (0.2%)
1	C	1.21	36/4423 (0.8%)	1.24	93/5942 (1.6%)
1	I	0.45	9/4423 (0.2%)	0.62	10/5942 (0.2%)
1	K	1.20	36/4423 (0.8%)	1.24	91/5942 (1.5%)
2	E	0.44	0/774	0.78	0/1193
2	M	0.30	0/774	0.72	0/1193
3	F	0.29	0/764	0.78	0/1176
3	N	0.29	0/764	0.78	0/1176
4	G	0.84	2/572 (0.3%)	1.15	1/880 (0.1%)
4	O	0.84	2/572 (0.3%)	1.15	2/880 (0.2%)
5	H	0.69	0/552	0.99	0/850
5	P	0.69	1/552 (0.2%)	0.98	0/850
All	All	0.84	95/23016 (0.4%)	0.96	207/31966 (0.6%)

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	A	0	2
1	C	0	3
1	I	0	2
1	K	0	3
4	O	0	1
5	H	0	1
All	All	0	12

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	20	ARG	CZ-NH2	-8.38	1.22	1.33
1	C	20	ARG	CZ-NH2	-8.33	1.22	1.33
1	K	70	ARG	CZ-NH2	-8.29	1.22	1.33
1	C	70	ARG	CZ-NH2	-8.23	1.22	1.33
1	K	144	ARG	CZ-NH2	-8.23	1.22	1.33
1	C	144	ARG	CZ-NH2	-8.20	1.22	1.33
1	K	28	ARG	CZ-NH2	-8.20	1.22	1.33
1	C	31	ARG	CZ-NH2	-8.17	1.22	1.33
1	A	28	ARG	CZ-NH2	-8.16	1.22	1.33
1	I	153	ARG	CZ-NH2	-8.16	1.22	1.33
1	K	153	ARG	CZ-NH2	-8.16	1.22	1.33
1	K	31	ARG	CZ-NH2	-8.15	1.22	1.33
1	C	95	ARG	CZ-NH2	-8.13	1.22	1.33
1	C	28	ARG	CZ-NH2	-8.12	1.22	1.33
1	I	28	ARG	CZ-NH2	-8.12	1.22	1.33
1	A	137	ARG	CZ-NH2	-8.11	1.23	1.33
1	A	153	ARG	CZ-NH2	-8.10	1.23	1.33
1	C	153	ARG	CZ-NH2	-8.10	1.23	1.33
1	K	95	ARG	CZ-NH2	-8.09	1.23	1.33
1	K	151	ARG	CZ-NH2	-8.09	1.23	1.33
1	I	137	ARG	CZ-NH2	-8.06	1.23	1.33
1	C	151	ARG	CZ-NH2	-8.05	1.23	1.33
1	K	144	ARG	CZ-NH1	-7.76	1.21	1.32
1	C	144	ARG	CZ-NH1	-7.73	1.22	1.32
1	C	104	ALA	CA-CB	-6.99	1.42	1.53
1	K	104	ALA	CA-CB	-6.92	1.42	1.53
1	C	143	ALA	CA-CB	-6.86	1.42	1.53
1	C	157	ALA	CA-CB	-6.86	1.42	1.53
1	K	143	ALA	CA-CB	-6.84	1.42	1.53
1	K	157	ALA	CA-CB	-6.83	1.42	1.53
1	C	31	ARG	CZ-NH1	-6.76	1.23	1.32
1	K	31	ARG	CZ-NH1	-6.72	1.23	1.32
1	A	153	ARG	CZ-NH1	-6.72	1.23	1.32
1	K	20	ARG	CZ-NH1	-6.70	1.23	1.32
1	I	153	ARG	CZ-NH1	-6.66	1.23	1.32
1	C	99	GLY	N-CA	-6.64	1.38	1.45
1	A	28	ARG	CZ-NH1	-6.61	1.23	1.32
1	C	20	ARG	CZ-NH1	-6.61	1.23	1.32
1	K	95	ARG	CZ-NH1	-6.61	1.23	1.32
1	A	137	ARG	CZ-NH1	-6.58	1.23	1.32
1	K	28	ARG	CZ-NH1	-6.58	1.23	1.32
1	C	28	ARG	CZ-NH1	-6.57	1.23	1.32
1	I	137	ARG	CZ-NH1	-6.57	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	70	ARG	CZ-NH1	-6.57	1.23	1.32
1	K	70	ARG	CZ-NH1	-6.56	1.23	1.32
1	C	95	ARG	CZ-NH1	-6.55	1.23	1.32
1	K	156	GLY	N-CA	-6.54	1.38	1.45
1	C	151	ARG	CZ-NH1	-6.51	1.23	1.32
1	I	28	ARG	CZ-NH1	-6.51	1.23	1.32
1	K	99	GLY	N-CA	-6.50	1.38	1.45
1	C	153	ARG	CZ-NH1	-6.49	1.23	1.32
1	K	153	ARG	CZ-NH1	-6.49	1.23	1.32
1	K	151	ARG	CZ-NH1	-6.42	1.23	1.32
1	C	156	GLY	N-CA	-6.37	1.38	1.45
1	C	70	ARG	CA-CB	-5.98	1.46	1.53
1	K	70	ARG	CA-CB	-5.97	1.46	1.53
1	C	144	ARG	CD-NE	-5.89	1.38	1.46
1	K	144	ARG	CD-NE	-5.88	1.38	1.46
1	C	20	ARG	CD-NE	-5.83	1.38	1.46
1	K	20	ARG	CD-NE	-5.76	1.38	1.46
1	C	95	ARG	CD-NE	-5.64	1.38	1.46
1	C	31	ARG	CD-NE	-5.60	1.38	1.46
1	K	95	ARG	CD-NE	-5.59	1.38	1.46
1	K	31	ARG	CD-NE	-5.58	1.38	1.46
1	K	170	GLY	N-CA	-5.58	1.38	1.45
1	C	170	GLY	N-CA	-5.55	1.38	1.45
1	A	137	ARG	CD-NE	-5.49	1.38	1.46
1	I	153	ARG	CD-NE	-5.41	1.38	1.46
1	A	153	ARG	CD-NE	-5.41	1.38	1.46
1	C	33	GLY	N-CA	-5.39	1.37	1.45
1	I	137	ARG	CD-NE	-5.37	1.38	1.46
1	K	33	GLY	N-CA	-5.35	1.37	1.45
1	K	151	ARG	CD-NE	-5.33	1.38	1.46
1	C	151	ARG	CD-NE	-5.31	1.38	1.46
1	K	28	ARG	CD-NE	-5.29	1.38	1.46
1	C	28	ARG	CD-NE	-5.29	1.38	1.46
1	I	28	ARG	CD-NE	-5.29	1.38	1.46
1	A	28	ARG	CD-NE	-5.25	1.39	1.46
1	C	153	ARG	CD-NE	-5.22	1.39	1.46
1	K	70	ARG	CD-NE	-5.18	1.39	1.46
1	C	70	ARG	CD-NE	-5.17	1.39	1.46
1	K	62	GLY	N-CA	-5.16	1.37	1.45
1	C	62	GLY	N-CA	-5.16	1.37	1.45
4	O	-4	DG	C2-N2	-5.15	1.24	1.34
1	C	64	GLY	N-CA	-5.14	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	153	ARG	CD-NE	-5.13	1.39	1.46
1	K	64	GLY	N-CA	-5.12	1.38	1.45
4	G	-4	DG	C2-N2	-5.11	1.24	1.34
1	K	178	LEU	CA-CB	-5.11	1.46	1.52
1	C	178	LEU	CA-CB	-5.10	1.46	1.52
1	C	69	GLY	N-CA	-5.06	1.37	1.45
1	K	69	GLY	N-CA	-5.04	1.37	1.45
4	O	-3	DA	C6-N6	-5.02	1.24	1.34
4	G	-3	DA	C6-N6	-5.01	1.24	1.34
5	P	4	DC	C4-N4	-5.00	1.24	1.34

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	69	GLY	CA-C-N	7.28	132.73	123.34
1	K	69	GLY	C-N-CA	7.28	132.73	123.34
1	C	69	GLY	CA-C-N	7.27	132.72	123.34
1	C	69	GLY	C-N-CA	7.27	132.72	123.34
1	C	147	PHE	CA-CB-CG	7.05	120.85	113.80
1	K	147	PHE	CA-CB-CG	7.04	120.83	113.80
1	C	18	TYR	CA-C-N	6.84	132.17	122.72
1	C	18	TYR	C-N-CA	6.84	132.17	122.72
1	K	18	TYR	CA-C-N	6.82	132.13	122.72
1	K	18	TYR	C-N-CA	6.82	132.13	122.72
1	I	101	TYR	CA-CB-CG	6.66	125.88	113.90
1	A	101	TYR	CA-CB-CG	6.63	125.84	113.90
1	K	103	ASP	CA-CB-CG	6.54	119.14	112.60
1	C	103	ASP	CA-CB-CG	6.50	119.10	112.60
1	K	35	ASP	CA-CB-CG	6.48	119.08	112.60
1	C	23	ARG	NE-CZ-NH2	6.47	125.02	119.20
1	K	165	GLY	CA-C-N	6.41	131.00	120.94
1	K	165	GLY	C-N-CA	6.41	131.00	120.94
1	C	35	ASP	CA-CB-CG	6.40	119.00	112.60
1	C	165	GLY	CA-C-N	6.35	130.91	120.94
1	C	165	GLY	C-N-CA	6.35	130.91	120.94
1	C	144	ARG	CD-NE-CZ	6.24	133.14	124.40
1	K	144	ARG	CD-NE-CZ	6.24	133.13	124.40
1	C	141	PHE	CA-CB-CG	6.17	119.97	113.80
1	K	141	PHE	CA-CB-CG	6.15	119.95	113.80
1	C	153	ARG	CD-NE-CZ	6.15	133.00	124.40
1	I	22	SER	CA-CB-OG	-6.07	98.96	111.10
1	K	153	ARG	CD-NE-CZ	6.07	132.90	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	SER	CA-CB-OG	-6.06	98.99	111.10
1	A	28	ARG	CD-NE-CZ	6.05	132.87	124.40
1	I	28	ARG	CD-NE-CZ	6.05	132.87	124.40
1	K	99	GLY	N-CA-C	5.98	121.38	112.41
1	C	99	GLY	N-CA-C	5.94	121.32	112.41
1	C	35	ASP	CA-C-N	5.92	128.14	120.44
1	C	35	ASP	C-N-CA	5.92	128.14	120.44
1	K	139	GLU	CA-C-N	5.90	128.11	120.44
1	K	139	GLU	C-N-CA	5.90	128.11	120.44
1	C	139	GLU	CA-C-N	5.88	128.09	120.44
1	C	139	GLU	C-N-CA	5.88	128.09	120.44
1	I	28	ARG	N-CA-CB	5.88	118.70	109.94
1	A	28	ARG	N-CA-CB	5.88	118.70	109.94
1	K	35	ASP	CA-C-N	5.87	128.08	120.44
1	K	35	ASP	C-N-CA	5.87	128.08	120.44
1	C	158	LYS	CA-C-N	5.86	128.45	120.54
1	C	158	LYS	C-N-CA	5.86	128.45	120.54
1	K	158	LYS	CA-C-N	5.85	128.44	120.54
1	K	158	LYS	C-N-CA	5.85	128.44	120.54
1	C	141	PHE	CA-C-N	5.83	128.01	120.44
1	C	141	PHE	C-N-CA	5.83	128.01	120.44
1	C	159	TYR	CA-C-N	5.81	128.38	120.54
1	C	159	TYR	C-N-CA	5.81	128.38	120.54
1	K	141	PHE	CA-C-N	5.81	127.99	120.44
1	K	141	PHE	C-N-CA	5.81	127.99	120.44
1	K	159	TYR	CA-C-N	5.79	128.35	120.54
1	K	159	TYR	C-N-CA	5.79	128.35	120.54
1	C	149	MET	CA-C-N	5.76	128.32	120.54
1	C	149	MET	C-N-CA	5.76	128.32	120.54
1	C	101	TYR	CA-CB-CG	5.76	124.27	113.90
1	K	101	TYR	CA-CB-CG	5.76	124.26	113.90
1	K	149	MET	CA-C-N	5.75	128.30	120.54
1	K	149	MET	C-N-CA	5.75	128.30	120.54
1	K	70	ARG	CA-CB-CG	5.72	125.54	114.10
1	C	70	ARG	CA-CB-CG	5.68	125.47	114.10
1	C	179	ASN	CA-C-N	5.63	128.39	120.28
1	C	179	ASN	C-N-CA	5.63	128.39	120.28
1	C	40	GLN	CA-C-N	5.63	128.14	120.54
1	C	40	GLN	C-N-CA	5.63	128.14	120.54
1	K	40	GLN	CA-C-N	5.63	128.13	120.54
1	K	40	GLN	C-N-CA	5.63	128.13	120.54
1	K	158	LYS	CB-CG-CD	5.62	124.22	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	167	TRP	N-CA-CB	5.62	119.57	110.42
1	C	158	LYS	CB-CG-CD	5.61	124.21	111.30
1	K	39	GLU	CA-C-N	5.61	128.11	120.54
1	K	39	GLU	C-N-CA	5.61	128.11	120.54
1	C	259	LYS	N-CA-CB	5.59	118.27	109.83
1	K	259	LYS	N-CA-CB	5.58	118.26	109.83
1	C	39	GLU	CA-C-N	5.57	128.06	120.54
1	C	39	GLU	C-N-CA	5.57	128.06	120.54
1	K	37	LEU	N-CA-CB	5.57	118.23	109.94
1	C	167	TRP	N-CA-CB	5.56	119.49	110.42
1	K	179	ASN	CA-C-N	5.55	128.28	120.28
1	K	179	ASN	C-N-CA	5.55	128.28	120.28
1	C	58	LYS	CA-C-N	5.55	130.82	123.05
1	C	58	LYS	C-N-CA	5.55	130.82	123.05
1	C	141	PHE	N-CA-CB	5.54	118.04	110.01
1	C	37	LEU	N-CA-CB	5.54	118.19	109.94
1	K	106	GLN	CA-C-N	5.52	127.72	120.60
1	K	106	GLN	C-N-CA	5.52	127.72	120.60
1	K	58	LYS	CA-C-N	5.51	130.76	123.05
1	K	58	LYS	C-N-CA	5.51	130.76	123.05
1	K	145	GLU	CA-C-N	5.50	127.97	120.54
1	K	145	GLU	C-N-CA	5.50	127.97	120.54
1	K	141	PHE	N-CA-CB	5.50	117.98	110.01
1	C	154	MET	CA-C-N	5.49	127.58	120.44
1	C	154	MET	C-N-CA	5.49	127.58	120.44
1	C	145	GLU	CA-C-N	5.49	127.95	120.54
1	C	145	GLU	C-N-CA	5.49	127.95	120.54
1	K	154	MET	CA-C-N	5.49	127.57	120.44
1	K	154	MET	C-N-CA	5.49	127.57	120.44
1	K	153	ARG	CA-C-N	5.47	128.40	120.79
1	K	153	ARG	C-N-CA	5.47	128.40	120.79
1	K	166	LYS	CA-C-N	5.46	130.04	122.77
1	K	166	LYS	C-N-CA	5.46	130.04	122.77
1	C	106	GLN	CA-C-N	5.46	127.64	120.60
1	C	106	GLN	C-N-CA	5.46	127.64	120.60
1	C	166	LYS	CA-C-N	5.45	130.02	122.77
1	C	166	LYS	C-N-CA	5.45	130.02	122.77
1	K	143	ALA	CA-C-N	5.44	127.52	120.44
1	K	143	ALA	C-N-CA	5.44	127.52	120.44
1	C	143	ALA	CA-C-N	5.44	127.51	120.44
1	C	143	ALA	C-N-CA	5.44	127.51	120.44
1	C	57	LEU	CA-C-N	5.42	130.73	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	LEU	C-N-CA	5.42	130.73	122.65
1	K	57	LEU	CA-C-N	5.42	130.73	122.65
1	K	57	LEU	C-N-CA	5.42	130.73	122.65
1	C	153	ARG	CA-C-N	5.41	128.31	120.79
1	C	153	ARG	C-N-CA	5.41	128.31	120.79
1	K	64	GLY	CA-C-N	5.40	127.96	120.29
1	K	64	GLY	C-N-CA	5.40	127.96	120.29
1	C	24	GLN	N-CA-CB	5.40	117.84	110.01
1	C	64	GLY	CA-C-N	5.37	127.91	120.29
1	C	64	GLY	C-N-CA	5.37	127.91	120.29
1	I	22	SER	N-CA-CB	5.35	118.75	110.46
1	K	144	ARG	N-CA-CB	5.35	117.77	110.01
1	A	22	SER	N-CA-CB	5.34	118.74	110.46
1	C	99	GLY	CA-C-N	5.34	131.74	121.54
1	C	99	GLY	C-N-CA	5.34	131.74	121.54
1	C	148	GLU	N-CA-CB	5.34	117.75	110.01
1	K	40	GLN	CA-CB-CG	5.34	124.78	114.10
1	K	99	GLY	CA-C-N	5.34	131.74	121.54
1	K	99	GLY	C-N-CA	5.34	131.74	121.54
1	K	26	MET	CA-C-N	5.34	127.43	120.28
1	K	26	MET	C-N-CA	5.34	127.43	120.28
1	K	148	GLU	N-CA-CB	5.34	117.75	110.01
1	C	40	GLN	CA-CB-CG	5.33	124.77	114.10
1	C	107	ILE	N-CA-CB	5.33	116.43	110.51
4	G	-3	DA	O5'-C5'-C4'	5.33	118.80	110.80
1	K	107	ILE	N-CA-CB	5.33	116.43	110.51
1	K	152	GLU	CA-C-N	5.33	127.36	120.44
1	K	152	GLU	C-N-CA	5.33	127.36	120.44
1	C	152	GLU	CA-C-N	5.32	127.36	120.44
1	C	152	GLU	C-N-CA	5.32	127.36	120.44
1	C	67	ILE	N-CA-CB	5.31	116.40	110.51
4	O	-3	DA	O5'-C5'-C4'	5.30	118.76	110.80
1	K	67	ILE	N-CA-CB	5.30	116.39	110.51
1	C	144	ARG	N-CA-CB	5.28	117.67	110.01
1	C	26	MET	CA-C-N	5.28	127.36	120.28
1	C	26	MET	C-N-CA	5.28	127.36	120.28
1	K	160	THR	CA-C-N	5.27	127.34	120.28
1	K	160	THR	C-N-CA	5.27	127.34	120.28
1	C	160	THR	CA-C-N	5.26	127.33	120.28
1	C	160	THR	C-N-CA	5.26	127.33	120.28
1	C	178	LEU	N-CA-CB	5.25	118.17	109.88
1	K	20	ARG	N-CA-C	5.24	116.96	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	178	LEU	N-CA-CB	5.24	118.15	109.88
1	C	20	ARG	N-CA-C	5.23	116.94	108.26
1	K	91	LYS	N-CA-CB	5.23	117.59	110.01
1	C	91	LYS	N-CA-CB	5.22	117.57	110.01
1	I	153	ARG	CA-CB-CG	5.21	124.52	114.10
1	K	70	ARG	CD-NE-CZ	5.21	131.69	124.40
1	A	153	ARG	CA-CB-CG	5.20	124.50	114.10
4	O	-2	DT	C5'-C4'-C3'	-5.19	107.12	114.90
1	C	70	ARG	CD-NE-CZ	5.17	131.64	124.40
1	C	94	THR	CA-C-N	5.16	127.20	120.28
1	C	94	THR	C-N-CA	5.16	127.20	120.28
1	I	137	ARG	CA-CB-CG	5.16	124.43	114.10
1	K	94	THR	CA-C-N	5.16	127.19	120.28
1	K	94	THR	C-N-CA	5.16	127.19	120.28
1	A	137	ARG	CA-CB-CG	5.15	124.40	114.10
1	C	153	ARG	CG-CD-NE	5.15	123.32	112.00
1	K	102	SER	N-CA-CB	5.14	117.60	109.94
1	C	157	ALA	CA-C-N	5.11	127.44	120.54
1	C	157	ALA	C-N-CA	5.11	127.44	120.54
1	K	29	GLU	CB-CG-CD	5.11	121.29	112.60
1	I	136	ILE	CA-C-N	5.11	127.44	120.54
1	I	136	ILE	C-N-CA	5.11	127.44	120.54
1	C	102	SER	N-CA-CB	5.11	117.58	109.82
1	K	101	TYR	CA-C-N	5.11	127.43	120.54
1	K	101	TYR	C-N-CA	5.11	127.43	120.54
1	C	29	GLU	CB-CG-CD	5.10	121.27	112.60
1	K	153	ARG	CG-CD-NE	5.09	123.21	112.00
1	K	157	ALA	CA-C-N	5.07	127.38	120.54
1	K	157	ALA	C-N-CA	5.07	127.38	120.54
1	K	259	LYS	CB-CG-CD	5.06	122.94	111.30
1	A	136	ILE	CA-C-N	5.06	127.37	120.54
1	A	136	ILE	C-N-CA	5.06	127.37	120.54
1	C	259	LYS	CB-CG-CD	5.06	122.94	111.30
1	K	149	MET	N-CA-CB	5.05	117.50	109.82
1	C	28	ARG	CD-NE-CZ	5.05	131.47	124.40
1	C	261	LYS	CG-CD-CE	5.05	122.92	111.30
1	K	146	GLU	CA-C-N	5.05	127.00	120.44
1	K	146	GLU	C-N-CA	5.05	127.00	120.44
1	I	28	ARG	CG-CD-NE	5.05	123.10	112.00
1	K	90	VAL	CA-C-N	5.04	126.99	120.44
1	K	90	VAL	C-N-CA	5.04	126.99	120.44
1	K	261	LYS	CG-CD-CE	5.04	122.89	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ARG	CG-CD-NE	5.04	123.08	112.00
1	C	144	ARG	CA-C-N	5.04	127.34	120.54
1	C	144	ARG	C-N-CA	5.04	127.34	120.54
1	C	41	LYS	CA-CB-CG	5.03	124.15	114.10
1	K	144	ARG	CA-C-N	5.02	127.32	120.54
1	K	144	ARG	C-N-CA	5.02	127.32	120.54
1	C	149	MET	N-CA-CB	5.01	117.43	109.82
1	C	150	THR	CA-C-N	5.00	126.94	120.44
1	C	150	THR	C-N-CA	5.00	126.94	120.44
1	C	90	VAL	CA-C-N	5.00	126.94	120.44
1	C	90	VAL	C-N-CA	5.00	126.94	120.44

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	TYR	Sidechain
1	A	516	ARG	Sidechain
1	C	23	ARG	Sidechain
1	C	444	ARG	Sidechain
1	C	95	ARG	Sidechain
5	H	3	DT	Sidechain
1	I	363	TYR	Sidechain
1	I	516	ARG	Sidechain
1	K	23	ARG	Sidechain
1	K	444	ARG	Sidechain
1	K	95	ARG	Sidechain
4	O	-2	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	4356	4425	4419	105	0
1	C	4356	4425	4419	111	0
1	I	4356	4425	4419	108	0
1	K	4356	4425	4419	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	694	393	392	38	0
2	M	694	393	393	37	0
3	F	679	373	373	39	0
3	N	679	373	373	41	0
4	G	511	285	277	23	0
4	O	511	285	277	24	0
5	H	493	274	271	19	0
5	P	493	274	271	20	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	22182	20350	20303	560	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 13.

All (560) 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:K:153:ARG:NE	4:O:-1:DT:O3'	2.12	0.83
1:C:153:ARG:NE	4:G:-1:DT:O3'	2.12	0.82
1:I:58:LYS:NZ	1:I:79:ASP:OD2	2.15	0.80
1:A:334:ARG:NH2	3:F:21:DT:O4	2.15	0.79
1:I:334:ARG:NH2	3:N:21:DT:O4	2.15	0.79
1:A:58:LYS:NZ	1:A:79:ASP:OD2	2.15	0.79
1:I:336:ARG:NH2	1:I:338:ASN:OD1	2.16	0.78
1:A:336:ARG:NH2	1:A:338:ASN:OD1	2.16	0.77
1:C:257:ARG:O	1:C:268:ARG:NH1	2.19	0.76
1:K:257:ARG:O	1:K:268:ARG:NH1	2.19	0.76
1:A:56:GLU:OE1	1:A:85:TYR:OH	2.08	0.71
1:K:243:LEU:O	1:K:293:GLN:NE2	2.21	0.71
1:C:243:LEU:O	1:C:293:GLN:NE2	2.21	0.70
1:I:56:GLU:OE1	1:I:85:TYR:OH	2.08	0.70
1:I:22:SER:OG	1:I:23:ARG:N	2.22	0.69
2:M:-23:DG:H2'	2:M:-22:DT:H71	1.74	0.69
2:E:-23:DG:H2'	2:E:-22:DT:H71	1.74	0.69
2:E:-24:DA:H2''	2:E:-23:DG:O4'	1.93	0.68
1:A:22:SER:OG	1:A:23:ARG:N	2.22	0.68
2:M:-24:DA:H2''	2:M:-23:DG:O4'	1.93	0.68
1:C:502:ARG:O	1:C:531:ARG:NE	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:LEU:HD12	4:G:-13:DA:C2	2.30	0.66
1:K:303:LEU:HD12	4:O:-13:DA:C2	2.30	0.66
1:K:502:ARG:O	1:K:531:ARG:NE	2.28	0.66
3:F:19:DC:H2'	3:F:20:DT:H71	1.79	0.65
1:C:135:GLN:NE2	1:K:135:GLN:NE2	2.45	0.65
2:E:-14:DT:C2'	2:E:-13:DT:H72	2.27	0.65
2:M:-14:DT:C2'	2:M:-13:DT:H72	2.27	0.64
3:N:19:DC:H2'	3:N:20:DT:H71	1.79	0.63
1:A:429:ASP:O	1:A:433:SER:OG	2.17	0.63
1:C:535:ILE:HG22	1:C:536:PHE:HD1	1.65	0.62
1:K:535:ILE:HG22	1:K:536:PHE:HD1	1.65	0.62
2:E:-3:DC:H2'	2:E:-2:DT:C5	2.34	0.62
1:K:477:VAL:HG13	1:K:535:ILE:HG23	1.81	0.62
1:C:477:VAL:HG13	1:C:535:ILE:HG23	1.81	0.61
2:M:-3:DC:H2'	2:M:-2:DT:C5	2.34	0.61
1:I:429:ASP:O	1:I:433:SER:OG	2.17	0.61
1:A:403:MET:HE2	1:A:403:MET:O	2.00	0.61
1:I:23:ARG:HG2	1:I:24:GLN:N	2.16	0.60
3:N:11:DT:H2'	3:N:12:DT:H71	1.84	0.60
3:F:11:DT:H2'	3:F:12:DT:H71	1.84	0.60
1:I:403:MET:HE2	1:I:403:MET:O	2.00	0.60
1:A:23:ARG:HG2	1:A:24:GLN:N	2.16	0.60
5:P:5:DT:H2''	5:P:6:DG:C8	2.37	0.59
1:A:16:LEU:O	1:A:88:ILE:HD12	2.02	0.59
5:H:5:DT:H2''	5:H:6:DG:C8	2.37	0.59
5:H:6:DG:H2'	5:H:7:DT:H71	1.84	0.59
1:I:21:ARG:HE	1:I:25:ASP:HB3	1.67	0.59
1:I:265:ARG:NH1	3:N:6:DG:N7	2.50	0.59
1:A:265:ARG:NH1	3:F:6:DG:N7	2.50	0.59
1:A:21:ARG:HE	1:A:25:ASP:HB3	1.68	0.59
5:P:6:DG:H2'	5:P:7:DT:H71	1.83	0.59
1:C:255:LYS:O	1:C:268:ARG:NE	2.35	0.59
1:K:255:LYS:O	1:K:268:ARG:NE	2.35	0.59
2:M:-26:DG:C2'	2:M:-25:DT:H71	2.33	0.59
2:M:-26:DG:H2''	2:M:-25:DT:H71	1.85	0.58
1:C:306:LYS:NZ	4:G:-11:DC:O3'	2.36	0.58
1:K:306:LYS:NZ	4:O:-11:DC:O3'	2.36	0.58
1:K:135:GLN:HA	1:K:138:PHE:CE2	2.38	0.58
1:C:135:GLN:HA	1:C:138:PHE:CE2	2.38	0.58
1:A:247:VAL:O	1:A:280:HIS:NE2	2.37	0.58
2:E:-26:DG:C2'	2:E:-25:DT:H71	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:LEU:O	1:I:88:ILE:HD12	2.02	0.58
1:I:247:VAL:O	1:I:280:HIS:NE2	2.37	0.58
3:N:16:DA:H2'	3:N:17:DT:C6	2.39	0.57
1:A:118:ILE:N	1:A:125:TYR:O	2.32	0.57
2:E:-26:DG:H2''	2:E:-25:DT:H71	1.85	0.57
3:F:16:DA:H2'	3:F:17:DT:C6	2.39	0.57
1:C:320:CYS:O	1:C:324:GLY:N	2.35	0.57
1:I:20:ARG:NH1	1:I:65:GLU:OE2	2.32	0.56
1:A:48:LEU:CD1	1:A:57:LEU:HD21	2.36	0.56
1:A:255:LYS:N	3:F:6:DG:OP1	2.38	0.56
1:C:213:TYR:HB2	1:C:236:GLN:HB2	1.87	0.56
1:I:255:LYS:N	3:N:6:DG:OP1	2.38	0.56
1:C:135:GLN:HE21	1:K:135:GLN:NE2	2.04	0.56
3:F:5:DT:H2'	3:F:6:DG:C8	2.41	0.56
1:A:477:VAL:HG21	1:A:535:ILE:HG23	1.88	0.56
1:A:20:ARG:NH1	1:A:65:GLU:OE2	2.31	0.56
2:E:-14:DT:H2'	2:E:-13:DT:H72	1.88	0.56
1:I:516:ARG:NH1	3:N:25:DA:O4'	2.39	0.56
1:K:213:TYR:HB2	1:K:236:GLN:HB2	1.87	0.56
1:C:135:GLN:NE2	1:K:135:GLN:HE21	2.03	0.56
1:C:393:LEU:O	1:C:397:GLU:HG3	2.06	0.55
2:M:-15:DC:H2'	2:M:-14:DT:H72	1.88	0.55
1:C:303:LEU:HD12	4:G:-13:DA:H2	1.70	0.55
1:I:477:VAL:HG21	1:I:535:ILE:HG23	1.88	0.55
1:A:516:ARG:NH1	3:F:25:DA:O4'	2.39	0.55
1:K:393:LEU:O	1:K:397:GLU:HG3	2.06	0.55
3:N:5:DT:H2'	3:N:6:DG:C8	2.41	0.55
1:I:48:LEU:CD1	1:I:57:LEU:HD21	2.36	0.55
2:M:-14:DT:H2'	2:M:-13:DT:H72	1.88	0.55
1:A:23:ARG:HD2	3:F:2:DA:N9	2.22	0.55
3:F:16:DA:H3'	3:F:17:DT:H71	1.89	0.55
1:K:165:GLY:HA3	1:K:279:ALA:HB1	1.89	0.54
1:I:168:ILE:HG23	2:M:-3:DC:H4'	1.88	0.54
1:K:516:ARG:CZ	4:O:-20:DC:H1'	2.37	0.54
3:N:16:DA:H3'	3:N:17:DT:H71	1.89	0.54
1:A:168:ILE:HG23	2:E:-3:DC:H4'	1.88	0.54
1:C:516:ARG:CZ	4:G:-20:DC:H1'	2.37	0.54
1:C:165:GLY:HA3	1:C:279:ALA:HB1	1.89	0.54
1:C:382:ASP:OD1	1:C:383:SER:N	2.41	0.54
1:I:248:TYR:O	1:I:283:ILE:N	2.36	0.54
1:I:373:TYR:HD2	1:I:528:PRO:HG2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:403:MET:HG3	1:I:406:LYS:HB2	1.89	0.54
1:K:320:CYS:O	1:K:324:GLY:N	2.35	0.54
2:E:-15:DC:H2'	2:E:-14:DT:H72	1.88	0.54
2:E:-3:DC:H2'	2:E:-2:DT:C6	2.42	0.54
2:M:-3:DC:H2'	2:M:-2:DT:C6	2.42	0.54
1:I:23:ARG:HD2	3:N:2:DA:N9	2.23	0.53
1:K:303:LEU:HD12	4:O:-13:DA:H2	1.70	0.53
1:A:403:MET:HG3	1:A:406:LYS:HB2	1.89	0.53
4:O:-24:DA:H2''	4:O:-23:DT:H71	1.90	0.53
1:A:225:ILE:O	1:A:234:TRP:NE1	2.42	0.53
1:A:373:TYR:HD2	1:A:528:PRO:HG2	1.73	0.53
2:E:-11:DA:H2'	2:E:-10:DT:H72	1.91	0.53
1:A:23:ARG:HB2	3:F:2:DA:C8	2.44	0.53
3:F:15:DG:H2''	3:F:16:DA:C8	2.44	0.53
2:M:-15:DC:H2'	2:M:-14:DT:C7	2.39	0.53
1:A:117:ILE:HD12	1:A:117:ILE:H	1.74	0.53
5:H:15:DT:H2'	5:H:16:DT:H71	1.91	0.53
2:E:-15:DC:H2'	2:E:-14:DT:C7	2.39	0.53
5:P:15:DT:H2'	5:P:16:DT:H71	1.91	0.53
1:K:535:ILE:HG22	1:K:536:PHE:CD1	2.43	0.52
1:K:115:ARG:NH1	1:K:126:ASP:OD2	2.41	0.52
1:I:202:PHE:O	1:I:295:LYS:NZ	2.40	0.52
4:G:-24:DA:H2''	4:G:-23:DT:H71	1.91	0.52
1:I:225:ILE:O	1:I:234:TRP:NE1	2.42	0.52
2:M:-11:DA:H2'	2:M:-10:DT:H72	1.91	0.52
1:C:115:ARG:NH1	1:C:126:ASP:OD2	2.41	0.52
1:K:202:PHE:O	1:K:295:LYS:NZ	2.36	0.52
1:C:247:VAL:HG13	1:C:280:HIS:CE1	2.45	0.52
5:H:16:DT:H2''	5:H:17:DA:C8	2.45	0.52
1:I:23:ARG:HB2	3:N:2:DA:C8	2.44	0.52
1:I:29:GLU:HG2	1:I:35:ASP:HA	1.92	0.52
3:N:15:DG:H2''	3:N:16:DA:C8	2.44	0.52
1:C:535:ILE:HG22	1:C:536:PHE:CD1	2.43	0.52
5:P:16:DT:H2''	5:P:17:DA:C8	2.45	0.52
1:A:29:GLU:HG2	1:A:35:ASP:HA	1.92	0.52
1:K:247:VAL:HG13	1:K:280:HIS:CE1	2.45	0.52
1:A:167:TRP:HB3	1:A:178:LEU:HD13	1.92	0.52
2:M:-28:DT:C2	3:N:29:DA:C2	2.98	0.52
1:C:101:TYR:HA	1:C:144:ARG:HH12	1.75	0.51
1:A:258:GLU:OE1	1:A:268:ARG:NH2	2.44	0.51
1:I:167:TRP:HB3	1:I:178:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:LEU:O	1:A:505:LEU:N	2.33	0.51
5:P:17:DA:H2''	5:P:18:DA:C8	2.46	0.51
1:C:215:ALA:N	4:G:-14:DT:OP2	2.28	0.51
2:E:-28:DT:C2	3:F:29:DA:C2	2.98	0.51
1:I:117:ILE:HD12	1:I:117:ILE:H	1.74	0.51
1:I:118:ILE:N	1:I:125:TYR:O	2.32	0.51
1:K:101:TYR:HA	1:K:144:ARG:HH12	1.75	0.51
1:C:167:TRP:HB3	1:C:178:LEU:HD13	1.93	0.51
1:I:228:PRO:HB2	3:N:8:DA:H5''	1.93	0.51
1:I:403:MET:HE2	1:I:403:MET:C	2.36	0.51
1:C:101:TYR:CA	1:C:144:ARG:HH12	2.24	0.51
1:K:417:GLU:HB2	1:K:455:LEU:HD21	1.93	0.51
1:A:23:ARG:HD2	3:F:2:DA:C8	2.46	0.50
1:A:403:MET:HE2	1:A:403:MET:C	2.36	0.50
1:A:432:GLU:OE2	1:C:444:ARG:NE	2.43	0.50
1:A:477:VAL:HG22	1:A:535:ILE:O	2.12	0.50
1:I:484:ILE:HG21	1:I:504:VAL:HG21	1.93	0.50
1:K:101:TYR:CA	1:K:144:ARG:HH12	2.25	0.50
3:N:20:DT:H4'	3:N:21:DT:OP1	2.12	0.50
1:A:105:GLY:HA2	1:C:101:TYR:HD2	1.77	0.50
3:F:20:DT:H4'	3:F:21:DT:OP1	2.12	0.50
5:H:9:DC:H2'	5:H:10:DT:C6	2.47	0.50
1:I:48:LEU:HD13	1:I:55:TYR:CD1	2.46	0.50
1:I:327:LEU:HB3	1:I:351:LEU:HG	1.93	0.50
1:A:120:THR:OG1	1:A:122:TYR:CD1	2.65	0.50
1:C:17:GLY:HA3	1:C:57:LEU:HD23	1.93	0.50
1:C:516:ARG:HH12	5:H:21:DA:H2	1.60	0.50
1:I:120:THR:OG1	1:I:122:TYR:CD1	2.65	0.50
5:H:17:DA:H2''	5:H:18:DA:C8	2.46	0.50
1:I:432:GLU:OE2	1:K:444:ARG:NE	2.43	0.50
1:I:477:VAL:HG22	1:I:535:ILE:O	2.12	0.50
1:K:250:GLY:O	1:K:279:ALA:N	2.45	0.50
1:K:516:ARG:HH12	5:P:21:DA:H2	1.60	0.50
1:A:48:LEU:HD13	1:A:55:TYR:CD1	2.46	0.50
1:A:327:LEU:HB3	1:A:351:LEU:HG	1.93	0.50
1:C:469:GLN:HB2	1:C:536:PHE:CD2	2.47	0.50
1:C:327:LEU:HB3	1:C:351:LEU:HG	1.94	0.50
1:K:469:GLN:HB2	1:K:536:PHE:CD2	2.47	0.50
1:I:501:LEU:O	1:I:505:LEU:N	2.32	0.50
1:C:161:TYR:O	1:C:164:GLN:O	2.29	0.50
1:I:258:GLU:OE1	1:I:268:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PRO:HB2	3:F:8:DA:H5''	1.93	0.49
2:E:-30:DT:C2'	2:E:-29:DT:H71	2.42	0.49
1:I:23:ARG:HD2	3:N:2:DA:C8	2.47	0.49
1:I:153:ARG:HE	2:M:-1:DT:H4'	1.77	0.49
1:K:161:TYR:O	1:K:164:GLN:O	2.29	0.49
1:K:167:TRP:HB3	1:K:178:LEU:HD13	1.93	0.49
1:K:382:ASP:OD1	1:K:383:SER:N	2.41	0.49
1:K:331:GLU:O	5:P:15:DT:H72	2.11	0.49
1:A:65:GLU:HG2	3:F:3:DG:OP2	2.12	0.49
1:A:229:SER:HB2	3:F:9:DT:H5'	1.94	0.49
1:C:250:GLY:O	1:C:279:ALA:N	2.45	0.49
1:I:229:SER:HB2	3:N:9:DT:H5'	1.94	0.49
1:K:484:ILE:HG21	1:K:504:VAL:HG21	1.94	0.49
1:A:302:LEU:HD23	2:E:-13:DT:OP1	2.12	0.49
1:A:511:ASN:O	1:A:525:GLU:N	2.39	0.49
1:C:331:GLU:O	5:H:15:DT:H72	2.11	0.49
1:I:302:LEU:HD23	2:M:-13:DT:OP1	2.12	0.49
1:K:17:GLY:HA3	1:K:57:LEU:HD23	1.93	0.49
1:A:484:ILE:HG21	1:A:504:VAL:HG21	1.93	0.49
1:K:327:LEU:HB3	1:K:351:LEU:HG	1.94	0.49
5:P:9:DC:H2'	5:P:10:DT:C6	2.47	0.49
1:C:417:GLU:HB2	1:C:455:LEU:HD21	1.93	0.49
1:I:105:GLY:HA2	1:K:101:TYR:HD2	1.77	0.49
2:M:-9:DA:C2	3:N:10:DA:C2	3.01	0.49
1:A:248:TYR:O	1:A:283:ILE:N	2.35	0.49
1:C:302:LEU:H	4:G:-13:DA:C1'	2.26	0.49
1:C:386:THR:HG23	1:C:472:ILE:HB	1.95	0.49
1:I:507:ASP:OD1	1:I:508:VAL:N	2.46	0.49
1:I:65:GLU:HG2	3:N:3:DG:OP2	2.13	0.48
1:K:309:PHE:CG	5:P:14:DA:H5'	2.48	0.48
1:K:302:LEU:H	4:O:-13:DA:C1'	2.26	0.48
2:M:-30:DT:C2'	2:M:-29:DT:H71	2.42	0.48
1:A:432:GLU:HG2	1:C:444:ARG:NH1	2.29	0.48
2:M:-7:DA:C2	3:N:8:DA:C2	3.02	0.48
1:C:309:PHE:CG	5:H:14:DA:H5'	2.48	0.48
1:I:432:GLU:HG2	1:K:444:ARG:NH1	2.29	0.48
1:K:60:GLU:CD	1:K:72:VAL:HB	2.39	0.48
1:C:60:GLU:CD	1:C:72:VAL:HB	2.39	0.48
2:E:-7:DA:C2	3:F:8:DA:C2	3.02	0.48
2:E:-12:DA:C6	2:E:-11:DA:C6	3.02	0.48
1:I:310:GLU:O	3:N:17:DT:H5''	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:ILE:HG21	1:C:504:VAL:HG21	1.94	0.48
2:E:-9:DA:C2	3:F:10:DA:C2	3.01	0.48
3:F:19:DC:H2'	3:F:20:DT:C7	2.44	0.48
3:N:19:DC:H2'	3:N:20:DT:C7	2.44	0.48
1:K:320:CYS:HB2	1:K:327:LEU:HD21	1.96	0.47
1:C:203:LEU:HD21	1:C:292:SER:N	2.29	0.47
1:I:346:TYR:OH	2:M:-25:DT:OP2	2.26	0.47
1:C:268:ARG:HH12	5:H:5:DT:H5''	1.79	0.47
1:I:320:CYS:O	1:I:324:GLY:N	2.45	0.47
1:K:386:THR:HG23	1:K:472:ILE:HB	1.95	0.47
1:A:487:GLN:O	1:A:491:GLU:N	2.42	0.47
1:I:203:LEU:HD21	1:I:292:SER:N	2.29	0.47
1:K:6:ILE:O	1:K:9:SER:OG	2.31	0.47
1:K:111:LEU:HD23	1:K:116:LEU:HB2	1.96	0.47
1:K:175:GLY:O	1:K:283:ILE:HD11	2.15	0.47
1:A:310:GLU:O	3:F:17:DT:H5''	2.14	0.47
1:C:175:GLY:O	1:C:283:ILE:HD11	2.15	0.47
4:G:-7:DA:C2	5:H:8:DA:C2	3.02	0.47
2:M:-12:DA:C6	2:M:-11:DA:C6	3.02	0.47
2:M:-20:DA:H2''	2:M:-19:DG:O4'	2.15	0.47
4:O:-7:DA:C2	5:P:8:DA:C2	3.02	0.47
1:A:507:ASP:OD1	1:A:508:VAL:N	2.46	0.47
1:C:111:LEU:HD23	1:C:116:LEU:HB2	1.96	0.47
2:E:-20:DA:H2''	2:E:-19:DG:O4'	2.15	0.47
3:F:18:DA:H2'	3:F:19:DC:O4'	2.15	0.47
1:I:213:TYR:CB	1:I:236:GLN:HB2	2.45	0.47
1:K:203:LEU:HD21	1:K:292:SER:N	2.29	0.47
4:G:-25:DC:C2	4:G:-24:DA:C8	3.03	0.47
1:I:147:PHE:CZ	3:N:2:DA:H4'	2.50	0.47
4:O:-25:DC:C2	4:O:-24:DA:C8	3.03	0.47
1:A:203:LEU:HD21	1:A:292:SER:N	2.29	0.47
1:A:329:LYS:NZ	3:F:18:DA:OP2	2.41	0.47
1:C:320:CYS:HB2	1:C:327:LEU:HD21	1.96	0.47
1:A:18:TYR:O	1:A:90:VAL:HG12	2.15	0.47
1:A:213:TYR:CB	1:A:236:GLN:HB2	2.45	0.47
1:K:215:ALA:N	4:O:-14:DT:OP2	2.28	0.47
1:A:346:TYR:OH	2:E:-25:DT:OP2	2.26	0.46
1:C:176:TYR:CE2	1:C:283:ILE:HD12	2.51	0.46
1:C:202:PHE:CZ	1:C:296:ILE:HG13	2.50	0.46
1:K:268:ARG:HH12	5:P:5:DT:H5''	1.79	0.46
4:G:-19:DA:H2'	4:G:-18:DT:H71	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:-24:DA:C2'	4:O:-23:DT:H71	2.45	0.46
4:G:-24:DA:C2'	4:G:-23:DT:H71	2.46	0.46
1:I:295:LYS:O	1:I:299:LYS:N	2.49	0.46
1:I:329:LYS:NZ	3:N:18:DA:OP2	2.41	0.46
1:I:393:LEU:HD13	1:I:536:PHE:CZ	2.50	0.46
1:A:60:GLU:HA	1:A:72:VAL:HB	1.97	0.46
1:A:147:PHE:CZ	3:F:2:DA:H4'	2.50	0.46
5:H:22:DC:H2''	5:H:23:DA:C8	2.51	0.46
1:I:511:ASN:O	1:I:525:GLU:N	2.39	0.46
1:K:202:PHE:CZ	1:K:296:ILE:HG13	2.50	0.46
1:I:58:LYS:NZ	1:I:75:GLU:OE2	2.42	0.46
1:I:247:VAL:HG13	1:I:280:HIS:CE1	2.51	0.46
1:K:302:LEU:HD22	4:O:-14:DT:O2	2.16	0.46
1:A:295:LYS:O	1:A:299:LYS:N	2.49	0.46
1:A:393:LEU:HD13	1:A:536:PHE:CZ	2.50	0.46
1:C:44:MET:HB3	1:C:57:LEU:HD21	1.98	0.46
3:N:22:DA:C4	3:N:23:DC:C6	3.04	0.46
1:C:92:GLU:OE1	1:C:95:ARG:NH2	2.46	0.46
1:K:176:TYR:CE2	1:K:283:ILE:HD12	2.50	0.46
1:A:417:GLU:HB2	1:A:455:LEU:HD21	1.98	0.46
2:E:-11:DA:C2'	2:E:-10:DT:H72	2.46	0.46
1:I:60:GLU:HA	1:I:72:VAL:HB	1.98	0.46
1:I:314:LEU:CG	1:I:363:TYR:HE1	2.29	0.46
3:N:27:DA:H2''	3:N:28:DA:C8	2.51	0.46
1:A:101:TYR:CZ	1:C:101:TYR:HE1	2.34	0.45
1:A:246:GLU:O	1:A:249:ILE:HG12	2.16	0.45
1:A:247:VAL:HG13	1:A:280:HIS:CE1	2.51	0.45
3:F:22:DA:C4	3:F:23:DC:C6	3.04	0.45
3:F:27:DA:H2''	3:F:28:DA:C8	2.51	0.45
1:K:92:GLU:OE1	1:K:95:ARG:NH2	2.46	0.45
1:A:118:ILE:O	1:A:125:TYR:N	2.50	0.45
1:I:101:TYR:CZ	1:K:101:TYR:HE1	2.34	0.45
3:N:18:DA:H2'	3:N:19:DC:O4'	2.15	0.45
1:I:18:TYR:O	1:I:90:VAL:HG12	2.15	0.45
1:I:37:LEU:HD23	1:I:37:LEU:O	2.17	0.45
1:I:313:GLU:CD	1:I:313:GLU:H	2.25	0.45
1:K:319:THR:HA	1:K:326:PRO:HA	1.99	0.45
5:P:22:DC:H2''	5:P:23:DA:C8	2.51	0.45
1:A:115:ARG:NH1	1:C:258:GLU:OE2	2.45	0.45
1:C:48:LEU:HB3	1:C:55:TYR:CD1	2.52	0.45
1:I:19:LEU:HD12	1:I:59:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:417:GLU:HB2	1:I:455:LEU:HD21	1.98	0.45
1:K:44:MET:HB3	1:K:57:LEU:HD21	1.98	0.45
4:O:-19:DA:H2'	4:O:-18:DT:H71	1.97	0.45
1:A:21:ARG:HH21	1:A:21:ARG:HB2	1.81	0.45
1:A:129:ASN:OD1	1:A:131:VAL:HG22	2.16	0.45
1:I:118:ILE:O	1:I:125:TYR:N	2.49	0.45
1:I:129:ASN:OD1	1:I:131:VAL:HG22	2.16	0.45
1:A:87:ALA:HA	1:A:117:ILE:O	2.16	0.45
1:C:504:VAL:O	1:C:531:ARG:N	2.34	0.45
1:I:246:GLU:O	1:I:249:ILE:HG12	2.16	0.45
1:K:179:ASN:O	1:K:183:SER:N	2.50	0.45
1:K:302:LEU:HD13	4:O:-14:DT:O2	2.17	0.45
2:M:-11:DA:C2'	2:M:-10:DT:H72	2.46	0.45
1:A:427:ILE:HD12	1:A:448:LEU:HD11	1.99	0.45
3:F:17:DT:H2''	3:F:18:DA:C8	2.52	0.45
3:N:11:DT:H2'	3:N:12:DT:C6	2.52	0.45
1:C:202:PHE:O	1:C:295:LYS:NZ	2.36	0.44
1:C:265:ARG:NH1	5:H:6:DG:N7	2.63	0.44
1:C:302:LEU:HD13	4:G:-14:DT:O2	2.17	0.44
2:E:-28:DT:H2'	2:E:-27:DT:H71	1.99	0.44
1:I:225:ILE:HG22	1:I:234:TRP:HZ2	1.83	0.44
1:A:313:GLU:CD	1:A:313:GLU:H	2.25	0.44
1:C:179:ASN:O	1:C:183:SER:N	2.50	0.44
1:C:302:LEU:HD22	4:G:-14:DT:O2	2.16	0.44
1:I:21:ARG:HH21	1:I:21:ARG:HB2	1.81	0.44
1:I:360:TYR:HB3	2:M:-22:DT:OP2	2.18	0.44
1:I:427:ILE:HD12	1:I:448:LEU:HD11	1.99	0.44
3:N:18:DA:C2'	3:N:19:DC:O4'	2.66	0.44
1:A:37:LEU:O	1:A:37:LEU:HD23	2.17	0.44
1:A:252:VAL:HG23	1:A:279:ALA:HB3	1.98	0.44
1:I:87:ALA:HA	1:I:117:ILE:O	2.17	0.44
1:A:314:LEU:CG	1:A:363:TYR:HE1	2.29	0.44
1:I:252:VAL:HG23	1:I:279:ALA:HB3	1.98	0.44
3:N:17:DT:H2''	3:N:18:DA:C8	2.52	0.44
1:A:153:ARG:HE	2:E:-1:DT:H4'	1.82	0.44
1:A:401:SER:OG	1:A:403:MET:SD	2.72	0.44
1:C:389:ILE:HD11	1:C:477:VAL:HG11	2.00	0.44
4:G:-19:DA:C2	5:H:20:DG:C2	3.06	0.44
1:I:111:LEU:HD22	1:I:118:ILE:HD11	2.00	0.44
1:K:321:SER:HA	1:K:509:ILE:HG23	2.00	0.44
2:E:-27:DT:O2	3:F:28:DA:C2	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:11:DT:H2'	3:F:12:DT:C6	2.52	0.44
1:K:123:LYS:HB3	1:K:125:TYR:HE1	1.82	0.44
1:K:389:ILE:HD11	1:K:477:VAL:HG11	2.00	0.44
2:M:-28:DT:H2'	2:M:-27:DT:H71	1.99	0.44
1:C:123:LYS:HB3	1:C:125:TYR:HE1	1.82	0.44
1:C:175:GLY:N	1:C:191:GLU:OE1	2.50	0.44
4:G:-25:DC:C2	4:G:-24:DA:N7	2.86	0.44
4:O:-17:DT:H2'	4:O:-16:DA:C8	2.52	0.44
1:A:175:GLY:HA2	1:A:191:GLU:CB	2.48	0.44
1:A:320:CYS:O	1:A:324:GLY:N	2.45	0.44
1:A:420:LEU:HD21	1:A:451:GLU:HB3	2.00	0.44
2:E:-21:DA:C2	3:F:22:DA:C2	3.06	0.44
1:I:254:TYR:CG	1:I:255:LYS:N	2.86	0.44
3:N:3:DG:OP1	3:N:3:DG:H4'	2.18	0.44
4:G:-24:DA:N1	5:H:25:DG:C6	2.86	0.43
4:G:-17:DT:H2'	4:G:-16:DA:C8	2.52	0.43
1:K:48:LEU:HB3	1:K:55:TYR:CD1	2.52	0.43
2:M:-27:DT:O2	3:N:28:DA:C2	2.71	0.43
4:O:-19:DA:C2	5:P:20:DG:C2	3.06	0.43
1:C:60:GLU:OE1	1:C:70:ARG:HB3	2.18	0.43
1:I:122:TYR:HD1	1:I:123:LYS:N	2.16	0.43
1:I:487:GLN:O	1:I:491:GLU:N	2.42	0.43
4:O:-24:DA:N1	5:P:25:DG:C6	2.86	0.43
1:A:111:LEU:HD22	1:A:118:ILE:HD11	2.00	0.43
2:M:-21:DA:C2	3:N:22:DA:C2	3.06	0.43
4:O:-25:DC:C2	4:O:-24:DA:N7	2.86	0.43
1:C:6:ILE:O	1:C:9:SER:OG	2.31	0.43
1:C:319:THR:HA	1:C:326:PRO:HA	1.99	0.43
3:F:3:DG:H4'	3:F:3:DG:OP1	2.18	0.43
1:K:537:ASP:OD1	1:K:537:ASP:C	2.62	0.43
1:C:321:SER:HA	1:C:509:ILE:HG23	2.00	0.43
1:K:265:ARG:NH1	5:P:6:DG:N7	2.63	0.43
3:N:20:DT:H2'	3:N:21:DT:C6	2.53	0.43
3:F:20:DT:H2'	3:F:21:DT:C6	2.53	0.43
1:K:60:GLU:OE1	1:K:70:ARG:HB3	2.18	0.43
1:A:19:LEU:HD12	1:A:59:MET:HG3	1.99	0.43
1:C:389:ILE:HG21	1:C:536:PHE:CE1	2.54	0.43
1:I:70:ARG:HB3	1:I:73:PHE:CB	2.48	0.43
1:I:146:GLU:O	1:I:150:THR:HG23	2.18	0.43
2:M:-26:DG:H2'	2:M:-25:DT:H71	2.00	0.43
2:M:-19:DG:H2'	2:M:-18:DT:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ILE:HG22	1:A:234:TRP:HZ2	1.83	0.43
1:A:360:TYR:HB3	2:E:-22:DT:OP2	2.18	0.43
1:C:48:LEU:HB3	1:C:55:TYR:CG	2.54	0.43
1:C:516:ARG:CZ	1:C:518:GLY:O	2.67	0.43
3:F:18:DA:C2'	3:F:19:DC:O4'	2.66	0.43
1:K:175:GLY:N	1:K:191:GLU:OE1	2.50	0.43
4:O:-22:DG:N1	5:P:23:DA:C2	2.87	0.43
1:A:122:TYR:HD1	1:A:123:LYS:N	2.16	0.43
1:A:254:TYR:CG	1:A:255:LYS:N	2.86	0.43
1:C:381:ASN:ND2	1:C:382:ASP:OD1	2.52	0.43
2:E:-19:DG:H2'	2:E:-18:DT:C6	2.54	0.43
1:I:213:TYR:HB2	1:I:236:GLN:HB2	2.01	0.43
1:K:516:ARG:CZ	1:K:518:GLY:O	2.67	0.43
2:M:-12:DA:C2	3:N:13:DA:C2	3.07	0.43
1:C:413:LEU:HD21	1:C:458:ALA:HB1	2.01	0.43
1:C:436:TYR:OH	1:C:444:ARG:NH2	2.49	0.43
2:E:-12:DA:C2	3:F:13:DA:C2	3.07	0.43
1:A:70:ARG:HB3	1:A:73:PHE:CB	2.49	0.42
1:C:13:THR:OG1	1:C:86:GLN:NE2	2.52	0.42
2:E:-3:DC:H2'	2:E:-2:DT:H72	2.01	0.42
4:G:-22:DG:N1	5:H:23:DA:C2	2.87	0.42
1:I:175:GLY:HA2	1:I:191:GLU:CB	2.48	0.42
3:N:10:DA:C2	3:N:11:DT:C2	3.07	0.42
1:C:16:LEU:HD13	1:C:58:LYS:HE3	2.01	0.42
1:K:13:THR:OG1	1:K:86:GLN:NE2	2.52	0.42
1:K:16:LEU:HD13	1:K:58:LYS:HE3	2.01	0.42
1:K:48:LEU:HB3	1:K:55:TYR:CG	2.54	0.42
1:K:389:ILE:HG21	1:K:536:PHE:CE1	2.54	0.42
5:P:17:DA:H2''	5:P:18:DA:H8	1.84	0.42
1:A:146:GLU:O	1:A:150:THR:HG23	2.18	0.42
1:C:537:ASP:OD1	1:C:537:ASP:C	2.62	0.42
1:I:154:MET:SD	2:M:-2:DT:H2''	2.59	0.42
1:K:385:LEU:HD23	1:K:478:ARG:HG3	2.01	0.42
1:K:404:LYS:C	1:K:406:LYS:H	2.28	0.42
1:C:530:LEU:CB	1:C:535:ILE:HD11	2.49	0.42
1:K:227:THR:HG21	1:K:233:ARG:O	2.19	0.42
1:K:334:ARG:NH1	4:O:-18:DT:O4	2.50	0.42
1:K:386:THR:OG1	1:K:472:ILE:HG21	2.19	0.42
1:K:466:GLN:CD	1:K:467:ASP:N	2.78	0.42
2:M:-3:DC:H2'	2:M:-2:DT:H72	2.01	0.42
1:A:176:TYR:CE2	1:A:283:ILE:HD12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:VAL:O	1:C:280:HIS:NE2	2.52	0.42
1:I:176:TYR:CE2	1:I:283:ILE:HD12	2.54	0.42
1:A:176:TYR:HB3	1:A:185:LEU:HB3	2.02	0.42
3:F:10:DA:C2	3:F:11:DT:C2	3.07	0.42
1:I:105:GLY:CA	1:K:101:TYR:HD2	2.33	0.42
1:K:302:LEU:HD23	1:K:303:LEU:HG	2.02	0.42
1:K:381:ASN:ND2	1:K:382:ASP:OD1	2.52	0.42
1:K:504:VAL:O	1:K:531:ARG:N	2.34	0.42
1:A:179:ASN:O	1:A:183:SER:N	2.52	0.42
1:C:385:LEU:HD23	1:C:478:ARG:HG3	2.02	0.42
1:C:466:GLN:CD	1:C:467:ASP:N	2.78	0.42
1:C:530:LEU:HB3	1:C:535:ILE:HD11	2.02	0.42
2:E:-26:DG:H2'	2:E:-25:DT:H71	2.00	0.42
1:I:420:LEU:HD21	1:I:451:GLU:HB3	2.00	0.42
1:K:247:VAL:O	1:K:280:HIS:NE2	2.52	0.42
1:I:179:ASN:O	1:I:183:SER:N	2.52	0.42
1:K:138:PHE:CD1	1:K:138:PHE:C	2.98	0.42
1:K:413:LEU:HD21	1:K:458:ALA:HB1	2.01	0.42
1:K:464:GLY:HA2	1:K:468:THR:OG1	2.20	0.42
1:C:59:MET:SD	1:C:59:MET:N	2.93	0.42
1:K:131:VAL:O	1:K:135:GLN:HG2	2.20	0.42
1:A:154:MET:SD	2:E:-2:DT:H2''	2.59	0.42
1:C:334:ARG:NH2	4:G:-18:DT:O4	2.48	0.42
1:C:371:LEU:HD21	1:C:488:TYR:CE1	2.55	0.42
1:C:386:THR:OG1	1:C:472:ILE:HG21	2.19	0.42
1:I:176:TYR:HB3	1:I:185:LEU:HB3	2.02	0.42
1:I:403:MET:SD	1:I:403:MET:N	2.93	0.42
1:K:371:LEU:HD21	1:K:488:TYR:CE1	2.55	0.42
1:A:403:MET:SD	1:A:403:MET:N	2.93	0.41
1:C:227:THR:HG21	1:C:233:ARG:O	2.19	0.41
1:K:48:LEU:HD13	1:K:55:TYR:CD2	2.55	0.41
1:K:516:ARG:NH1	4:O:-21:DT:O2	2.54	0.41
1:A:25:ASP:HB3	1:A:36:THR:OG1	2.21	0.41
1:A:213:TYR:HB2	1:A:236:GLN:HB2	2.01	0.41
1:C:138:PHE:CD1	1:C:138:PHE:C	2.98	0.41
1:C:210:ASP:OD1	1:C:295:LYS:NZ	2.47	0.41
1:C:353:CYS:O	1:C:357:LYS:N	2.52	0.41
1:C:245:ASN:OD1	1:C:247:VAL:HG23	2.20	0.41
5:H:17:DA:H2''	5:H:18:DA:H8	1.84	0.41
1:K:115:ARG:HG3	1:K:128:ARG:CG	2.50	0.41
1:K:334:ARG:NH2	4:O:-18:DT:O4	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:HD13	1:A:119:ILE:HD11	2.02	0.41
1:C:48:LEU:HD13	1:C:55:TYR:CD2	2.55	0.41
1:C:247:VAL:HA	1:C:251:THR:O	2.20	0.41
1:C:389:ILE:HG21	1:C:536:PHE:HE1	1.85	0.41
1:C:404:LYS:C	1:C:406:LYS:H	2.28	0.41
1:C:516:ARG:NH1	4:G:-21:DT:O2	2.54	0.41
1:I:12:ILE:HD13	1:I:119:ILE:HD11	2.02	0.41
1:K:59:MET:SD	1:K:59:MET:N	2.93	0.41
1:K:257:ARG:HB3	1:K:265:ARG:CG	2.51	0.41
1:K:530:LEU:CB	1:K:535:ILE:HD11	2.49	0.41
2:M:-13:DT:H2''	2:M:-12:DA:C8	2.56	0.41
5:P:11:DG:C2	5:P:12:DA:C5	3.08	0.41
1:I:173:PRO:HG3	3:N:7:DT:H5''	2.02	0.41
1:I:513:THR:H	1:I:524:PHE:HA	1.86	0.41
1:K:247:VAL:HA	1:K:251:THR:O	2.21	0.41
1:A:105:GLY:CA	1:C:101:TYR:HD2	2.33	0.41
1:A:118:ILE:HB	1:A:125:TYR:HB2	2.03	0.41
1:C:115:ARG:HG3	1:C:128:ARG:CG	2.50	0.41
1:C:131:VAL:O	1:C:135:GLN:HG2	2.20	0.41
2:E:-16:DT:C2'	2:E:-15:DC:C6	3.04	0.41
2:E:-14:DT:H2''	2:E:-13:DT:C7	2.51	0.41
2:E:-13:DT:H2''	2:E:-12:DA:C8	2.56	0.41
1:I:118:ILE:HB	1:I:125:TYR:HB2	2.03	0.41
1:K:245:ASN:OD1	1:K:247:VAL:HG23	2.20	0.41
1:K:389:ILE:HG21	1:K:536:PHE:HE1	1.85	0.41
1:K:530:LEU:HB3	1:K:535:ILE:HD11	2.02	0.41
2:M:-14:DT:H2''	2:M:-13:DT:C7	2.51	0.41
2:M:-4:DG:H2''	2:M:-3:DC:H6	1.84	0.41
4:O:-22:DG:C2	5:P:23:DA:C2	3.09	0.41
1:A:201:ILE:O	1:A:205:GLY:N	2.54	0.41
5:H:11:DG:C2	5:H:12:DA:C5	3.08	0.41
1:A:366:VAL:HG22	1:A:524:PHE:CE2	2.56	0.41
1:C:257:ARG:HB3	1:C:265:ARG:CG	2.51	0.41
1:I:145:GLU:O	1:I:148:GLU:HG3	2.20	0.41
1:I:366:VAL:HG22	1:I:524:PHE:CE2	2.56	0.41
1:I:401:SER:OG	1:I:403:MET:SD	2.72	0.41
3:N:11:DT:C2'	3:N:12:DT:C6	3.04	0.41
1:A:16:LEU:HB2	1:A:85:TYR:CG	2.56	0.41
1:A:131:VAL:HG23	1:A:132:ASP:N	2.36	0.41
1:C:175:GLY:HA2	1:C:191:GLU:CB	2.50	0.41
1:C:176:TYR:CE2	1:C:247:VAL:HG12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:GLY:HA2	1:C:468:THR:OG1	2.20	0.41
2:E:-4:DG:H2''	2:E:-3:DC:H6	1.84	0.41
2:E:-3:DC:H2'	2:E:-2:DT:C7	2.51	0.41
1:I:25:ASP:HB3	1:I:36:THR:OG1	2.21	0.41
1:I:70:ARG:HB3	1:I:73:PHE:HB2	2.03	0.41
1:I:115:ARG:NH1	1:K:258:GLU:OE2	2.45	0.41
1:K:477:VAL:HG22	1:K:535:ILE:CG2	2.51	0.41
3:N:15:DG:H2''	3:N:16:DA:H8	1.84	0.41
1:I:174:TYR:O	1:I:248:TYR:CE1	2.74	0.41
1:I:201:ILE:O	1:I:205:GLY:N	2.54	0.41
1:K:176:TYR:CE2	1:K:247:VAL:HG12	2.56	0.41
1:K:463:ASN:O	1:K:466:GLN:HG3	2.21	0.41
2:M:-30:DT:H2'	2:M:-29:DT:H71	2.02	0.41
1:A:68:ASP:HA	1:A:74:LYS:HE3	2.03	0.40
1:A:173:PRO:HG3	3:F:7:DT:H5''	2.02	0.40
1:A:513:THR:H	1:A:524:PHE:HA	1.86	0.40
1:C:396:TYR:HB3	1:C:532:PHE:CE2	2.56	0.40
1:C:463:ASN:O	1:C:466:GLN:HG3	2.21	0.40
1:K:175:GLY:HA2	1:K:191:GLU:CB	2.50	0.40
3:N:17:DT:H2''	3:N:18:DA:H8	1.86	0.40
1:A:105:GLY:HA2	1:C:101:TYR:CD2	2.56	0.40
1:A:145:GLU:O	1:A:148:GLU:HG3	2.20	0.40
1:C:43:LEU:HD13	1:I:164:GLN:NE2	2.36	0.40
1:C:166:LYS:HA	1:C:183:SER:O	2.22	0.40
1:C:175:GLY:HA2	1:C:191:GLU:HB3	2.03	0.40
2:E:-32:DT:C6	2:E:-31:DT:H72	2.56	0.40
2:E:-30:DT:H2'	2:E:-29:DT:H71	2.02	0.40
5:H:15:DT:C2'	5:H:16:DT:H71	2.51	0.40
1:I:68:ASP:HA	1:I:74:LYS:HE3	2.03	0.40
1:I:422:ASN:ND2	1:K:12:ILE:O	2.54	0.40
2:M:-16:DT:C2'	2:M:-15:DC:C6	3.04	0.40
4:G:-22:DG:H2'	4:G:-21:DT:H71	2.03	0.40
1:I:518:GLY:HA2	3:N:25:DA:C2	2.56	0.40
1:K:175:GLY:HA2	1:K:191:GLU:HB3	2.02	0.40
1:K:353:CYS:O	1:K:357:LYS:N	2.52	0.40
4:O:-22:DG:H2'	4:O:-21:DT:H71	2.03	0.40
5:P:15:DT:C2'	5:P:16:DT:H71	2.51	0.40
1:A:70:ARG:HB3	1:A:73:PHE:HB2	2.03	0.40
3:F:11:DT:C2'	3:F:12:DT:C6	3.04	0.40
1:I:16:LEU:HB2	1:I:85:TYR:CG	2.56	0.40
1:K:392:MET:O	1:K:396:TYR:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:-3:DC:H2'	2:M:-2:DT:C7	2.51	0.40
1:A:174:TYR:O	1:A:248:TYR:CE1	2.74	0.40
1:C:334:ARG:NH1	4:G:-18:DT:O4	2.50	0.40
1:C:477:VAL:HG22	1:C:535:ILE:CG2	2.51	0.40
3:F:15:DG:H2''	3:F:16:DA:H8	1.85	0.40
1:K:472:ILE:HG23	1:K:474:SER:H	1.87	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%)	501 (94%)	32 (6%)	0	100	100
1	C	533/545 (98%)	501 (94%)	28 (5%)	4 (1%)	16	53
1	I	533/545 (98%)	501 (94%)	32 (6%)	0	100	100
1	K	533/545 (98%)	502 (94%)	27 (5%)	4 (1%)	16	53
All	All	2132/2180 (98%)	2005 (94%)	119 (6%)	8 (0%)	31	67

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	35	ASP
1	C	100	SER
1	K	35	ASP
1	K	100	SER
1	C	62	GLY
1	K	62	GLY
1	C	303	LEU
1	K	303	LEU

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	490/499 (98%)	478 (98%)	12 (2%)	43	63
1	C	490/499 (98%)	472 (96%)	18 (4%)	30	51
1	I	490/499 (98%)	478 (98%)	12 (2%)	43	63
1	K	490/499 (98%)	473 (96%)	17 (4%)	32	54
All	All	1960/1996 (98%)	1901 (97%)	59 (3%)	37	57

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	23	ARG
1	A	92	GLU
1	A	101	TYR
1	A	122	TYR
1	A	126	ASP
1	A	360	TYR
1	A	403	MET
1	A	407	LYS
1	A	433	SER
1	A	472	ILE
1	A	484	ILE
1	C	26	MET
1	C	34	GLU
1	C	168	ILE
1	C	199	PHE
1	C	262	ASP
1	C	288	GLN
1	C	302	LEU
1	C	304	PRO
1	C	306	LYS
1	C	362	ARG
1	C	380	LEU
1	C	381	ASN

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Mol	Chain	Res	Type
1	C	383	SER
1	C	384	THR
1	C	385	LEU
1	C	465	LEU
1	C	472	ILE
1	C	537	ASP
1	I	21	ARG
1	I	23	ARG
1	I	92	GLU
1	I	101	TYR
1	I	122	TYR
1	I	126	ASP
1	I	360	TYR
1	I	403	MET
1	I	407	LYS
1	I	433	SER
1	I	472	ILE
1	I	484	ILE
1	K	34	GLU
1	K	168	ILE
1	K	199	PHE
1	K	262	ASP
1	K	288	GLN
1	K	302	LEU
1	K	304	PRO
1	K	306	LYS
1	K	362	ARG
1	K	380	LEU
1	K	381	ASN
1	K	383	SER
1	K	384	THR
1	K	385	LEU
1	K	465	LEU
1	K	472	ILE
1	K	537	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	388	HIS
1	A	402	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	469	GLN
1	A	498	ASN
1	C	11	ASN
1	C	135	GLN
1	C	356	ASN
1	C	408	GLN
1	I	135	GLN
1	I	388	HIS
1	I	402	ASN
1	I	469	GLN
1	I	498	ASN
1	K	11	ASN
1	K	356	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

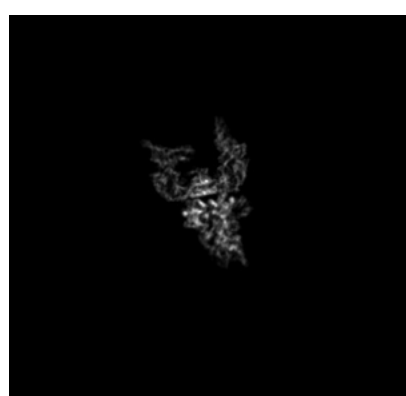
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47289. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

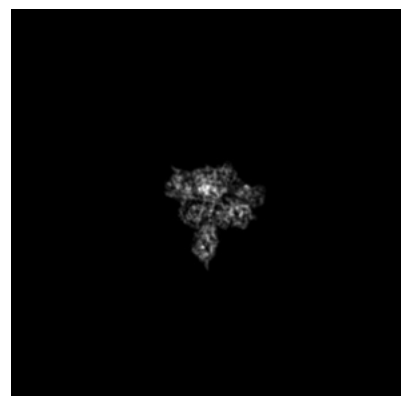
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 228



Y Index: 222

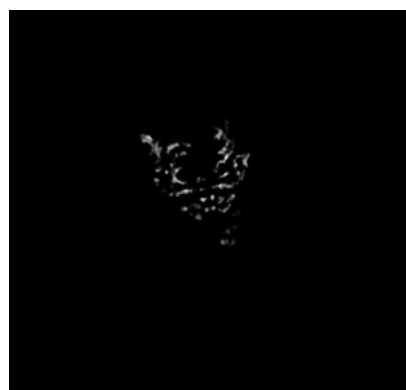


Z Index: 213

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: 223



Y Index: 239



Z Index: 230

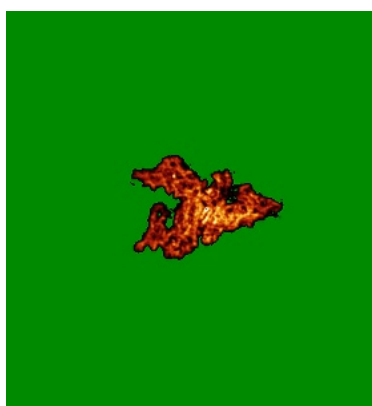
The images above show the largest variance slices of the map in three orthogonal directions.

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

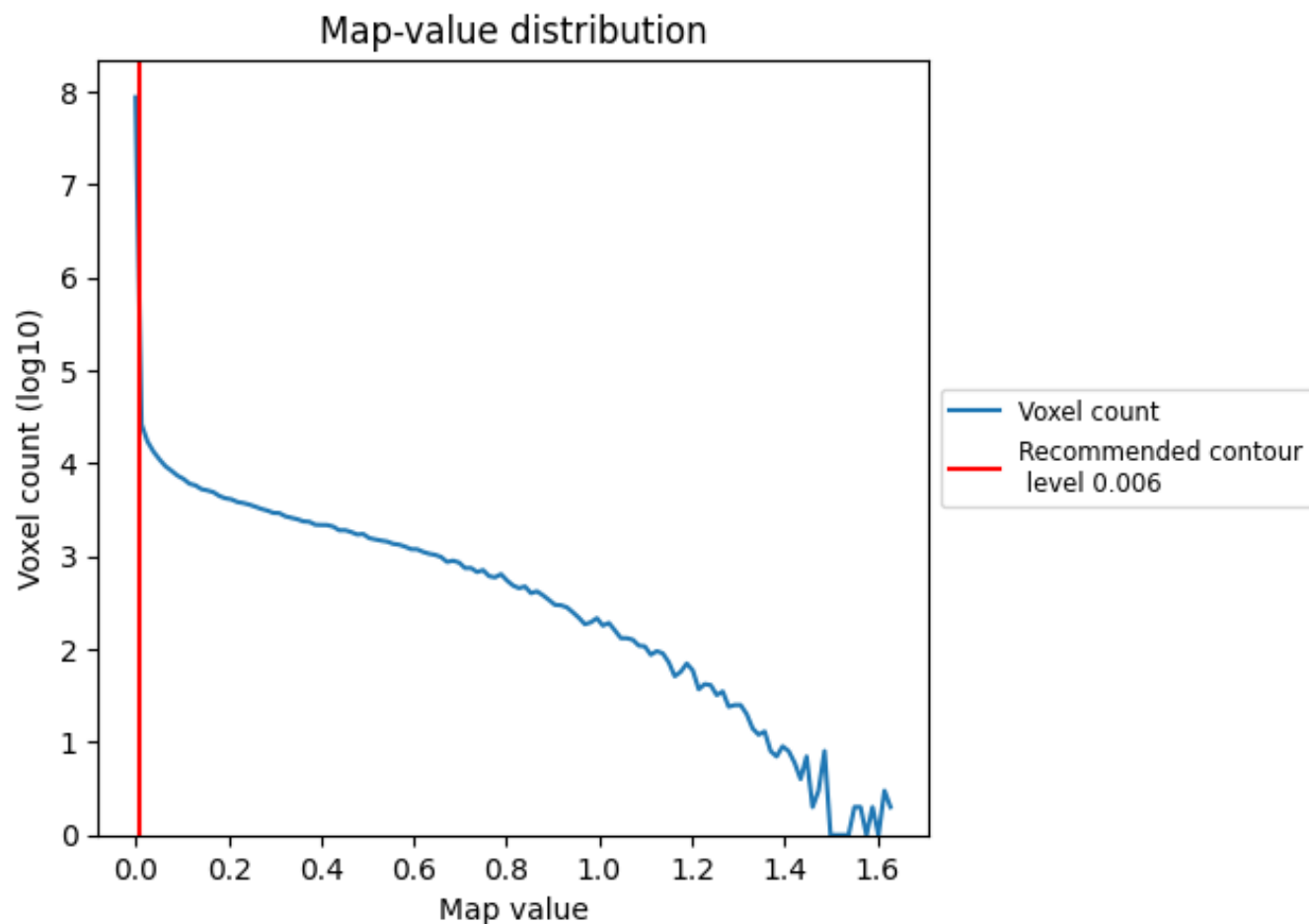
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

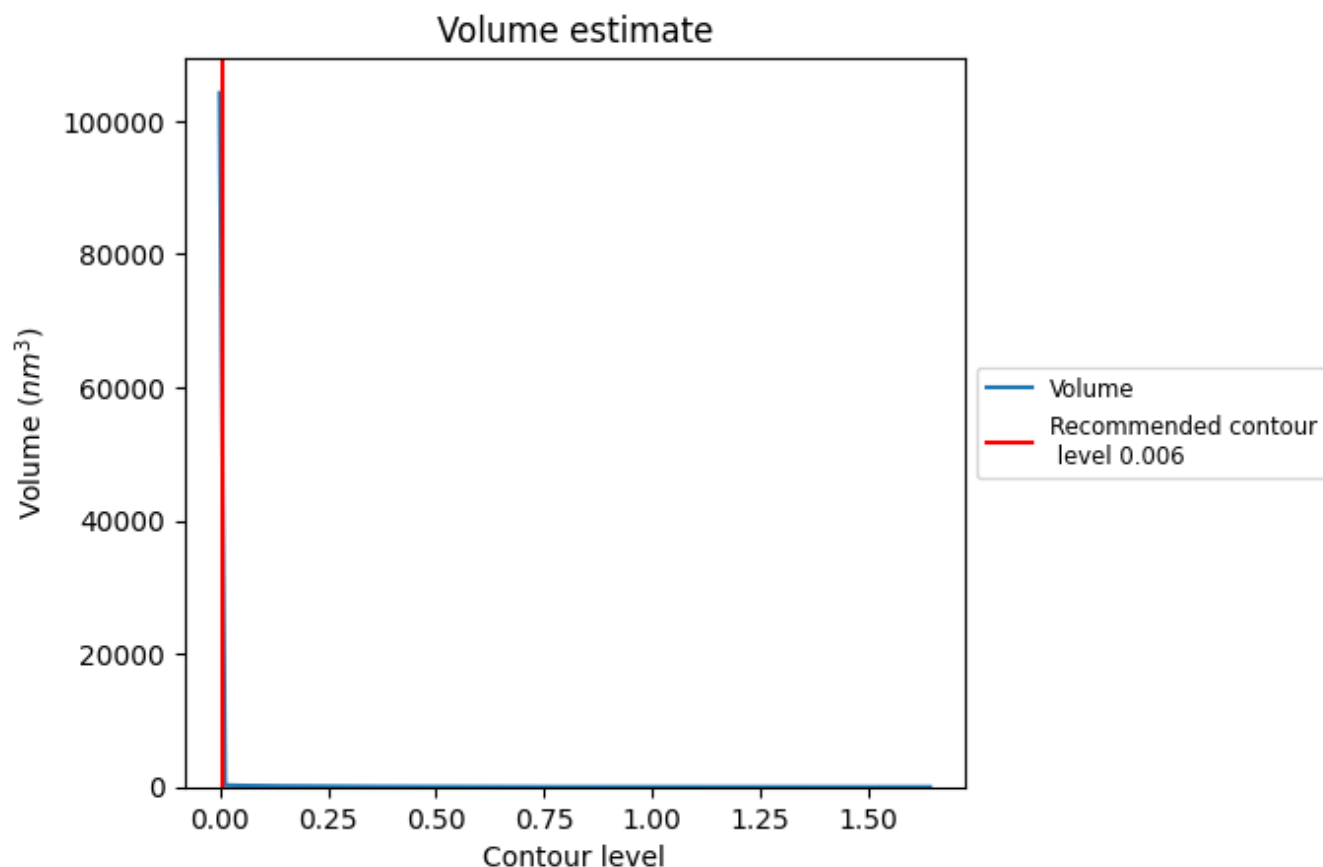
This section contains the results of statistical analysis of the map.

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 51913 nm³; this corresponds to an approximate mass of 46894 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.

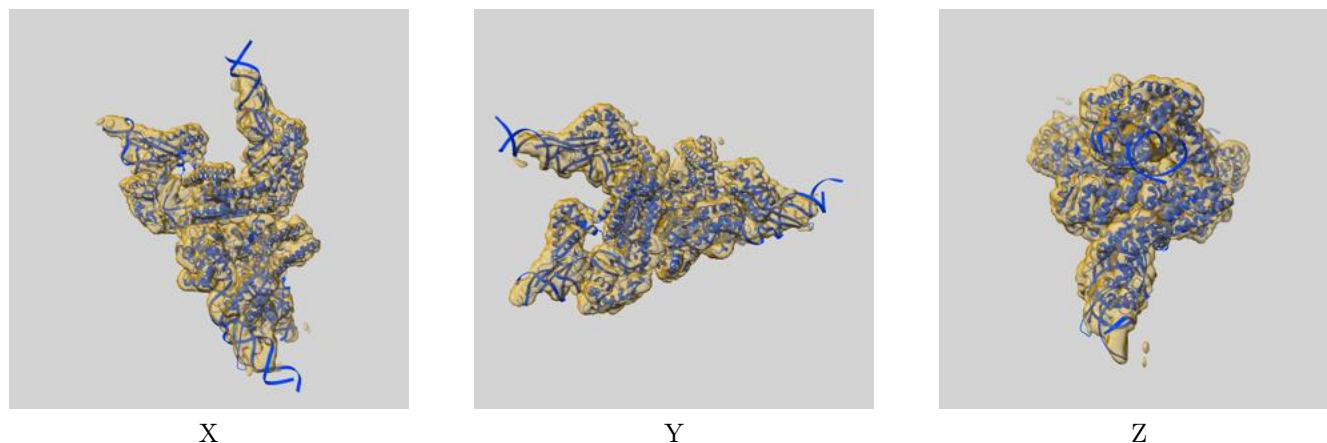
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

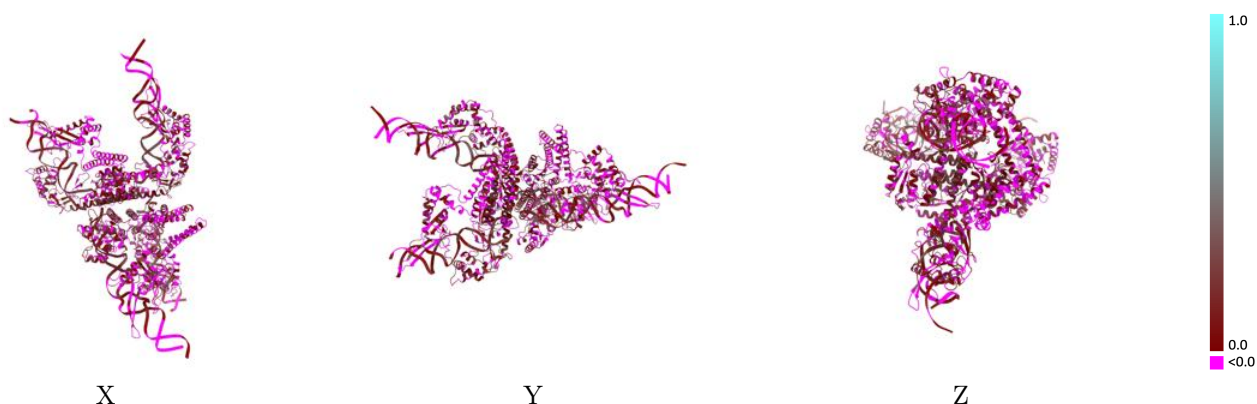
This section contains information regarding the fit between EMDB map EMD-47289 and PDB model 9DXJ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



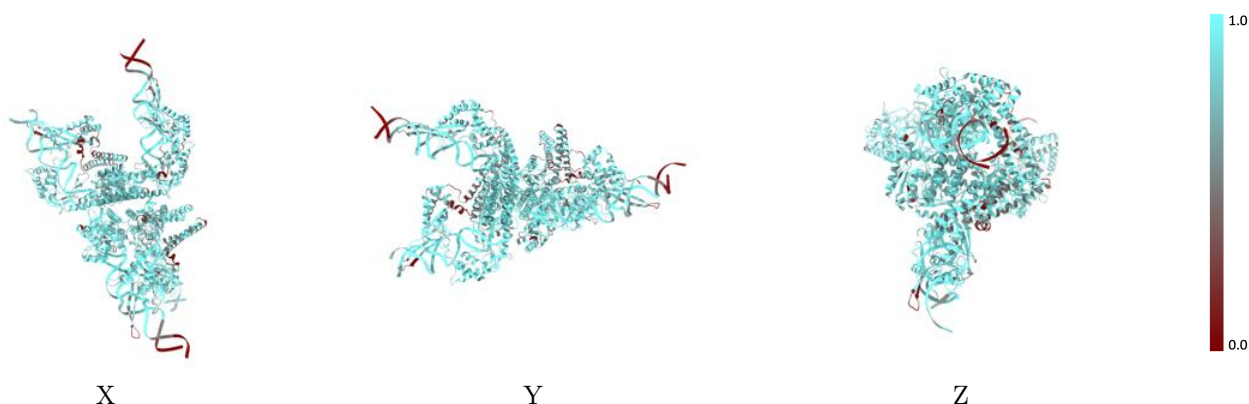
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



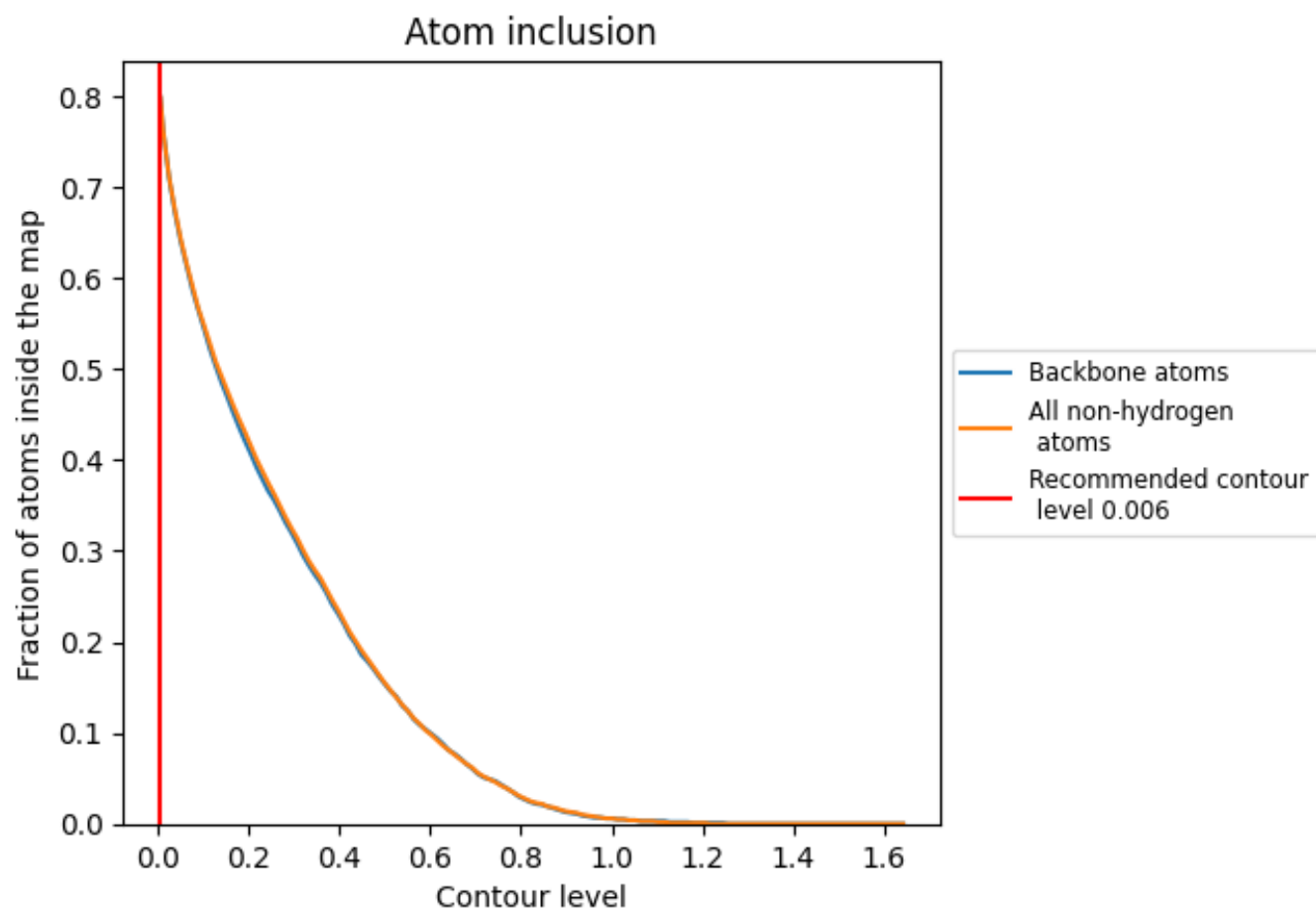
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).



























9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7980	 0.0560
A	 0.7970	 0.0340
C	 0.7840	 0.0310
E	 0.7900	 0.1100
F	 0.7450	 0.1150
G	 0.9430	 0.1500
H	 0.8800	 0.1470
I	 0.8300	 0.0410
K	 0.8150	 0.0390
M	 0.7980	 0.1140
N	 0.7580	 0.1200
O	 0.9510	 0.1530
P	 0.8940	 0.1510

