



Full wwPDB EM Validation Report ⓘ

Jul 29, 2026 – 03:14 PM JST

PDB ID : 23OR / pdb_000023or
EMDB ID : EMD-69132
Title : Cryo-EM structure of the Retron-Eco8-SSB complex
Authors : Zhang, J.T.; Ji, C.G.; Li, Z.L.; Wei, X.Y.; Jia, N.
Deposited on : 2026-02-12
Resolution : 3.11 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:

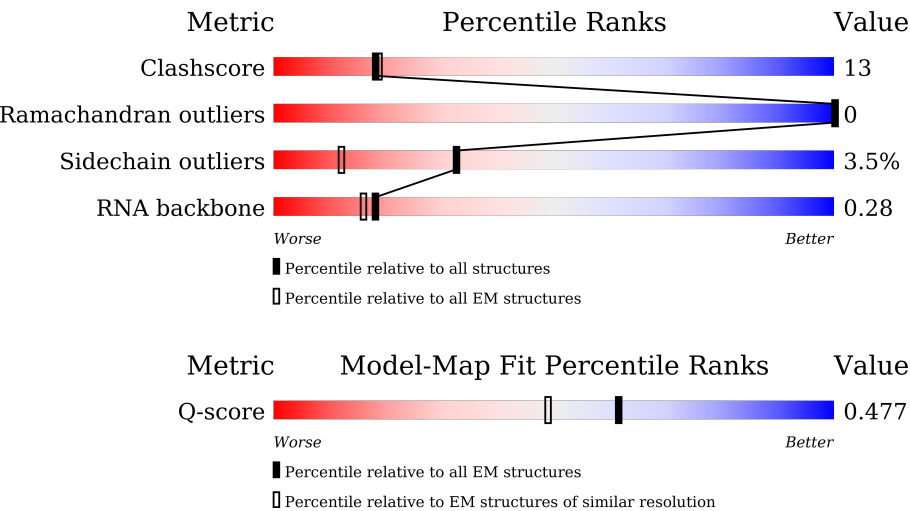
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.11 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.



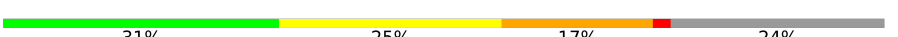
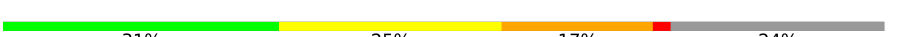
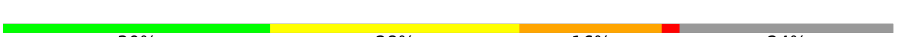
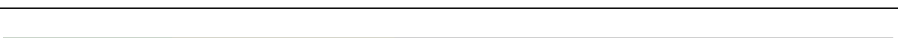
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14465 (2.61 - 3.61)

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	374	80%14%...
1	E	374	79%14%...
1	I	374	80%14%...

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Mol	Chain	Length	Quality of chain
1	M	374	
2	B	750	
2	F	750	
2	J	750	
2	N	750	
3	C	83	
3	G	83	
3	K	83	
3	O	83	
4	D	75	
4	H	75	
4	L	75	
4	P	75	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 42224 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Retron Eco8 reverse transcriptase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	367	Total	C	N	O	S	0	0
			2981	1921	503	546	11		
1	E	367	Total	C	N	O	S	0	0
			2981	1921	503	546	11		
1	I	367	Total	C	N	O	S	0	0
			2981	1921	503	546	11		
1	M	367	Total	C	N	O	S	0	0
			2981	1921	503	546	11		

- Molecule 2 is a protein called Retron Eco8 OLD nuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	671	Total	C	N	O	S	0	0
			5549	3594	918	1030	7		
2	F	669	Total	C	N	O	S	0	0
			5540	3591	915	1027	7		
2	J	672	Total	C	N	O	S	0	0
			5561	3603	919	1032	7		
2	N	674	Total	C	N	O	S	0	0
			5578	3615	921	1035	7		

- Molecule 3 is a RNA chain called RNA (83-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	63	Total	C	N	O	P	0	0
			1346	602	244	437	63		
3	G	63	Total	C	N	O	P	0	0
			1346	602	244	437	63		
3	K	63	Total	C	N	O	P	0	0
			1346	602	244	437	63		
3	O	63	Total	C	N	O	P	0	0
			1346	602	244	437	63		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	A	-	expression tag	GB 1881611662
C	0	G	-	expression tag	GB 1881611662
G	-1	A	-	expression tag	GB 1881611662
G	0	G	-	expression tag	GB 1881611662
K	-1	A	-	expression tag	GB 1881611662
K	0	G	-	expression tag	GB 1881611662
O	-1	A	-	expression tag	GB 1881611662
O	0	G	-	expression tag	GB 1881611662

- Molecule 4 is a DNA chain called DNA (75-MER).

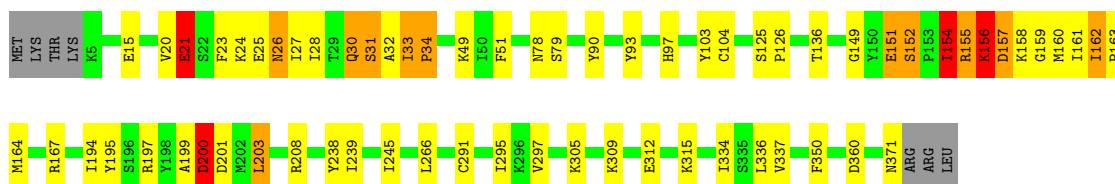
Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	33	Total	C	N	O	P	0	0
			672	323	115	201	33		
4	H	33	Total	C	N	O	P	0	0
			672	323	115	201	33		
4	L	33	Total	C	N	O	P	0	0
			672	323	115	201	33		
4	P	33	Total	C	N	O	P	0	0
			672	323	115	201	33		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

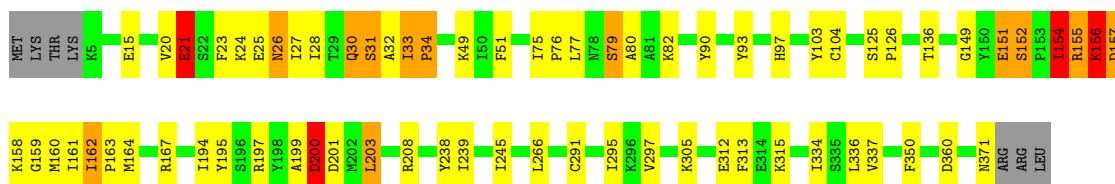
- Molecule 1: Retron Eco8 reverse transcriptase

Chain A: 



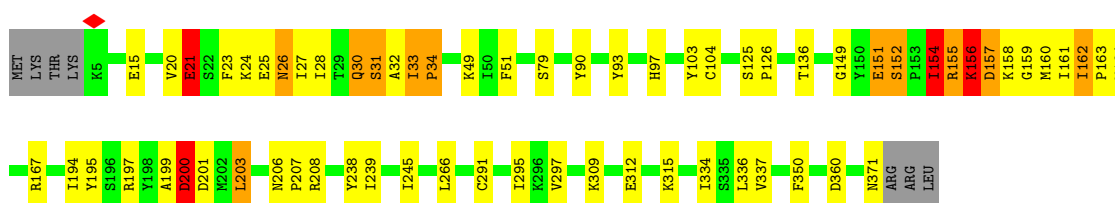
- Molecule 1: Retron Eco8 reverse transcriptase

Chain E: 



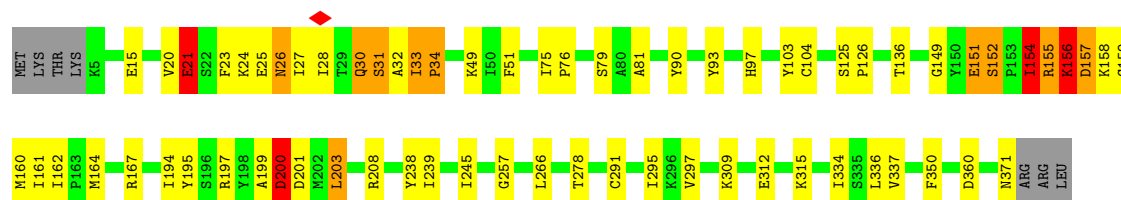
- Molecule 1: Retron Eco8 reverse transcriptase

Chain I: 

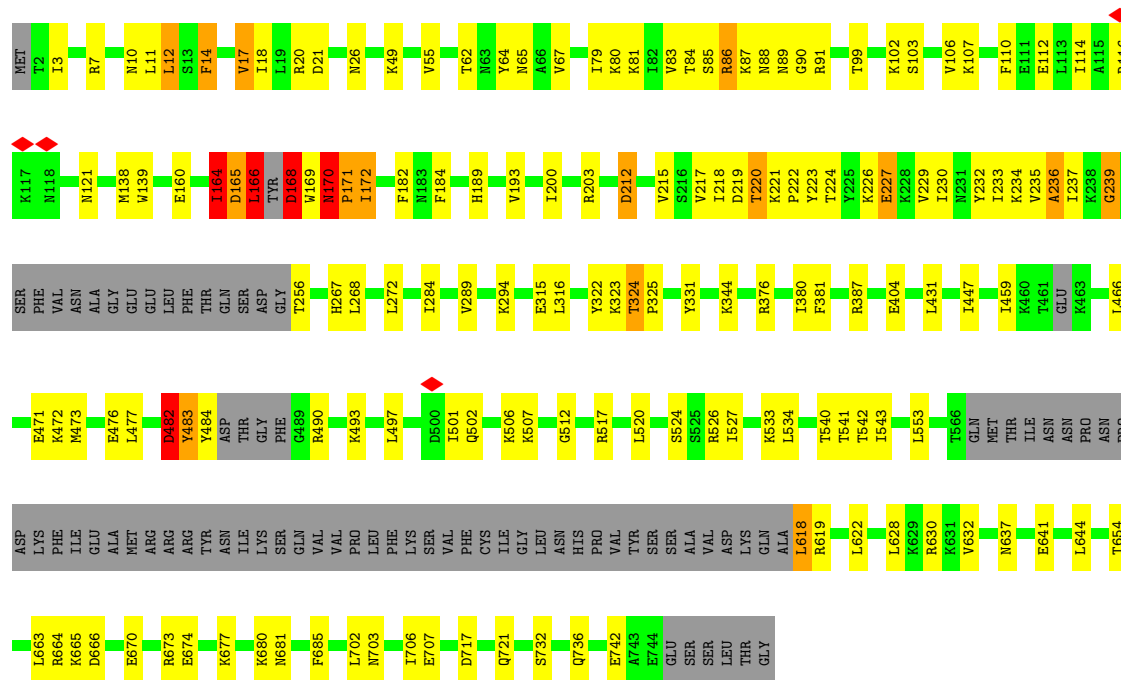


- Molecule 1: Retron Eco8 reverse transcriptase

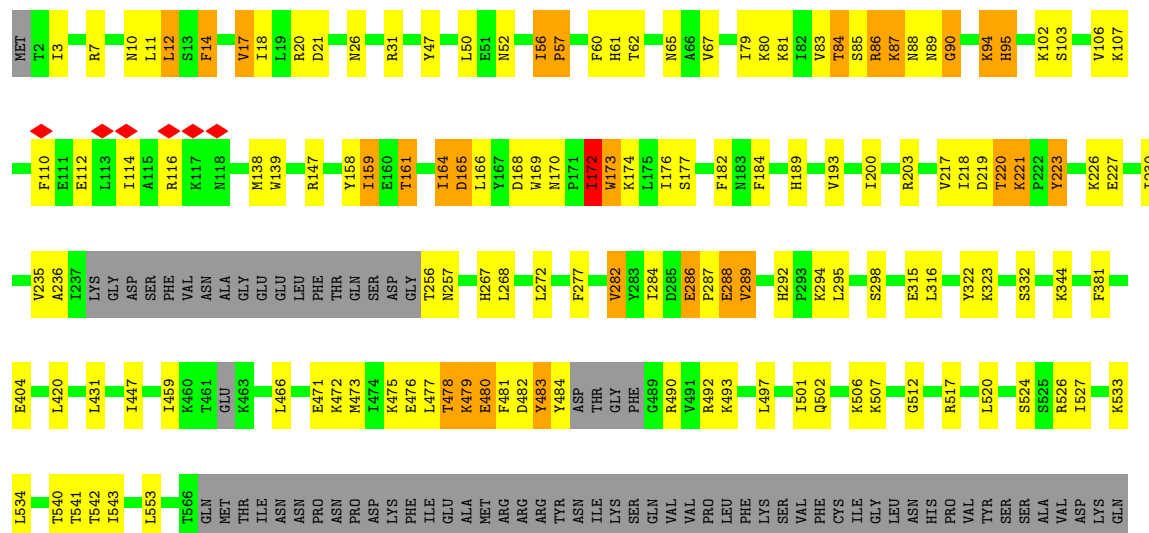
Chain M: 



• Molecule 2: Retron Eco8 OLD nuclease

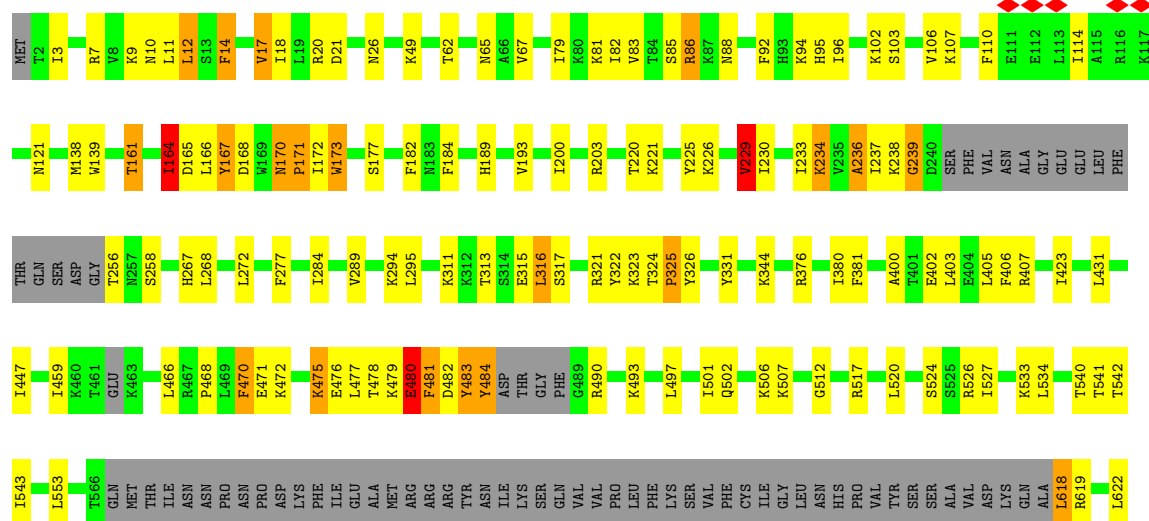


• Molecule 2: Retron Eco8 OLD nuclease

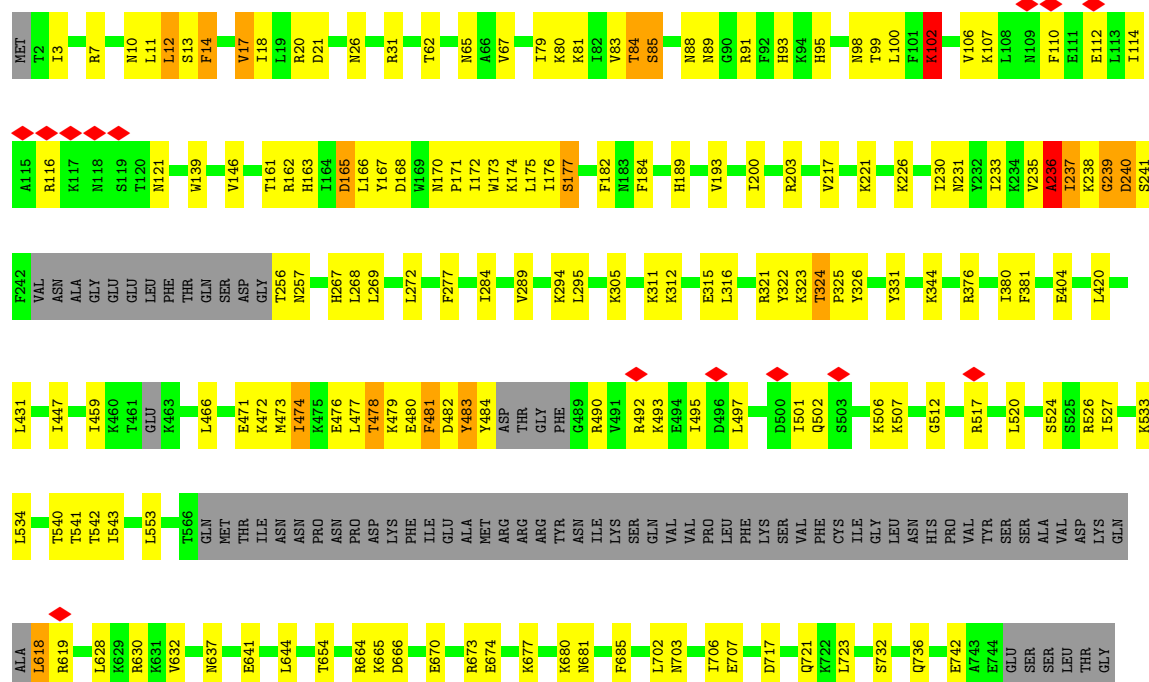




• Molecule 2: Retron Eco8 OLD nuclease

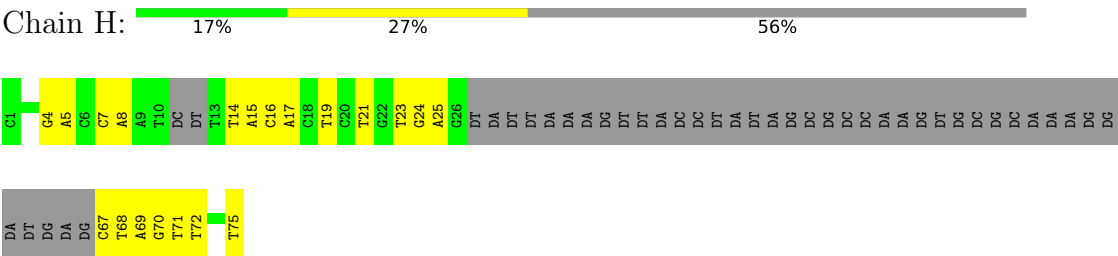


• Molecule 2: Retron Eco8 OLD nuclease

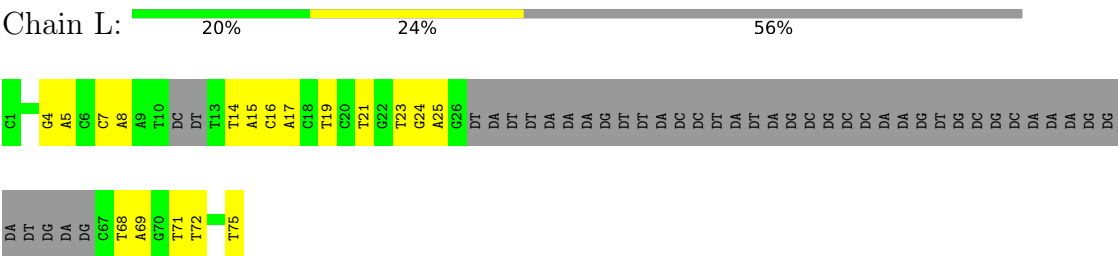


[illegible]

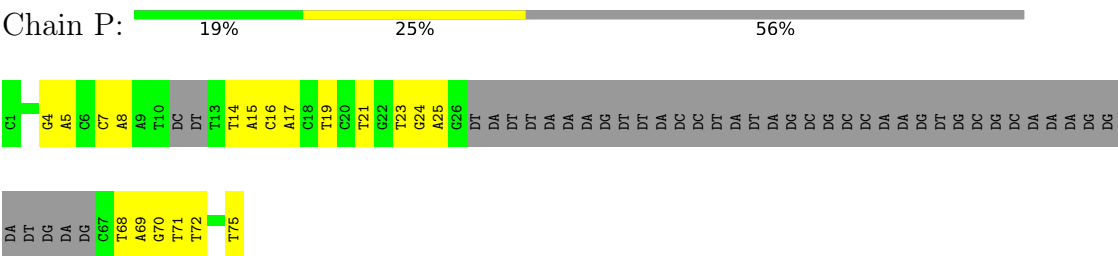
• Molecule 4: DNA (75-MER)



• Molecule 4: DNA (75-MER)



• Molecule 4: DNA (75-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114917	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.939	Depositor
Minimum map value	-1.644	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	469.28, 469.28, 469.28	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.838, 0.838, 0.838	Depositor

5 Model quality

5.1 Standard geometry

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	0.76	11/3038 (0.4%)	0.84	27/4080 (0.7%)
1	E	0.83	14/3038 (0.5%)	0.88	28/4080 (0.7%)
1	I	0.76	11/3038 (0.4%)	0.84	28/4080 (0.7%)
1	M	0.84	13/3038 (0.4%)	0.86	27/4080 (0.7%)
2	B	0.78	22/5663 (0.4%)	0.84	27/7632 (0.4%)
2	F	0.84	20/5656 (0.4%)	0.88	32/7626 (0.4%)
2	J	0.83	22/5677 (0.4%)	0.87	35/7653 (0.5%)
2	N	0.80	21/5695 (0.4%)	0.81	31/7677 (0.4%)
3	C	0.71	1/1505 (0.1%)	0.88	8/2341 (0.3%)
3	G	0.70	1/1505 (0.1%)	0.89	7/2341 (0.3%)
3	K	0.72	2/1505 (0.1%)	0.89	8/2341 (0.3%)
3	O	0.71	1/1505 (0.1%)	0.89	9/2341 (0.4%)
4	D	0.28	0/749	0.50	0/1148
4	H	0.27	0/749	0.49	0/1148
4	L	0.29	0/749	0.50	0/1148
4	P	0.26	0/749	0.47	0/1148
All	All	0.77	139/43859 (0.3%)	0.84	267/60864 (0.4%)

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
2	B	0	1
2	F	0	1
2	J	0	1
2	N	0	2
All	All	0	5

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	177	SER	CA-C	-10.39	1.39	1.52
2	F	286	GLU	C-O	-9.83	1.19	1.23
2	J	165	ASP	CA-C	-9.37	1.41	1.52
1	M	155	ARG	CA-C	-8.65	1.42	1.52
1	I	155	ARG	CA-C	-8.62	1.42	1.52
1	A	155	ARG	CA-C	-8.62	1.42	1.52
1	E	155	ARG	CA-C	-8.57	1.42	1.52
2	N	236	ALA	C-O	-8.11	1.14	1.24
2	B	165	ASP	CA-C	-7.83	1.42	1.53
2	J	170	ASN	CA-C	-7.58	1.43	1.52
1	I	152	SER	CA-C	-7.34	1.42	1.52
1	A	21	GLU	CA-C	-7.34	1.43	1.52
1	I	21	GLU	CA-C	-7.34	1.43	1.52
1	E	21	GLU	CA-C	-7.33	1.43	1.52
1	M	81	ALA	CA-C	-7.33	1.43	1.52
1	M	21	GLU	CA-C	-7.33	1.43	1.52
1	A	152	SER	CA-C	-7.32	1.42	1.52
1	E	152	SER	CA-C	-7.31	1.42	1.52
1	A	159	GLY	CA-C	-7.30	1.44	1.52
1	M	152	SER	CA-C	-7.30	1.42	1.52
1	I	159	GLY	CA-C	-7.30	1.44	1.52
1	M	159	GLY	CA-C	-7.28	1.44	1.52
1	E	159	GLY	CA-C	-7.26	1.44	1.52
2	J	324	THR	C-N	-6.82	1.24	1.33
2	J	400	ALA	N-CA	-6.80	1.37	1.46
2	B	164	ILE	CA-C	-6.74	1.44	1.52
1	I	151	GLU	CA-C	-6.62	1.44	1.52
1	E	151	GLU	CA-C	-6.59	1.44	1.52
1	M	151	GLU	CA-C	-6.58	1.44	1.52
1	A	151	GLU	CA-C	-6.57	1.44	1.52
2	J	324	THR	CA-C	-6.48	1.46	1.52
2	F	221	LYS	CA-C	-6.47	1.46	1.53
3	K	17	A	C1'-N9	-6.41	1.38	1.48
3	C	17	A	C1'-N9	-6.38	1.38	1.48
3	O	17	A	C1'-N9	-6.38	1.38	1.48
3	G	17	A	C1'-N9	-6.35	1.38	1.48
2	B	169	TRP	N-CA	-6.30	1.38	1.46
2	B	166	LEU	CA-C	-6.28	1.39	1.52
2	N	325	PRO	CA-C	6.16	1.60	1.52
2	N	324	THR	C-N	-6.14	1.25	1.33
2	J	479	LYS	N-CA	6.12	1.55	1.46
2	N	478	THR	C-O	-6.07	1.17	1.24
2	B	221	LYS	C-N	-6.04	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	79	SER	C-O	-6.01	1.16	1.24
2	N	241	SER	CA-C	-5.99	1.45	1.52
2	B	234	LYS	C-O	-5.96	1.17	1.24
1	A	199	ALA	C-O	-5.95	1.18	1.24
1	E	199	ALA	C-O	-5.94	1.18	1.24
2	B	227	GLU	CA-C	-5.94	1.45	1.52
1	M	199	ALA	C-O	-5.94	1.18	1.24
2	N	89	ASN	CA-C	-5.94	1.45	1.52
1	I	199	ALA	C-O	-5.92	1.18	1.24
2	N	102	LYS	C-N	-5.91	1.25	1.33
2	F	284	ILE	C-O	-5.89	1.17	1.24
2	B	324	THR	CA-C	-5.85	1.46	1.53
2	F	475	LYS	C-N	-5.85	1.25	1.34
2	J	173	TRP	CA-C	-5.84	1.44	1.52
2	F	292	HIS	CA-C	-5.81	1.46	1.53
1	E	195	TYR	CA-C	5.79	1.59	1.52
1	I	195	TYR	CA-C	5.78	1.59	1.52
1	A	195	TYR	CA-C	5.77	1.59	1.52
1	M	195	TYR	CA-C	5.77	1.59	1.52
2	J	17	VAL	C-O	-5.64	1.18	1.23
2	F	17	VAL	C-O	-5.63	1.18	1.23
2	B	17	VAL	C-O	-5.62	1.18	1.23
2	N	17	VAL	C-O	-5.57	1.18	1.23
2	B	10	ASN	C-N	-5.56	1.26	1.33
2	J	10	ASN	C-N	-5.54	1.26	1.33
2	F	10	ASN	C-N	-5.54	1.26	1.33
2	F	61	HIS	C-N	-5.54	1.25	1.33
2	B	325	PRO	CA-CB	-5.53	1.46	1.53
2	N	10	ASN	C-N	-5.53	1.26	1.33
2	F	322	TYR	CA-C	5.47	1.59	1.52
2	J	164	ILE	CA-C	-5.45	1.45	1.52
1	M	81	ALA	CA-CB	-5.45	1.46	1.53
2	F	7	ARG	C-O	-5.40	1.18	1.24
2	J	7	ARG	C-O	-5.38	1.18	1.24
2	N	239	GLY	C-O	-5.38	1.18	1.24
2	N	7	ARG	C-O	-5.37	1.18	1.24
2	B	7	ARG	C-O	-5.37	1.18	1.24
2	N	93	HIS	C-N	-5.36	1.26	1.33
2	J	478	THR	CA-C	5.34	1.59	1.52
2	F	286	GLU	CA-C	-5.29	1.49	1.53
1	E	80	ALA	C-O	-5.29	1.18	1.24
2	B	236	ALA	C-O	-5.29	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	95	HIS	C-O	-5.29	1.18	1.24
2	F	18	ILE	C-O	-5.24	1.18	1.24
2	B	90	GLY	CA-C	-5.23	1.46	1.51
3	K	44	A	O3'-P	5.22	1.69	1.61
2	N	12	LEU	C-O	-5.22	1.19	1.24
2	J	18	ILE	C-O	-5.21	1.18	1.24
2	F	12	LEU	C-O	-5.21	1.19	1.24
2	J	12	LEU	C-O	-5.21	1.19	1.24
1	E	31	SER	CA-C	-5.19	1.46	1.52
1	I	21	GLU	N-CA	-5.19	1.40	1.46
2	B	172	ILE	C-O	-5.19	1.18	1.24
2	B	212	ASP	C-O	-5.19	1.18	1.24
1	A	21	GLU	N-CA	-5.18	1.40	1.46
2	F	170	ASN	C-O	-5.18	1.19	1.24
2	B	12	LEU	C-O	-5.17	1.19	1.24
2	B	160	GLU	C-N	-5.17	1.26	1.33
1	E	21	GLU	N-CA	-5.17	1.40	1.46
2	J	407	ARG	CA-C	5.17	1.59	1.52
1	M	21	GLU	N-CA	-5.17	1.40	1.46
2	B	18	ILE	C-O	-5.16	1.18	1.24
1	I	31	SER	CA-C	-5.16	1.46	1.52
2	N	18	ILE	C-O	-5.16	1.18	1.24
2	F	221	LYS	C-N	-5.16	1.26	1.33
2	J	475	LYS	C-O	-5.15	1.18	1.24
2	N	98	ASN	N-CA	-5.15	1.40	1.46
2	J	324	THR	N-CA	-5.14	1.39	1.45
2	J	476	GLU	C-O	-5.14	1.18	1.24
1	M	31	SER	CA-C	-5.14	1.46	1.52
2	N	162	ARG	C-O	-5.14	1.18	1.24
2	J	470	PHE	C-O	-5.14	1.18	1.24
1	A	31	SER	CA-C	-5.13	1.46	1.52
1	A	194	ILE	C-N	5.12	1.40	1.33
1	M	194	ILE	C-N	5.12	1.40	1.33
2	F	480	GLU	CA-C	-5.11	1.46	1.53
1	I	194	ILE	C-N	5.11	1.40	1.33
2	B	89	ASN	N-CA	-5.10	1.39	1.46
2	N	11	LEU	N-CA	-5.10	1.40	1.46
2	F	14	PHE	C-O	-5.10	1.17	1.23
2	J	11	LEU	N-CA	-5.10	1.40	1.46
1	E	194	ILE	C-N	5.10	1.40	1.33
2	N	14	PHE	C-O	-5.09	1.17	1.23
2	F	11	LEU	N-CA	-5.09	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	11	LEU	N-CA	-5.08	1.40	1.46
2	B	14	PHE	C-O	-5.08	1.17	1.23
1	E	82	LYS	C-O	-5.07	1.18	1.23
2	J	14	PHE	C-O	-5.07	1.17	1.23
2	N	13	SER	C-O	-5.06	1.18	1.24
2	F	95	HIS	C-O	-5.05	1.18	1.24
2	F	289	VAL	C-O	-5.02	1.18	1.24
1	E	77	LEU	C-O	-5.02	1.17	1.23
1	A	157	ASP	CA-C	-5.02	1.46	1.52
1	I	157	ASP	CA-C	-5.02	1.46	1.52
2	J	9	LYS	C-O	-5.01	1.18	1.24
1	M	157	ASP	CA-C	-5.01	1.46	1.52

All (267) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	483	TYR	N-CA-C	19.08	132.16	111.36
2	B	239	GLY	N-CA-C	16.27	133.18	112.68
2	F	483	TYR	N-CA-C	16.17	128.90	111.28
2	J	479	LYS	N-CA-C	15.91	133.80	111.52
2	B	164	ILE	N-CA-C	-15.32	86.66	108.11
2	F	479	LYS	N-CA-C	14.04	131.18	111.52
2	J	478	THR	N-CA-C	13.72	126.23	111.28
2	B	220	THR	N-CA-C	13.66	129.77	110.50
2	J	483	TYR	N-CA-C	13.13	130.14	112.68
2	F	478	THR	N-CA-C	11.60	123.92	111.28
2	B	483	TYR	N-CA-C	11.51	123.91	111.36
2	F	288	GLU	N-CA-C	11.45	126.75	113.01
2	B	14	PHE	N-CA-C	11.07	126.66	110.28
2	J	14	PHE	N-CA-C	11.06	126.66	110.28
2	F	14	PHE	N-CA-C	11.05	126.63	110.28
2	N	14	PHE	N-CA-C	11.05	126.63	110.28
2	B	218	ILE	N-CA-C	10.09	120.91	110.72
1	A	157	ASP	N-CA-C	-10.03	95.69	110.23
1	E	157	ASP	N-CA-C	-10.02	95.71	110.23
1	M	157	ASP	N-CA-C	-10.01	95.71	110.23
1	I	157	ASP	N-CA-C	-10.00	95.72	110.23
2	B	168	ASP	N-CA-C	-9.82	83.51	111.00
2	B	236	ALA	N-CA-C	9.81	122.05	111.36
2	J	170	ASN	CA-C-N	-9.74	108.24	119.05
2	J	170	ASN	C-N-CA	-9.74	108.24	119.05
2	N	479	LYS	N-CA-C	9.72	124.87	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	238	LYS	N-CA-C	9.59	121.73	111.28
1	I	33	ILE	N-CA-C	9.58	117.93	109.02
1	M	33	ILE	N-CA-C	9.56	117.91	109.02
1	A	33	ILE	N-CA-C	9.55	117.90	109.02
1	E	33	ILE	N-CA-C	9.52	117.87	109.02
2	N	322	TYR	N-CA-C	9.30	124.20	109.50
2	F	322	TYR	N-CA-C	9.25	123.56	109.23
2	J	239	GLY	N-CA-C	8.98	123.99	112.68
2	F	172	ILE	N-CA-C	8.78	119.57	110.62
2	N	478	THR	N-CA-C	8.73	120.80	111.28
2	J	236	ALA	N-CA-C	8.64	120.78	111.36
1	E	32	ALA	N-CA-C	8.60	122.62	110.50
1	M	32	ALA	N-CA-C	8.60	122.62	110.50
1	A	32	ALA	N-CA-C	8.58	122.60	110.50
1	I	32	ALA	N-CA-C	8.58	122.59	110.50
2	J	324	THR	N-CA-C	-8.55	95.64	109.58
2	J	172	ILE	N-CA-C	8.52	119.31	110.62
1	I	195	TYR	N-CA-C	8.41	122.61	108.90
1	A	195	TYR	N-CA-C	8.40	122.58	108.90
1	E	195	TYR	N-CA-C	8.39	122.58	108.90
1	M	195	TYR	N-CA-C	8.37	122.55	108.90
2	J	161	THR	N-CA-C	8.36	120.48	111.36
1	I	26	ASN	N-CA-C	-8.34	102.19	111.28
1	E	26	ASN	N-CA-C	-8.32	102.21	111.28
1	M	26	ASN	N-CA-C	-8.31	102.22	111.28
1	A	26	ASN	N-CA-C	-8.30	102.23	111.28
1	M	149	GLY	N-CA-C	8.25	123.89	111.18
1	E	149	GLY	N-CA-C	8.25	123.89	111.18
1	A	149	GLY	N-CA-C	8.24	123.87	111.18
1	I	149	GLY	N-CA-C	8.23	123.85	111.18
2	N	236	ALA	N-CA-C	8.20	120.21	111.28
2	F	219	ASP	N-CA-C	8.05	122.50	111.39
2	B	322	TYR	N-CA-C	7.79	122.18	109.72
1	E	34	PRO	N-CA-C	7.69	123.26	111.57
2	B	91	ARG	N-CA-C	7.69	119.66	111.28
1	M	34	PRO	N-CA-C	7.68	123.25	111.57
1	A	34	PRO	N-CA-C	7.67	123.23	111.57
1	I	34	PRO	N-CA-C	7.67	123.22	111.57
2	B	169	TRP	N-CA-C	-7.65	103.52	112.92
2	N	85	SER	N-CA-C	7.55	121.18	110.23
1	A	200	ASP	N-CA-C	7.44	119.39	111.28
2	N	240	ASP	N-CA-C	7.44	122.55	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	200	ASP	N-CA-C	7.43	119.38	111.28
2	N	177	SER	N-CA-C	-7.43	103.26	111.36
1	M	200	ASP	N-CA-C	7.42	119.37	111.28
1	I	200	ASP	N-CA-C	7.41	119.36	111.28
2	F	165	ASP	N-CA-C	7.41	119.43	111.36
2	F	223	TYR	CA-CB-CG	7.33	127.08	113.90
2	N	172	ILE	N-CA-C	7.32	118.09	110.62
1	I	27	ILE	N-CA-C	7.32	118.09	110.62
1	M	197	ARG	N-CA-C	7.31	121.11	108.76
1	A	27	ILE	N-CA-C	7.30	118.07	110.62
2	F	220	THR	N-CA-C	7.30	121.39	109.85
1	A	197	ARG	N-CA-C	7.28	121.06	108.76
1	E	197	ARG	N-CA-C	7.28	121.06	108.76
1	I	197	ARG	N-CA-C	7.27	121.05	108.76
2	J	322	TYR	N-CA-C	7.27	120.79	109.52
2	B	237	ILE	N-CA-C	7.27	117.97	110.05
1	M	27	ILE	N-CA-C	7.26	118.03	110.62
1	E	27	ILE	N-CA-C	7.25	118.01	110.62
2	B	482	ASP	N-CA-C	7.22	121.79	110.17
2	J	165	ASP	N-CA-C	-7.22	96.75	108.52
2	J	407	ARG	CA-C-N	7.16	130.91	120.82
2	J	407	ARG	C-N-CA	7.16	130.91	120.82
2	F	218	ILE	N-CA-C	7.11	122.38	112.35
2	B	219	ASP	N-CA-C	7.10	121.33	111.74
2	B	220	THR	N-CA-CB	-7.09	99.95	110.17
1	E	152	SER	N-CA-C	7.07	119.87	109.62
1	A	152	SER	N-CA-C	7.07	119.87	109.62
1	M	152	SER	N-CA-C	7.06	119.86	109.62
1	I	152	SER	N-CA-C	7.05	119.84	109.62
2	N	167	TYR	N-CA-C	6.94	118.84	111.28
2	J	475	LYS	N-CA-C	6.91	118.81	111.28
2	J	481	PHE	N-CA-C	6.71	123.26	113.40
2	N	237	ILE	N-CA-C	6.63	118.70	109.55
1	I	34	PRO	CB-CA-C	-6.62	101.46	110.60
1	A	34	PRO	CB-CA-C	-6.61	101.48	110.60
2	B	86	ARG	N-CA-C	6.61	118.48	111.28
1	M	34	PRO	CB-CA-C	-6.61	101.48	110.60
1	E	34	PRO	CB-CA-C	-6.59	101.50	110.60
2	J	168	ASP	N-CA-C	6.56	119.80	109.96
1	E	21	GLU	N-CA-C	-6.53	107.18	114.62
1	I	21	GLU	N-CA-C	-6.51	107.20	114.62
1	A	21	GLU	N-CA-C	-6.51	107.20	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	21	GLU	N-CA-C	-6.49	107.22	114.62
2	J	173	TRP	CA-C-N	-6.47	111.11	120.29
2	J	173	TRP	C-N-CA	-6.47	111.11	120.29
1	E	201	ASP	N-CA-C	6.46	119.85	110.28
1	I	201	ASP	N-CA-C	6.46	119.84	110.28
1	A	201	ASP	N-CA-C	6.46	119.83	110.28
1	M	201	ASP	N-CA-C	6.45	119.82	110.28
2	J	406	PHE	CB-CA-C	6.43	121.78	110.85
2	N	99	THR	N-CA-C	6.35	118.28	111.36
2	B	223	TYR	N-CA-C	6.33	119.40	110.23
3	G	26	G	C4'-C3'-O3'	-6.32	103.52	113.00
2	F	478	THR	CB-CA-C	-6.32	100.30	110.79
3	K	26	G	C4'-C3'-O3'	-6.30	103.55	113.00
3	C	26	G	C4'-C3'-O3'	-6.29	103.56	113.00
3	O	26	G	C4'-C3'-O3'	-6.29	103.57	113.00
2	F	161	THR	N-CA-C	6.28	118.20	111.36
3	G	66	C	C2'-C3'-O3'	-6.23	104.36	113.70
3	C	66	C	C2'-C3'-O3'	-6.23	104.36	113.70
3	O	66	C	C2'-C3'-O3'	-6.22	104.37	113.70
2	F	90	GLY	N-CA-C	-6.21	98.96	110.83
3	K	66	C	C2'-C3'-O3'	-6.20	104.40	113.70
1	I	33	ILE	CA-C-N	6.20	126.38	120.31
1	I	33	ILE	C-N-CA	6.20	126.38	120.31
1	A	33	ILE	CA-C-N	6.18	126.36	120.31
1	A	33	ILE	C-N-CA	6.18	126.36	120.31
2	B	171	PRO	N-CA-C	-6.17	104.96	113.53
1	M	33	ILE	CA-C-N	6.17	126.35	120.31
1	M	33	ILE	C-N-CA	6.17	126.35	120.31
1	E	33	ILE	CA-C-N	6.15	126.34	120.31
1	E	33	ILE	C-N-CA	6.15	126.34	120.31
1	E	156	LYS	CA-C-N	-6.12	112.02	120.71
1	E	156	LYS	C-N-CA	-6.12	112.02	120.71
1	M	156	LYS	CA-C-N	-6.12	112.02	120.71
1	M	156	LYS	C-N-CA	-6.12	112.02	120.71
1	M	25	GLU	N-CA-C	6.12	117.95	111.28
1	A	156	LYS	CA-C-N	-6.11	112.04	120.71
1	A	156	LYS	C-N-CA	-6.11	112.04	120.71
1	I	156	LYS	CA-C-N	-6.11	112.04	120.71
1	I	156	LYS	C-N-CA	-6.11	112.04	120.71
1	I	25	GLU	N-CA-C	6.10	117.93	111.28
2	F	282	VAL	N-CA-C	6.09	116.90	108.12
1	E	25	GLU	N-CA-C	6.09	117.92	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	GLU	N-CA-C	6.08	117.91	111.28
2	N	326	TYR	N-CA-C	6.07	118.67	110.29
2	F	56	ILE	CA-C-N	5.90	125.81	119.85
2	F	56	ILE	C-N-CA	5.90	125.81	119.85
2	N	240	ASP	CB-CA-C	-5.88	100.27	110.09
2	F	173	TRP	CA-C-N	-5.85	112.37	120.38
2	F	173	TRP	C-N-CA	-5.85	112.37	120.38
1	E	162	ILE	CA-C-N	5.83	125.74	119.85
1	E	162	ILE	C-N-CA	5.83	125.74	119.85
1	M	162	ILE	CA-C-N	5.81	125.72	119.85
1	M	162	ILE	C-N-CA	5.81	125.72	119.85
2	B	222	PRO	N-CA-C	5.80	120.11	111.41
1	A	162	ILE	CA-C-N	5.80	125.70	119.85
1	A	162	ILE	C-N-CA	5.80	125.70	119.85
1	I	162	ILE	CA-C-N	5.76	125.67	119.85
1	I	162	ILE	C-N-CA	5.76	125.67	119.85
2	N	161	THR	N-CA-C	5.75	117.63	111.36
1	I	154	ILE	N-CA-C	5.74	116.47	110.62
2	F	88	ASN	N-CA-C	5.73	117.64	108.41
1	A	154	ILE	N-CA-C	5.72	116.45	110.62
1	E	154	ILE	N-CA-C	5.72	116.45	110.62
1	M	154	ILE	N-CA-C	5.72	116.45	110.62
2	N	176	ILE	N-CA-C	5.66	116.44	110.72
2	B	85	SER	N-CA-C	5.66	118.66	110.28
2	N	481	PHE	N-CA-C	5.66	119.38	111.74
2	F	89	ASN	N-CA-C	-5.63	99.24	108.76
2	B	170	ASN	CA-C-N	-5.61	112.82	119.05
2	B	170	ASN	C-N-CA	-5.61	112.82	119.05
3	K	50	U	C2'-C3'-O3'	-5.61	105.28	113.70
2	N	177	SER	CA-C-N	-5.60	112.33	120.29
2	N	177	SER	C-N-CA	-5.60	112.33	120.29
3	C	67	C	C2'-C3'-O3'	-5.60	105.30	113.70
3	G	67	C	C2'-C3'-O3'	-5.60	105.30	113.70
3	G	50	U	C2'-C3'-O3'	-5.59	105.31	113.70
3	C	50	U	C2'-C3'-O3'	-5.59	105.31	113.70
3	K	67	C	C2'-C3'-O3'	-5.59	105.32	113.70
3	O	67	C	C2'-C3'-O3'	-5.59	105.32	113.70
3	O	50	U	C2'-C3'-O3'	-5.58	105.33	113.70
2	F	60	PHE	CA-CB-CG	5.57	119.36	113.80
2	J	483	TYR	CB-CA-C	-5.56	100.95	110.24
1	M	23	PHE	N-CA-C	5.56	119.37	112.59
2	J	479	LYS	CB-CA-C	-5.55	104.42	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	407	ARG	N-CA-C	5.55	119.91	113.20
1	A	23	PHE	N-CA-C	5.51	119.32	112.59
2	N	165	ASP	N-CA-C	-5.51	99.53	108.52
1	I	23	PHE	N-CA-C	5.51	119.31	112.59
2	J	317	SER	N-CA-C	5.50	119.30	112.59
1	E	23	PHE	N-CA-C	5.50	119.30	112.59
2	N	479	LYS	CB-CA-C	-5.49	103.93	111.73
2	J	326	TYR	N-CA-C	5.46	117.82	110.29
2	J	402	GLU	N-CA-C	5.46	117.23	111.28
2	J	171	PRO	N-CA-C	-5.44	105.97	113.53
2	J	234	LYS	N-CA-C	5.41	117.17	111.28
2	B	217	VAL	N-CA-C	5.38	116.15	110.72
2	F	323	LYS	N-CA-C	5.37	119.94	113.17
3	O	45	U	C2'-C3'-O3'	-5.35	105.67	113.70
1	A	26	ASN	CA-C-N	-5.34	113.14	120.46
1	A	26	ASN	C-N-CA	-5.34	113.14	120.46
1	I	26	ASN	CA-C-N	-5.34	113.15	120.46
1	I	26	ASN	C-N-CA	-5.34	113.15	120.46
1	E	26	ASN	CA-C-N	-5.33	113.15	120.46
1	E	26	ASN	C-N-CA	-5.33	113.15	120.46
2	F	85	SER	N-CA-C	5.33	117.95	110.23
2	N	12	LEU	CA-C-N	5.32	127.85	120.29
2	N	12	LEU	C-N-CA	5.32	127.85	120.29
1	M	26	ASN	CA-C-N	-5.31	113.18	120.46
1	M	26	ASN	C-N-CA	-5.31	113.18	120.46
2	B	12	LEU	CA-C-N	5.31	127.83	120.29
2	B	12	LEU	C-N-CA	5.31	127.83	120.29
2	J	12	LEU	CA-C-N	5.30	127.82	120.29
2	J	12	LEU	C-N-CA	5.30	127.82	120.29
2	N	322	TYR	CA-CB-CG	5.28	123.40	113.90
2	F	12	LEU	CA-C-N	5.27	127.77	120.29
2	F	12	LEU	C-N-CA	5.27	127.77	120.29
2	F	57	PRO	N-CA-C	5.25	119.73	111.38
2	F	52	ASN	N-CA-C	5.25	118.87	111.52
2	F	169	TRP	N-CA-C	-5.23	106.14	112.88
2	F	219	ASP	CB-CA-C	-5.22	104.48	111.89
2	J	325	PRO	N-CA-CB	-5.21	98.48	103.33
2	B	169	TRP	CB-CA-C	5.20	119.34	110.56
2	F	47	TYR	N-CA-C	5.18	117.83	111.82
2	N	168	ASP	N-CA-C	5.16	117.69	109.96
1	I	151	GLU	N-CA-C	-5.14	100.79	109.07
2	N	239	GLY	N-CA-C	5.13	120.38	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	GLU	N-CA-C	-5.13	100.81	109.07
1	M	151	GLU	N-CA-C	-5.12	100.83	109.07
2	N	163	HIS	N-CA-C	5.11	118.55	112.72
1	I	33	ILE	N-CA-CB	-5.11	104.73	109.99
3	C	19	A	C4'-C3'-O3'	-5.10	105.34	113.00
1	E	151	GLU	N-CA-C	-5.10	100.86	109.07
3	K	19	A	C4'-C3'-O3'	-5.10	105.35	113.00
2	N	325	PRO	O-C-N	-5.10	116.86	123.03
3	O	19	A	C4'-C3'-O3'	-5.10	105.35	113.00
3	G	19	A	C4'-C3'-O3'	-5.08	105.37	113.00
1	M	33	ILE	N-CA-CB	-5.08	104.76	109.99
3	O	62	C	C4'-C3'-O3'	-5.07	105.40	113.00
1	A	33	ILE	N-CA-CB	-5.06	104.78	109.99
2	J	229	VAL	N-CA-C	5.06	115.78	110.62
2	N	239	GLY	CA-C-O	-5.05	115.86	121.37
3	G	62	C	C4'-C3'-O3'	-5.05	105.43	113.00
3	C	62	C	C4'-C3'-O3'	-5.05	105.43	113.00
1	E	33	ILE	N-CA-CB	-5.05	104.79	109.99
3	K	62	C	C4'-C3'-O3'	-5.04	105.44	113.00
3	G	55	G	C4'-C3'-O3'	-5.04	105.44	113.00
2	J	480	GLU	N-CA-CB	-5.04	102.64	110.04
3	C	55	G	C4'-C3'-O3'	-5.03	105.45	113.00
3	K	55	G	C4'-C3'-O3'	-5.03	105.45	113.00
3	O	55	G	C4'-C3'-O3'	-5.03	105.45	113.00
3	C	70	A	C4'-C3'-O3'	-5.03	105.46	113.00
1	I	155	ARG	N-CA-C	-5.03	101.05	109.24
2	B	322	TYR	N-CA-CB	-5.02	102.49	111.08
3	K	70	A	C4'-C3'-O3'	-5.02	105.47	113.00
2	J	167	TYR	N-CA-C	5.02	116.75	111.28
3	O	70	A	C4'-C3'-O3'	-5.01	105.48	113.00
1	E	155	ARG	N-CA-C	-5.00	101.08	109.24

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	12	LEU	Mainchain
2	F	12	LEU	Mainchain
2	J	12	LEU	Mainchain
2	N	12	LEU	Mainchain
2	N	236	ALA	Mainchain

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	2981	0	3063	51	0
1	E	2981	0	3063	47	0
1	I	2981	0	3063	50	0
1	M	2981	0	3063	57	0
2	B	5549	0	5622	150	0
2	F	5540	0	5612	182	0
2	J	5561	0	5632	174	0
2	N	5578	0	5646	196	0
3	C	1346	0	680	63	0
3	G	1346	0	680	61	0
3	K	1346	0	680	60	0
3	O	1346	0	680	68	0
4	D	672	0	378	40	0
4	H	672	0	378	33	0
4	L	672	0	378	42	0
4	P	672	0	378	40	0
All	All	42224	0	38996	1057	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 (1057) 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)
4:D:21:DT:O4	2:N:203:ARG:HD2	1.26	1.35
2:F:203:ARG:HD2	4:L:21:DT:C4	1.67	1.28
2:F:203:ARG:HD2	4:L:21:DT:O4	1.10	1.26
2:B:404:GLU:OE2	2:N:376:ARG:NH1	1.70	1.23
2:F:31:ARG:NH1	2:J:294:LYS:HD3	1.55	1.21
2:F:404:GLU:OE2	2:J:376:ARG:NH1	1.73	1.21
2:B:376:ARG:NH1	2:N:404:GLU:OE2	1.77	1.17
2:F:31:ARG:HH12	2:J:294:LYS:HD3	1.05	1.16
2:F:404:GLU:OE2	2:J:376:ARG:HG3	1.45	1.15
2:F:166:LEU:HD11	2:F:257:ASN:HB3	1.27	1.15
4:D:21:DT:C4	2:N:203:ARG:HD2	1.82	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:175:LEU:HD11	2:N:269:LEU:HD13	1.30	1.11
2:F:420:LEU:CD2	2:J:294:LYS:HZ1	1.64	1.09
2:F:420:LEU:HD22	2:J:294:LYS:NZ	1.65	1.09
2:F:404:GLU:HG3	2:J:380:ILE:HD11	1.36	1.07
2:F:203:ARG:CD	4:L:21:DT:O4	2.03	1.06
2:B:294:LYS:CE	2:N:420:LEU:HD22	1.85	1.06
2:F:166:LEU:CD1	2:F:257:ASN:HB3	1.86	1.05
2:F:420:LEU:HD22	2:J:294:LYS:CE	1.86	1.05
1:A:79:SER:CB	2:B:65:ASN:HD21	1.68	1.05
1:I:79:SER:CB	2:J:65:ASN:HD21	1.68	1.05
2:F:200:ILE:HG23	2:N:182:PHE:HB3	1.40	1.04
2:F:404:GLU:CG	2:J:380:ILE:HD11	1.88	1.04
2:B:294:LYS:NZ	2:N:420:LEU:HD22	1.73	1.03
2:B:380:ILE:HD11	2:N:404:GLU:CG	1.88	1.03
2:B:404:GLU:CG	2:N:380:ILE:HD11	1.88	1.02
2:B:294:LYS:HZ1	2:N:420:LEU:CD2	1.72	1.02
1:I:20:VAL:HG23	1:I:21:GLU:HG3	1.42	1.02
1:A:20:VAL:HG23	1:A:21:GLU:HG3	1.42	1.02
4:L:25:DA:OP1	2:N:81:LYS:NZ	1.92	1.02
2:F:200:ILE:CG2	2:N:182:PHE:HB3	1.91	1.01
2:B:404:GLU:HG3	2:N:380:ILE:HD11	1.42	1.00
2:F:182:PHE:HB3	2:N:200:ILE:HG23	1.43	1.00
2:F:420:LEU:HD22	2:J:294:LYS:HZ1	1.16	1.00
3:O:39:A:H2'	3:O:40:C:C6	1.98	0.99
3:G:39:A:H2'	3:G:40:C:C6	1.98	0.99
2:F:203:ARG:HD3	4:L:21:DT:H72	1.44	0.99
1:M:20:VAL:HG23	1:M:21:GLU:HG3	1.42	0.98
4:D:21:DT:H72	2:N:203:ARG:HD3	1.42	0.98
3:K:39:A:H2'	3:K:40:C:C6	1.98	0.98
3:C:39:A:H2'	3:C:40:C:C6	1.98	0.97
1:E:20:VAL:HG23	1:E:21:GLU:HG3	1.42	0.97
1:I:79:SER:OG	2:J:65:ASN:ND2	1.97	0.97
2:F:182:PHE:HB3	2:N:200:ILE:CG2	1.94	0.97
1:A:79:SER:OG	2:B:65:ASN:ND2	1.97	0.97
2:F:166:LEU:HD11	2:F:257:ASN:CB	1.94	0.97
2:B:380:ILE:HD11	2:N:404:GLU:HG3	1.46	0.96
2:B:404:GLU:OE2	2:N:376:ARG:HG3	1.66	0.96
2:B:294:LYS:HZ1	2:N:420:LEU:HD22	1.26	0.95
2:B:294:LYS:HD3	2:N:31:ARG:NH1	1.82	0.94
2:F:203:ARG:NH1	4:L:21:DT:C5	2.35	0.94
4:D:21:DT:C5	2:N:203:ARG:NH1	2.35	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:81:LYS:NZ	4:P:25:DA:OP1	2.02	0.93
2:F:203:ARG:CD	4:L:21:DT:C4	2.49	0.93
3:G:28:A:H2'	3:G:29:G:C8	2.05	0.92
3:O:28:A:H2'	3:O:29:G:C8	2.05	0.92
3:C:28:A:H2'	3:C:29:G:C8	2.04	0.92
4:D:21:DT:O4	2:N:203:ARG:CD	2.18	0.92
3:K:28:A:H2'	3:K:29:G:C8	2.05	0.92
4:D:25:DA:OP1	2:F:81:LYS:NZ	2.04	0.90
2:B:294:LYS:HD3	2:N:31:ARG:HH12	1.33	0.90
2:F:189:HIS:CE1	2:N:236:ALA:O	2.27	0.88
2:J:403:LEU:HD12	2:J:423:ILE:HG22	1.53	0.88
2:F:203:ARG:NH1	4:L:21:DT:C6	2.41	0.87
3:O:35:U:H3'	3:O:36:U:H6	1.40	0.86
3:G:35:U:H3'	3:G:36:U:H6	1.41	0.86
2:F:203:ARG:HD3	4:L:21:DT:C7	2.06	0.86
4:D:21:DT:C6	2:N:203:ARG:NH1	2.45	0.85
2:F:404:GLU:OE2	2:J:376:ARG:CG	2.23	0.85
2:B:81:LYS:NZ	4:H:25:DA:OP1	2.09	0.85
2:F:165:ASP:HB2	2:F:168:ASP:OD1	1.77	0.84
2:B:294:LYS:NZ	2:N:420:LEU:CD2	2.38	0.84
2:B:380:ILE:HD11	2:N:404:GLU:HG2	1.58	0.83
2:F:236:ALA:O	2:N:189:HIS:CE1	2.31	0.83
2:F:483:TYR:O	2:F:484:TYR:HB2	1.78	0.83
3:C:35:U:H3'	3:C:36:U:H6	1.41	0.83
4:H:21:DT:H72	2:J:203:ARG:HD3	1.60	0.82
1:M:257:GLY:N	2:N:107:LYS:HE3	1.93	0.82
2:F:459:ILE:HD11	2:F:512:GLY:HA3	1.61	0.82
1:I:79:SER:CB	2:J:65:ASN:ND2	2.42	0.82
2:N:478:THR:O	2:N:492:ARG:NH2	2.12	0.82
2:B:376:ARG:HG3	2:N:404:GLU:OE2	1.80	0.82
2:J:459:ILE:HD11	2:J:512:GLY:HA3	1.61	0.82
3:K:35:U:H3'	3:K:36:U:H6	1.41	0.82
2:N:459:ILE:HD11	2:N:512:GLY:HA3	1.61	0.82
2:F:31:ARG:HH12	2:J:294:LYS:CD	1.92	0.82
4:D:21:DT:C7	2:N:203:ARG:HD3	2.09	0.82
2:B:459:ILE:HD11	2:B:512:GLY:HA3	1.61	0.81
1:A:79:SER:CB	2:B:65:ASN:ND2	2.42	0.81
2:J:86:ARG:HH11	2:J:86:ARG:H	1.26	0.81
4:H:21:DT:O4	2:J:203:ARG:HD2	1.80	0.80
2:B:239:GLY:HA3	2:J:220:THR:CG2	2.12	0.80
2:J:177:SER:HB2	2:J:230:ILE:HD11	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:236:ALA:O	2:N:189:HIS:NE2	2.14	0.79
2:B:483:TYR:O	2:B:484:TYR:HB2	1.81	0.79
2:B:404:GLU:HG2	2:N:380:ILE:HD11	1.62	0.79
2:F:166:LEU:CD1	2:F:257:ASN:CB	2.57	0.79
2:F:200:ILE:CD1	2:N:184:PHE:CE1	2.65	0.79
4:H:21:DT:C4	2:J:203:ARG:HD2	2.18	0.79
1:M:257:GLY:H	2:N:107:LYS:HE3	1.45	0.78
4:D:21:DT:C4	2:N:203:ARG:CD	2.63	0.78
2:B:239:GLY:HA3	2:J:220:THR:HG23	1.66	0.78
4:L:71:DT:C6	4:L:72:DT:H72	2.19	0.78
2:N:102:LYS:O	2:N:106:VAL:HG23	1.82	0.78
2:B:203:ARG:HD3	4:P:21:DT:H72	1.67	0.77
4:D:21:DT:C7	2:N:203:ARG:CD	2.61	0.77
1:M:208:ARG:NH2	2:N:139:TRP:O	2.17	0.77
1:E:208:ARG:NH2	2:F:139:TRP:O	2.17	0.77
2:F:287:PRO:HD2	2:F:332:SER:O	1.86	0.76
2:F:420:LEU:HD22	2:J:294:LYS:HE3	1.66	0.76
2:F:203:ARG:CD	4:L:21:DT:C7	2.64	0.76
1:A:208:ARG:NH2	2:B:139:TRP:O	2.17	0.76
1:I:208:ARG:NH2	2:J:139:TRP:O	2.17	0.76
3:C:34:G:H1	3:C:40:C:H42	1.34	0.75
2:F:184:PHE:CE1	2:N:200:ILE:CD1	2.69	0.75
3:K:34:G:H1	3:K:40:C:H42	1.35	0.75
3:C:28:A:H2'	3:C:29:G:H8	1.50	0.75
2:F:200:ILE:HD11	2:N:184:PHE:CD1	2.22	0.75
3:G:28:A:H2'	3:G:29:G:H8	1.50	0.75
2:N:166:LEU:HD22	2:N:257:ASN:HB3	1.69	0.75
2:F:200:ILE:HD11	2:N:184:PHE:CE1	2.22	0.74
3:K:28:A:H2'	3:K:29:G:H8	1.50	0.74
1:M:257:GLY:N	2:N:107:LYS:CD	2.50	0.74
2:B:203:ARG:CD	4:P:21:DT:H72	2.18	0.74
2:F:203:ARG:HD2	4:L:21:DT:C5	2.22	0.74
2:F:404:GLU:CG	2:J:380:ILE:CD1	2.65	0.74
2:B:200:ILE:CD1	2:J:184:PHE:CE1	2.71	0.74
1:M:257:GLY:CA	2:N:107:LYS:HE3	2.18	0.74
2:F:220:THR:HG21	2:N:239:GLY:O	1.87	0.74
2:F:420:LEU:CD2	2:J:294:LYS:NZ	2.36	0.73
3:G:34:G:H1	3:G:40:C:H42	1.34	0.73
3:O:34:G:H1	3:O:40:C:H42	1.34	0.73
3:O:39:A:H2'	3:O:40:C:N1	2.03	0.73
2:F:50:LEU:HD22	2:F:147:ARG:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:39:A:H2'	3:G:40:C:N1	2.03	0.73
1:A:79:SER:HB3	2:B:65:ASN:ND2	2.03	0.73
1:I:79:SER:HB3	2:J:65:ASN:ND2	2.03	0.73
3:C:39:A:H2'	3:C:40:C:N1	2.03	0.73
3:K:39:A:H2'	3:K:40:C:N1	2.03	0.73
3:O:28:A:H2'	3:O:29:G:H8	1.50	0.73
2:B:477:LEU:HD21	2:B:534:LEU:HD11	1.70	0.73
3:G:40:C:H2'	3:G:41:U:H6	1.53	0.73
3:K:40:C:H2'	3:K:41:U:H6	1.53	0.73
3:O:40:C:H2'	3:O:41:U:H6	1.53	0.73
3:K:35:U:H3'	3:K:36:U:C6	2.23	0.72
3:C:35:U:H3'	3:C:36:U:C6	2.23	0.72
2:F:404:GLU:HG2	2:J:380:ILE:HD11	1.70	0.72
3:C:40:C:H2'	3:C:41:U:H6	1.53	0.72
2:J:482:ASP:OD2	2:J:483:TYR:N	2.23	0.71
2:J:226:LYS:HA	2:J:229:VAL:HG13	1.73	0.71
2:J:618:LEU:HB2	2:J:619:ARG:HE	1.55	0.71
3:G:35:U:H3'	3:G:36:U:C6	2.23	0.71
2:B:618:LEU:HB2	2:B:619:ARG:HE	1.55	0.71
2:F:184:PHE:CD1	2:N:200:ILE:HD11	2.26	0.71
3:O:35:U:H3'	3:O:36:U:C6	2.23	0.70
2:F:31:ARG:NH1	2:J:294:LYS:CD	2.47	0.70
2:F:404:GLU:HG3	2:J:380:ILE:CD1	2.18	0.70
2:F:618:LEU:HB2	2:F:619:ARG:HE	1.55	0.70
2:J:173:TRP:HB3	2:J:230:ILE:HD12	1.72	0.70
1:M:155:ARG:HD3	1:M:161:ILE:HG21	1.74	0.70
2:N:618:LEU:HB2	2:N:619:ARG:HE	1.55	0.70
1:E:155:ARG:HD3	1:E:161:ILE:HG21	1.74	0.70
2:F:184:PHE:CE1	2:N:200:ILE:HD11	2.27	0.70
2:F:217:VAL:HG13	2:N:267:HIS:CG	2.26	0.70
4:H:21:DT:H72	2:J:203:ARG:CD	2.21	0.70
2:B:239:GLY:C	2:J:220:THR:HG21	2.16	0.69
4:D:21:DT:C5	2:N:203:ARG:HD2	2.25	0.69
2:B:315:GLU:HG2	2:B:316:LEU:HD22	1.74	0.69
2:J:86:ARG:H	2:J:86:ARG:HD3	1.56	0.69
1:M:79:SER:CB	2:N:65:ASN:HD21	2.05	0.69
2:B:200:ILE:HD13	2:J:184:PHE:CE1	2.27	0.69
2:F:203:ARG:CD	4:L:21:DT:C5	2.77	0.68
2:N:315:GLU:HG2	2:N:316:LEU:HD22	1.74	0.68
2:B:165:ASP:O	2:B:166:LEU:C	2.34	0.68
2:F:315:GLU:HG2	2:F:316:LEU:HD22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:LYS:HE3	2:N:420:LEU:HD22	1.74	0.68
2:F:267:HIS:CG	2:N:217:VAL:HG13	2.28	0.68
1:I:155:ARG:HD3	1:I:161:ILE:HG21	1.74	0.68
2:F:223:TYR:HD1	2:F:227:GLU:OE1	1.77	0.68
2:F:404:GLU:CD	2:J:376:ARG:HG3	2.19	0.67
2:J:644:LEU:HD21	2:J:654:THR:HG22	1.77	0.67
3:K:39:A:C8	3:K:39:A:H3'	2.30	0.67
2:B:644:LEU:HD21	2:B:654:THR:HG22	1.77	0.67
2:N:80:LYS:O	2:N:84:THR:HB	1.94	0.67
3:C:39:A:C8	3:C:39:A:H3'	2.30	0.67
2:F:404:GLU:OE2	2:J:376:ARG:CZ	2.41	0.67
2:F:506:LYS:HE3	2:F:507:LYS:H	1.60	0.67
2:J:86:ARG:HH11	2:J:86:ARG:N	1.93	0.67
2:N:644:LEU:HD21	2:N:654:THR:HG22	1.77	0.67
3:O:39:A:C8	3:O:39:A:H3'	2.30	0.67
1:A:155:ARG:HD3	1:A:161:ILE:HG21	1.74	0.67
2:B:404:GLU:CG	2:N:380:ILE:CD1	2.71	0.67
3:G:39:A:C8	3:G:39:A:H3'	2.30	0.67
2:N:506:LYS:HE3	2:N:507:LYS:H	1.60	0.67
1:A:24:LYS:HZ2	1:A:28:ILE:HG13	1.60	0.67
2:F:644:LEU:HD21	2:F:654:THR:HG22	1.77	0.67
1:M:257:GLY:N	2:N:107:LYS:CE	2.58	0.67
2:B:203:ARG:HD2	4:P:21:DT:C7	2.25	0.66
3:C:34:G:C6	3:C:35:U:C4	2.83	0.66
3:G:34:G:C6	3:G:35:U:C4	2.83	0.66
3:K:34:G:C6	3:K:35:U:C4	2.83	0.66
3:O:34:G:C6	3:O:35:U:C4	2.83	0.66
2:N:484:TYR:CZ	4:P:69:DA:C5	2.84	0.66
2:F:166:LEU:HD13	2:F:257:ASN:HB3	1.78	0.65
2:J:506:LYS:HE3	2:J:507:LYS:H	1.60	0.65
2:B:229:VAL:O	2:B:233:ILE:HG13	1.96	0.65
1:M:24:LYS:HZ2	1:M:28:ILE:HG13	1.62	0.65
2:N:483:TYR:O	2:N:484:TYR:HB2	1.97	0.65
2:B:506:LYS:HE3	2:B:507:LYS:H	1.60	0.65
3:O:34:G:H8	3:O:34:G:OP2	1.80	0.65
2:F:404:GLU:HG2	2:J:380:ILE:CD1	2.25	0.65
2:F:189:HIS:NE2	2:N:236:ALA:HA	2.11	0.65
3:G:34:G:H8	3:G:34:G:OP2	1.80	0.65
2:B:404:GLU:HG2	2:N:380:ILE:CD1	2.26	0.65
2:J:313:THR:HB	2:J:316:LEU:HD23	1.79	0.65
3:K:34:G:OP2	3:K:34:G:H8	1.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:A:H3'	3:C:39:A:H8	1.62	0.64
3:C:34:G:H8	3:C:34:G:OP2	1.80	0.64
2:J:277:PHE:CD2	4:P:16:DC:C4	2.85	0.64
3:K:39:A:H3'	3:K:39:A:H8	1.62	0.64
3:G:39:A:C8	3:G:40:C:C5	2.86	0.64
2:B:184:PHE:CE1	2:J:200:ILE:CD1	2.81	0.64
2:F:235:VAL:HG11	2:N:235:VAL:HG11	1.80	0.64
3:K:39:A:C8	3:K:40:C:C5	2.86	0.64
3:O:39:A:C8	3:O:40:C:C5	2.86	0.64
4:D:21:DT:C7	2:N:203:ARG:HD2	2.27	0.64
2:N:166:LEU:HD13	2:N:257:ASN:HD22	1.62	0.64
1:E:79:SER:CB	2:F:65:ASN:HD21	2.09	0.64
2:B:404:GLU:OE2	2:N:376:ARG:CZ	2.46	0.64
3:C:39:A:C8	3:C:40:C:C5	2.86	0.64
2:F:472:LYS:O	2:F:476:GLU:HG2	1.98	0.64
3:G:39:A:H3'	3:G:39:A:H8	1.62	0.64
2:F:189:HIS:HE1	2:N:236:ALA:O	1.81	0.63
1:A:156:LYS:O	1:A:157:ASP:C	2.39	0.63
2:F:480:GLU:HG3	2:F:481:PHE:CD1	2.33	0.63
3:O:39:A:H3'	3:O:39:A:H8	1.62	0.63
3:C:32:C:H2'	3:C:33:A:C8	2.34	0.63
2:J:480:GLU:OE1	2:J:481:PHE:N	2.32	0.63
1:M:24:LYS:NZ	1:M:28:ILE:HG13	2.14	0.63
3:C:40:C:H2'	3:C:41:U:C6	2.34	0.63
1:E:24:LYS:NZ	1:E:28:ILE:HG13	2.14	0.63
3:K:32:C:H2'	3:K:33:A:C8	2.34	0.63
4:H:21:DT:C7	2:J:203:ARG:HD2	2.29	0.63
3:K:40:C:H2'	3:K:41:U:C6	2.34	0.63
3:O:32:C:H2'	3:O:33:A:C8	2.34	0.63
3:G:32:C:H2'	3:G:33:A:C8	2.34	0.62
1:M:257:GLY:HA2	2:N:107:LYS:CE	2.29	0.62
2:F:50:LEU:CD2	2:F:147:ARG:HB3	2.28	0.62
2:F:203:ARG:NH1	4:L:21:DT:C4	2.66	0.62
1:I:156:LYS:O	1:I:157:ASP:C	2.39	0.62
2:F:161:THR:O	2:F:164:ILE:HG22	1.99	0.62
2:F:420:LEU:CB	2:J:294:LYS:HZ1	2.11	0.62
3:C:33:A:N1	3:C:34:G:C6	2.68	0.62
3:G:40:C:H2'	3:G:41:U:C6	2.34	0.62
3:K:33:A:N1	3:K:34:G:C6	2.68	0.62
3:O:33:A:N1	3:O:34:G:C6	2.68	0.62
3:C:42:G:H4'	3:C:42:G:OP1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:33:A:N1	3:G:34:G:C6	2.68	0.62
3:O:40:C:H2'	3:O:41:U:C6	2.34	0.62
3:G:35:U:O4	3:G:39:A:C2	2.53	0.62
1:I:24:LYS:NZ	1:I:28:ILE:HG13	2.14	0.62
3:O:35:U:O4	3:O:39:A:C2	2.53	0.62
1:A:24:LYS:NZ	1:A:28:ILE:HG13	2.14	0.62
3:K:35:U:O4	3:K:39:A:C2	2.53	0.62
2:F:189:HIS:NE2	2:N:236:ALA:O	2.33	0.61
2:B:203:ARG:HD2	4:P:21:DT:C4	2.35	0.61
2:J:403:LEU:HD12	2:J:423:ILE:CG2	2.26	0.61
3:K:42:G:H4'	3:K:42:G:OP1	1.99	0.61
2:B:380:ILE:CD1	2:N:404:GLU:HG2	2.29	0.61
4:L:71:DT:C4	4:L:72:DT:O4	2.53	0.61
3:C:35:U:O4	3:C:39:A:C2	2.53	0.61
1:M:156:LYS:O	1:M:157:ASP:C	2.39	0.61
3:G:32:C:H2'	3:G:33:A:H8	1.65	0.61
1:M:291:CYS:HB3	1:M:297:VAL:HG12	1.83	0.61
2:N:474:ILE:HG12	2:N:495:ILE:CD1	2.31	0.61
3:O:34:G:OP2	3:O:34:G:C8	2.54	0.61
1:E:291:CYS:HB3	1:E:297:VAL:HG12	1.83	0.61
3:G:34:G:OP2	3:G:34:G:C8	2.54	0.61
3:O:42:G:H4'	3:O:42:G:OP1	2.00	0.61
2:B:431:LEU:HD21	2:B:447:ILE:HD13	1.83	0.60
1:I:24:LYS:HZ2	1:I:28:ILE:HG13	1.65	0.60
2:J:431:LEU:HD21	2:J:447:ILE:HD13	1.83	0.60
3:O:32:C:H2'	3:O:33:A:H8	1.65	0.60
2:F:172:ILE:O	2:F:176:ILE:HG13	2.01	0.60
2:J:225:TYR:O	2:J:229:VAL:HG12	2.01	0.60
4:D:21:DT:C5	2:N:203:ARG:CD	2.84	0.60
3:C:34:G:OP2	3:C:34:G:C8	2.54	0.60
1:E:156:LYS:O	1:E:157:ASP:C	2.39	0.60
2:F:477:LEU:HD21	2:F:534:LEU:HD11	1.82	0.60
2:F:431:LEU:HD21	2:F:447:ILE:HD13	1.83	0.60
2:J:226:LYS:HA	2:J:229:VAL:CG1	2.31	0.60
3:K:34:G:OP2	3:K:34:G:C8	2.54	0.60
2:J:311:LYS:O	2:J:321:ARG:HG2	2.02	0.60
3:K:32:C:H2'	3:K:33:A:H8	1.65	0.60
2:F:404:GLU:CD	2:J:376:ARG:NH1	2.58	0.60
3:G:42:G:H4'	3:G:42:G:OP1	2.00	0.60
2:N:540:THR:HG23	2:N:541:THR:HG23	1.83	0.60
2:B:483:TYR:CZ	3:C:79:U:C4	2.89	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:540:THR:HG23	2:F:541:THR:HG23	1.84	0.60
2:N:431:LEU:HD21	2:N:447:ILE:HD13	1.83	0.60
2:N:484:TYR:CE2	4:P:69:DA:C6	2.90	0.60
3:C:32:C:H2'	3:C:33:A:H8	1.65	0.60
2:J:161:THR:O	2:J:164:ILE:HG12	2.02	0.60
2:J:468:PRO:HA	2:J:471:GLU:CD	2.27	0.59
2:J:540:THR:HG23	2:J:541:THR:HG23	1.83	0.59
2:B:540:THR:HG23	2:B:541:THR:HG23	1.84	0.59
1:M:79:SER:HB3	2:N:65:ASN:ND2	2.16	0.59
2:N:474:ILE:HG12	2:N:495:ILE:HD13	1.84	0.59
2:N:166:LEU:HD13	2:N:257:ASN:ND2	2.17	0.59
1:A:291:CYS:HB3	1:A:297:VAL:HG12	1.83	0.59
3:G:40:C:C5	3:G:41:U:C5	2.91	0.59
1:I:291:CYS:HB3	1:I:297:VAL:HG12	1.83	0.59
3:O:40:C:C5	3:O:41:U:C5	2.91	0.59
2:J:315:GLU:HG2	2:J:316:LEU:HD13	1.83	0.59
2:N:472:LYS:O	2:N:476:GLU:HG2	2.02	0.59
2:B:184:PHE:CE1	2:J:200:ILE:HD13	2.37	0.59
2:F:31:ARG:HH21	2:J:295:LEU:HD11	1.68	0.59
2:N:231:ASN:O	2:N:235:VAL:HG13	2.03	0.59
3:C:40:C:C5	3:C:41:U:C5	2.91	0.59
4:H:21:DT:C7	2:J:203:ARG:CD	2.81	0.59
4:D:24:DG:H3'	2:F:81:LYS:NZ	2.18	0.58
4:H:67:DC:O5'	4:H:67:DC:H6	1.85	0.58
3:K:40:C:C5	3:K:41:U:C5	2.91	0.58
3:C:34:G:H1	3:C:40:C:N4	2.01	0.58
3:C:39:A:C8	3:C:39:A:C3'	2.86	0.58
3:K:34:G:H1	3:K:40:C:N4	2.01	0.58
1:E:20:VAL:HG23	1:E:21:GLU:CG	2.27	0.58
3:K:39:A:C8	3:K:39:A:C3'	2.86	0.58
1:I:156:LYS:NZ	1:I:156:LYS:HA	2.19	0.58
2:J:226:LYS:O	2:J:229:VAL:HG13	2.03	0.58
1:A:20:VAL:HG23	1:A:21:GLU:CG	2.26	0.58
2:B:236:ALA:O	2:J:189:HIS:CE1	2.56	0.58
1:A:156:LYS:HA	1:A:156:LYS:NZ	2.19	0.58
2:J:472:LYS:HB2	2:J:472:LYS:NZ	2.18	0.58
1:M:20:VAL:HG23	1:M:21:GLU:CG	2.26	0.58
2:F:717:ASP:O	2:F:721:GLN:HG2	2.04	0.58
1:I:20:VAL:HG23	1:I:21:GLU:CG	2.27	0.58
2:N:717:ASP:O	2:N:721:GLN:HG2	2.04	0.58
3:O:36:U:O2	3:O:39:A:N3	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:483:TYR:O	2:B:484:TYR:CB	2.51	0.58
2:N:79:ILE:O	2:N:83:VAL:HG22	2.04	0.58
3:C:26:G:H5''	3:C:26:G:H8	1.69	0.57
2:J:323:LYS:O	2:J:323:LYS:HG3	2.04	0.57
2:B:224:THR:OG1	2:B:227:GLU:HG3	2.04	0.57
1:E:156:LYS:NZ	1:E:156:LYS:HA	2.19	0.57
3:K:26:G:H8	3:K:26:G:H5''	1.70	0.57
1:M:156:LYS:HA	1:M:156:LYS:NZ	2.19	0.57
3:G:36:U:O2	3:G:39:A:N3	2.37	0.57
4:H:16:DC:H2''	4:H:17:DA:C8	2.39	0.57
2:J:403:LEU:CD1	2:J:423:ILE:HG22	2.29	0.57
4:P:16:DC:H2''	4:P:17:DA:C8	2.39	0.57
2:B:482:ASP:N	2:B:482:ASP:OD1	2.36	0.57
2:B:86:ARG:O	2:B:86:ARG:HD3	2.04	0.57
3:C:36:U:O2	3:C:39:A:C2	2.58	0.57
3:K:36:U:O2	3:K:39:A:C2	2.58	0.57
2:J:717:ASP:O	2:J:721:GLN:HG2	2.04	0.57
4:L:16:DC:H2''	4:L:17:DA:C8	2.39	0.57
1:M:257:GLY:CA	2:N:107:LYS:CE	2.82	0.57
2:B:102:LYS:O	2:B:106:VAL:HG23	2.05	0.57
2:B:200:ILE:HD11	2:J:184:PHE:CE1	2.38	0.57
2:B:203:ARG:HD2	4:P:21:DT:O4	2.03	0.57
2:B:220:THR:HG21	2:J:238:LYS:O	2.05	0.57
2:B:717:ASP:O	2:B:721:GLN:HG2	2.04	0.57
3:C:36:U:O2	3:C:39:A:N3	2.37	0.57
4:H:21:DT:C5	2:J:203:ARG:HD2	2.39	0.57
3:O:26:G:H5''	3:O:26:G:H8	1.70	0.57
3:O:39:A:C8	3:O:39:A:C3'	2.86	0.57
1:A:200:ASP:OD2	1:A:200:ASP:N	2.38	0.57
3:G:26:G:H8	3:G:26:G:H5''	1.69	0.57
1:I:200:ASP:OD2	1:I:200:ASP:N	2.38	0.57
2:J:102:LYS:O	2:J:106:VAL:HG23	2.05	0.57
3:O:36:U:O2	3:O:39:A:C2	2.58	0.57
4:D:21:DT:C4	2:N:203:ARG:NH1	2.73	0.57
3:K:36:U:O2	3:K:39:A:N3	2.37	0.57
3:C:17:A:C2	3:C:18:G:C4	2.93	0.57
4:D:16:DC:H2''	4:D:17:DA:C8	2.39	0.57
3:G:39:A:C8	3:G:39:A:C3'	2.86	0.57
3:K:17:A:C2	3:K:18:G:C4	2.93	0.57
2:F:102:LYS:O	2:F:106:VAL:HG23	2.05	0.56
3:G:36:U:O2	3:G:39:A:C2	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:GLU:OE2	2:N:376:ARG:CG	2.45	0.56
2:F:200:ILE:HD13	2:N:184:PHE:CE1	2.41	0.56
3:G:17:A:C2	3:G:18:G:C4	2.93	0.56
3:O:17:A:C2	3:O:18:G:C4	2.93	0.56
3:C:33:A:H2'	3:C:34:G:C8	2.40	0.56
3:K:33:A:H2'	3:K:34:G:C8	2.40	0.56
2:F:173:TRP:O	2:F:174:LYS:C	2.48	0.56
2:F:703:ASN:O	2:F:707:GLU:HG2	2.05	0.56
3:O:34:G:H1	3:O:40:C:N4	2.01	0.56
1:A:26:ASN:HB3	1:A:31:SER:O	2.05	0.56
2:J:484:TYR:CE1	4:L:69:DA:C6	2.93	0.56
2:N:703:ASN:O	2:N:707:GLU:HG2	2.05	0.56
2:F:493:LYS:O	2:F:497:LEU:HG	2.06	0.56
2:N:493:LYS:O	2:N:497:LEU:HG	2.06	0.56
1:E:26:ASN:HB3	1:E:31:SER:O	2.05	0.56
3:G:35:U:H2'	3:G:36:U:O4'	2.06	0.56
3:G:40:C:C4	3:G:41:U:C4	2.94	0.56
1:I:26:ASN:HB3	1:I:31:SER:O	2.05	0.56
3:O:35:U:H2'	3:O:36:U:O4'	2.06	0.56
2:B:703:ASN:O	2:B:707:GLU:HG2	2.05	0.55
3:G:34:G:H1	3:G:40:C:N4	2.01	0.55
1:E:200:ASP:OD2	1:E:200:ASP:N	2.38	0.55
3:G:33:A:H2'	3:G:34:G:C8	2.41	0.55
1:M:200:ASP:OD2	1:M:200:ASP:N	2.38	0.55
3:O:40:C:C4	3:O:41:U:C4	2.95	0.55
3:K:35:U:H2'	3:K:36:U:O4'	2.06	0.55
1:M:26:ASN:HB3	1:M:31:SER:O	2.05	0.55
3:O:33:A:H2'	3:O:34:G:C8	2.40	0.55
2:B:493:LYS:O	2:B:497:LEU:HG	2.06	0.55
3:G:39:A:H3'	3:G:39:A:OP2	2.06	0.55
2:J:703:ASN:O	2:J:707:GLU:HG2	2.05	0.55
1:E:24:LYS:HE3	1:E:28:ILE:HD11	1.88	0.55
2:B:226:LYS:O	2:B:229:VAL:HG22	2.07	0.55
2:F:200:ILE:CG2	2:N:182:PHE:CB	2.77	0.55
2:J:405:LEU:HD21	2:J:730:ILE:HD13	1.89	0.55
2:B:677:LYS:O	2:B:681:ASN:HB2	2.07	0.55
3:C:40:C:C4	3:C:41:U:C4	2.94	0.55
2:J:480:GLU:O	2:J:481:PHE:HB2	2.07	0.55
2:J:493:LYS:O	2:J:497:LEU:HG	2.06	0.55
3:O:39:A:H3'	3:O:39:A:OP2	2.06	0.55
1:M:24:LYS:HE3	1:M:28:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ARG:HA	2:B:86:ARG:NE	2.22	0.55
3:C:35:U:H2'	3:C:36:U:O4'	2.06	0.55
2:N:482:ASP:C	2:N:482:ASP:OD2	2.48	0.55
3:C:35:U:H2'	3:C:36:U:C1'	2.37	0.54
4:D:16:DC:C4	2:F:277:PHE:CD2	2.95	0.54
3:K:40:C:C4	3:K:41:U:C4	2.94	0.54
2:N:175:LEU:HD11	2:N:269:LEU:CD1	2.22	0.54
3:C:39:A:H3'	3:C:39:A:OP2	2.06	0.54
1:I:24:LYS:HE3	1:I:28:ILE:HD11	1.88	0.54
2:J:677:LYS:O	2:J:681:ASN:HB2	2.07	0.54
3:K:35:U:H2'	3:K:36:U:C1'	2.37	0.54
2:N:677:LYS:O	2:N:681:ASN:HB2	2.07	0.54
2:F:235:VAL:HG12	2:N:231:ASN:HB3	1.88	0.54
2:J:483:TYR:O	2:J:484:TYR:HB2	2.07	0.54
2:N:173:TRP:HB3	2:N:230:ILE:CD1	2.38	0.54
3:K:39:A:H3'	3:K:39:A:OP2	2.06	0.54
3:O:44:A:C6	3:O:45:U:C4	2.95	0.54
3:O:35:U:H2'	3:O:36:U:C1'	2.37	0.54
1:A:24:LYS:HE3	1:A:28:ILE:HD11	1.88	0.54
2:F:677:LYS:O	2:F:681:ASN:HB2	2.07	0.54
2:J:166:LEU:HD12	2:J:167:TYR:N	2.23	0.54
1:M:312:GLU:HA	1:M:315:LYS:NZ	2.23	0.54
2:J:313:THR:HB	2:J:316:LEU:CD2	2.38	0.54
1:M:151:GLU:HG2	1:M:160:MET:HG2	1.90	0.54
1:E:312:GLU:HA	1:E:315:LYS:NZ	2.23	0.54
3:G:35:U:H2'	3:G:36:U:C1'	2.37	0.54
1:E:151:GLU:HG2	1:E:160:MET:HG2	1.90	0.54
4:L:16:DC:C4	2:N:277:PHE:CD2	2.96	0.54
3:O:44:A:C2	3:O:45:U:C2	2.95	0.54
2:B:55:VAL:HA	2:F:56:ILE:HD11	1.90	0.53
2:B:164:ILE:C	2:B:166:LEU:H	2.16	0.53
2:F:484:TYR:CZ	4:H:69:DA:C6	2.95	0.53
2:F:478:THR:O	2:F:492:ARG:NH2	2.41	0.53
2:F:480:GLU:HG3	2:F:481:PHE:CG	2.44	0.53
2:J:277:PHE:HD2	4:P:16:DC:C4	2.25	0.53
2:N:542:THR:HG22	2:N:543:ILE:H	1.74	0.53
2:B:164:ILE:HG22	2:B:166:LEU:H	1.73	0.53
2:F:484:TYR:CE2	4:H:69:DA:N1	2.76	0.53
2:F:542:THR:HG22	2:F:543:ILE:H	1.74	0.53
2:J:226:LYS:O	2:J:230:ILE:HG12	2.08	0.53
2:F:200:ILE:CD1	2:N:184:PHE:CD1	2.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:312:GLU:HA	1:I:315:LYS:NZ	2.23	0.53
1:A:156:LYS:O	1:A:158:LYS:HD2	2.09	0.53
1:E:305:LYS:HB2	4:H:67:DC:O2	2.09	0.53
2:F:203:ARG:HD2	4:L:21:DT:C7	2.36	0.53
2:J:316:LEU:HD22	2:J:316:LEU:H	1.74	0.53
2:N:497:LEU:O	2:N:501:ILE:HG13	2.09	0.53
1:E:24:LYS:HZ2	1:E:28:ILE:HG13	1.73	0.52
1:I:156:LYS:O	1:I:158:LYS:HD2	2.09	0.52
2:F:184:PHE:CE1	2:N:200:ILE:HD13	2.45	0.52
2:J:88:ASN:ND2	4:P:24:DG:H21	2.07	0.52
2:J:170:ASN:O	2:J:171:PRO:C	2.46	0.52
1:A:151:GLU:HG2	1:A:160:MET:HG2	1.90	0.52
1:A:312:GLU:HA	1:A:315:LYS:NZ	2.23	0.52
2:B:200:ILE:HG23	2:J:182:PHE:HB3	1.90	0.52
2:F:420:LEU:CG	2:J:294:LYS:HZ1	2.21	0.52
2:F:497:LEU:O	2:F:501:ILE:HG13	2.09	0.52
1:M:156:LYS:O	1:M:158:LYS:HD2	2.09	0.52
2:N:312:LYS:HD2	2:N:323:LYS:HG3	1.91	0.52
2:F:217:VAL:HG13	2:N:267:HIS:CD2	2.44	0.52
2:B:189:HIS:HE2	2:J:236:ALA:HA	1.75	0.52
2:B:542:THR:HG22	2:B:543:ILE:H	1.74	0.52
3:C:40:C:C4	3:C:41:U:C5	2.98	0.52
2:J:164:ILE:HD11	2:J:258:SER:CB	2.40	0.52
2:J:542:THR:HG22	2:J:543:ILE:H	1.74	0.52
3:K:40:C:C4	3:K:41:U:C5	2.98	0.52
3:O:33:A:C6	3:O:34:G:C6	2.98	0.52
2:B:483:TYR:CE2	3:C:79:U:N3	2.77	0.52
2:B:497:LEU:O	2:B:501:ILE:HG13	2.09	0.52
3:G:33:A:C6	3:G:34:G:C6	2.98	0.52
1:I:151:GLU:HG2	1:I:160:MET:HG2	1.90	0.52
1:E:156:LYS:O	1:E:158:LYS:HD2	2.09	0.52
2:J:277:PHE:HE2	4:P:16:DC:C2	2.27	0.52
1:M:257:GLY:N	2:N:107:LYS:HD2	2.24	0.52
2:N:482:ASP:OD2	2:N:483:TYR:N	2.43	0.52
2:F:31:ARG:NH2	2:J:295:LEU:CD1	2.73	0.52
2:F:484:TYR:CE2	4:H:69:DA:C2	2.97	0.52
2:B:387:ARG:HH22	2:N:294:LYS:NZ	2.07	0.51
2:J:480:GLU:O	2:J:481:PHE:CB	2.58	0.51
2:J:497:LEU:O	2:J:501:ILE:HG13	2.09	0.51
2:J:484:TYR:CZ	4:L:69:DA:C6	2.97	0.51
3:O:40:C:C4	3:O:41:U:C5	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:DT:H2''	4:D:69:DA:H5''	1.93	0.51
2:F:267:HIS:CD2	2:N:217:VAL:HG13	2.45	0.51
2:B:732:SER:O	2:B:736:GLN:HG3	2.11	0.51
2:F:189:HIS:NE2	2:N:236:ALA:C	2.69	0.51
2:J:732:SER:O	2:J:736:GLN:HG3	2.11	0.51
4:L:16:DC:C2	2:N:277:PHE:HE2	2.28	0.51
2:B:294:LYS:HZ1	2:N:420:LEU:CB	2.24	0.51
2:F:158:TYR:C	2:F:159:ILE:HG13	2.34	0.51
2:B:203:ARG:HD2	4:P:21:DT:C5	2.45	0.51
3:G:40:C:C4	3:G:41:U:C5	2.98	0.51
3:K:33:A:C6	3:K:34:G:C6	2.98	0.51
4:L:69:DA:H8	4:L:69:DA:H5''	1.74	0.51
3:C:41:U:H3'	3:C:42:G:O4'	2.10	0.51
3:G:41:U:H3'	3:G:42:G:O4'	2.10	0.51
2:J:81:LYS:NZ	4:P:24:DG:H3'	2.26	0.51
3:K:41:U:H3'	3:K:42:G:O4'	2.10	0.51
2:N:480:GLU:CD	2:N:481:PHE:H	2.18	0.51
3:O:41:U:H3'	3:O:42:G:O4'	2.10	0.51
2:J:533:LYS:NZ	2:J:533:LYS:HB3	2.26	0.51
2:B:533:LYS:NZ	2:B:533:LYS:HB3	2.26	0.50
2:F:80:LYS:O	2:F:84:THR:HB	2.11	0.50
2:N:480:GLU:O	2:N:481:PHE:HB2	2.10	0.50
1:A:104:CYS:O	1:A:203:LEU:HD23	2.12	0.50
3:C:33:A:C6	3:C:34:G:C6	2.98	0.50
2:N:484:TYR:CE2	4:P:69:DA:C5	2.98	0.50
3:G:73:A:H2'	3:G:74:A:H8	1.77	0.50
1:I:104:CYS:O	1:I:203:LEU:HD23	2.12	0.50
4:D:24:DG:H3'	2:F:81:LYS:HZ2	1.75	0.50
1:A:156:LYS:HA	1:A:156:LYS:HZ2	1.75	0.50
2:F:479:LYS:N	2:F:479:LYS:HD2	2.26	0.50
2:F:732:SER:O	2:F:736:GLN:HG3	2.11	0.50
3:O:39:A:H3'	3:O:39:A:P	2.51	0.50
3:O:73:A:H2'	3:O:74:A:H8	1.77	0.50
2:F:404:GLU:OE2	2:J:376:ARG:CD	2.59	0.50
2:J:484:TYR:CZ	4:L:69:DA:N1	2.80	0.50
3:K:73:A:H2'	3:K:74:A:H8	1.77	0.50
3:C:39:A:H3'	3:C:39:A:P	2.51	0.50
4:D:16:DC:C4	2:F:277:PHE:HD2	2.30	0.50
3:G:39:A:H3'	3:G:39:A:P	2.51	0.50
4:P:68:DT:H71	4:P:69:DA:N6	2.27	0.50
1:A:305:LYS:HB2	4:D:67:DC:O2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:533:LYS:NZ	2:N:533:LYS:HB3	2.26	0.50
2:F:184:PHE:CD1	2:N:200:ILE:CD1	2.92	0.49
2:F:533:LYS:NZ	2:F:533:LYS:HB3	2.26	0.49
3:K:39:A:H3'	3:K:39:A:P	2.51	0.49
4:L:71:DT:C5	4:L:72:DT:H72	2.47	0.49
1:M:104:CYS:O	1:M:203:LEU:HD23	2.12	0.49
3:C:73:A:H2'	3:C:74:A:H8	1.77	0.49
1:E:79:SER:HB3	2:F:65:ASN:ND2	2.27	0.49
2:F:217:VAL:CG1	2:N:267:HIS:CG	2.95	0.49
2:F:482:ASP:C	2:F:482:ASP:OD2	2.55	0.49
2:B:380:ILE:CD1	2:N:404:GLU:CG	2.75	0.49
2:N:732:SER:O	2:N:736:GLN:HG3	2.11	0.49
1:A:97:HIS:CD2	1:A:203:LEU:HD13	2.47	0.49
1:E:154:ILE:HG12	1:E:155:ARG:N	2.28	0.49
2:J:226:LYS:CA	2:J:229:VAL:HG13	2.40	0.49
2:B:184:PHE:CE1	2:J:200:ILE:HD11	2.46	0.49
2:B:220:THR:OG1	2:J:239:GLY:HA3	2.13	0.49
1:E:26:ASN:HA	1:E:31:SER:OG	2.12	0.49
1:E:97:HIS:CD2	1:E:203:LEU:HD13	2.47	0.49
1:E:104:CYS:O	1:E:203:LEU:HD23	2.12	0.49
1:E:313:PHE:CD2	4:H:67:DC:N4	2.80	0.49
1:M:97:HIS:CD2	1:M:203:LEU:HD13	2.47	0.49
2:B:168:ASP:OD1	2:B:168:ASP:N	2.46	0.48
2:F:182:PHE:CB	2:N:200:ILE:CG2	2.81	0.48
2:F:203:ARG:CZ	4:L:21:DT:C4	2.96	0.48
1:M:154:ILE:HG12	1:M:155:ARG:N	2.28	0.48
2:B:630:ARG:HA	2:B:630:ARG:NE	2.29	0.48
4:D:70:DG:H2'	4:D:71:DT:H71	1.94	0.48
1:I:97:HIS:CD2	1:I:203:LEU:HD13	2.47	0.48
2:N:477:LEU:HD21	2:N:534:LEU:HD11	1.96	0.48
2:N:483:TYR:CZ	3:O:79:U:C4	3.01	0.48
1:A:26:ASN:HA	1:A:31:SER:OG	2.12	0.48
4:D:21:DT:C7	2:N:203:ARG:HH11	2.22	0.48
2:F:630:ARG:NE	2:F:630:ARG:HA	2.29	0.48
1:M:26:ASN:HA	1:M:31:SER:OG	2.12	0.48
1:I:26:ASN:HA	1:I:31:SER:OG	2.12	0.48
2:J:630:ARG:HA	2:J:630:ARG:NE	2.29	0.48
1:A:154:ILE:HG12	1:A:155:ARG:N	2.28	0.48
2:F:200:ILE:HG22	2:N:182:PHE:CD1	2.48	0.48
3:G:26:G:H5''	3:G:26:G:C8	2.49	0.48
2:J:110:PHE:O	2:J:114:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:257:GLY:CA	2:N:107:LYS:HD2	2.44	0.48
2:N:630:ARG:HA	2:N:630:ARG:NE	2.29	0.48
2:B:387:ARG:NH2	2:N:294:LYS:NZ	2.62	0.48
4:H:19:DT:H5'	4:H:19:DT:H6	1.79	0.48
2:J:482:ASP:OD2	2:J:482:ASP:C	2.56	0.48
2:N:482:ASP:OD1	3:O:79:U:N3	2.47	0.48
2:B:110:PHE:O	2:B:114:ILE:HG12	2.14	0.48
1:I:154:ILE:HG12	1:I:155:ARG:N	2.28	0.48
1:E:79:SER:CB	2:F:65:ASN:ND2	2.76	0.48
3:O:26:G:H5''	3:O:26:G:C8	2.49	0.48
2:F:501:ILE:HD11	2:F:526:ARG:HH12	1.79	0.48
2:B:212:ASP:HA	2:B:215:VAL:HG22	1.96	0.47
2:F:31:ARG:NH2	2:J:295:LEU:HD12	2.29	0.47
2:F:267:HIS:CG	2:N:217:VAL:CG1	2.96	0.47
2:B:182:PHE:HB3	2:J:200:ILE:HG23	1.95	0.47
2:F:86:ARG:HE	2:F:86:ARG:HA	1.79	0.47
2:F:173:TRP:HB3	2:F:230:ILE:CD1	2.44	0.47
2:N:501:ILE:HD11	2:N:526:ARG:HH12	1.79	0.47
2:B:294:LYS:CD	2:N:31:ARG:HH12	2.16	0.47
2:J:277:PHE:CE2	4:P:16:DC:C5	3.03	0.47
2:N:20:ARG:HG2	2:N:21:ASP:N	2.30	0.47
2:N:170:ASN:N	2:N:171:PRO:HD2	2.29	0.47
4:P:19:DT:H6	4:P:19:DT:H5'	1.79	0.47
2:F:20:ARG:HG2	2:F:21:ASP:N	2.30	0.47
2:F:110:PHE:O	2:F:114:ILE:HG12	2.14	0.47
3:G:44:A:O2'	3:G:45:U:H5'	2.14	0.47
2:J:233:ILE:O	2:J:237:ILE:HG23	2.15	0.47
2:F:480:GLU:O	2:F:481:PHE:HB2	2.14	0.47
2:N:173:TRP:HB3	2:N:230:ILE:HD11	1.95	0.47
2:B:484:TYR:CG	2:B:484:TYR:O	2.63	0.47
2:F:490:ARG:HA	2:F:493:LYS:NZ	2.30	0.47
2:N:110:PHE:O	2:N:114:ILE:HG12	2.14	0.47
2:N:490:ARG:HA	2:N:493:LYS:NZ	2.30	0.47
1:A:136:THR:HG22	1:A:136:THR:O	2.15	0.47
1:A:152:SER:HB3	1:A:155:ARG:HG2	1.97	0.47
3:C:33:A:H8	3:C:33:A:O5'	1.97	0.47
4:D:23:DT:H2''	4:D:24:DG:C8	2.50	0.47
2:F:479:LYS:HD2	2:F:479:LYS:H	1.80	0.47
4:H:21:DT:C5	2:J:203:ARG:NH1	2.82	0.47
4:H:23:DT:H2''	4:H:24:DG:C8	2.50	0.47
2:J:166:LEU:HD12	2:J:167:TYR:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:475:LYS:HZ2	2:J:475:LYS:HB3	1.80	0.47
2:J:506:LYS:HZ3	2:J:517:ARG:HD2	1.79	0.47
4:L:23:DT:H2''	4:L:24:DG:C8	2.50	0.47
3:O:33:A:H8	3:O:33:A:O5'	1.97	0.47
2:B:404:GLU:CD	2:N:376:ARG:NH1	2.65	0.47
2:F:628:LEU:HD12	2:F:628:LEU:HA	1.78	0.47
4:L:24:DG:H3'	2:N:81:LYS:NZ	2.30	0.47
1:M:257:GLY:HA2	2:N:107:LYS:HE3	1.91	0.47
4:P:23:DT:H2''	4:P:24:DG:C8	2.50	0.47
4:P:24:DG:H8	4:P:24:DG:H5''	1.80	0.47
3:G:33:A:H8	3:G:33:A:O5'	1.97	0.47
1:I:136:THR:HG22	1:I:136:THR:O	2.15	0.47
1:I:152:SER:HB3	1:I:155:ARG:HG2	1.97	0.47
3:K:26:G:H5''	3:K:26:G:C8	2.49	0.47
4:H:24:DG:H5''	4:H:24:DG:H8	1.80	0.47
1:M:136:THR:O	1:M:136:THR:HG22	2.15	0.47
3:C:26:G:H5''	3:C:26:G:C8	2.49	0.46
1:E:136:THR:O	1:E:136:THR:HG22	2.15	0.46
3:K:33:A:H8	3:K:33:A:O5'	1.97	0.46
2:J:82:ILE:HG23	4:P:24:DG:C2	2.50	0.46
2:J:477:LEU:HD21	2:J:534:LEU:HD11	1.96	0.46
4:L:19:DT:H6	4:L:19:DT:H5'	1.79	0.46
2:N:221:LYS:HD2	2:N:221:LYS:N	2.30	0.46
1:A:309:LYS:HB2	1:A:309:LYS:HE3	1.54	0.46
2:B:20:ARG:HG2	2:B:21:ASP:N	2.30	0.46
2:B:490:ARG:HA	2:B:493:LYS:NZ	2.30	0.46
2:F:182:PHE:CD1	2:N:200:ILE:HG22	2.50	0.46
4:L:24:DG:H8	4:L:24:DG:H5''	1.80	0.46
1:M:152:SER:HB3	1:M:155:ARG:HG2	1.97	0.46
4:D:24:DG:H8	4:D:24:DG:H5''	1.80	0.46
1:I:312:GLU:HA	1:I:315:LYS:HZ1	1.80	0.46
2:B:387:ARG:NH2	2:N:294:LYS:HZ3	2.14	0.46
2:B:506:LYS:HZ3	2:B:517:ARG:HD2	1.80	0.46
4:D:19:DT:H6	4:D:19:DT:H5'	1.79	0.46
4:D:26:DG:O6	2:F:87:LYS:NZ	2.48	0.46
1:A:162:ILE:HA	1:A:163:PRO:HD3	1.78	0.46
4:L:24:DG:H21	2:N:88:ASN:ND2	2.14	0.46
2:N:166:LEU:CD1	2:N:257:ASN:HD22	2.26	0.46
3:O:35:U:C4	3:O:36:U:N3	2.84	0.46
3:G:35:U:C4	3:G:36:U:N3	2.84	0.46
2:J:221:LYS:HD2	2:J:221:LYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:501:ILE:HD11	2:J:526:ARG:HH12	1.79	0.46
3:K:35:U:C4	3:K:36:U:N3	2.84	0.46
1:E:371:ASN:C	1:E:371:ASN:OD1	2.58	0.46
2:F:484:TYR:OH	4:H:69:DA:C6	2.69	0.46
1:I:309:LYS:HB2	1:I:309:LYS:HE3	1.54	0.46
1:I:371:ASN:OD1	1:I:371:ASN:C	2.58	0.46
1:M:371:ASN:OD1	1:M:371:ASN:C	2.59	0.46
1:A:371:ASN:OD1	1:A:371:ASN:C	2.58	0.46
2:B:501:ILE:HD11	2:B:526:ARG:HH12	1.79	0.46
1:E:152:SER:HB3	1:E:155:ARG:HG2	1.97	0.46
2:J:20:ARG:HG2	2:J:21:ASP:N	2.30	0.46
2:B:164:ILE:O	2:B:166:LEU:N	2.49	0.45
3:C:17:A:O2'	3:C:18:G:P	2.74	0.45
3:C:35:U:C4	3:C:36:U:N3	2.84	0.45
2:B:166:LEU:HD23	2:B:166:LEU:HA	1.67	0.45
2:B:542:THR:HG22	2:B:543:ILE:N	2.32	0.45
4:D:4:DG:H5'	4:D:4:DG:H8	1.81	0.45
2:F:506:LYS:HE3	2:F:507:LYS:N	2.29	0.45
1:I:160:MET:HB3	1:I:160:MET:HE2	1.66	0.45
2:J:277:PHE:CE2	4:P:16:DC:C4	3.04	0.45
2:J:490:ARG:HA	2:J:493:LYS:NZ	2.30	0.45
4:L:4:DG:H5'	4:L:4:DG:H8	1.81	0.45
2:N:480:GLU:HG3	2:N:481:PHE:CD2	2.51	0.45
3:O:17:A:O2'	3:O:18:G:P	2.74	0.45
4:P:4:DG:H2''	4:P:5:DA:O5'	2.17	0.45
4:P:7:DC:H2''	4:P:8:DA:C8	2.51	0.45
3:G:40:C:H2'	3:G:41:U:O4'	2.16	0.45
2:J:482:ASP:OD1	3:K:79:U:C2	2.69	0.45
2:J:553:LEU:HD23	2:J:553:LEU:HA	1.79	0.45
3:K:17:A:O2'	3:K:18:G:P	2.74	0.45
1:M:51:PHE:CE1	1:M:164:MET:HE3	2.51	0.45
2:N:628:LEU:HD12	2:N:628:LEU:HA	1.78	0.45
1:A:51:PHE:CE1	1:A:164:MET:HE3	2.51	0.45
2:B:230:ILE:HD13	2:B:230:ILE:HA	1.85	0.45
1:E:51:PHE:CE1	1:E:164:MET:HE3	2.51	0.45
4:H:4:DG:H2''	4:H:5:DA:O5'	2.17	0.45
1:I:156:LYS:HA	1:I:156:LYS:HZ2	1.81	0.45
2:J:542:THR:HG22	2:J:543:ILE:N	2.32	0.45
2:B:472:LYS:HB2	2:B:472:LYS:NZ	2.31	0.45
3:C:22:C:N4	3:C:23:U:O4	2.50	0.45
4:D:14:DT:H2''	4:D:15:DA:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:TYR:HB2	1:E:245:ILE:HD12	1.98	0.45
2:F:542:THR:HG22	2:F:543:ILE:N	2.32	0.45
3:G:17:A:O2'	3:G:18:G:P	2.74	0.45
4:L:68:DT:H2''	4:L:69:DA:O5'	2.17	0.45
2:N:480:GLU:OE1	2:N:480:GLU:HA	2.17	0.45
2:N:506:LYS:HE3	2:N:507:LYS:N	2.29	0.45
3:O:40:C:H2'	3:O:41:U:O4'	2.16	0.45
2:B:103:SER:O	2:B:107:LYS:HG2	2.17	0.45
1:E:49:LYS:HE3	4:H:75:DT:H1'	1.99	0.45
2:J:277:PHE:CE2	4:P:16:DC:C6	3.04	0.45
2:J:316:LEU:HD22	2:J:316:LEU:N	2.31	0.45
3:K:22:C:N4	3:K:23:U:O4	2.50	0.45
3:K:40:C:H2'	3:K:41:U:O4'	2.16	0.45
4:L:14:DT:H2''	4:L:15:DA:C8	2.52	0.45
1:M:49:LYS:HE3	4:P:75:DT:H1'	1.99	0.45
1:M:103:TYR:HB2	1:M:245:ILE:HD12	1.98	0.45
1:M:291:CYS:HA	1:M:295:ILE:HG12	1.99	0.45
2:N:472:LYS:HB2	2:N:472:LYS:NZ	2.31	0.45
2:N:542:THR:HG22	2:N:543:ILE:N	2.32	0.45
1:A:155:ARG:O	1:A:156:LYS:NZ	2.50	0.45
1:A:167:ARG:HA	3:C:74:A:O2'	2.17	0.45
2:B:294:LYS:NZ	2:N:420:LEU:HD23	2.30	0.45
4:D:7:DC:H2''	4:D:8:DA:C8	2.51	0.45
2:F:90:GLY:O	2:F:94:LYS:HG3	2.16	0.45
2:F:742:GLU:OE1	2:F:742:GLU:HA	2.17	0.45
1:I:51:PHE:CE1	1:I:164:MET:HE3	2.51	0.45
1:M:160:MET:HE2	1:M:160:MET:HB3	1.66	0.45
2:B:189:HIS:CE1	2:J:236:ALA:O	2.70	0.45
1:E:155:ARG:O	1:E:156:LYS:NZ	2.50	0.45
1:E:291:CYS:HA	1:E:295:ILE:HG12	1.99	0.45
4:H:7:DC:H2''	4:H:8:DA:C8	2.51	0.45
1:I:155:ARG:O	1:I:156:LYS:NZ	2.50	0.45
2:J:103:SER:O	2:J:107:LYS:HG2	2.17	0.45
2:N:742:GLU:OE1	2:N:742:GLU:HA	2.17	0.45
4:D:4:DG:H2''	4:D:5:DA:O5'	2.17	0.45
2:F:103:SER:O	2:F:107:LYS:HG2	2.17	0.45
1:I:167:ARG:HA	3:K:74:A:O2'	2.17	0.45
2:N:177:SER:OG	2:N:226:LYS:HD2	2.16	0.45
2:B:742:GLU:HA	2:B:742:GLU:OE1	2.17	0.45
3:C:40:C:H2'	3:C:41:U:O4'	2.16	0.45
4:H:14:DT:H2''	4:H:15:DA:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:472:LYS:HB2	2:F:472:LYS:NZ	2.31	0.44
3:G:22:C:N4	3:G:23:U:O4	2.50	0.44
3:G:46:A:N6	3:G:66:C:C6	2.85	0.44
2:N:520:LEU:HD23	2:N:520:LEU:HA	1.83	0.44
2:B:506:LYS:HE3	2:B:507:LYS:N	2.29	0.44
3:G:17:A:C6	3:G:18:G:C5	3.06	0.44
4:H:4:DG:H5'	4:H:4:DG:H8	1.81	0.44
2:J:267:HIS:C	2:J:267:HIS:HD1	2.25	0.44
2:J:742:GLU:HA	2:J:742:GLU:OE1	2.17	0.44
1:M:79:SER:CB	2:N:65:ASN:ND2	2.71	0.44
1:M:155:ARG:O	1:M:156:LYS:NZ	2.50	0.44
2:N:267:HIS:HD1	2:N:267:HIS:C	2.25	0.44
2:N:506:LYS:HZ3	2:N:517:ARG:HD2	1.82	0.44
3:O:44:A:C6	3:O:45:U:N3	2.85	0.44
1:E:167:ARG:HA	3:G:74:A:O2'	2.17	0.44
2:F:484:TYR:OH	4:H:69:DA:N6	2.50	0.44
2:J:226:LYS:C	2:J:229:VAL:HG13	2.42	0.44
1:M:167:ARG:HA	3:O:74:A:O2'	2.17	0.44
3:O:40:C:HO2'	3:O:41:U:P	2.40	0.44
2:B:267:HIS:HD1	2:B:267:HIS:C	2.25	0.44
2:F:267:HIS:C	2:F:267:HIS:HD1	2.25	0.44
4:L:7:DC:H2''	4:L:8:DA:C8	2.51	0.44
3:O:17:A:C6	3:O:18:G:C5	3.06	0.44
1:E:75:ILE:HA	1:E:76:PRO:HD3	1.87	0.44
1:I:291:CYS:HA	1:I:295:ILE:HG12	1.99	0.44
2:J:164:ILE:HD11	2:J:258:SER:HB3	2.00	0.44
2:J:164:ILE:HD11	2:J:258:SER:OG	2.17	0.44
3:K:35:U:C5	3:K:36:U:C4	3.06	0.44
2:N:553:LEU:HA	2:N:553:LEU:HD23	1.78	0.44
3:O:22:C:N4	3:O:23:U:O4	2.50	0.44
1:I:162:ILE:HA	1:I:163:PRO:HD3	1.78	0.44
4:L:4:DG:H2''	4:L:5:DA:O5'	2.17	0.44
2:N:175:LEU:HD21	2:N:269:LEU:HB2	2.00	0.44
1:A:291:CYS:HA	1:A:295:ILE:HG12	1.99	0.44
1:A:312:GLU:HA	1:A:315:LYS:HZ1	1.82	0.44
2:B:49:LYS:HD2	2:B:49:LYS:HA	1.78	0.44
2:B:200:ILE:HD11	2:J:184:PHE:CD1	2.52	0.44
2:B:553:LEU:HD23	2:B:553:LEU:HA	1.78	0.44
2:F:702:LEU:O	2:F:706:ILE:HG13	2.18	0.44
4:H:68:DT:H2''	4:H:69:DA:C8	2.53	0.44
1:I:103:TYR:HB2	1:I:245:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:663:LEU:HD23	2:J:663:LEU:HA	1.89	0.44
2:N:702:LEU:O	2:N:706:ILE:HG13	2.18	0.44
4:P:4:DG:H5'	4:P:4:DG:H8	1.81	0.44
4:P:14:DT:H2''	4:P:15:DA:C8	2.52	0.44
1:A:49:LYS:HE3	4:D:75:DT:H1'	1.99	0.44
1:A:160:MET:HE2	1:A:160:MET:HB3	1.66	0.44
3:C:35:U:C5	3:C:36:U:C4	3.06	0.44
4:D:21:DT:C4	2:N:203:ARG:CZ	3.01	0.44
2:F:506:LYS:HZ3	2:F:517:ARG:HD2	1.82	0.44
2:F:664:ARG:HA	2:F:673:ARG:CZ	2.48	0.44
2:J:506:LYS:HE3	2:J:507:LYS:N	2.29	0.44
2:N:484:TYR:CZ	4:P:69:DA:N7	2.86	0.44
2:B:387:ARG:HH22	2:N:294:LYS:HZ3	1.66	0.44
2:F:166:LEU:HD13	2:F:257:ASN:CB	2.44	0.44
1:I:49:LYS:HE3	4:L:75:DT:H1'	1.99	0.44
2:N:664:ARG:HA	2:N:673:ARG:CZ	2.48	0.44
3:O:35:U:C5	3:O:36:U:C4	3.06	0.44
2:B:79:ILE:O	2:B:83:VAL:HG22	2.18	0.43
3:C:17:A:C6	3:C:18:G:C5	3.06	0.43
3:G:35:U:C5	3:G:36:U:C4	3.06	0.43
2:J:177:SER:OG	2:J:226:LYS:HD2	2.18	0.43
3:K:17:A:C6	3:K:18:G:C5	3.05	0.43
1:M:24:LYS:O	1:M:24:LYS:HG3	2.18	0.43
1:M:309:LYS:HE3	1:M:309:LYS:HB2	1.54	0.43
1:A:266:LEU:HB2	1:A:350:PHE:CZ	2.54	0.43
2:B:170:ASN:N	2:B:171:PRO:HD2	2.33	0.43
3:C:33:A:C2	3:C:34:G:C5	3.07	0.43
1:E:30:GLN:HE21	1:E:30:GLN:HB2	1.55	0.43
2:F:685:PHE:HD1	2:F:685:PHE:O	2.01	0.43
1:I:266:LEU:HB2	1:I:350:PHE:CZ	2.54	0.43
2:J:79:ILE:O	2:J:83:VAL:HG22	2.18	0.43
2:J:86:ARG:CZ	2:J:86:ARG:HB2	2.48	0.43
4:L:68:DT:C7	4:L:69:DA:N6	2.81	0.43
3:O:42:G:C8	3:O:42:G:H5''	2.54	0.43
3:O:44:A:N1	3:O:45:U:N3	2.66	0.43
2:B:702:LEU:O	2:B:706:ILE:HG13	2.18	0.43
1:E:156:LYS:HA	1:E:156:LYS:HZ2	1.82	0.43
2:F:79:ILE:O	2:F:83:VAL:HG22	2.18	0.43
2:J:277:PHE:HE2	4:P:16:DC:C6	2.36	0.43
2:J:665:LYS:HE2	2:J:665:LYS:HB2	1.85	0.43
2:J:702:LEU:O	2:J:706:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:33:A:C2	3:K:34:G:C5	3.07	0.43
1:A:103:TYR:HB2	1:A:245:ILE:HD12	1.98	0.43
2:B:203:ARG:CD	4:P:21:DT:C7	2.84	0.43
2:B:466:LEU:HG	2:B:502:GLN:HG2	2.01	0.43
2:B:685:PHE:HD1	2:B:685:PHE:O	2.01	0.43
2:F:177:SER:OG	2:F:226:LYS:HD2	2.18	0.43
3:G:42:G:C8	3:G:42:G:H5''	2.54	0.43
4:H:21:DT:C6	2:J:203:ARG:NH1	2.86	0.43
2:J:685:PHE:HD1	2:J:685:PHE:O	2.01	0.43
1:M:257:GLY:H	2:N:107:LYS:CE	2.18	0.43
2:B:138:MET:HE3	2:B:138:MET:HB3	1.87	0.43
2:B:404:GLU:HG3	2:N:380:ILE:CD1	2.29	0.43
2:F:294:LYS:HB3	2:F:294:LYS:HE3	1.64	0.43
3:G:33:A:C2	3:G:34:G:C5	3.07	0.43
2:J:466:LEU:HG	2:J:502:GLN:HG2	2.01	0.43
3:O:33:A:C2	3:O:34:G:C5	3.07	0.43
2:B:232:TYR:O	2:B:235:VAL:HG22	2.18	0.43
1:E:24:LYS:O	1:E:24:LYS:HG3	2.18	0.43
4:H:71:DT:H2'	4:H:72:DT:C6	2.53	0.43
1:M:75:ILE:HA	1:M:76:PRO:HD3	1.73	0.43
2:N:685:PHE:HD1	2:N:685:PHE:O	2.01	0.43
2:B:664:ARG:HA	2:B:673:ARG:CZ	2.48	0.43
2:F:723:LEU:HD23	2:F:723:LEU:HA	1.85	0.43
4:H:24:DG:C8	4:H:24:DG:H5''	2.54	0.43
2:J:138:MET:HE3	2:J:138:MET:HB3	1.87	0.43
3:K:42:G:C8	3:K:42:G:H5''	2.53	0.43
3:O:36:U:O2	3:O:36:U:H2'	2.19	0.43
1:A:90:TYR:O	1:A:93:TYR:HB3	2.19	0.43
1:E:160:MET:HE2	1:E:160:MET:HB3	1.66	0.43
3:G:56:C:H6	3:G:56:C:H2'	1.67	0.43
2:J:490:ARG:HA	2:J:493:LYS:HZ3	1.83	0.43
1:M:266:LEU:HB2	1:M:350:PHE:CZ	2.54	0.43
2:B:476:GLU:OE1	2:B:476:GLU:HA	2.19	0.43
3:C:40:C:C6	3:C:41:U:C5	3.07	0.43
4:D:24:DG:C8	4:D:24:DG:H5''	2.54	0.43
1:I:90:TYR:O	1:I:93:TYR:HB3	2.19	0.43
4:P:71:DT:H2'	4:P:72:DT:C6	2.53	0.43
4:D:71:DT:H2'	4:D:72:DT:C6	2.53	0.43
2:F:165:ASP:O	2:F:166:LEU:HB2	2.17	0.43
3:K:40:C:C6	3:K:41:U:C5	3.07	0.43
2:N:100:LEU:CD2	2:N:146:VAL:HG13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:70:DG:C2'	4:D:71:DT:H71	2.49	0.42
1:E:33:ILE:HG23	1:E:34:PRO:HD2	2.01	0.42
3:G:36:U:O2	3:G:36:U:H2'	2.19	0.42
3:G:40:C:C6	3:G:41:U:C5	3.07	0.42
4:L:24:DG:C8	4:L:24:DG:H5''	2.54	0.42
4:P:24:DG:C8	4:P:24:DG:H5''	2.54	0.42
1:A:26:ASN:HA	1:A:31:SER:HG	1.84	0.42
3:C:42:G:C8	3:C:42:G:H5''	2.54	0.42
2:F:166:LEU:CD1	2:F:257:ASN:HB2	2.47	0.42
4:L:16:DC:C4	2:N:277:PHE:HD2	2.36	0.42
3:O:40:C:C6	3:O:41:U:C5	3.07	0.42
2:B:88:ASN:ND2	4:H:24:DG:H21	2.18	0.42
2:B:520:LEU:HD23	2:B:520:LEU:HA	1.83	0.42
3:C:17:A:C6	3:C:18:G:C6	3.08	0.42
2:F:520:LEU:HD23	2:F:520:LEU:HA	1.83	0.42
4:H:19:DT:H5'	4:H:19:DT:C6	2.54	0.42
2:J:664:ARG:HA	2:J:673:ARG:CZ	2.48	0.42
3:K:17:A:C6	3:K:18:G:C6	3.08	0.42
2:N:473:MET:HE3	2:N:473:MET:HB2	1.84	0.42
4:P:19:DT:H5'	4:P:19:DT:C6	2.54	0.42
2:B:164:ILE:C	2:B:166:LEU:N	2.72	0.42
2:B:294:LYS:NZ	2:N:420:LEU:HA	2.33	0.42
1:E:266:LEU:HB2	1:E:350:PHE:CZ	2.54	0.42
2:F:553:LEU:HD23	2:F:553:LEU:HA	1.78	0.42
2:J:49:LYS:HD2	2:J:49:LYS:HA	1.78	0.42
1:M:33:ILE:HG23	1:M:34:PRO:HD2	2.01	0.42
1:A:238:TYR:O	1:A:239:ILE:HD13	2.20	0.42
2:B:268:LEU:O	2:B:272:LEU:HG	2.19	0.42
2:B:663:LEU:HD23	2:B:663:LEU:HA	1.89	0.42
3:C:35:U:N3	3:C:36:U:C2	2.88	0.42
4:D:16:DC:C6	2:F:277:PHE:CE2	3.08	0.42
2:F:56:ILE:HA	2:F:57:PRO:HD3	1.75	0.42
1:I:238:TYR:O	1:I:239:ILE:HD13	2.20	0.42
2:J:344:LYS:HD2	2:J:381:PHE:HB3	2.02	0.42
3:K:34:G:C5	3:K:35:U:C5	3.08	0.42
2:N:506:LYS:HD2	2:N:506:LYS:HA	1.96	0.42
1:A:33:ILE:HG23	1:A:34:PRO:HD2	2.01	0.42
2:B:344:LYS:HD2	2:B:381:PHE:HB3	2.02	0.42
2:F:189:HIS:O	2:F:193:VAL:HG23	2.20	0.42
2:F:466:LEU:HG	2:F:502:GLN:HG2	2.01	0.42
2:F:482:ASP:OD2	2:F:483:TYR:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:268:LEU:O	2:J:272:LEU:HG	2.20	0.42
2:J:284:ILE:O	2:J:331:TYR:HA	2.20	0.42
2:N:189:HIS:O	2:N:193:VAL:HG23	2.20	0.42
2:N:233:ILE:O	2:N:237:ILE:HG23	2.19	0.42
3:O:34:G:C5	3:O:35:U:C5	3.08	0.42
3:G:17:A:C6	3:G:18:G:C6	3.08	0.42
2:J:189:HIS:O	2:J:193:VAL:HG23	2.20	0.42
2:J:484:TYR:CE1	4:L:69:DA:C5	3.07	0.42
1:M:90:TYR:O	1:M:93:TYR:HB3	2.19	0.42
2:N:483:TYR:CE2	3:O:79:U:N3	2.87	0.42
2:N:723:LEU:HD23	2:N:723:LEU:HA	1.84	0.42
3:O:17:A:C6	3:O:18:G:C6	3.08	0.42
3:O:56:C:H6	3:O:56:C:H2'	1.67	0.42
2:B:189:HIS:O	2:B:193:VAL:HG23	2.20	0.42
2:B:284:ILE:O	2:B:331:TYR:HA	2.20	0.42
2:B:294:LYS:HZ1	2:N:420:LEU:HA	1.84	0.42
3:C:34:G:C5	3:C:35:U:C5	3.08	0.42
3:C:36:U:O2	3:C:36:U:H2'	2.19	0.42
3:K:35:U:N3	3:K:36:U:C2	2.88	0.42
2:N:466:LEU:HG	2:N:502:GLN:HG2	2.01	0.42
2:B:665:LYS:HE2	2:B:665:LYS:HB2	1.85	0.42
3:C:62:C:O2'	3:C:63:U:C5	2.69	0.42
3:G:34:G:C5	3:G:35:U:C5	3.08	0.42
1:I:30:GLN:HE21	1:I:30:GLN:HB2	1.55	0.42
2:J:506:LYS:HD2	2:J:506:LYS:HA	1.96	0.42
3:K:36:U:O2	3:K:36:U:H2'	2.19	0.42
2:F:203:ARG:NE	4:L:21:DT:C4	2.88	0.42
2:F:268:LEU:O	2:F:272:LEU:HG	2.19	0.42
3:G:35:U:N3	3:G:36:U:C2	2.88	0.42
3:K:63:U:H3'	3:K:64:A:C8	2.55	0.42
1:M:30:GLN:HE21	1:M:30:GLN:HB2	1.55	0.42
2:N:524:SER:HA	2:N:527:ILE:HG22	2.02	0.42
3:O:35:U:N3	3:O:36:U:C2	2.88	0.42
3:O:41:U:H3'	3:O:42:G:H8	1.85	0.42
2:B:622:LEU:HD12	2:B:622:LEU:HA	1.86	0.41
3:C:63:U:H3'	3:C:64:A:C8	2.55	0.41
1:E:90:TYR:O	1:E:93:TYR:HB3	2.19	0.41
2:F:524:SER:HA	2:F:527:ILE:HG22	2.02	0.41
3:G:41:U:H3'	3:G:42:G:H8	1.85	0.41
3:G:56:C:H4'	3:G:57:C:OP2	2.20	0.41
1:I:33:ILE:HG23	1:I:34:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:524:SER:HA	2:J:527:ILE:HG22	2.02	0.41
2:N:670:GLU:O	2:N:674:GLU:HG2	2.20	0.41
1:A:78:ASN:ND2	2:B:64:TYR:O	2.52	0.41
2:B:628:LEU:HA	2:B:628:LEU:HD12	1.78	0.41
4:L:19:DT:H5'	4:L:19:DT:C6	2.54	0.41
2:B:490:ARG:HA	2:B:493:LYS:HZ3	1.84	0.41
3:C:41:U:C3'	3:C:42:G:O4'	2.68	0.41
4:D:16:DC:C2	2:F:277:PHE:HE2	2.38	0.41
4:D:19:DT:H5'	4:D:19:DT:C6	2.54	0.41
2:F:641:GLU:OE2	2:F:641:GLU:HA	2.20	0.41
2:J:88:ASN:HD21	4:P:24:DG:H21	1.69	0.41
2:N:284:ILE:O	2:N:331:TYR:HA	2.20	0.41
1:A:125:SER:OG	1:A:126:PRO:HD3	2.20	0.41
2:B:524:SER:HA	2:B:527:ILE:HG22	2.02	0.41
2:F:344:LYS:HD2	2:F:381:PHE:HB3	2.02	0.41
2:F:670:GLU:O	2:F:674:GLU:HG2	2.21	0.41
3:K:41:U:C3'	3:K:42:G:O4'	2.68	0.41
1:M:125:SER:OG	1:M:126:PRO:HD3	2.20	0.41
1:M:257:GLY:HA2	2:N:107:LYS:HD2	2.02	0.41
3:O:56:C:H4'	3:O:57:C:OP2	2.20	0.41
2:F:506:LYS:HD2	2:F:506:LYS:HA	1.96	0.41
1:I:125:SER:OG	1:I:126:PRO:HD3	2.20	0.41
2:J:622:LEU:HD12	2:J:622:LEU:HA	1.86	0.41
3:K:39:A:C8	3:K:39:A:OP2	2.74	0.41
2:N:305:LYS:HZ2	2:N:305:LYS:HG2	1.77	0.41
2:B:170:ASN:OD1	2:B:170:ASN:O	2.38	0.41
2:B:404:GLU:CD	2:N:376:ARG:HG3	2.41	0.41
2:B:641:GLU:HA	2:B:641:GLU:OE2	2.20	0.41
3:C:39:A:C8	3:C:39:A:OP2	2.74	0.41
2:J:277:PHE:HE2	4:P:16:DC:N1	2.19	0.41
1:M:238:TYR:O	1:M:239:ILE:HD13	2.20	0.41
2:N:268:LEU:O	2:N:272:LEU:HG	2.19	0.41
2:N:641:GLU:OE2	2:N:641:GLU:HA	2.20	0.41
2:B:200:ILE:CG2	2:J:182:PHE:HB3	2.50	0.41
1:E:125:SER:OG	1:E:126:PRO:HD3	2.20	0.41
3:G:63:U:H3'	3:G:64:A:C8	2.55	0.41
2:N:100:LEU:HD21	2:N:146:VAL:HG13	2.02	0.41
2:N:311:LYS:O	2:N:321:ARG:HG2	2.20	0.41
1:A:158:LYS:HE3	1:A:158:LYS:HA	2.02	0.41
2:B:506:LYS:HD2	2:B:506:LYS:HA	1.96	0.41
2:B:670:GLU:O	2:B:674:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:TYR:O	1:E:239:ILE:HD13	2.20	0.41
1:I:206:ASN:HA	1:I:207:PRO:HD3	1.88	0.41
2:J:641:GLU:OE2	2:J:641:GLU:HA	2.20	0.41
2:J:670:GLU:O	2:J:674:GLU:HG2	2.21	0.41
2:N:344:LYS:HD2	2:N:381:PHE:HB3	2.02	0.41
1:A:157:ASP:O	1:A:157:ASP:CG	2.63	0.41
1:A:334:ILE:O	1:A:337:VAL:HG22	2.21	0.41
2:B:80:LYS:O	2:B:84:THR:HB	2.21	0.41
1:E:162:ILE:HA	1:E:163:PRO:HD3	1.78	0.41
2:F:168:ASP:O	2:F:168:ASP:CG	2.63	0.41
2:F:473:MET:HE3	2:F:473:MET:HB2	1.84	0.41
1:I:158:LYS:HE3	1:I:158:LYS:HA	2.02	0.41
2:J:95:HIS:CE1	4:P:15:DA:N6	2.89	0.41
2:J:520:LEU:HD23	2:J:520:LEU:HA	1.83	0.41
3:K:56:C:H4'	3:K:57:C:OP2	2.20	0.41
3:O:63:U:H3'	3:O:64:A:C8	2.55	0.41
2:B:121:ASN:OD1	2:B:121:ASN:C	2.64	0.41
2:B:482:ASP:HA	3:C:79:U:O2	2.21	0.41
3:C:56:C:H4'	3:C:57:C:OP2	2.20	0.41
3:G:41:U:C3'	3:G:42:G:O4'	2.68	0.41
1:I:158:LYS:HA	1:I:158:LYS:CE	2.51	0.41
1:I:334:ILE:O	1:I:337:VAL:HG22	2.21	0.41
2:J:92:PHE:O	2:J:96:ILE:HG13	2.21	0.41
2:N:112:GLU:O	2:N:116:ARG:HG2	2.21	0.41
2:N:478:THR:O	2:N:478:THR:HG22	2.20	0.41
2:F:112:GLU:O	2:F:116:ARG:HG2	2.21	0.40
2:B:112:GLU:O	2:B:116:ARG:HG2	2.21	0.40
1:E:158:LYS:CE	1:E:158:LYS:HA	2.51	0.40
2:F:164:ILE:HD13	2:F:164:ILE:HG21	1.69	0.40
1:I:26:ASN:HA	1:I:31:SER:HG	1.86	0.40
2:J:121:ASN:OD1	2:J:121:ASN:C	2.64	0.40
1:A:30:GLN:HE21	1:A:30:GLN:HB2	1.55	0.40
1:A:158:LYS:HA	1:A:158:LYS:CE	2.51	0.40
2:B:473:MET:HE3	2:B:473:MET:HB2	1.84	0.40
3:C:53:U:H5''	3:C:54:C:H5	1.87	0.40
4:D:15:DA:N6	2:F:95:HIS:CE1	2.89	0.40
2:F:138:MET:HE3	2:F:138:MET:HB3	1.87	0.40
3:K:41:U:H3'	3:K:42:G:H8	1.85	0.40
1:M:158:LYS:CE	1:M:158:LYS:HA	2.51	0.40
1:M:334:ILE:O	1:M:337:VAL:HG22	2.21	0.40
3:O:41:U:C3'	3:O:42:G:O4'	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:U:H3'	3:C:42:G:H8	1.85	0.40
1:E:158:LYS:HA	1:E:158:LYS:HE3	2.02	0.40
2:F:165:ASP:OD1	2:F:165:ASP:N	2.53	0.40
3:G:39:A:C8	3:G:39:A:OP2	2.74	0.40
4:H:70:DG:H2'	4:H:71:DT:C6	2.57	0.40
1:I:24:LYS:O	1:I:24:LYS:HG3	2.18	0.40
2:J:86:ARG:HD3	2:J:86:ARG:N	2.30	0.40
3:K:53:U:H5''	3:K:54:C:H5	1.87	0.40
2:N:121:ASN:OD1	2:N:121:ASN:C	2.64	0.40
2:N:665:LYS:HE2	2:N:665:LYS:HB2	1.85	0.40
4:P:68:DT:C7	4:P:69:DA:N6	2.85	0.40
1:A:24:LYS:O	1:A:24:LYS:HG3	2.18	0.40
1:E:334:ILE:O	1:E:337:VAL:HG22	2.21	0.40
2:F:665:LYS:HE2	2:F:665:LYS:HB2	1.85	0.40
1:I:157:ASP:O	1:I:157:ASP:CG	2.63	0.40
2:J:628:LEU:HD12	2:J:628:LEU:HA	1.78	0.40
1:M:158:LYS:HA	1:M:158:LYS:HE3	2.02	0.40
1:M:257:GLY:CA	2:N:107:LYS:CD	2.99	0.40
3:O:39:A:C8	3:O:39:A:OP2	2.74	0.40
3:O:53:U:H5''	3:O:54:C:H5	1.87	0.40
4:P:70:DG:H2'	4:P:71:DT:C6	2.57	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	365/374 (98%)	355 (97%)	10 (3%)	0	100	100
1	E	365/374 (98%)	355 (97%)	10 (3%)	0	100	100
1	I	365/374 (98%)	355 (97%)	10 (3%)	0	100	100
1	M	365/374 (98%)	355 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	659/750 (88%)	638 (97%)	21 (3%)	0	100	100
2	F	659/750 (88%)	638 (97%)	21 (3%)	0	100	100
2	J	662/750 (88%)	639 (96%)	23 (4%)	0	100	100
2	N	664/750 (88%)	644 (97%)	20 (3%)	0	100	100
All	All	4104/4496 (91%)	3979 (97%)	125 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	338/345 (98%)	329 (97%)	9 (3%)	39	65
1	E	338/345 (98%)	329 (97%)	9 (3%)	39	65
1	I	338/345 (98%)	329 (97%)	9 (3%)	39	65
1	M	338/345 (98%)	328 (97%)	10 (3%)	36	63
2	B	631/701 (90%)	607 (96%)	24 (4%)	29	58
2	F	630/701 (90%)	603 (96%)	27 (4%)	26	55
2	J	632/701 (90%)	608 (96%)	24 (4%)	29	58
2	N	634/701 (90%)	610 (96%)	24 (4%)	29	58
All	All	3879/4184 (93%)	3743 (96%)	136 (4%)	32	60

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	21	GLU
1	A	30	GLN
1	A	154	ILE
1	A	156	LYS
1	A	200	ASP

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Mol	Chain	Res	Type
1	A	203	LEU
1	A	336	LEU
1	A	360	ASP
2	B	3	ILE
2	B	14	PHE
2	B	17	VAL
2	B	26	ASN
2	B	62	THR
2	B	67	VAL
2	B	87	LYS
2	B	99	THR
2	B	164	ILE
2	B	166	LEU
2	B	168	ASP
2	B	170	ASN
2	B	172	ILE
2	B	256	THR
2	B	289	VAL
2	B	323	LYS
2	B	324	THR
2	B	471	GLU
2	B	482	ASP
2	B	618	LEU
2	B	632	VAL
2	B	637	ASN
2	B	666	ASP
2	B	680	LYS
1	E	15	GLU
1	E	21	GLU
1	E	30	GLN
1	E	154	ILE
1	E	156	LYS
1	E	200	ASP
1	E	203	LEU
1	E	336	LEU
1	E	360	ASP
2	F	3	ILE
2	F	14	PHE
2	F	17	VAL
2	F	26	ASN
2	F	62	THR
2	F	67	VAL

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Mol	Chain	Res	Type
2	F	84	THR
2	F	86	ARG
2	F	87	LYS
2	F	94	LYS
2	F	159	ILE
2	F	164	ILE
2	F	172	ILE
2	F	221	LYS
2	F	256	THR
2	F	282	VAL
2	F	286	GLU
2	F	288	GLU
2	F	289	VAL
2	F	295	LEU
2	F	298	SER
2	F	471	GLU
2	F	618	LEU
2	F	632	VAL
2	F	637	ASN
2	F	666	ASP
2	F	680	LYS
1	I	15	GLU
1	I	21	GLU
1	I	30	GLN
1	I	154	ILE
1	I	156	LYS
1	I	200	ASP
1	I	203	LEU
1	I	336	LEU
1	I	360	ASP
2	J	3	ILE
2	J	14	PHE
2	J	17	VAL
2	J	26	ASN
2	J	62	THR
2	J	67	VAL
2	J	85	SER
2	J	86	ARG
2	J	94	LYS
2	J	164	ILE
2	J	229	VAL
2	J	234	LYS

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Mol	Chain	Res	Type
2	J	256	THR
2	J	289	VAL
2	J	316	LEU
2	J	325	PRO
2	J	470	PHE
2	J	480	GLU
2	J	484	TYR
2	J	618	LEU
2	J	632	VAL
2	J	637	ASN
2	J	666	ASP
2	J	680	LYS
1	M	15	GLU
1	M	21	GLU
1	M	30	GLN
1	M	154	ILE
1	M	156	LYS
1	M	200	ASP
1	M	203	LEU
1	M	278	THR
1	M	336	LEU
1	M	360	ASP
2	N	3	ILE
2	N	14	PHE
2	N	17	VAL
2	N	26	ASN
2	N	62	THR
2	N	67	VAL
2	N	84	THR
2	N	85	SER
2	N	91	ARG
2	N	102	LYS
2	N	165	ASP
2	N	174	LYS
2	N	240	ASP
2	N	256	THR
2	N	289	VAL
2	N	295	LEU
2	N	324	THR
2	N	471	GLU
2	N	474	ILE
2	N	618	LEU

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Mol	Chain	Res	Type
2	N	632	VAL
2	N	637	ASN
2	N	666	ASP
2	N	680	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	74	HIS
1	A	113	ASN
1	A	114	ASN
2	B	38	ASN
2	B	65	ASN
2	B	88	ASN
2	B	304	ASN
2	B	384	ASN
2	B	657	GLN
2	B	690	GLN
1	E	64	GLN
1	E	74	HIS
1	E	113	ASN
1	E	114	ASN
2	F	38	ASN
2	F	52	ASN
2	F	61	HIS
2	F	65	ASN
2	F	88	ASN
2	F	89	ASN
2	F	95	HIS
2	F	170	ASN
2	F	304	ASN
2	F	657	GLN
2	F	690	GLN
1	I	74	HIS
1	I	113	ASN
1	I	114	ASN
1	I	279	HIS
2	J	38	ASN
2	J	65	ASN
2	J	88	ASN
2	J	304	ASN

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Mol	Chain	Res	Type
2	J	657	GLN
2	J	690	GLN
1	M	26	ASN
1	M	64	GLN
1	M	74	HIS
1	M	113	ASN
1	M	114	ASN
2	N	38	ASN
2	N	65	ASN
2	N	88	ASN
2	N	257	ASN
2	N	304	ASN
2	N	384	ASN
2	N	657	GLN
2	N	690	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	62/83 (74%)	19 (30%)	4 (6%)
3	G	62/83 (74%)	20 (32%)	4 (6%)
3	K	62/83 (74%)	19 (30%)	4 (6%)
3	O	62/83 (74%)	19 (30%)	4 (6%)
All	All	248/332 (74%)	77 (31%)	16 (6%)

All (77) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	18	G
3	C	19	A
3	C	26	G
3	C	29	G
3	C	31	C
3	C	34	G
3	C	35	U
3	C	36	U
3	C	40	C
3	C	41	U
3	C	42	G
3	C	43	G
3	C	46	A

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Mol	Chain	Res	Type
3	C	53	U
3	C	54	C
3	C	56	C
3	C	63	U
3	C	76	A
3	C	80	A
3	G	18	G
3	G	19	A
3	G	26	G
3	G	29	G
3	G	31	C
3	G	34	G
3	G	35	U
3	G	36	U
3	G	40	C
3	G	41	U
3	G	42	G
3	G	43	G
3	G	44	A
3	G	46	A
3	G	53	U
3	G	54	C
3	G	56	C
3	G	63	U
3	G	76	A
3	G	80	A
3	K	18	G
3	K	19	A
3	K	26	G
3	K	29	G
3	K	31	C
3	K	34	G
3	K	35	U
3	K	36	U
3	K	40	C
3	K	41	U
3	K	42	G
3	K	43	G
3	K	46	A
3	K	53	U
3	K	54	C
3	K	56	C

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Mol	Chain	Res	Type
3	K	63	U
3	K	76	A
3	K	80	A
3	O	18	G
3	O	19	A
3	O	26	G
3	O	29	G
3	O	31	C
3	O	34	G
3	O	35	U
3	O	36	U
3	O	40	C
3	O	41	U
3	O	42	G
3	O	43	G
3	O	46	A
3	O	53	U
3	O	54	C
3	O	56	C
3	O	63	U
3	O	76	A
3	O	80	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	17	A
3	C	35	U
3	C	42	G
3	C	56	C
3	G	17	A
3	G	35	U
3	G	42	G
3	G	56	C
3	K	17	A
3	K	35	U
3	K	42	G
3	K	56	C
3	O	17	A
3	O	35	U
3	O	42	G
3	O	56	C

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](#)

There are no ligands in this entry.

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.

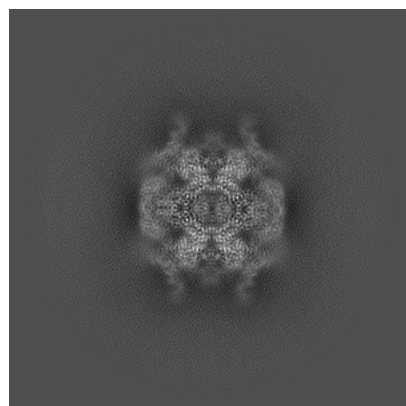
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-69132. These allow visual inspection of the internal detail of the map and identification of artifacts.

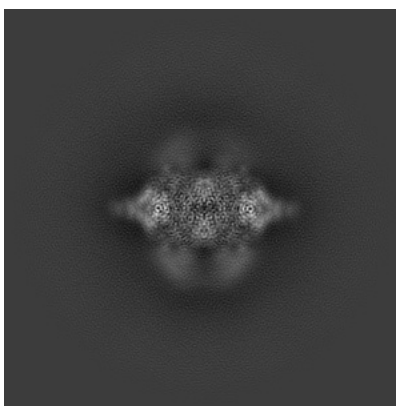
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

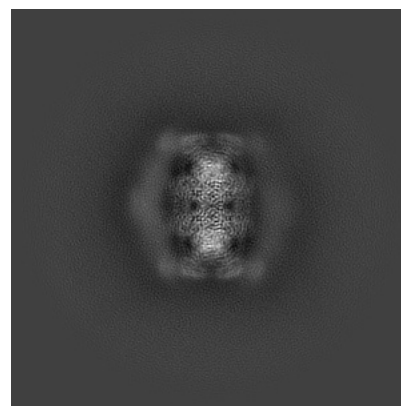
6.1.1 Primary map



X

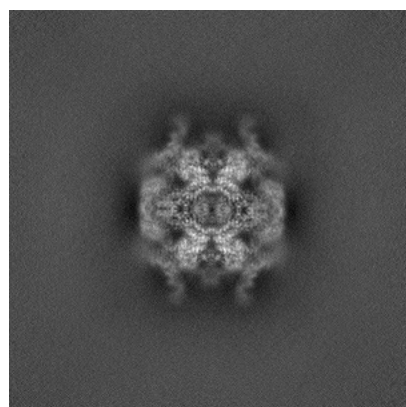


Y

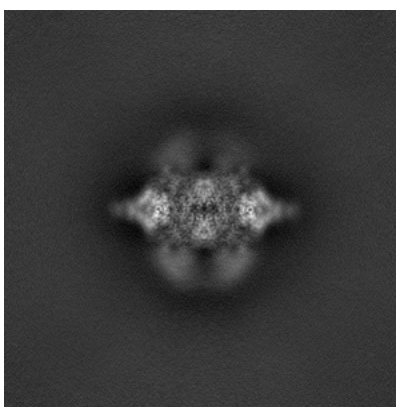


Z

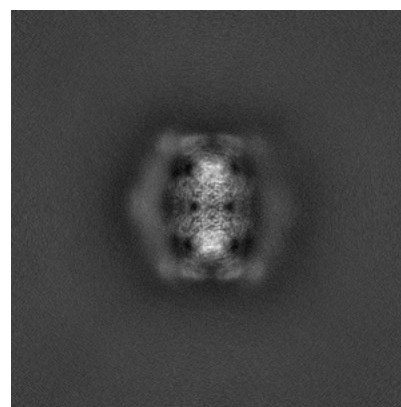
6.1.2 Raw map



X



Y

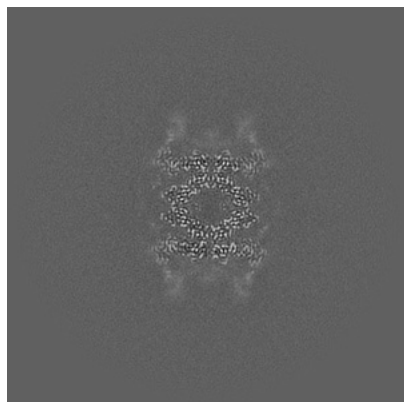


Z

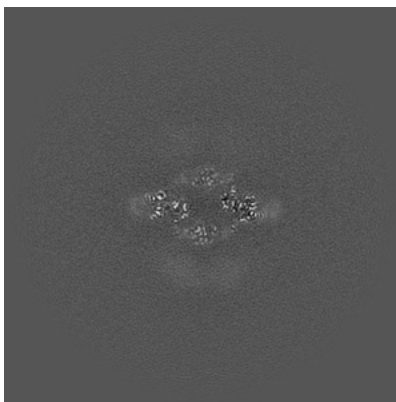
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

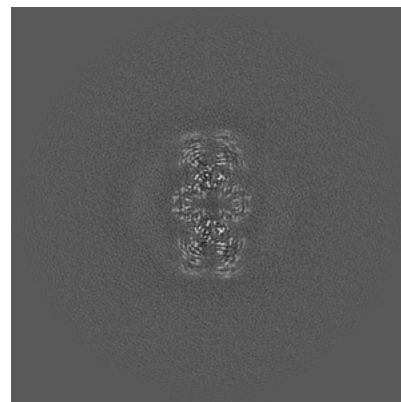
6.2.1 Primary map



X Index: 280

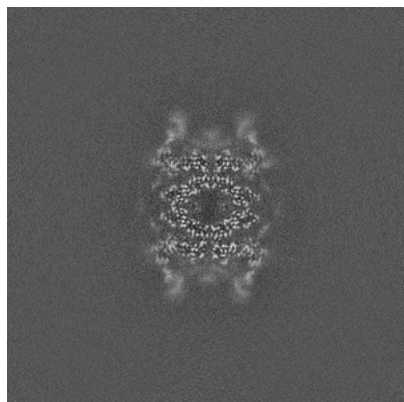


Y Index: 280

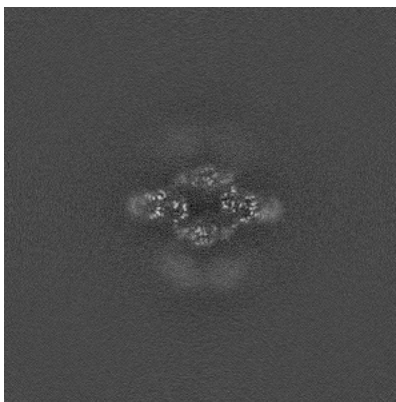


Z Index: 280

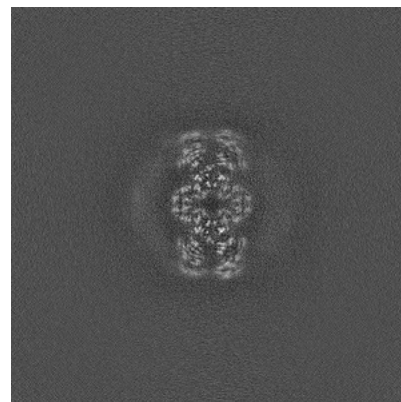
6.2.2 Raw map



X Index: 280



Y Index: 280

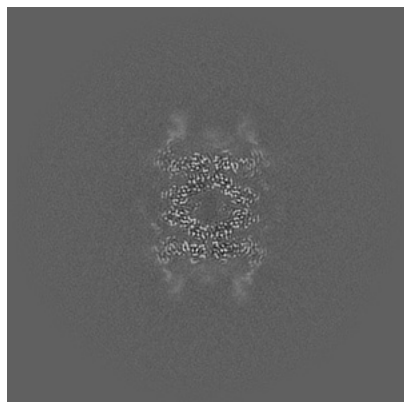


Z Index: 280

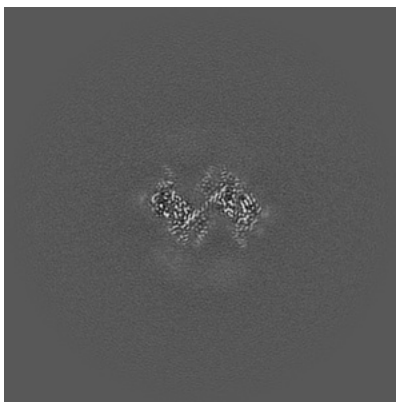
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

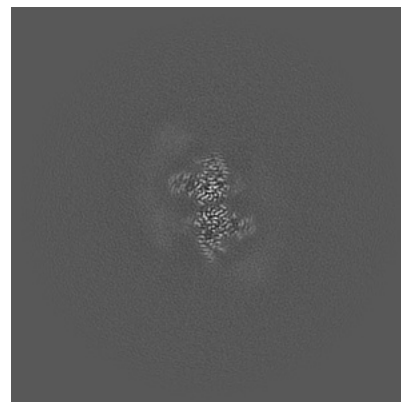
6.3.1 Primary map



X Index: 282

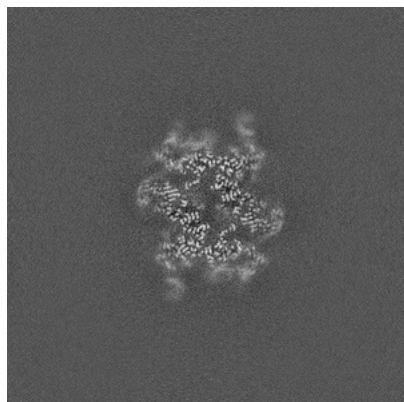


Y Index: 266

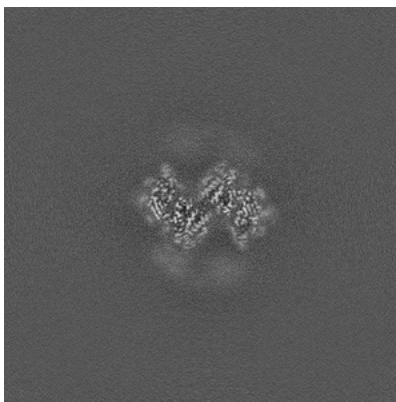


Z Index: 224

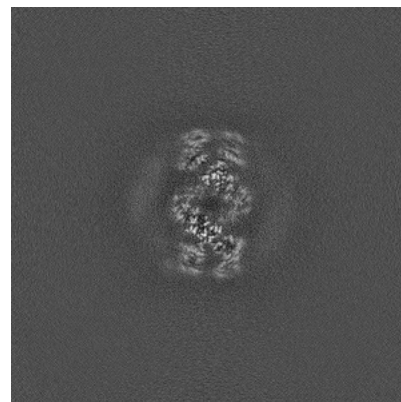
6.3.2 Raw map



X Index: 269



Y Index: 261

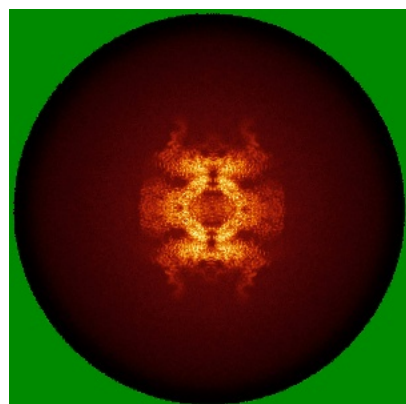


Z Index: 274

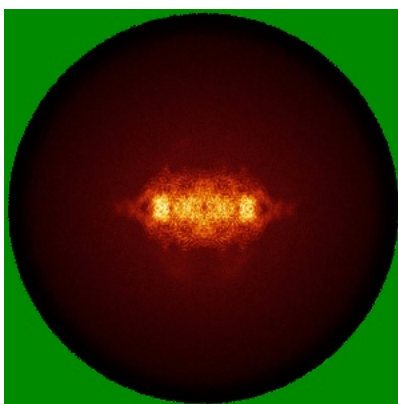
The images above show the largest variance slices of the map in three orthogonal directions.

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

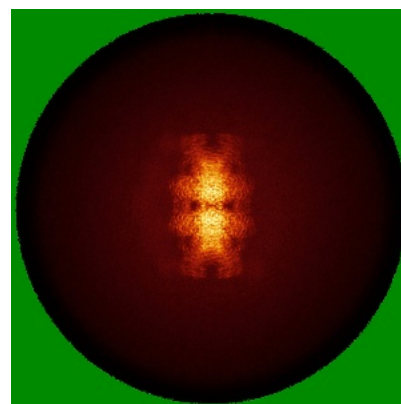
6.4.1 Primary map



X

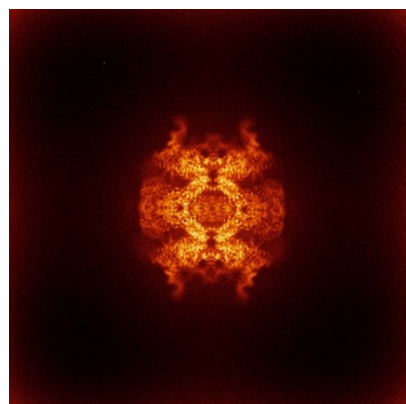


Y

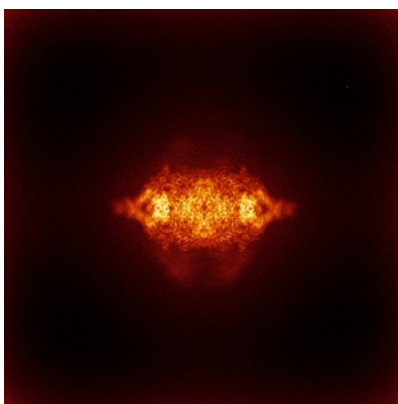


Z

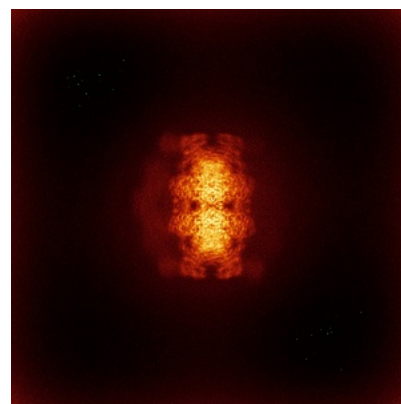
6.4.2 Raw map



X



Y

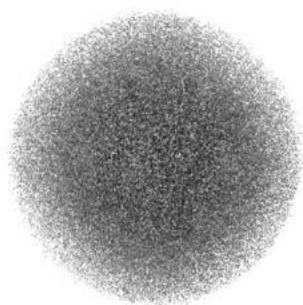


Z

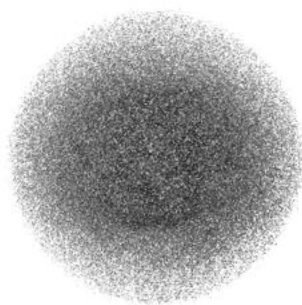
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

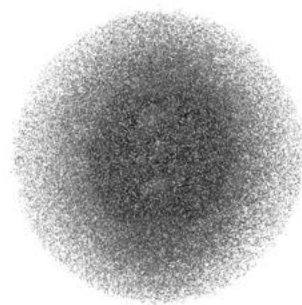
6.5.1 Primary map



X



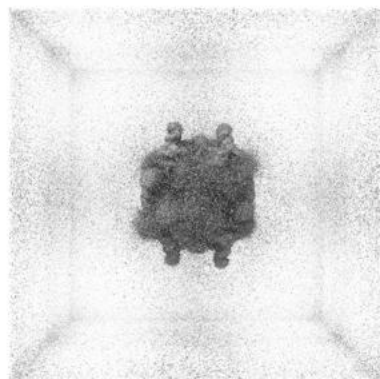
Y



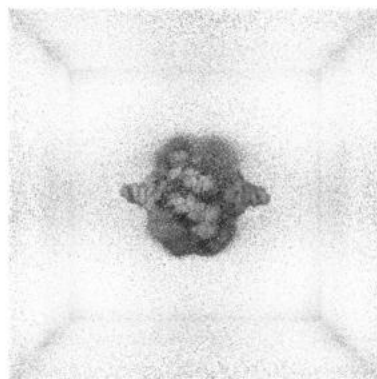
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

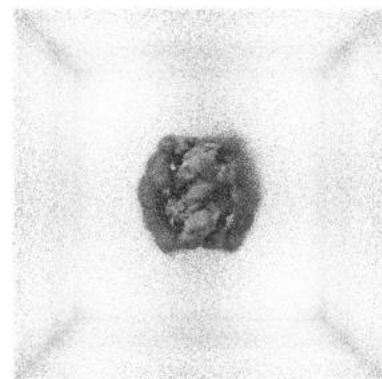
6.5.2 Raw map



X



Y



Z

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

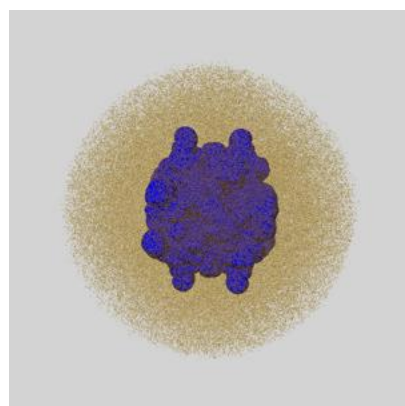
6.6 Mask visualisation [i](#)

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

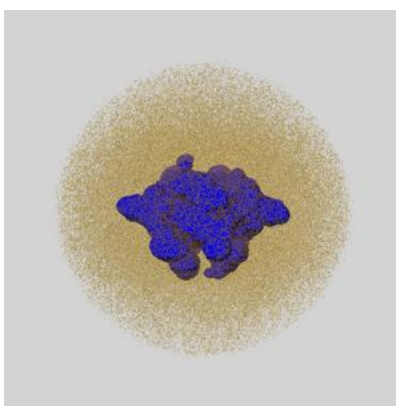
A mask typically either:

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

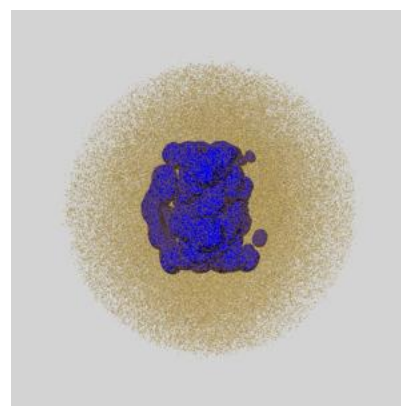
6.6.1 emd_69132_msk_1.map [i](#)



X



Y

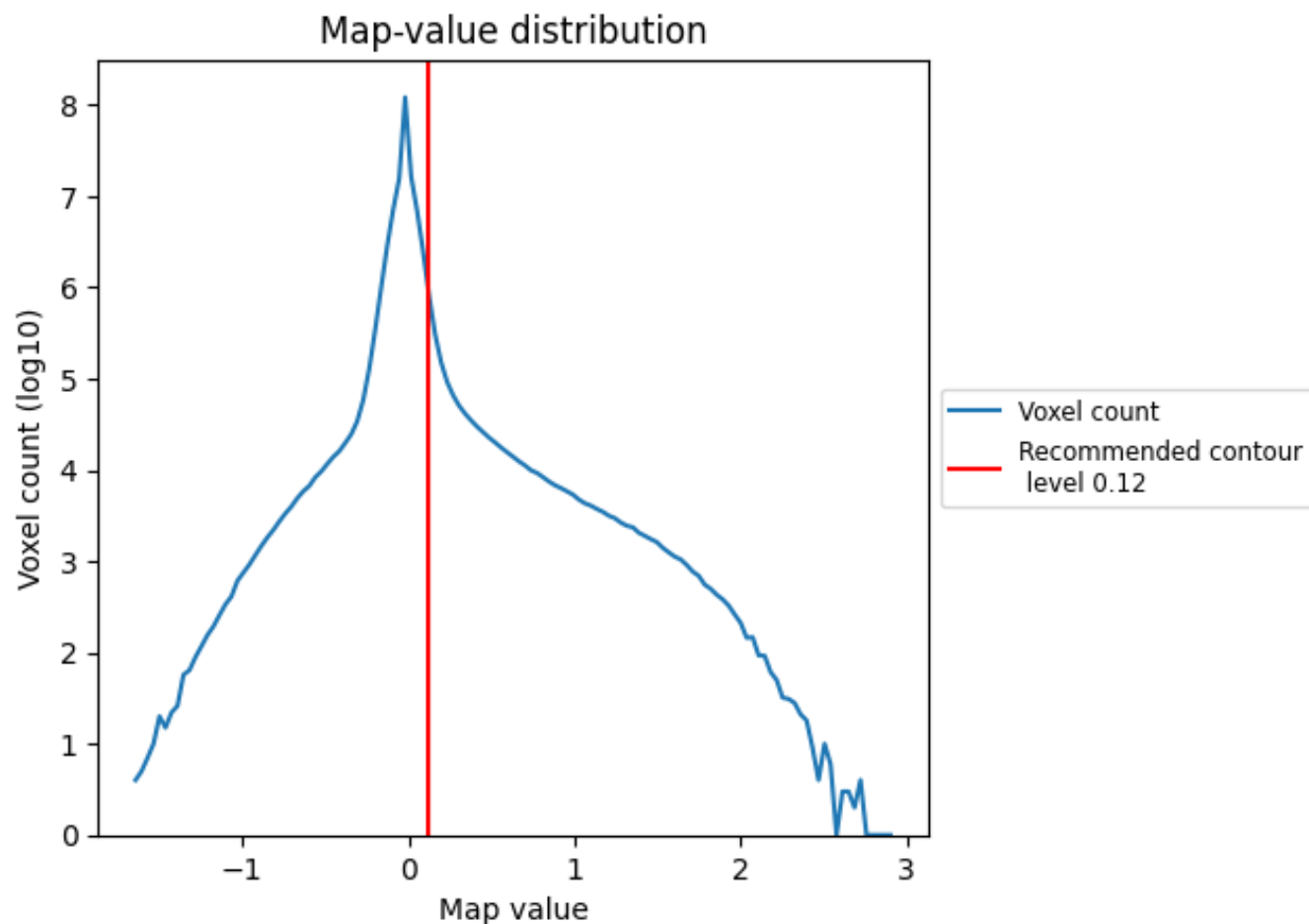


Z

7 Map analysis [i](#)

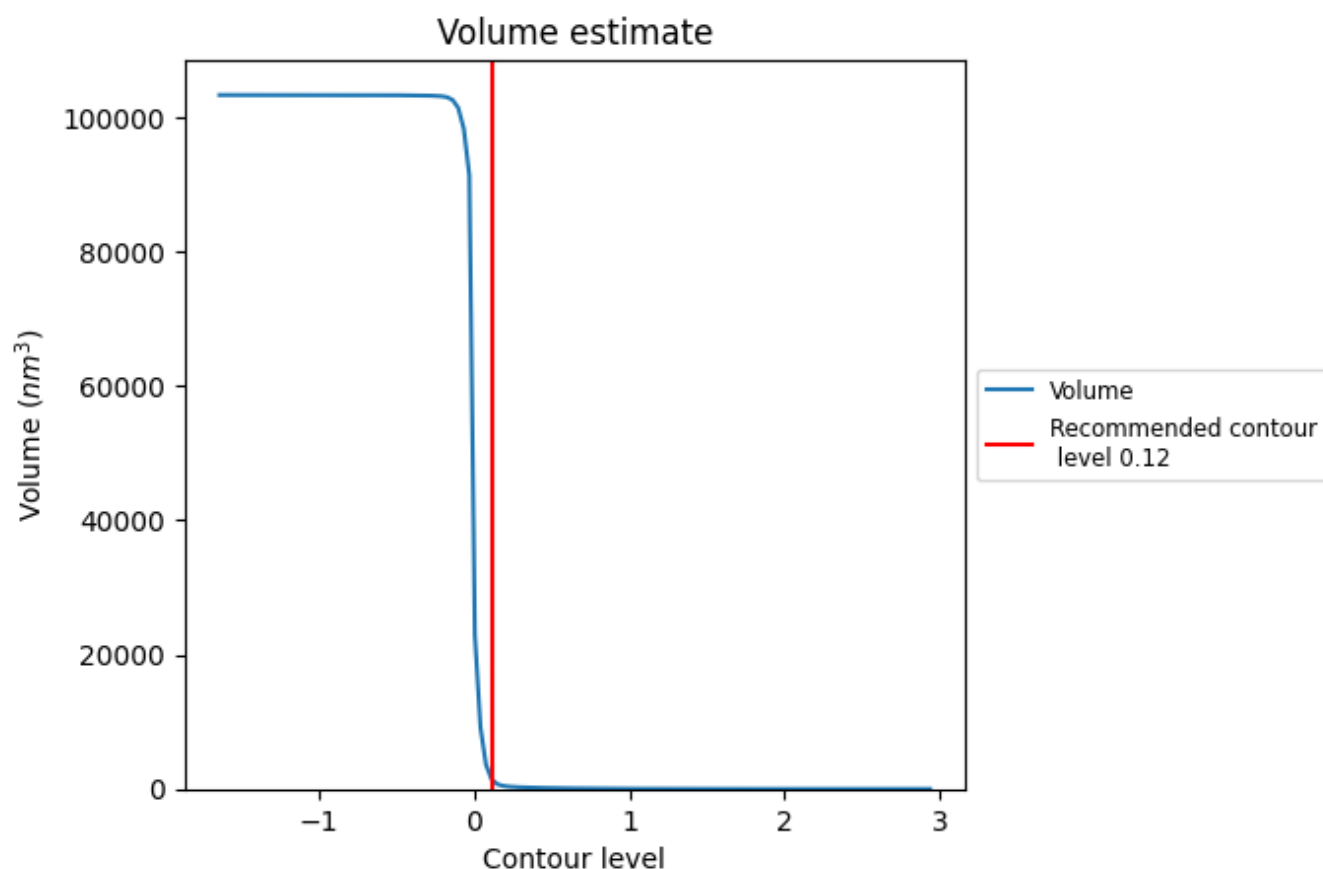
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

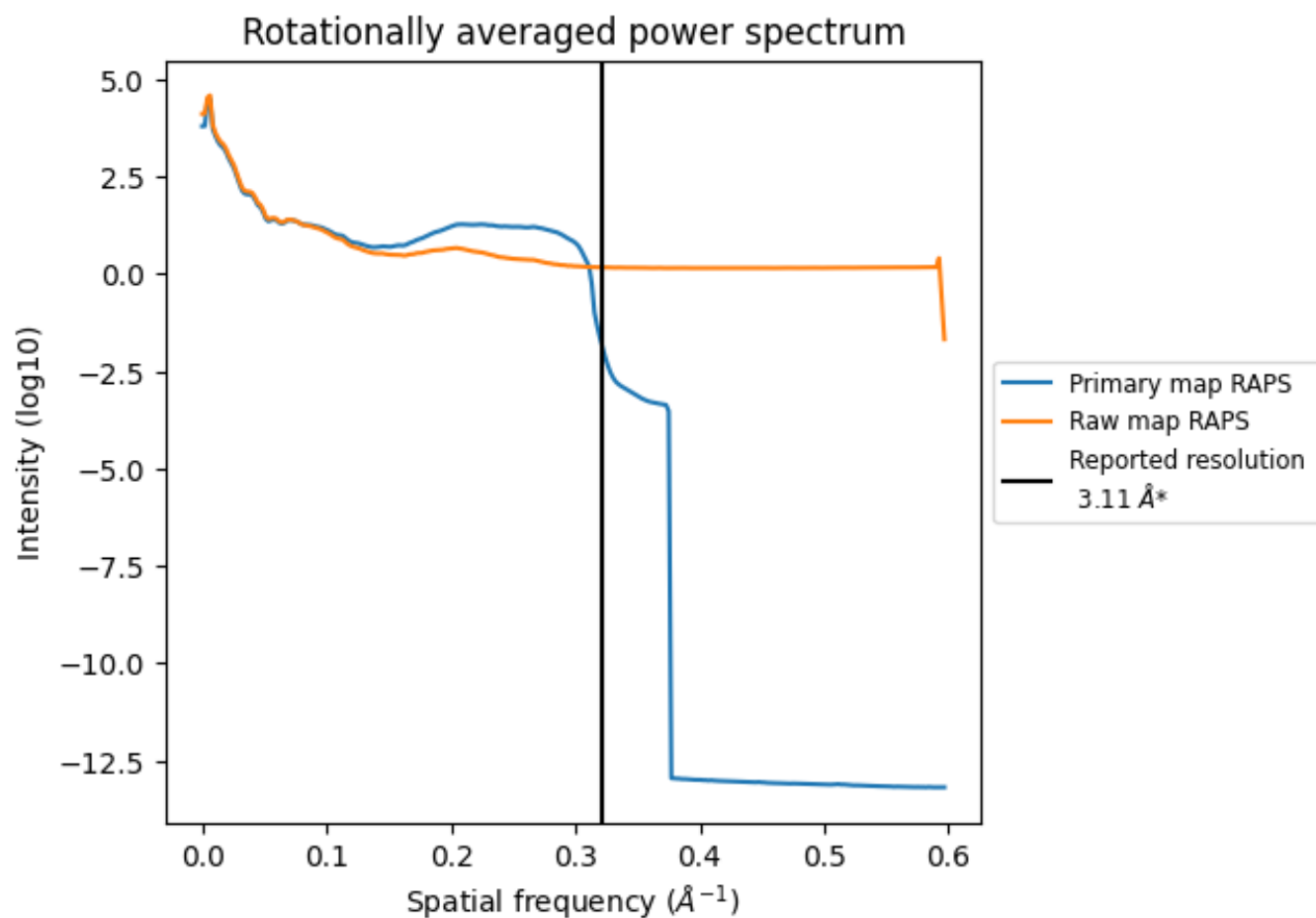
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1258 nm^3 ; this corresponds to an approximate mass of 1137 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

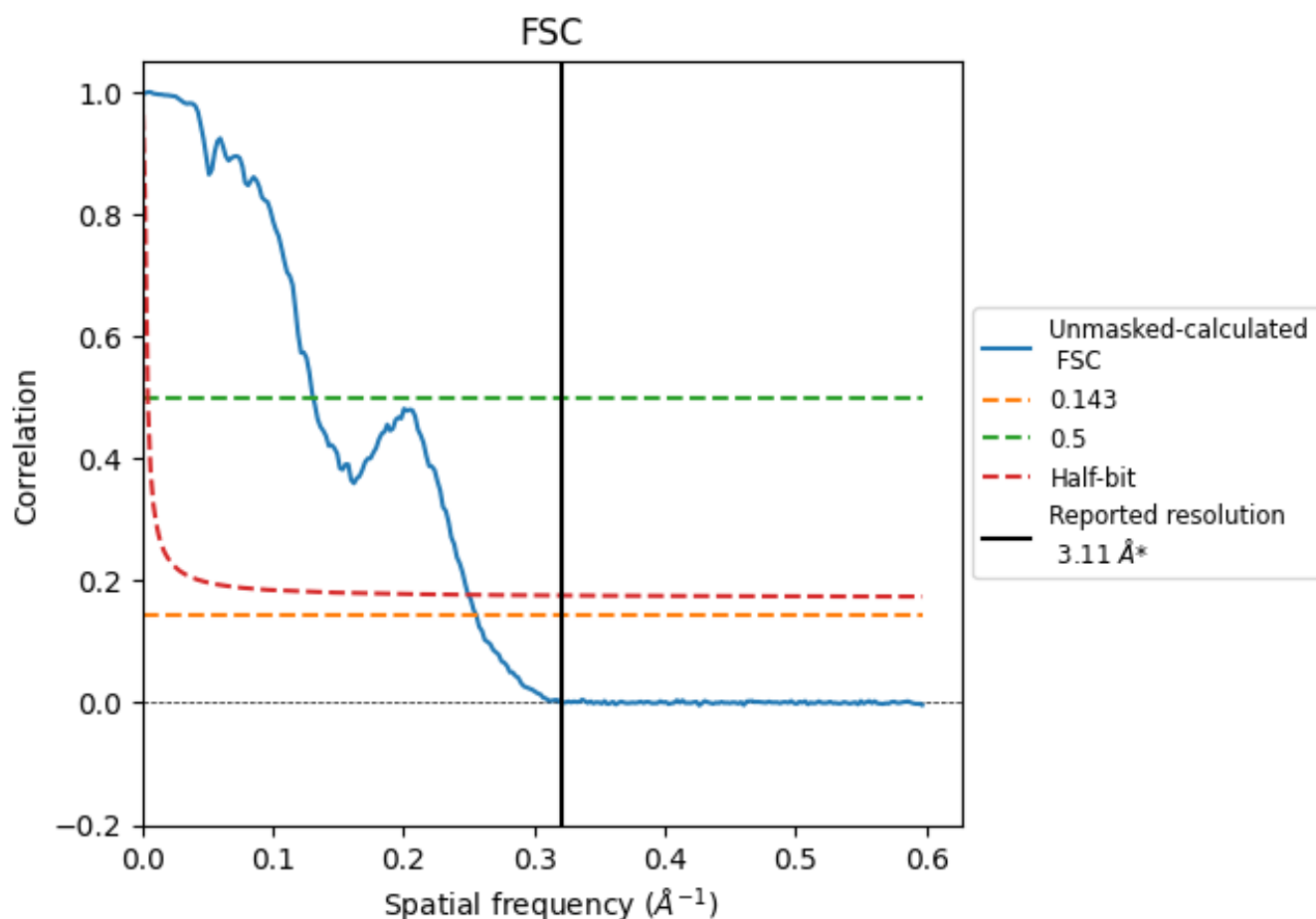


*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

8.2 Resolution estimates [i](#)

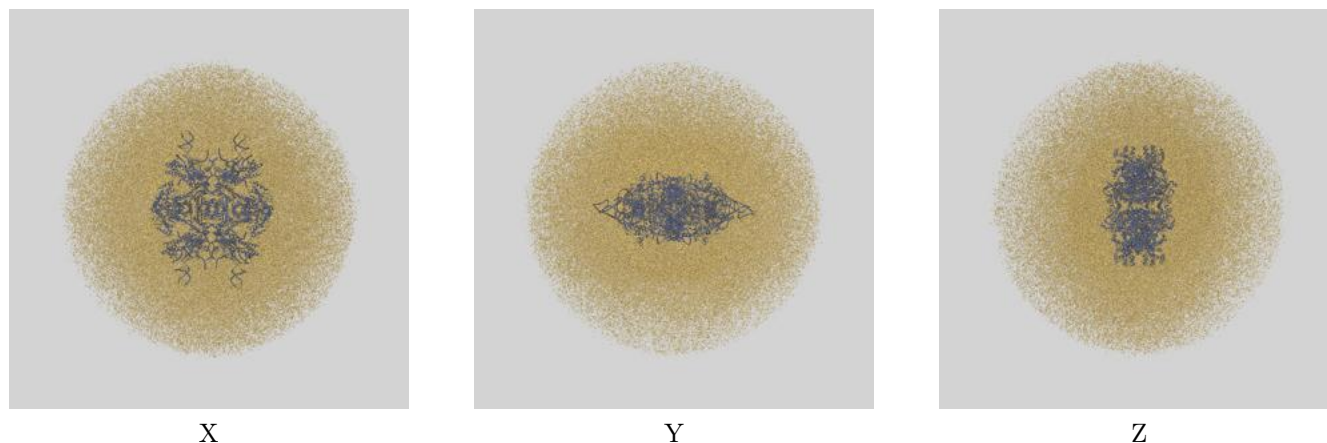
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	7.65	4.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.11 by more than 10 %

9 Map-model fit [i](#)

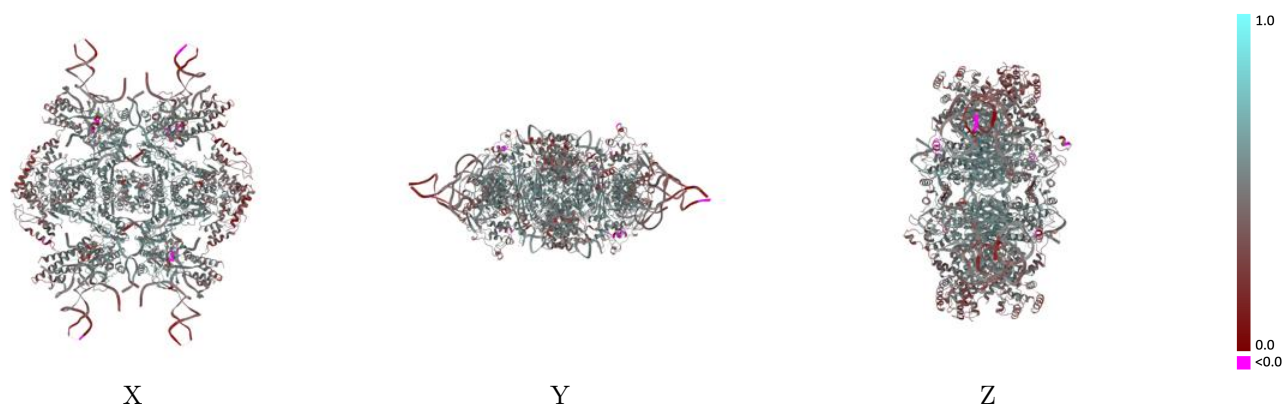
This section contains information regarding the fit between EMDB map EMD-69132 and PDB model 23OR. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



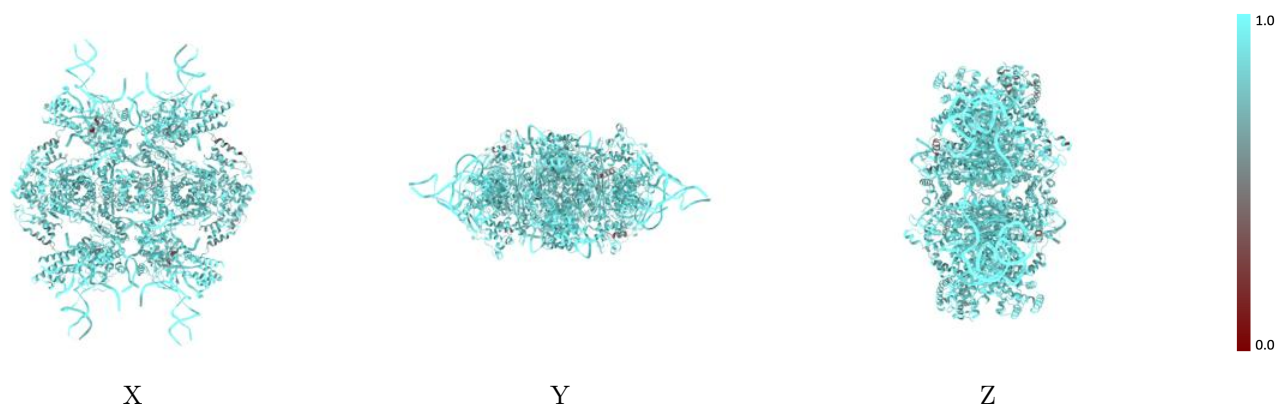
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



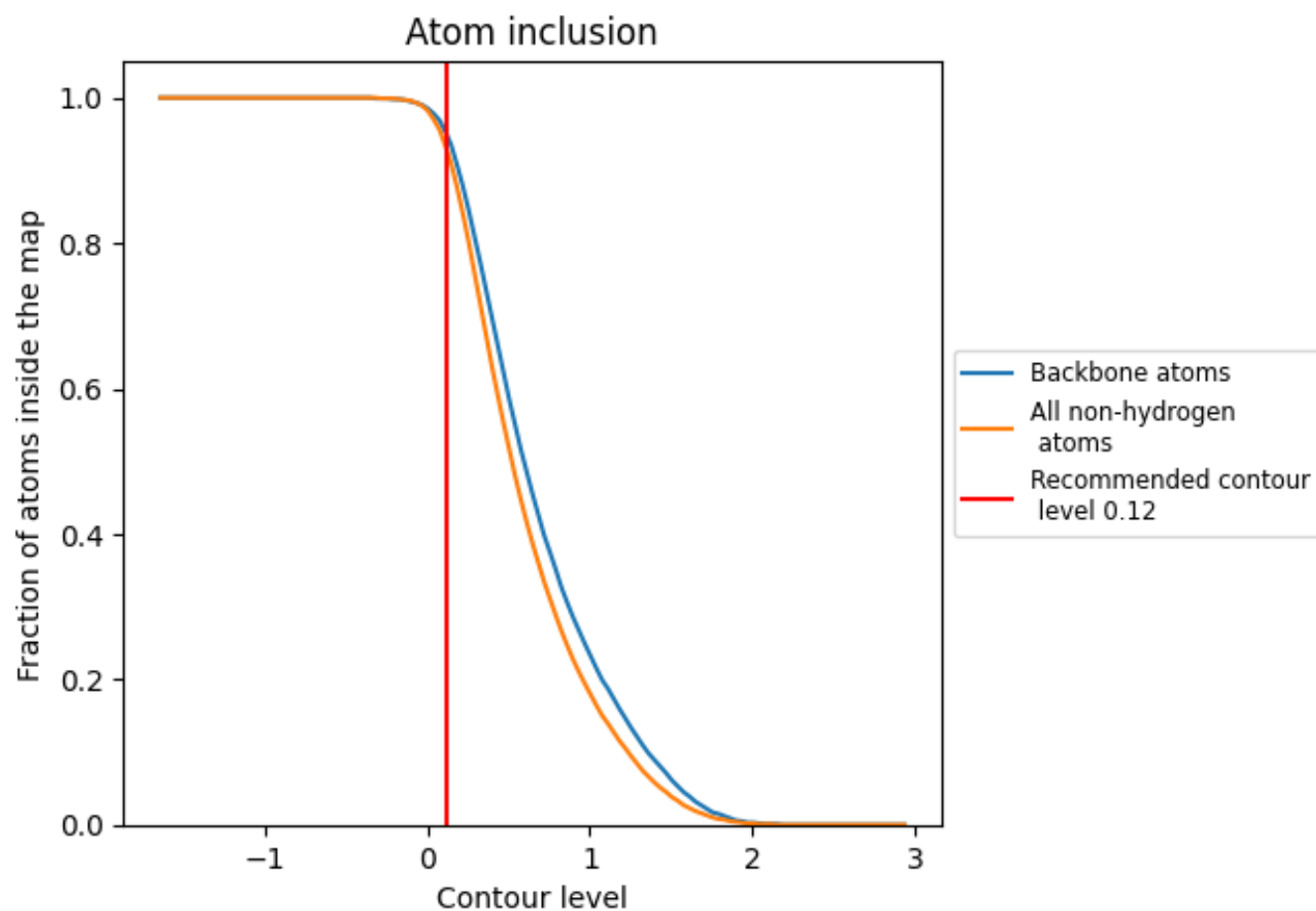
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9280	 0.4770
A	 0.9390	 0.4950
B	 0.9260	 0.5060
C	 0.9700	 0.3850
D	 0.9600	 0.4930
E	 0.9320	 0.4880
F	 0.9220	 0.4990
G	 0.9700	 0.4000
H	 0.9580	 0.5000
I	 0.9350	 0.4890
J	 0.9150	 0.4900
K	 0.9730	 0.3810
L	 0.9640	 0.5100
M	 0.9170	 0.4700
N	 0.8930	 0.4770
O	 0.9590	 0.3550
P	 0.9450	 0.4840

