



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 03:40 AM UTC

PDB ID : 9M9E / pdb_00009m9e
EMDB ID : EMD-63731
Title : Structural Basis of Pausing During Transcription Initiation in Mycobacterium tuberculosis
Authors : Zheng, L.T.
Deposited on : 2025-03-13
Resolution : 3.31 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

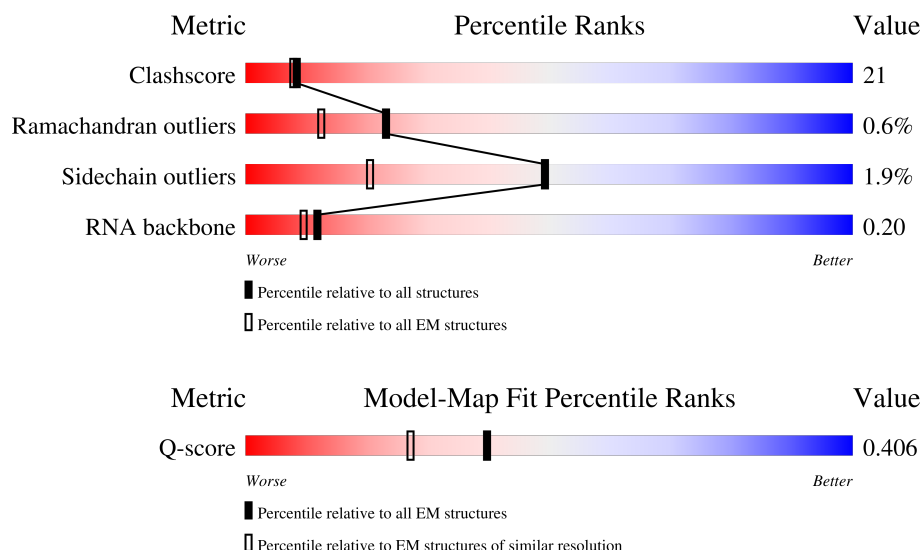
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.31 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.



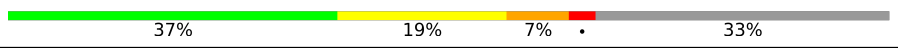
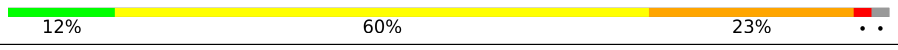
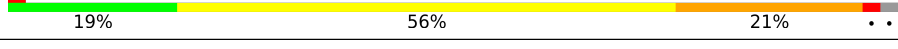
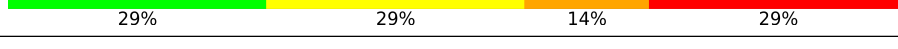
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14550 (2.81 - 3.81)

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	347	50% 12% 38%
1	B	347	46% 21% 33%
2	C	1178	71% 23% ••

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Mol	Chain	Length	Quality of chain
3	D	1326	
4	E	110	
5	F	263	
6	G	48	
7	H	48	
8	I	7	
9	M	169	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 26920 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	215	Total	C	N	O	S	0	0
			1622	1024	278	318	2		
1	B	233	Total	C	N	O	S	0	0
			1753	1103	303	345	2		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1125	Total	C	N	O	S	0	0
			8530	5345	1496	1650	39		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1256	Total	C	N	O	S	0	0
			9743	6108	1767	1828	40		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP P9WGY7
D	1318	HIS	-	expression tag	UNP P9WGY7
D	1319	HIS	-	expression tag	UNP P9WGY7
D	1320	HIS	-	expression tag	UNP P9WGY7
D	1321	HIS	-	expression tag	UNP P9WGY7
D	1322	HIS	-	expression tag	UNP P9WGY7
D	1323	HIS	-	expression tag	UNP P9WGY7
D	1324	HIS	-	expression tag	UNP P9WGY7
D	1325	HIS	-	expression tag	UNP P9WGY7
D	1326	HIS	-	expression tag	UNP P9WGY7

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	76	Total	C	N	O	0	0
			600	383	101	116		

- Molecule 5 is a protein called ECF RNA polymerase sigma factor SigE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	176	Total	C	N	O	S	0	0
			1414	883	263	264	4		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	MET	-	initiating methionine	UNP P9WGG7
F	-4	HIS	-	expression tag	UNP P9WGG7
F	-3	HIS	-	expression tag	UNP P9WGG7
F	-2	HIS	-	expression tag	UNP P9WGG7
F	-1	HIS	-	expression tag	UNP P9WGG7
F	0	HIS	-	expression tag	UNP P9WGG7
F	1	HIS	-	expression tag	UNP P9WGG7

- Molecule 6 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	47	Total	C	N	O	P	0	0
			938	447	165	279	47		

- Molecule 7 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	47	Total	C	N	O	P	0	0
			942	450	169	277	46		

- Molecule 8 is a RNA chain called RNA (5'-R(*CP*CP*CP*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	7	Total	C	N	O	P	0	0
			141	65	24	46	6		

- Molecule 9 is a protein called RNA polymerase-binding transcription factor CarD.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	159	Total	C	N	O	S	0	0
			1234	771	224	238	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-6	MET	-	initiating methionine	UNP P9WJG3
M	-5	GLY	-	expression tag	UNP P9WJG3
M	-4	HIS	-	expression tag	UNP P9WJG3
M	-3	HIS	-	expression tag	UNP P9WJG3
M	-2	HIS	-	expression tag	UNP P9WJG3
M	-1	HIS	-	expression tag	UNP P9WJG3
M	0	HIS	-	expression tag	UNP P9WJG3
M	1	HIS	-	expression tag	UNP P9WJG3

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	

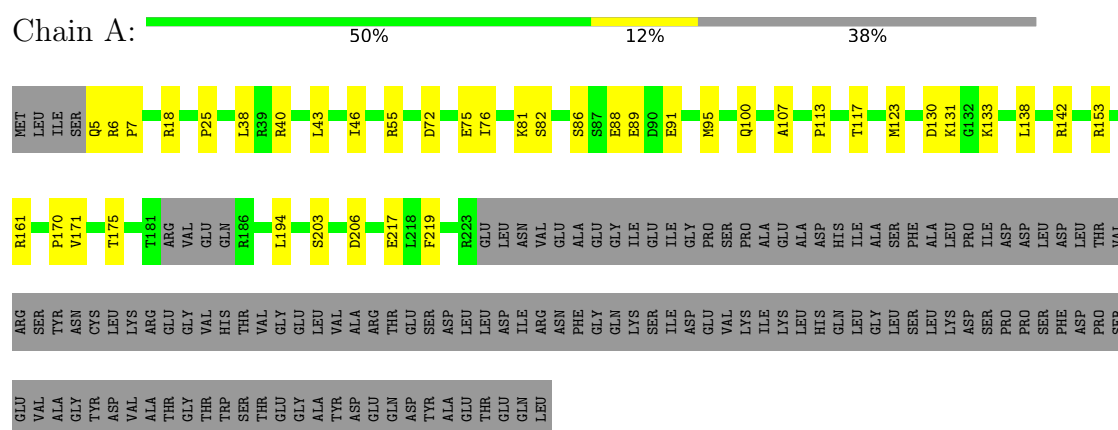
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	D	2	Total	Zn	0
			2	2	

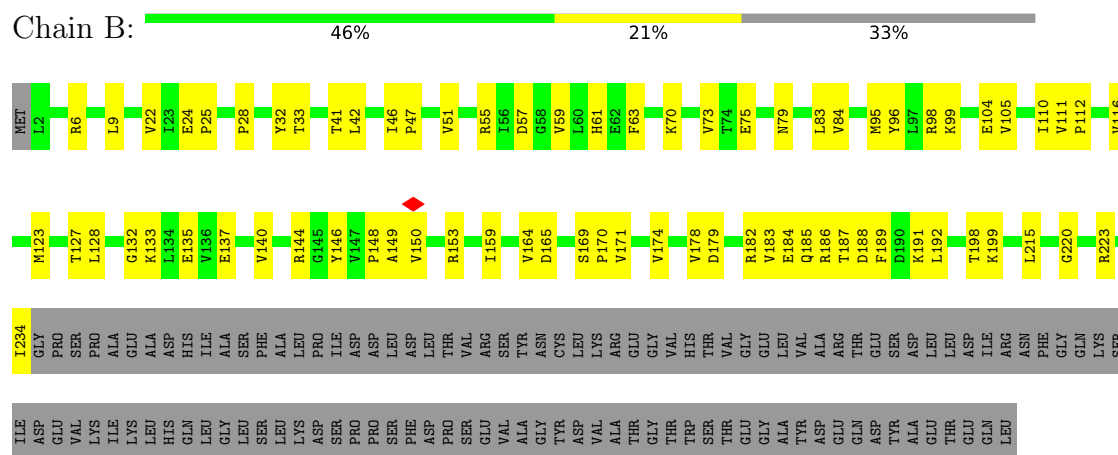
3 Residue-property plots

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

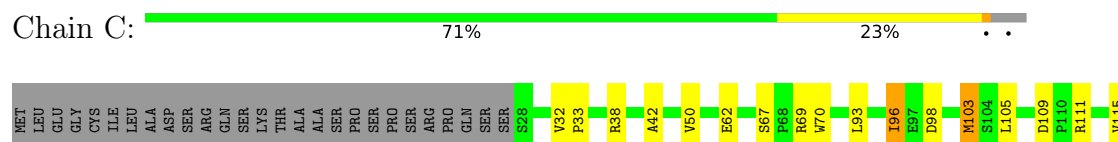
• Molecule 1: DNA-directed RNA polymerase subunit alpha

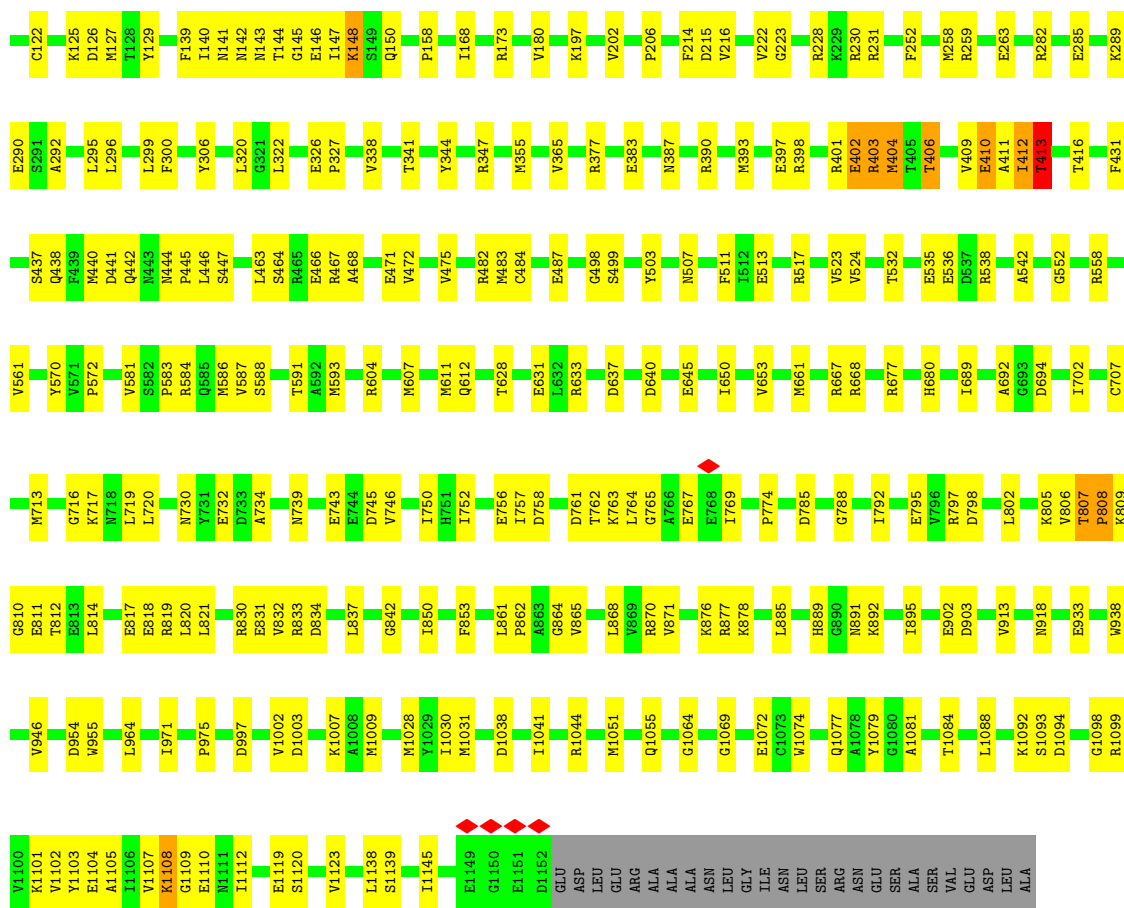


• Molecule 1: DNA-directed RNA polymerase subunit alpha

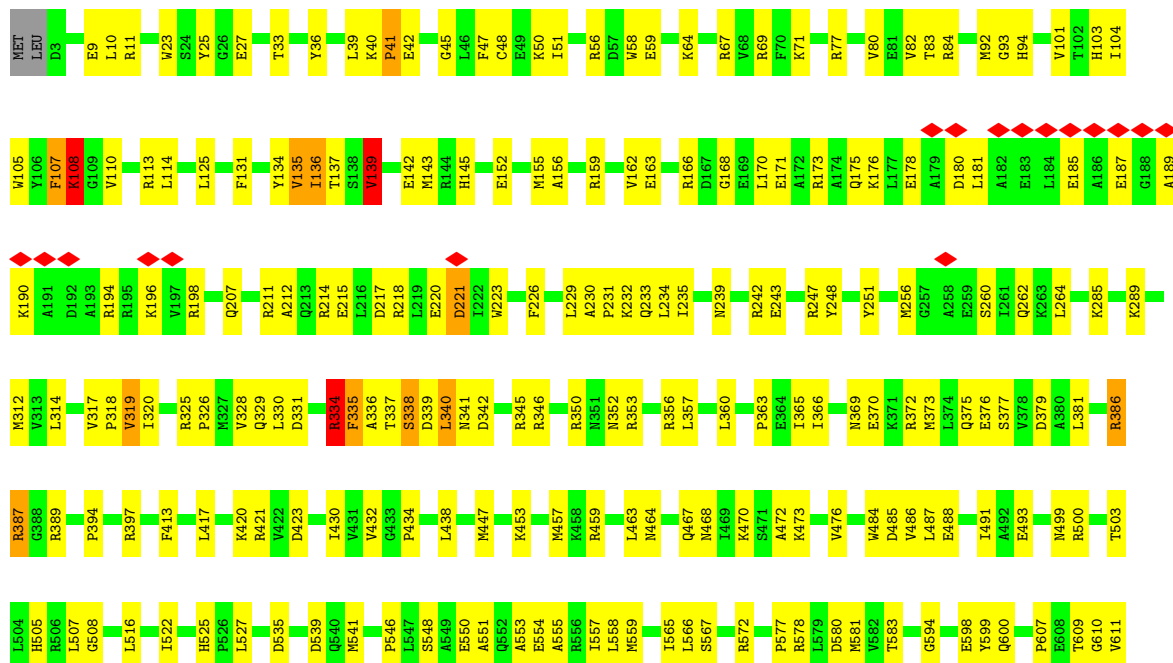


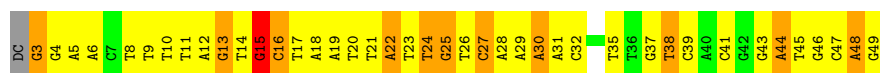
• Molecule 2: DNA-directed RNA polymerase subunit beta



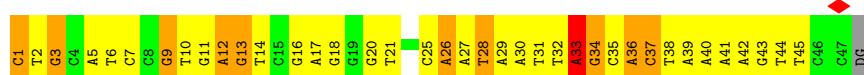
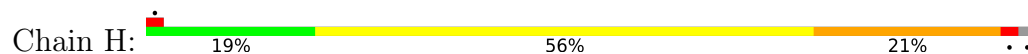


• Molecule 3: DNA-directed RNA polymerase subunit beta'

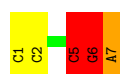
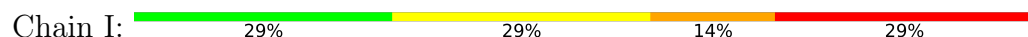




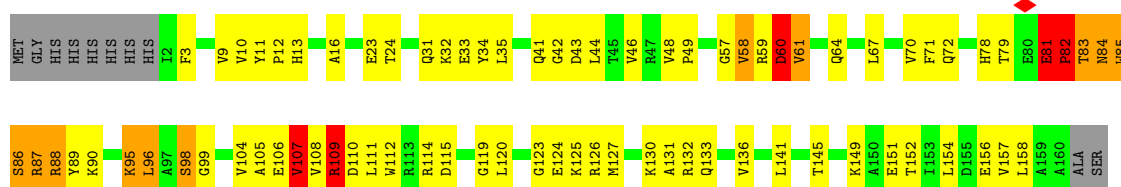
• Molecule 7: DNA (48-MER)



• Molecule 8: RNA (5'-R(*CP*CP*CP*UP*CP*GP*A)-3')



• Molecule 9: RNA polymerase-binding transcription factor CarD



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65908	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.844	Depositor
Minimum map value	-0.341	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	284.8, 284.8, 284.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89, 0.89, 0.89	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/1647	0.35	0/2241
1	B	0.17	0/1779	0.40	0/2423
2	C	0.24	1/8687 (0.0%)	0.51	8/11799 (0.1%)
3	D	0.30	1/9906 (0.0%)	0.62	14/13400 (0.1%)
4	E	0.17	0/612	0.37	0/833
5	F	1.09	5/1444 (0.3%)	1.57	19/1959 (1.0%)
6	G	0.76	5/1051 (0.5%)	1.51	29/1619 (1.8%)
7	H	0.75	3/1056 (0.3%)	1.35	21/1627 (1.3%)
8	I	0.76	0/156	1.40	3/241 (1.2%)
9	M	0.64	2/1249 (0.2%)	1.51	13/1689 (0.8%)
All	All	0.43	17/27587 (0.1%)	0.81	107/37831 (0.3%)

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	C	0	1
3	D	0	1
6	G	0	1
7	H	0	1
9	M	0	2
All	All	0	6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	160	PRO	N-CA	19.70	1.70	1.47
3	D	41	PRO	N-CA	17.80	1.70	1.47
9	M	82	PRO	N-CA	16.93	1.69	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	9	DG	O3'-P	-13.41	1.41	1.61
5	F	166	VAL	C-N	13.21	1.50	1.33
6	G	3	DG	O3'-P	-12.29	1.42	1.61
5	F	135	TRP	C-O	-9.65	1.13	1.24
5	F	159	LEU	C-N	9.24	1.45	1.33
7	H	2	DT	O3'-P	-8.43	1.48	1.61
6	G	19	DA	O3'-P	-8.26	1.48	1.61
5	F	172	ASN	C-N	6.83	1.49	1.33
2	C	413	THR	C-N	6.76	1.49	1.33
6	G	25	DG	O3'-P	5.74	1.69	1.61
7	H	3	DG	O3'-P	-5.30	1.53	1.61
6	G	27	DC	O3'-P	-5.24	1.53	1.61
9	M	81	GLU	C-N	5.06	1.45	1.33
6	G	24	DT	O3'-P	-5.01	1.53	1.61

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	33	THR	O-C-N	-26.15	91.33	122.19
9	M	84	ASN	CA-C-N	-23.96	88.20	120.54
9	M	84	ASN	C-N-CA	-23.96	88.20	120.54
3	D	33	THR	CA-C-N	19.34	151.55	121.95
3	D	33	THR	C-N-CA	19.34	151.55	121.95
9	M	84	ASN	O-C-N	18.48	147.17	122.59
6	G	3	DG	O3'-P-O5'	18.10	131.14	104.00
5	F	159	LEU	CA-C-N	17.60	137.85	119.90
5	F	159	LEU	C-N-CA	17.60	137.85	119.90
9	M	82	PRO	N-CA-C	-16.16	79.19	112.47
9	M	81	GLU	CA-C-N	15.96	139.78	119.84
9	M	81	GLU	C-N-CA	15.96	139.78	119.84
5	F	166	VAL	CA-C-N	15.05	135.05	119.85
5	F	166	VAL	C-N-CA	15.05	135.05	119.85
2	C	413	THR	CA-C-N	14.77	138.30	119.84
2	C	413	THR	C-N-CA	14.77	138.30	119.84
3	D	40	LYS	CA-C-N	14.50	137.97	119.84
3	D	40	LYS	C-N-CA	14.50	137.97	119.84
6	G	25	DG	C2'-C3'-O3'	-13.45	91.33	111.50
2	C	180	VAL	CA-C-N	-13.18	104.54	122.72
2	C	180	VAL	C-N-CA	-13.18	104.54	122.72
9	M	60	ASP	CA-C-N	12.18	143.89	121.97
9	M	60	ASP	C-N-CA	12.18	143.89	121.97
8	I	5	C	C4'-C3'-O3'	11.65	130.48	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	180	VAL	O-C-N	11.59	137.06	122.57
7	H	33	DA	C4'-C3'-O3'	11.29	126.94	110.00
6	G	18	DA	C4-N9-C1'	-11.16	110.31	127.05
7	H	37	DC	C2'-C3'-O3'	10.81	127.71	111.50
7	H	34	DG	C4'-C3'-O3'	10.72	126.08	110.00
6	G	3	DG	P-O3'-C3'	10.71	136.27	120.20
7	H	33	DA	C2'-C3'-O3'	-10.71	95.44	111.50
6	G	22	DA	C4-N9-C1'	-10.33	111.55	127.05
6	G	22	DA	C8-N9-C1'	10.21	142.36	127.05
6	G	18	DA	N9-C1'-C2'	10.18	128.77	113.50
6	G	18	DA	C8-N9-C1'	9.99	142.04	127.05
7	H	29	DA	C2'-C3'-O3'	-9.65	97.03	111.50
5	F	221	LYS	CB-CA-C	9.64	126.00	109.51
6	G	15	DG	C2'-C3'-O3'	-9.61	97.09	111.50
5	F	172	ASN	CA-C-N	9.58	131.81	119.84
5	F	172	ASN	C-N-CA	9.58	131.81	119.84
7	H	13	DG	C2'-C3'-O3'	-9.47	97.29	111.50
3	D	221	ASP	N-CA-C	-9.35	99.99	111.40
9	M	82	PRO	CA-N-CD	-9.30	98.97	112.00
2	C	406	THR	CA-CB-OG1	-8.95	96.18	109.60
3	D	108	LYS	CB-CA-C	8.85	125.03	109.72
7	H	33	DA	N9-C1'-C2'	-8.83	100.26	113.50
5	F	135	TRP	CA-C-O	-8.68	111.70	120.82
6	G	3	DG	OP1-P-O3'	-8.55	82.35	108.00
8	I	6	G	C4'-C3'-O3'	-8.54	100.19	113.00
6	G	22	DA	N9-C1'-C2'	8.52	126.28	113.50
3	D	334	ARG	CB-CA-C	-8.28	96.64	114.10
6	G	48	DA	C4-N9-C1'	-8.18	114.78	127.05
7	H	13	DG	C4'-C3'-O3'	8.17	122.26	110.00
5	F	160	PRO	N-CA-C	-8.16	98.25	111.15
6	G	13	DG	C2'-C3'-O3'	8.05	123.57	111.50
5	F	135	TRP	CA-C-N	7.96	130.79	120.44
5	F	135	TRP	C-N-CA	7.96	130.79	120.44
6	G	48	DA	C8-N9-C1'	7.94	138.96	127.05
5	F	129	PRO	O-C-N	7.73	132.71	122.89
7	H	12	DA	C2'-C3'-O3'	-7.60	100.10	111.50
7	H	26	DA	C2'-C3'-O3'	7.58	122.88	111.50
7	H	29	DA	C4'-C3'-O3'	7.49	121.24	110.00
6	G	19	DA	C2'-C3'-O3'	-7.42	100.38	111.50
3	D	41	PRO	CA-N-CD	-7.38	101.67	112.00
7	H	2	DT	P-O3'-C3'	-7.37	109.15	120.20
5	F	160	PRO	CA-N-CD	-7.22	101.89	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	44	DA	C2'-C3'-O3'	-7.07	100.89	111.50
7	H	36	DA	C4'-C3'-O3'	7.01	120.51	110.00
7	H	1	DC	P-O3'-C3'	6.88	130.51	120.20
6	G	16	DC	C4'-C3'-O3'	6.44	119.66	110.00
9	M	58	VAL	O-C-N	-6.40	115.47	122.64
6	G	13	DG	N9-C1'-C2'	6.20	122.81	113.50
3	D	334	ARG	N-CA-C	6.16	116.14	108.19
7	H	13	DG	N9-C1'-C2'	-6.13	104.30	113.50
3	D	221	ASP	CA-C-N	-6.12	114.72	122.37
3	D	221	ASP	C-N-CA	-6.12	114.72	122.37
7	H	31	DT	C2'-C3'-O3'	-6.12	102.33	111.50
6	G	48	DA	N9-C1'-C2'	6.10	122.65	113.50
5	F	144	PHE	CA-CB-CG	-6.10	107.70	113.80
7	H	28	DT	C4'-C3'-O3'	-6.00	101.00	110.00
6	G	44	DA	P-O3'-C3'	5.97	129.15	120.20
5	F	143	LEU	N-CA-C	-5.90	104.85	111.28
5	F	166	VAL	CA-C-O	-5.84	115.85	119.12
6	G	16	DC	C2'-C3'-O3'	-5.83	102.76	111.50
9	M	107	VAL	N-CA-CB	5.78	117.97	110.57
6	G	24	DT	P-O3'-C3'	5.74	128.81	120.20
6	G	18	DA	C3'-C2'-C1'	-5.73	93.01	101.60
2	C	402	GLU	CA-C-O	-5.63	114.91	120.82
6	G	22	DA	C3'-C2'-C1'	-5.62	93.17	101.60
3	D	107	PHE	CA-C-N	-5.61	115.26	123.00
3	D	107	PHE	C-N-CA	-5.61	115.26	123.00
7	H	37	DC	C4'-C3'-O3'	-5.45	101.82	110.00
2	C	406	THR	CB-CA-C	5.39	118.11	109.27
6	G	38	DT	C2'-C3'-O3'	-5.37	103.45	111.50
6	G	48	DA	C3'-C2'-C1'	-5.24	93.73	101.60
6	G	30	DA	C2'-C3'-O3'	5.18	119.27	111.50
5	F	165	ARG	N-CA-C	-5.18	106.07	114.09
5	F	132	PHE	CA-C-N	5.17	127.20	120.28
5	F	132	PHE	C-N-CA	5.17	127.20	120.28
7	H	12	DA	C5'-C4'-O4'	-5.15	101.67	109.40
9	M	109	ARG	N-CA-C	-5.11	105.79	111.36
6	G	44	DA	O3'-P-O5'	5.05	111.57	104.00
9	M	107	VAL	CB-CA-C	-5.04	105.42	112.02
6	G	24	DT	C4'-C3'-O3'	-5.04	102.44	110.00
7	H	30	DA	C4'-C3'-O3'	5.03	117.55	110.00
7	H	12	DA	C3'-C2'-C1'	5.02	109.13	101.60
8	I	6	G	O4'-C1'-C2'	-5.00	102.60	107.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	807	THR	Peptide
3	D	23	TRP	Peptide
6	G	15	DG	Sidechain
7	H	33	DA	Sidechain
9	M	58	VAL	Mainchain
9	M	81	GLU	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	1622	0	1651	34	0
1	B	1753	0	1771	62	0
2	C	8530	0	8323	275	0
3	D	9743	0	9764	321	0
4	E	600	0	592	20	0
5	F	1414	0	1378	194	0
6	G	938	0	516	138	0
7	H	942	0	521	91	0
8	I	141	0	74	16	0
9	M	1234	0	1252	163	0
10	D	1	0	0	0	0
11	D	2	0	0	0	0
All	All	26920	0	25842	1123	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 21.

All (1123) 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)
2:C:817:GLU:CG	5:F:182:LEU:HD23	1.31	1.60
2:C:817:GLU:HG3	5:F:182:LEU:CD2	1.37	1.52
9:M:85:TRP:CZ3	9:M:89:TYR:HB2	1.45	1.51
5:F:159:LEU:HD12	5:F:160:PRO:CD	1.44	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:41:PRO:N	3:D:41:PRO:CA	1.70	1.44
9:M:82:PRO:N	9:M:82:PRO:CA	1.69	1.43
5:F:160:PRO:CA	5:F:160:PRO:N	1.70	1.33
9:M:85:TRP:CH2	9:M:89:TYR:HB2	1.67	1.28
5:F:101:ARG:HD3	6:G:29:DA:C1'	1.70	1.20
9:M:16:ALA:HB2	9:M:141:LEU:CD1	1.70	1.19
6:G:8:DT:C2'	6:G:9:DT:H72	1.74	1.17
9:M:95:LYS:HE2	9:M:107:VAL:CG1	1.74	1.16
5:F:101:ARG:CZ	6:G:29:DA:C8	2.31	1.14
9:M:79:THR:HG21	9:M:110:ASP:OD1	1.48	1.14
2:C:146:GLU:CG	9:M:46:VAL:HG21	1.77	1.14
9:M:82:PRO:N	9:M:82:PRO:C	2.05	1.14
5:F:159:LEU:CD1	5:F:160:PRO:HD3	1.79	1.13
6:G:8:DT:H2''	6:G:9:DT:C7	1.79	1.12
2:C:817:GLU:HG2	5:F:182:LEU:HA	1.28	1.12
9:M:16:ALA:HB2	9:M:141:LEU:HD13	1.19	1.10
5:F:159:LEU:CD1	5:F:160:PRO:CD	2.29	1.10
9:M:85:TRP:HH2	9:M:89:TYR:CD2	1.70	1.09
2:C:96:ILE:HD11	2:C:401:ARG:HE	1.17	1.09
9:M:10:VAL:HG22	9:M:141:LEU:HD21	1.35	1.07
2:C:103:MET:HE2	2:C:404:MET:HE2	1.29	1.07
2:C:146:GLU:HG2	9:M:46:VAL:HG21	1.12	1.05
9:M:87:ARG:HG2	9:M:90:LYS:CE	1.86	1.04
5:F:101:ARG:NE	6:G:29:DA:C8	2.26	1.04
5:F:67:GLN:HA	5:F:71:VAL:CG2	1.87	1.04
9:M:95:LYS:HE2	9:M:107:VAL:HG12	1.35	1.04
9:M:85:TRP:CH2	9:M:89:TYR:CB	2.40	1.03
3:D:366:ILE:HD11	5:F:88:VAL:HG11	1.42	1.02
5:F:97:ARG:HD3	6:G:29:DA:N6	1.73	1.02
9:M:85:TRP:CZ3	9:M:89:TYR:CB	2.41	1.02
2:C:150:GLN:HE22	9:M:43:ASP:C	1.67	1.02
9:M:95:LYS:HD3	9:M:107:VAL:HB	1.37	1.01
5:F:116:THR:HG23	5:F:139:ILE:CG2	1.90	1.00
5:F:101:ARG:HD3	6:G:29:DA:C8	1.95	1.00
9:M:87:ARG:CG	9:M:90:LYS:HE2	1.91	1.00
5:F:101:ARG:CZ	6:G:29:DA:H8	1.76	0.99
5:F:67:GLN:HA	5:F:71:VAL:HG23	1.45	0.99
9:M:95:LYS:HZ2	9:M:95:LYS:HB2	1.24	0.99
5:F:161:GLU:HG2	8:I:1:C:C5	1.98	0.98
9:M:10:VAL:HG21	9:M:61:VAL:HA	1.44	0.98
5:F:156:MET:SD	5:F:156:MET:N	2.31	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:88:ARG:HE	9:M:114:ARG:NH1	1.61	0.97
2:C:146:GLU:HG2	9:M:46:VAL:CG2	1.94	0.97
5:F:101:ARG:HD3	6:G:29:DA:O4'	1.63	0.97
5:F:101:ARG:HD3	6:G:29:DA:N9	1.79	0.96
5:F:101:ARG:CD	6:G:29:DA:C8	2.49	0.95
9:M:87:ARG:HG2	9:M:90:LYS:HE2	0.96	0.95
6:G:48:DA:P	6:G:48:DA:H2'	2.07	0.95
2:C:148:LYS:H	2:C:148:LYS:HE2	1.31	0.95
6:G:8:DT:C1'	6:G:9:DT:H72	1.96	0.95
6:G:49:DG:N2	7:H:1:DC:H42	1.64	0.95
6:G:37:DG:H8	6:G:37:DG:H5''	1.30	0.94
3:D:326:PRO:HD2	3:D:338:SER:OG	1.67	0.94
5:F:128:GLN:OE1	9:M:85:TRP:HD1	1.49	0.94
9:M:10:VAL:HG22	9:M:141:LEU:CD2	1.98	0.94
2:C:148:LYS:HZ3	2:C:148:LYS:HB3	1.33	0.94
5:F:101:ARG:NH1	6:G:29:DA:H8	1.66	0.94
5:F:159:LEU:CD1	5:F:160:PRO:HD2	1.98	0.93
5:F:84:TRP:CZ3	5:F:120:VAL:HG12	2.04	0.93
6:G:8:DT:C2'	6:G:9:DT:C7	2.42	0.93
9:M:85:TRP:HZ3	9:M:89:TYR:HB2	1.19	0.92
3:D:346:ARG:NH2	5:F:107:HIS:HB3	1.84	0.92
5:F:159:LEU:HD12	5:F:160:PRO:HD2	1.51	0.92
9:M:95:LYS:HE2	9:M:104:VAL:HA	1.51	0.92
9:M:95:LYS:HE2	9:M:107:VAL:HG11	1.50	0.92
9:M:87:ARG:HB3	9:M:87:ARG:NH2	1.83	0.92
2:C:764:LEU:HD12	2:C:809:LYS:HG3	1.52	0.91
2:C:401:ARG:HH11	2:C:401:ARG:HG2	1.36	0.91
5:F:116:THR:HG23	5:F:139:ILE:HG23	1.53	0.91
9:M:9:VAL:HG23	9:M:60:ASP:HB3	1.53	0.91
6:G:8:DT:H2''	6:G:9:DT:H73	1.53	0.90
5:F:145:LEU:HD21	7:H:27:DA:H5'	1.51	0.90
2:C:139:PHE:HB3	2:C:148:LYS:HD3	1.52	0.90
9:M:85:TRP:CH2	9:M:89:TYR:CD2	2.60	0.90
9:M:95:LYS:CE	9:M:107:VAL:CG1	2.50	0.89
8:I:2:C:H5''	8:I:2:C:C6	2.08	0.89
5:F:128:GLN:OE1	9:M:85:TRP:CD1	2.25	0.89
9:M:79:THR:CG2	9:M:110:ASP:OD1	2.20	0.88
2:C:398:ARG:HG3	2:C:398:ARG:HH11	1.38	0.88
9:M:10:VAL:HG21	9:M:61:VAL:CA	2.04	0.87
2:C:812:THR:CG2	3:D:39:LEU:HB2	2.04	0.87
8:I:2:C:H5''	8:I:2:C:H6	1.35	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:85:TRP:HH2	9:M:89:TYR:CG	1.93	0.86
3:D:108:LYS:O	3:D:108:LYS:NZ	2.08	0.86
2:C:1108:LYS:O	2:C:1108:LYS:NZ	2.08	0.86
5:F:68:GLY:O	5:F:82:PRO:HG3	1.75	0.86
2:C:821:LEU:HD21	5:F:186:LEU:HD13	1.57	0.85
5:F:160:PRO:HB3	5:F:165:ARG:HG3	1.57	0.85
5:F:145:LEU:CD2	7:H:27:DA:H5'	2.07	0.85
7:H:36:DA:C8	7:H:36:DA:H3'	2.12	0.84
3:D:387:ARG:HA	3:D:387:ARG:HH11	1.38	0.84
2:C:817:GLU:CG	5:F:182:LEU:HA	2.07	0.84
9:M:95:LYS:CE	9:M:107:VAL:HG11	2.06	0.84
5:F:142:ASN:ND2	7:H:28:DT:C6	2.45	0.84
6:G:37:DG:H5''	6:G:37:DG:C8	2.13	0.84
3:D:230:ALA:HB3	3:D:233:GLN:HE22	1.43	0.83
5:F:159:LEU:HD12	5:F:160:PRO:HD3	0.83	0.82
6:G:26:DT:P	6:G:26:DT:H3'	2.18	0.82
9:M:16:ALA:CB	9:M:141:LEU:HD13	2.08	0.82
2:C:820:LEU:HD23	5:F:186:LEU:HD21	1.62	0.82
5:F:97:ARG:HD3	6:G:29:DA:H61	1.45	0.82
5:F:226:ARG:CZ	7:H:38:DT:H73	2.10	0.82
5:F:226:ARG:NH1	7:H:38:DT:C7	2.43	0.81
6:G:8:DT:N1	6:G:9:DT:H72	1.95	0.81
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.60	0.81
2:C:150:GLN:NE2	9:M:43:ASP:C	2.39	0.81
3:D:346:ARG:HH22	5:F:107:HIS:HB3	1.46	0.80
2:C:412:ILE:HD12	2:C:412:ILE:H	1.45	0.80
5:F:159:LEU:CG	5:F:160:PRO:HD2	2.11	0.80
5:F:145:LEU:HD23	7:H:27:DA:OP2	1.80	0.79
2:C:230:ARG:HG3	2:C:230:ARG:HH11	1.47	0.79
2:C:769:ILE:HG13	2:C:806:VAL:H	1.48	0.79
6:G:48:DA:H2'	6:G:48:DA:OP2	1.80	0.79
5:F:100:TYR:HE2	6:G:31:DA:OP1	1.64	0.79
9:M:87:ARG:HB3	9:M:87:ARG:CZ	2.10	0.79
2:C:96:ILE:CD1	2:C:401:ARG:HE	1.97	0.78
9:M:60:ASP:OD1	9:M:60:ASP:N	2.15	0.78
3:D:346:ARG:HH22	5:F:107:HIS:CB	1.97	0.78
2:C:148:LYS:H	2:C:148:LYS:CE	1.95	0.78
3:D:326:PRO:CD	3:D:338:SER:OG	2.30	0.78
2:C:168:ILE:HD13	2:C:431:PHE:HB3	1.65	0.77
5:F:68:GLY:O	5:F:82:PRO:CG	2.32	0.77
9:M:104:VAL:HA	9:M:107:VAL:HG12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:228:ARG:NH2	6:G:35:DT:H2'	2.00	0.77
5:F:226:ARG:NH1	7:H:38:DT:H73	2.00	0.77
6:G:3:DG:H2'	6:G:3:DG:P	2.25	0.77
3:D:352:ASN:HB2	3:D:356:ARG:HH12	1.49	0.76
3:D:139:VAL:HG11	3:D:229:LEU:O	1.85	0.76
9:M:88:ARG:HB3	9:M:88:ARG:HH11	1.49	0.76
2:C:146:GLU:CD	9:M:46:VAL:HG21	2.10	0.76
1:B:182:ARG:HG3	1:B:187:THR:HG22	1.67	0.76
7:H:11:DG:H2''	7:H:12:DA:H5'	1.68	0.76
2:C:891:ASN:HD21	2:C:1028:MET:HE1	1.51	0.75
3:D:92:MET:HE3	3:D:93:GLY:H	1.49	0.75
5:F:160:PRO:N	5:F:160:PRO:C	2.44	0.75
3:D:328:VAL:O	3:D:335:PHE:HB3	1.86	0.75
9:M:10:VAL:HB	9:M:59:ARG:O	1.86	0.75
2:C:410:GLU:OE2	9:M:13:HIS:HB2	1.85	0.75
3:D:1228:GLU:OE2	7:H:11:DG:H5''	1.87	0.75
7:H:20:DG:C8	7:H:20:DG:H5''	2.20	0.75
5:F:162:ASP:OD2	5:F:165:ARG:NE	2.20	0.75
8:I:6:G:H8	8:I:6:G:C5'	2.00	0.74
5:F:73:ASP:CG	5:F:130:GLY:O	2.30	0.74
5:F:84:TRP:HZ3	5:F:120:VAL:HG12	1.48	0.74
2:C:139:PHE:HB3	2:C:148:LYS:CD	2.18	0.74
5:F:153:ARG:HG2	5:F:154:ILE:HD13	1.68	0.74
5:F:144:PHE:CE2	5:F:148:VAL:HG21	2.22	0.74
9:M:88:ARG:NE	9:M:114:ARG:NH1	2.34	0.74
2:C:103:MET:CE	2:C:404:MET:HE2	2.14	0.74
5:F:101:ARG:CD	6:G:29:DA:O4'	2.35	0.74
9:M:87:ARG:O	9:M:87:ARG:NE	2.19	0.74
9:M:95:LYS:CE	9:M:107:VAL:HG12	2.17	0.73
2:C:125:LYS:HD2	2:C:853:PHE:CE1	2.23	0.73
2:C:719:LEU:HD12	2:C:1030:ILE:HD11	1.68	0.73
6:G:47:DC:H4'	6:G:48:DA:H5'	1.70	0.73
7:H:13:DG:C8	7:H:13:DG:H3'	2.23	0.73
5:F:142:ASN:O	5:F:146:ASP:HB2	1.89	0.73
6:G:37:DG:H8	6:G:37:DG:C5'	2.01	0.73
1:A:95:MET:HB3	1:A:138:LEU:HB2	1.70	0.73
5:F:141:THR:O	5:F:144:PHE:N	2.22	0.73
3:D:386:ARG:HH11	3:D:386:ARG:HG2	1.54	0.73
9:M:88:ARG:HH21	9:M:114:ARG:NH2	1.87	0.73
6:G:23:DT:H2''	6:G:24:DT:H5''	1.69	0.72
9:M:57:GLY:O	9:M:59:ARG:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1112:ILE:HD13	3:D:548:SER:HA	1.72	0.72
9:M:88:ARG:HH21	9:M:114:ARG:CZ	2.03	0.72
2:C:401:ARG:HG2	2:C:401:ARG:NH1	2.03	0.72
9:M:16:ALA:CB	9:M:141:LEU:CD1	2.61	0.72
3:D:370:GLU:OE1	5:F:114:GLN:CD	2.31	0.72
3:D:1265:ASN:HA	3:D:1268:ARG:HG2	1.71	0.72
9:M:96:LEU:C	9:M:96:LEU:HD23	2.14	0.72
9:M:85:TRP:CH2	9:M:89:TYR:CG	2.74	0.71
5:F:161:GLU:HG2	8:I:1:C:C6	2.24	0.71
9:M:115:ASP:OD2	9:M:124:GLU:HB3	1.89	0.71
5:F:84:TRP:CH2	5:F:124:VAL:HB	2.26	0.71
3:D:42:GLU:HA	3:D:42:GLU:OE1	1.91	0.71
9:M:124:GLU:N	9:M:124:GLU:OE1	2.24	0.71
5:F:159:LEU:HG	5:F:160:PRO:HD2	1.70	0.71
9:M:10:VAL:H	9:M:60:ASP:HA	1.56	0.71
2:C:1069:GLY:N	2:C:1072:GLU:OE2	2.24	0.70
2:C:1108:LYS:C	2:C:1108:LYS:HD3	2.16	0.70
3:D:247:ARG:HD2	3:D:248:TYR:HD1	1.57	0.70
3:D:577:PRO:HA	3:D:581:MET:HE3	1.73	0.70
2:C:764:LEU:HD13	2:C:808:PRO:HA	1.74	0.70
5:F:84:TRP:CZ2	5:F:124:VAL:HG11	2.27	0.70
5:F:142:ASN:O	5:F:146:ASP:N	2.20	0.70
9:M:95:LYS:HD3	9:M:107:VAL:CB	2.19	0.70
2:C:398:ARG:HG3	2:C:398:ARG:NH1	2.07	0.70
5:F:97:ARG:HD3	6:G:29:DA:C6	2.26	0.70
3:D:320:ILE:O	3:D:325:ARG:NH1	2.25	0.70
5:F:182:LEU:HD22	5:F:186:LEU:HD23	1.74	0.70
6:G:13:DG:P	6:G:13:DG:H3'	2.32	0.70
9:M:104:VAL:O	9:M:107:VAL:HG13	1.92	0.69
2:C:126:ASP:OD2	2:C:870:ARG:NH2	2.24	0.69
3:D:366:ILE:HD11	5:F:88:VAL:CG1	2.22	0.69
3:D:387:ARG:HB2	3:D:387:ARG:CZ	2.19	0.69
6:G:49:DG:N2	7:H:1:DC:N4	2.38	0.69
3:D:136:ILE:HD11	3:D:234:LEU:N	2.07	0.69
9:M:95:LYS:HZ2	9:M:95:LYS:CB	2.04	0.69
5:F:170:GLU:OE1	5:F:171:PRO:HD2	1.92	0.69
6:G:4:DG:H2''	6:G:5:DA:H5''	1.75	0.69
5:F:84:TRP:CH2	5:F:120:VAL:HG12	2.27	0.69
2:C:892:LYS:HE3	8:I:7:A:OP1	1.93	0.68
5:F:143:LEU:N	5:F:143:LEU:HD23	2.07	0.68
3:D:1264:ILE:HG22	3:D:1266:ARG:H	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:13:DG:H3'	6:G:13:DG:OP2	1.92	0.68
2:C:146:GLU:OE2	9:M:46:VAL:HG21	1.92	0.68
2:C:821:LEU:HD21	5:F:186:LEU:CD1	2.23	0.68
3:D:334:ARG:HD3	3:D:334:ARG:N	2.09	0.68
5:F:67:GLN:HA	5:F:71:VAL:HG21	1.72	0.68
5:F:142:ASN:HA	5:F:145:LEU:HB2	1.74	0.68
8:I:2:C:H6	8:I:2:C:C5'	2.07	0.68
2:C:139:PHE:HD2	2:C:148:LYS:HE3	1.59	0.68
2:C:148:LYS:HB3	2:C:148:LYS:NZ	2.08	0.68
7:H:36:DA:O5'	7:H:36:DA:H8	1.76	0.68
2:C:146:GLU:OE2	9:M:46:VAL:CG2	2.42	0.68
2:C:410:GLU:OE2	9:M:13:HIS:CG	2.47	0.68
2:C:320:LEU:HB3	2:C:322:LEU:HD23	1.75	0.68
9:M:16:ALA:HB2	9:M:141:LEU:HD11	1.70	0.68
2:C:139:PHE:CD2	2:C:148:LYS:HE3	2.29	0.67
3:D:363:PRO:HD3	5:F:121:PHE:HE2	1.59	0.67
9:M:132:ARG:HH21	9:M:151:GLU:HG2	1.59	0.67
2:C:412:ILE:HD12	2:C:412:ILE:N	2.05	0.67
9:M:10:VAL:CG2	9:M:61:VAL:CA	2.72	0.67
7:H:17:DA:N3	7:H:17:DA:H2'	2.08	0.67
9:M:125:LYS:HD3	9:M:125:LYS:N	2.08	0.67
2:C:812:THR:HG21	3:D:39:LEU:HB2	1.76	0.67
5:F:226:ARG:HH11	7:H:38:DT:H72	1.59	0.67
1:A:89:GLU:HG3	1:A:91:GLU:HG3	1.77	0.67
1:B:55:ARG:NH2	1:B:159:ILE:O	2.25	0.67
2:C:125:LYS:HB2	2:C:127:MET:HE1	1.77	0.67
6:G:12:DA:OP2	6:G:12:DA:H3'	1.93	0.67
3:D:50:LYS:HA	3:D:80:VAL:HG22	1.77	0.67
3:D:377:SER:O	3:D:379:ASP:N	2.27	0.66
3:D:925:LEU:HD12	3:D:942:GLN:HB2	1.76	0.66
2:C:148:LYS:HE2	2:C:148:LYS:N	2.07	0.66
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.78	0.66
1:A:95:MET:HE1	1:A:113:PRO:HD2	1.77	0.66
3:D:328:VAL:CG2	3:D:336:ALA:HB3	2.25	0.66
5:F:145:LEU:HD13	7:H:28:DT:H5''	1.77	0.66
9:M:120:LEU:HB2	9:M:124:GLU:HG2	1.77	0.66
1:B:95:MET:HE2	1:B:110:ILE:HG23	1.76	0.66
2:C:146:GLU:OE1	2:C:148:LYS:NZ	2.28	0.66
5:F:101:ARG:NH1	6:G:29:DA:C8	2.51	0.66
9:M:105:ALA:O	9:M:109:ARG:HG2	1.96	0.66
9:M:108:VAL:HG12	9:M:131:ALA:HB1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:93:LEU:HD22	2:C:393:MET:HB3	1.77	0.66
3:D:143:MET:HE1	3:D:251:TYR:HD1	1.60	0.66
6:G:46:DG:N2	7:H:5:DA:C2	2.64	0.66
9:M:79:THR:HB	9:M:109:ARG:HH22	1.60	0.66
3:D:525:HIS:HE1	3:D:527:LEU:HD23	1.59	0.66
5:F:161:GLU:OE2	5:F:161:GLU:N	2.29	0.66
9:M:85:TRP:CH2	9:M:89:TYR:HD2	2.13	0.66
7:H:36:DA:C8	7:H:36:DA:C3'	2.79	0.65
3:D:637:LEU:O	3:D:661:ALA:HA	1.96	0.65
5:F:221:LYS:HE2	6:G:9:DT:H3'	1.78	0.65
3:D:239:ASN:OD1	3:D:242:ARG:NH2	2.30	0.65
5:F:133:GLU:CD	5:F:133:GLU:H	2.03	0.65
2:C:612:GLN:HG2	2:C:1031:MET:HE1	1.77	0.65
2:C:661:MET:SD	2:C:667:ARG:NH2	2.69	0.65
2:C:767:GLU:HG2	2:C:769:ILE:HG12	1.78	0.65
3:D:329:GLN:OE1	3:D:335:PHE:CD2	2.49	0.65
5:F:226:ARG:NH1	7:H:38:DT:H72	2.11	0.65
3:D:993:GLU:OE1	3:D:993:GLU:HA	1.97	0.65
3:D:1052:ARG:HE	3:D:1102:GLY:HA2	1.62	0.65
9:M:106:GLU:HG2	9:M:109:ARG:HE	1.61	0.65
3:D:328:VAL:HG23	3:D:336:ALA:HB3	1.79	0.65
6:G:16:DC:N3	7:H:34:DG:O6	2.30	0.65
5:F:156:MET:HE2	5:F:156:MET:C	2.22	0.65
2:C:1051:MET:HE2	5:F:168:ALA:HA	1.76	0.65
3:D:387:ARG:HH11	3:D:387:ARG:CA	2.10	0.65
7:H:16:DG:O5'	7:H:16:DG:H8	1.78	0.65
1:B:24:GLU:HG3	1:B:191:LYS:HA	1.78	0.64
2:C:830:ARG:NH1	2:C:831:GLU:O	2.31	0.64
3:D:113:ARG:NH2	3:D:1235:ASP:OD1	2.28	0.64
3:D:965:VAL:HG13	3:D:974:VAL:HG11	1.79	0.64
3:D:64:LYS:HB2	3:D:77:ARG:HH21	1.61	0.64
2:C:168:ILE:CD1	2:C:431:PHE:HB3	2.27	0.64
7:H:13:DG:C8	7:H:13:DG:C3'	2.81	0.64
5:F:205:ASP:OD1	5:F:233:ARG:NH2	2.28	0.64
2:C:139:PHE:O	2:C:148:LYS:HD2	1.98	0.64
5:F:138:ARG:HG3	6:G:25:DG:O5'	1.97	0.64
1:B:24:GLU:HG3	1:B:192:LEU:H	1.61	0.63
3:D:363:PRO:HD3	5:F:121:PHE:CE2	2.32	0.63
5:F:226:ARG:HD3	7:H:38:DT:H72	1.80	0.63
2:C:148:LYS:HD2	2:C:148:LYS:O	1.97	0.63
3:D:413:PHE:HA	3:D:417:LEU:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:897:ILE:HA	3:D:1128:ARG:HH22	1.64	0.63
9:M:88:ARG:HH11	9:M:88:ARG:CB	2.12	0.63
1:A:153:ARG:NE	2:C:795:GLU:OE2	2.31	0.63
6:G:31:DA:N3	6:G:31:DA:H2'	2.13	0.63
2:C:96:ILE:HD11	2:C:401:ARG:NE	2.01	0.63
9:M:107:VAL:HG22	9:M:111:LEU:HD23	1.80	0.63
6:G:27:DC:H2''	6:G:28:DA:C8	2.34	0.62
5:F:101:ARG:CD	6:G:29:DA:C1'	2.63	0.62
9:M:104:VAL:HA	9:M:107:VAL:CG1	2.29	0.62
9:M:125:LYS:HD3	9:M:125:LYS:H	1.63	0.62
2:C:732:GLU:OE2	3:D:578:ARG:NH1	2.32	0.62
5:F:138:ARG:O	5:F:138:ARG:HD3	1.99	0.62
5:F:170:GLU:HG2	5:F:171:PRO:HD2	1.81	0.62
1:B:99:LYS:NZ	1:B:104:GLU:O	2.32	0.62
2:C:230:ARG:HH11	2:C:230:ARG:CG	2.13	0.62
3:D:365:ILE:HG22	5:F:85:ASP:OD1	1.99	0.62
3:D:27:GLU:HB3	3:D:94:HIS:CE1	2.35	0.62
3:D:142:GLU:O	3:D:145:HIS:ND1	2.24	0.62
3:D:939:GLU:OE2	3:D:942:GLN:NE2	2.32	0.61
3:D:330:LEU:HD22	3:D:336:ALA:HB2	1.81	0.61
5:F:226:ARG:HD3	7:H:38:DT:C7	2.30	0.61
3:D:387:ARG:HA	3:D:387:ARG:NH1	2.13	0.61
3:D:623:ASP:OD1	3:D:624:ARG:N	2.33	0.61
6:G:46:DG:C2	7:H:5:DA:C2	2.89	0.61
9:M:79:THR:HG21	9:M:110:ASP:CG	2.24	0.61
2:C:817:GLU:CB	5:F:182:LEU:HD23	2.25	0.61
3:D:539:ASP:OD1	8:I:7:A:O3'	2.18	0.61
3:D:904:ARG:NH1	3:D:909:THR:O	2.34	0.61
5:F:84:TRP:CZ2	5:F:124:VAL:CG1	2.83	0.61
6:G:10:DT:N3	7:H:41:DA:C2	2.69	0.61
7:H:21:DT:OP2	7:H:21:DT:H6	1.84	0.61
2:C:507:ASN:OD1	2:C:511:PHE:N	2.33	0.61
9:M:95:LYS:HB2	9:M:95:LYS:NZ	2.07	0.61
3:D:688:MET:HE2	3:D:688:MET:HA	1.82	0.61
2:C:403:ARG:HH11	2:C:403:ARG:CG	2.14	0.60
2:C:750:ILE:HG22	2:C:876:LYS:HD2	1.83	0.60
3:D:339:ASP:C	3:D:341:ASN:H	2.09	0.60
1:B:184:GLU:CD	1:B:185:GLN:H	2.09	0.60
5:F:97:ARG:CD	6:G:29:DA:N6	2.59	0.60
9:M:10:VAL:CG2	9:M:61:VAL:N	2.65	0.60
2:C:103:MET:HE2	2:C:404:MET:CE	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:607:MET:O	2:C:611:MET:HG2	2.01	0.60
5:F:97:ARG:HH11	6:G:29:DA:H61	1.47	0.60
5:F:166:VAL:HG22	5:F:166:VAL:O	2.02	0.60
1:B:75:GLU:OE1	1:B:79:ASN:ND2	2.33	0.60
2:C:150:GLN:NE2	9:M:43:ASP:O	2.33	0.60
2:C:410:GLU:OE2	9:M:13:HIS:CB	2.50	0.60
3:D:387:ARG:HB2	3:D:387:ARG:NH1	2.17	0.60
2:C:484:CYS:HB2	2:C:588:SER:HB3	1.82	0.60
3:D:171:GLU:OE1	3:D:175:GLN:NE2	2.34	0.60
3:D:421:ARG:NH2	7:H:17:DA:OP1	2.33	0.60
5:F:98:LEU:HD22	5:F:137:HIS:CD2	2.37	0.60
6:G:22:DA:H2'	6:G:22:DA:O5'	2.01	0.60
9:M:106:GLU:HG2	9:M:109:ARG:NE	2.17	0.60
2:C:146:GLU:OE2	2:C:148:LYS:HB3	2.02	0.60
3:D:328:VAL:O	3:D:335:PHE:CA	2.50	0.60
7:H:20:DG:C8	7:H:20:DG:C5'	2.85	0.60
2:C:802:LEU:HD21	2:C:871:VAL:HG21	1.83	0.60
5:F:84:TRP:HH2	5:F:124:VAL:HB	1.64	0.60
2:C:50:VAL:HG12	2:C:503:TYR:CE1	2.37	0.60
2:C:145:GLY:O	9:M:49:PRO:HD2	2.02	0.60
3:D:107:PHE:HE1	3:D:125:LEU:HB3	1.67	0.60
3:D:110:VAL:HG22	7:H:9:DG:H21	1.66	0.60
6:G:12:DA:N1	7:H:39:DA:C2	2.70	0.60
3:D:340:LEU:HD12	3:D:340:LEU:O	2.02	0.59
7:H:44:DT:H2'	7:H:45:DT:H71	1.84	0.59
3:D:488:GLU:HA	3:D:491:ILE:HG22	1.83	0.59
3:D:1265:ASN:OD1	3:D:1269:ASN:ND2	2.35	0.59
5:F:103:SER:HA	5:F:144:PHE:HE1	1.67	0.59
5:F:155:ARG:O	5:F:155:ARG:HG3	2.00	0.59
5:F:226:ARG:CZ	7:H:38:DT:C7	2.79	0.59
5:F:101:ARG:CZ	6:G:29:DA:N7	2.65	0.59
5:F:160:PRO:CB	5:F:165:ARG:HG3	2.30	0.59
6:G:28:DA:OP2	6:G:28:DA:H2'	2.03	0.59
2:C:62:GLU:HG3	2:C:67:SER:HB3	1.85	0.59
2:C:148:LYS:H	2:C:148:LYS:CD	2.14	0.59
2:C:1138:LEU:HB2	3:D:9:GLU:HB3	1.84	0.59
3:D:217:ASP:O	3:D:221:ASP:N	2.36	0.59
7:H:38:DT:H2''	7:H:39:DA:C8	2.37	0.59
9:M:88:ARG:NH2	9:M:114:ARG:NH2	2.51	0.59
7:H:18:DG:C5'	7:H:18:DG:C8	2.85	0.59
3:D:137:THR:HA	3:D:264:LEU:HD21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:260:SER:OG	3:D:262:GLN:OE1	2.21	0.59
3:D:369:ASN:HD22	5:F:114:GLN:NE2	1.99	0.59
3:D:394:PRO:HG2	3:D:397:ARG:HH21	1.68	0.59
3:D:1038:ARG:HH21	6:G:41:DC:H5''	1.67	0.59
2:C:475:VAL:HG23	3:D:857:ARG:HD2	1.85	0.58
5:F:67:GLN:CA	5:F:71:VAL:HG23	2.28	0.58
4:E:69:GLN:NE2	4:E:70:LEU:O	2.37	0.58
6:G:29:DA:H2''	6:G:30:DA:H8	1.69	0.58
1:B:6:ARG:NH2	1:B:234:ILE:O	2.32	0.58
3:D:58:TRP:HA	3:D:82:VAL:HB	1.85	0.58
3:D:335:PHE:CD1	3:D:335:PHE:N	2.72	0.58
6:G:48:DA:H2'	6:G:48:DA:O5'	2.04	0.58
3:D:1228:GLU:OE1	7:H:11:DG:H4'	2.04	0.58
6:G:27:DC:H2'	6:G:27:DC:O2	2.03	0.58
2:C:139:PHE:HD2	2:C:148:LYS:HD3	1.69	0.57
3:D:913:ASP:HB3	3:D:916:ILE:HG13	1.85	0.57
5:F:116:THR:CG2	5:F:139:ILE:CG2	2.75	0.57
7:H:26:DA:H2''	7:H:27:DA:H5''	1.86	0.57
8:I:6:G:C5'	8:I:6:G:C8	2.85	0.57
3:D:369:ASN:HD22	5:F:114:GLN:HE21	1.52	0.57
3:D:1044:ALA:HB1	3:D:1112:MET:HB3	1.87	0.57
1:B:179:ASP:N	1:B:191:LYS:O	2.33	0.57
2:C:62:GLU:OE1	2:C:69:ARG:NH2	2.37	0.57
6:G:26:DT:P	6:G:26:DT:C3'	2.90	0.57
3:D:110:VAL:CG2	7:H:9:DG:H21	2.18	0.57
3:D:714:ASP:OD1	3:D:715:LYS:N	2.37	0.57
3:D:737:LEU:HB2	3:D:793:TYR:HE1	1.67	0.57
5:F:170:GLU:CD	5:F:171:PRO:HD2	2.30	0.57
3:D:1228:GLU:CD	7:H:11:DG:H5''	2.30	0.57
9:M:95:LYS:CD	9:M:107:VAL:HB	2.24	0.57
5:F:98:LEU:CD2	5:F:137:HIS:CD2	2.87	0.57
3:D:331:ASP:CB	3:D:334:ARG:HH11	2.17	0.57
2:C:403:ARG:NH1	2:C:403:ARG:HG3	2.20	0.57
3:D:328:VAL:O	3:D:335:PHE:CB	2.52	0.57
2:C:650:ILE:HD12	2:C:694:ASP:HB2	1.85	0.57
5:F:132:PHE:CE2	5:F:136:LEU:HD21	2.39	0.57
2:C:50:VAL:HG12	2:C:503:TYR:HE1	1.69	0.57
2:C:717:LYS:NZ	2:C:746:VAL:O	2.37	0.57
3:D:430:ILE:HG21	3:D:541:MET:HG3	1.86	0.57
7:H:18:DG:O5'	7:H:18:DG:H8	1.88	0.56
2:C:103:MET:HE1	2:C:404:MET:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1270:ILE:HG12	4:E:107:GLU:HA	1.88	0.56
4:E:40:ASP:OD1	4:E:41:GLU:N	2.37	0.56
6:G:16:DC:N3	7:H:34:DG:C6	2.73	0.56
7:H:20:DG:H5''	7:H:20:DG:H8	1.63	0.56
2:C:810:GLY:O	2:C:830:ARG:NH2	2.39	0.56
6:G:3:DG:P	6:G:3:DG:C3'	2.94	0.56
3:D:369:ASN:ND2	5:F:114:GLN:HE21	2.04	0.56
4:E:43:LEU:HD11	4:E:49:LYS:HG3	1.87	0.56
1:A:219:PHE:HE2	1:B:215:LEU:HD13	1.71	0.56
3:D:152:GLU:HA	3:D:155:MET:HG2	1.87	0.56
3:D:173:ARG:HD2	3:D:176:LYS:HD2	1.88	0.56
2:C:820:LEU:HD23	5:F:186:LEU:CD2	2.35	0.56
3:D:41:PRO:N	3:D:41:PRO:C	2.59	0.56
3:D:58:TRP:HE1	3:D:84:ARG:NH2	2.04	0.56
3:D:162:VAL:O	3:D:166:ARG:HG3	2.05	0.56
3:D:386:ARG:HH11	3:D:386:ARG:CG	2.14	0.56
3:D:821:LYS:HB3	3:D:836:VAL:HG23	1.88	0.56
5:F:170:GLU:CG	5:F:171:PRO:HD2	2.35	0.56
9:M:107:VAL:CG2	9:M:111:LEU:HD23	2.36	0.56
2:C:125:LYS:CD	2:C:853:PHE:CE1	2.89	0.56
2:C:215:ASP:O	2:C:223:GLY:N	2.38	0.56
2:C:811:GLU:HA	2:C:814:LEU:HG	1.88	0.56
6:G:13:DG:OP2	6:G:13:DG:H2'	2.05	0.56
6:G:44:DA:C8	6:G:45:DT:H72	2.40	0.56
6:G:44:DA:H2	7:H:7:DC:O2	1.87	0.56
9:M:104:VAL:O	9:M:108:VAL:HG13	2.05	0.56
2:C:223:GLY:HA2	2:C:231:ARG:HH11	1.71	0.56
3:D:928:ASP:HA	3:D:940:ARG:NH2	2.21	0.56
1:B:24:GLU:HB3	1:B:25:PRO:HA	1.87	0.56
1:B:182:ARG:NH2	3:D:488:GLU:OE2	2.37	0.56
3:D:346:ARG:NH2	5:F:107:HIS:CB	2.59	0.56
1:A:5:GLN:O	1:A:6:ARG:NE	2.37	0.55
2:C:833:ARG:HH12	3:D:329:GLN:HG2	1.71	0.55
6:G:3:DG:P	6:G:3:DG:C2'	2.94	0.55
3:D:611:VAL:HG12	3:D:634:LYS:HB2	1.88	0.55
9:M:106:GLU:O	9:M:109:ARG:HG3	2.07	0.55
1:B:146:TYR:HB2	3:D:620:MET:HE2	1.89	0.55
1:B:148:PRO:HB2	1:B:150:VAL:HG12	1.88	0.55
2:C:818:GLU:HG3	2:C:831:GLU:HG2	1.89	0.55
2:C:1139:SER:HB2	2:C:1145:ILE:HD11	1.89	0.55
6:G:47:DC:OP2	6:G:47:DC:H3'	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:3:DG:OP2	6:G:3:DG:H3'	2.06	0.55
6:G:25:DG:H2''	9:M:89:TYR:HE2	1.71	0.55
1:B:55:ARG:HB2	1:B:137:GLU:HG2	1.87	0.55
5:F:221:LYS:HB3	6:G:9:DT:H5''	1.89	0.55
9:M:32:LYS:NZ	9:M:33:GLU:O	2.39	0.55
3:D:217:ASP:OD1	3:D:218:ARG:N	2.39	0.55
3:D:555:ALA:HA	3:D:559:MET:HB2	1.89	0.55
3:D:135:VAL:CG1	3:D:256:MET:HB3	2.37	0.55
3:D:346:ARG:O	3:D:350:ARG:HG2	2.06	0.55
6:G:48:DA:C2	7:H:3:DG:N1	2.74	0.55
3:D:328:VAL:O	3:D:335:PHE:HA	2.07	0.55
5:F:84:TRP:CH2	5:F:124:VAL:CB	2.90	0.55
5:F:133:GLU:N	5:F:133:GLU:OE2	2.40	0.55
9:M:23:GLU:O	9:M:34:TYR:N	2.40	0.55
9:M:95:LYS:CD	9:M:107:VAL:CG1	2.85	0.55
3:D:432:VAL:HG22	3:D:434:PRO:HD3	1.88	0.55
6:G:12:DA:H3'	6:G:12:DA:P	2.46	0.55
6:G:38:DT:H1'	6:G:39:DC:H5'	1.89	0.55
2:C:745:ASP:OD1	2:C:878:LYS:NZ	2.33	0.54
2:C:797:ARG:HG2	2:C:798:ASP:H	1.71	0.54
3:D:189:ALA:HA	3:D:194:ARG:HD3	1.88	0.54
3:D:525:HIS:CE1	3:D:527:LEU:HD23	2.39	0.54
5:F:134:GLY:HA2	6:G:26:DT:O2	2.07	0.54
2:C:141:ASN:H	2:C:147:ILE:HG12	1.73	0.54
2:C:535:GLU:OE1	2:C:538:ARG:NH2	2.37	0.54
3:D:925:LEU:HB3	3:D:940:ARG:NH1	2.22	0.54
5:F:91:HIS:HB3	5:F:136:LEU:HD13	1.89	0.54
2:C:139:PHE:CD2	2:C:148:LYS:HD3	2.42	0.54
6:G:11:DT:H2''	6:G:12:DA:H2'	1.89	0.54
7:H:18:DG:C8	7:H:18:DG:H5''	2.42	0.54
2:C:523:VAL:HG13	2:C:552:GLY:HA3	1.89	0.54
2:C:611:MET:HE1	2:C:892:LYS:HD3	1.89	0.54
5:F:103:SER:HA	5:F:144:PHE:CE1	2.43	0.54
2:C:403:ARG:NH2	2:C:416:THR:O	2.40	0.54
2:C:812:THR:HG21	3:D:39:LEU:CB	2.37	0.54
3:D:938:VAL:O	3:D:940:ARG:NH2	2.39	0.54
3:D:1078:ASP:OD1	3:D:1079:LYS:N	2.38	0.54
4:E:42:LEU:HD11	4:E:98:ILE:HG23	1.89	0.54
7:H:20:DG:C5'	7:H:20:DG:H8	2.20	0.54
9:M:95:LYS:C	9:M:95:LYS:HZ1	2.15	0.54
2:C:441:ASP:OD1	2:C:680:HIS:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:204:CYS:SG	5:F:211:TYR:HE1	2.31	0.54
9:M:10:VAL:CG2	9:M:61:VAL:HB	2.38	0.54
1:B:96:TYR:HD1	1:B:137:GLU:HB3	1.73	0.54
2:C:173:ARG:HG3	2:C:438:GLN:O	2.08	0.54
2:C:228:ARG:HH21	6:G:35:DT:C1'	2.21	0.54
3:D:778:TRP:CE3	3:D:835:PRO:HG3	2.42	0.54
9:M:88:ARG:NE	9:M:114:ARG:HH12	2.05	0.54
1:B:95:MET:HE1	1:B:111:VAL:C	2.33	0.54
2:C:446:LEU:HB2	2:C:713:MET:HE3	1.89	0.54
2:C:524:VAL:HG12	2:C:552:GLY:HA2	1.90	0.54
2:C:1103:TYR:OH	3:D:473:LYS:NZ	2.33	0.54
6:G:13:DG:P	6:G:13:DG:C3'	2.96	0.54
6:G:26:DT:H3'	6:G:26:DT:OP2	2.07	0.54
1:B:179:ASP:HB2	1:B:191:LYS:HB3	1.90	0.53
6:G:14:DT:H2''	6:G:15:DG:C8	2.43	0.53
6:G:49:DG:H22	7:H:1:DC:N4	2.03	0.53
9:M:10:VAL:CG2	9:M:61:VAL:H	2.21	0.53
1:B:128:LEU:HD12	1:B:132:GLY:HA3	1.90	0.53
2:C:42:ALA:HB2	2:C:975:PRO:HG2	1.90	0.53
3:D:365:ILE:CG2	5:F:85:ASP:OD1	2.56	0.53
5:F:69:THR:O	5:F:72:PHE:N	2.40	0.53
9:M:10:VAL:HG23	9:M:61:VAL:N	2.23	0.53
2:C:821:LEU:CD2	5:F:186:LEU:CD1	2.86	0.53
3:D:56:ARG:HB3	3:D:59:GLU:HB2	1.89	0.53
3:D:178:GLU:OE1	3:D:198:ARG:NH2	2.38	0.53
7:H:42:DA:H2'	7:H:43:DG:C8	2.43	0.53
9:M:87:ARG:CZ	9:M:87:ARG:CB	2.85	0.53
9:M:96:LEU:HD11	9:M:130:LYS:HD2	1.91	0.53
2:C:814:LEU:O	2:C:819:ARG:NH1	2.41	0.53
4:E:55:TYR:HE2	4:E:105:HIS:HB3	1.73	0.53
2:C:173:ARG:HD3	2:C:437:SER:OG	2.08	0.53
3:D:905:ALA:HB2	3:D:911:ILE:HG23	1.90	0.53
2:C:259:ARG:O	2:C:263:GLU:HG2	2.09	0.53
2:C:885:LEU:HG	2:C:895:ILE:HD11	1.90	0.53
3:D:103:HIS:CE1	3:D:105:TRP:HB3	2.44	0.53
2:C:216:VAL:HA	2:C:222:VAL:HA	1.90	0.53
5:F:161:GLU:CG	8:I:1:C:C6	2.91	0.53
2:C:402:GLU:O	2:C:406:THR:HG22	2.09	0.53
6:G:12:DA:H2''	6:G:13:DG:C8	2.44	0.53
5:F:100:TYR:OH	6:G:31:DA:OP2	2.27	0.53
6:G:31:DA:N3	6:G:31:DA:C2'	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:84:ASN:ND2	9:M:86:SER:HB3	2.24	0.53
2:C:862:PRO:HG2	2:C:865:VAL:HG21	1.91	0.52
3:D:900:GLU:OE1	3:D:959:GLN:NE2	2.28	0.52
5:F:138:ARG:HD3	5:F:138:ARG:C	2.27	0.52
9:M:125:LYS:N	9:M:125:LYS:CD	2.72	0.52
1:A:206:ASP:OD1	1:A:206:ASP:N	2.41	0.52
2:C:140:ILE:HA	2:C:147:ILE:HG23	1.91	0.52
2:C:806:VAL:HB	2:C:832:VAL:HG23	1.90	0.52
2:C:861:LEU:HD13	2:C:865:VAL:HG12	1.91	0.52
3:D:457:MET:HE1	3:D:473:LYS:HD2	1.92	0.52
3:D:862:ASP:O	3:D:866:ARG:HG2	2.09	0.52
5:F:163:TYR:N	5:F:163:TYR:CD1	2.73	0.52
2:C:62:GLU:HG2	2:C:70:TRP:HB2	1.92	0.52
5:F:142:ASN:HB2	6:G:24:DT:H72	1.90	0.52
3:D:181:LEU:HD23	3:D:185:GLU:HG2	1.92	0.52
3:D:1054:ARG:HB3	3:D:1065:THR:HB	1.92	0.52
3:D:1086:LEU:HD23	3:D:1099:LEU:HD23	1.92	0.52
5:F:73:ASP:HB3	5:F:130:GLY:O	2.10	0.52
5:F:68:GLY:C	5:F:82:PRO:HG3	2.35	0.52
9:M:81:GLU:C	9:M:82:PRO:C	2.77	0.52
2:C:143:ASN:OD1	2:C:144:THR:N	2.43	0.52
2:C:758:ASP:O	2:C:805:LYS:NZ	2.43	0.52
2:C:817:GLU:O	2:C:821:LEU:HG	2.09	0.52
3:D:342:ASP:OD1	3:D:345:ARG:NH2	2.43	0.52
3:D:108:LYS:CA	3:D:108:LYS:HE3	2.36	0.51
5:F:138:ARG:HG3	6:G:24:DT:H2'	1.92	0.51
5:F:141:THR:OG1	6:G:24:DT:H71	2.09	0.51
6:G:37:DG:C8	6:G:37:DG:C5'	2.85	0.51
8:I:6:G:H8	8:I:6:G:O5'	1.92	0.51
1:B:51:VAL:HG22	1:B:140:VAL:HG22	1.91	0.51
2:C:410:GLU:O	2:C:410:GLU:HG3	2.04	0.51
4:E:42:LEU:HB3	4:E:52:LEU:HD11	1.91	0.51
5:F:84:TRP:HZ3	5:F:120:VAL:CG1	2.18	0.51
5:F:172:ASN:HD21	5:F:174:GLU:HB3	1.76	0.51
6:G:3:DG:P	6:G:3:DG:H3'	2.50	0.51
5:F:169:ASP:OD1	5:F:169:ASP:N	2.43	0.51
6:G:47:DC:H3'	6:G:47:DC:P	2.50	0.51
2:C:122:CYS:HA	2:C:127:MET:SD	2.50	0.51
2:C:444:ASN:O	2:C:447:SER:OG	2.26	0.51
3:D:248:TYR:HB2	3:D:251:TYR:CE2	2.45	0.51
3:D:778:TRP:CD2	3:D:835:PRO:HG3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:88:ARG:CB	9:M:88:ARG:NH1	2.73	0.51
1:B:112:PRO:HB2	1:B:116:VAL:HG23	1.91	0.51
3:D:215:GLU:HG3	3:D:218:ARG:HH12	1.76	0.51
2:C:103:MET:CE	2:C:404:MET:HG3	2.40	0.51
2:C:463:LEU:HD13	2:C:468:ALA:HB2	1.92	0.51
2:C:806:VAL:HG12	2:C:834:ASP:HA	1.93	0.51
3:D:558:LEU:HD23	4:E:49:LYS:NZ	2.26	0.51
3:D:890:ASP:OD1	3:D:963:ARG:NH2	2.44	0.51
3:D:893:THR:O	3:D:963:ARG:NH1	2.44	0.51
2:C:471:GLU:HG2	2:C:472:VAL:HG13	1.93	0.51
4:E:39:ILE:HG13	4:E:43:LEU:HD23	1.93	0.51
7:H:13:DG:H3'	7:H:13:DG:H8	1.74	0.51
2:C:761:ASP:N	2:C:864:GLY:O	2.43	0.51
2:C:774:PRO:HD3	2:C:806:VAL:HG11	1.93	0.51
2:C:125:LYS:HE3	2:C:853:PHE:CD1	2.45	0.51
2:C:139:PHE:HD2	2:C:148:LYS:CE	2.23	0.51
2:C:817:GLU:OE2	5:F:181:ARG:C	2.54	0.50
6:G:14:DT:H2''	6:G:15:DG:H8	1.76	0.50
2:C:282:ARG:HB2	2:C:285:GLU:HG3	1.93	0.50
2:C:593:MET:HE1	2:C:631:GLU:HA	1.94	0.50
3:D:386:ARG:CG	3:D:386:ARG:NH1	2.73	0.50
3:D:901:LEU:HB3	3:D:958:THR:HA	1.93	0.50
2:C:587:VAL:HG22	2:C:591:THR:HG23	1.93	0.50
3:D:101:VAL:HG13	3:D:375:GLN:OE1	2.11	0.50
3:D:320:ILE:HG23	3:D:325:ARG:HH11	1.76	0.50
3:D:642:PRO:HD3	3:D:656:TRP:CD1	2.46	0.50
5:F:68:GLY:C	5:F:82:PRO:CG	2.84	0.50
1:A:219:PHE:CE2	1:B:215:LEU:HD13	2.45	0.50
2:C:730:ASN:O	2:C:918:ASN:ND2	2.34	0.50
2:C:1108:LYS:C	2:C:1108:LYS:CD	2.85	0.50
3:D:331:ASP:HB2	3:D:334:ARG:HH11	1.76	0.50
3:D:938:VAL:HG13	3:D:940:ARG:HH22	1.76	0.50
3:D:1089:PHE:CE2	3:D:1099:LEU:HB2	2.47	0.50
3:D:1254:ILE:HD11	3:D:1256:LYS:HE3	1.92	0.50
5:F:156:MET:C	5:F:156:MET:CE	2.85	0.50
3:D:580:ASP:O	3:D:583:THR:HB	2.10	0.50
3:D:760:PHE:HA	3:D:765:LEU:HB2	1.94	0.50
8:I:2:C:C6	8:I:2:C:C5'	2.85	0.50
1:A:86:SER:OG	1:A:117:THR:OG1	2.27	0.50
3:D:114:LEU:HD21	3:D:312:MET:HG2	1.93	0.50
6:G:48:DA:H2	7:H:3:DG:N1	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:95:LYS:CE	9:M:104:VAL:HA	2.32	0.50
1:B:183:VAL:HG12	1:B:184:GLU:HG3	1.92	0.50
3:D:927:THR:O	3:D:940:ARG:NH1	2.45	0.50
3:D:1062:TYR:HB2	3:D:1080:ILE:HB	1.93	0.50
3:D:1169:ASP:H	3:D:1202:ALA:HB3	1.77	0.50
6:G:26:DT:H1'	6:G:27:DC:C2	2.47	0.50
1:A:43:LEU:HA	1:A:171:VAL:HG11	1.93	0.50
2:C:756:GLU:HB3	2:C:870:ARG:HG2	1.94	0.50
2:C:938:TRP:HE1	2:C:1002:VAL:HG11	1.76	0.50
2:C:206:PRO:HB3	2:C:306:TYR:CZ	2.47	0.50
2:C:633:ARG:NH1	2:C:637:ASP:OD2	2.45	0.50
3:D:58:TRP:HZ3	3:D:71:LYS:HA	1.76	0.50
3:D:876:ARG:NH2	3:D:1032:GLN:OE1	2.45	0.50
5:F:139:ILE:HG23	5:F:139:ILE:O	2.11	0.50
2:C:817:GLU:CG	5:F:182:LEU:CD2	2.28	0.49
5:F:139:ILE:HA	6:G:24:DT:C4	2.47	0.49
6:G:16:DC:H2'	6:G:17:DT:C6	2.46	0.49
9:M:3:PHE:CE1	9:M:60:ASP:OD2	2.65	0.49
3:D:187:GLU:OE2	3:D:190:LYS:NZ	2.45	0.49
1:A:46:ILE:HG23	1:A:170:PRO:HD2	1.95	0.49
2:C:282:ARG:NH1	2:C:295:LEU:HD21	2.27	0.49
5:F:144:PHE:CE2	5:F:148:VAL:CG2	2.95	0.49
1:A:82:SER:HB2	1:A:123:MET:HE1	1.94	0.49
2:C:398:ARG:NH1	2:C:398:ARG:CG	2.72	0.49
3:D:223:TRP:O	3:D:226:PHE:HB2	2.12	0.49
3:D:328:VAL:O	3:D:336:ALA:N	2.42	0.49
3:D:353:ARG:O	3:D:357:LEU:N	2.45	0.49
3:D:493:GLU:HA	4:E:34:ILE:HD11	1.94	0.49
5:F:131:THR:C	5:F:133:GLU:OE2	2.55	0.49
5:F:138:ARG:HG2	6:G:25:DG:H5''	1.94	0.49
3:D:554:GLU:HB2	3:D:558:LEU:HD12	1.94	0.49
3:D:557:ILE:HG22	4:E:49:LYS:NZ	2.27	0.49
6:G:20:DT:H2''	6:G:21:DT:H5'	1.94	0.49
3:D:231:PRO:O	3:D:232:LYS:HG2	2.13	0.49
3:D:387:ARG:NH1	3:D:387:ARG:CB	2.75	0.49
3:D:689:HIS:O	3:D:693:GLN:NE2	2.44	0.49
9:M:104:VAL:O	9:M:107:VAL:CG1	2.60	0.49
3:D:108:LYS:C	3:D:108:LYS:CD	2.86	0.49
5:F:156:MET:SD	5:F:156:MET:C	2.94	0.49
9:M:154:LEU:HA	9:M:157:VAL:HG22	1.95	0.49
1:B:153:ARG:HH22	3:D:607:PRO:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:135:VAL:HG11	3:D:256:MET:HB3	1.95	0.49
3:D:487:LEU:HD23	3:D:516:LEU:HD21	1.93	0.49
3:D:1173:THR:OG1	3:D:1200:PRO:O	2.30	0.49
1:A:7:PRO:HA	1:A:25:PRO:HD2	1.94	0.49
2:C:215:ASP:OD1	2:C:216:VAL:N	2.46	0.49
3:D:190:LYS:HB2	3:D:194:ARG:H	1.76	0.49
3:D:904:ARG:NH1	3:D:907:ASP:O	2.35	0.49
1:A:217:GLU:OE2	1:B:234:ILE:N	2.44	0.49
2:C:757:ILE:HG23	2:C:837:LEU:HD12	1.95	0.49
2:C:817:GLU:HG2	5:F:182:LEU:HD23	1.69	0.49
3:D:334:ARG:N	3:D:334:ARG:CD	2.72	0.49
3:D:838:SER:HB2	3:D:844:LEU:HD23	1.94	0.49
7:H:6:DT:H2''	7:H:7:DC:H5'	1.95	0.49
9:M:120:LEU:HB2	9:M:124:GLU:CG	2.43	0.49
2:C:158:PRO:HG2	2:C:431:PHE:CE2	2.48	0.48
3:D:982:SER:HG	3:D:985:THR:HG1	1.53	0.48
8:I:6:G:C8	8:I:6:G:C4'	2.96	0.48
3:D:464:ASN:O	3:D:467:GLN:NE2	2.42	0.48
3:D:1162:LEU:C	3:D:1183:ARG:HH21	2.21	0.48
5:F:145:LEU:CD2	7:H:27:DA:OP2	2.58	0.48
6:G:8:DT:C6	6:G:9:DT:H72	2.48	0.48
6:G:25:DG:OP1	6:G:25:DG:C8	2.66	0.48
9:M:84:ASN:O	9:M:85:TRP:C	2.49	0.48
2:C:558:ARG:HG2	2:C:572:PRO:HA	1.96	0.48
3:D:387:ARG:CA	3:D:387:ARG:NH1	2.73	0.48
6:G:12:DA:N1	7:H:39:DA:H2	2.10	0.48
5:F:84:TRP:CZ2	5:F:124:VAL:HB	2.48	0.48
5:F:162:ASP:OD1	5:F:164:ASP:HB2	2.13	0.48
6:G:39:DC:C2	7:H:11:DG:N2	2.77	0.48
7:H:32:DT:H2'	7:H:33:DA:C8	2.48	0.48
3:D:503:THR:HG23	3:D:508:GLY:HA3	1.94	0.48
7:H:20:DG:H8	7:H:20:DG:OP2	1.97	0.48
9:M:124:GLU:N	9:M:124:GLU:CD	2.71	0.48
5:F:101:ARG:HD3	6:G:29:DA:H1'	1.83	0.48
2:C:1079:TYR:HD2	3:D:559:MET:SD	2.36	0.48
3:D:207:GLN:HB3	3:D:211:ARG:HH22	1.79	0.48
3:D:366:ILE:CD1	5:F:88:VAL:HG11	2.27	0.48
9:M:95:LYS:CB	9:M:95:LYS:NZ	2.73	0.48
3:D:557:ILE:HG22	4:E:49:LYS:HZ3	1.79	0.48
3:D:1222:SER:OG	3:D:1250:GLU:OE2	2.20	0.48
5:F:138:ARG:C	5:F:138:ARG:CD	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ARG:HH21	1:A:161:ARG:HB2	1.79	0.48
2:C:1088:LEU:HD12	2:C:1092:LYS:HD2	1.95	0.48
3:D:217:ASP:O	3:D:220:GLU:N	2.47	0.48
5:F:138:ARG:CG	6:G:25:DG:C5'	2.91	0.48
1:A:40:ARG:HH12	1:B:32:TYR:HB2	1.79	0.47
1:A:100:GLN:OE1	1:A:133:LYS:HE2	2.14	0.47
2:C:150:GLN:NE2	9:M:44:LEU:N	2.62	0.47
5:F:91:HIS:HB3	5:F:136:LEU:CD1	2.44	0.47
7:H:40:DA:H1'	7:H:41:DA:H5'	1.96	0.47
1:B:83:LEU:HA	1:B:123:MET:HE1	1.95	0.47
2:C:228:ARG:NH2	6:G:35:DT:C2'	2.75	0.47
2:C:403:ARG:HH11	2:C:403:ARG:HG3	1.78	0.47
2:C:798:ASP:OD2	2:C:842:GLY:N	2.41	0.47
3:D:459:ARG:HG3	3:D:486:VAL:HG13	1.97	0.47
3:D:1038:ARG:HH21	6:G:41:DC:C5'	2.27	0.47
4:E:55:TYR:CE2	4:E:105:HIS:HB3	2.49	0.47
9:M:81:GLU:C	9:M:83:THR:N	2.72	0.47
3:D:105:TRP:NE1	3:D:1230:THR:OG1	2.47	0.47
3:D:468:ASN:OD1	3:D:470:LYS:HG3	2.13	0.47
3:D:565:ILE:HG13	3:D:566:LEU:HD22	1.95	0.47
3:D:1087:ARG:HD3	3:D:1110:GLN:OE1	2.13	0.47
5:F:133:GLU:CD	5:F:133:GLU:N	2.72	0.47
9:M:10:VAL:HG23	9:M:61:VAL:HB	1.96	0.47
9:M:16:ALA:CB	9:M:141:LEU:HD11	2.37	0.47
2:C:762:THR:HG21	2:C:808:PRO:HG3	1.96	0.47
5:F:131:THR:HB	5:F:133:GLU:OE2	2.13	0.47
2:C:202:VAL:HG13	2:C:214:PHE:HB3	1.97	0.47
2:C:292:ALA:O	2:C:296:LEU:HD23	2.14	0.47
2:C:440:MET:HG3	2:C:442:GLN:HG3	1.95	0.47
2:C:812:THR:HG23	3:D:39:LEU:HB2	1.92	0.47
3:D:108:LYS:C	3:D:108:LYS:HD2	2.40	0.47
4:E:50:TYR:HA	4:E:53:VAL:HG12	1.96	0.47
5:F:73:ASP:CB	5:F:130:GLY:O	2.62	0.47
5:F:87:LEU:HD22	5:F:132:PHE:CZ	2.50	0.47
1:B:47:PRO:HB3	1:B:144:ARG:HD2	1.96	0.47
1:B:110:ILE:HG22	1:B:112:PRO:HD3	1.96	0.47
2:C:148:LYS:H	2:C:148:LYS:HD2	1.79	0.47
2:C:393:MET:HE3	2:C:393:MET:HA	1.96	0.47
2:C:401:ARG:NH1	2:C:401:ARG:CG	2.72	0.47
2:C:583:PRO:O	2:C:584:ARG:HG2	2.15	0.47
2:C:604:ARG:NH1	2:C:607:MET:HE1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:104:ILE:HB	3:D:379:ASP:OD1	2.15	0.47
3:D:285:LYS:HA	3:D:289:LYS:HE2	1.96	0.47
3:D:550:GLU:O	3:D:553:ALA:N	2.48	0.47
3:D:580:ASP:OD1	3:D:581:MET:N	2.47	0.47
4:E:59:ARG:HH21	4:E:63:ILE:HD11	1.79	0.47
9:M:85:TRP:C	9:M:85:TRP:CD2	2.92	0.47
1:B:24:GLU:HG3	1:B:192:LEU:N	2.28	0.47
2:C:347:ARG:HD2	2:C:355:MET:HG2	1.96	0.47
3:D:180:ASP:OD1	3:D:181:LEU:N	2.47	0.47
3:D:318:PRO:O	3:D:319:VAL:HG12	2.15	0.47
5:F:159:LEU:CG	5:F:160:PRO:CD	2.81	0.47
6:G:16:DC:O2	7:H:34:DG:N1	2.42	0.47
2:C:653:VAL:HG22	2:C:692:ALA:HB2	1.97	0.47
1:A:72:ASP:O	1:A:76:ILE:HG12	2.15	0.47
2:C:148:LYS:CE	2:C:148:LYS:N	2.73	0.47
2:C:792:ILE:HG13	2:C:850:ILE:HD12	1.97	0.47
3:D:166:ARG:HG2	3:D:212:ALA:HB1	1.95	0.47
5:F:91:HIS:CG	5:F:136:LEU:CD1	2.98	0.47
5:F:137:HIS:ND1	5:F:137:HIS:C	2.72	0.47
6:G:31:DA:OP1	6:G:31:DA:H8	1.98	0.47
7:H:20:DG:H8	7:H:20:DG:P	2.38	0.47
9:M:87:ARG:NE	9:M:87:ARG:C	2.72	0.47
6:G:25:DG:H4'	6:G:26:DT:H5''	1.97	0.46
1:A:72:ASP:OD1	1:A:75:GLU:HG2	2.16	0.46
2:C:228:ARG:HH21	6:G:35:DT:C2'	2.28	0.46
2:C:466:GLU:OE1	2:C:467:ARG:NH2	2.47	0.46
3:D:168:GLY:O	3:D:171:GLU:HG3	2.16	0.46
6:G:24:DT:O2	6:G:24:DT:O4'	2.33	0.46
9:M:79:THR:HB	9:M:109:ARG:NH2	2.30	0.46
1:A:153:ARG:HB2	2:C:795:GLU:OE2	2.14	0.46
2:C:830:ARG:NH1	2:C:831:GLU:HG3	2.30	0.46
3:D:143:MET:HE1	3:D:251:TYR:CD1	2.47	0.46
5:F:204:CYS:O	5:F:208:GLY:HA2	2.14	0.46
7:H:10:DT:H2'	7:H:11:DG:C8	2.49	0.46
2:C:542:ALA:HA	2:C:561:VAL:HG12	1.97	0.46
3:D:181:LEU:HD22	3:D:198:ARG:HH22	1.79	0.46
9:M:81:GLU:HA	9:M:82:PRO:HD2	1.47	0.46
2:C:139:PHE:HD2	2:C:148:LYS:CD	2.28	0.46
3:D:350:ARG:NH2	3:D:350:ARG:HG3	2.30	0.46
3:D:499:ASN:OD1	3:D:500:ARG:N	2.49	0.46
1:B:186:ARG:NH2	1:B:188:ASP:OD2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:230:ARG:CG	2:C:230:ARG:NH1	2.73	0.46
9:M:85:TRP:CE3	9:M:85:TRP:O	2.68	0.46
9:M:95:LYS:NZ	9:M:95:LYS:C	2.73	0.46
2:C:483:MET:HE3	2:C:498:GLY:HA3	1.98	0.46
3:D:196:LYS:HA	3:D:196:LYS:HD3	1.65	0.46
3:D:223:TRP:HA	3:D:226:PHE:CD1	2.50	0.46
3:D:594:GLY:N	3:D:598:GLU:OE2	2.47	0.46
6:G:25:DG:OP2	6:G:25:DG:C4	2.69	0.46
9:M:57:GLY:O	9:M:59:ARG:CG	2.61	0.46
1:B:70:LYS:HB2	1:B:127:THR:HG23	1.98	0.46
2:C:338:VAL:HA	2:C:341:THR:HG22	1.98	0.46
6:G:13:DG:H1	7:H:37:DC:H41	1.62	0.46
6:G:31:DA:H3'	6:G:31:DA:C4	2.51	0.46
6:G:46:DG:N2	7:H:5:DA:N3	2.63	0.46
9:M:84:ASN:CG	9:M:86:SER:HB3	2.41	0.46
2:C:487:GLU:OE2	2:C:499:SER:N	2.49	0.46
5:F:155:ARG:HA	5:F:155:ARG:CZ	2.46	0.46
8:I:6:G:H8	8:I:6:G:H5''	1.77	0.46
1:B:96:TYR:CD1	1:B:137:GLU:HB3	2.51	0.46
3:D:749:TYR:CD2	3:D:781:ALA:HB2	2.51	0.46
3:D:826:ASN:OD1	3:D:827:PRO:HD2	2.16	0.46
6:G:48:DA:H2	7:H:3:DG:N2	2.14	0.46
2:C:326:GLU:N	2:C:327:PRO:HD3	2.31	0.45
2:C:442:GLN:H	2:C:680:HIS:CD2	2.34	0.45
3:D:137:THR:O	3:D:231:PRO:HB3	2.16	0.45
3:D:558:LEU:HA	4:E:49:LYS:HZ2	1.80	0.45
2:C:230:ARG:HB3	2:C:230:ARG:CZ	2.46	0.45
3:D:642:PRO:HG3	3:D:662:TRP:CE2	2.52	0.45
3:D:798:PRO:HA	3:D:801:THR:HG22	1.97	0.45
5:F:69:THR:O	5:F:71:VAL:N	2.50	0.45
9:M:71:PHE:CE1	9:M:157:VAL:HG21	2.51	0.45
3:D:110:VAL:O	6:G:43:DG:H4'	2.16	0.45
3:D:339:ASP:C	3:D:341:ASN:N	2.75	0.45
3:D:1218:ASP:O	3:D:1241:ARG:NH1	2.48	0.45
7:H:25:DC:C2	7:H:25:DC:OP1	2.69	0.45
7:H:26:DA:OP1	7:H:26:DA:C8	2.70	0.45
1:B:63:PHE:HB3	1:B:73:VAL:HG21	1.99	0.45
2:C:197:LYS:HA	2:C:197:LYS:HD3	1.81	0.45
2:C:289:LYS:HG3	2:C:290:GLU:N	2.32	0.45
2:C:409:VAL:C	2:C:411:ALA:H	2.24	0.45
3:D:10:LEU:HD23	3:D:1245:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:163:GLU:HG3	3:D:166:ARG:HH21	1.81	0.45
3:D:329:GLN:OE1	3:D:329:GLN:HA	2.17	0.45
3:D:928:ASP:HA	3:D:940:ARG:CZ	2.46	0.45
5:F:193:LEU:HD11	5:F:236:LEU:HG	1.98	0.45
1:B:9:LEU:HA	1:B:22:VAL:O	2.17	0.45
2:C:558:ARG:NH1	2:C:570:TYR:HD2	2.15	0.45
2:C:716:GLY:HA3	2:C:1030:ILE:O	2.17	0.45
3:D:45:GLY:H	3:D:48:CYS:HB2	1.81	0.45
3:D:248:TYR:HB2	3:D:251:TYR:HE2	1.81	0.45
3:D:927:THR:HG21	3:D:961:LYS:HD3	1.99	0.45
3:D:1007:GLY:HA2	3:D:1010:LEU:HD13	1.98	0.45
9:M:95:LYS:HD3	9:M:107:VAL:CG1	2.46	0.45
1:B:24:GLU:HG3	1:B:191:LYS:HD2	1.99	0.45
2:C:38:ARG:NH1	2:C:971:ILE:HB	2.31	0.45
2:C:98:ASP:OD1	2:C:98:ASP:N	2.49	0.45
2:C:148:LYS:NZ	2:C:148:LYS:CB	2.73	0.45
3:D:459:ARG:HH22	3:D:463:LEU:HD21	1.82	0.45
3:D:629:VAL:HG23	3:D:630:ARG:HG3	1.99	0.45
7:H:42:DA:H2'	7:H:43:DG:H8	1.81	0.45
1:A:107:ALA:N	1:A:123:MET:O	2.44	0.45
1:A:203:SER:OG	1:A:206:ASP:OD1	2.28	0.45
1:B:32:TYR:CZ	1:B:178:VAL:HG11	2.51	0.45
2:C:1081:ALA:HB1	3:D:554:GLU:HG3	1.99	0.45
6:G:4:DG:C8	6:G:4:DG:O5'	2.70	0.45
1:B:185:GLN:OE1	3:D:484:TRP:NE1	2.50	0.45
2:C:739:ASN:ND2	2:C:743:GLU:OE2	2.49	0.45
3:D:676:LEU:HD22	3:D:715:LYS:HB3	1.99	0.45
9:M:127:MET:HA	9:M:130:LYS:HG2	1.99	0.45
1:B:169:SER:OG	3:D:620:MET:HE1	2.17	0.44
9:M:83:THR:O	9:M:84:ASN:C	2.60	0.44
2:C:148:LYS:CD	2:C:148:LYS:N	2.78	0.44
6:G:39:DC:N3	7:H:11:DG:N2	2.62	0.44
7:H:36:DA:C8	7:H:36:DA:OP2	2.70	0.44
1:B:179:ASP:O	1:B:191:LYS:N	2.45	0.44
1:B:182:ARG:NH2	3:D:485:ASP:OD1	2.38	0.44
2:C:115:VAL:HG11	2:C:129:TYR:CE2	2.52	0.44
2:C:946:VAL:HG11	2:C:964:LEU:HD22	1.99	0.44
3:D:243:GLU:N	3:D:243:GLU:OE1	2.50	0.44
5:F:145:LEU:HD22	7:H:27:DA:H4'	1.99	0.44
5:F:162:ASP:H	5:F:165:ARG:HD2	1.83	0.44
5:F:165:ARG:HE	5:F:165:ARG:HB3	1.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:20:DG:C8	7:H:20:DG:OP2	2.70	0.44
9:M:11:TYR:CD1	9:M:12:PRO:HD2	2.52	0.44
9:M:78:HIS:CD2	9:M:78:HIS:O	2.70	0.44
1:B:42:LEU:HD22	1:B:174:VAL:HG21	2.00	0.44
2:C:1041:ILE:HD11	3:D:447:MET:HG3	1.99	0.44
3:D:1108:GLY:HA3	3:D:1125:GLN:HE21	1.82	0.44
6:G:4:DG:C8	6:G:4:DG:OP2	2.71	0.44
6:G:31:DA:C8	6:G:31:DA:O5'	2.70	0.44
2:C:758:ASP:HB3	2:C:868:LEU:HD13	1.99	0.44
3:D:376:GLU:OE1	3:D:376:GLU:HA	2.16	0.44
9:M:112:TRP:CH2	9:M:158:LEU:HB3	2.53	0.44
1:A:40:ARG:NH1	1:B:32:TYR:HB2	2.32	0.44
3:D:215:GLU:HG3	3:D:218:ARG:NH1	2.32	0.44
5:F:69:THR:O	5:F:70:ALA:C	2.58	0.44
5:F:142:ASN:ND2	7:H:28:DT:C5	2.79	0.44
6:G:30:DA:OP2	6:G:30:DA:C8	2.70	0.44
9:M:85:TRP:HZ3	9:M:89:TYR:CB	2.05	0.44
1:A:175:THR:O	1:A:194:LEU:HD12	2.18	0.44
1:B:41:THR:HG21	1:B:215:LEU:HG	1.99	0.44
2:C:1120:SER:HA	2:C:1123:VAL:HG22	2.00	0.44
3:D:389:ARG:HG3	3:D:389:ARG:HH11	1.83	0.44
3:D:700:LEU:HD23	3:D:709:VAL:HG22	2.00	0.44
7:H:36:DA:H3'	7:H:36:DA:H8	1.73	0.44
2:C:228:ARG:HH21	6:G:35:DT:H2'	1.78	0.44
2:C:1044:ARG:NE	3:D:423:ASP:OD1	2.51	0.44
3:D:1218:ASP:HA	3:D:1241:ARG:HH22	1.83	0.44
2:C:587:VAL:CG2	2:C:591:THR:HG23	2.47	0.44
2:C:1138:LEU:HD11	3:D:11:ARG:HD3	1.98	0.44
3:D:430:ILE:HG22	3:D:522:ILE:HB	1.99	0.44
3:D:546:PRO:HB3	3:D:551:ALA:HB1	1.98	0.44
3:D:756:VAL:HG12	3:D:770:ARG:HG3	1.99	0.44
3:D:885:ILE:HG13	3:D:993:GLU:O	2.17	0.44
5:F:84:TRP:HZ2	5:F:124:VAL:CG1	2.30	0.44
5:F:142:ASN:HD22	7:H:28:DT:C7	2.31	0.44
2:C:103:MET:HG3	2:C:142:ASN:HA	1.99	0.43
3:D:131:PHE:CD2	3:D:372:ARG:HB3	2.52	0.43
1:B:171:VAL:HG22	1:B:198:THR:HG22	2.00	0.43
3:D:214:ARG:HA	3:D:217:ASP:OD2	2.18	0.43
3:D:381:LEU:HD23	3:D:381:LEU:H	1.84	0.43
3:D:535:ASP:N	3:D:539:ASP:OD2	2.48	0.43
3:D:966:LEU:HG	3:D:1155:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1108:GLY:HA3	3:D:1125:GLN:NE2	2.33	0.43
3:D:1168:ILE:HG13	3:D:1203:GLY:HA2	1.99	0.43
5:F:142:ASN:CB	6:G:24:DT:H72	2.48	0.43
9:M:78:HIS:O	9:M:78:HIS:CG	2.70	0.43
1:A:18:ARG:HH22	2:C:997:ASP:CG	2.25	0.43
2:C:202:VAL:CG1	2:C:214:PHE:HB3	2.49	0.43
2:C:1093:SER:C	2:C:1099:ARG:HH22	2.23	0.43
2:C:1094:ASP:HB3	2:C:1119:GLU:H	1.83	0.43
3:D:226:PHE:HA	3:D:248:TYR:OH	2.18	0.43
3:D:944:LEU:HA	3:D:948:GLU:HG2	2.00	0.43
6:G:5:DA:H2''	6:G:6:DA:H8	1.82	0.43
6:G:16:DC:C4	7:H:34:DG:O6	2.70	0.43
7:H:20:DG:C8	7:H:20:DG:C4'	3.01	0.43
2:C:258:MET:SD	2:C:259:ARG:N	2.91	0.43
2:C:628:THR:N	2:C:631:GLU:OE2	2.39	0.43
3:D:103:HIS:HD2	3:D:314:LEU:HD11	1.83	0.43
6:G:26:DT:H3'	6:G:26:DT:OP1	2.18	0.43
9:M:145:THR:O	9:M:149:LYS:HE3	2.19	0.43
9:M:152:THR:O	9:M:156:GLU:OE1	2.37	0.43
2:C:146:GLU:CD	2:C:148:LYS:NZ	2.77	0.43
2:C:1084:THR:OG1	3:D:554:GLU:OE2	2.28	0.43
3:D:41:PRO:HB3	3:D:47:PHE:O	2.19	0.43
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	2.01	0.43
1:B:220:GLY:HA2	1:B:223:ARG:HB3	2.01	0.43
2:C:464:SER:OG	2:C:467:ARG:HG2	2.18	0.43
2:C:689:ILE:HG12	2:C:702:ILE:O	2.19	0.43
7:H:26:DA:O4'	7:H:26:DA:P	2.76	0.43
9:M:106:GLU:HA	9:M:109:ARG:CG	2.49	0.43
2:C:730:ASN:HA	2:C:734:ALA:HB3	2.01	0.43
3:D:181:LEU:HD22	3:D:198:ARG:NH2	2.33	0.43
3:D:360:LEU:HD23	3:D:360:LEU:H	1.84	0.43
9:M:10:VAL:CG2	9:M:141:LEU:CD2	2.85	0.43
9:M:87:ARG:HB3	9:M:87:ARG:HH21	1.76	0.43
9:M:133:GLN:HA	9:M:136:VAL:HG12	2.00	0.43
1:B:149:ALA:HB2	1:B:164:VAL:C	2.43	0.43
2:C:109:ASP:O	2:C:111:ARG:NH1	2.46	0.43
3:D:868:ALA:HB2	7:H:14:DT:H71	2.01	0.43
3:D:1109:GLN:OE1	3:D:1110:GLN:N	2.51	0.43
3:D:1233:LEU:HD23	3:D:1233:LEU:HA	1.89	0.43
6:G:25:DG:OP1	6:G:25:DG:C3'	2.66	0.43
6:G:48:DA:H2	7:H:3:DG:H22	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:64:GLN:O	9:M:67:LEU:HG	2.19	0.43
2:C:1055:GLN:HE21	3:D:420:LYS:HD2	1.83	0.43
2:C:1104:GLU:HA	2:C:1107:VAL:HG12	2.01	0.43
3:D:25:TYR:O	3:D:51:ILE:HG23	2.18	0.43
3:D:125:LEU:HD23	3:D:125:LEU:HA	1.86	0.43
3:D:233:GLN:HG2	3:D:234:LEU:N	2.34	0.43
3:D:352:ASN:O	3:D:356:ARG:NH1	2.52	0.43
2:C:677:ARG:NE	2:C:752:ILE:O	2.48	0.43
2:C:785:ASP:OD1	2:C:788:GLY:N	2.52	0.43
2:C:821:LEU:CD2	5:F:186:LEU:HD13	2.36	0.43
3:D:453:LYS:O	3:D:457:MET:HG3	2.19	0.43
6:G:21:DT:H2''	6:G:22:DA:N7	2.33	0.43
9:M:44:LEU:H	9:M:44:LEU:HD23	1.84	0.43
1:B:182:ARG:HA	1:B:187:THR:HA	2.00	0.42
2:C:441:ASP:HA	2:C:680:HIS:HE2	1.84	0.42
2:C:889:HIS:NE2	2:C:933:GLU:OE1	2.47	0.42
3:D:159:ARG:O	3:D:162:VAL:N	2.52	0.42
4:E:45:ARG:NH1	4:E:101:ASP:HB2	2.34	0.42
6:G:20:DT:C2'	6:G:21:DT:H5'	2.49	0.42
9:M:115:ASP:HA	9:M:119:GLY:HA2	1.99	0.42
2:C:377:ARG:NH2	2:C:383:GLU:OE2	2.31	0.42
2:C:586:MET:HE3	3:D:850:PHE:HB2	2.00	0.42
2:C:807:THR:OG1	2:C:808:PRO:HD3	2.18	0.42
2:C:1003:ASP:OD1	2:C:1007:LYS:N	2.51	0.42
3:D:1087:ARG:HG3	3:D:1113:GLU:HA	2.01	0.42
9:M:95:LYS:O	9:M:98:SER:OG	2.33	0.42
1:B:28:PRO:HD3	1:B:189:PHE:CE1	2.54	0.42
1:B:149:ALA:N	1:B:165:ASP:OD1	2.39	0.42
2:C:125:LYS:HD2	2:C:853:PHE:HE1	1.82	0.42
2:C:762:THR:OG1	2:C:763:LYS:N	2.50	0.42
3:D:135:VAL:HA	3:D:235:ILE:HD13	2.00	0.42
7:H:38:DT:H2''	7:H:39:DA:H5''	2.01	0.42
1:A:130:ASP:OD1	1:A:131:LYS:N	2.53	0.42
1:B:57:ASP:OD2	1:B:135:GLU:HG3	2.19	0.42
2:C:809:LYS:HA	2:C:830:ARG:HE	1.84	0.42
3:D:136:ILE:HG12	3:D:234:LEU:HB2	2.01	0.42
3:D:317:VAL:HA	3:D:318:PRO:HD3	1.90	0.42
5:F:161:GLU:OE1	7:H:21:DT:O4	2.37	0.42
7:H:18:DG:H4'	7:H:18:DG:OP1	2.19	0.42
9:M:24:THR:HG22	9:M:31:GLN:OE1	2.20	0.42
9:M:79:THR:CG2	9:M:109:ARG:HH22	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLU:CD	1:B:234:ILE:H	2.26	0.42
2:C:645:GLU:HG3	2:C:668:ARG:HH21	1.84	0.42
2:C:1074:TRP:HA	2:C:1077:GLN:OE1	2.20	0.42
3:D:136:ILE:CD1	3:D:234:LEU:N	2.79	0.42
5:F:162:ASP:OD2	5:F:165:ARG:CD	2.67	0.42
5:F:226:ARG:CD	7:H:38:DT:H72	2.47	0.42
6:G:49:DG:H21	7:H:1:DC:H42	1.58	0.42
9:M:87:ARG:CG	9:M:90:LYS:CE	2.73	0.42
1:A:40:ARG:HD3	1:B:33:THR:HG22	2.02	0.42
2:C:105:LEU:HD23	2:C:105:LEU:HA	1.86	0.42
2:C:513:GLU:HG2	2:C:532:THR:HG22	2.02	0.42
3:D:108:LYS:CA	3:D:108:LYS:CE	2.97	0.42
3:D:134:TYR:O	3:D:135:VAL:HG12	2.19	0.42
3:D:873:LEU:O	3:D:877:LEU:HD23	2.19	0.42
3:D:983:MET:HE2	3:D:983:MET:HB2	1.82	0.42
5:F:98:LEU:HD21	5:F:137:HIS:CD2	2.55	0.42
5:F:138:ARG:HD3	5:F:138:ARG:HA	1.71	0.42
1:A:38:LEU:HD23	1:A:38:LEU:HA	1.86	0.42
1:A:88:GLU:HA	1:A:142:ARG:NH2	2.34	0.42
6:G:31:DA:N3	6:G:31:DA:H3'	2.34	0.42
9:M:124:GLU:HA	9:M:127:MET:HG2	2.02	0.42
3:D:894:GLU:O	3:D:961:LYS:NZ	2.52	0.42
2:C:762:THR:H	2:C:765:GLY:CA	2.33	0.42
3:D:114:LEU:HD23	3:D:114:LEU:HA	1.87	0.42
3:D:156:ALA:HA	3:D:159:ARG:HE	1.85	0.42
3:D:247:ARG:HD2	3:D:248:TYR:CD1	2.46	0.42
5:F:101:ARG:CD	6:G:29:DA:H8	2.18	0.42
6:G:38:DT:H2'	6:G:38:DT:O5'	2.20	0.42
9:M:82:PRO:O	9:M:82:PRO:HG2	2.20	0.42
1:A:100:GLN:HB2	1:A:133:LYS:NZ	2.35	0.42
2:C:413:THR:OG1	9:M:44:LEU:HD13	2.19	0.42
3:D:386:ARG:HD2	3:D:386:ARG:HA	1.58	0.42
3:D:904:ARG:NH1	3:D:905:ALA:O	2.53	0.42
3:D:1091:HIS:NE2	3:D:1099:LEU:HA	2.35	0.42
5:F:116:THR:HG23	5:F:139:ILE:HG22	1.92	0.42
9:M:10:VAL:N	9:M:60:ASP:HA	2.28	0.42
2:C:482:ARG:NH2	2:C:536:GLU:OE1	2.42	0.41
2:C:902:GLU:HG2	2:C:903:ASP:N	2.35	0.41
2:C:1044:ARG:HH11	2:C:1064:GLY:HA2	1.84	0.41
3:D:901:LEU:N	3:D:958:THR:O	2.36	0.41
3:D:557:ILE:HD12	4:E:53:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1055:LEU:HB3	3:D:1101:ASP:HB2	2.01	0.41
5:F:141:THR:OG1	6:G:24:DT:C7	2.68	0.41
6:G:47:DC:OP2	6:G:47:DC:C3'	2.68	0.41
7:H:25:DC:O4'	7:H:25:DC:P	2.78	0.41
2:C:252:PHE:O	2:C:258:MET:HG2	2.21	0.41
3:D:472:ALA:O	3:D:476:VAL:HG22	2.20	0.41
9:M:10:VAL:CG2	9:M:61:VAL:CB	2.97	0.41
3:D:600:GLN:HB2	3:D:609:THR:OG1	2.20	0.41
3:D:672:MET:O	3:D:675:GLU:HG3	2.20	0.41
3:D:1191:ARG:H	3:D:1191:ARG:HD3	1.85	0.41
4:E:45:ARG:CZ	4:E:101:ASP:HB2	2.50	0.41
1:A:95:MET:CE	1:A:113:PRO:HD2	2.48	0.41
2:C:517:ARG:HG3	2:C:581:VAL:HA	2.02	0.41
3:D:917:GLU:HA	3:D:921:TYR:CD1	2.55	0.41
9:M:41:GLN:HG2	9:M:42:GLY:N	2.36	0.41
1:B:46:ILE:HD12	1:B:47:PRO:HD2	2.03	0.41
3:D:9:GLU:HG2	3:D:1243:ASP:O	2.21	0.41
3:D:166:ARG:O	3:D:170:LEU:HG	2.21	0.41
3:D:214:ARG:HB3	3:D:218:ARG:HH21	1.84	0.41
3:D:438:LEU:HD12	3:D:438:LEU:O	2.19	0.41
5:F:97:ARG:CD	6:G:29:DA:H61	2.22	0.41
2:C:146:GLU:OE2	9:M:46:VAL:CB	2.68	0.41
2:C:148:LYS:N	2:C:148:LYS:HD2	2.36	0.41
2:C:445:PRO:HG3	2:C:640:ASP:OD2	2.20	0.41
3:D:67:ARG:HG3	3:D:69:ARG:HH21	1.86	0.41
3:D:386:ARG:HH21	7:H:10:DT:H5'	1.86	0.41
3:D:505:HIS:CD2	3:D:507:LEU:HB2	2.55	0.41
3:D:599:TYR:HA	3:D:610:GLY:HA3	2.02	0.41
3:D:696:ILE:HD13	3:D:696:ILE:HA	1.96	0.41
5:F:221:LYS:O	5:F:224:THR:N	2.52	0.41
6:G:48:DA:O5'	6:G:48:DA:C2'	2.69	0.41
9:M:67:LEU:HA	9:M:70:VAL:HG22	2.03	0.41
9:M:79:THR:CB	9:M:109:ARG:HH22	2.31	0.41
9:M:106:GLU:HA	9:M:109:ARG:HG2	2.03	0.41
1:B:59:VAL:HG23	1:B:61:HIS:CE1	2.55	0.41
1:B:98:ARG:HG2	1:B:135:GLU:HB2	2.02	0.41
2:C:299:LEU:HD12	2:C:300:PHE:CD1	2.56	0.41
2:C:1098:GLY:O	2:C:1102:VAL:HG23	2.20	0.41
2:C:1101:LYS:O	2:C:1104:GLU:HG3	2.20	0.41
5:F:96:TYR:OH	5:F:106:GLN:HG3	2.21	0.41
1:A:81:LYS:HE3	1:A:81:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:PHE:CB	2:C:148:LYS:HD3	2.37	0.41
2:C:344:TYR:CE1	2:C:365:VAL:HG13	2.56	0.41
2:C:387:ASN:O	2:C:390:ARG:HG2	2.21	0.41
2:C:445:PRO:HD2	2:C:707:CYS:SG	2.61	0.41
3:D:567:SER:N	3:D:572:ARG:O	2.47	0.41
3:D:904:ARG:HH22	3:D:908:GLY:HA2	1.85	0.41
5:F:135:TRP:O	5:F:139:ILE:N	2.46	0.41
5:F:142:ASN:O	5:F:146:ASP:CB	2.66	0.41
6:G:48:DA:H2	7:H:3:DG:C2	2.38	0.41
9:M:35:LEU:HB2	9:M:48:VAL:HG12	2.03	0.41
1:A:95:MET:HE2	1:A:95:MET:HA	2.03	0.41
2:C:146:GLU:OE2	9:M:46:VAL:HB	2.21	0.41
3:D:83:THR:OG1	3:D:84:ARG:N	2.53	0.41
3:D:135:VAL:HG22	3:D:136:ILE:H	1.86	0.41
3:D:645:GLU:HG2	3:D:646:ILE:N	2.36	0.41
3:D:1182:ASP:OD1	3:D:1183:ARG:N	2.54	0.41
4:E:88:GLU:OE1	4:E:92:SER:HB2	2.20	0.41
5:F:138:ARG:CG	6:G:25:DG:H5''	2.51	0.41
8:I:5:C:O2	8:I:5:C:H2'	2.20	0.41
2:C:877:ARG:NH1	2:C:1038:ASP:OD2	2.54	0.40
2:C:1112:ILE:HD12	2:C:1112:ILE:H	1.86	0.40
3:D:328:VAL:HG22	3:D:336:ALA:O	2.21	0.40
5:F:160:PRO:HB3	5:F:165:ARG:CG	2.41	0.40
6:G:32:DC:O2	6:G:32:DC:C2'	2.69	0.40
9:M:11:TYR:CG	9:M:12:PRO:HD2	2.56	0.40
1:B:84:VAL:HG22	1:B:199:LYS:HD2	2.02	0.40
2:C:32:VAL:HA	2:C:33:PRO:HD3	1.98	0.40
2:C:954:ASP:OD1	2:C:955:TRP:N	2.54	0.40
2:C:1009:MET:HA	2:C:1009:MET:HE2	2.03	0.40
2:C:1105:ALA:O	2:C:1109:GLY:N	2.44	0.40
3:D:1052:ARG:NE	3:D:1102:GLY:HA2	2.31	0.40
6:G:22:DA:O5'	6:G:22:DA:C2'	2.67	0.40
7:H:18:DG:C5'	7:H:18:DG:H8	2.32	0.40
2:C:127:MET:SD	2:C:127:MET:N	2.95	0.40
2:C:762:THR:H	2:C:765:GLY:HA2	1.86	0.40
7:H:35:DC:H2'	7:H:36:DA:C8	2.56	0.40
9:M:123:GLY:HA2	9:M:126:ARG:NH1	2.36	0.40
3:D:897:ILE:HG13	3:D:1128:ARG:NH2	2.36	0.40
3:D:1039:VAL:HA	3:D:1040:PRO:HD3	1.96	0.40
5:F:153:ARG:HE	5:F:153:ARG:HB2	1.59	0.40
7:H:36:DA:C8	7:H:36:DA:P	3.15	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:6:G:C8	8:I:6:G:H5''	2.55	0.40
9:M:71:PHE:HE1	9:M:157:VAL:HG21	1.86	0.40
1:B:105:VAL:HG23	1:B:128:LEU:HD22	2.02	0.40
1:B:133:LYS:HA	1:B:133:LYS:HD2	1.87	0.40
1:B:170:PRO:HA	1:B:199:LYS:HE3	2.04	0.40
2:C:158:PRO:HG2	2:C:431:PHE:HE2	1.85	0.40
2:C:821:LEU:CD2	5:F:186:LEU:HD11	2.50	0.40
3:D:173:ARG:HA	3:D:176:LYS:HG2	2.04	0.40
3:D:1154:ILE:HA	3:D:1157:ILE:HG22	2.04	0.40
3:D:1220:TRP:CD1	3:D:1220:TRP:H	2.40	0.40
3:D:1251:ASN:ND2	3:D:1259:PRO:HD3	2.36	0.40
5:F:156:MET:HE2	5:F:157:GLU:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/347 (61%)	205 (97%)	6 (3%)	0	100	100
1	B	231/347 (67%)	218 (94%)	13 (6%)	0	100	100
2	C	1123/1178 (95%)	1073 (96%)	49 (4%)	1 (0%)	48	76
3	D	1250/1326 (94%)	1208 (97%)	38 (3%)	4 (0%)	36	66
4	E	72/110 (66%)	69 (96%)	3 (4%)	0	100	100
5	F	174/263 (66%)	162 (93%)	5 (3%)	7 (4%)	2	16
9	M	157/169 (93%)	141 (90%)	9 (6%)	7 (4%)	2	14
All	All	3218/3740 (86%)	3076 (96%)	123 (4%)	19 (1%)	23	52

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	135	VAL
5	F	141	THR
9	M	60	ASP
9	M	61	VAL
3	D	319	VAL
3	D	340	LEU
9	M	86	SER
5	F	70	ALA
5	F	164	ASP
5	F	171	PRO
9	M	82	PRO
2	C	808	PRO
5	F	163	TYR
5	F	169	ASP
9	M	83	THR
9	M	98	SER
3	D	139	VAL
5	F	170	GLU
9	M	99	GLY

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	181/297 (61%)	181 (100%)	0	100	100
1	B	193/297 (65%)	193 (100%)	0	100	100
2	C	901/998 (90%)	890 (99%)	11 (1%)	63	74
3	D	1023/1105 (93%)	1012 (99%)	11 (1%)	65	74
4	E	64/90 (71%)	64 (100%)	0	100	100
5	F	146/225 (65%)	127 (87%)	19 (13%)	4	17
9	M	128/137 (93%)	119 (93%)	9 (7%)	14	41
All	All	2636/3149 (84%)	2586 (98%)	50 (2%)	49	68

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	96	ILE
2	C	103	MET
2	C	148	LYS
2	C	397	GLU
2	C	403	ARG
2	C	404	MET
2	C	410	GLU
2	C	412	ILE
2	C	413	THR
2	C	1108	LYS
2	C	1110	GLU
3	D	36	TYR
3	D	108	LYS
3	D	136	ILE
3	D	139	VAL
3	D	334	ARG
3	D	335	PHE
3	D	337	THR
3	D	338	SER
3	D	373	MET
3	D	386	ARG
3	D	387	ARG
5	F	67	GLN
5	F	121	PHE
5	F	124	VAL
5	F	133	GLU
5	F	138	ARG
5	F	139	ILE
5	F	140	THR
5	F	143	LEU
5	F	154	ILE
5	F	155	ARG
5	F	156	MET
5	F	159	LEU
5	F	161	GLU
5	F	164	ASP
5	F	165	ARG
5	F	166	VAL
5	F	169	ASP
5	F	172	ASN
5	F	221	LYS
9	M	60	ASP
9	M	72	GLN

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Mol	Chain	Res	Type
9	M	85	TRP
9	M	87	ARG
9	M	88	ARG
9	M	95	LYS
9	M	96	LEU
9	M	107	VAL
9	M	109	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	151	GLN
2	C	150	GLN
2	C	493	ASN
2	C	539	HIS
2	C	612	GLN
2	C	967	GLN
2	C	981	GLN
2	C	1129	GLN
3	D	351	ASN
3	D	369	ASN
3	D	494	HIS
3	D	540	GLN
3	D	693	GLN
3	D	792	HIS
3	D	889	HIS
3	D	1265	ASN
3	D	1269	ASN
4	E	68	ASN
4	E	69	GLN
5	F	107	HIS
9	M	78	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	6/7 (85%)	3 (50%)	1 (16%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	5	C
8	I	6	G
8	I	7	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	I	5	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

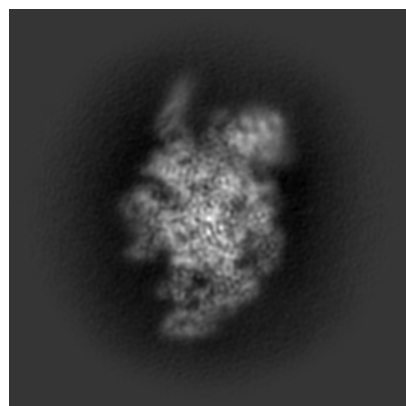
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63731. These allow visual inspection of the internal detail of the map and identification of artifacts.

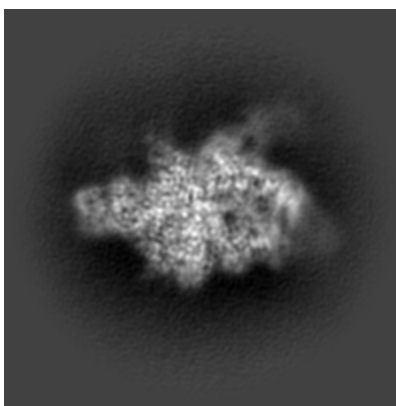
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

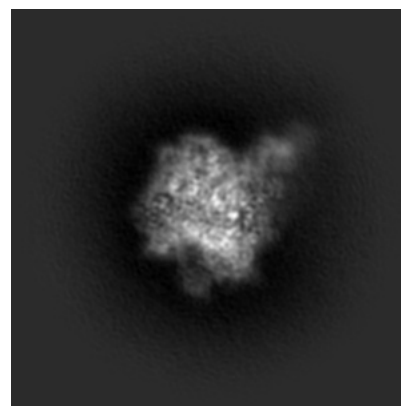
6.1.1 Primary map



X

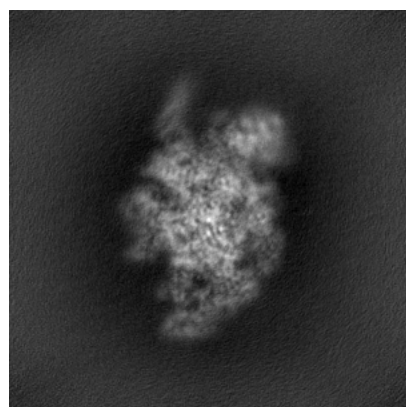


Y

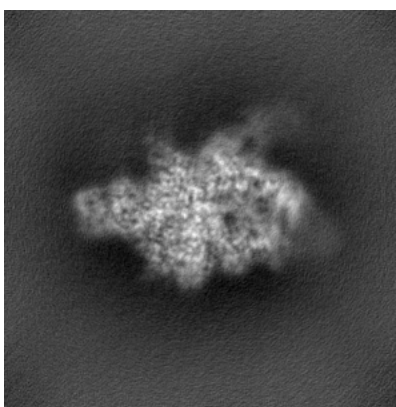


Z

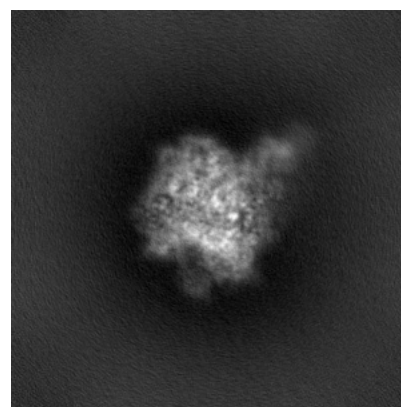
6.1.2 Raw map



X



Y

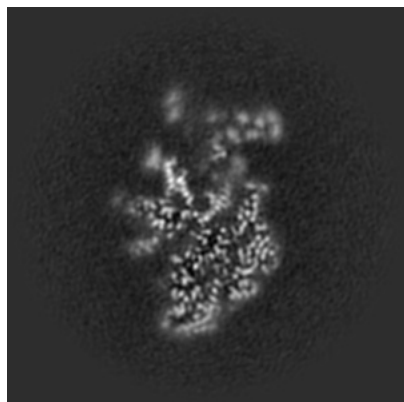


Z

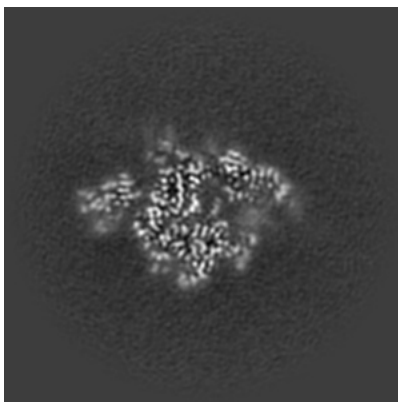
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

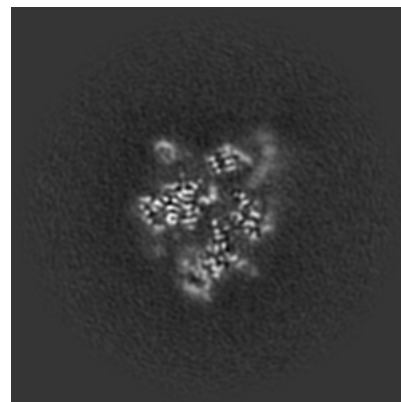
6.2.1 Primary map



X Index: 160

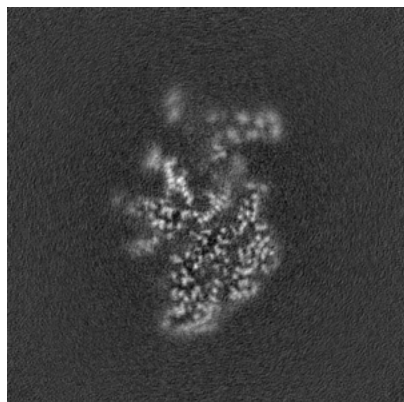


Y Index: 160

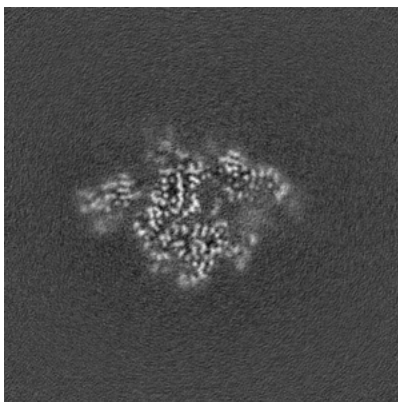


Z Index: 160

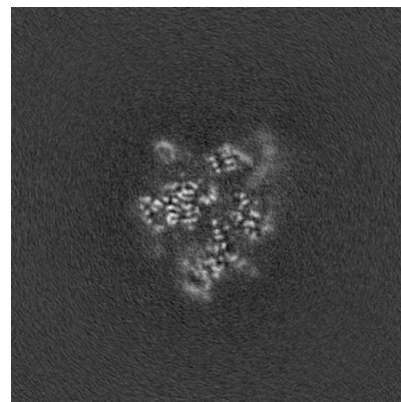
6.2.2 Raw map



X Index: 160



Y Index: 160

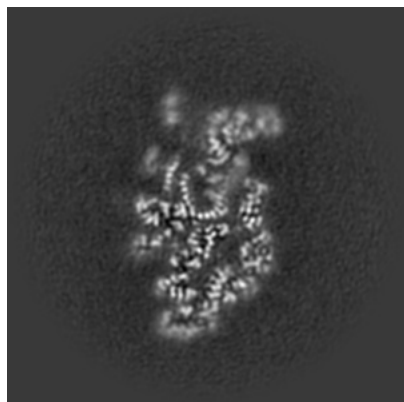


Z Index: 160

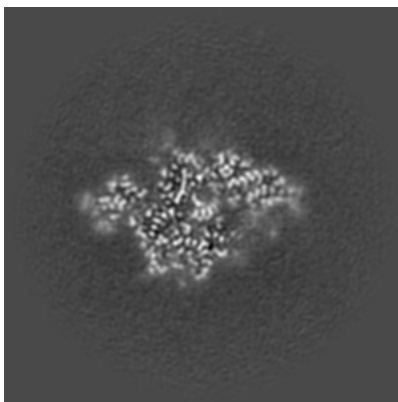
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

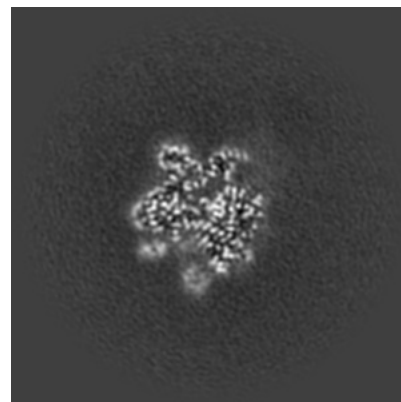
6.3.1 Primary map



X Index: 164

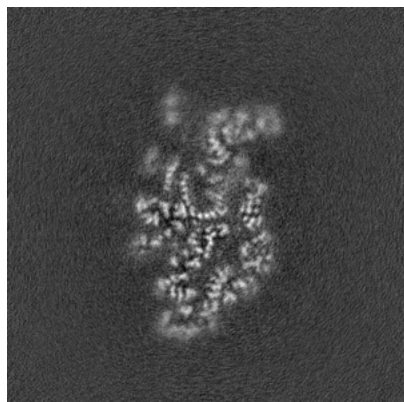


Y Index: 165

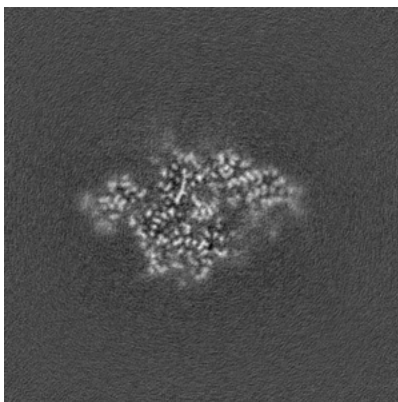


Z Index: 152

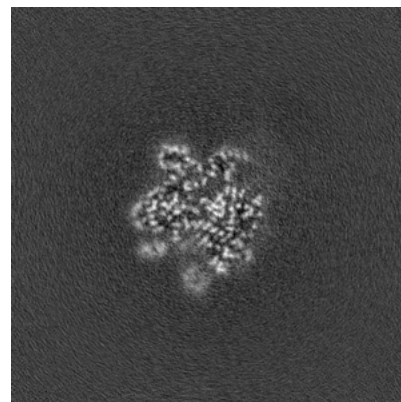
6.3.2 Raw map



X Index: 164



Y Index: 165

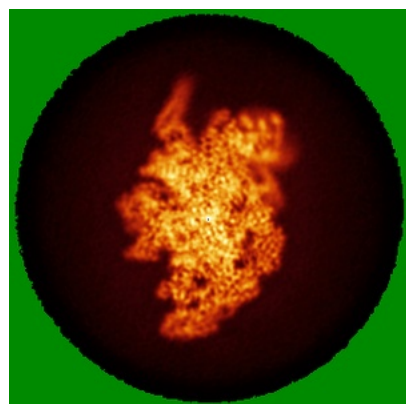


Z Index: 152

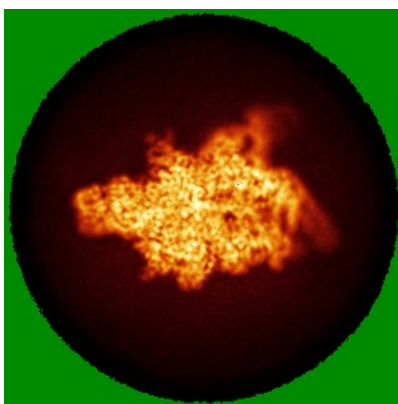
The images above show the largest variance slices of the map in three orthogonal directions.

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

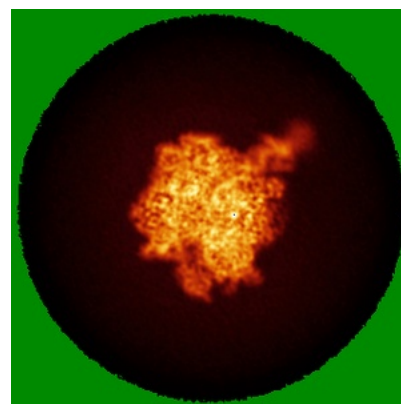
6.4.1 Primary map



X

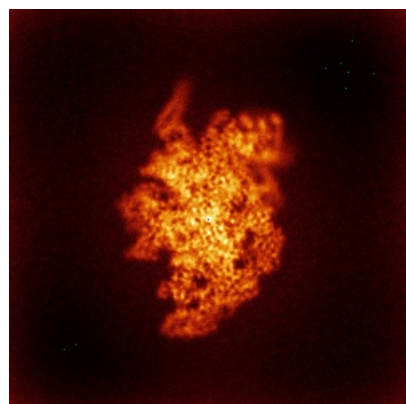


Y

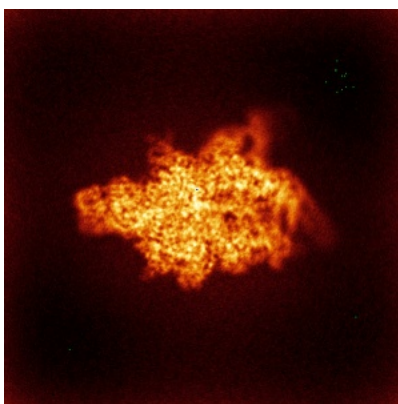


Z

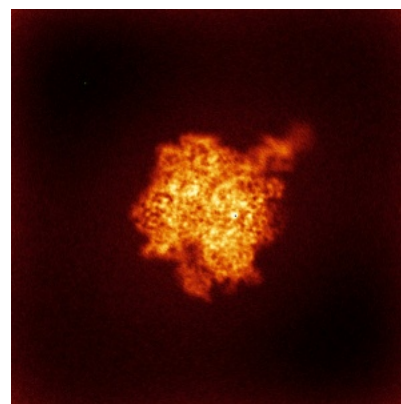
6.4.2 Raw map



X



Y

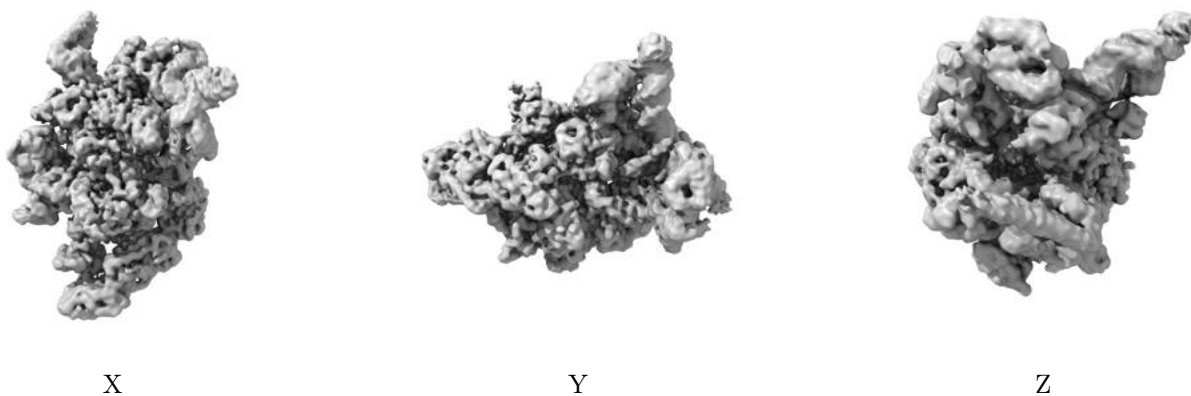


Z

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.

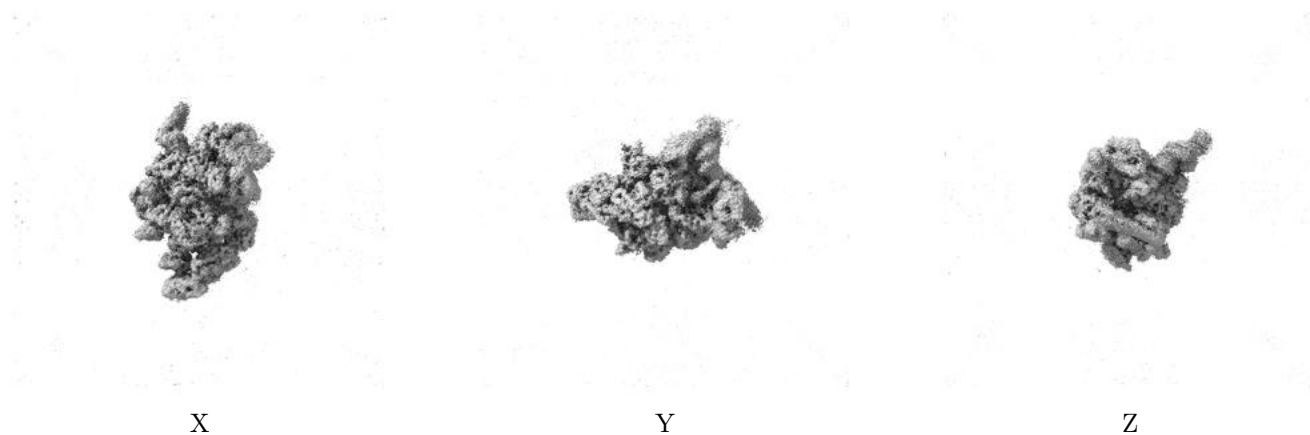
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

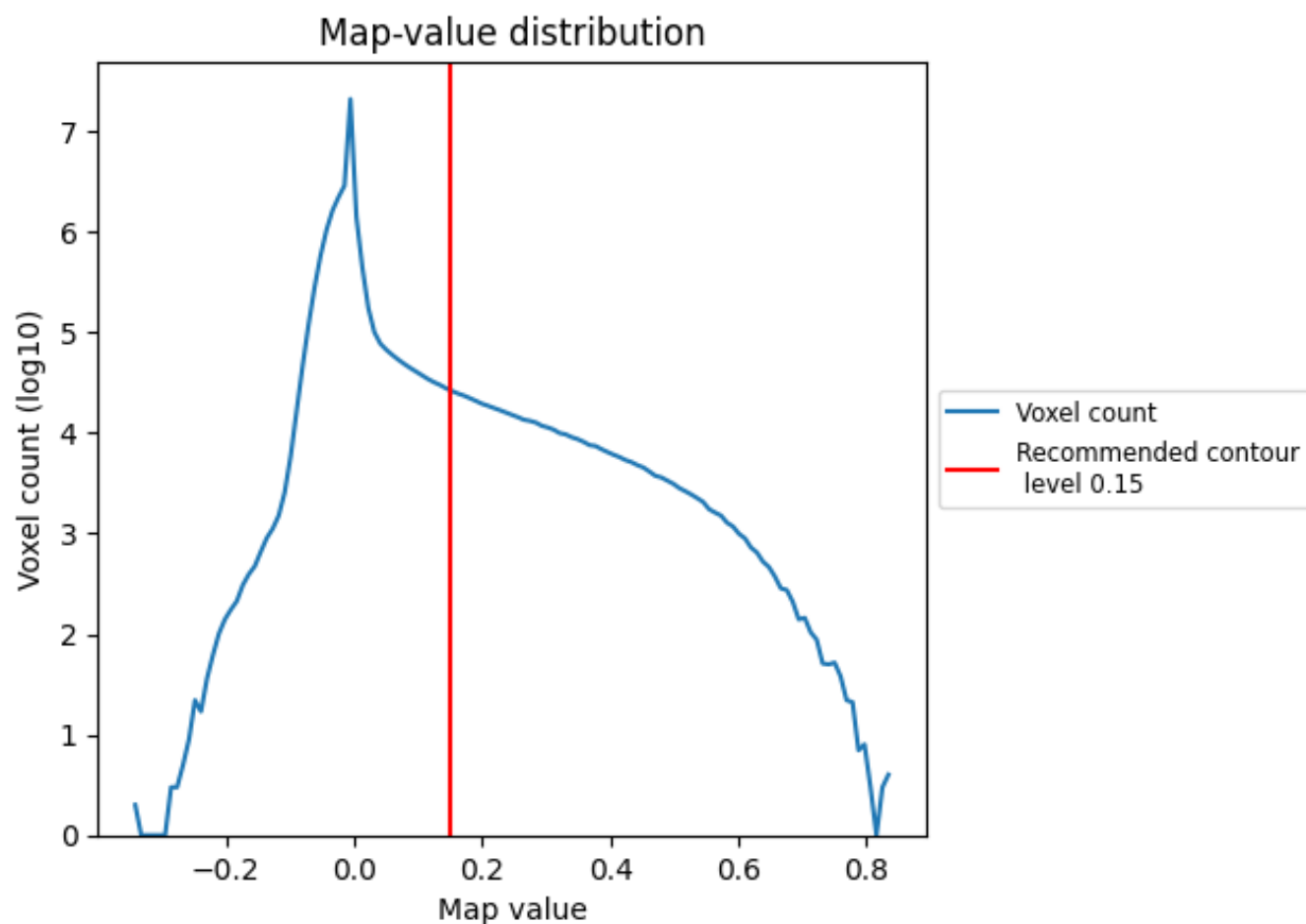
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

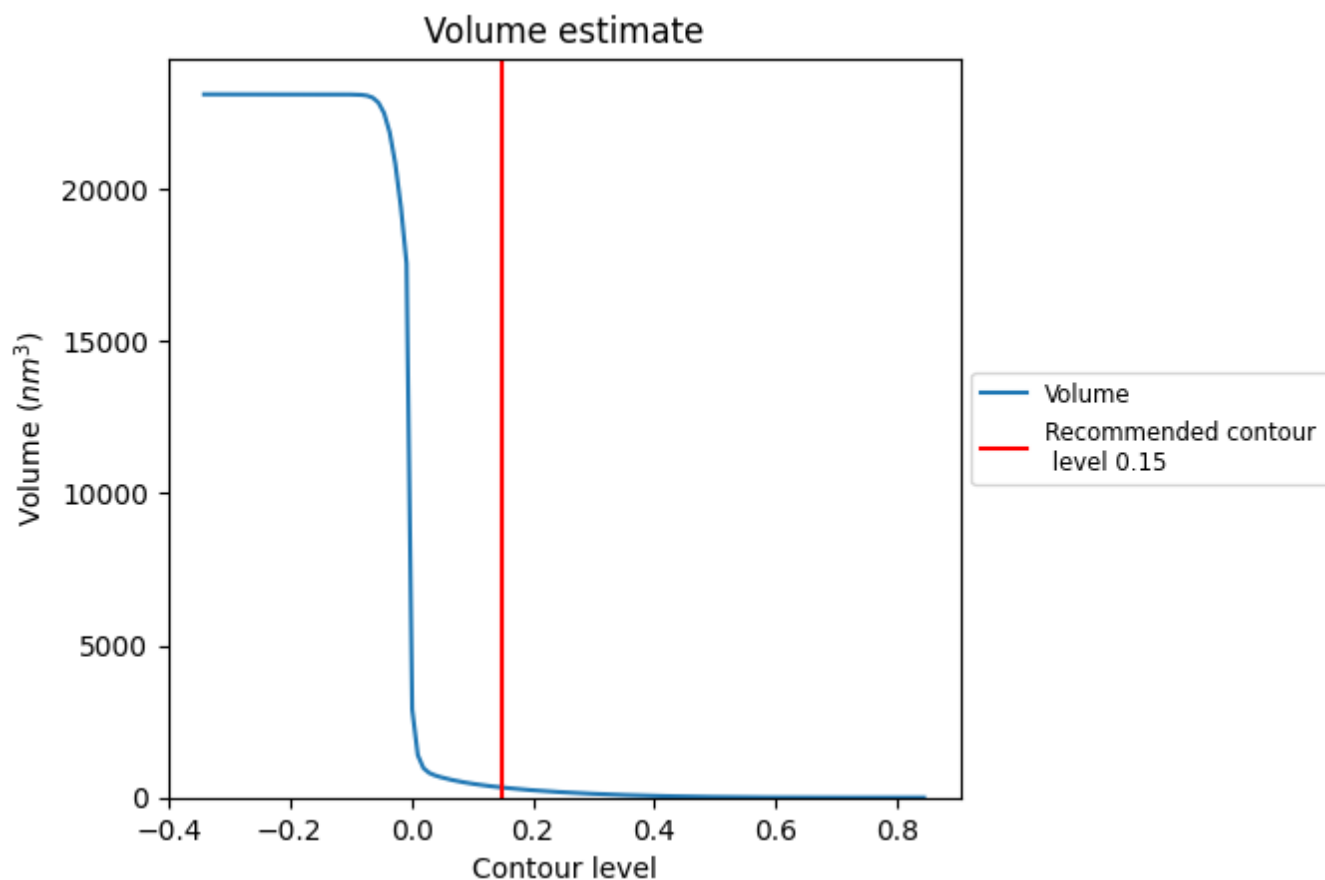
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

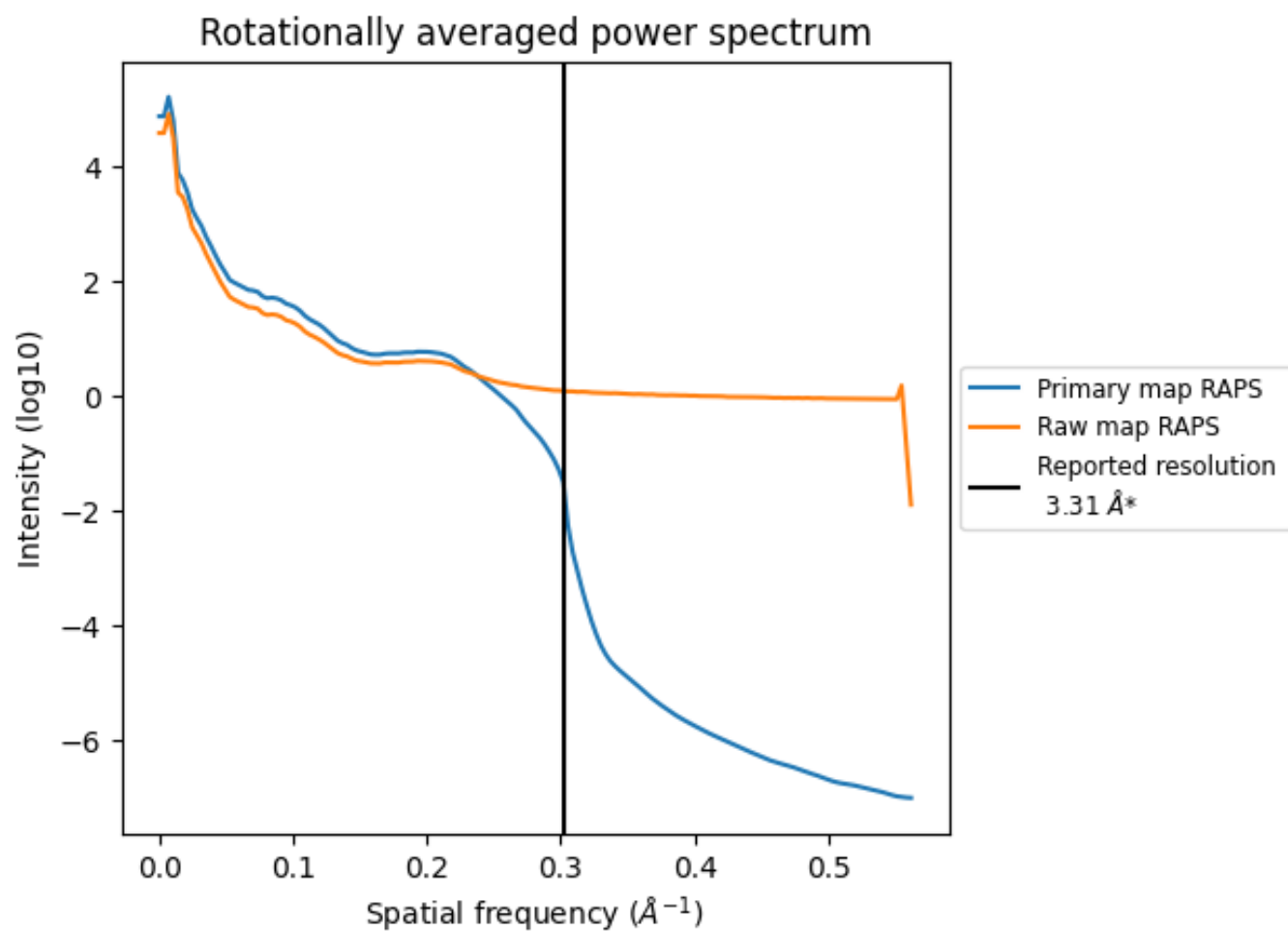
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 329 nm³; this corresponds to an approximate mass of 297 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

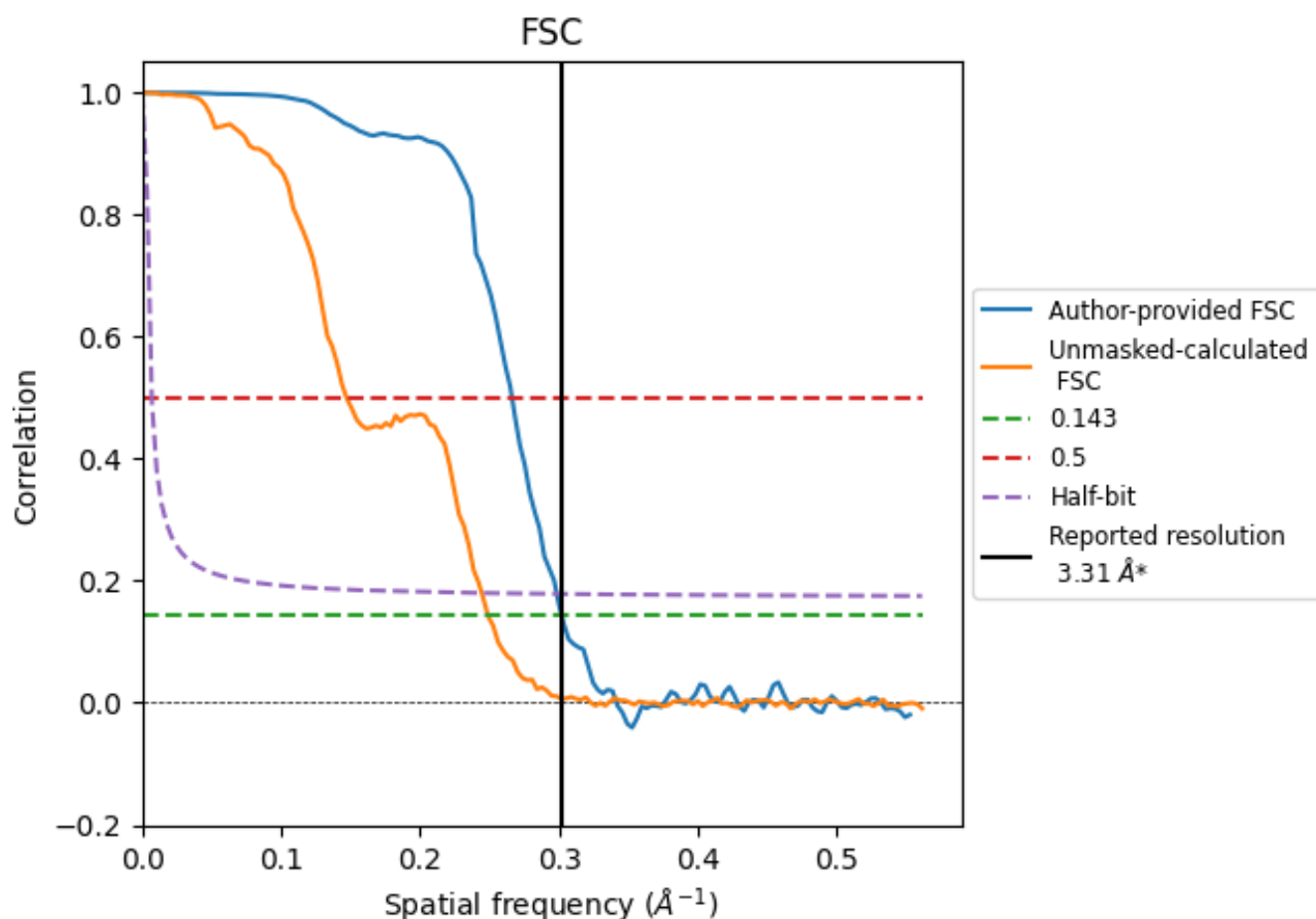


*Reported resolution corresponds to spatial frequency of 0.302 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.302 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

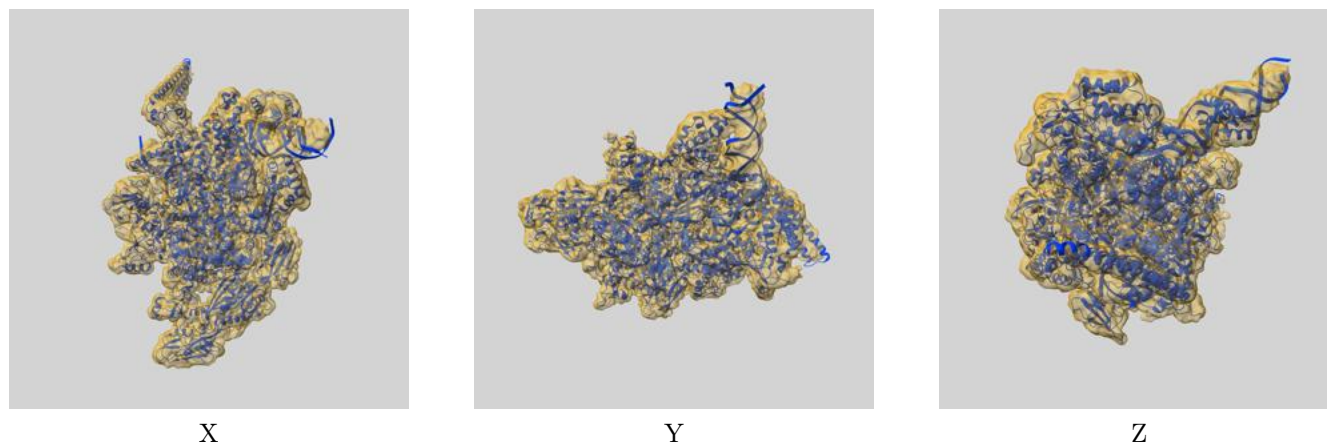
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.31	-	-
Author-provided FSC curve	3.31	3.75	3.35
Unmasked-calculated*	4.01	6.79	4.09

*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 4.01 differs from the reported value 3.31 by more than 10 %

9 Map-model fit [i](#)

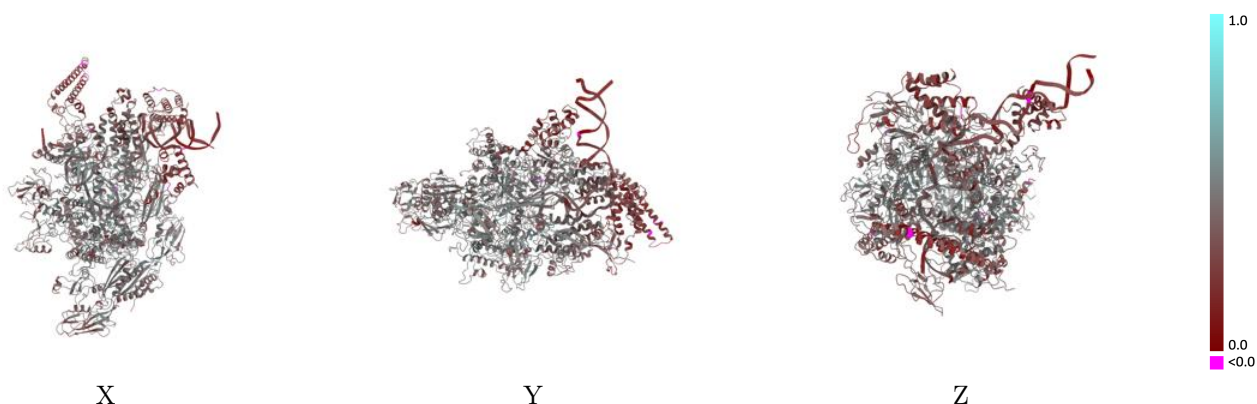
This section contains information regarding the fit between EMDB map EMD-63731 and PDB model 9M9E. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



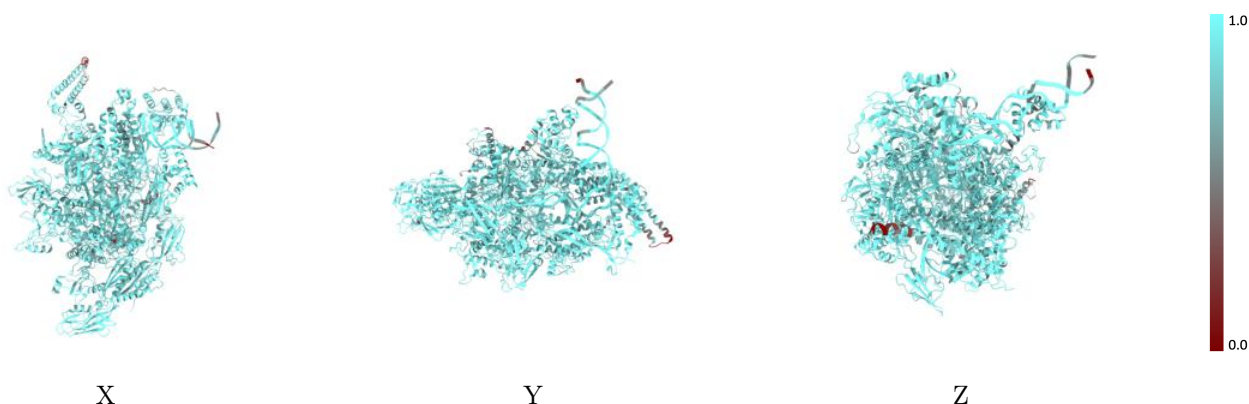
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



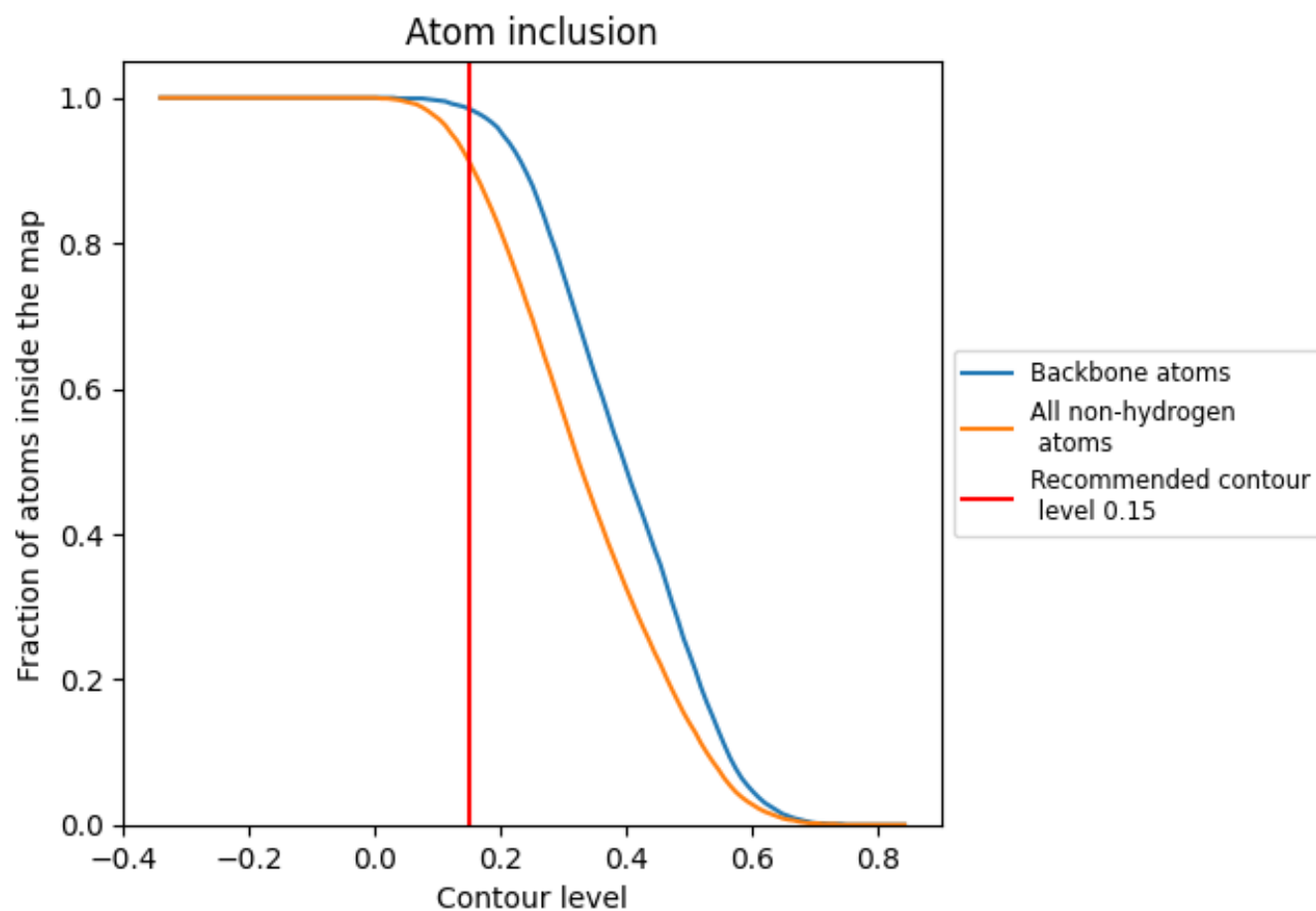
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9130	0.4060
A	0.9320	0.4410
B	0.9290	0.4050
C	0.9240	0.4470
D	0.9130	0.4140
E	0.7420	0.3890
F	0.8710	0.3170
G	0.9250	0.2980
H	0.9100	0.3210
I	0.9930	0.4830
M	0.8950	0.2630

1.0

0.0

<0.0