



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:28 PM UTC

PDB ID : 8W9F / pdb_00008w9f
EMDB ID : EMD-37367
Title : Cryo-EM structure of the Rpd3S-nucleosome complex from budding yeast in State 3
Authors : Wang, C.; Zhan, X.
Deposited on : 2023-09-05
Resolution : 4.40 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:

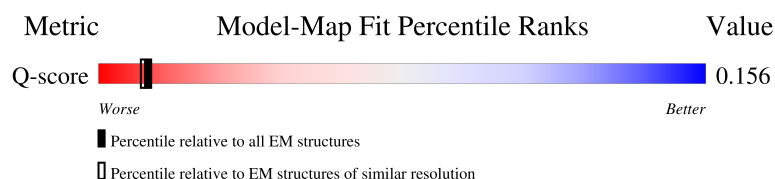
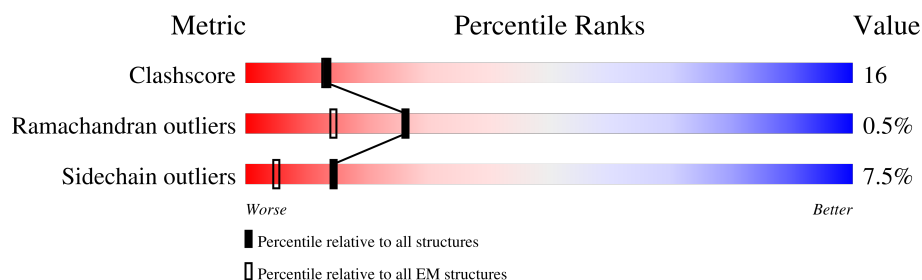
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

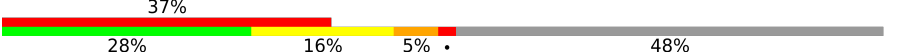
The reported resolution of this entry is 4.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	1536	 22% 25% 13% 61%
2	E	684	 37% 28% 16% 5% 48%
2	F	684	 20% 16% 6% 77%
3	B	433	 23% 57% 26% 6% 11%

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Mol	Chain	Length	Quality of chain
4	C	401	
4	D	401	
4	G	401	
5	a	136	
5	e	136	
6	b	103	
6	f	103	
7	c	130	
7	g	130	
8	d	126	
8	h	126	
9	i	147	
10	j	147	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 27868 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 Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	606	Total	C	N	O	S	0	0
			5066	3253	860	938	15		

- Molecule 2 is a protein called Transcriptional regulatory protein RCO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	353	Total	C	N	O	S	0	0
			2884	1837	493	536	18		
2	F	156	Total	C	N	O	S	0	0
			1282	822	211	239	10		

- Molecule 3 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	385	Total	C	N	O	S	0	0
			3057	1948	513	571	25		

- Molecule 4 is a protein called Chromatin modification-related protein EAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	183	Total	C	N	O	S	0	0
			1483	950	239	285	9		
4	D	185	Total	C	N	O	S	0	0
			1497	959	241	288	9		
4	G	69	Total	C	N	O	S	0	0
			570	371	98	97	4		

- Molecule 5 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	97	Total	C	N	O	S	0	0
			801	505	155	137	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	99	Total	C	N	O	S	0	0
			816	514	158	140	4		

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	79	Total	C	N	O	S	0	0
			627	395	121	110	1		
6	f	82	Total	C	N	O	S	0	0
			653	412	127	113	1		

- Molecule 7 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	107	Total	C	N	O		0	0
			817	516	158	143			
7	g	107	Total	C	N	O		0	0
			817	516	158	143			

- Molecule 8 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	94	Total	C	N	O	S	0	0
			735	461	134	138	2		
8	h	94	Total	C	N	O	S	0	0
			735	461	134	138	2		

- Molecule 9 is a DNA chain called 5-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	147	Total	C	N	O	P	0	0
			3011	1440	546	879	146		

- Molecule 10 is a DNA chain called 3-DNA.

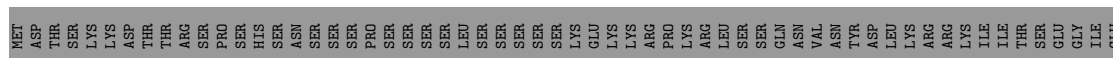
Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	147	Total	C	N	O	P	0	0
			3010	1440	543	881	146		

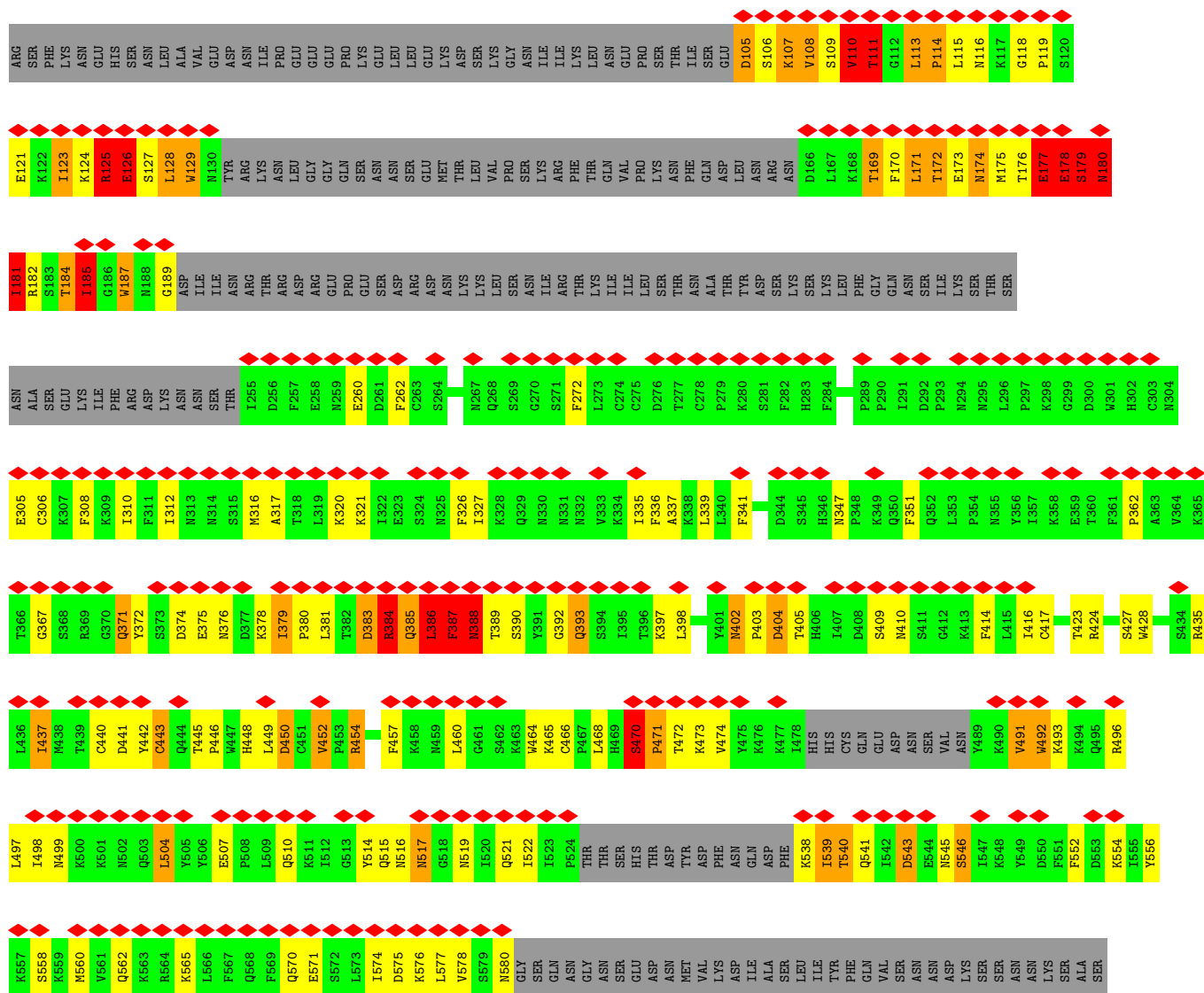
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	E	4	Total 4	Zn 4	0
11	B	1	Total 1	Zn 1	0
11	F	2	Total 2	Zn 2	0

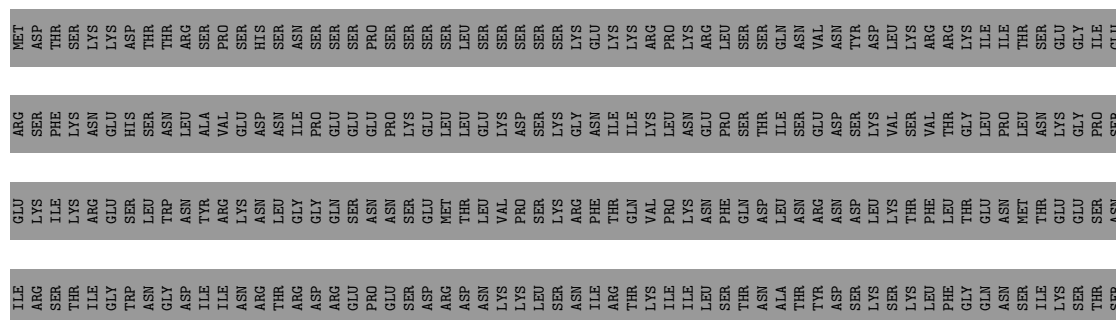


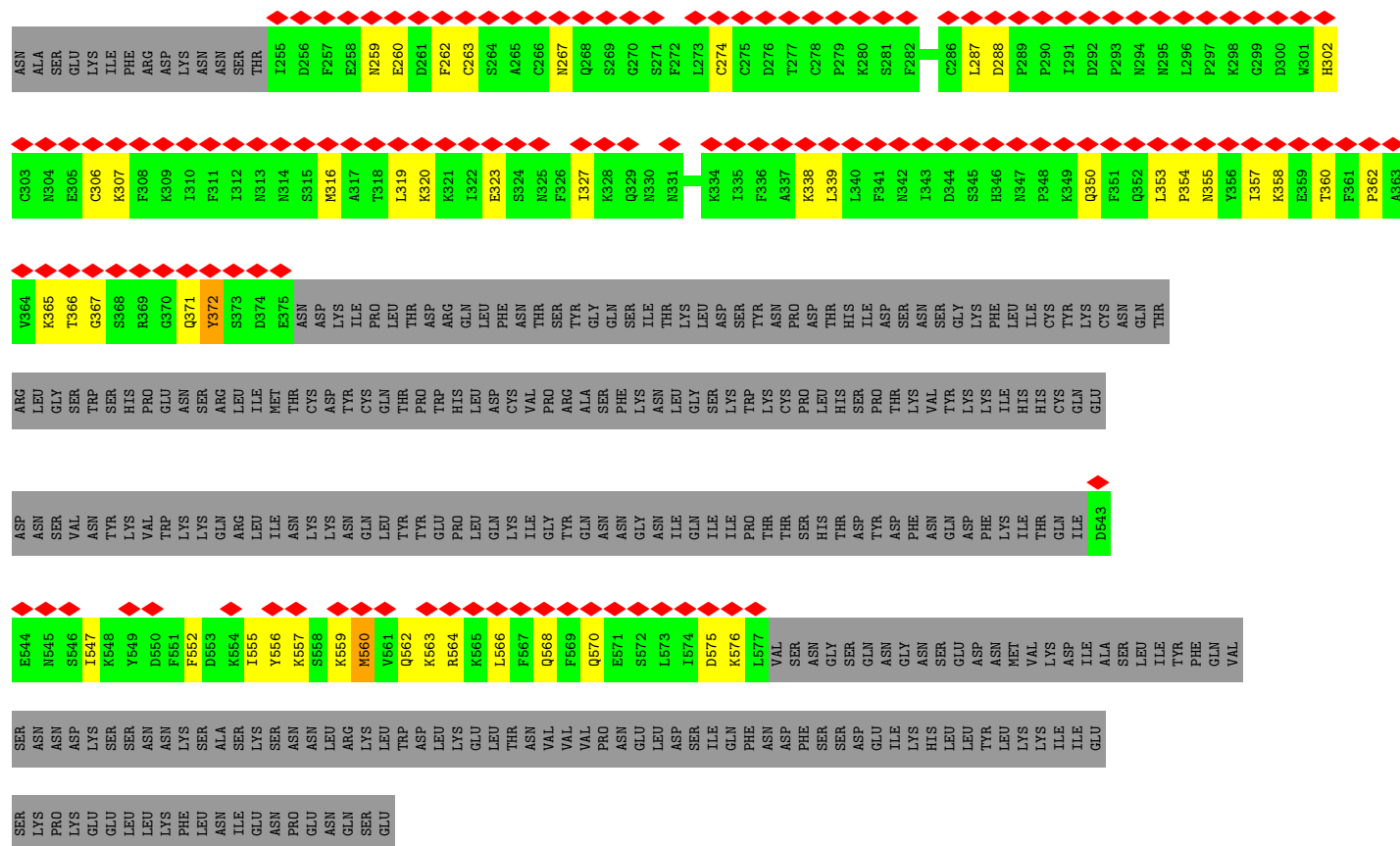
Frequency	Percentage
Daily	37%
Often	28%
Sometimes	16%
Not at all	5%
Never	48%



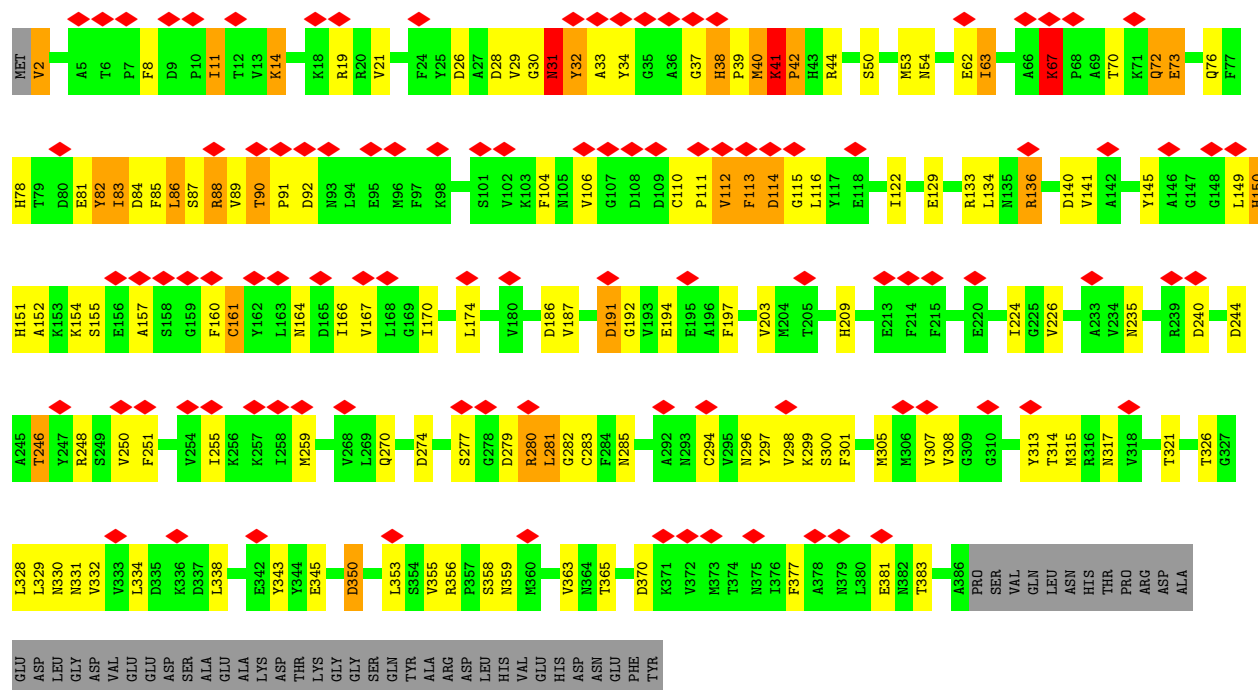


• Molecule 2: Transcriptional regulatory protein RCO1

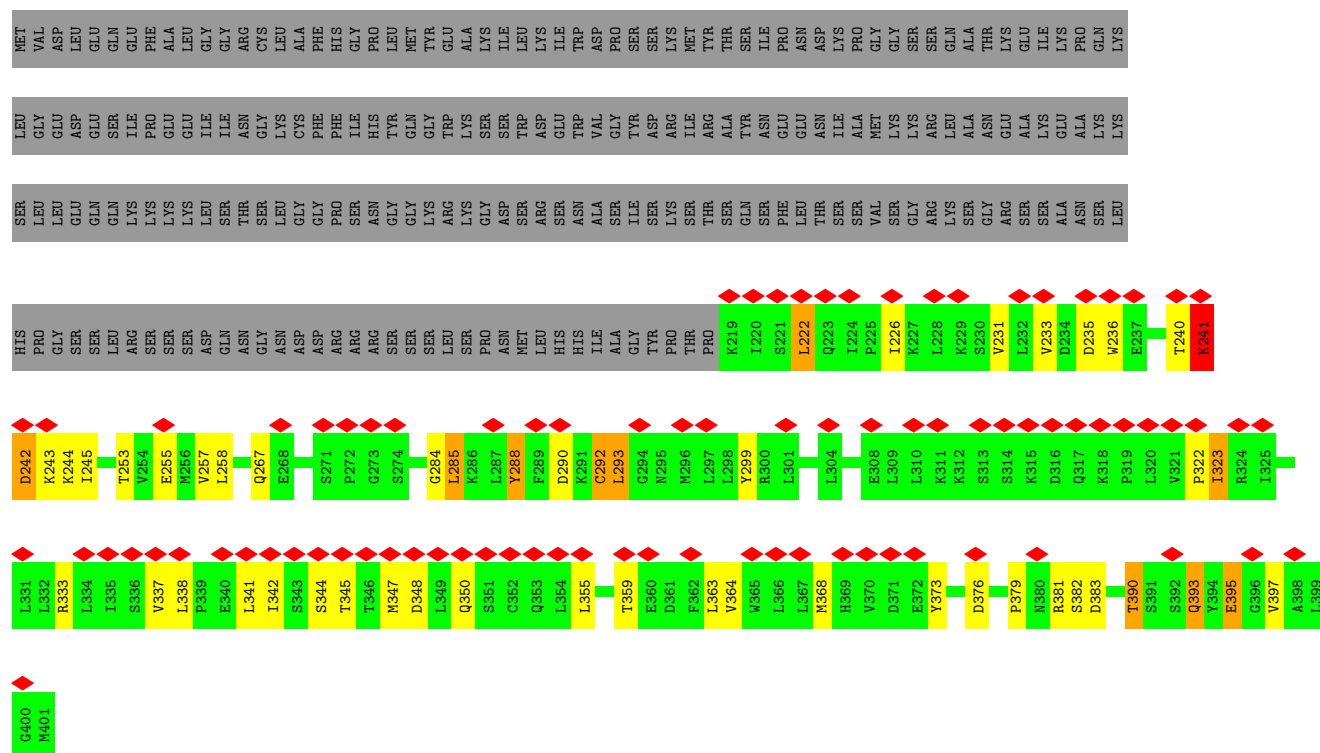




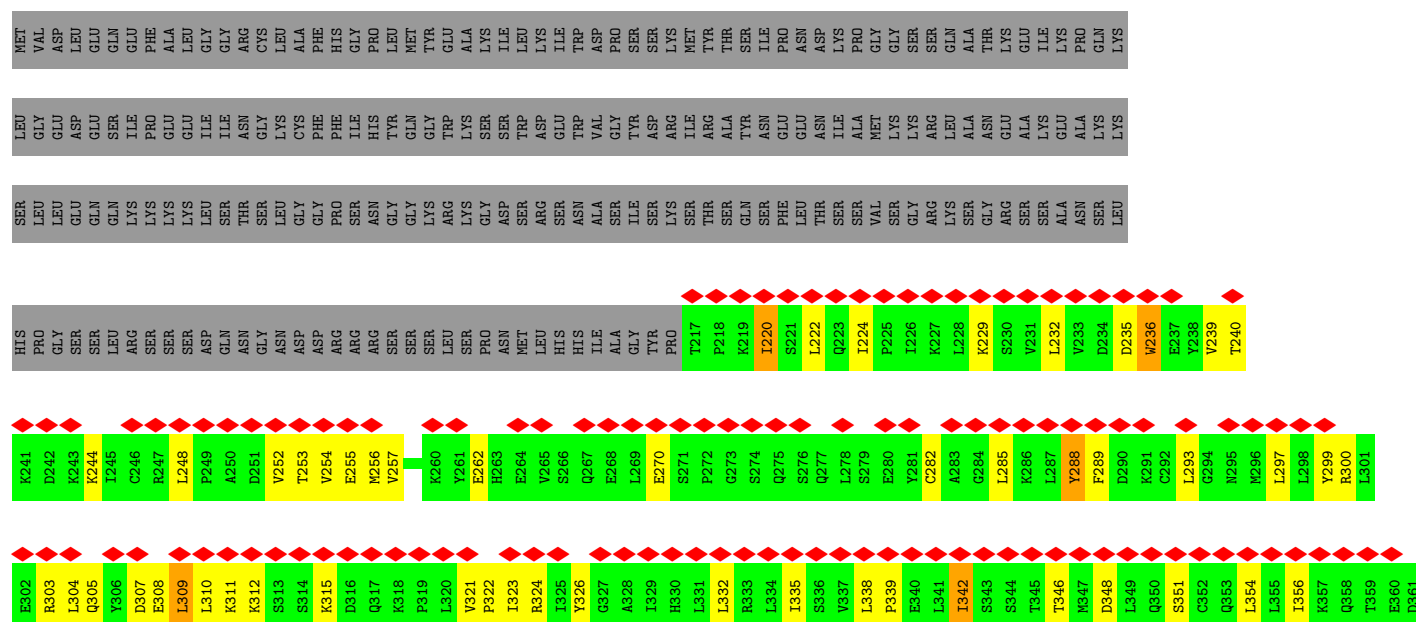
• Molecule 3: Histone deacetylase RPD3

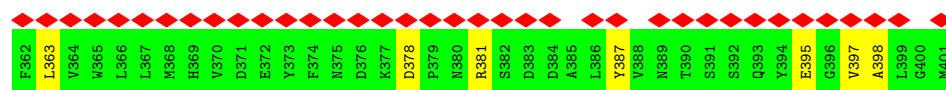


Chain C:

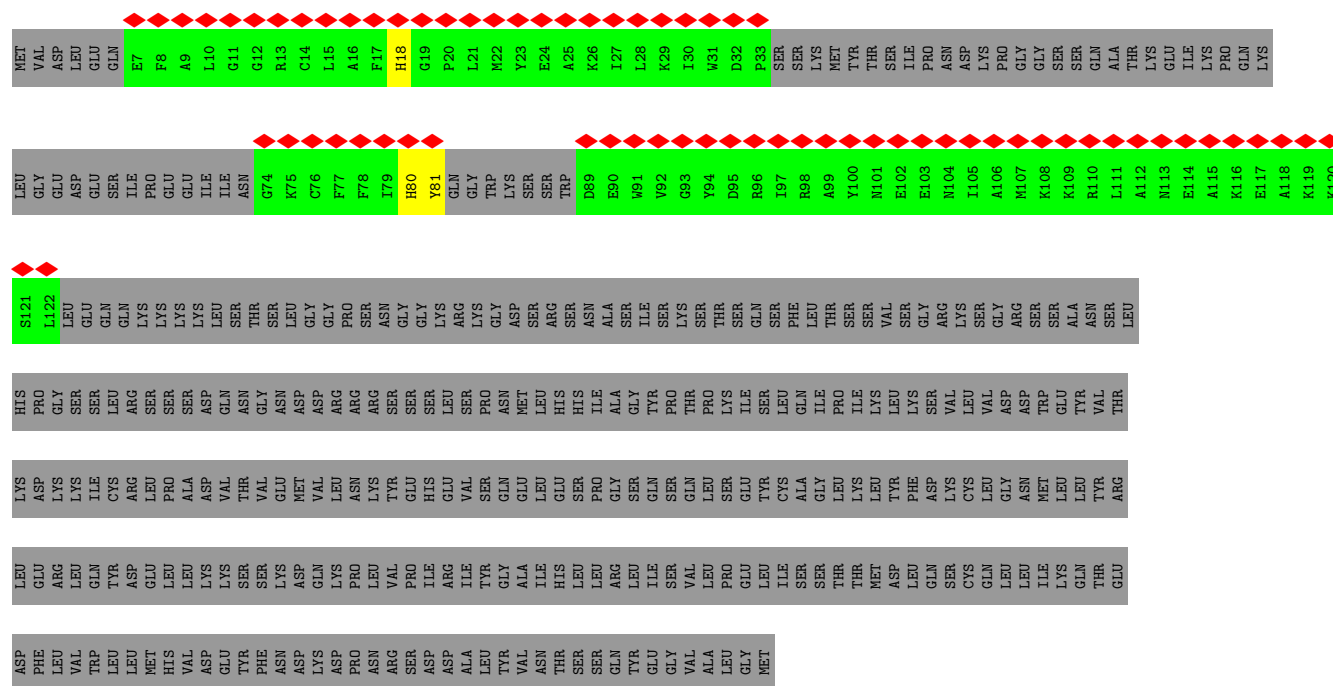


Chain D: 40% 31% 13% . 54%

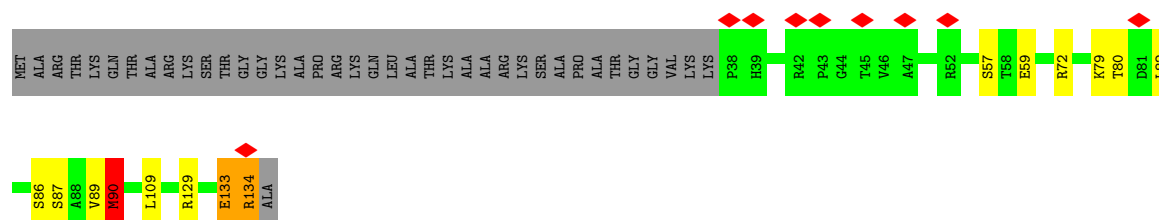




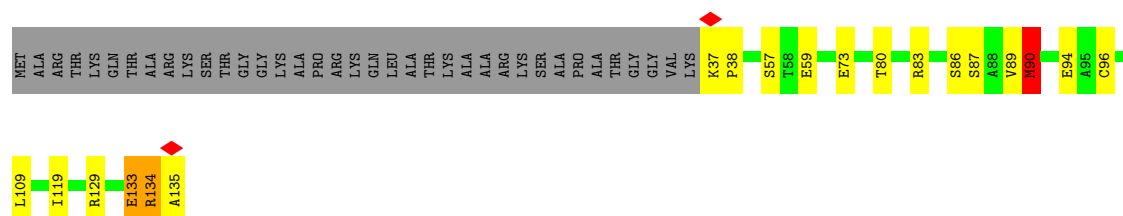
• Molecule 4: Chromatin modification-related protein EAF3



• Molecule 5: Histone H3.1



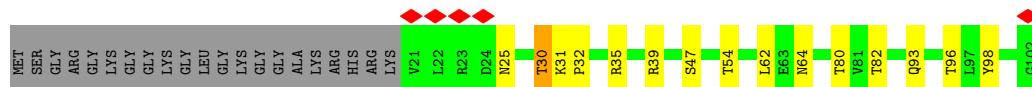
• Molecule 5: Histone H3.1



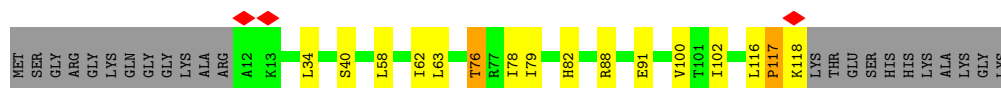
- Molecule 6: Histone H4



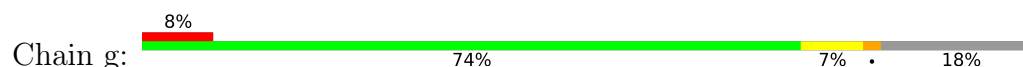
- Molecule 6: Histone H4



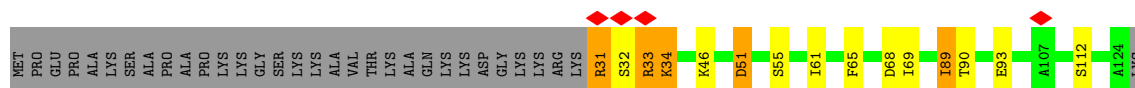
- Molecule 7: Histone H2A type 1-B/E



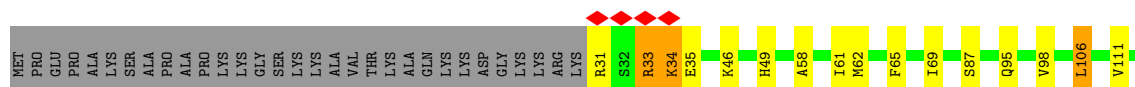
- Molecule 7: Histone H2A type 1-B/E



- Molecule 8: Histone H2B type 1-K

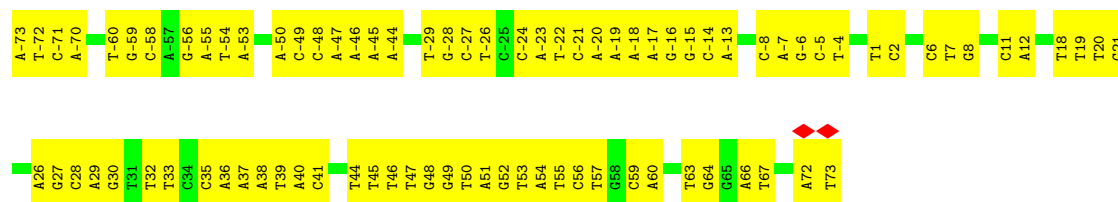


- Molecule 8: Histone H2B type 1-K



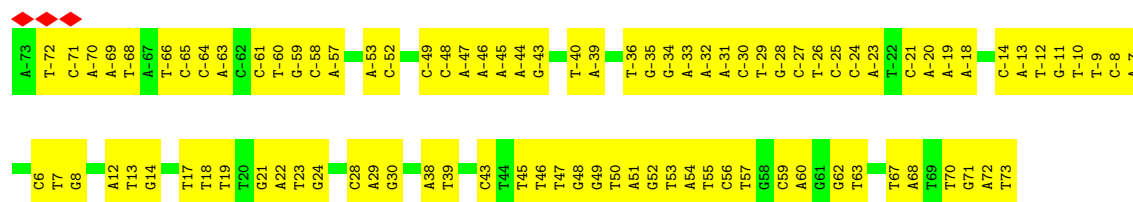
- Molecule 9: 5-DNA

Chain i:  41% 59%



• Molecule 10: 3-DNA

Chain j:  37% 63%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	213127	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size ($\text{\AA}$)	304.36002, 304.36002, 304.36002	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/5180	0.40	1/6984 (0.0%)
2	E	0.73	15/2952 (0.5%)	1.17	42/3978 (1.1%)
2	F	1.54	3/1313 (0.2%)	0.52	2/1763 (0.1%)
3	B	0.54	3/3137 (0.1%)	0.88	16/4246 (0.4%)
4	C	0.17	0/1509	0.50	3/2039 (0.1%)
4	D	1.22	6/1524 (0.4%)	0.41	1/2061 (0.0%)
4	G	0.70	0/583	1.14	0/777
5	a	0.44	0/813	0.65	2/1090 (0.2%)
5	e	0.49	0/828	0.61	2/1109 (0.2%)
6	b	0.43	0/634	0.51	0/848
6	f	0.40	0/660	0.48	0/883
7	c	0.80	2/827 (0.2%)	0.95	3/1116 (0.3%)
7	g	0.41	0/827	0.53	0/1116
8	d	0.44	0/746	0.59	1/1003 (0.1%)
8	h	0.38	0/746	0.51	0/1003
9	i	0.32	0/3378	0.45	0/5212
10	j	0.33	0/3376	0.44	0/5209
All	All	0.60	29/29033 (0.1%)	0.66	73/40437 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	E	0	1
3	B	0	1
All	All	0	3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	372	TYR	CB-CG	54.81	2.72	1.51
4	D	236	TRP	CE3-CZ3	29.57	2.27	1.38
4	D	236	TRP	CE2-CZ2	20.45	1.82	1.39
4	D	236	TRP	CZ3-CH2	18.12	1.85	1.40
7	c	117	PRO	N-CA	18.06	1.69	1.47
4	D	236	TRP	CD2-CE2	14.83	1.66	1.41
3	B	41	LYS	C-N	14.72	1.50	1.34
4	D	236	TRP	CZ2-CH2	14.59	1.65	1.37
4	D	236	TRP	CD2-CE3	13.65	1.62	1.40
3	B	67	LYS	C-N	13.02	1.50	1.33
2	E	177	GLU	C-O	-8.23	1.14	1.24
7	c	116	LEU	C-N	8.12	1.44	1.33
2	E	184	THR	C-O	-7.77	1.13	1.23
2	E	114	PRO	C-O	-7.72	1.14	1.23
2	E	179	SER	CA-CB	-7.23	1.43	1.53
2	E	182	ARG	C-O	-7.12	1.15	1.24
2	F	372	TYR	CG-CD1	7.12	1.54	1.39
2	E	111	THR	C-O	-6.28	1.16	1.24
2	F	372	TYR	CG-CD2	6.22	1.52	1.39
2	E	178	GLU	C-O	-6.10	1.16	1.23
2	E	109	SER	C-O	-5.90	1.16	1.24
2	E	123	ILE	C-O	-5.74	1.17	1.24
2	E	385	GLN	C-O	5.47	1.30	1.24
2	E	387	PHE	N-CA	5.46	1.52	1.46
2	E	110	VAL	C-O	-5.45	1.17	1.24
2	E	108	VAL	C-O	-5.32	1.17	1.24
3	B	277	SER	CA-CB	-5.21	1.45	1.53
2	E	128	LEU	C-O	-5.11	1.19	1.24
2	E	109	SER	CA-CB	-5.06	1.45	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	384	ARG	CB-CA-C	18.62	142.05	109.65
7	c	116	LEU	CA-C-N	18.25	138.57	119.78
7	c	116	LEU	C-N-CA	18.25	138.57	119.78
3	B	67	LYS	CA-C-N	14.39	134.56	119.89
3	B	67	LYS	C-N-CA	14.39	134.56	119.89
3	B	41	LYS	CA-C-N	13.44	133.85	119.87
3	B	41	LYS	C-N-CA	13.44	133.85	119.87
2	F	372	TYR	CA-CB-CG	12.81	136.95	113.90
3	B	85	PHE	CB-CA-C	-11.00	92.53	110.79
2	E	389	THR	CB-CA-C	9.06	125.21	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	383	ASP	CB-CA-C	8.81	125.48	110.94
2	E	387	PHE	CA-CB-CG	8.70	122.50	113.80
2	E	181	ILE	N-CA-C	-8.55	104.11	113.43
5	a	133	GLU	CB-CA-C	-8.52	95.23	109.55
2	E	387	PHE	N-CA-CB	8.48	122.58	110.12
2	F	372	TYR	CD1-CG-CD2	-8.48	105.38	118.10
3	B	42	PRO	N-CA-C	-8.40	103.70	114.03
2	E	182	ARG	CB-CG-CD	-8.24	92.35	111.30
3	B	161	CYS	CA-C-O	-8.07	112.55	122.64
2	E	184	THR	OG1-CB-CG2	-8.02	93.25	109.30
2	E	385	GLN	N-CA-C	-7.96	102.68	111.36
2	E	386	LEU	CA-C-N	7.69	130.59	120.28
2	E	386	LEU	C-N-CA	7.69	130.59	120.28
2	E	172	THR	CA-CB-OG1	7.67	121.10	109.60
2	E	388	ASN	N-CA-C	-7.54	103.15	111.36
7	c	117	PRO	CA-N-CD	-7.34	101.72	112.00
2	E	169	THR	CB-CA-C	7.31	122.90	111.13
2	E	180	ASN	CA-C-N	7.26	131.31	122.16
2	E	180	ASN	C-N-CA	7.26	131.31	122.16
2	E	123	ILE	N-CA-CB	6.72	119.17	110.57
3	B	82	TYR	CB-CA-C	-6.60	100.52	110.88
2	E	170	PHE	CA-C-N	6.57	134.09	121.54
2	E	170	PHE	C-N-CA	6.57	134.09	121.54
2	E	169	THR	CA-C-N	6.52	129.01	120.28
2	E	169	THR	C-N-CA	6.52	129.01	120.28
1	A	787	VAL	N-CA-C	-6.47	107.56	113.71
4	C	242	ASP	N-CA-C	-6.47	103.66	113.89
2	E	125	ARG	CB-CA-C	-6.46	97.56	110.42
2	E	181	ILE	N-CA-CB	-6.36	105.21	112.21
2	E	388	ASN	CA-C-N	-6.35	111.80	120.44
2	E	388	ASN	C-N-CA	-6.35	111.80	120.44
3	B	42	PRO	N-CD-CG	-6.27	93.79	103.20
2	E	384	ARG	N-CA-C	-6.26	105.68	113.38
2	E	384	ARG	CB-CG-CD	6.21	125.59	111.30
4	D	236	TRP	CE3-CZ3-CH2	-6.18	113.06	121.10
2	E	129	TRP	N-CA-C	-6.16	105.67	113.43
2	E	114	PRO	N-CA-CB	-6.05	98.24	103.32
8	d	34	LYS	CB-CA-C	-5.87	98.08	109.76
4	C	381	ARG	CA-C-N	-5.75	114.65	121.90
4	C	381	ARG	C-N-CA	-5.75	114.65	121.90
2	E	185	ILE	CA-C-N	5.68	126.25	120.00
2	E	185	ILE	C-N-CA	5.68	126.25	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	184	THR	CA-C-O	-5.67	114.85	122.44
3	B	39	PRO	N-CA-C	5.66	122.18	113.75
3	B	113	PHE	CA-C-O	-5.60	114.93	120.70
2	E	126	GLU	CA-C-N	5.46	130.69	122.67
2	E	126	GLU	C-N-CA	5.46	130.69	122.67
5	e	133	GLU	CB-CA-C	-5.31	101.74	110.72
3	B	31	ASN	CA-C-N	-5.27	115.63	123.11
3	B	31	ASN	C-N-CA	-5.27	115.63	123.11
3	B	160	PHE	CA-CB-CG	5.21	119.01	113.80
2	E	182	ARG	CB-CA-C	-5.20	100.07	110.42
5	e	90	MET	CB-CG-SD	5.17	128.22	112.70
5	a	90	MET	CB-CG-SD	5.17	128.21	112.70
2	E	169	THR	OG1-CB-CG2	5.15	119.59	109.30
2	E	386	LEU	CA-C-O	-5.12	114.31	120.10
3	B	355	VAL	CA-C-N	-5.12	113.22	122.28
3	B	355	VAL	C-N-CA	-5.12	113.22	122.28
2	E	110	VAL	CA-C-N	5.12	128.78	120.60
2	E	110	VAL	C-N-CA	5.12	128.78	120.60
2	E	174	ASN	CB-CA-C	-5.09	100.29	110.42
2	E	108	VAL	CA-C-O	-5.06	116.52	121.58
2	E	178	GLU	CB-CA-C	-5.05	100.57	109.62

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1232	TYR	Peptide
3	B	157	ALA	Mainchain
2	E	470	SER	Peptide

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	5066	0	5024	208	0
2	E	2884	0	2831	200	0
2	F	1282	0	1239	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3057	0	2930	155	0
4	C	1483	0	1510	33	0
4	D	1497	0	1524	76	0
4	G	570	0	563	23	0
5	a	801	0	839	8	0
5	e	816	0	856	38	0
6	b	627	0	663	4	0
6	f	653	0	696	12	0
7	c	817	0	872	14	0
7	g	817	0	872	8	0
8	d	735	0	756	26	0
8	h	735	0	756	18	0
9	i	3011	0	1662	88	0
10	j	3010	0	1663	85	0
11	B	1	0	0	0	0
11	E	4	0	0	0	0
11	F	2	0	0	0	0
All	All	27868	0	25256	846	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 16.

All (846) 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:236:TRP:CE2	4:D:236:TRP:CZ2	1.82	1.65
4:D:236:TRP:CH2	4:D:236:TRP:CZ3	1.85	1.59
1:A:922:LYS:CE	2:E:129:TRP:CZ2	1.96	1.48
5:e:37:LYS:CD	5:e:38:PRO:HD3	1.41	1.46
1:A:922:LYS:HE3	2:E:129:TRP:CE2	1.49	1.44
7:c:117:PRO:CA	7:c:117:PRO:N	1.69	1.40
2:E:379:ILE:HD12	2:E:380:PRO:CD	1.53	1.39
1:A:798:HIS:CG	3:B:283:CYS:SG	2.17	1.38
1:A:819:PHE:CD2	3:B:33:ALA:HB2	1.61	1.34
1:A:922:LYS:HE3	2:E:129:TRP:CZ2	1.57	1.34
1:A:1190:GLN:NE2	2:E:129:TRP:CE3	1.95	1.33
4:D:236:TRP:CZ3	2:F:372:TYR:CG	2.16	1.33
3:B:152:ALA:HB2	3:B:161:CYS:O	1.27	1.32
4:D:236:TRP:CE3	2:F:372:TYR:CG	2.17	1.31
5:e:37:LYS:CG	4:G:18:HIS:CD2	2.14	1.30
4:D:236:TRP:CE3	2:F:372:TYR:CB	2.15	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:37:LYS:HD3	5:e:38:PRO:CD	1.64	1.27
3:B:151:HIS:N	3:B:161:CYS:SG	2.06	1.26
5:e:37:LYS:CE	4:G:18:HIS:CD2	2.18	1.26
1:A:798:HIS:CD2	3:B:283:CYS:SG	2.28	1.26
1:A:922:LYS:NZ	2:E:129:TRP:CZ2	2.02	1.26
1:A:1190:GLN:OE1	2:E:129:TRP:CH2	1.90	1.24
5:e:37:LYS:CG	4:G:18:HIS:HD2	1.46	1.23
5:e:37:LYS:HE3	4:G:18:HIS:CD2	1.72	1.23
5:e:37:LYS:HG2	4:G:18:HIS:CD2	1.71	1.23
1:A:922:LYS:CE	2:E:129:TRP:CE2	2.16	1.22
4:D:236:TRP:CZ3	2:F:372:TYR:CB	2.22	1.22
4:D:236:TRP:CZ3	4:D:236:TRP:CE3	2.27	1.21
4:D:236:TRP:CH2	2:F:372:TYR:CG	2.29	1.21
4:D:236:TRP:CD2	2:F:372:TYR:CG	2.28	1.21
1:A:918:GLU:OE2	2:E:128:LEU:HA	1.33	1.21
8:d:65:PHE:CE1	8:d:69:ILE:HD11	1.75	1.20
5:e:37:LYS:HB3	5:e:38:PRO:CD	1.71	1.19
4:D:236:TRP:CE3	2:F:372:TYR:HB3	1.76	1.18
4:D:236:TRP:CE2	2:F:372:TYR:CG	2.32	1.18
1:A:819:PHE:CE2	3:B:33:ALA:HB2	1.75	1.18
4:D:236:TRP:CE2	2:F:372:TYR:CB	2.27	1.17
4:D:236:TRP:CD2	2:F:372:TYR:CB	2.26	1.17
1:A:922:LYS:CE	2:E:129:TRP:HZ2	1.43	1.17
1:A:812:GLU:OE2	3:B:37:GLY:HA2	1.44	1.16
4:D:236:TRP:CE2	2:F:372:TYR:HB2	1.81	1.15
1:A:922:LYS:CE	2:E:129:TRP:NE1	2.09	1.14
1:A:819:PHE:CE2	3:B:33:ALA:CB	2.32	1.12
1:A:904:GLU:HG2	2:E:116:ASN:HB2	1.29	1.12
4:D:236:TRP:CZ2	2:F:372:TYR:CG	2.37	1.12
9:i:12:DA:P	4:G:80:HIS:CE1	2.44	1.11
2:E:381:LEU:HB3	2:E:384:ARG:HB2	1.33	1.07
1:A:819:PHE:HE2	3:B:33:ALA:N	1.52	1.07
2:E:179:SER:O	3:B:129:GLU:OE2	1.73	1.06
2:E:379:ILE:CD1	2:E:380:PRO:CD	2.33	1.05
5:e:37:LYS:HG3	4:G:18:HIS:HD2	1.21	1.05
2:E:379:ILE:CD1	2:E:380:PRO:HD3	1.84	1.05
1:A:922:LYS:CD	2:E:129:TRP:HZ2	1.71	1.04
1:A:922:LYS:NZ	2:E:129:TRP:CE2	2.24	1.04
1:A:813:GLU:OE1	2:E:110:VAL:HG12	1.56	1.03
4:D:236:TRP:CZ3	2:F:372:TYR:CD1	2.45	1.03
4:D:236:TRP:CZ2	2:F:372:TYR:CB	2.42	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:LYS:HE3	2:E:129:TRP:NE1	1.70	1.02
5:e:37:LYS:CB	5:e:38:PRO:HD2	1.90	1.01
1:A:922:LYS:CE	2:E:129:TRP:HE1	1.70	1.01
4:D:236:TRP:CE2	2:F:372:TYR:CD2	2.48	1.01
8:h:65:PHE:CE1	8:h:69:ILE:HD11	1.96	1.01
5:e:37:LYS:CB	5:e:38:PRO:CD	2.40	1.00
5:e:37:LYS:CD	5:e:38:PRO:CD	2.31	0.99
4:D:236:TRP:CH2	2:F:372:TYR:CB	2.45	0.99
2:E:189:GLY:HA2	3:B:72:GLN:HB2	1.41	0.98
1:A:798:HIS:CB	3:B:283:CYS:SG	2.51	0.98
5:e:37:LYS:HB3	5:e:38:PRO:HD2	0.99	0.98
1:A:1190:GLN:OE1	2:E:129:TRP:CZ2	2.17	0.97
1:A:798:HIS:HB2	3:B:283:CYS:SG	2.05	0.97
3:B:149:LEU:HB3	3:B:161:CYS:HB2	1.46	0.97
5:e:37:LYS:HG2	4:G:18:HIS:NE2	1.78	0.97
1:A:918:GLU:OE2	2:E:128:LEU:CA	2.14	0.96
3:B:151:HIS:CB	3:B:161:CYS:SG	2.46	0.95
8:d:31:ARG:HA	8:d:31:ARG:HH11	1.30	0.95
1:A:1190:GLN:NE2	2:E:129:TRP:CZ3	2.26	0.95
3:B:150:HIS:CE1	3:B:270:GLN:NE2	2.35	0.94
3:B:151:HIS:HB2	3:B:161:CYS:SG	2.07	0.94
5:e:96:CYS:SG	6:f:62:LEU:HD21	2.06	0.93
1:A:918:GLU:OE2	2:E:127:SER:O	1.87	0.93
1:A:918:GLU:CD	2:E:128:LEU:HD12	1.93	0.93
3:B:114:ASP:O	3:B:116:LEU:N	2.02	0.93
4:D:236:TRP:CD2	2:F:372:TYR:HB2	1.99	0.93
4:D:236:TRP:CZ2	2:F:372:TYR:CD2	2.57	0.92
8:d:65:PHE:CE1	8:d:69:ILE:CD1	2.52	0.92
8:d:65:PHE:CZ	8:d:69:ILE:CD1	2.52	0.92
1:A:819:PHE:HE2	3:B:33:ALA:H	0.93	0.91
1:A:904:GLU:CG	2:E:116:ASN:HB2	2.01	0.90
5:e:37:LYS:CD	4:G:18:HIS:CD2	2.54	0.90
1:A:918:GLU:OE2	2:E:128:LEU:HD12	1.72	0.90
9:i:12:DA:P	4:G:80:HIS:HE1	1.91	0.90
8:h:65:PHE:CZ	8:h:69:ILE:HD11	2.07	0.90
2:E:379:ILE:CD1	2:E:380:PRO:HD2	2.02	0.89
8:d:31:ARG:HA	8:d:31:ARG:NH1	1.85	0.89
8:h:65:PHE:CZ	8:h:69:ILE:CD1	2.55	0.89
8:d:65:PHE:CZ	8:d:69:ILE:HD11	2.08	0.89
4:D:236:TRP:CE3	2:F:372:TYR:CD1	2.60	0.88
3:B:28:ASP:HA	3:B:31:ASN:HD21	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:379:ILE:HD12	2:E:380:PRO:HD3	0.89	0.87
1:A:819:PHE:CE2	3:B:33:ALA:N	2.42	0.87
3:B:136:ARG:HG2	3:B:136:ARG:HH21	1.40	0.86
1:A:911:GLU:OE1	2:E:118:GLY:HA3	1.75	0.86
3:B:114:ASP:C	3:B:116:LEU:H	1.83	0.85
1:A:813:GLU:OE1	2:E:110:VAL:CG1	2.26	0.84
1:A:922:LYS:HE2	2:E:129:TRP:HE1	1.43	0.84
9:i:12:DA:OP2	4:G:80:HIS:HE1	1.61	0.82
1:A:918:GLU:OE1	2:E:128:LEU:HD12	1.78	0.82
4:D:255:GLU:HG2	4:D:323:ILE:HG12	1.61	0.82
3:B:31:ASN:HD22	3:B:31:ASN:H	1.25	0.82
1:A:922:LYS:HD2	2:E:129:TRP:HZ2	1.44	0.81
5:e:37:LYS:HE3	4:G:18:HIS:CG	2.17	0.80
5:e:37:LYS:HE2	4:G:18:HIS:CD2	2.17	0.80
1:A:819:PHE:CD2	3:B:33:ALA:CB	2.55	0.79
4:C:240:THR:O	4:C:242:ASP:N	2.14	0.79
1:A:812:GLU:OE2	3:B:37:GLY:CA	2.30	0.79
2:E:515:GLN:HG3	2:E:516:ASN:H	1.48	0.79
3:B:28:ASP:O	3:B:31:ASN:ND2	2.16	0.79
1:A:922:LYS:CD	2:E:129:TRP:CZ2	2.55	0.78
1:A:1190:GLN:OE1	2:E:129:TRP:CZ3	2.37	0.78
2:E:517:ASN:HB3	2:E:519:ASN:H	1.47	0.78
3:B:88:ARG:HG3	3:B:88:ARG:HH11	1.49	0.78
5:e:83:ARG:HB2	6:f:80:THR:HG22	1.66	0.78
1:A:921:GLN:NE2	1:A:1186:LEU:O	2.17	0.78
3:B:136:ARG:HG2	3:B:136:ARG:NH2	1.98	0.78
3:B:28:ASP:HA	3:B:31:ASN:ND2	1.99	0.77
1:A:911:GLU:OE1	2:E:119:PRO:CD	2.32	0.77
1:A:922:LYS:NZ	2:E:129:TRP:NE1	2.29	0.77
1:A:868:ARG:HD2	1:A:873:LYS:HE3	1.66	0.77
2:E:384:ARG:HA	2:E:387:PHE:HB3	1.65	0.77
2:F:260:GLU:HG3	2:F:262:PHE:H	1.48	0.77
2:E:491:VAL:HG12	2:E:492:TRP:HD1	1.51	0.75
9:i:12:DA:OP1	4:G:80:HIS:CE1	2.38	0.75
1:A:1190:GLN:CD	2:E:129:TRP:CZ3	2.64	0.75
1:A:918:GLU:CD	2:E:128:LEU:HA	2.11	0.74
1:A:946:LYS:HE2	9:i:-19:DA:OP1	1.87	0.74
4:D:293:LEU:HD23	4:D:322:PRO:HB3	1.68	0.74
5:e:37:LYS:CD	4:G:18:HIS:HD2	1.96	0.74
1:A:1190:GLN:NE2	2:E:129:TRP:CD2	2.54	0.74
3:B:280:ARG:HB2	3:B:313:TYR:HB2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:350:ASP:OD1	3:B:350:ASP:N	2.16	0.73
3:B:78:HIS:HD1	3:B:82:TYR:HD1	1.37	0.73
2:F:372:TYR:CG	2:F:372:TYR:CB	2.72	0.73
1:A:812:GLU:CD	3:B:37:GLY:HA2	2.14	0.73
4:C:288:TYR:O	4:C:292:CYS:HB2	1.89	0.72
1:A:1318:ALA:HB3	1:A:1321:ASP:HB2	1.72	0.72
8:d:31:ARG:HD3	8:d:32:SER:H	1.53	0.72
1:A:911:GLU:OE1	2:E:119:PRO:HD3	1.90	0.71
2:E:404:ASP:N	2:E:404:ASP:OD2	2.19	0.71
3:B:152:ALA:CB	3:B:161:CYS:O	2.23	0.71
4:D:236:TRP:CE2	2:F:372:TYR:HD2	2.07	0.71
2:F:354:PRO:HD2	2:F:357:ILE:HD12	1.72	0.71
2:E:113:LEU:HD12	2:E:113:LEU:N	2.07	0.70
2:E:570:GLN:HB2	2:F:564:ARG:HH22	1.56	0.70
3:B:149:LEU:HB3	3:B:161:CYS:CB	2.21	0.70
8:d:31:ARG:HH11	8:d:31:ARG:HG2	1.56	0.70
5:e:37:LYS:CG	5:e:38:PRO:HD3	2.19	0.70
8:d:31:ARG:HH11	8:d:31:ARG:CA	2.02	0.70
2:E:371:GLN:HA	4:C:240:THR:HG21	1.74	0.69
5:e:129:ARG:HG3	5:e:135:ALA:HB3	1.73	0.69
7:g:15:LYS:HG3	7:g:15:LYS:O	1.92	0.69
9:i:48:DC:N4	10:j:47:DT:O4	2.26	0.69
1:A:922:LYS:NZ	2:E:129:TRP:HZ2	1.65	0.69
3:B:2:VAL:N	3:B:370:ASP:OD1	2.26	0.69
2:E:187:TRP:HE3	2:E:187:TRP:N	1.91	0.69
2:E:372:TYR:OH	2:E:496:ARG:NH1	2.24	0.69
3:B:28:ASP:C	3:B:31:ASN:ND2	2.50	0.69
8:h:31:ARG:O	8:h:31:ARG:HD3	1.93	0.69
1:A:922:LYS:HD2	2:E:129:TRP:CZ2	2.25	0.69
8:d:33:ARG:O	8:d:33:ARG:HD3	1.93	0.69
8:d:65:PHE:CZ	8:d:69:ILE:HD12	2.28	0.68
2:E:384:ARG:HG3	2:E:387:PHE:HB3	1.75	0.68
5:a:79:LYS:NZ	6:b:74:GLU:OE1	2.26	0.68
2:E:414:PHE:HB3	2:E:423:THR:HG21	1.76	0.67
9:i:12:DA:O5'	4:G:80:HIS:NE2	2.27	0.67
5:e:37:LYS:HG3	4:G:18:HIS:CD2	2.07	0.67
5:e:37:LYS:HD3	5:e:38:PRO:HD3	0.68	0.67
2:E:180:ASN:C	2:E:180:ASN:HD22	2.00	0.67
2:E:184:THR:O	3:B:73:GLU:OE1	2.13	0.67
10:j:72:DA:H2''	10:j:73:DT:H5''	1.76	0.67
2:E:179:SER:C	3:B:129:GLU:OE2	2.38	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:d:31:ARG:HH11	8:d:31:ARG:CG	2.08	0.66
10:j:-48:DC:H4'	10:j:-47:DA:H5'	1.77	0.66
4:D:236:TRP:CH2	2:F:372:TYR:CA	2.79	0.66
1:A:812:GLU:CD	3:B:37:GLY:CA	2.68	0.66
2:E:384:ARG:HB3	2:E:387:PHE:HD2	1.61	0.66
3:B:299:LYS:NZ	3:B:331:ASN:OD1	2.28	0.66
1:A:813:GLU:CD	2:E:110:VAL:HG12	2.19	0.66
2:E:181:ILE:HG13	3:B:136:ARG:HD2	1.77	0.66
3:B:88:ARG:HH11	3:B:88:ARG:CG	2.08	0.66
5:e:37:LYS:CG	5:e:38:PRO:CD	2.74	0.65
2:E:180:ASN:HB2	2:E:185:ILE:HD12	1.78	0.65
4:C:293:LEU:HD22	4:C:322:PRO:HB3	1.78	0.65
8:d:51:ASP:N	8:d:51:ASP:OD1	2.30	0.65
2:E:440:CYS:SG	2:E:441:ASP:N	2.70	0.65
3:B:91:PRO:HD2	3:B:114:ASP:OD1	1.97	0.65
2:E:379:ILE:CG1	2:E:380:PRO:HD2	2.26	0.64
3:B:150:HIS:CE1	3:B:270:GLN:HE22	2.13	0.64
7:c:117:PRO:N	7:c:117:PRO:C	2.52	0.64
8:h:65:PHE:CE1	8:h:69:ILE:CD1	2.74	0.64
4:D:236:TRP:CZ3	2:F:372:TYR:HB3	2.28	0.64
1:A:819:PHE:CE2	3:B:33:ALA:HB3	2.32	0.64
2:E:381:LEU:CB	2:E:384:ARG:HB2	2.20	0.63
2:E:424:ARG:HD3	2:E:435:ARG:HG3	1.80	0.63
4:D:236:TRP:CH2	2:F:372:TYR:HA	2.33	0.63
1:A:929:ASP:OD1	3:B:359:ASN:ND2	2.26	0.63
3:B:209:HIS:HE1	3:B:235:ASN:HB3	1.61	0.63
2:E:121:GLU:O	2:E:125:ARG:HG2	1.98	0.63
8:h:34:LYS:HB2	9:i:50:DT:OP1	1.98	0.63
8:h:33:ARG:HH21	8:h:35:GLU:HG2	1.61	0.63
10:j:17:DT:H2'	10:j:18:DT:H71	1.81	0.63
2:E:178:GLU:HG2	3:B:67:LYS:HZ2	1.63	0.63
4:D:308:GLU:HA	4:D:311:LYS:HE2	1.81	0.63
8:h:65:PHE:CZ	8:h:69:ILE:HD12	2.34	0.63
3:B:285:ASN:OD1	3:B:358:SER:OG	2.14	0.62
2:E:124:LYS:O	2:E:124:LYS:HG3	1.98	0.62
3:B:81:GLU:CG	3:B:104:PHE:HZ	2.11	0.62
8:d:31:ARG:NH1	8:d:31:ARG:HG2	2.12	0.62
2:E:189:GLY:HA3	3:B:70:THR:HB	1.82	0.62
1:A:912:TRP:CH2	2:E:111:THR:HG23	2.34	0.62
1:A:1007:LYS:O	1:A:1011:LYS:HG3	1.99	0.62
3:B:90:THR:HG23	3:B:92:ASP:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:a:129:ARG:HB2	5:a:134:ARG:HH22	1.63	0.62
5:e:57:SER:OG	5:e:59:GLU:OE2	2.18	0.62
2:E:507:GLU:HB2	2:E:541:GLN:HE21	1.63	0.62
10:j:-29:DT:H2''	10:j:-28:DG:C8	2.35	0.61
3:B:136:ARG:HH21	3:B:136:ARG:CG	2.13	0.61
3:B:28:ASP:CA	3:B:31:ASN:ND2	2.62	0.61
10:j:28:DC:H2''	10:j:29:DA:C8	2.35	0.61
3:B:44:ARG:HB3	3:B:315:MET:HG2	1.83	0.61
3:B:81:GLU:CG	3:B:104:PHE:CZ	2.83	0.61
5:e:96:CYS:SG	6:f:62:LEU:CD2	2.84	0.61
3:B:149:LEU:CB	3:B:161:CYS:HB2	2.28	0.61
1:A:663:ASN:HB3	2:F:547:ILE:HG23	1.81	0.61
9:i:26:DA:H2''	9:i:27:DG:C8	2.35	0.61
2:E:516:ASN:ND2	2:E:540:THR:OG1	2.34	0.61
4:D:253:THR:OG1	4:D:323:ILE:O	2.19	0.61
5:e:73:GLU:OE1	6:f:25:ASN:ND2	2.25	0.61
3:B:81:GLU:HG3	3:B:104:PHE:CZ	2.36	0.60
5:a:90:MET:HA	5:a:90:MET:HE2	1.83	0.60
6:b:47:SER:OG	6:b:48:GLY:N	2.32	0.60
9:i:12:DA:OP1	4:G:81:TYR:O	2.18	0.60
2:E:367:GLY:HA3	2:E:371:GLN:HG3	1.83	0.60
1:A:665:GLU:HB3	2:E:552:PHE:CZ	2.36	0.60
1:A:808:PHE:CZ	3:B:280:ARG:HA	2.36	0.60
2:E:416:ILE:HA	2:E:423:THR:HG22	1.83	0.60
1:A:798:HIS:CD2	3:B:283:CYS:HG	2.16	0.60
3:B:106:VAL:HG12	3:B:106:VAL:O	2.00	0.60
1:A:1181:ALA:HB1	1:A:1186:LEU:HB2	1.84	0.60
4:D:300:ARG:NH2	4:D:397:VAL:O	2.34	0.60
5:e:90:MET:HE2	5:e:90:MET:HA	1.83	0.60
1:A:901:LYS:HZ3	2:E:105:ASP:N	2.00	0.60
9:i:63:DT:H2''	9:i:64:DG:H5''	1.83	0.59
1:A:1076:LYS:HG2	1:A:1079:ARG:HH22	1.66	0.59
3:B:326:THR:O	3:B:330:ASN:ND2	2.35	0.59
2:E:543:ASP:O	2:E:546:SER:OG	2.21	0.59
1:A:911:GLU:OE1	2:E:118:GLY:CA	2.51	0.59
1:A:904:GLU:CD	2:E:116:ASN:HB2	2.28	0.59
9:i:-14:DC:H2''	9:i:-13:DA:C8	2.38	0.59
2:E:379:ILE:HG13	2:E:380:PRO:HD2	1.83	0.59
4:C:236:TRP:CD1	4:C:299:TYR:HH	2.21	0.59
2:E:492:TRP:CD1	2:E:492:TRP:H	2.21	0.59
3:B:150:HIS:HE1	3:B:270:GLN:NE2	1.97	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:31:ASN:H	3:B:31:ASN:ND2	1.98	0.59
2:E:171:LEU:O	2:E:173:GLU:N	2.36	0.58
8:d:33:ARG:HB2	10:j:50:DT:H5'	1.85	0.58
1:A:1190:GLN:CD	2:E:129:TRP:CE3	2.77	0.58
1:A:959:GLN:NE2	1:A:972:LYS:O	2.27	0.58
2:E:172:THR:HG22	3:B:63:ILE:HD13	1.86	0.58
7:c:76:THR:O	7:c:76:THR:OG1	2.17	0.58
3:B:31:ASN:HD22	3:B:31:ASN:N	2.00	0.58
1:A:770:ARG:HH22	3:B:154:LYS:HZ1	1.52	0.58
2:E:187:TRP:N	2:E:187:TRP:CE3	2.71	0.58
9:i:12:DA:O5'	4:G:80:HIS:CE1	2.57	0.58
1:A:819:PHE:CE2	3:B:33:ALA:CA	2.86	0.57
1:A:952:ILE:HA	1:A:955:ILE:HD12	1.86	0.57
1:A:911:GLU:OE1	2:E:119:PRO:HD2	2.04	0.57
2:E:107:LYS:HG3	2:E:107:LYS:O	2.05	0.57
2:E:317:ALA:O	2:E:321:LYS:HG3	2.04	0.57
5:a:57:SER:OG	5:a:59:GLU:OE2	2.18	0.57
2:E:387:PHE:CD1	2:E:387:PHE:C	2.82	0.57
2:E:181:ILE:HG21	3:B:133:ARG:HG2	1.87	0.57
4:D:253:THR:HG23	4:D:256:MET:H	1.69	0.57
2:E:543:ASP:OD1	2:E:543:ASP:N	2.38	0.57
2:E:172:THR:HG22	3:B:63:ILE:CD1	2.34	0.57
2:E:443:CYS:HB2	2:E:445:THR:HG22	1.86	0.57
4:D:304:LEU:HD22	4:D:397:VAL:HG21	1.86	0.57
2:E:180:ASN:ND2	2:E:180:ASN:O	2.35	0.57
3:B:32:TYR:CD2	3:B:32:TYR:N	2.72	0.57
1:A:1206:GLN:OE1	1:A:1209:ARG:NH2	2.37	0.56
10:j:28:DC:H2''	10:j:29:DA:H8	1.70	0.56
1:A:675:TYR:CZ	1:A:713:ASN:HB2	2.40	0.56
9:i:12:DA:P	4:G:80:HIS:NE2	2.78	0.56
4:D:303:ARG:HH21	2:F:350:GLN:HA	1.70	0.56
10:j:51:DA:C6	10:j:52:DG:C6	2.93	0.56
10:j:55:DT:H2''	10:j:56:DC:C6	2.40	0.56
1:A:918:GLU:OE1	2:E:128:LEU:CD1	2.53	0.56
4:C:244:LYS:HE2	4:C:379:PRO:HG2	1.88	0.56
9:i:46:DT:H2''	9:i:47:DT:H71	1.87	0.56
1:A:696:ILE:HG21	2:E:493:LYS:HB2	1.86	0.56
10:j:-60:DT:H2''	10:j:-59:DG:N7	2.20	0.56
1:A:812:GLU:OE1	3:B:280:ARG:NH1	2.19	0.56
3:B:297:TYR:O	3:B:300:SER:OG	2.21	0.56
1:A:912:TRP:CZ3	2:E:111:THR:HG23	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:402:ASN:HA	2:E:405:THR:HB	1.87	0.56
2:E:562:GLN:HA	2:E:565:LYS:HD3	1.88	0.56
4:C:364:VAL:HG12	4:C:368:MET:HE1	1.88	0.56
2:F:302:HIS:HB2	2:F:307:LYS:HD3	1.88	0.56
2:E:379:ILE:CG1	2:E:380:PRO:CD	2.82	0.56
2:F:355:ASN:HA	2:F:358:LYS:HG3	1.88	0.56
3:B:91:PRO:HG2	3:B:113:PHE:O	2.06	0.56
9:i:-8:DC:H2''	9:i:-7:DA:C8	2.41	0.56
3:B:38:HIS:C	3:B:38:HIS:CD2	2.85	0.55
1:A:1075:GLN:HA	1:A:1078:LYS:HG2	1.87	0.55
4:C:255:GLU:HB2	4:C:323:ILE:HG12	1.88	0.55
9:i:12:DA:C5'	4:G:80:HIS:NE2	2.69	0.55
1:A:755:TYR:OH	3:B:194:GLU:OE1	2.24	0.55
7:c:102:ILE:HG23	8:d:61:ILE:HD12	1.88	0.55
1:A:1194:MET:HB2	1:A:1196:LEU:HG	1.88	0.55
8:d:90:THR:OG1	8:d:93:GLU:OE1	2.25	0.55
1:A:1229:ARG:O	1:A:1233:ASN:HA	2.06	0.55
2:E:106:SER:O	2:E:106:SER:OG	2.18	0.55
10:j:-53:DA:H1'	10:j:-52:DC:H5'	1.88	0.55
1:A:999:THR:HG22	1:A:1001:ALA:H	1.71	0.55
1:A:1219:LEU:HD11	1:A:1223:TRP:HB2	1.89	0.55
3:B:81:GLU:HG2	3:B:104:PHE:HZ	1.71	0.55
4:D:305:GLN:O	4:D:308:GLU:HB3	2.06	0.55
9:i:47:DT:H2''	9:i:48:DG:N7	2.22	0.55
1:A:886:HIS:O	1:A:890:THR:OG1	2.23	0.55
1:A:913:ASN:ND2	3:B:345:GLU:OE2	2.39	0.55
2:E:449:LEU:HD11	2:E:457:PHE:HE1	1.72	0.54
2:E:327:ILE:HG22	2:E:337:ALA:HB1	1.88	0.54
2:E:491:VAL:HG12	2:E:492:TRP:CD1	2.38	0.54
8:d:68:ASP:OD1	6:f:98:TYR:OH	2.25	0.54
9:i:7:DT:H2''	9:i:8:DG:C8	2.43	0.54
2:E:452:VAL:HG21	2:E:464:TRP:HZ2	1.71	0.54
4:C:290:ASP:HA	4:C:322:PRO:HD2	1.89	0.54
9:i:-29:DT:H2''	9:i:-28:DG:C8	2.42	0.54
1:A:851:LEU:HD13	1:A:855:LEU:HG	1.89	0.54
1:A:1178:VAL:HG12	1:A:1181:ALA:H	1.73	0.54
2:E:402:ASN:H	2:E:428:TRP:HZ2	1.54	0.54
9:i:-49:DC:N4	10:j:48:DG:O6	2.41	0.54
9:i:72:DA:H2''	9:i:73:DT:H5''	1.90	0.54
10:j:7:DT:H2''	10:j:8:DG:C8	2.43	0.54
2:E:184:THR:O	2:E:184:THR:OG1	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:492:TRP:HD1	2:E:492:TRP:H	1.55	0.54
4:D:236:TRP:HH2	2:F:366:THR:HA	1.73	0.54
9:i:-16:DG:H2''	9:i:-15:DG:N7	2.23	0.54
2:E:184:THR:HG21	3:B:76:GLN:HE22	1.72	0.54
3:B:70:THR:OG1	3:B:73:GLU:OE2	2.26	0.54
4:D:307:ASP:O	4:D:310:LEU:HB2	2.07	0.54
4:D:378:ASP:OD2	4:D:381:ARG:NH2	2.34	0.54
9:i:6:DC:H2''	9:i:7:DT:H72	1.89	0.54
9:i:12:DA:H5''	4:G:80:HIS:NE2	2.23	0.54
1:A:990:CYS:O	1:A:994:THR:HG23	2.08	0.54
4:D:335:ILE:HG21	4:D:363:LEU:HD21	1.89	0.53
1:A:954:SER:HA	2:E:414:PHE:CE2	2.44	0.53
3:B:28:ASP:O	3:B:32:TYR:CE2	2.62	0.53
2:E:189:GLY:CA	3:B:72:GLN:HB2	2.27	0.53
3:B:8:PHE:HD2	3:B:248:ARG:HD2	1.74	0.53
5:a:134:ARG:HH21	5:a:134:ARG:HB2	1.73	0.53
9:i:11:DC:H2''	9:i:12:DA:C8	2.44	0.53
1:A:666:VAL:O	1:A:670:GLU:HG2	2.09	0.53
2:E:498:ILE:HG21	4:C:226:ILE:HD13	1.90	0.53
3:B:150:HIS:O	3:B:192:GLY:HA3	2.09	0.53
8:d:33:ARG:CB	10:j:50:DT:H5'	2.39	0.53
4:D:293:LEU:HD12	4:D:297:LEU:HB3	1.91	0.53
7:g:35:ARG:NH2	9:i:39:DT:OP2	2.33	0.53
4:D:236:TRP:CZ3	2:F:372:TYR:HD1	2.20	0.52
3:B:307:VAL:HG21	3:B:329:LEU:HD11	1.90	0.52
4:C:342:ILE:O	4:C:345:THR:OG1	2.20	0.52
4:D:244:LYS:HB3	4:D:387:TYR:HB3	1.90	0.52
9:i:-50:DA:H1'	9:i:-49:DC:H5'	1.92	0.52
1:A:1280:ALA:O	1:A:1284:ILE:HG13	2.10	0.52
2:F:263:CYS:O	2:F:267:ASN:N	2.43	0.52
1:A:1287:ARG:HD2	1:A:1323:THR:HG22	1.90	0.52
2:E:126:GLU:O	2:E:126:GLU:HG3	2.08	0.52
2:E:384:ARG:HA	2:E:387:PHE:CB	2.38	0.52
9:i:-47:DA:N6	10:j:46:DT:O4	2.43	0.52
1:A:917:ARG:CZ	1:A:1186:LEU:HD22	2.40	0.52
2:E:317:ALA:O	2:E:320:LYS:HG3	2.10	0.52
4:D:312:LYS:O	4:D:315:LYS:HG3	2.09	0.52
9:i:-27:DC:H2''	9:i:-26:DT:H71	1.91	0.52
3:B:50:SER:O	3:B:54:ASN:ND2	2.40	0.52
3:B:274:ASP:OD1	3:B:274:ASP:N	2.34	0.52
7:g:102:ILE:HG23	8:h:61:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:-6:DG:H2''	9:i:-5:DC:C5	2.45	0.52
2:E:470:SER:HB2	2:E:471:PRO:CD	2.40	0.52
3:B:167:VAL:HG22	3:B:197:PHE:HE2	1.73	0.52
2:F:562:GLN:O	2:F:566:LEU:HG	2.09	0.52
9:i:53:DT:H1'	9:i:54:DA:H5'	1.91	0.52
1:A:875:ARG:O	1:A:879:ILE:HG12	2.10	0.51
3:B:377:PHE:O	3:B:381:GLU:HG2	2.10	0.51
4:D:236:TRP:CD1	4:D:299:TYR:HH	2.28	0.51
3:B:150:HIS:HB3	3:B:166:ILE:HD12	1.91	0.51
4:C:222:LEU:HD21	4:C:363:LEU:HD11	1.92	0.51
1:A:782:TRP:CE2	3:B:226:VAL:HG21	2.46	0.51
1:A:1300:MET:O	1:A:1317:ILE:HB	2.10	0.51
10:j:-21:DC:C2	10:j:-20:DA:N7	2.79	0.51
10:j:-14:DC:H2''	10:j:-13:DA:C8	2.45	0.51
1:A:794:GLY:HA2	2:E:460:LEU:HD13	1.92	0.51
3:B:114:ASP:C	3:B:116:LEU:N	2.54	0.51
9:i:1:DT:H1'	9:i:2:DC:H5'	1.93	0.51
3:B:78:HIS:ND1	3:B:82:TYR:CD1	2.77	0.51
10:j:54:DA:H1'	10:j:55:DT:H5'	1.91	0.51
2:E:449:LEU:HD11	2:E:457:PHE:CE1	2.46	0.51
3:B:294:CYS:O	3:B:298:VAL:HG23	2.11	0.51
3:B:338:LEU:HD21	3:B:353:LEU:HD13	1.93	0.51
5:e:134:ARG:NE	5:e:134:ARG:HA	2.26	0.51
9:i:59:DC:H2''	9:i:60:DA:N7	2.25	0.51
2:E:308:PHE:O	2:E:312:ILE:HG12	2.11	0.51
2:E:169:THR:HG22	3:B:53:MET:CE	2.41	0.50
3:B:26:ASP:HB3	3:B:29:VAL:HG13	1.93	0.50
9:i:-48:DC:H1'	9:i:-47:DA:C8	2.46	0.50
9:i:54:DA:H1'	9:i:55:DT:H5'	1.92	0.50
10:j:46:DT:H2''	10:j:47:DT:H72	1.93	0.50
1:A:874:GLU:O	1:A:878:GLU:HG3	2.11	0.50
1:A:1140:ALA:HB1	1:A:1144:ILE:HB	1.92	0.50
2:E:504:LEU:HB3	2:E:538:LYS:HG3	1.92	0.50
2:E:558:SER:O	2:E:562:GLN:HG3	2.10	0.50
3:B:281:LEU:HB2	3:B:313:TYR:CD2	2.46	0.50
4:D:236:TRP:CZ3	2:F:372:TYR:CA	2.94	0.50
5:e:119:ILE:O	6:f:47:SER:OG	2.27	0.50
1:A:864:LYS:HG2	1:A:880:ILE:HD13	1.94	0.50
1:A:1184:LEU:HB2	1:A:1186:LEU:HG	1.93	0.50
9:i:51:DA:H2''	9:i:52:DG:H5''	1.93	0.50
2:F:559:LYS:O	2:F:563:LYS:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:-8:DC:H2''	10:j:-7:DA:C8	2.47	0.50
5:e:134:ARG:HA	5:e:134:ARG:HE	1.76	0.50
3:B:279:ASP:OD2	3:B:314:THR:HG22	2.12	0.50
2:E:111:THR:HG22	2:E:113:LEU:H	1.77	0.49
2:F:355:ASN:HA	2:F:358:LYS:HZ3	1.76	0.49
1:A:842:THR:HG23	1:A:845:GLU:H	1.77	0.49
1:A:951:GLU:HG2	2:E:427:SER:HA	1.93	0.49
3:B:246:THR:O	3:B:250:VAL:HG23	2.12	0.49
4:D:236:TRP:CH2	2:F:366:THR:HA	2.47	0.49
2:F:302:HIS:HB3	2:F:306:CYS:HB2	1.94	0.49
2:E:326:PHE:CD1	2:E:341:PHE:HB2	2.46	0.49
2:E:385:GLN:OE1	2:E:385:GLN:HA	2.12	0.49
2:E:510:GLN:HG3	4:D:354:LEU:HD22	1.94	0.49
9:i:-60:DT:H2''	9:i:-59:DG:C8	2.48	0.49
9:i:28:DC:H1'	9:i:29:DA:H5'	1.93	0.49
10:j:21:DG:H1'	10:j:22:DA:H5'	1.95	0.49
2:E:385:GLN:CD	2:E:385:GLN:N	2.71	0.49
2:E:521:GLN:HB2	2:E:539:ILE:HD11	1.93	0.49
2:E:560:MET:HG2	2:F:557:LYS:HE3	1.93	0.49
7:g:16:THR:HA	10:j:-43:DG:H5''	1.94	0.49
10:j:29:DA:H2''	10:j:30:DG:H8	1.78	0.49
1:A:1018:ILE:HD12	1:A:1022:PHE:HE2	1.77	0.49
2:F:259:ASN:ND2	2:F:274:CYS:SG	2.86	0.49
1:A:1139:PHE:CE1	1:A:1287:ARG:HG3	2.47	0.49
2:E:362:PRO:HG3	2:E:499:ASN:HB2	1.94	0.49
1:A:1203:ALA:O	1:A:1207:VAL:HG23	2.12	0.49
1:A:1294:MET:HE1	1:A:1300:MET:HE3	1.94	0.49
3:B:40:MET:SD	3:B:313:TYR:HE1	2.36	0.49
4:D:254:VAL:HA	4:D:257:VAL:HG12	1.94	0.49
9:i:-48:DC:H4'	9:i:-47:DA:H5'	1.95	0.49
2:E:571:GLU:HA	2:E:574:ILE:HG22	1.95	0.49
10:j:-48:DC:H1'	10:j:-47:DA:C5	2.48	0.48
10:j:59:DC:H2''	10:j:60:DA:C8	2.48	0.48
1:A:862:ILE:HG13	1:A:863:TYR:N	2.28	0.48
1:A:1202:ASP:OD2	1:A:1205:LYS:NZ	2.39	0.48
2:E:372:TYR:CZ	2:E:374:ASP:HB3	2.48	0.48
9:i:-45:DA:H2''	9:i:-44:DA:C8	2.48	0.48
1:A:981:ASP:OD2	1:A:984:ILE:HG13	2.14	0.48
3:B:155:SER:HB3	4:C:393:GLN:HE22	1.79	0.48
3:B:279:ASP:CG	3:B:314:THR:HG22	2.38	0.48
2:E:437:ILE:HG12	2:E:448:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:37:LYS:HE3	4:G:18:HIS:HD2	1.53	0.48
1:A:1063:MET:HE1	1:A:1074:TYR:CD2	2.48	0.48
4:D:229:LYS:HD3	2:F:360:THR:HG21	1.96	0.48
6:f:31:LYS:HE2	6:f:35:ARG:HH21	1.78	0.48
1:A:675:TYR:CE2	1:A:713:ASN:HB2	2.49	0.48
4:D:236:TRP:CZ2	2:F:372:TYR:HD2	2.25	0.48
4:D:288:TYR:OH	2:F:339:LEU:HB3	2.14	0.48
2:F:316:MET:N	2:F:316:MET:SD	2.85	0.48
8:d:33:ARG:HB3	10:j:50:DT:C5'	2.44	0.48
4:C:393:GLN:O	4:C:397:VAL:HG23	2.13	0.48
3:B:11:ILE:HD13	3:B:11:ILE:H	1.78	0.48
2:F:327:ILE:HD11	2:F:338:LYS:HD2	1.96	0.48
1:A:872:ASP:O	1:A:874:GLU:N	2.47	0.48
3:B:82:TYR:C	3:B:82:TYR:CD2	2.85	0.48
10:j:50:DT:C2	10:j:51:DA:N7	2.82	0.48
1:A:1137:ASN:HD22	1:A:1283:GLN:NE2	2.13	0.47
2:E:180:ASN:ND2	2:E:180:ASN:N	2.58	0.47
3:B:28:ASP:CA	3:B:31:ASN:HD21	2.17	0.47
4:D:222:LEU:HG	4:D:339:PRO:HG3	1.95	0.47
1:A:1168:VAL:HG21	1:A:1232:TYR:CE1	2.48	0.47
8:h:31:ARG:HG2	8:h:31:ARG:HH11	1.79	0.47
10:j:-26:DT:H2''	10:j:-25:DC:C6	2.50	0.47
10:j:-19:DA:H2''	10:j:-18:DA:C8	2.49	0.47
1:A:937:GLN:O	1:A:941:LYS:HE2	2.14	0.47
1:A:1021:PHE:HE1	1:A:1305:PHE:HB2	1.79	0.47
3:B:281:LEU:HB2	3:B:313:TYR:CE2	2.49	0.47
1:A:978:ASP:OD1	1:A:1311:HIS:ND1	2.47	0.47
1:A:1131:GLN:HG3	1:A:1132:ASN:OD1	2.15	0.47
1:A:1261:LYS:HA	1:A:1261:LYS:HD3	1.71	0.47
9:i:-46:DA:H2''	9:i:-45:DA:H8	1.78	0.47
10:j:-58:DC:H2''	10:j:-57:DA:N7	2.30	0.47
10:j:6:DC:H2''	10:j:7:DT:H71	1.97	0.47
1:A:1189:SER:O	1:A:1193:GLU:N	2.46	0.47
3:B:296:ASN:HB2	3:B:328:LEU:HD21	1.97	0.47
5:a:82:LEU:HD23	5:a:82:LEU:HA	1.74	0.47
9:i:-47:DA:H1'	9:i:-46:DA:C8	2.50	0.47
9:i:36:DA:H2''	9:i:37:DA:C8	2.50	0.47
10:j:62:DG:H1'	10:j:63:DT:H5'	1.96	0.47
1:A:901:LYS:NZ	2:E:105:ASP:HB3	2.30	0.47
3:B:30:GLY:HA2	3:B:42:PRO:HB2	1.95	0.47
3:B:31:ASN:ND2	3:B:31:ASN:N	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:34:TYR:CE1	3:B:113:PHE:HE1	2.33	0.47
3:B:285:ASN:ND2	3:B:285:ASN:O	2.48	0.47
4:C:245:ILE:HG12	4:C:390:THR:HG23	1.95	0.47
4:D:321:VAL:HG21	4:D:324:ARG:HD2	1.96	0.47
10:j:-72:DT:H2''	10:j:-71:DC:C6	2.50	0.47
10:j:-48:DC:H1'	10:j:-47:DA:C4	2.49	0.47
1:A:696:ILE:O	2:E:474:VAL:HG11	2.14	0.47
1:A:904:GLU:CD	2:E:116:ASN:CB	2.88	0.47
3:B:332:VAL:HG12	3:B:334:LEU:HD12	1.96	0.47
1:A:1343:LEU:HG	1:A:1344:PRO:HD2	1.97	0.47
2:E:556:TYR:HD2	2:F:557:LYS:HE2	1.79	0.47
1:A:1161:ILE:HG22	1:A:1204:TYR:HD2	1.80	0.47
3:B:149:LEU:HD22	3:B:161:CYS:HA	1.97	0.47
10:j:49:DG:H2''	10:j:50:DT:H71	1.97	0.47
4:D:232:LEU:HD13	2:F:353:LEU:HD22	1.97	0.46
8:h:34:LYS:HD3	8:h:34:LYS:N	2.31	0.46
2:E:517:ASN:HB3	2:E:519:ASN:N	2.21	0.46
4:C:333:ARG:O	4:C:337:VAL:HG23	2.15	0.46
7:g:50:TYR:OH	8:h:95:GLN:NE2	2.48	0.46
8:h:106:LEU:HD12	8:h:106:LEU:HA	1.77	0.46
1:A:867:ILE:O	1:A:871:TYR:HB2	2.14	0.46
1:A:922:LYS:NZ	2:E:129:TRP:HE1	2.06	0.46
1:A:979:PHE:HZ	1:A:1152:THR:HG22	1.81	0.46
1:A:1034:TYR:O	1:A:1038:GLN:HG3	2.16	0.46
2:E:351:PHE:CD1	4:C:333:ARG:HD3	2.51	0.46
2:E:417:CYS:HA	2:E:446:PRO:O	2.14	0.46
7:c:91:GLU:CD	7:c:91:GLU:H	2.23	0.46
8:d:33:ARG:HD3	8:d:33:ARG:C	2.39	0.46
4:D:252:VAL:HG13	4:D:256:MET:HE2	1.98	0.46
8:d:33:ARG:CB	10:j:50:DT:C5'	2.94	0.46
2:E:576:LYS:O	2:E:580:ASN:ND2	2.48	0.46
2:F:287:LEU:HD12	2:F:288:ASP:H	1.81	0.46
2:E:398:LEU:HD12	2:E:457:PHE:CE2	2.51	0.46
2:E:423:THR:O	2:E:423:THR:OG1	2.33	0.46
3:B:28:ASP:HB3	3:B:32:TYR:OH	2.15	0.46
2:E:383:ASP:HA	2:E:386:LEU:HB2	1.97	0.46
10:j:12:DA:H1'	10:j:13:DT:H5''	1.98	0.46
10:j:-70:DA:H1'	10:j:-69:DA:H5'	1.98	0.46
4:D:348:ASP:CG	4:D:351:SER:HG	2.20	0.46
9:i:18:DT:H1'	9:i:19:DT:H5'	1.98	0.46
10:j:-69:DA:H2''	10:j:-68:DT:H5''	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:-44:DA:H2''	10:j:-43:DG:H8	1.81	0.46
1:A:799:ARG:HD2	1:A:799:ARG:HA	1.53	0.46
3:B:240:ASP:OD1	3:B:240:ASP:N	2.48	0.46
2:F:353:LEU:HB2	2:F:372:TYR:OH	2.15	0.46
9:i:-71:DC:H2''	9:i:-70:DA:C8	2.51	0.46
10:j:-24:DC:H2''	10:j:-23:DA:C8	2.51	0.46
1:A:1252:HIS:O	1:A:1255:THR:HB	2.16	0.45
10:j:-64:DC:C2	10:j:-63:DA:N7	2.84	0.45
10:j:-28:DG:H2''	10:j:-27:DC:C5	2.51	0.45
3:B:191:ASP:OD1	3:B:191:ASP:N	2.34	0.45
1:A:767:CYS:SG	1:A:770:ARG:HD2	2.56	0.45
2:E:189:GLY:CA	3:B:72:GLN:OE1	2.65	0.45
3:B:186:ASP:OD1	3:B:187:VAL:N	2.50	0.45
9:i:46:DT:C2'	9:i:47:DT:H71	2.46	0.45
9:i:51:DA:C6	9:i:52:DG:C6	3.05	0.45
1:A:1324:LEU:HD12	1:A:1325:LYS:H	1.81	0.45
2:E:384:ARG:CG	2:E:387:PHE:HB3	2.44	0.45
2:E:578:VAL:HG11	2:F:575:ASP:CG	2.40	0.45
3:B:224:ILE:HG12	3:B:224:ILE:O	2.16	0.45
10:j:50:DT:H2''	10:j:51:DA:H8	1.82	0.45
2:E:260:GLU:HG2	2:E:262:PHE:H	1.80	0.45
7:c:78:ILE:O	8:d:55:SER:OG	2.29	0.45
7:c:88:ARG:HA	7:c:88:ARG:HD3	1.75	0.45
3:B:41:LYS:HA	3:B:42:PRO:HD3	1.74	0.45
4:C:285:LEU:HD23	4:C:285:LEU:HA	1.80	0.45
4:D:299:TYR:O	4:D:303:ARG:HG3	2.16	0.45
10:j:-49:DC:H2''	10:j:-48:DC:C6	2.51	0.45
1:A:941:LYS:HG2	1:A:942:LEU:HD23	1.99	0.45
1:A:1289:GLN:O	1:A:1292:SER:OG	2.35	0.45
2:E:472:THR:O	2:E:473:LYS:HG3	2.17	0.45
9:i:-21:DC:H2''	9:i:-20:DA:H8	1.82	0.45
2:E:189:GLY:N	3:B:72:GLN:OE1	2.50	0.45
2:E:470:SER:HB2	2:E:471:PRO:HD2	1.98	0.45
1:A:972:LYS:HE3	1:A:972:LYS:HB2	1.79	0.45
1:A:1129:ILE:HG12	1:A:1279:SER:HB2	1.99	0.45
4:D:293:LEU:HA	4:D:297:LEU:HB2	2.00	0.44
10:j:13:DT:H5'	10:j:13:DT:H6	1.83	0.44
10:j:38:DA:C8	10:j:39:DT:H72	2.52	0.44
1:A:770:ARG:CG	1:A:774:CYS:HB2	2.47	0.44
10:j:-47:DA:C5	10:j:-46:DA:C5	3.06	0.44
10:j:70:DT:H2''	10:j:71:DG:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:THR:HG21	1:A:866:VAL:HG21	1.98	0.44
2:E:187:TRP:HB3	3:B:72:GLN:HB3	1.98	0.44
2:E:450:ASP:OD1	2:E:450:ASP:N	2.50	0.44
9:i:-24:DC:H2''	9:i:-23:DA:C8	2.52	0.44
10:j:-45:DA:H2''	10:j:-44:DA:H8	1.83	0.44
1:A:1175:ARG:NH2	1:A:1230:GLN:O	2.46	0.44
1:A:1142:THR:O	1:A:1146:ILE:HG12	2.18	0.44
1:A:1171:GLU:O	1:A:1174:THR:HG22	2.17	0.44
1:A:1340:SER:HB3	1:A:1347:THR:HG23	1.98	0.44
4:C:348:ASP:OD2	4:C:350:GLN:HG3	2.18	0.44
9:i:-59:DG:H2''	9:i:-58:DC:C6	2.52	0.44
9:i:-48:DC:H1'	9:i:-47:DA:C4	2.53	0.44
2:E:381:LEU:HB3	2:E:384:ARG:CB	2.25	0.44
2:E:554:LYS:HE3	2:E:554:LYS:HB3	1.65	0.44
2:F:556:TYR:OH	2:F:560:MET:SD	2.68	0.44
1:A:872:ASP:O	1:A:875:ARG:N	2.50	0.44
1:A:931:LEU:HD12	1:A:931:LEU:HA	1.83	0.44
1:A:965:HIS:CE1	1:A:967:LEU:HB2	2.53	0.44
2:E:180:ASN:ND2	2:E:180:ASN:H	2.16	0.44
2:E:452:VAL:O	2:E:454:ARG:N	2.51	0.44
3:B:14:LYS:H	3:B:14:LYS:HD2	1.83	0.44
3:B:274:ASP:O	3:B:282:GLY:HA3	2.18	0.44
10:j:-61:DC:H5'	10:j:-61:DC:C6	2.52	0.44
10:j:-45:DA:H2''	10:j:-44:DA:C8	2.53	0.44
10:j:50:DT:H2''	10:j:51:DA:C8	2.52	0.44
4:C:395:GLU:OE1	4:C:395:GLU:N	2.50	0.44
4:D:254:VAL:HG21	4:D:289:PHE:CZ	2.53	0.44
8:h:46:LYS:HA	8:h:46:LYS:HD3	1.72	0.44
9:i:51:DA:C4	9:i:52:DG:C5	3.06	0.44
10:j:45:DT:H2''	10:j:46:DT:H72	1.99	0.43
1:A:942:LEU:HD13	2:E:428:TRP:CG	2.53	0.43
2:E:176:THR:HG22	3:B:63:ILE:HG12	2.01	0.43
2:F:576:LYS:HD3	2:F:576:LYS:HA	1.85	0.43
5:a:90:MET:HA	5:a:90:MET:CE	2.48	0.43
9:i:-46:DA:H2''	9:i:-45:DA:C8	2.53	0.43
1:A:945:THR:O	1:A:949:ILE:HG12	2.18	0.43
4:C:382:SER:O	4:C:383:ASP:HB2	2.17	0.43
9:i:41:DC:H5'	9:i:41:DC:C6	2.53	0.43
9:i:66:DA:H2'	9:i:67:DT:H71	2.00	0.43
10:j:-20:DA:H2''	10:j:-19:DA:H8	1.83	0.43
1:A:698:ASP:OD2	1:A:699:LEU:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:MET:HE3	1:A:773:MET:HB2	1.87	0.43
1:A:871:TYR:HE2	1:A:894:VAL:HG23	1.83	0.43
1:A:1020:LEU:HG	1:A:1273:ARG:HG2	2.00	0.43
2:E:397:LYS:HA	2:E:397:LYS:HD3	1.73	0.43
3:B:86:LEU:HD21	3:B:116:LEU:HG	2.00	0.43
4:C:355:LEU:O	4:C:359:THR:HG23	2.19	0.43
9:i:-46:DA:C6	9:i:-45:DA:C6	3.05	0.43
10:j:-40:DT:H2"	10:j:-39:DA:N7	2.33	0.43
1:A:871:TYR:CE2	1:A:894:VAL:HG23	2.53	0.43
2:E:372:TYR:HD1	4:C:241:LYS:HE3	1.84	0.43
4:C:257:VAL:HG22	4:C:373:TYR:CZ	2.54	0.43
1:A:663:ASN:HA	2:F:547:ILE:HG12	1.99	0.43
1:A:866:VAL:O	1:A:870:VAL:HG23	2.18	0.43
4:C:345:THR:HB	4:C:347:MET:H	1.84	0.43
9:i:-48:DC:H2"	9:i:-47:DA:C8	2.53	0.43
10:j:23:DT:H2"	10:j:24:DG:C8	2.53	0.43
1:A:928:LEU:HD21	3:B:356:ARG:HB2	2.01	0.43
2:E:381:LEU:N	2:E:381:LEU:HD23	2.32	0.43
3:B:150:HIS:O	3:B:164:ASN:ND2	2.48	0.43
3:B:197:PHE:CD1	3:B:203:VAL:HG21	2.54	0.43
4:D:285:LEU:HD21	4:D:335:ILE:HD11	1.99	0.43
5:e:37:LYS:HD2	5:e:38:PRO:HD3	1.71	0.43
5:e:90:MET:HA	5:e:90:MET:CE	2.48	0.43
9:i:-55:DA:H1'	9:i:-54:DT:H5'	1.99	0.43
1:A:1037:LYS:HA	1:A:1037:LYS:HD3	1.69	0.43
1:A:1315:GLN:HE22	1:A:1325:LYS:HD3	1.83	0.43
8:d:65:PHE:HE1	8:d:69:ILE:HD11	1.62	0.43
10:j:50:DT:C2	10:j:51:DA:C5	3.07	0.43
1:A:770:ARG:HH12	3:B:154:LYS:NZ	2.17	0.43
1:A:930:HIS:HD2	2:E:393:GLN:NE2	2.17	0.43
3:B:112:VAL:O	3:B:112:VAL:HG13	2.18	0.43
4:D:236:TRP:CZ2	2:F:372:TYR:CA	3.00	0.43
10:j:-28:DG:H2"	10:j:-27:DC:C6	2.54	0.43
1:A:984:ILE:O	1:A:988:ILE:HG13	2.18	0.43
2:E:388:ASN:HD22	2:E:388:ASN:HA	1.37	0.43
4:D:240:THR:HG21	2:F:371:GLN:HA	2.01	0.43
4:D:309:LEU:HD13	4:D:309:LEU:HA	1.91	0.43
4:D:395:GLU:HA	4:D:398:ALA:HB3	2.01	0.43
7:c:58:LEU:O	7:c:62:ILE:HG22	2.19	0.43
9:i:53:DT:C2	9:i:54:DA:C8	3.07	0.43
1:A:955:ILE:O	1:A:959:GLN:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:LEU:O	1:A:1232:TYR:HB2	2.19	0.42
1:A:1299:ASN:ND2	1:A:1299:ASN:H	2.17	0.42
3:B:145:TYR:OH	3:B:326:THR:OG1	2.19	0.42
5:a:72:ARG:HH22	9:i:-23:DA:P	2.42	0.42
9:i:39:DT:H2''	9:i:40:DA:H8	1.83	0.42
1:A:813:GLU:CD	2:E:110:VAL:CG1	2.85	0.42
1:A:1009:ARG:HH12	1:A:1071:ARG:HB3	1.84	0.42
1:A:1300:MET:HG2	1:A:1317:ILE:HG13	2.01	0.42
4:D:220:ILE:HB	4:D:356:ILE:HD11	2.01	0.42
9:i:38:DA:C2'	9:i:39:DT:H71	2.49	0.42
9:i:50:DT:C2	9:i:51:DA:C5	3.07	0.42
3:B:19:ARG:HB2	3:B:140:ASP:HB2	2.01	0.42
9:i:-22:DT:H2''	9:i:-21:DC:H5''	2.01	0.42
10:j:13:DT:H2''	10:j:14:DG:C8	2.55	0.42
1:A:770:ARG:HG2	1:A:774:CYS:HB2	2.01	0.42
1:A:1076:LYS:HA	1:A:1079:ARG:HH12	1.84	0.42
1:A:1151:TRP:HE3	1:A:1249:LEU:HD11	1.85	0.42
3:B:83:ILE:HA	3:B:83:ILE:HD13	1.49	0.42
4:D:293:LEU:HD21	4:D:326:TYR:CE2	2.54	0.42
4:D:338:LEU:O	4:D:342:ILE:HG22	2.19	0.42
2:F:367:GLY:HA3	2:F:371:GLN:HE21	1.84	0.42
10:j:-33:DA:C2	10:j:-32:DA:C5	3.07	0.42
10:j:56:DC:H2''	10:j:57:DT:C6	2.55	0.42
3:B:50:SER:HG	3:B:343:TYR:HE2	1.66	0.42
2:F:564:ARG:O	2:F:568:GLN:HG2	2.19	0.42
6:b:24:ASP:HB3	6:b:25:ASN:H	1.47	0.42
8:h:65:PHE:CE2	8:h:69:ILE:HD12	2.55	0.42
9:i:-5:DC:H2''	9:i:-4:DT:C7	2.50	0.42
1:A:1078:LYS:HE2	1:A:1078:LYS:HB2	1.92	0.42
2:E:187:TRP:HE3	2:E:187:TRP:H	1.60	0.42
2:E:440:CYS:HB2	2:E:466:CYS:SG	2.60	0.42
3:B:88:ARG:CG	3:B:88:ARG:NH1	2.72	0.42
4:C:243:LYS:O	4:C:390:THR:OG1	2.37	0.42
4:D:224:ILE:HB	4:D:229:LYS:HE3	2.01	0.42
2:F:552:PHE:HA	2:F:555:ILE:HG22	2.01	0.42
6:f:35:ARG:O	6:f:39:ARG:HG2	2.20	0.42
9:i:-54:DT:H1'	9:i:-53:DA:H5'	2.01	0.42
9:i:44:DT:H1'	9:i:45:DT:H5'	2.01	0.42
1:A:826:ARG:O	1:A:829:GLN:HG2	2.20	0.42
2:E:177:GLU:OE1	3:B:62:GLU:OE2	2.38	0.42
3:B:29:VAL:HG12	3:B:122:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:40:SER:OG	8:d:89:ILE:HG13	2.20	0.42
9:i:-50:DA:N6	10:j:49:DG:C6	2.88	0.42
9:i:-18:DA:H2''	9:i:-17:DA:C8	2.55	0.42
1:A:798:HIS:HD2	1:A:800:LYS:NZ	2.17	0.42
1:A:1136:PHE:CD1	1:A:1273:ARG:HD2	2.55	0.42
4:D:270:GLU:HB3	2:F:556:TYR:HE1	1.85	0.42
10:j:-36:DT:H2''	10:j:-35:DG:N7	2.34	0.42
1:A:690:ASN:HA	1:A:693:SER:OG	2.20	0.42
1:A:862:ILE:O	1:A:866:VAL:HG13	2.19	0.42
1:A:975:LEU:HB2	1:A:1314:ILE:HB	2.02	0.42
1:A:996:ILE:HG22	1:A:1007:LYS:HG3	2.01	0.42
4:D:253:THR:OG1	4:D:254:VAL:N	2.52	0.42
4:D:297:LEU:HD12	4:D:297:LEU:HA	1.86	0.42
6:f:30:THR:HB	6:f:32:PRO:HD2	2.00	0.42
7:g:67:GLY:HA3	8:h:49:HIS:CD2	2.55	0.42
9:i:50:DT:H1'	9:i:51:DA:H5'	2.01	0.42
10:j:-20:DA:C6	10:j:-19:DA:N6	2.88	0.42
1:A:871:TYR:O	1:A:876:GLY:N	2.52	0.42
1:A:1233:ASN:OD1	1:A:1235:LYS:HE2	2.20	0.42
5:e:134:ARG:C	5:e:134:ARG:HD3	2.45	0.42
9:i:-73:DA:C8	9:i:-72:DT:H72	2.55	0.42
9:i:48:DG:H1'	9:i:49:DG:C8	2.55	0.42
10:j:-60:DT:H2''	10:j:-59:DG:C8	2.55	0.42
10:j:-40:DT:H2''	10:j:-39:DA:C8	2.54	0.42
1:A:1003:SER:O	1:A:1007:LYS:N	2.47	0.41
1:A:1014:LEU:O	1:A:1018:ILE:HG12	2.19	0.41
2:E:107:LYS:NZ	2:E:107:LYS:HB2	2.35	0.41
2:E:574:ILE:O	2:E:578:VAL:HG22	2.19	0.41
3:B:141:VAL:HA	3:B:305:MET:O	2.20	0.41
7:g:35:ARG:HH12	9:i:39:DT:P	2.43	0.41
10:j:-35:DG:H2''	10:j:-34:DG:C8	2.54	0.41
1:A:1257:MET:HE2	1:A:1257:MET:HB2	1.88	0.41
2:E:351:PHE:CE1	4:C:333:ARG:HD3	2.54	0.41
4:D:254:VAL:HG12	4:D:323:ILE:HG13	2.02	0.41
8:d:46:LYS:HA	8:d:46:LYS:HD3	1.68	0.41
9:i:-48:DC:H1'	9:i:-47:DA:N9	2.35	0.41
10:j:-32:DA:C6	10:j:-31:DA:N6	2.88	0.41
1:A:918:GLU:OE2	2:E:128:LEU:CD1	2.55	0.41
2:E:113:LEU:HD12	2:E:113:LEU:H	1.82	0.41
9:i:56:DC:H2''	9:i:57:DT:H72	2.02	0.41
10:j:-20:DA:H2''	10:j:-19:DA:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:372:TYR:HB3	4:C:241:LYS:HD2	2.02	0.41
3:B:34:TYR:HD2	3:B:41:LYS:HA	1.86	0.41
3:B:40:MET:SD	3:B:313:TYR:CE1	3.13	0.41
2:F:365:LYS:HA	2:F:365:LYS:HD3	1.77	0.41
9:i:-56:DG:H2''	9:i:-55:DA:C8	2.55	0.41
2:E:409:SER:OG	2:E:410:ASN:N	2.53	0.41
2:E:493:LYS:HA	2:E:493:LYS:HD2	1.73	0.41
3:B:8:PHE:CD2	3:B:248:ARG:HD2	2.54	0.41
2:F:362:PRO:O	2:F:365:LYS:NZ	2.46	0.41
10:j:18:DT:H2'	10:j:19:DT:H71	2.03	0.41
10:j:22:DA:H1'	10:j:23:DT:H5'	2.01	0.41
1:A:684:GLU:O	1:A:688:ILE:HG13	2.21	0.41
1:A:910:ARG:HG3	1:A:911:GLU:N	2.36	0.41
1:A:1028:LYS:O	1:A:1031:GLU:HG2	2.21	0.41
1:A:1078:LYS:HA	1:A:1081:ASN:HD21	1.85	0.41
1:A:1165:ASN:OD1	1:A:1204:TYR:N	2.51	0.41
1:A:1190:GLN:CD	2:E:129:TRP:CH2	2.76	0.41
3:B:251:PHE:CZ	3:B:255:ILE:HG13	2.55	0.41
7:c:100:VAL:HG22	6:f:96:THR:HB	2.02	0.41
8:h:111:VAL:O	8:h:115:THR:OG1	2.34	0.41
3:B:86:LEU:HA	3:B:86:LEU:HD23	1.76	0.41
4:D:236:TRP:CD2	2:F:372:TYR:CD2	2.97	0.41
7:g:68:ASN:OD1	7:g:71:ARG:NH2	2.54	0.41
9:i:47:DT:O4	10:j:-48:DC:N4	2.53	0.41
9:i:55:DT:H2''	9:i:56:DC:C6	2.56	0.41
2:E:442:TYR:CE2	2:E:465:LYS:HB2	2.56	0.41
9:i:-60:DT:H2''	9:i:-59:DG:N7	2.35	0.41
9:i:32:DT:H1'	9:i:33:DT:H5'	2.02	0.41
9:i:50:DT:H5'	9:i:50:DT:C6	2.56	0.41
1:A:664:GLU:O	1:A:667:THR:OG1	2.25	0.41
1:A:808:PHE:O	1:A:811:GLU:HG3	2.21	0.41
1:A:842:THR:O	1:A:846:LYS:HG3	2.21	0.41
1:A:1149:ARG:HA	1:A:1149:ARG:HD2	1.87	0.41
1:A:1223:TRP:HA	1:A:1226:GLU:HG3	2.02	0.41
2:E:305:GLU:HB2	2:E:347:ASN:HD21	1.85	0.41
2:E:402:ASN:N	2:E:403:PRO:HD3	2.36	0.41
3:B:40:MET:HG3	3:B:44:ARG:HH21	1.86	0.41
3:B:259:MET:HE2	3:B:301:PHE:CG	2.56	0.41
4:D:235:ASP:O	4:D:239:VAL:HG12	2.20	0.41
7:c:100:VAL:HG11	6:f:98:TYR:CE2	2.56	0.41
5:e:37:LYS:HD2	5:e:38:PRO:CD	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:58:ALA:O	8:h:62:MET:HG2	2.20	0.41
9:i:-48:DC:C2	9:i:-47:DA:C6	3.09	0.41
10:j:-12:DT:H2''	10:j:-11:DG:C8	2.56	0.41
10:j:-12:DT:H2''	10:j:-11:DG:H8	1.86	0.41
10:j:-10:DT:H2'	10:j:-9:DT:H71	2.01	0.41
1:A:1009:ARG:HG2	1:A:1074:TYR:CZ	2.56	0.41
1:A:1228:LEU:HD13	1:A:1232:TYR:CD2	2.56	0.41
2:E:126:GLU:O	2:E:126:GLU:CG	2.69	0.41
2:E:184:THR:OG1	3:B:73:GLU:CG	2.69	0.41
2:E:450:ASP:OD2	3:B:365:THR:OG1	2.36	0.41
9:i:50:DT:C2	9:i:51:DA:N7	2.89	0.41
10:j:-31:DA:H1'	10:j:-30:DC:H5'	2.03	0.41
10:j:43:DC:H5'	10:j:43:DC:C6	2.56	0.41
10:j:67:DT:H2''	10:j:68:DA:C8	2.55	0.41
2:E:177:GLU:H	2:E:177:GLU:HG2	1.52	0.40
2:E:316:MET:SD	2:E:316:MET:N	2.94	0.40
2:E:466:CYS:C	2:E:468:LEU:H	2.30	0.40
3:B:113:PHE:CE2	3:B:116:LEU:HA	2.57	0.40
4:C:258:LEU:HD23	4:C:258:LEU:HA	1.93	0.40
4:C:341:LEU:O	4:C:344:SER:OG	2.32	0.40
2:F:320:LYS:HA	2:F:323:GLU:HG3	2.03	0.40
6:b:62:LEU:HA	6:b:62:LEU:HD23	1.73	0.40
10:j:-66:DT:H2''	10:j:-65:DC:C6	2.56	0.40
3:B:174:LEU:HD11	3:B:203:VAL:CG2	2.51	0.40
7:c:34:LEU:HD23	7:c:34:LEU:HA	1.92	0.40
7:c:79:ILE:HG12	7:c:82:HIS:CE1	2.56	0.40
5:e:90:MET:O	5:e:94:GLU:HG2	2.21	0.40
9:i:20:DT:C2	9:i:21:DG:C8	3.10	0.40
1:A:959:GLN:OE1	1:A:974:GLN:NE2	2.54	0.40
2:E:184:THR:OG1	3:B:73:GLU:HG2	2.21	0.40
2:E:306:CYS:O	2:E:310:ILE:HG12	2.22	0.40
2:E:375:GLU:OE1	2:E:376:ASN:ND2	2.54	0.40
7:c:63:LEU:HD23	7:c:63:LEU:HA	1.79	0.40
10:j:52:DG:C5	10:j:53:DT:C4	3.10	0.40
1:A:767:CYS:SG	1:A:770:ARG:HB2	2.61	0.40
1:A:823:SER:O	1:A:827:THR:HG23	2.21	0.40
2:E:339:LEU:HB3	4:C:288:TYR:OH	2.20	0.40
3:B:317:ASN:O	3:B:321:THR:OG1	2.28	0.40
9:i:-24:DC:H2''	9:i:-23:DA:H8	1.86	0.40
1:A:1005:PRO:O	1:A:1009:ARG:HG3	2.21	0.40
2:E:336:PHE:HD2	4:C:284:GLY:HA3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:374:ASP:C	2:E:376:ASN:H	2.29	0.40
2:E:387:PHE:O	2:E:390:SER:HB2	2.21	0.40
4:C:338:LEU:O	4:C:342:ILE:HG13	2.21	0.40
4:D:248:LEU:HD21	4:D:326:TYR:CZ	2.56	0.40
4:D:262:GLU:HB2	4:D:282:CYS:SG	2.61	0.40
6:f:64:ASN:O	6:f:93:GLN:NE2	2.52	0.40
9:i:30:DG:N2	10:j:-29:DT:O2	2.55	0.40
9:i:35:DC:H2''	9:i:36:DA:N7	2.37	0.40
10:j:-47:DA:C6	10:j:-46:DA:C6	3.09	0.40
10:j:-27:DC:H1'	10:j:-26:DT:C6	2.56	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	598/1536 (39%)	573 (96%)	24 (4%)	1 (0%)	43	77
2	E	343/684 (50%)	293 (85%)	41 (12%)	9 (3%)	4	25
2	F	152/684 (22%)	150 (99%)	2 (1%)	0	100	100
3	B	383/433 (88%)	362 (94%)	18 (5%)	3 (1%)	16	52
4	C	181/401 (45%)	171 (94%)	9 (5%)	1 (1%)	21	58
4	D	183/401 (46%)	179 (98%)	4 (2%)	0	100	100
4	G	63/401 (16%)	62 (98%)	1 (2%)	0	100	100
5	a	95/136 (70%)	95 (100%)	0	0	100	100
5	e	97/136 (71%)	96 (99%)	1 (1%)	0	100	100
6	b	77/103 (75%)	72 (94%)	5 (6%)	0	100	100
6	f	80/103 (78%)	77 (96%)	3 (4%)	0	100	100
7	c	105/130 (81%)	101 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	g	105/130 (81%)	103 (98%)	2 (2%)	0	100	100
8	d	92/126 (73%)	89 (97%)	3 (3%)	0	100	100
8	h	92/126 (73%)	88 (96%)	4 (4%)	0	100	100
All	All	2646/5530 (48%)	2511 (95%)	121 (5%)	14 (0%)	26	62

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	171	LEU
2	E	174	ASN
2	E	470	SER
3	B	114	ASP
3	B	115	GLY
1	A	873	LYS
2	E	125	ARG
2	E	392	GLY
2	E	517	ASN
4	C	241	LYS
2	E	378	LYS
2	E	471	PRO
2	E	393	GLN
3	B	110	CYS

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	560/1391 (40%)	531 (95%)	29 (5%)	21	43
2	E	332/653 (51%)	285 (86%)	47 (14%)	3	15
2	F	148/653 (23%)	145 (98%)	3 (2%)	48	66
3	B	326/367 (89%)	291 (89%)	35 (11%)	6	22
4	C	172/359 (48%)	156 (91%)	16 (9%)	8	26
4	D	174/359 (48%)	168 (97%)	6 (3%)	32	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	56/359 (16%)	56 (100%)	0	100	100
5	a	85/111 (77%)	77 (91%)	8 (9%)	8	26
5	e	86/111 (78%)	78 (91%)	8 (9%)	8	26
6	b	64/79 (81%)	58 (91%)	6 (9%)	8	26
6	f	67/79 (85%)	64 (96%)	3 (4%)	24	46
7	c	83/100 (83%)	81 (98%)	2 (2%)	43	63
7	g	83/100 (83%)	78 (94%)	5 (6%)	17	39
8	d	80/105 (76%)	74 (92%)	6 (8%)	12	33
8	h	80/105 (76%)	74 (92%)	6 (8%)	12	33
All	All	2396/4931 (49%)	2216 (92%)	180 (8%)	14	33

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	690	ASN
1	A	697	LEU
1	A	707	ASP
1	A	777	VAL
1	A	781	GLU
1	A	783	VAL
1	A	796	ILE
1	A	799	ARG
1	A	802	GLN
1	A	805	GLU
1	A	811	GLU
1	A	813	GLU
1	A	825	LEU
1	A	828	ILE
1	A	893	VAL
1	A	903	GLU
1	A	929	ASP
1	A	951	GLU
1	A	1012	ASP
1	A	1065	LEU
1	A	1152	THR
1	A	1153	THR
1	A	1179	THR
1	A	1228	LEU
1	A	1241	THR

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Mol	Chain	Res	Type
1	A	1278	THR
1	A	1299	ASN
1	A	1316	TYR
1	A	1341	TYR
2	E	105	ASP
2	E	107	LYS
2	E	108	VAL
2	E	110	VAL
2	E	111	THR
2	E	113	LEU
2	E	114	PRO
2	E	115	LEU
2	E	123	ILE
2	E	125	ARG
2	E	126	GLU
2	E	175	MET
2	E	177	GLU
2	E	178	GLU
2	E	179	SER
2	E	180	ASN
2	E	181	ILE
2	E	185	ILE
2	E	187	TRP
2	E	272	PHE
2	E	335	ILE
2	E	371	GLN
2	E	379	ILE
2	E	384	ARG
2	E	386	LEU
2	E	387	PHE
2	E	388	ASN
2	E	402	ASN
2	E	404	ASP
2	E	437	ILE
2	E	443	CYS
2	E	450	ASP
2	E	452	VAL
2	E	454	ARG
2	E	491	VAL
2	E	492	TRP
2	E	497	LEU
2	E	504	LEU

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Mol	Chain	Res	Type
2	E	514	TYR
2	E	522	ILE
2	E	539	ILE
2	E	540	THR
2	E	543	ASP
2	E	545	ASN
2	E	546	SER
2	E	575	ASP
2	E	577	LEU
3	B	2	VAL
3	B	11	ILE
3	B	14	LYS
3	B	21	VAL
3	B	31	ASN
3	B	32	TYR
3	B	38	HIS
3	B	40	MET
3	B	41	LYS
3	B	63	ILE
3	B	67	LYS
3	B	72	GLN
3	B	73	GLU
3	B	83	ILE
3	B	84	ASP
3	B	86	LEU
3	B	87	SER
3	B	88	ARG
3	B	89	VAL
3	B	90	THR
3	B	111	PRO
3	B	112	VAL
3	B	134	LEU
3	B	136	ARG
3	B	150	HIS
3	B	170	ILE
3	B	191	ASP
3	B	244	ASP
3	B	246	THR
3	B	280	ARG
3	B	281	LEU
3	B	308	VAL
3	B	350	ASP

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Mol	Chain	Res	Type
3	B	363	VAL
3	B	383	THR
4	C	222	LEU
4	C	231	VAL
4	C	233	VAL
4	C	235	ASP
4	C	241	LYS
4	C	253	THR
4	C	267	GLN
4	C	285	LEU
4	C	288	TYR
4	C	292	CYS
4	C	293	LEU
4	C	323	ILE
4	C	376	ASP
4	C	390	THR
4	C	393	GLN
4	C	395	GLU
4	D	220	ILE
4	D	288	TYR
4	D	309	LEU
4	D	332	LEU
4	D	342	ILE
4	D	346	THR
2	F	319	LEU
2	F	560	MET
2	F	570	GLN
5	a	80	THR
5	a	86	SER
5	a	87	SER
5	a	89	VAL
5	a	90	MET
5	a	109	LEU
5	a	133	GLU
5	a	134	ARG
6	b	30	THR
6	b	49	LEU
6	b	73	THR
6	b	80	THR
6	b	92	ARG
6	b	96	THR
7	c	76	THR

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Mol	Chain	Res	Type
7	c	118	LYS
8	d	31	ARG
8	d	33	ARG
8	d	34	LYS
8	d	51	ASP
8	d	89	ILE
8	d	112	SER
5	e	80	THR
5	e	86	SER
5	e	87	SER
5	e	89	VAL
5	e	90	MET
5	e	109	LEU
5	e	133	GLU
5	e	134	ARG
6	f	30	THR
6	f	54	THR
6	f	82	THR
7	g	13	LYS
7	g	15	LYS
7	g	16	THR
7	g	62	ILE
7	g	76	THR
8	h	33	ARG
8	h	34	LYS
8	h	87	SER
8	h	98	VAL
8	h	106	LEU
8	h	115	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	779	ASN
1	A	798	HIS
1	A	829	GLN
1	A	884	HIS
1	A	930	HIS
1	A	965	HIS
1	A	1081	ASN
1	A	1127	GLN
1	A	1137	ASN

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Mol	Chain	Res	Type
1	A	1299	ASN
2	E	130	ASN
2	E	314	ASN
2	E	325	ASN
2	E	347	ASN
2	E	350	GLN
2	E	352	GLN
2	E	355	ASN
2	E	376	ASN
2	E	388	ASN
2	E	516	ASN
2	E	521	GLN
2	E	541	GLN
2	E	580	ASN
3	B	31	ASN
3	B	76	GLN
3	B	150	HIS
3	B	188	HIS
3	B	270	GLN
4	C	263	HIS
4	C	305	GLN
4	C	380	ASN
4	C	389	ASN
4	C	393	GLN
4	D	305	GLN
4	D	317	GLN
4	D	375	ASN
4	D	380	ASN
2	F	259	ASN
2	F	331	ASN
2	F	355	ASN
2	F	568	GLN
2	F	570	GLN
5	a	125	GLN
6	b	27	GLN
6	b	93	GLN
7	c	38	ASN
8	d	49	HIS
8	d	109	HIS
5	e	125	GLN
8	h	49	HIS
8	h	95	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	G	18	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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.

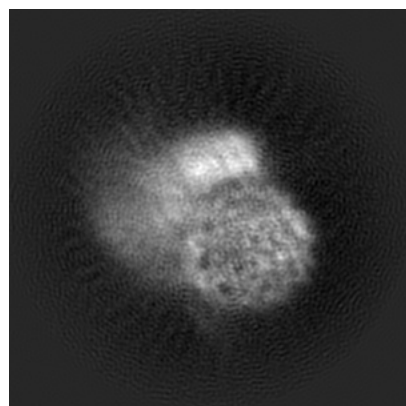
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37367. These allow visual inspection of the internal detail of the map and identification of artifacts.

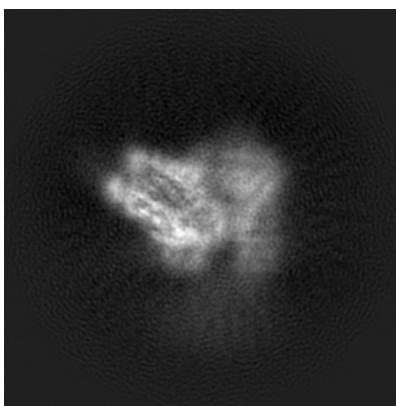
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

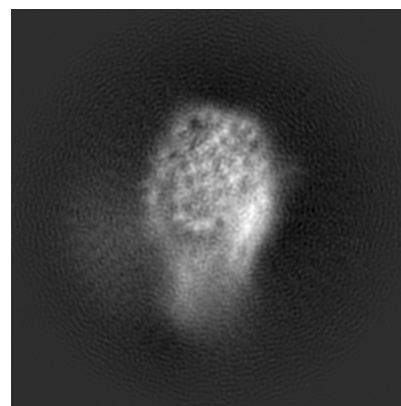
6.1.1 Primary map



X

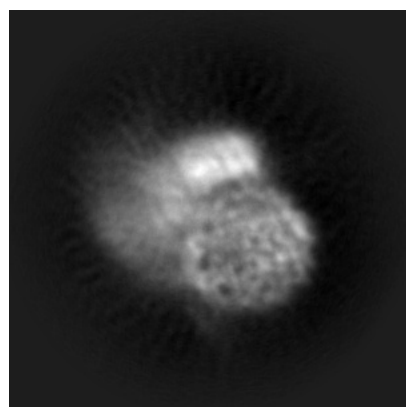


Y

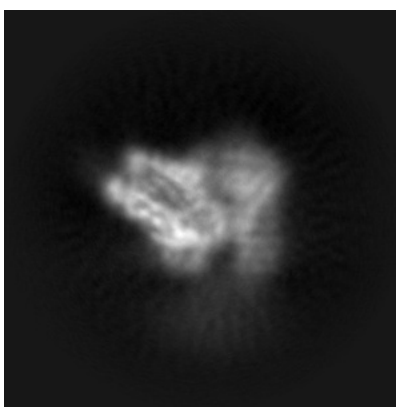


Z

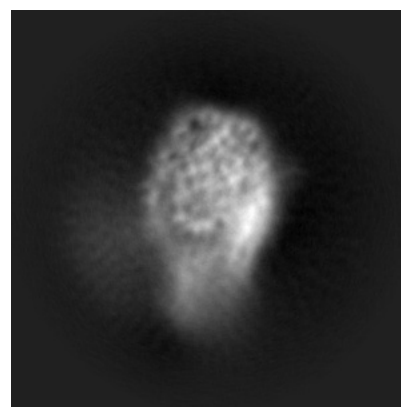
6.1.2 Raw map



X



Y

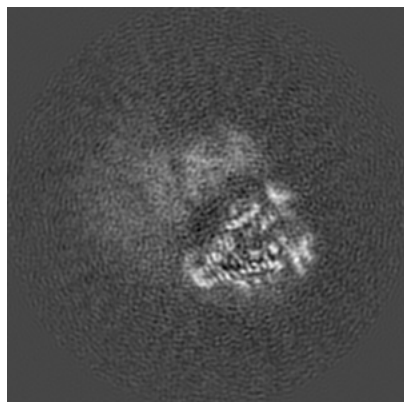


Z

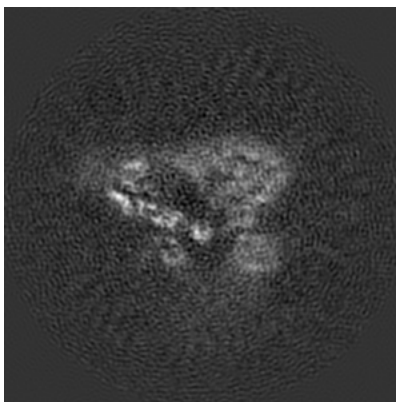
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

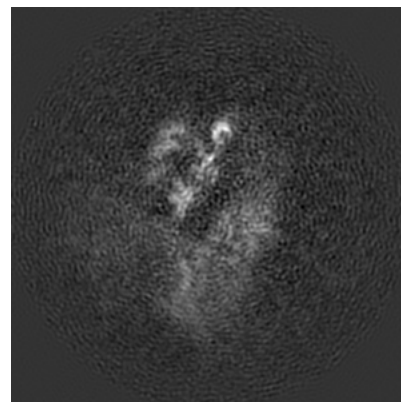
6.2.1 Primary map



X Index: 140

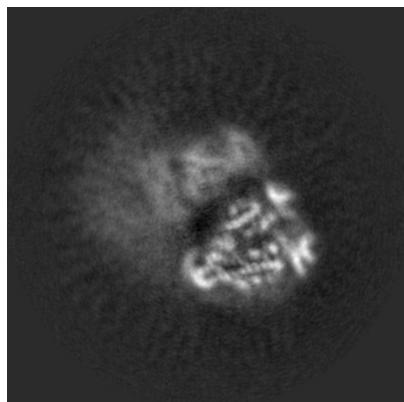


Y Index: 140

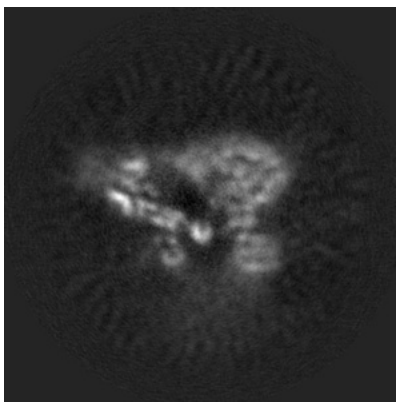


Z Index: 140

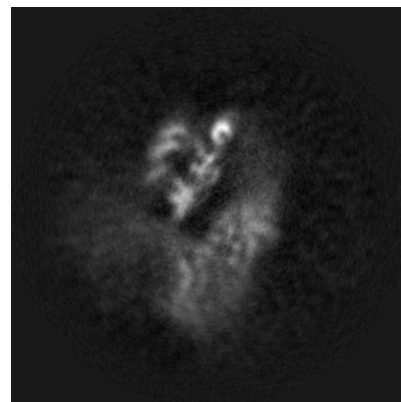
6.2.2 Raw map



X Index: 140



Y Index: 140

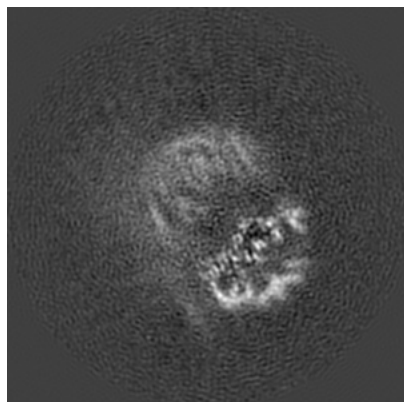


Z Index: 140

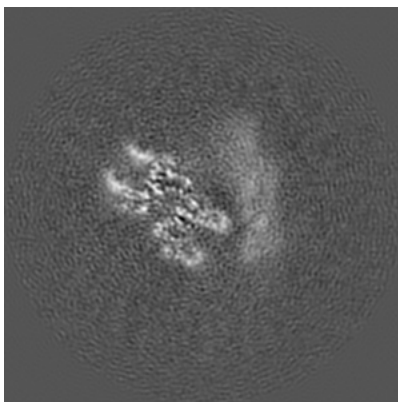
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

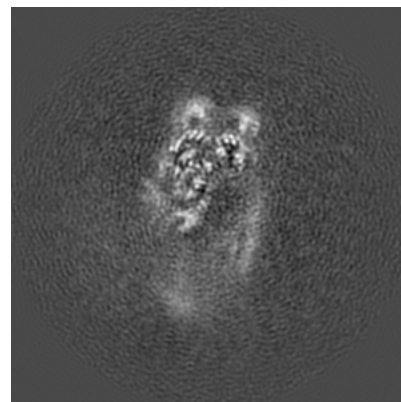
6.3.1 Primary map



X Index: 154

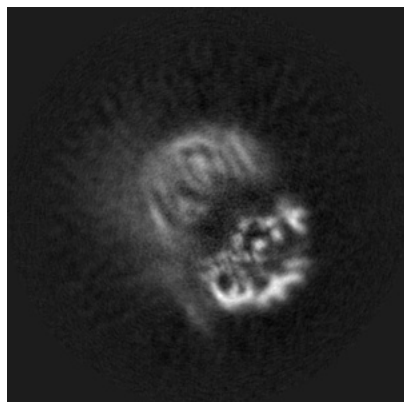


Y Index: 168

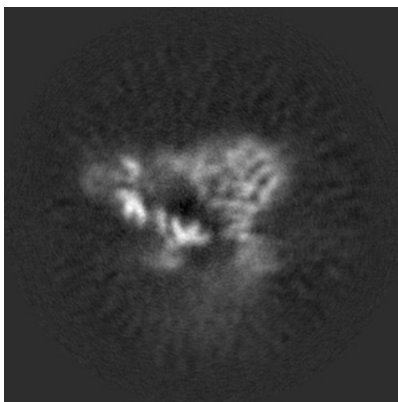


Z Index: 121

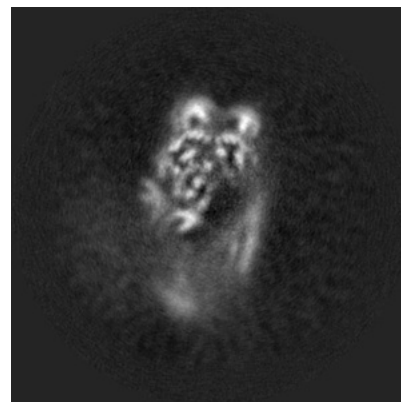
6.3.2 Raw map



X Index: 154



Y Index: 134

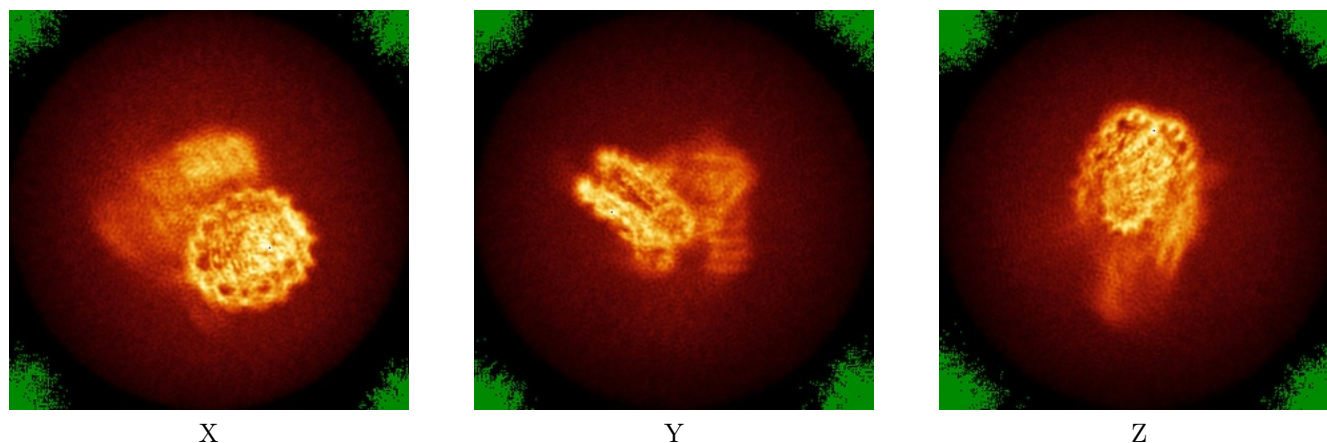


Z Index: 121

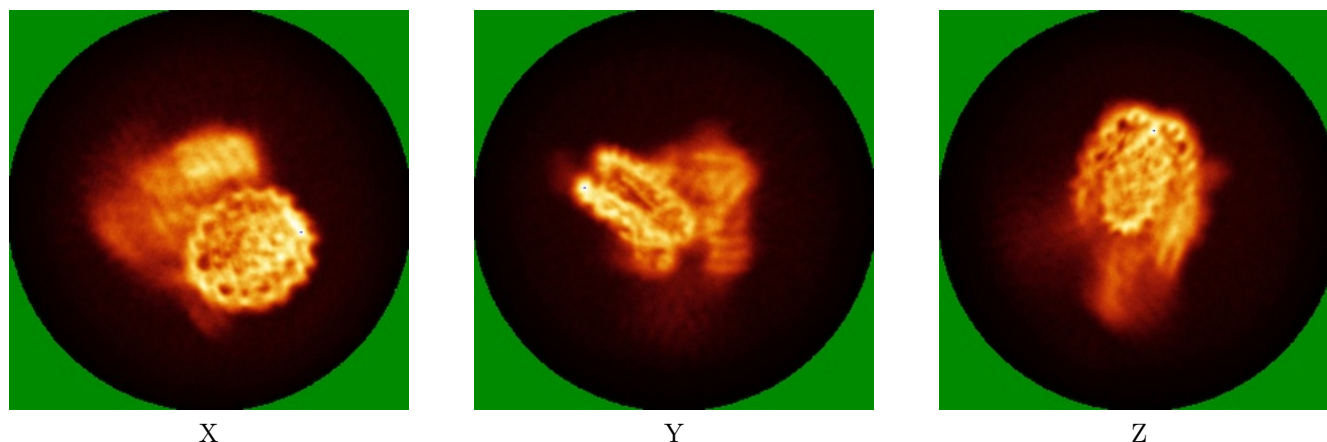
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

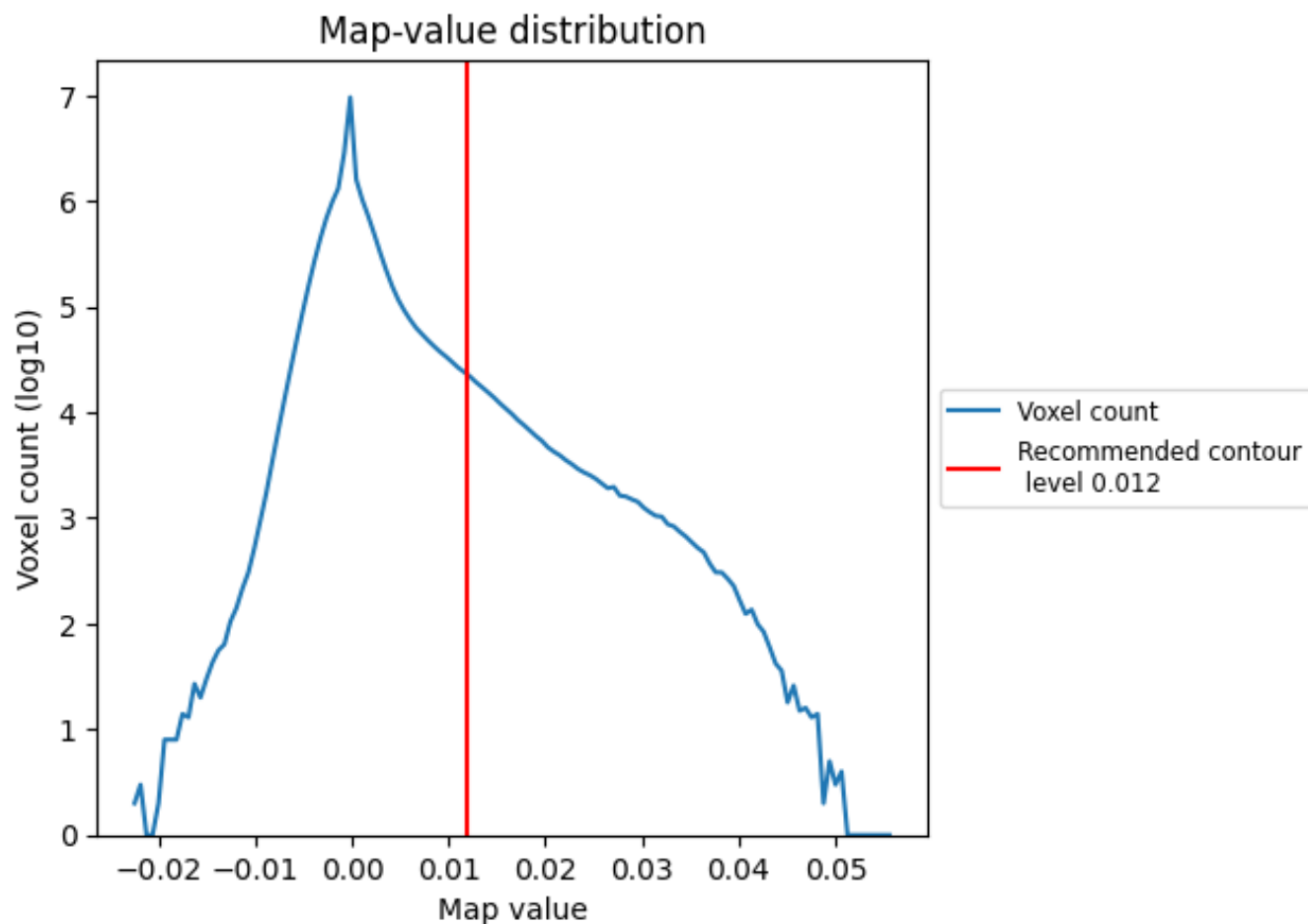
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

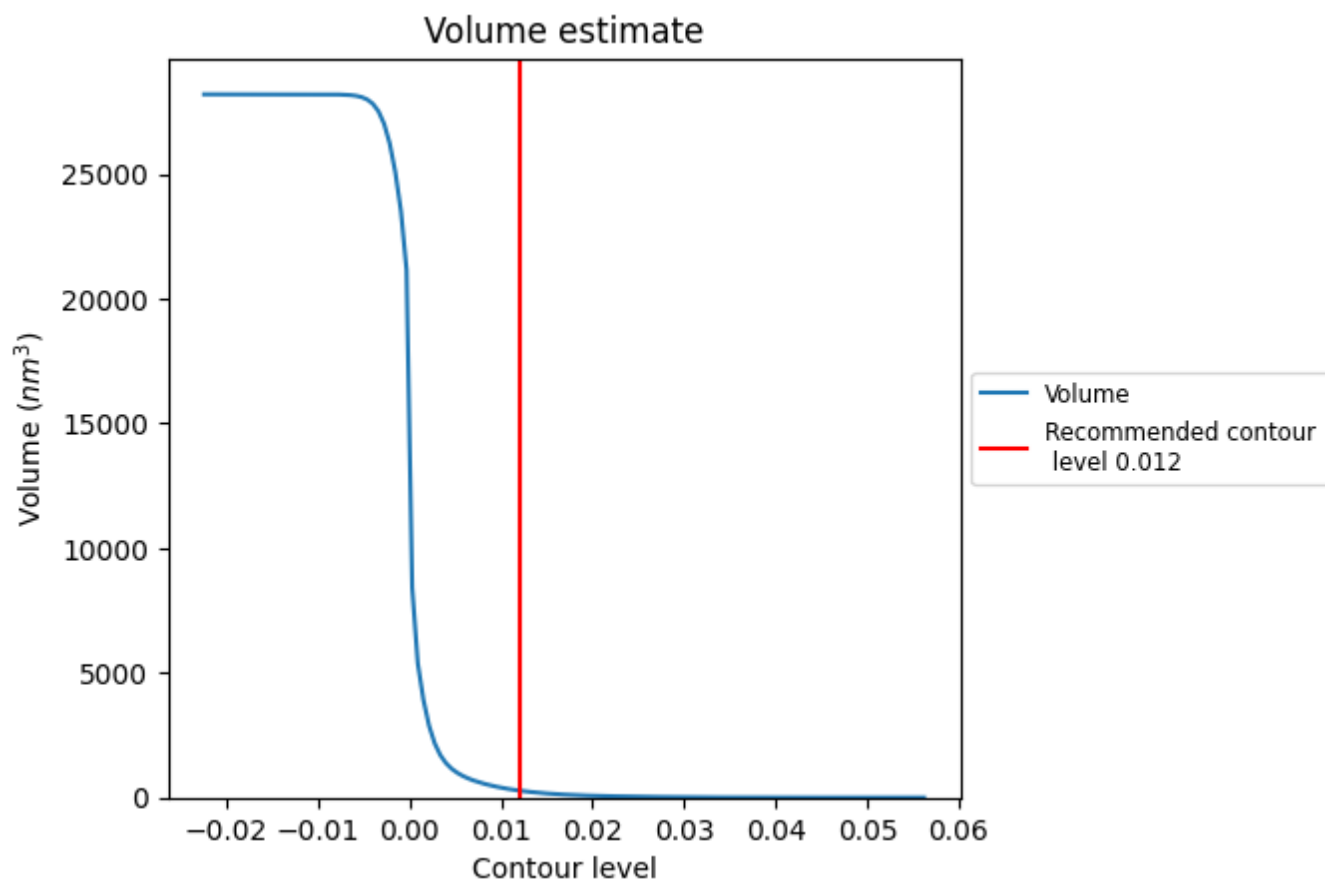
This section contains the results of statistical analysis of the map.

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.

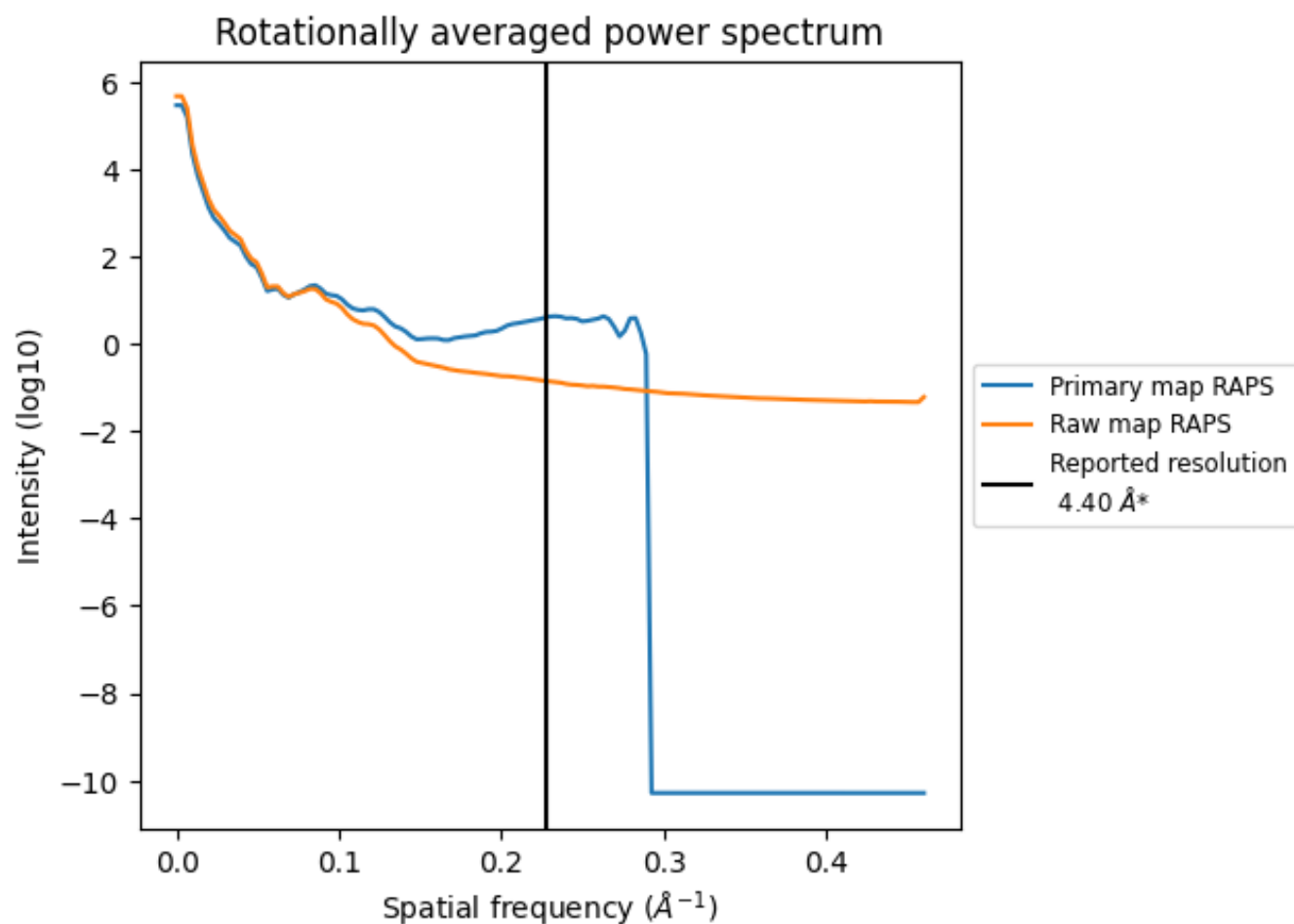
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 279 nm³; this corresponds to an approximate mass of 252 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 ⓘ

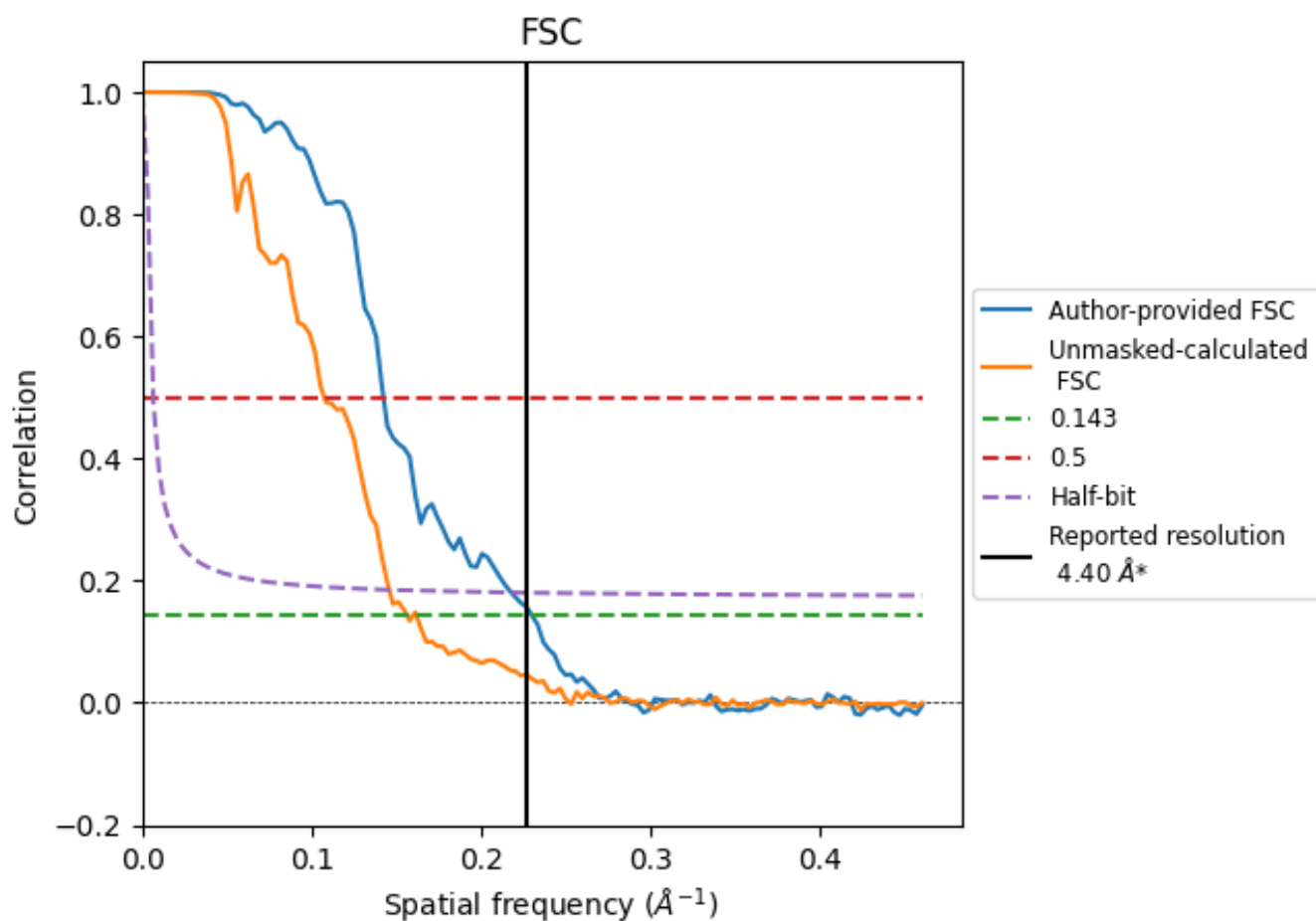


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.35	7.03	4.59
Unmasked-calculated*	6.41	9.30	6.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.41 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37367 and PDB model 8W9F. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

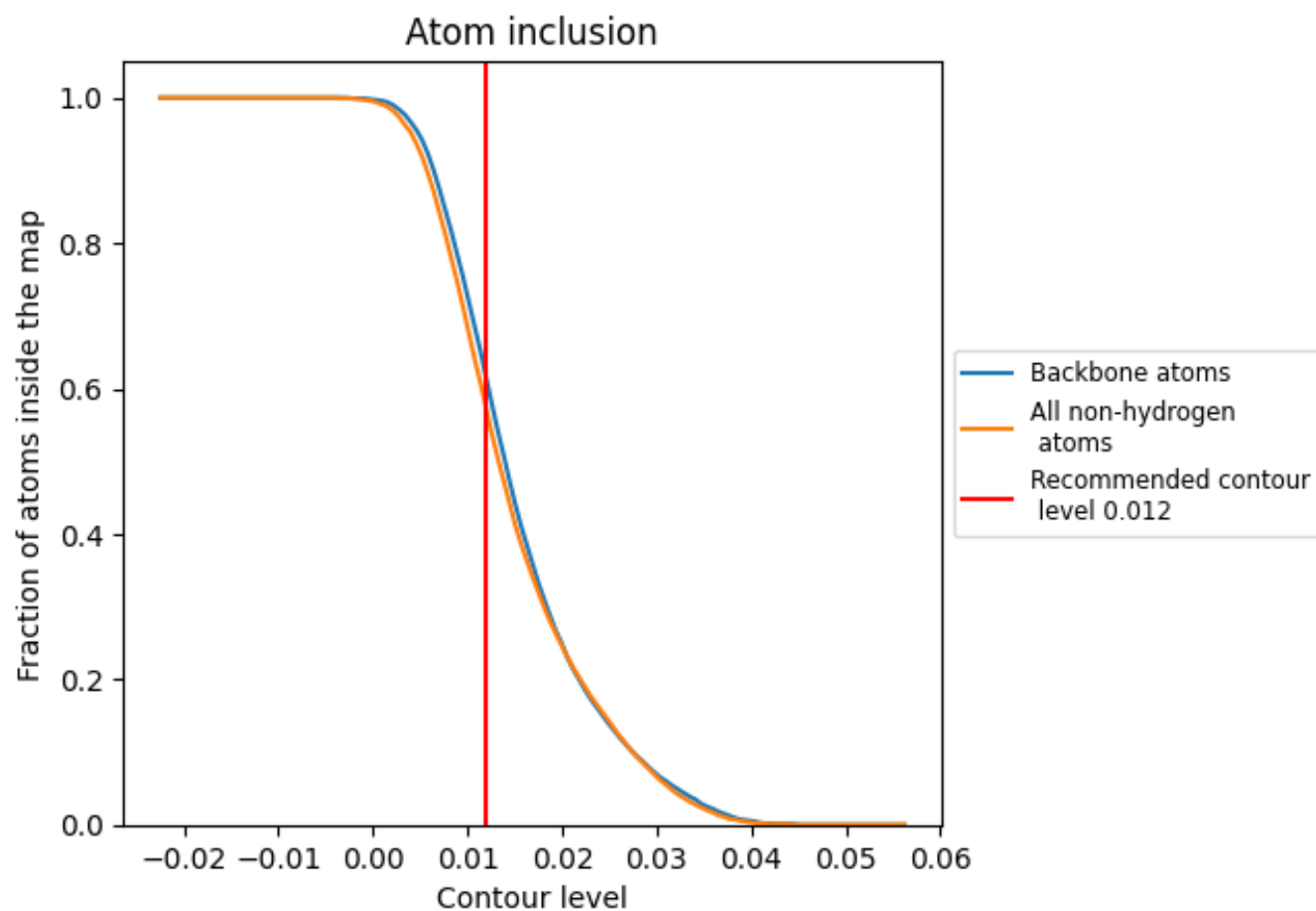


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 57% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5710	0.1560
A	0.3860	0.0520
B	0.6130	0.0480
C	0.4590	0.0390
D	0.1660	0.0200
E	0.2740	0.0410
F	0.0950	0.0210
G	0.0290	0.0430
a	0.7360	0.3290
b	0.7980	0.3710
c	0.8160	0.3750
d	0.8030	0.3820
e	0.8340	0.3790
f	0.8600	0.4020
g	0.7880	0.3750
h	0.8230	0.3800
i	0.8890	0.2500
j	0.9020	0.2260

1.0

0.0

<0.0