



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:43 PM UTC

PDB ID : 8P4E / pdb_00008p4e
EMDB ID : EMD-17407
Title : Structural insights into human co-transcriptional capping - structure 5
Authors : Garg, G.; Dienemann, C.; Farnung, L.; Schwarz, J.; Linden, A.; Urlaub, H.; Cramer, P.
Deposited on : 2023-05-20
Resolution : 3.90 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
Mogul : 2022.3.0, CSD as543be (2022)
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

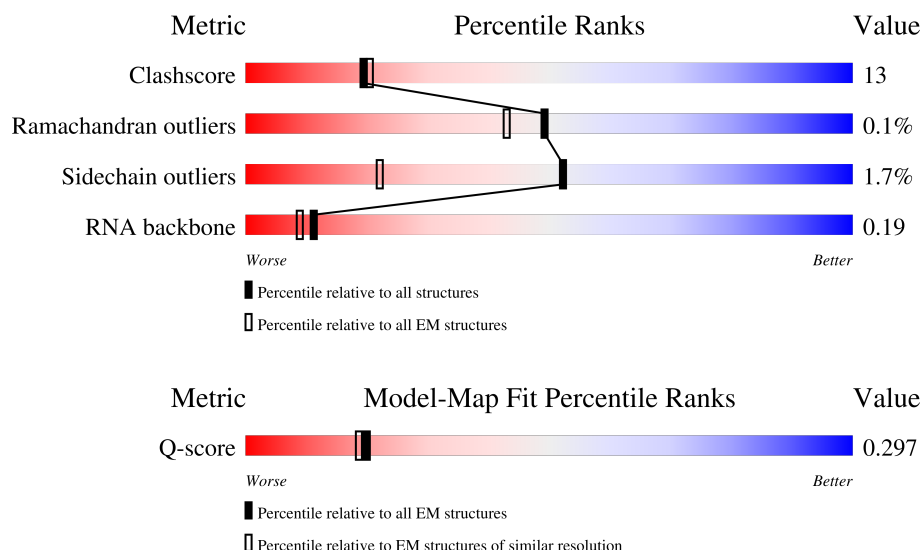
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.



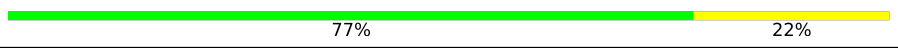
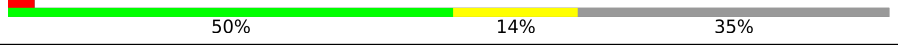
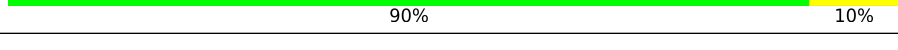
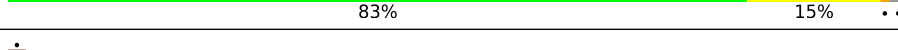
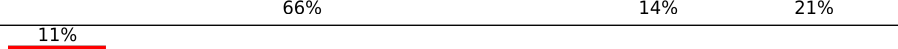
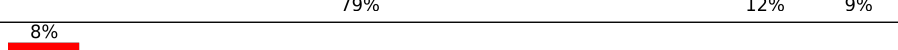
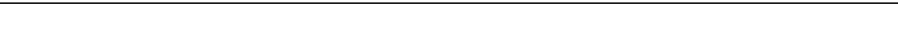
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	Z	1087	
2	M	597	
3	A	1970	

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Mol	Chain	Length	Quality of chain
4	B	1174	
5	C	275	
6	E	210	
7	F	127	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	D	142	
14	G	172	
15	O	835	
16	P	21	
17	N	26	
18	T	35	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 41213 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 Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	52	Total	C	N	O	S	0	0
			397	243	73	80	1		

- Molecule 2 is a protein called mRNA-capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	329	Total	C	N	O	S	0	0
			2649	1689	456	483	21		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1407	Total	C	N	O	S	0	0
			11142	7014	1997	2063	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	1116	Total	C	N	O	S	0	0
			8928	5652	1568	1644	64		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	258	Total	C	N	O	S	0	0
			2071	1301	353	411	6		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	209	Total	C	N	O	S	0	0
			1721	1089	300	324	8		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	82	Total	C	N	O	S	0	0
			658	418	113	122	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total	C	N	O	S	0	0
			950	587	169	183	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			389	241	75	67	6		

- Molecule 13 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	129	Total	C	N	O	S	0	1
			998	629	170	195	4		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	171	Total	C	N	O	S	0	0
			1305	852	205	240	8		

- Molecule 15 is a protein called Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	695	Total	C	N	O	S	0	0
			5643	3606	962	1040	35		

- Molecule 16 is a RNA chain called RNA (5'-D(*(MGT))-R(P*GP*AP*CP*AP*UP*AP*C P*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	21	Total	C	N	O	P	0	0
			462	204	89	146	23		

- Molecule 17 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	26	Total	C	N	O	P	0	0
			538	257	100	155	26		

- Molecule 18 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	35	Total	C	N	O	P	0	0
			714	342	126	211	35		

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mg	0
			1	1	

- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	

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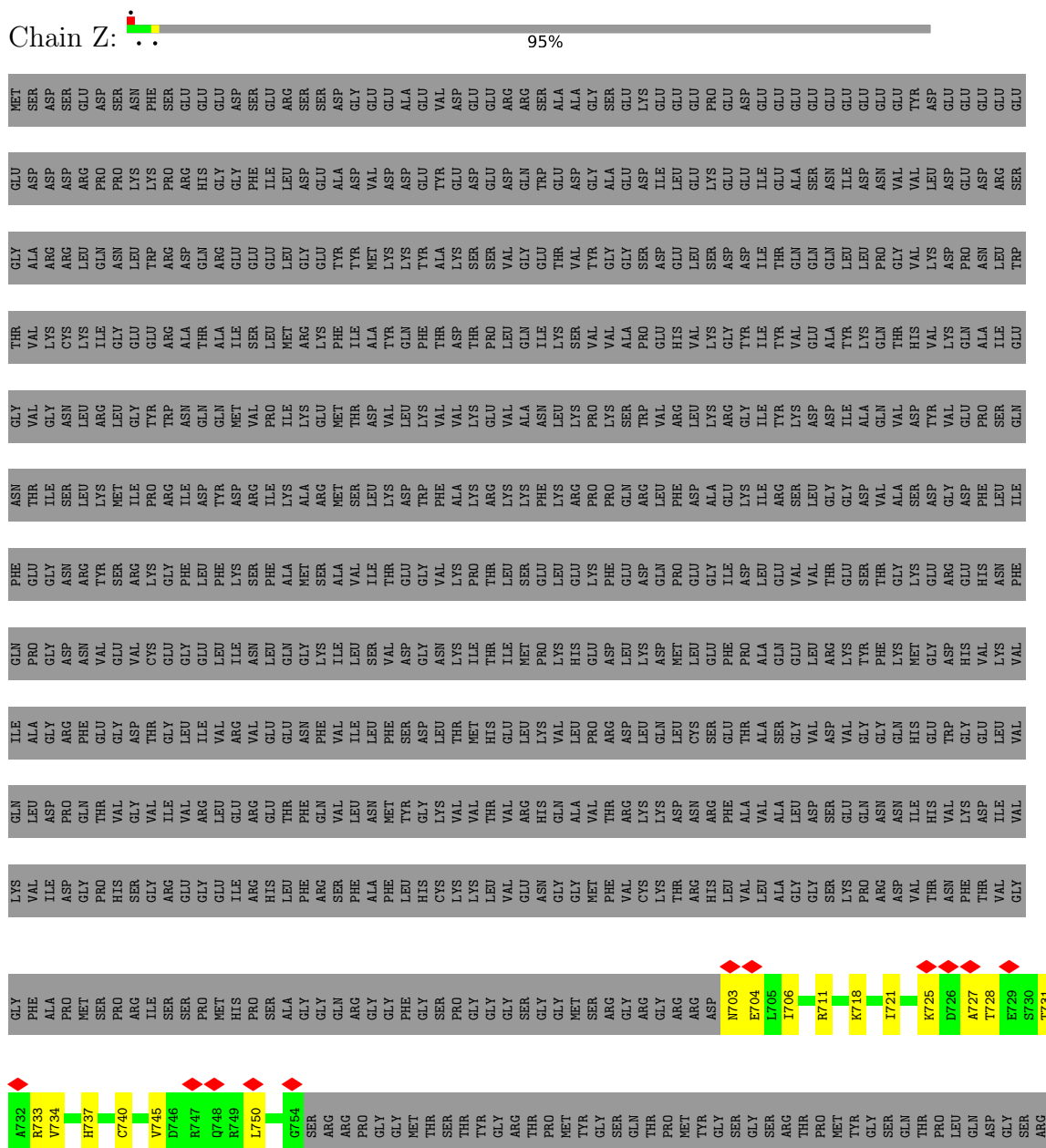
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Mol	Chain	Residues	Atoms		AltConf
20	C	1	Total 1	Zn 1	0
20	I	2	Total 2	Zn 2	0
20	J	1	Total 1	Zn 1	0
20	L	1	Total 1	Zn 1	0

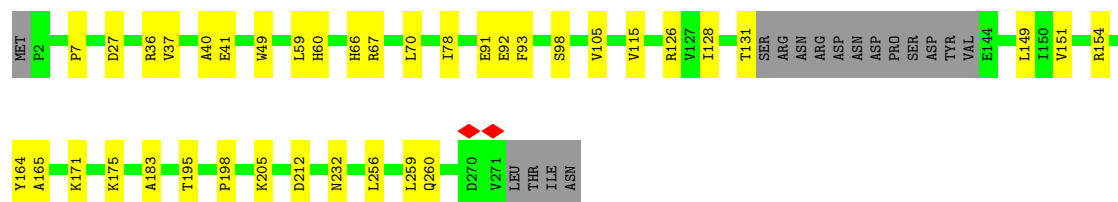
3 Residue-property plots

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.

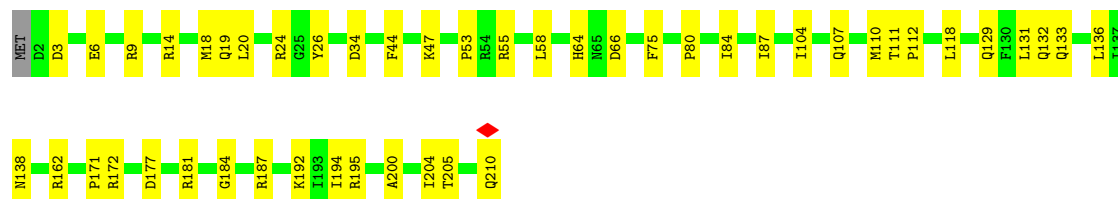
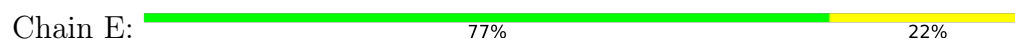
- Molecule 1: Transcription elongation factor SPT5



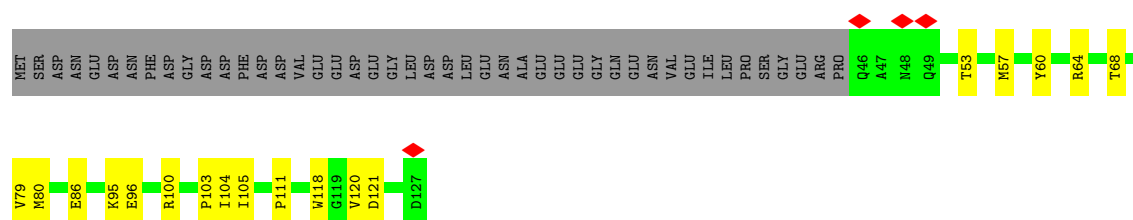




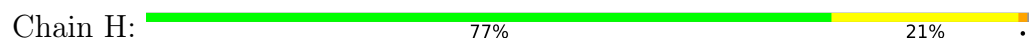
• Molecule 6: DNA-directed RNA polymerase II subunit E



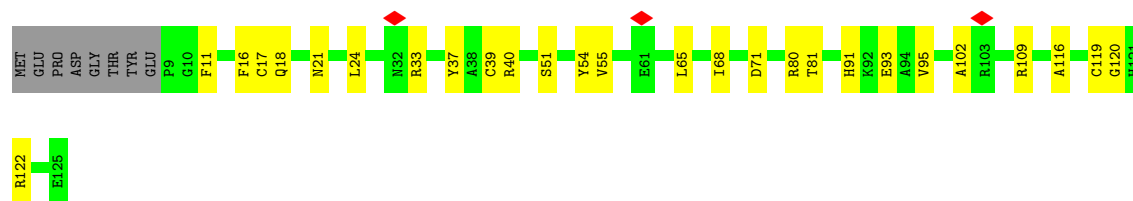
• Molecule 7: DNA-directed RNA polymerase II subunit F



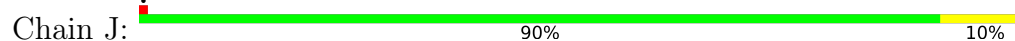
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



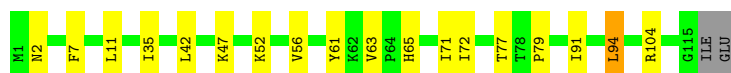
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5





- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 83% 15% ..



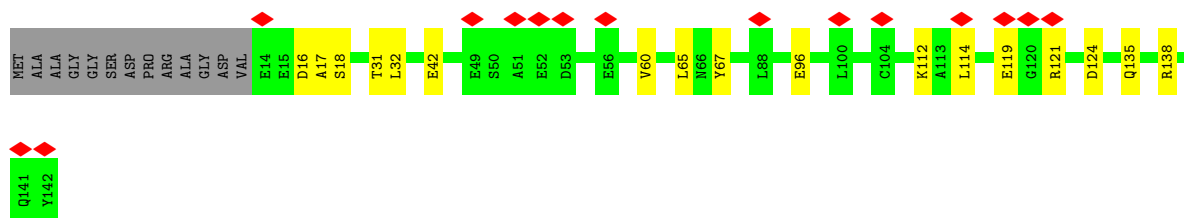
- Molecule 12: RNA polymerase II subunit K

Chain L: 66% 14% 21%



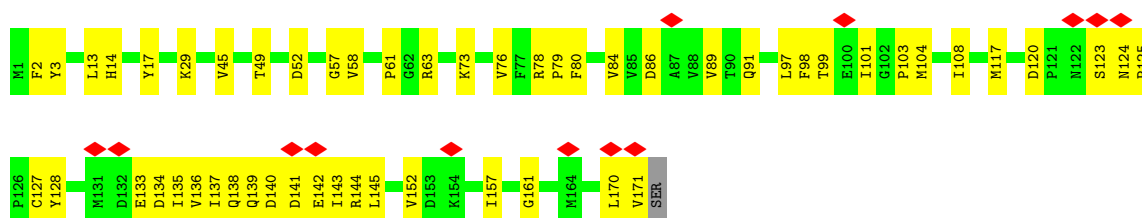
- Molecule 13: RNA polymerase II subunit D

Chain D: 11% 79% 12% 9%



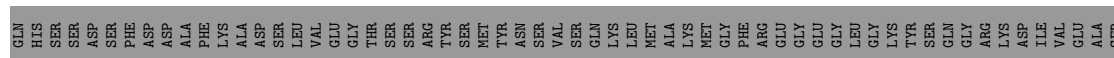
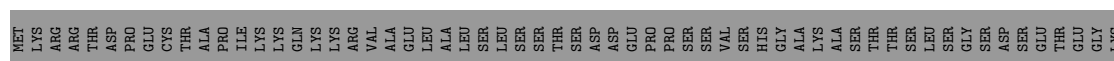
- Molecule 14: DNA-directed RNA polymerase II subunit RPB7

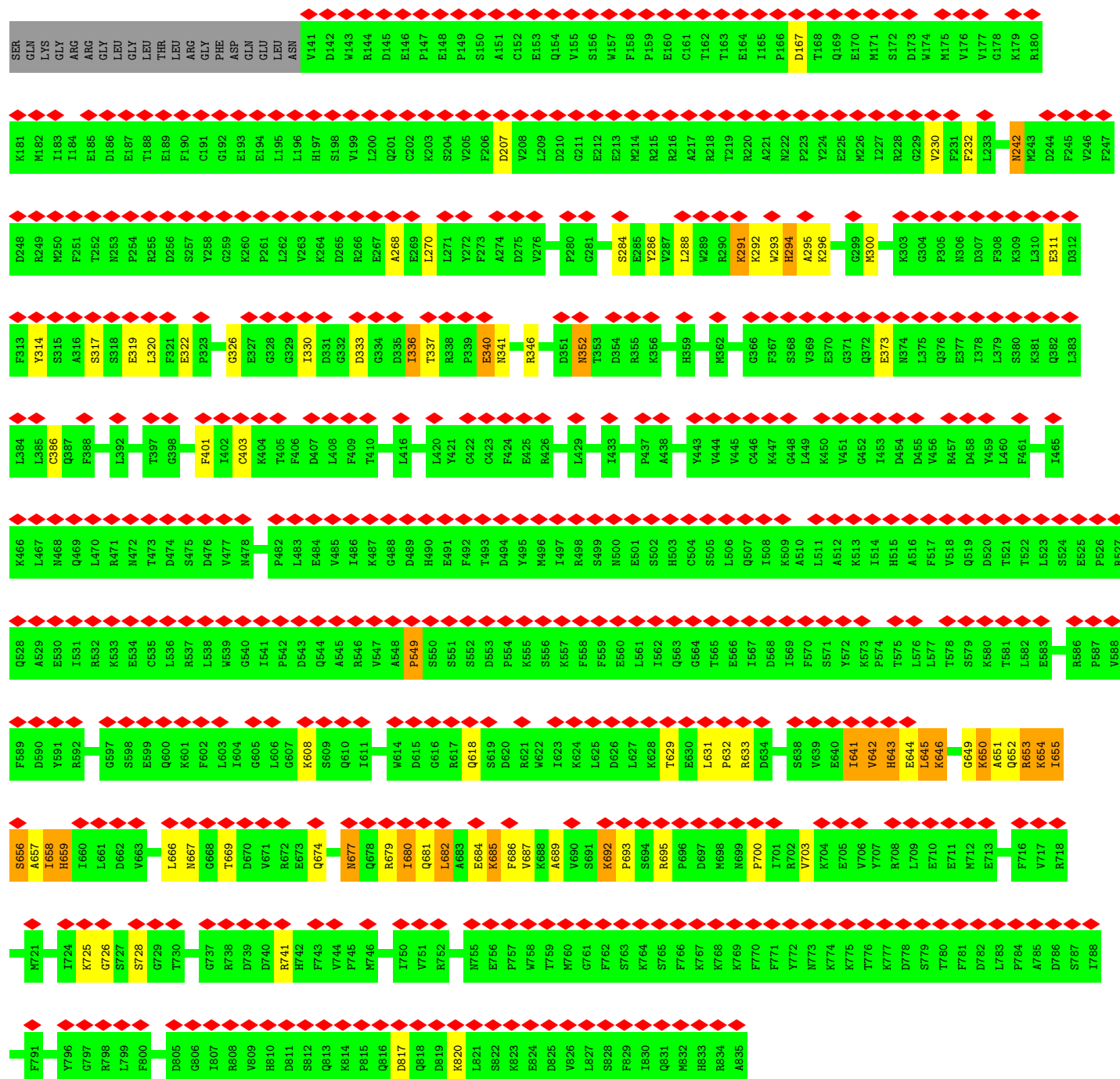
Chain G: 8% 68% 31%



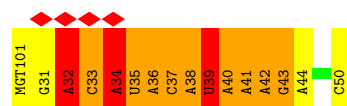
- Molecule 15: Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase 1

Chain O: 62% 73% 7% 17%

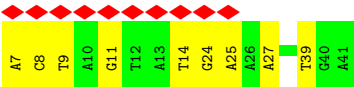




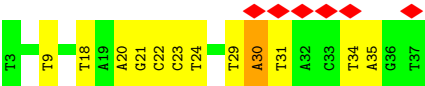
- Molecule 16: RNA (5'-D*(MGT))-R(P*GP*AP*CP*AP*UP*AP*CP*AP*UP*AP*AP*AP*G P*AP*CP*CP*AP*GP*GP*C)-3')



- Molecule 17: DNA (26-MER)



• Molecule 18: DNA (35-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48148	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0221	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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, MG, MGT

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	Z	0.30	0/400	0.46	0/541
2	M	0.70	0/2706	1.12	13/3646 (0.4%)
3	A	0.36	0/11345	0.61	0/15315
4	B	0.39	0/9105	0.60	0/12290
5	C	0.39	0/2114	0.59	2/2873 (0.1%)
6	E	0.33	0/1752	0.58	0/2366
7	F	0.33	0/668	0.49	0/901
8	H	0.36	0/1207	0.59	0/1628
9	I	0.28	0/973	0.51	0/1316
10	J	0.40	0/542	0.54	0/730
11	K	0.41	0/939	0.56	2/1271 (0.2%)
12	L	0.37	0/395	0.59	0/524
13	D	0.17	0/1012	0.43	0/1366
14	G	0.22	0/1336	0.46	0/1820
15	O	2.30	4/5775 (0.1%)	1.47	10/7785 (0.1%)
16	P	0.49	0/482	1.17	4/749 (0.5%)
17	N	0.33	0/603	0.78	0/927
18	T	0.44	0/799	0.73	1/1230 (0.1%)
All	All	0.93	4/42153 (0.0%)	0.82	32/57278 (0.1%)

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
3	A	0	5
4	B	0	1
14	G	0	1
15	O	0	1
16	P	1	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	1	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	659	HIS	CE1-NE2	120.55	2.53	1.32
15	O	659	HIS	ND1-CE1	83.32	2.15	1.32
15	O	659	HIS	CD2-NE2	69.86	2.14	1.37
15	O	549	PRO	C-N	23.94	1.66	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	549	PRO	O-C-N	39.14	165.65	122.98
15	O	549	PRO	CA-C-N	-30.38	76.05	121.31
15	O	549	PRO	C-N-CA	-30.38	76.05	121.31
15	O	659	HIS	ND1-CE1-NE2	-23.43	84.97	108.40
15	O	659	HIS	CG-CD2-NE2	21.59	128.79	107.20
15	O	659	HIS	CE1-NE2-CD2	-21.51	87.49	109.00
16	P	34	A	O5'-P-OP1	-16.64	58.09	108.00
16	P	34	A	O5'-P-OP2	-14.03	65.92	108.00
15	O	659	HIS	CG-ND1-CE1	12.24	130.10	109.30
2	M	479	GLU	N-CA-C	-8.17	102.77	114.12
2	M	365	ILE	N-CA-C	7.33	117.94	110.82
2	M	310	VAL	N-CA-C	7.01	118.06	109.30
2	M	268	PHE	CA-C-N	6.53	126.23	119.64
2	M	268	PHE	C-N-CA	6.53	126.23	119.64
15	O	242	ASN	CA-CB-CG	6.35	118.95	112.60
2	M	390	SER	CA-C-N	6.33	125.55	118.97
2	M	390	SER	C-N-CA	6.33	125.55	118.97
2	M	508	LYS	N-CA-C	6.00	117.50	111.07
18	T	30	DA	C2'-C3'-O3'	-6.00	102.50	111.50
16	P	39	U	C4'-C3'-O3'	5.74	118.01	109.40
2	M	521	ASN	N-CA-C	5.71	119.22	112.72
2	M	481	LEU	N-CA-CB	-5.56	101.95	110.01
2	M	327	PHE	CA-C-N	5.51	125.44	119.76
2	M	327	PHE	C-N-CA	5.51	125.44	119.76
2	M	362	TYR	CB-CA-C	5.41	119.07	109.65
11	K	79	PRO	CA-C-N	5.27	135.41	125.66
11	K	79	PRO	C-N-CA	5.27	135.41	125.66
15	O	618	GLN	OE1-CD-NE2	-5.26	117.34	122.60
16	P	32	A	C2'-C3'-O3'	5.20	121.51	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	91	GLU	CA-C-N	5.05	131.18	121.54
5	C	91	GLU	C-N-CA	5.05	131.18	121.54
15	O	167	ASP	CA-CB-CG	5.03	117.63	112.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	P	40	A	C4'

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1108	HIS	Peptide
3	A	1112	VAL	Peptide
3	A	1467	GLY	Peptide
3	A	412	GLN	Peptide
3	A	910	LYS	Peptide
4	B	629	GLU	Peptide
14	G	124	ASN	Peptide
15	O	314	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	397	0	403	31	0
2	M	2649	0	2658	195	0
3	A	11142	0	11286	222	0
4	B	8928	0	8946	225	0
5	C	2071	0	2016	42	0
6	E	1721	0	1737	43	0
7	F	658	0	684	18	0
8	H	1186	0	1147	26	0
9	I	950	0	880	20	0
10	J	533	0	553	7	0
11	K	920	0	942	14	0
12	L	389	0	395	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	D	998	0	953	14	0
14	G	1305	0	1264	157	0
15	O	5643	0	5592	223	0
16	P	462	0	234	39	0
17	N	538	0	296	33	0
18	T	714	0	397	47	0
19	A	1	0	0	0	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
All	All	41213	0	40383	1031	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1031) 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)
14:G:125:PRO:HG3	15:O:655:ILE:CG1	1.18	1.60
14:G:170:LEU:CD2	15:O:650:LYS:HA	1.36	1.53
14:G:170:LEU:HD23	15:O:650:LYS:CA	1.32	1.53
6:E:112:PRO:CG	18:T:9:DT:H5''	1.47	1.45
14:G:137:ILE:HA	15:O:725:LYS:NZ	1.11	1.38
1:Z:711:ARG:NH2	5:C:93:PHE:CD2	1.91	1.38
3:A:854:THR:HG21	18:T:20:DA:C6	1.61	1.36
14:G:134:ASP:O	15:O:651:ALA:N	1.60	1.35
1:Z:711:ARG:NH2	5:C:93:PHE:HD2	1.22	1.31
6:E:112:PRO:CB	18:T:9:DT:H5''	1.62	1.30
14:G:125:PRO:CG	15:O:655:ILE:CG1	2.08	1.29
14:G:137:ILE:CA	15:O:725:LYS:NZ	1.98	1.25
14:G:125:PRO:CG	15:O:655:ILE:HG13	1.66	1.25
4:B:222:ARG:NH1	17:N:24:DG:O6	1.68	1.24
14:G:134:ASP:C	15:O:651:ALA:HB2	1.61	1.22
4:B:222:ARG:NH2	17:N:24:DG:C5	2.08	1.20
6:E:112:PRO:HG3	18:T:9:DT:C5'	1.75	1.17
15:O:659:HIS:NE2	15:O:659:HIS:CD2	2.14	1.15
15:O:311:GLU:O	15:O:608:LYS:NZ	1.78	1.14
3:A:854:THR:CG2	18:T:20:DA:C6	2.30	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:317:SER:OG	15:O:667:ASN:ND2	1.81	1.14
15:O:659:HIS:CE1	15:O:659:HIS:ND1	2.15	1.14
14:G:138:GLN:OE1	15:O:653:ARG:CB	1.95	1.13
15:O:317:SER:HB3	15:O:632:PRO:HB3	1.25	1.13
4:B:222:ARG:NH1	17:N:24:DG:C6	2.15	1.13
3:A:854:THR:HG21	18:T:20:DA:N6	1.61	1.12
14:G:134:ASP:OD2	15:O:650:LYS:NZ	1.82	1.12
6:E:112:PRO:CG	18:T:9:DT:C5'	2.27	1.12
4:B:1077:GLY:HA2	18:T:24:DT:OP1	1.49	1.11
14:G:135:ILE:HA	15:O:650:LYS:HB2	1.17	1.11
15:O:330:ILE:HG12	15:O:695:ARG:HD3	1.27	1.11
4:B:1089:MET:HE2	18:T:21:DG:C4'	1.78	1.11
14:G:125:PRO:CG	15:O:655:ILE:HG12	1.75	1.11
14:G:127:CYS:SG	15:O:653:ARG:CZ	2.38	1.11
14:G:134:ASP:O	15:O:651:ALA:CB	2.00	1.10
15:O:319:GLU:HG2	15:O:631:LEU:C	1.76	1.09
15:O:322:GLU:OE1	15:O:693:PRO:CD	2.00	1.09
1:Z:711:ARG:CZ	5:C:92:GLU:OE1	2.01	1.09
6:E:112:PRO:HG3	18:T:9:DT:H5''	1.17	1.09
14:G:142:GLU:HB2	15:O:726:GLY:HA3	1.34	1.08
15:O:319:GLU:HB2	15:O:632:PRO:HD3	1.33	1.08
14:G:138:GLN:OE1	15:O:653:ARG:HB3	1.53	1.08
15:O:207:ASP:OD1	16:P:101:MGT:N1	1.86	1.07
15:O:330:ILE:HG12	15:O:695:ARG:CD	1.85	1.06
14:G:134:ASP:CA	15:O:651:ALA:HB2	1.85	1.06
4:B:1089:MET:HE2	18:T:21:DG:H4'	1.10	1.05
1:Z:740:CYS:HA	4:B:859:ARG:HH22	1.17	1.04
14:G:123:SER:CB	15:O:653:ARG:HH22	1.70	1.04
3:A:331:LYS:O	18:T:30:DA:N1	1.91	1.03
14:G:125:PRO:HG3	15:O:655:ILE:HG13	1.06	1.03
15:O:319:GLU:OE2	15:O:632:PRO:HA	1.58	1.03
15:O:319:GLU:CB	15:O:632:PRO:HD3	1.87	1.03
14:G:139:GLN:O	15:O:654:LYS:CD	2.06	1.02
1:Z:733:ARG:NH1	3:A:411:SER:OG	1.93	1.02
15:O:319:GLU:HB2	15:O:632:PRO:CD	1.88	1.02
14:G:134:ASP:O	15:O:651:ALA:CA	2.06	1.02
3:A:331:LYS:O	18:T:30:DA:C2	2.12	1.02
4:B:489:ILE:CD1	17:N:25:DA:N7	2.23	1.01
14:G:127:CYS:SG	15:O:653:ARG:NH1	2.33	1.01
15:O:317:SER:CB	15:O:632:PRO:HB3	1.91	1.01
4:B:489:ILE:HD11	17:N:25:DA:C5	1.95	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:322:GLU:OE1	15:O:693:PRO:HD2	1.62	1.00
14:G:137:ILE:HA	15:O:725:LYS:HZ2	1.19	0.98
1:Z:711:ARG:NE	5:C:92:GLU:OE1	1.96	0.98
2:M:473:ILE:HD12	2:M:503:VAL:HG21	1.42	0.98
14:G:170:LEU:HD21	15:O:649:GLY:O	1.64	0.98
4:B:1150:ARG:HD3	14:G:63:ARG:HH22	1.25	0.97
14:G:134:ASP:O	15:O:651:ALA:HB2	1.58	0.97
14:G:135:ILE:CA	15:O:650:LYS:HB2	1.94	0.96
14:G:133:GLU:O	15:O:651:ALA:HB1	1.64	0.96
4:B:489:ILE:HD11	17:N:25:DA:N7	1.81	0.95
2:M:496:ARG:HB3	2:M:497:PRO:HD2	1.49	0.95
1:Z:711:ARG:NH2	5:C:93:PHE:CE2	2.33	0.94
14:G:125:PRO:CD	15:O:655:ILE:HG13	1.97	0.94
3:A:331:LYS:HB3	18:T:30:DA:H61	1.33	0.93
14:G:139:GLN:O	15:O:654:LYS:HD3	1.65	0.93
1:Z:740:CYS:HA	4:B:859:ARG:NH2	1.84	0.93
1:Z:725:LYS:NZ	4:B:864:ASP:OD1	2.02	0.92
4:B:1077:GLY:HA2	18:T:24:DT:P	2.08	0.92
2:M:481:LEU:HD11	14:G:13:LEU:HA	1.50	0.92
14:G:138:GLN:OE1	15:O:653:ARG:CA	2.06	0.92
15:O:317:SER:HB3	15:O:632:PRO:CB	1.99	0.91
14:G:170:LEU:HD23	15:O:650:LYS:N	1.84	0.91
1:Z:740:CYS:HB2	4:B:901:THR:HG21	1.51	0.90
14:G:125:PRO:HG3	15:O:655:ILE:HG12	0.92	0.90
3:A:331:LYS:O	18:T:30:DA:C6	2.25	0.90
4:B:489:ILE:CD1	17:N:25:DA:C5	2.55	0.90
14:G:135:ILE:HA	15:O:650:LYS:CB	2.01	0.90
4:B:83:ARG:HH12	4:B:139:GLN:HB3	1.37	0.89
15:O:330:ILE:CG1	15:O:695:ARG:HD3	2.03	0.88
14:G:133:GLU:O	15:O:651:ALA:CB	2.22	0.88
7:F:64:ARG:HH22	14:G:61:PRO:HG3	1.39	0.87
15:O:311:GLU:HA	15:O:608:LYS:NZ	1.89	0.87
15:O:296:LYS:HD3	15:O:689:ALA:HA	1.57	0.87
2:M:420:THR:HG23	2:M:423:LYS:HE2	1.55	0.87
14:G:136:VAL:N	15:O:651:ALA:HA	1.89	0.87
15:O:311:GLU:HA	15:O:608:LYS:CE	2.04	0.87
15:O:319:GLU:HG2	15:O:631:LEU:CA	2.05	0.87
15:O:311:GLU:HA	15:O:608:LYS:HE2	1.57	0.86
2:M:496:ARG:NH2	3:A:437:ASP:HB3	1.89	0.86
2:M:293:TRP:HD1	2:M:424:LEU:HD21	1.40	0.86
14:G:139:GLN:O	15:O:654:LYS:HD2	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:24:ARG:HH12	6:E:184:GLY:HA3	1.42	0.85
2:M:233:LEU:HD21	2:M:348:ILE:HD11	1.55	0.85
15:O:319:GLU:CG	15:O:631:LEU:C	2.50	0.85
14:G:135:ILE:HA	15:O:650:LYS:C	2.01	0.84
15:O:643:HIS:HA	15:O:656:SER:HA	1.60	0.84
18:T:29:DT:H2"	18:T:30:DA:OP1	1.77	0.84
7:F:64:ARG:NH2	14:G:61:PRO:HG3	1.94	0.83
14:G:123:SER:HB2	15:O:653:ARG:HH22	1.41	0.83
3:A:481:THR:H	3:A:483:ARG:HH12	1.26	0.83
2:M:246:THR:HG22	2:M:248:PRO:HD2	1.58	0.83
14:G:137:ILE:CA	15:O:725:LYS:HZ1	1.91	0.83
14:G:134:ASP:C	15:O:651:ALA:CB	2.44	0.82
3:A:1474:LEU:HA	14:G:57:GLY:O	1.80	0.82
14:G:135:ILE:HG12	15:O:650:LYS:CB	2.09	0.82
2:M:314:ASP:HB3	2:M:316:ASP:H	1.44	0.81
14:G:170:LEU:CD2	15:O:649:GLY:O	2.28	0.81
6:E:112:PRO:CB	18:T:9:DT:C5'	2.52	0.81
15:O:311:GLU:C	15:O:608:LYS:HZ1	1.87	0.81
2:M:309:GLU:OE1	2:M:309:GLU:HA	1.81	0.80
4:B:1150:ARG:CD	14:G:63:ARG:HH22	1.94	0.80
14:G:137:ILE:HA	15:O:725:LYS:HZ1	1.40	0.80
4:B:222:ARG:NH2	17:N:24:DG:C6	2.46	0.80
4:B:489:ILE:HD11	17:N:25:DA:C6	2.15	0.80
1:Z:718:LYS:HE3	5:C:92:GLU:HA	1.62	0.80
15:O:311:GLU:CA	15:O:608:LYS:HZ3	1.94	0.80
3:A:854:THR:HG22	18:T:20:DA:C5	2.17	0.80
14:G:170:LEU:HD22	15:O:650:LYS:HA	1.63	0.80
3:A:854:THR:CG2	18:T:20:DA:C5	2.66	0.79
15:O:300:MET:HE3	15:O:336:ILE:HG12	1.63	0.79
4:B:222:ARG:CZ	17:N:24:DG:C6	2.66	0.79
14:G:137:ILE:CG1	15:O:725:LYS:HZ1	1.95	0.79
14:G:142:GLU:HB2	15:O:726:GLY:CA	2.11	0.79
2:M:398:THR:OG1	2:M:400:LEU:HD13	1.82	0.79
4:B:1077:GLY:CA	18:T:24:DT:OP1	2.29	0.79
13:D:135:GLN:HE22	13:D:138:ARG:HH11	1.30	0.79
3:A:481:THR:OG1	3:A:483:ARG:NH1	2.15	0.78
14:G:170:LEU:CD2	15:O:650:LYS:CA	2.16	0.78
3:A:331:LYS:HB3	18:T:30:DA:N6	1.97	0.78
5:C:7:PRO:O	11:K:104:ARG:NH1	2.17	0.78
14:G:142:GLU:OE1	15:O:726:GLY:O	2.01	0.78
2:M:481:LEU:HB3	14:G:29:LYS:CD	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:171:VAL:HB	15:O:726:GLY:HA2	1.66	0.78
3:A:132:LYS:HG2	6:E:187:ARG:HH12	1.47	0.78
14:G:123:SER:CB	15:O:653:ARG:NH2	2.47	0.78
14:G:140:ASP:HB3	15:O:654:LYS:HE3	1.65	0.78
2:M:481:LEU:HB2	14:G:17:TYR:HD2	1.49	0.77
17:N:7:DA:H8	17:N:7:DA:P	2.07	0.77
3:A:1053:ARG:NE	3:A:1057:GLU:OE2	2.15	0.77
16:P:39:U:C6	16:P:39:U:H5''	2.19	0.77
15:O:311:GLU:C	15:O:608:LYS:NZ	2.42	0.77
15:O:659:HIS:NE2	15:O:659:HIS:CE1	2.53	0.77
2:M:545:VAL:HG12	2:M:549:ILE:HD11	1.66	0.77
15:O:311:GLU:CA	15:O:608:LYS:NZ	2.47	0.77
14:G:123:SER:HB2	15:O:653:ARG:NH2	2.01	0.76
2:M:554:THR:OG1	2:M:557:MET:HB2	1.86	0.76
4:B:1089:MET:CE	18:T:21:DG:C4'	2.62	0.76
2:M:496:ARG:NH2	3:A:437:ASP:CB	2.49	0.75
14:G:137:ILE:HA	15:O:725:LYS:HZ3	0.92	0.75
16:P:43:G:H8	16:P:43:G:OP2	1.69	0.75
1:Z:711:ARG:CZ	5:C:92:GLU:CD	2.59	0.75
2:M:514:ILE:HD12	2:M:533:LYS:HB3	1.67	0.75
14:G:170:LEU:HB2	15:O:725:LYS:HE3	1.67	0.74
14:G:134:ASP:HA	15:O:651:ALA:HB2	1.68	0.74
4:B:489:ILE:HD12	17:N:25:DA:N7	2.01	0.74
3:A:38:GLU:H	3:A:61:ARG:HH12	1.36	0.73
15:O:293:TRP:HA	15:O:320:LEU:HD13	1.70	0.73
1:Z:740:CYS:HB2	4:B:901:THR:CG2	2.19	0.73
15:O:319:GLU:OE2	15:O:632:PRO:CA	2.36	0.73
4:B:1150:ARG:HD3	14:G:63:ARG:NH2	2.02	0.72
7:F:86:GLU:OE2	7:F:95:LYS:NZ	2.21	0.72
1:Z:711:ARG:HH22	5:C:93:PHE:HD2	1.03	0.72
14:G:134:ASP:OD2	15:O:650:LYS:CE	2.38	0.72
3:A:36:VAL:HG23	4:B:1138:ARG:HH12	1.55	0.72
14:G:141:ASP:CG	15:O:725:LYS:HD3	2.13	0.72
2:M:481:LEU:HD23	14:G:29:LYS:HG2	1.71	0.72
4:B:1078:ARG:N	18:T:24:DT:OP1	2.23	0.72
3:A:853:LYS:NZ	3:A:1103:THR:OG1	2.20	0.72
14:G:170:LEU:CB	15:O:725:LYS:HE3	2.19	0.72
2:M:332:ASP:OD2	2:M:335:MET:HG3	1.90	0.71
14:G:137:ILE:CA	15:O:725:LYS:HZ3	1.79	0.71
15:O:293:TRP:HB3	15:O:667:ASN:HB3	1.72	0.71
6:E:112:PRO:HG3	18:T:9:DT:C4'	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:322:GLU:OE1	15:O:693:PRO:N	2.24	0.71
4:B:851:ASP:OD2	12:L:17:TYR:OH	2.08	0.71
14:G:135:ILE:HG12	15:O:650:LYS:HB2	1.72	0.71
16:P:41:A:H3'	16:P:42:A:C8	2.26	0.71
15:O:549:PRO:HG2	15:O:633:ARG:NH2	2.05	0.71
3:A:869:GLU:OE1	4:B:1091:ARG:NH1	2.21	0.70
15:O:319:GLU:CD	15:O:632:PRO:HA	2.15	0.70
4:B:200:MET:HE2	17:N:24:DG:N2	2.06	0.70
14:G:170:LEU:CD2	15:O:649:GLY:C	2.64	0.70
2:M:514:ILE:HD11	2:M:535:PHE:O	1.89	0.70
2:M:481:LEU:HB2	14:G:17:TYR:CD2	2.26	0.70
15:O:268:ALA:HB2	15:O:681:GLN:HB3	1.74	0.70
2:M:420:THR:HG23	2:M:423:LYS:CE	2.20	0.70
4:B:230:ARG:NH1	4:B:231:PRO:O	2.25	0.70
15:O:311:GLU:HA	15:O:608:LYS:HZ3	1.52	0.70
14:G:125:PRO:HD3	15:O:655:ILE:HG13	1.72	0.70
2:M:276:MET:HA	2:M:280:ASN:HD22	1.57	0.69
16:P:35:U:H6	16:P:35:U:H5'	1.57	0.69
14:G:135:ILE:CG1	15:O:650:LYS:HB2	2.23	0.69
15:O:319:GLU:HB2	15:O:632:PRO:CG	2.23	0.69
15:O:682:LEU:HA	15:O:685:LYS:HD3	1.75	0.69
1:Z:711:ARG:NH2	5:C:92:GLU:OE1	2.25	0.68
2:M:278:LYS:HG2	2:M:557:MET:HE1	1.76	0.68
14:G:136:VAL:N	15:O:651:ALA:CA	2.57	0.68
15:O:340:GLU:H	15:O:340:GLU:CD	2.01	0.68
2:M:496:ARG:HB3	2:M:497:PRO:CD	2.22	0.68
2:M:395:LYS:HB3	2:M:401:ILE:HG13	1.76	0.68
16:P:35:U:H5'	16:P:35:U:C6	2.28	0.68
14:G:127:CYS:SG	15:O:653:ARG:NH2	2.67	0.67
1:Z:721:ILE:HG13	12:L:54:VAL:HG21	1.77	0.67
3:A:94:VAL:HG13	3:A:311:GLN:HG2	1.76	0.67
15:O:319:GLU:HG2	15:O:631:LEU:N	2.10	0.67
2:M:422:ARG:NH1	2:M:566:THR:HG21	2.10	0.66
2:M:471:LEU:HB2	2:M:515:ILE:HD13	1.78	0.66
3:A:1218:ARG:NH1	3:A:1252:ALA:O	2.29	0.66
5:C:37:VAL:HG13	5:C:41:GLU:HB2	1.76	0.66
2:M:481:LEU:HD11	14:G:13:LEU:CA	2.23	0.66
2:M:392:ARG:O	2:M:396:MET:HG3	1.95	0.66
4:B:385:ARG:NH1	17:N:24:DG:H1'	2.11	0.66
16:P:36:A:N3	16:P:36:A:H5'	2.11	0.66
3:A:291:ARG:O	3:A:295:GLN:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:329:PHE:CE2	2:M:331:LYS:HB2	2.31	0.65
4:B:387:HIS:NE2	4:B:671:GLU:OE2	2.29	0.65
15:O:319:GLU:OE1	15:O:608:LYS:N	2.23	0.65
2:M:496:ARG:HH22	3:A:421:ARG:NH2	1.94	0.65
2:M:494:TYR:CD1	2:M:539:TYR:CE1	2.84	0.65
2:M:541:THR:O	2:M:545:VAL:HG23	1.95	0.65
16:P:43:G:OP2	16:P:43:G:C8	2.50	0.65
4:B:790:GLN:O	4:B:968:ASN:ND2	2.30	0.64
18:T:30:DA:H2'	18:T:31:DT:C6	2.33	0.64
3:A:999:ARG:NH1	8:H:103:GLU:OE1	2.31	0.64
6:E:112:PRO:HB2	18:T:9:DT:H5''	1.69	0.64
3:A:1141:VAL:HB	3:A:1336:LEU:HB2	1.77	0.64
6:E:24:ARG:NH1	6:E:184:GLY:HA3	2.11	0.64
1:Z:703:ASN:OD1	1:Z:704:GLU:N	2.31	0.64
1:Z:740:CYS:CA	4:B:859:ARG:HH22	2.03	0.64
2:M:327:PHE:CD1	2:M:392:ARG:HD2	2.32	0.64
3:A:691:ASP:OD2	3:A:765:ASN:ND2	2.28	0.64
14:G:136:VAL:O	15:O:725:LYS:NZ	2.30	0.64
2:M:278:LYS:HE3	2:M:552:PRO:O	1.98	0.64
4:B:116:ARG:NH1	4:B:118:LEU:HD11	2.12	0.64
15:O:293:TRP:CZ3	15:O:666:LEU:HD13	2.33	0.64
14:G:137:ILE:HG12	15:O:725:LYS:HZ1	1.63	0.64
3:A:329:MET:HE3	3:A:333:GLY:HA2	1.80	0.64
6:E:112:PRO:HG3	18:T:9:DT:H4'	1.78	0.64
16:P:42:A:H8	16:P:42:A:C5'	2.11	0.64
2:M:485:ASN:OD1	2:M:485:ASN:N	2.26	0.64
4:B:489:ILE:HD11	17:N:25:DA:N6	2.12	0.64
14:G:170:LEU:HD21	15:O:649:GLY:C	2.23	0.63
2:M:479:GLU:HG2	14:G:14:HIS:CE1	2.34	0.63
2:M:420:THR:O	2:M:420:THR:HG22	1.98	0.63
14:G:170:LEU:HD23	15:O:650:LYS:HA	0.65	0.63
16:P:42:A:C8	16:P:42:A:O5'	2.52	0.63
15:O:293:TRP:HH2	15:O:682:LEU:HB3	1.63	0.63
2:M:329:PHE:HE2	2:M:331:LYS:HB2	1.64	0.63
2:M:463:SER:HB2	2:M:464:LEU:HD23	1.81	0.63
4:B:792:ASP:OD2	4:B:975:ARG:NH2	2.26	0.63
4:B:222:ARG:NH2	17:N:24:DG:N7	2.47	0.63
14:G:45:VAL:HA	14:G:76:VAL:HG12	1.81	0.63
2:M:425:LEU:HD11	2:M:559:PHE:HE1	1.64	0.62
15:O:293:TRP:HA	15:O:320:LEU:CD1	2.28	0.62
16:P:34:A:H2'	16:P:34:A:N3	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:393:HIS:HA	2:M:396:MET:HE2	1.81	0.62
15:O:330:ILE:HG12	15:O:695:ARG:HD2	1.75	0.62
14:G:137:ILE:HG12	15:O:725:LYS:NZ	2.14	0.62
2:M:484:GLN:NE2	2:M:484:GLN:HA	2.15	0.62
4:B:334:LYS:HZ3	4:B:337:LYS:NZ	1.98	0.62
4:B:507:GLY:HA3	4:B:623:ARG:NH1	2.15	0.62
4:B:130:LYS:O	4:B:141:GLN:HA	2.00	0.61
14:G:170:LEU:HD22	15:O:725:LYS:HD2	1.82	0.61
2:M:377:PHE:HD1	2:M:380:ARG:HH21	1.48	0.61
3:A:419:ILE:HG23	3:A:427:ILE:HB	1.82	0.61
4:B:274:ARG:NH1	4:B:312:GLN:HA	2.15	0.61
2:M:358:ARG:HH11	2:M:411:ARG:CZ	2.13	0.61
14:G:137:ILE:CG1	15:O:725:LYS:NZ	2.63	0.61
2:M:312:MET:C	2:M:313:ILE:HD12	2.25	0.61
2:M:363:ASP:OD1	2:M:448:TYR:HD1	1.84	0.61
2:M:489:LEU:CD2	2:M:515:ILE:HD11	2.31	0.61
4:B:417:ILE:HG22	4:B:421:LYS:NZ	2.15	0.61
4:B:861:SER:N	4:B:864:ASP:OD2	2.32	0.61
6:E:129:GLN:O	6:E:181:ARG:NH2	2.33	0.61
15:O:322:GLU:OE1	15:O:692:LYS:HA	2.01	0.61
8:H:49:PRO:O	8:H:147:LYS:NZ	2.34	0.60
15:O:293:TRP:CE3	15:O:686:PHE:HD2	2.19	0.60
2:M:358:ARG:HD3	2:M:411:ARG:CD	2.31	0.60
2:M:361:ILE:HG22	2:M:384:ILE:HD13	1.83	0.60
4:B:65:ILE:HD11	4:B:86:LEU:HD12	1.83	0.60
4:B:489:ILE:HD12	17:N:25:DA:C5	2.36	0.60
3:A:102:LYS:NZ	3:A:141:LEU:HD22	2.16	0.60
3:A:896:LEU:HB2	3:A:1396:ARG:HH21	1.66	0.60
4:B:65:ILE:HB	4:B:416:ARG:HH11	1.65	0.60
3:A:520:MET:HB3	3:A:522:PRO:HD2	1.82	0.60
4:B:1150:ARG:CD	14:G:63:ARG:NH2	2.64	0.60
3:A:102:LYS:HZ3	3:A:141:LEU:HD22	1.64	0.60
3:A:932:ARG:HH12	8:H:108:ALA:HA	1.67	0.60
4:B:780:VAL:HG12	4:B:965:ILE:HB	1.84	0.60
15:O:326:GLY:HA3	15:O:341:ASN:HA	1.82	0.60
16:P:42:A:H8	16:P:42:A:O5'	1.85	0.60
17:N:11:DG:H8	17:N:11:DG:OP2	1.84	0.60
2:M:247:GLN:OE1	2:M:247:GLN:HA	2.01	0.60
2:M:464:LEU:HD23	2:M:464:LEU:N	2.16	0.60
3:A:1468:THR:HG23	7:F:64:ARG:HB2	1.84	0.60
4:B:1135:TYR:HB3	4:B:1146:ILE:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:115:SER:HB3	3:A:227:ARG:HD3	1.84	0.59
4:B:205:VAL:O	4:B:371:ARG:NH1	2.35	0.59
4:B:777:ASN:O	10:J:47:ARG:NH1	2.35	0.59
14:G:170:LEU:HD23	15:O:649:GLY:C	2.25	0.59
15:O:330:ILE:CG1	15:O:695:ARG:CD	2.68	0.59
1:Z:745:VAL:HG21	1:Z:750:LEU:HD21	1.84	0.59
3:A:886:VAL:HG23	6:E:171:PRO:HD3	1.82	0.59
16:P:42:A:H2'	16:P:43:G:O4'	2.02	0.59
2:M:518:LYS:HG2	2:M:519:PHE:H	1.67	0.59
2:M:496:ARG:NH1	3:A:439:HIS:NE2	2.48	0.59
14:G:135:ILE:CB	15:O:650:LYS:HB2	2.32	0.59
4:B:603:MET:HG3	4:B:614:ILE:HG12	1.83	0.59
4:B:924:ARG:NH1	5:C:60:HIS:HB2	2.17	0.59
1:Z:711:ARG:NE	5:C:92:GLU:CD	2.60	0.59
3:A:1209:PRO:HB3	9:I:33:ARG:HH21	1.68	0.59
2:M:313:ILE:HD12	2:M:313:ILE:N	2.18	0.59
8:H:14:ASP:HB2	8:H:29:HIS:HB2	1.85	0.59
9:I:119:CYS:SG	9:I:120:GLY:N	2.76	0.59
18:T:29:DT:C2'	18:T:30:DA:OP1	2.51	0.59
3:A:539:GLN:NE2	4:B:790:GLN:O	2.35	0.59
3:A:1468:THR:H	7:F:60:TYR:HB3	1.68	0.59
15:O:319:GLU:CD	15:O:631:LEU:C	2.71	0.59
3:A:552:ASP:HB2	8:H:24:ARG:HB2	1.85	0.59
13:D:114:LEU:HD22	14:G:84:VAL:HG11	1.85	0.59
1:Z:718:LYS:CE	5:C:92:GLU:HA	2.32	0.58
15:O:319:GLU:CB	15:O:632:PRO:CD	2.62	0.58
2:M:246:THR:HG22	2:M:248:PRO:CD	2.31	0.58
2:M:268:PHE:CD1	2:M:269:PRO:HD2	2.38	0.58
3:A:78:MET:O	4:B:1072:ARG:NH2	2.36	0.58
9:I:68:ILE:O	9:I:122:ARG:NH1	2.36	0.58
2:M:236:VAL:HG12	2:M:237:THR:O	2.04	0.58
2:M:314:ASP:HB3	2:M:316:ASP:N	2.18	0.58
4:B:750:VAL:HG23	4:B:809:VAL:HG13	1.85	0.58
4:B:754:PRO:HB2	4:B:773:PRO:HG2	1.86	0.58
3:A:905:ASN:ND2	3:A:975:SER:OG	2.36	0.58
15:O:319:GLU:HB3	15:O:632:PRO:HD3	1.79	0.58
4:B:1062:ARG:NH1	4:B:1074:PRO:HB3	2.19	0.58
4:B:1089:MET:CE	18:T:21:DG:O4'	2.52	0.58
17:N:9:DT:H3	18:T:35:DA:H61	1.52	0.58
15:O:319:GLU:HB2	15:O:632:PRO:HG3	1.86	0.57
2:M:306:GLY:CA	2:M:309:GLU:HB2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:957:GLU:OE2	3:A:960:ARG:NH2	2.37	0.57
6:E:80:PRO:HA	6:E:107:GLN:HB2	1.86	0.57
15:O:330:ILE:CD1	15:O:695:ARG:HD3	2.34	0.57
8:H:40:ILE:O	8:H:123:MET:HA	2.05	0.57
3:A:75:ALA:HB1	4:B:1131:ARG:HH11	1.69	0.57
4:B:229:SER:HA	4:B:405:ARG:HD3	1.86	0.57
10:J:10:CYS:SG	10:J:42:ARG:NE	2.77	0.57
3:A:894:ASP:OD2	3:A:1396:ARG:NH2	2.38	0.57
4:B:274:ARG:NH2	4:B:281:ASP:OD1	2.36	0.57
4:B:334:LYS:NZ	4:B:337:LYS:NZ	2.53	0.57
13:D:60:VAL:HG13	14:G:103:PRO:HG3	1.86	0.57
14:G:120:ASP:OD2	14:G:123:SER:N	2.34	0.57
3:A:331:LYS:HA	17:N:14:DT:C4	2.39	0.57
3:A:655:ILE:HG12	3:A:985:ARG:NH1	2.20	0.57
15:O:340:GLU:OE2	15:O:340:GLU:N	2.32	0.57
4:B:764:MET:HE1	4:B:938:ARG:NH1	2.19	0.57
3:A:689:ILE:HG21	4:B:985:LEU:HD22	1.86	0.56
15:O:319:GLU:CG	15:O:632:PRO:N	2.67	0.56
2:M:481:LEU:CD2	14:G:13:LEU:HG	2.35	0.56
8:H:39:LEU:HD12	8:H:125:LEU:HD13	1.88	0.56
14:G:134:ASP:C	15:O:651:ALA:CA	2.75	0.56
2:M:247:GLN:N	2:M:248:PRO:HD2	2.20	0.56
2:M:316:ASP:O	2:M:317:ASN:HB2	2.04	0.56
2:M:467:VAL:HG22	2:M:545:VAL:HG21	1.88	0.56
15:O:293:TRP:CZ3	15:O:685:LYS:NZ	2.73	0.56
2:M:467:VAL:HG23	2:M:545:VAL:HG11	1.87	0.56
3:A:814:ASP:OD2	4:B:689:TYR:OH	2.22	0.56
4:B:748:ALA:HB3	4:B:811:TYR:HB2	1.86	0.56
16:P:39:U:H5'	16:P:39:U:H6	1.70	0.56
4:B:760:THR:OG1	4:B:764:MET:SD	2.61	0.56
15:O:319:GLU:CD	15:O:632:PRO:CA	2.79	0.56
4:B:677:MET:HE2	4:B:700:PRO:HB3	1.88	0.56
15:O:293:TRP:H	15:O:293:TRP:CD1	2.23	0.56
2:M:273:PRO:HB3	2:M:456:ILE:HG22	1.87	0.56
12:L:56:ASP:CG	12:L:58:ARG:HH11	2.13	0.56
14:G:142:GLU:CB	15:O:726:GLY:HA3	2.21	0.56
3:A:228:ILE:O	3:A:244:ARG:NH2	2.39	0.56
3:A:394:VAL:HG21	3:A:440:LEU:HD22	1.87	0.56
3:A:1175:ILE:HG12	9:I:54:TYR:HB3	1.86	0.56
4:B:636:LYS:H	4:B:639:HIS:HD2	1.54	0.56
15:O:682:LEU:N	15:O:682:LEU:HD23	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:293:TRP:CD1	2:M:424:LEU:HD21	2.29	0.56
3:A:894:ASP:HB3	6:E:200:ALA:HB2	1.86	0.56
4:B:1119:CYS:HA	4:B:1146:ILE:HA	1.88	0.56
14:G:170:LEU:CD2	15:O:725:LYS:CD	2.81	0.56
3:A:1163:HIS:HE1	3:A:1297:THR:HG22	1.71	0.56
3:A:111:CYS:HB3	3:A:116:LYS:H	1.70	0.55
2:M:374:ASP:HA	2:M:447:LYS:HB3	1.87	0.55
2:M:481:LEU:CD1	14:G:13:LEU:HA	2.31	0.55
2:M:492:GLY:O	2:M:539:TYR:N	2.39	0.55
2:M:517:CYS:HA	2:M:525:VAL:O	2.06	0.55
3:A:197:GLU:OE2	3:A:311:GLN:NE2	2.39	0.55
14:G:108:ILE:HD11	14:G:145:LEU:HD22	1.86	0.55
2:M:481:LEU:CD2	14:G:29:LYS:HG2	2.35	0.55
3:A:331:LYS:CB	18:T:30:DA:H61	2.14	0.55
4:B:924:ARG:HH12	5:C:60:HIS:HB2	1.72	0.55
4:B:1089:MET:HE1	18:T:21:DG:C1'	2.37	0.55
5:C:78:ILE:HD11	5:C:126:ARG:HD2	1.88	0.55
3:A:140:ARG:HH11	3:A:237:GLY:HA2	1.70	0.55
4:B:371:ARG:NE	4:B:380:ARG:HH11	2.04	0.55
14:G:137:ILE:CA	15:O:725:LYS:HZ2	1.96	0.55
15:O:682:LEU:O	15:O:685:LYS:HG2	2.06	0.55
3:A:420:ILE:HB	3:A:445:LYS:HB2	1.87	0.55
4:B:1089:MET:CE	18:T:21:DG:H4'	2.06	0.55
14:G:136:VAL:C	15:O:725:LYS:HZ2	2.15	0.55
15:O:293:TRP:C	15:O:295:ALA:H	2.15	0.55
3:A:331:LYS:HA	17:N:14:DT:N3	2.21	0.55
4:B:942:LYS:HE3	16:P:50:C:OP1	2.06	0.55
3:A:902:GLU:OE2	3:A:985:ARG:NH1	2.40	0.55
15:O:270:LEU:HD21	15:O:685:LYS:HG3	1.88	0.55
15:O:319:GLU:CD	15:O:632:PRO:N	2.65	0.55
1:Z:711:ARG:NH1	5:C:92:GLU:OE2	2.40	0.55
2:M:235:GLY:O	2:M:236:VAL:HG23	2.07	0.55
3:A:330:GLN:HB3	3:A:336:LEU:HD21	1.89	0.55
3:A:1427:LEU:HB2	3:A:1456:GLU:HG3	1.89	0.55
2:M:424:LEU:O	2:M:425:LEU:HG	2.07	0.54
2:M:481:LEU:CD1	14:G:17:TYR:HB2	2.37	0.54
11:K:63:VAL:HG12	11:K:71:ILE:HG22	1.89	0.54
3:A:36:VAL:HA	4:B:1138:ARG:NH1	2.22	0.54
2:M:380:ARG:HH12	2:M:448:TYR:N	2.05	0.54
14:G:138:GLN:NE2	15:O:654:LYS:HG3	2.23	0.54
2:M:389:ILE:HG22	2:M:390:SER:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:469:PHE:CG	2:M:489:LEU:HB3	2.43	0.54
3:A:1093:GLN:HE22	4:B:1093:CYS:HA	1.73	0.54
4:B:1062:ARG:NH2	4:B:1066:PRO:O	2.36	0.54
2:M:246:THR:CG2	2:M:248:PRO:HD2	2.32	0.54
2:M:367:PHE:O	2:M:370:GLN:HB2	2.06	0.54
4:B:200:MET:CE	17:N:24:DG:N2	2.71	0.54
15:O:352:ASN:N	15:O:352:ASN:HD22	2.06	0.54
16:P:38:A:OP2	16:P:38:A:H3'	2.07	0.54
3:A:76:GLY:HA3	3:A:81:CYS:HB2	1.88	0.54
4:B:354:SER:OG	4:B:357:CYS:SG	2.65	0.54
4:B:1031:GLY:O	5:C:36:ARG:NH1	2.39	0.54
3:A:1372:GLU:OE2	6:E:195:ARG:NH1	2.41	0.54
4:B:92:TYR:HB2	4:B:125:TYR:HB2	1.89	0.54
4:B:229:SER:HA	4:B:405:ARG:HH11	1.73	0.54
15:O:645:LEU:HD23	15:O:654:LYS:HB3	1.90	0.54
2:M:566:THR:HG22	2:M:566:THR:O	2.08	0.54
8:H:42:ASP:OD2	8:H:122:LEU:N	2.38	0.54
17:N:7:DA:P	17:N:7:DA:C8	2.97	0.53
2:M:233:LEU:C	2:M:233:LEU:HD23	2.33	0.53
2:M:307:THR:HG23	2:M:336:HIS:CE1	2.43	0.53
6:E:19:GLN:OE1	6:E:138:ASN:ND2	2.40	0.53
13:D:67:TYR:OH	14:G:86:ASP:O	2.26	0.53
2:M:300:TYR:HA	2:M:313:ILE:O	2.08	0.53
3:A:510:GLU:OE2	4:B:1101:GLN:NE2	2.42	0.53
14:G:137:ILE:CB	15:O:725:LYS:NZ	2.69	0.53
2:M:481:LEU:HD21	14:G:13:LEU:HG	1.89	0.53
4:B:99:TRP:HE1	4:B:105:PRO:HG3	1.74	0.53
4:B:489:ILE:HD12	17:N:25:DA:C8	2.44	0.53
13:D:16:ASP:OD2	13:D:18:SER:OG	2.20	0.53
15:O:629:THR:HG21	15:O:658:ILE:HD11	1.90	0.53
2:M:375:CYS:HB3	2:M:379:VAL:HG11	1.90	0.53
16:P:42:A:O2'	16:P:43:G:H5'	2.07	0.53
2:M:494:TYR:HB2	2:M:539:TYR:HD1	1.73	0.53
3:A:760:LEU:HG	3:A:767:LYS:HB2	1.89	0.53
4:B:334:LYS:HZ3	4:B:337:LYS:HD2	1.74	0.53
6:E:112:PRO:HB3	18:T:9:DT:H5''	1.75	0.53
2:M:360:LEU:HA	2:M:411:ARG:O	2.08	0.53
3:A:880:ARG:NH1	7:F:111:PRO:HB2	2.24	0.53
8:H:7:GLU:HG3	8:H:59:VAL:HG22	1.90	0.53
3:A:1103:THR:HG22	3:A:1105:ASN:H	1.73	0.53
3:A:1169:VAL:HG12	3:A:1216:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:721:ILE:HG13	12:L:54:VAL:CG2	2.39	0.53
3:A:461:GLN:OE1	3:A:502:ASN:ND2	2.42	0.53
4:B:899:SER:OG	4:B:1078:ARG:NH2	2.42	0.53
4:B:1016:SER:HB2	4:B:1022:LEU:HD23	1.91	0.53
3:A:395:THR:HG23	3:A:397:PHE:H	1.74	0.52
2:M:419:CYS:HB3	2:M:566:THR:HG23	1.92	0.52
3:A:461:GLN:NE2	4:B:1090:GLU:OE2	2.40	0.52
4:B:483:ARG:O	4:B:525:ASN:ND2	2.42	0.52
15:O:293:TRP:HE3	15:O:686:PHE:HD2	1.57	0.52
3:A:496:PHE:HD2	4:B:791:GLU:HB3	1.74	0.52
3:A:892:GLY:HA3	3:A:1396:ARG:HG3	1.91	0.52
2:M:494:TYR:HD2	2:M:496:ARG:O	1.91	0.52
3:A:922:PHE:HA	3:A:1052:ARG:HD3	1.91	0.52
5:C:260:GLN:HB2	11:K:91:ILE:HG21	1.91	0.52
15:O:322:GLU:CD	15:O:692:LYS:HA	2.34	0.52
15:O:646:LYS:N	15:O:653:ARG:O	2.40	0.52
2:M:388:ILE:HG22	2:M:388:ILE:O	2.09	0.52
4:B:501:LEU:HD12	4:B:505:LEU:HD13	1.92	0.52
6:E:20:LEU:HD21	6:E:24:ARG:HH21	1.74	0.52
8:H:20:LYS:HE2	8:H:23:ASP:HA	1.91	0.52
13:D:112:LYS:HB3	13:D:119:GLU:OE2	2.10	0.52
15:O:317:SER:OG	15:O:667:ASN:CG	2.50	0.52
2:M:496:ARG:NH2	3:A:437:ASP:HB2	2.25	0.52
3:A:693:ILE:HG21	4:B:1023:ARG:HH21	1.73	0.52
15:O:684:GLU:HA	15:O:703:VAL:HG21	1.92	0.52
3:A:655:ILE:HG12	3:A:985:ARG:HH11	1.75	0.52
4:B:1089:MET:HE1	18:T:21:DG:O4'	2.10	0.52
9:I:39:CYS:SG	9:I:40:ARG:N	2.83	0.52
15:O:642:VAL:O	15:O:657:ALA:N	2.40	0.52
1:Z:737:HIS:CE1	12:L:53:VAL:HB	2.45	0.52
2:M:233:LEU:HD21	2:M:348:ILE:CD1	2.35	0.52
15:O:645:LEU:HA	15:O:654:LYS:HA	1.92	0.52
3:A:1030:SER:OG	6:E:162:ARG:NE	2.42	0.51
4:B:417:ILE:HG22	4:B:421:LYS:HZ2	1.75	0.51
2:M:356:VAL:CG1	2:M:358:ARG:HH21	2.23	0.51
3:A:1366:PHE:HB2	3:A:1374:VAL:HG21	1.93	0.51
3:A:1244:ASN:O	3:A:1259:ILE:HA	2.10	0.51
4:B:639:HIS:O	4:B:643:LEU:HB2	2.10	0.51
3:A:46:THR:OG1	3:A:273:GLN:NE2	2.43	0.51
4:B:222:ARG:CZ	17:N:24:DG:C5	2.88	0.51
4:B:474:THR:OG1	4:B:732:ALA:O	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:644:GLU:HB3	15:O:741:ARG:HB3	1.92	0.51
16:P:43:G:H2'	16:P:44:A:O4'	2.11	0.51
3:A:904:GLN:NE2	3:A:981:CYS:O	2.44	0.51
4:B:94:SER:HB3	4:B:123:PRO:HG2	1.92	0.51
4:B:199:LYS:NZ	4:B:202:THR:HG23	2.25	0.51
2:M:556:GLU:CD	2:M:556:GLU:H	2.18	0.51
2:M:230:ALA:HA	2:M:243:GLN:OE1	2.11	0.51
2:M:268:PHE:CE1	2:M:301:MET:HG3	2.46	0.51
2:M:533:LYS:HG2	2:M:535:PHE:O	2.11	0.51
2:M:538:ALA:HB3	2:M:541:THR:OG1	2.10	0.51
3:A:508:SER:HB3	3:A:511:THR:HG22	1.93	0.51
7:F:100:ARG:NH2	7:F:121:ASP:O	2.44	0.51
16:P:34:A:N3	16:P:34:A:C2'	2.73	0.51
2:M:542:ALA:O	2:M:545:VAL:HB	2.11	0.51
3:A:801:GLY:HA3	4:B:503:ASN:HB2	1.92	0.51
4:B:905:ASP:HB2	4:B:924:ARG:HB2	1.93	0.51
4:B:1038:THR:HA	5:C:195:THR:HA	1.93	0.50
5:C:259:LEU:HG	11:K:42:LEU:HD21	1.91	0.50
14:G:170:LEU:CD2	15:O:725:LYS:HD2	2.41	0.50
15:O:373:GLU:HG2	16:P:101:MGT:C4	2.41	0.50
2:M:239:LYS:O	2:M:407:PRO:HB3	2.10	0.50
4:B:585:ASN:OD1	4:B:588:ARG:NH2	2.45	0.50
16:P:42:A:O4'	16:P:42:A:OP1	2.29	0.50
4:B:817:GLN:HB3	4:B:918:PHE:HD1	1.76	0.50
3:A:686:THR:OG1	3:A:687:ILE:N	2.43	0.50
4:B:41:ARG:O	4:B:45:ASP:HB2	2.11	0.50
4:B:380:ARG:HH21	4:B:609:GLU:HG2	1.76	0.50
2:M:268:PHE:CZ	2:M:301:MET:HG3	2.46	0.50
3:A:320:ASN:ND2	3:A:336:LEU:O	2.44	0.50
4:B:873:LEU:HD22	4:B:874:PRO:HD2	1.94	0.50
2:M:293:TRP:O	2:M:293:TRP:CE3	2.65	0.50
2:M:358:ARG:HD3	2:M:411:ARG:HD3	1.92	0.50
4:B:1062:ARG:HE	4:B:1065:GLY:H	1.59	0.50
2:M:396:MET:HG2	2:M:401:ILE:HB	1.93	0.50
3:A:75:ALA:HB1	4:B:1131:ARG:NH1	2.26	0.50
6:E:112:PRO:HB2	18:T:9:DT:C5'	2.34	0.50
2:M:232:PHE:HB2	2:M:320:PHE:CE2	2.47	0.50
3:A:723:ASN:OD1	9:I:109:ARG:NE	2.44	0.50
3:A:901:VAL:HA	3:A:980:PRO:HA	1.92	0.50
3:A:932:ARG:NH1	8:H:108:ALA:HA	2.26	0.50
3:A:331:LYS:HB3	18:T:30:DA:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:135:ILE:C	15:O:651:ALA:HA	2.36	0.50
2:M:347:ILE:HG13	2:M:347:ILE:O	2.12	0.49
2:M:468:ASP:HB2	2:M:537:ASN:OD1	2.12	0.49
3:A:1239:PHE:HB3	3:A:1243:LEU:HD23	1.93	0.49
4:B:59:VAL:HG21	4:B:91:ILE:HD12	1.94	0.49
15:O:311:GLU:CB	15:O:608:LYS:HZ3	2.25	0.49
3:A:392:GLU:OE2	3:A:401:ARG:NH2	2.37	0.49
3:A:480:SER:HB3	11:K:2:ASN:HB2	1.93	0.49
15:O:293:TRP:HB3	15:O:667:ASN:CB	2.42	0.49
2:M:236:VAL:HG12	2:M:237:THR:N	2.27	0.49
3:A:551:ARG:HH12	8:H:27:ARG:HH21	1.59	0.49
3:A:756:ALA:HB2	3:A:786:ALA:HB2	1.95	0.49
3:A:762:GLU:OE2	3:A:767:LYS:NZ	2.36	0.49
15:O:654:LYS:O	15:O:654:LYS:NZ	2.33	0.49
2:M:232:PHE:CD1	2:M:238:VAL:HG21	2.47	0.49
3:A:1073:GLU:OE2	3:A:1077:ASN:ND2	2.46	0.49
3:A:1473:LEU:HD23	7:F:104:ILE:HG21	1.94	0.49
4:B:494:LYS:HZ2	17:N:27:DA:H5'	1.77	0.49
6:E:44:PHE:HB3	6:E:53:PRO:HB3	1.93	0.49
15:O:207:ASP:OD1	16:P:101:MGT:C2	2.58	0.49
6:E:131:LEU:HD23	6:E:133:GLN:H	1.76	0.49
14:G:170:LEU:CG	15:O:725:LYS:HE3	2.17	0.49
15:O:650:LYS:H	15:O:650:LYS:HD2	1.77	0.49
7:F:64:ARG:NH2	14:G:61:PRO:CG	2.69	0.49
14:G:170:LEU:HD22	15:O:725:LYS:CD	2.41	0.49
15:O:293:TRP:HE1	15:O:669:THR:CB	2.25	0.49
6:E:26:TYR:HD1	6:E:64:HIS:HA	1.77	0.49
12:L:56:ASP:OD1	12:L:58:ARG:NH1	2.46	0.49
14:G:97:LEU:HD23	14:G:108:ILE:HD12	1.93	0.49
14:G:145:LEU:HD13	14:G:161:GLY:HA3	1.94	0.49
12:L:17:TYR:HB3	12:L:44:MET:HB3	1.94	0.49
14:G:136:VAL:HG23	15:O:651:ALA:HB1	1.91	0.49
1:Z:721:ILE:CG1	12:L:54:VAL:HG21	2.41	0.49
4:B:873:LEU:HD13	4:B:875:GLU:H	1.78	0.49
14:G:170:LEU:CD2	15:O:650:LYS:C	2.83	0.49
15:O:293:TRP:CH2	15:O:666:LEU:CD1	2.96	0.49
3:A:375:ILE:HG12	3:A:666:ARG:HG3	1.94	0.49
4:B:591:ARG:HD3	4:B:603:MET:HE1	1.95	0.49
7:F:53:THR:HG1	7:F:118:TRP:HE1	1.61	0.49
9:I:11:PHE:HA	9:I:55:VAL:HG11	1.94	0.49
15:O:293:TRP:CH2	15:O:685:LYS:NZ	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:657:ALA:HB3	15:O:659:HIS:NE2	2.28	0.49
6:E:3:ASP:OD2	6:E:47:LYS:HA	2.12	0.48
2:M:496:ARG:HH22	3:A:421:ARG:HH22	1.60	0.48
3:A:381:PRO:HD2	3:A:384:ILE:HD12	1.95	0.48
3:A:805:ARG:NH2	4:B:670:GLU:O	2.47	0.48
4:B:506:TRP:HZ2	4:B:677:MET:HE1	1.76	0.48
15:O:293:TRP:CH2	15:O:666:LEU:HD12	2.48	0.48
3:A:241:ARG:NH1	3:A:242:TYR:OH	2.46	0.48
4:B:384:ASP:O	4:B:390:ASN:ND2	2.46	0.48
16:P:31:G:N3	16:P:31:G:H2'	2.28	0.48
2:M:358:ARG:HG3	2:M:409:SER:HB3	1.94	0.48
3:A:383:SER:H	11:K:2:ASN:HD21	1.60	0.48
4:B:280:SER:OG	9:I:21:ASN:O	2.29	0.48
15:O:653:ARG:HB3	15:O:653:ARG:HH11	1.78	0.48
3:A:1461:GLY:HA3	4:B:1152:PRO:HD3	1.94	0.48
6:E:111:THR:HG21	17:N:39:DT:OP1	2.13	0.48
11:K:61:TYR:HA	11:K:72:ILE:O	2.14	0.48
2:M:325:LEU:HA	2:M:406:GLU:HG2	1.95	0.48
3:A:576:GLN:HE21	3:A:580:LEU:HD21	1.78	0.48
3:A:680:LEU:HD21	4:B:784:SER:HB3	1.96	0.48
5:C:105:VAL:HG11	5:C:115:VAL:HG22	1.96	0.48
8:H:27:ARG:HA	8:H:41:LEU:O	2.14	0.48
3:A:370:ASP:OD2	11:K:65:HIS:NE2	2.32	0.48
3:A:613:GLU:OE2	3:A:623:PRO:HD2	2.13	0.48
4:B:796:MET:HB2	4:B:948:GLN:HG2	1.93	0.48
2:M:235:GLY:O	2:M:236:VAL:CG2	2.62	0.48
3:A:1097:GLU:O	3:A:1101:GLN:NE2	2.47	0.48
8:H:89:GLU:OE2	8:H:147:LYS:HG2	2.14	0.48
2:M:316:ASP:O	2:M:317:ASN:CB	2.61	0.48
3:A:30:GLU:HA	3:A:33:ARG:HG2	1.95	0.48
2:M:358:ARG:HH11	2:M:411:ARG:NH1	2.12	0.47
2:M:424:LEU:O	2:M:425:LEU:CB	2.62	0.47
2:M:475:ARG:HA	2:M:485:ASN:HA	1.96	0.47
3:A:457:ILE:HD11	3:A:515:ILE:HD12	1.95	0.47
5:C:175:LYS:HZ2	12:L:57:ALA:HB3	1.79	0.47
6:E:55:ARG:NH1	6:E:107:GLN:HE21	2.12	0.47
11:K:56:VAL:HG22	11:K:77:THR:HG22	1.95	0.47
16:P:42:A:C8	16:P:42:A:C5'	2.94	0.47
2:M:461:PRO:HG2	2:M:464:LEU:HG	1.96	0.47
2:M:494:TYR:CD1	2:M:539:TYR:CD1	3.02	0.47
3:A:866:LYS:HD3	4:B:1091:ARG:HH22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:977:VAL:HG21	3:A:1040:LEU:HD21	1.96	0.47
3:A:1474:LEU:HB2	7:F:105:ILE:HB	1.95	0.47
13:D:112:LYS:NZ	13:D:124:ASP:OD2	2.42	0.47
2:M:377:PHE:O	2:M:381:LEU:HB2	2.14	0.47
3:A:460:ARG:NH2	16:P:50:C:O2'	2.47	0.47
5:C:67:ARG:NH2	5:C:149:LEU:O	2.38	0.47
13:D:42:GLU:HG2	13:D:65:LEU:HD11	1.96	0.47
2:M:306:GLY:C	2:M:309:GLU:HB2	2.39	0.47
3:A:331:LYS:CB	18:T:30:DA:N6	2.75	0.47
3:A:367:ILE:HG22	3:A:482:PHE:HB2	1.96	0.47
4:B:718:GLN:HG2	4:B:720:PRO:HD2	1.96	0.47
18:T:23:DC:H2''	18:T:24:DT:H5'	1.96	0.47
2:M:329:PHE:HD2	2:M:331:LYS:H	1.63	0.47
5:C:259:LEU:HD21	11:K:35:ILE:HD12	1.96	0.47
6:E:195:ARG:HH12	6:E:205:THR:HG21	1.80	0.47
9:I:24:LEU:HB3	9:I:37:TYR:HB3	1.96	0.47
15:O:270:LEU:HG	15:O:685:LYS:HB2	1.95	0.47
2:M:287:LYS:HB2	2:M:288:PRO:CD	2.45	0.47
3:A:221:VAL:HG12	3:A:249:ILE:HD11	1.96	0.47
3:A:1428:MET:HB2	3:A:1456:GLU:OE2	2.15	0.47
2:M:420:THR:O	2:M:420:THR:CG2	2.61	0.47
2:M:422:ARG:HH21	2:M:423:LYS:NZ	2.12	0.47
2:M:521:ASN:O	2:M:522:ASN:HB2	2.15	0.47
3:A:566:PHE:HB2	3:A:675:VAL:HG12	1.96	0.47
3:A:1218:ARG:NH1	3:A:1253:GLU:HA	2.30	0.47
4:B:200:MET:HE2	17:N:24:DG:C2	2.49	0.47
13:D:138:ARG:HH22	15:O:728:SER:CB	2.27	0.47
14:G:134:ASP:C	15:O:650:LYS:HD3	2.39	0.47
14:G:135:ILE:HG12	15:O:650:LYS:HB3	1.94	0.47
16:P:42:A:C2'	16:P:43:G:H5'	2.45	0.47
2:M:473:ILE:HD11	2:M:485:ASN:HB2	1.97	0.47
3:A:481:THR:H	3:A:483:ARG:NH1	2.04	0.47
3:A:1141:VAL:HA	3:A:1357:THR:HG23	1.97	0.47
4:B:931:ILE:HA	4:B:945:CYS:HB3	1.97	0.47
14:G:49:THR:N	14:G:73:LYS:O	2.47	0.47
14:G:142:GLU:OE1	15:O:726:GLY:C	2.57	0.47
1:Z:706:ILE:HD11	1:Z:727:ALA:H	1.79	0.47
3:A:186:ARG:HG2	3:A:202:TRP:HD1	1.80	0.47
3:A:556:GLU:OE1	3:A:583:ARG:NH2	2.47	0.47
3:A:854:THR:CG2	18:T:20:DA:N1	2.77	0.47
4:B:1077:GLY:C	18:T:24:DT:OP1	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:40:ALA:HB1	5:C:171:LYS:HG3	1.95	0.47
6:E:64:HIS:ND1	6:E:66:ASP:O	2.48	0.47
7:F:57:MET:HE1	7:F:120:VAL:HG13	1.97	0.47
2:M:278:LYS:HD2	2:M:551:ASN:OD1	2.14	0.47
2:M:496:ARG:HH22	3:A:437:ASP:HB2	1.80	0.47
3:A:875:TYR:HA	3:A:1083:PRO:HB3	1.96	0.47
5:C:256:LEU:HD13	11:K:94:LEU:HB3	1.97	0.47
13:D:31:THR:HG22	14:G:3:TYR:HE1	1.80	0.47
1:Z:711:ARG:CZ	5:C:92:GLU:OE2	2.62	0.46
1:Z:728:THR:OG1	1:Z:731:THR:N	2.47	0.46
2:M:293:TRP:O	2:M:293:TRP:HE3	1.98	0.46
3:A:880:ARG:HH11	7:F:111:PRO:HB2	1.80	0.46
3:A:1184:THR:HG23	3:A:1187:ALA:H	1.80	0.46
15:O:293:TRP:C	15:O:295:ALA:N	2.73	0.46
4:B:567:ILE:HA	4:B:612:ILE:O	2.15	0.46
4:B:937:SER:OG	4:B:938:ARG:N	2.49	0.46
15:O:326:GLY:CA	15:O:341:ASN:HA	2.45	0.46
2:M:363:ASP:OD1	2:M:448:TYR:CD1	2.68	0.46
6:E:194:ILE:HG13	6:E:204:ILE:HG12	1.98	0.46
14:G:134:ASP:OD2	15:O:650:LYS:CD	2.64	0.46
15:O:401:PHE:CZ	15:O:403:CYS:HB2	2.51	0.46
3:A:913:ASN:OD1	3:A:963:ARG:NH1	2.45	0.46
4:B:411:LEU:HD21	4:B:435:ILE:HG23	1.98	0.46
4:B:573:TRP:NE1	4:B:575:GLY:O	2.49	0.46
4:B:584:MET:HG3	4:B:605:ARG:HB2	1.96	0.46
13:D:17:ALA:HB2	14:G:80:PHE:HB3	1.97	0.46
14:G:134:ASP:O	15:O:650:LYS:HD3	2.16	0.46
14:G:136:VAL:C	15:O:725:LYS:NZ	2.74	0.46
14:G:137:ILE:N	15:O:725:LYS:NZ	2.61	0.46
3:A:1005:HIS:HD2	3:A:1006:PRO:HD2	1.80	0.46
6:E:9:ARG:HG3	6:E:136:LEU:HD21	1.97	0.46
14:G:152:VAL:HA	14:G:157:ILE:HA	1.97	0.46
2:M:481:LEU:HD12	14:G:17:TYR:HD2	1.81	0.46
3:A:833:PRO:HB2	4:B:506:TRP:HH2	1.80	0.46
4:B:438:ARG:O	4:B:442:ASP:HB2	2.16	0.46
4:B:834:ARG:NH1	16:P:33:C:H2'	2.31	0.46
6:E:107:GLN:HA	6:E:132:GLN:HG3	1.98	0.46
14:G:135:ILE:HA	15:O:650:LYS:CA	2.44	0.46
15:O:293:TRP:CZ2	15:O:294:HIS:CE1	3.04	0.46
2:M:278:LYS:HB2	2:M:551:ASN:HD21	1.81	0.46
2:M:309:GLU:OE1	2:M:309:GLU:CA	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:491:VAL:HG11	2:M:498:PHE:HD1	1.81	0.46
4:B:282:ARG:HH11	9:I:16:PHE:HD2	1.61	0.46
4:B:778:SER:HA	10:J:47:ARG:HH12	1.79	0.46
4:B:907:VAL:HG22	4:B:921:ILE:HG12	1.98	0.46
5:C:27:ASP:OD2	11:K:52:LYS:HD2	2.16	0.46
5:C:183:ALA:HB3	5:C:232:ASN:HB3	1.97	0.46
5:C:205:LYS:HZ1	5:C:212:ASP:C	2.24	0.46
9:I:81:THR:O	9:I:93:GLU:HA	2.15	0.46
15:O:232:PHE:CE1	15:O:286:TYR:HA	2.51	0.46
1:Z:721:ILE:HB	12:L:54:VAL:HB	1.97	0.46
2:M:550:SER:O	2:M:552:PRO:HD3	2.16	0.46
4:B:601:VAL:HG22	4:B:616:THR:HG23	1.98	0.46
4:B:1094:GLN:HB2	4:B:1103:LEU:HD13	1.98	0.46
5:C:154:ARG:HD3	10:J:64:PRO:HD3	1.98	0.46
14:G:134:ASP:OD2	15:O:650:LYS:HD3	2.15	0.46
14:G:136:VAL:HB	15:O:652:GLN:O	2.16	0.46
3:A:61:ARG:HA	3:A:72:GLN:HB3	1.97	0.46
3:A:631:GLU:OE2	3:A:992:LYS:NZ	2.28	0.46
4:B:124:LEU:HB3	4:B:150:GLY:O	2.16	0.46
4:B:438:ARG:HD2	4:B:442:ASP:OD2	2.16	0.46
2:M:314:ASP:C	2:M:316:ASP:N	2.72	0.45
3:A:997:ASN:ND2	8:H:136:GLU:OE1	2.49	0.45
4:B:842:HIS:HD2	16:P:37:C:N3	2.14	0.45
4:B:180:ASP:OD1	4:B:472:ARG:NH2	2.50	0.45
4:B:489:ILE:HD11	17:N:25:DA:H62	1.80	0.45
1:Z:711:ARG:HH21	5:C:93:PHE:HE2	1.53	0.45
4:B:483:ARG:NH2	4:B:527:ALA:O	2.49	0.45
15:O:646:LYS:HE3	15:O:646:LYS:HB3	1.52	0.45
2:M:546:CYS:HA	2:M:549:ILE:HD12	1.97	0.45
3:A:1188:GLU:OE2	3:A:1258:ARG:HD2	2.17	0.45
4:B:84:TYR:HA	4:B:131:THR:O	2.16	0.45
15:O:333:ASP:OD1	15:O:341:ASN:ND2	2.48	0.45
2:M:314:ASP:HB2	2:M:318:SER:HB2	1.99	0.45
3:A:397:PHE:HZ	3:A:1486:ILE:HG12	1.81	0.45
3:A:554:PHE:HB3	3:A:585:LEU:HG	1.99	0.45
5:C:131:THR:HG21	10:J:16:ASN:HD22	1.81	0.45
15:O:680:ILE:HD12	15:O:680:ILE:HA	1.86	0.45
2:M:347:ILE:CD1	2:M:360:LEU:HD11	2.46	0.45
3:A:200:ALA:O	3:A:213:LYS:HA	2.17	0.45
4:B:626:LEU:HD23	4:B:662:VAL:HG12	1.98	0.45
4:B:636:LYS:HG3	4:B:638:ARG:HH12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:674:GLN:O	15:O:679:ARG:NH1	2.50	0.45
3:A:690:GLY:HA2	4:B:1023:ARG:HG2	1.99	0.45
4:B:779:ILE:HD13	4:B:1045:PRO:HB3	1.99	0.45
2:M:244:VAL:O	2:M:244:VAL:HG12	2.16	0.45
2:M:516:GLU:HG2	2:M:527:MET:HG3	1.99	0.45
3:A:579:ILE:HB	3:A:585:LEU:HB3	1.99	0.45
3:A:1186:VAL:HG11	3:A:1213:ARG:HH12	1.81	0.45
3:A:1353:ASP:O	3:A:1357:THR:OG1	2.30	0.45
8:H:60:ILE:HG21	8:H:135:PHE:HE1	1.80	0.45
9:I:17:CYS:SG	9:I:18:GLN:N	2.90	0.45
14:G:134:ASP:CG	15:O:650:LYS:CE	2.90	0.45
3:A:684:GLY:HA3	4:B:1037:ILE:HG23	1.99	0.45
3:A:902:GLU:OE1	3:A:982:ASN:ND2	2.49	0.45
14:G:170:LEU:HD22	15:O:650:LYS:O	2.17	0.45
2:M:365:ILE:N	2:M:365:ILE:HD12	2.32	0.45
2:M:368:ASN:O	2:M:369:SER:HB2	2.17	0.45
2:M:230:ALA:HB2	2:M:243:GLN:OE1	2.17	0.44
3:A:481:THR:N	3:A:483:ARG:HH12	2.04	0.44
4:B:714:PRO:HD2	4:B:1001:PRO:HB3	1.99	0.44
15:O:373:GLU:HG2	16:P:101:MGT:N9	2.32	0.44
16:P:32:A:OP2	16:P:32:A:C8	2.71	0.44
2:M:395:LYS:HB3	2:M:401:ILE:CG1	2.46	0.44
2:M:402:ASP:O	2:M:403:LYS:C	2.60	0.44
3:A:61:ARG:O	3:A:73:THR:OG1	2.35	0.44
4:B:801:VAL:HG13	4:B:929:PRO:HD2	1.99	0.44
5:C:59:LEU:HD12	5:C:151:VAL:HG23	1.99	0.44
17:N:8:DC:OP2	17:N:8:DC:H2'	2.16	0.44
3:A:36:VAL:HG23	4:B:1138:ARG:NH1	2.26	0.44
3:A:1309:MET:HB3	3:A:1336:LEU:HD23	2.00	0.44
3:A:1472:ASP:OD2	14:G:58:VAL:HG13	2.16	0.44
4:B:86:LEU:HD23	4:B:130:LYS:HB3	2.00	0.44
4:B:222:ARG:NH2	17:N:24:DG:C4	2.60	0.44
4:B:760:THR:O	4:B:999:ALA:N	2.50	0.44
2:M:278:LYS:HG2	2:M:557:MET:CE	2.46	0.44
3:A:1212:LEU:HB2	3:A:1285:LEU:HD21	2.00	0.44
6:E:192:LYS:HE2	6:E:194:ILE:HD11	1.98	0.44
14:G:123:SER:HB3	15:O:653:ARG:HH22	1.68	0.44
2:M:462:PRO:HD2	2:M:555:LYS:HE2	1.99	0.44
2:M:481:LEU:HD12	14:G:17:TYR:CD2	2.53	0.44
3:A:487:SER:OG	3:A:673:GLN:NE2	2.50	0.44
3:A:1186:VAL:HG11	3:A:1213:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:744:MET:HE1	4:B:906:GLN:HG3	1.99	0.44
4:B:807:ARG:NH1	5:C:66:HIS:HD2	2.15	0.44
2:M:390:SER:O	2:M:394:GLU:HG3	2.18	0.44
3:A:26:LEU:HD12	4:B:1166:SER:HA	1.99	0.44
15:O:337:THR:HA	15:O:386:CYS:SG	2.58	0.44
2:M:230:ALA:CA	2:M:243:GLN:OE1	2.65	0.44
4:B:50:PHE:HB2	4:B:397:GLY:HA2	2.00	0.44
4:B:84:TYR:HB3	4:B:132:VAL:HG23	1.98	0.44
7:F:80:MET:HG3	7:F:103:PRO:HD3	2.00	0.44
15:O:650:LYS:N	15:O:650:LYS:HD2	2.32	0.44
16:P:36:A:N3	16:P:36:A:C5'	2.79	0.44
18:T:34:DT:H2'	18:T:34:DT:OP2	2.18	0.44
3:A:18:ILE:HD12	4:B:1171:MET:HB2	1.99	0.44
3:A:1020:LEU:O	3:A:1034:GLN:NE2	2.51	0.44
3:A:1286:ARG:HH21	9:I:54:TYR:HB2	1.82	0.44
4:B:87:LYS:HB3	4:B:129:THR:HG23	1.99	0.44
4:B:94:SER:OG	4:B:95:LYS:N	2.49	0.44
4:B:699:HIS:HD2	4:B:701:SER:H	1.65	0.44
4:B:1022:LEU:HD13	4:B:1023:ARG:NH1	2.32	0.44
5:C:98:SER:HA	5:C:165:ALA:O	2.17	0.44
2:M:501:ILE:CD1	2:M:524:TRP:O	2.66	0.44
3:A:1212:LEU:HB3	3:A:1259:ILE:HB	2.00	0.44
2:M:392:ARG:HH21	2:M:406:GLU:CD	2.25	0.43
2:M:481:LEU:HD13	14:G:17:TYR:HB2	1.99	0.43
3:A:603:ILE:HG12	3:A:629:VAL:HG22	2.00	0.43
4:B:330:VAL:HG12	4:B:331:THR:HG23	1.99	0.43
8:H:28:LEU:O	8:H:40:ILE:HA	2.18	0.43
16:P:39:U:C6	16:P:39:U:OP2	2.71	0.43
2:M:244:VAL:HG12	2:M:250:LEU:HB2	1.99	0.43
2:M:390:SER:N	2:M:391:PRO:CD	2.81	0.43
4:B:737:ILE:HG21	4:B:743:ARG:HD3	2.00	0.43
4:B:756:LYS:O	4:B:777:ASN:ND2	2.50	0.43
8:H:64:LEU:HB3	8:H:83:SER:HB2	1.99	0.43
15:O:641:ILE:HD13	15:O:641:ILE:HA	1.81	0.43
2:M:269:PRO:HG2	2:M:301:MET:CE	2.48	0.43
2:M:380:ARG:NH1	2:M:448:TYR:N	2.66	0.43
3:A:695:ASP:N	3:A:695:ASP:OD1	2.51	0.43
3:A:1027:ASP:OD1	3:A:1027:ASP:N	2.52	0.43
16:P:35:U:C6	16:P:35:U:C3'	3.01	0.43
2:M:303:LEU:HD12	2:M:303:LEU:C	2.44	0.43
3:A:417:LYS:HD3	3:A:430:ARG:HH21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:97:LEU:HB3	14:G:108:ILE:HB	2.01	0.43
2:M:367:PHE:CZ	2:M:387:GLU:HB3	2.53	0.43
3:A:628:VAL:HA	3:A:638:GLY:HA3	2.00	0.43
4:B:65:ILE:HB	4:B:416:ARG:NH1	2.30	0.43
4:B:334:LYS:HZ3	4:B:337:LYS:CD	2.31	0.43
6:E:75:PHE:HB2	6:E:104:ILE:HG22	2.00	0.43
14:G:136:VAL:HB	15:O:652:GLN:C	2.43	0.43
16:P:39:U:OP2	16:P:39:U:C5	2.71	0.43
2:M:402:ASP:OD2	2:M:404:THR:HB	2.19	0.43
3:A:110:VAL:HG21	3:A:228:ILE:HD11	2.00	0.43
3:A:1168:LYS:HE2	3:A:1224:ARG:HH21	1.83	0.43
4:B:131:THR:HG22	4:B:141:GLN:HB3	2.00	0.43
7:F:79:VAL:HG23	7:F:96:GLU:OE2	2.19	0.43
14:G:52:ASP:OD2	14:G:73:LYS:HG2	2.19	0.43
2:M:269:PRO:HG2	2:M:301:MET:HE1	2.01	0.43
3:A:863:ARG:HB3	3:A:1414:ILE:HG22	2.01	0.43
2:M:380:ARG:O	2:M:384:ILE:HG13	2.18	0.43
3:A:809:HIS:HE1	4:B:506:TRP:CE2	2.37	0.43
4:B:274:ARG:HH11	4:B:312:GLN:HA	1.83	0.43
14:G:135:ILE:CA	15:O:650:LYS:C	2.78	0.43
3:A:38:GLU:H	3:A:61:ARG:NH1	2.11	0.43
3:A:229:SER:OG	3:A:230:ASP:N	2.52	0.43
3:A:467:MET:HG3	3:A:524:MET:HB3	1.99	0.43
3:A:551:ARG:HH12	8:H:27:ARG:NH2	2.16	0.43
5:C:70:LEU:HD12	10:J:6:ARG:HD2	2.00	0.43
3:A:420:ILE:HD11	3:A:426:ARG:NH1	2.34	0.43
3:A:715:GLU:HA	3:A:718:GLU:HG2	2.01	0.43
3:A:869:GLU:OE2	3:A:1455:SER:HB2	2.18	0.43
4:B:494:LYS:NZ	17:N:27:DA:H5'	2.33	0.43
2:M:377:PHE:CZ	2:M:443:GLN:HG2	2.54	0.42
3:A:1433:GLU:HB2	18:T:18:DT:C5'	2.48	0.42
4:B:42:GLN:HE22	4:B:483:ARG:HA	1.84	0.42
4:B:494:LYS:NZ	17:N:27:DA:C5'	2.82	0.42
6:E:112:PRO:CG	18:T:9:DT:H5'	2.36	0.42
16:P:31:G:N3	16:P:31:G:C2'	2.81	0.42
3:A:330:GLN:HG3	3:A:332:SER:H	1.83	0.42
3:A:1365:ILE:O	3:A:1369:LEU:N	2.45	0.42
4:B:83:ARG:NH1	4:B:139:GLN:HB3	2.19	0.42
4:B:378:GLY:HA3	9:I:102:ALA:HB3	2.00	0.42
4:B:610:ARG:NH1	9:I:71:ASP:OD2	2.52	0.42
10:J:6:ARG:HG2	10:J:13:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:78:ARG:HD2	14:G:79:PRO:HD2	2.01	0.42
14:G:99:THR:HG21	14:G:143:ILE:HD11	2.00	0.42
1:Z:734:VAL:HG21	1:Z:750:LEU:HD21	1.99	0.42
2:M:402:ASP:O	2:M:405:GLN:HG2	2.19	0.42
2:M:418:ILE:HD12	2:M:418:ILE:HA	1.75	0.42
2:M:545:VAL:O	2:M:549:ILE:HG13	2.19	0.42
2:M:247:GLN:N	2:M:248:PRO:CD	2.82	0.42
3:A:196:LEU:HD22	3:A:311:GLN:HE22	1.84	0.42
3:A:505:LEU:O	4:B:1106:ARG:NH2	2.52	0.42
3:A:514:GLU:OE2	4:B:1099:ALA:HA	2.18	0.42
7:F:64:ARG:NH2	14:G:61:PRO:HB3	2.34	0.42
8:H:27:ARG:HH11	8:H:40:ILE:CG2	2.32	0.42
13:D:135:GLN:HE22	13:D:138:ARG:NH1	2.08	0.42
15:O:330:ILE:HG21	15:O:695:ARG:HD2	2.01	0.42
2:M:235:GLY:C	2:M:236:VAL:HG23	2.45	0.42
3:A:41:ILE:HG22	3:A:88:ILE:HG12	2.01	0.42
3:A:606:HIS:CE1	3:A:641:CYS:HB3	2.54	0.42
3:A:1210:TRP:HD1	3:A:1285:LEU:HD13	1.85	0.42
3:A:1411:LEU:HD23	3:A:1411:LEU:HA	1.89	0.42
4:B:84:TYR:HE1	4:B:423:ILE:HD12	1.84	0.42
4:B:285:LEU:HD23	9:I:16:PHE:HZ	1.84	0.42
4:B:334:LYS:HZ3	4:B:337:LYS:HZ2	1.66	0.42
7:F:53:THR:OG1	7:F:118:TRP:NE1	2.52	0.42
9:I:65:LEU:HD22	9:I:122:ARG:HG2	2.00	0.42
11:K:7:PHE:HB2	11:K:11:LEU:HD12	2.01	0.42
2:M:250:LEU:O	2:M:251:GLY:C	2.62	0.42
2:M:402:ASP:CG	2:M:404:THR:HB	2.44	0.42
2:M:473:ILE:HA	2:M:486:VAL:O	2.19	0.42
3:A:902:GLU:O	3:A:978:VAL:HA	2.20	0.42
4:B:347:MET:HE3	4:B:348:LEU:HD13	2.02	0.42
4:B:1040:GLN:NE2	5:C:195:THR:OG1	2.53	0.42
8:H:98:ARG:HB3	8:H:115:TYR:HB2	2.02	0.42
15:O:677:ASN:OD1	15:O:677:ASN:N	2.52	0.42
16:P:40:A:H5'	16:P:41:A:H4'	2.00	0.42
2:M:402:ASP:HB3	2:M:405:GLN:CG	2.49	0.42
3:A:1170:THR:HA	3:A:1216:LEU:HD13	2.00	0.42
3:A:1185:VAL:HG11	9:I:51:SER:HB2	2.01	0.42
4:B:236:TRP:HB2	4:B:259:THR:HB	2.02	0.42
4:B:908:MET:HE2	12:L:43:ILE:HG23	2.01	0.42
8:H:27:ARG:HH11	8:H:40:ILE:HG22	1.84	0.42
13:D:32:LEU:N	14:G:2:PHE:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:328:PRO:HD2	2:M:392:ARG:HG2	2.01	0.42
3:A:470:MET:HB3	3:A:521:VAL:HG12	2.02	0.42
3:A:1153:ARG:NH1	3:A:1156:ASP:OD2	2.48	0.42
14:G:101:ILE:HB	14:G:104:MET:HE2	2.02	0.42
2:M:518:LYS:HG2	2:M:519:PHE:N	2.34	0.42
3:A:340:LYS:HG2	3:A:1436:VAL:HG21	2.02	0.42
4:B:334:LYS:HZ3	4:B:337:LYS:CE	2.33	0.42
5:C:49:TRP:HB3	5:C:164:TYR:HB2	2.00	0.42
14:G:117:MET:HE3	14:G:128:TYR:HB3	2.02	0.42
15:O:311:GLU:HB2	15:O:608:LYS:HZ3	1.84	0.42
2:M:333:LEU:O	2:M:395:LYS:HE3	2.20	0.41
2:M:481:LEU:HD21	14:G:13:LEU:HA	2.02	0.41
2:M:494:TYR:HB2	2:M:539:TYR:CD1	2.54	0.41
3:A:35:SER:OG	3:A:87:HIS:ND1	2.50	0.41
3:A:457:ILE:HD13	3:A:457:ILE:HA	1.96	0.41
4:B:483:ARG:HH12	4:B:528:LEU:HA	1.85	0.41
4:B:807:ARG:NH1	5:C:66:HIS:CD2	2.87	0.41
6:E:34:ASP:N	6:E:34:ASP:OD1	2.54	0.41
16:P:35:U:H6	16:P:35:U:C5'	2.30	0.41
2:M:233:LEU:HD12	2:M:346:MET:HB3	2.02	0.41
2:M:556:GLU:CD	2:M:556:GLU:N	2.78	0.41
4:B:507:GLY:HA3	4:B:623:ARG:HH12	1.81	0.41
6:E:6:GLU:OE2	6:E:9:ARG:NH1	2.53	0.41
13:D:96:GLU:OE2	13:D:121:ARG:NH1	2.53	0.41
14:G:89:VAL:HA	14:G:99:THR:HG22	2.02	0.41
3:A:418:TYR:HB2	3:A:447:GLU:HB2	2.02	0.41
4:B:706:VAL:HG23	4:B:767:LEU:HD22	2.01	0.41
2:M:376:ASP:O	2:M:379:VAL:HB	2.20	0.41
2:M:521:ASN:O	2:M:522:ASN:CB	2.69	0.41
3:A:618:TYR:HB3	3:A:623:PRO:HD3	2.02	0.41
3:A:1321:ILE:HG12	3:A:1331:LEU:HD13	2.01	0.41
4:B:934:LYS:HG2	4:B:1051:LEU:HD12	2.00	0.41
8:H:41:LEU:HG	8:H:43:VAL:HG13	2.02	0.41
9:I:80:ARG:HG3	9:I:95:VAL:HG12	2.01	0.41
2:M:321:HIS:HE1	2:M:323:SER:HA	1.85	0.41
3:A:230:ASP:HA	3:A:240:PRO:HG2	2.03	0.41
3:A:763:TYR:HD2	5:C:198:PRO:HB3	1.85	0.41
3:A:763:TYR:OH	8:H:23:ASP:OD2	2.38	0.41
3:A:1371:ILE:HG22	6:E:177:ASP:OD2	2.20	0.41
4:B:285:LEU:HA	4:B:285:LEU:HD12	1.85	0.41
4:B:806:PHE:HB3	4:B:1050:ARG:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:14:ARG:HE	6:E:18:MET:HE2	1.85	0.41
6:E:172:ARG:HD3	6:E:210:GLN:HB2	2.01	0.41
15:O:293:TRP:O	15:O:295:ALA:N	2.53	0.41
2:M:293:TRP:HD1	2:M:424:LEU:CD2	2.23	0.41
3:A:129:ILE:HG23	3:A:143:HIS:HD1	1.86	0.41
6:E:84:ILE:HA	6:E:87:ILE:HG12	2.02	0.41
6:E:110:MET:HE1	6:E:118:LEU:HD11	2.02	0.41
14:G:123:SER:OG	15:O:653:ARG:NH2	2.53	0.41
16:P:35:U:OP1	16:P:35:U:O3'	2.39	0.41
3:A:79:THR:HA	4:B:1072:ARG:HH22	1.85	0.41
3:A:1128:ILE:HD13	3:A:1128:ILE:HA	1.87	0.41
4:B:93:LEU:HD23	4:B:124:LEU:HD13	2.03	0.41
4:B:116:ARG:HH11	4:B:118:LEU:HD11	1.83	0.41
4:B:393:LEU:HD22	4:B:485:LEU:HD22	2.03	0.41
4:B:715:ASP:OD1	4:B:715:ASP:N	2.53	0.41
4:B:954:MET:HG3	4:B:963:PRO:HD2	2.00	0.41
2:M:361:ILE:CG2	2:M:384:ILE:HD13	2.49	0.41
16:P:38:A:H1'	16:P:39:U:O2	2.20	0.41
2:M:333:LEU:HD23	2:M:333:LEU:HA	1.89	0.41
2:M:367:PHE:O	2:M:368:ASN:HB2	2.21	0.41
3:A:522:PRO:HB2	3:A:662:HIS:HD2	1.85	0.41
3:A:1038:THR:O	3:A:1042:ASN:ND2	2.54	0.41
3:A:1473:LEU:HD22	7:F:68:THR:HG21	2.02	0.41
4:B:26:CYS:O	4:B:30:ILE:HG12	2.21	0.41
4:B:27:TRP:CD1	4:B:762:ARG:NH1	2.89	0.41
4:B:271:ILE:HG21	4:B:320:PHE:HD2	1.86	0.41
4:B:506:TRP:CD1	4:B:623:ARG:HH22	2.39	0.41
14:G:86:ASP:OD1	14:G:144:ARG:NH1	2.54	0.41
3:A:486:LEU:HB3	3:A:538:VAL:HG21	2.01	0.41
3:A:928:ARG:HH11	8:H:107:GLU:HG3	1.86	0.41
4:B:149:ILE:HG22	4:B:440:ILE:HG21	2.02	0.41
11:K:47:LYS:HD3	11:K:61:TYR:HD1	1.85	0.41
14:G:117:MET:HE2	14:G:137:ILE:HD12	2.03	0.41
14:G:136:VAL:HG23	15:O:651:ALA:HA	1.02	0.41
3:A:1423:ASP:OD1	3:A:1423:ASP:N	2.51	0.40
4:B:1151:MET:HE2	4:B:1151:MET:HB3	1.98	0.40
15:O:291:LYS:HD2	15:O:291:LYS:HA	1.77	0.40
15:O:817:ASP:OD2	15:O:820:LYS:HE3	2.21	0.40
2:M:329:PHE:HD2	2:M:331:LYS:N	2.19	0.40
2:M:469:PHE:CB	2:M:489:LEU:HB3	2.51	0.40
4:B:377:LEU:HD13	4:B:377:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:807:ARG:HA	4:B:929:PRO:HD3	2.03	0.40
15:O:288:LEU:HD23	15:O:288:LEU:HA	1.85	0.40
4:B:113:ALA:HA	4:B:118:LEU:HB2	2.03	0.40
4:B:192:LYS:HE3	4:B:449:ALA:HA	2.02	0.40
4:B:334:LYS:NZ	4:B:337:LYS:HZ2	2.18	0.40
4:B:622:CYS:HA	4:B:666:ASP:HA	2.04	0.40
4:B:1028:LEU:HD21	4:B:1043:ILE:HD12	2.02	0.40
9:I:91:HIS:CG	9:I:116:ALA:HB2	2.57	0.40
14:G:136:VAL:HG23	15:O:651:ALA:CB	2.04	0.40
14:G:152:VAL:HB	14:G:157:ILE:HG12	2.04	0.40
15:O:657:ALA:CB	15:O:700:PRO:HG2	2.51	0.40
2:M:377:PHE:CE2	2:M:381:LEU:HD22	2.55	0.40
3:A:57:LEU:O	3:A:261:ARG:NH2	2.55	0.40
3:A:1148:ALA:HB1	3:A:1333:GLU:HB2	2.03	0.40
4:B:285:LEU:HD11	4:B:289:ILE:HD12	2.03	0.40
4:B:348:LEU:HB3	4:B:351:VAL:HG22	2.02	0.40
8:H:100:GLU:HG2	8:H:115:TYR:HE2	1.86	0.40
14:G:91:GLN:HB3	14:G:98:PHE:HB2	2.02	0.40
15:O:674:GLN:O	15:O:679:ARG:HG3	2.22	0.40
2:M:236:VAL:CG1	2:M:237:THR:N	2.84	0.40
2:M:489:LEU:HD11	2:M:501:ILE:HB	2.04	0.40
3:A:76:GLY:HA2	3:A:80:GLU:HG3	2.03	0.40
4:B:1085:ARG:HD3	18:T:22:DC:H5''	2.03	0.40
14:G:140:ASP:HB3	15:O:654:LYS:CE	2.42	0.40
15:O:322:GLU:OE1	15:O:693:PRO:HD3	2.11	0.40
15:O:654:LYS:HB2	15:O:654:LYS:HE2	1.47	0.40
18:T:30:DA:H2''	18:T:31:DT:H5'	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	50/1087 (5%)	48 (96%)	2 (4%)	0	100	100
2	M	325/597 (54%)	308 (95%)	17 (5%)	0	100	100
3	A	1395/1970 (71%)	1298 (93%)	96 (7%)	1 (0%)	48	80
4	B	1102/1174 (94%)	1030 (94%)	72 (6%)	0	100	100
5	C	254/275 (92%)	242 (95%)	12 (5%)	0	100	100
6	E	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
7	F	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
8	H	146/150 (97%)	138 (94%)	8 (6%)	0	100	100
9	I	115/125 (92%)	107 (93%)	8 (7%)	0	100	100
10	J	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
11	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
12	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
13	D	127/142 (89%)	120 (94%)	7 (6%)	0	100	100
14	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
15	O	693/835 (83%)	666 (96%)	25 (4%)	2 (0%)	36	69
All	All	4885/7106 (69%)	4611 (94%)	271 (6%)	3 (0%)	49	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	O	294	HIS
3	A	1108	HIS
15	O	230	VAL

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	Z	45/940 (5%)	45 (100%)	0	100	100
2	M	297/534 (56%)	264 (89%)	33 (11%)	6	23
3	A	1238/1749 (71%)	1228 (99%)	10 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	979/1027 (95%)	977 (100%)	2 (0%)	87	87
5	C	235/252 (93%)	234 (100%)	1 (0%)	84	83
6	E	191/192 (100%)	190 (100%)	1 (0%)	81	82
7	F	71/111 (64%)	71 (100%)	0	100	100
8	H	129/131 (98%)	127 (98%)	2 (2%)	55	69
9	I	105/112 (94%)	105 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	103 (99%)	1 (1%)	68	75
12	L	43/55 (78%)	43 (100%)	0	100	100
13	D	104/126 (82%)	104 (100%)	0	100	100
14	G	138/153 (90%)	138 (100%)	0	100	100
15	O	623/741 (84%)	598 (96%)	25 (4%)	28	51
All	All	4358/6285 (69%)	4283 (98%)	75 (2%)	52	68

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	286	LEU
2	M	308	ASN
2	M	309	GLU
2	M	313	ILE
2	M	314	ASP
2	M	362	TYR
2	M	366	LYS
2	M	381	LEU
2	M	385	GLU
2	M	389	ILE
2	M	390	SER
2	M	405	GLN
2	M	411	ARG
2	M	418	ILE
2	M	445	THR
2	M	447	LYS
2	M	464	LEU
2	M	471	LEU
2	M	473	ILE
2	M	474	THR
2	M	475	ARG

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Mol	Chain	Res	Type
2	M	476	MET
2	M	481	LEU
2	M	482	LEU
2	M	484	GLN
2	M	485	ASN
2	M	514	ILE
2	M	518	LYS
2	M	533	LYS
2	M	543	MET
2	M	556	GLU
2	M	562	ILE
2	M	565	CYS
3	A	118	LEU
3	A	214	ILE
3	A	368	THR
3	A	405	LEU
3	A	521	VAL
3	A	706	ILE
3	A	1087	VAL
3	A	1166	LEU
3	A	1374	VAL
3	A	1378	LEU
4	B	163	LEU
4	B	809	VAL
5	C	128	ILE
6	E	58	LEU
8	H	60	ILE
8	H	96	VAL
11	K	94	LEU
15	O	242	ASN
15	O	284	SER
15	O	291	LYS
15	O	292	LYS
15	O	336	ILE
15	O	340	GLU
15	O	346	ARG
15	O	352	ASN
15	O	641	ILE
15	O	642	VAL
15	O	643	HIS
15	O	645	LEU
15	O	646	LYS

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Mol	Chain	Res	Type
15	O	650	LYS
15	O	653	ARG
15	O	654	LYS
15	O	655	ILE
15	O	656	SER
15	O	658	ILE
15	O	677	ASN
15	O	680	ILE
15	O	682	LEU
15	O	685	LYS
15	O	687	VAL
15	O	692	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	280	ASN
2	M	393	HIS
2	M	484	GLN
2	M	540	ASN
3	A	123	ASN
3	A	152	ASN
3	A	188	GLN
3	A	272	ASN
3	A	273	GLN
3	A	278	HIS
3	A	311	GLN
3	A	330	GLN
3	A	472	HIS
3	A	529	GLN
3	A	539	GLN
3	A	576	GLN
3	A	654	HIS
3	A	662	HIS
3	A	678	ASN
3	A	711	GLN
3	A	861	GLN
3	A	905	ASN
3	A	989	ASN
3	A	1005	HIS
3	A	1032	GLN
3	A	1093	GLN

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Mol	Chain	Res	Type
3	A	1129	ASN
3	A	1163	HIS
3	A	1244	ASN
3	A	1248	ASN
3	A	1299	GLN
3	A	1332	GLN
3	A	1384	HIS
3	A	1417	HIS
3	A	1457	ASN
4	B	111	ASN
4	B	227	ASN
4	B	254	GLN
4	B	420	GLN
4	B	486	ASN
4	B	518	HIS
4	B	639	HIS
4	B	650	ASN
4	B	699	HIS
4	B	842	HIS
4	B	986	GLN
4	B	1003	ASN
4	B	1025	ASN
4	B	1145	GLN
5	C	55	ASN
5	C	66	HIS
6	E	95	GLN
6	E	107	GLN
6	E	132	GLN
6	E	168	ASN
8	H	44	ASN
8	H	76	ASN
9	I	22	ASN
9	I	41	ASN
11	K	2	ASN
11	K	29	ASN
11	K	49	GLN
12	L	26	ASN
13	D	43	HIS
13	D	47	GLN
13	D	48	ASN
13	D	66	ASN
13	D	129	GLN

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Mol	Chain	Res	Type
13	D	135	GLN
14	G	14	HIS
15	O	352	ASN
15	O	372	GLN
15	O	478	ASN
15	O	515	HIS
15	O	667	ASN
15	O	681	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	19/21 (90%)	12 (63%)	7 (36%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	32	A
16	P	33	C
16	P	34	A
16	P	35	U
16	P	36	A
16	P	37	C
16	P	38	A
16	P	39	U
16	P	40	A
16	P	41	A
16	P	42	A
16	P	43	G

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	33	C
16	P	35	U
16	P	36	A
16	P	37	C
16	P	39	U
16	P	40	A
16	P	42	A

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 9 ligands modelled in this entry, 9 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	P	1
17	N	1
15	O	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	101:MGT	O3'	31:G	P	51.64
1	N	14:DT	O3'	24:DG	P	27.51
1	O	549:PRO	C	550:SER	N	1.66

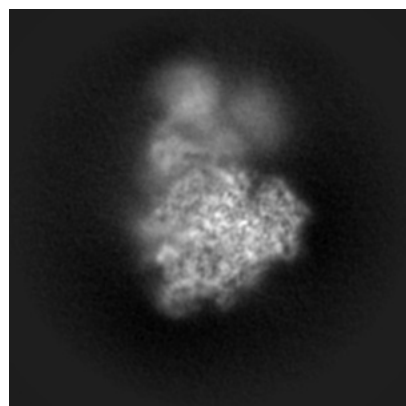
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17407. These allow visual inspection of the internal detail of the map and identification of artifacts.

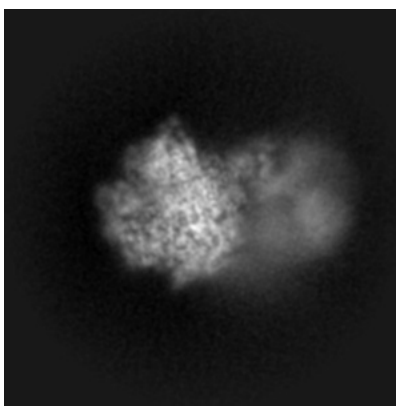
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

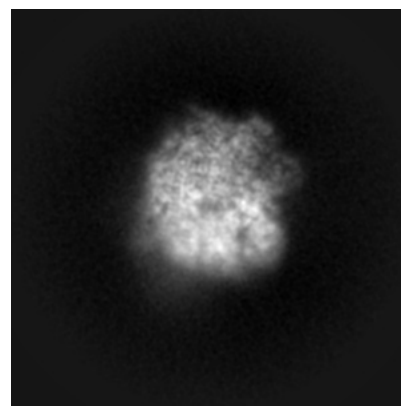
6.1.1 Primary map



X

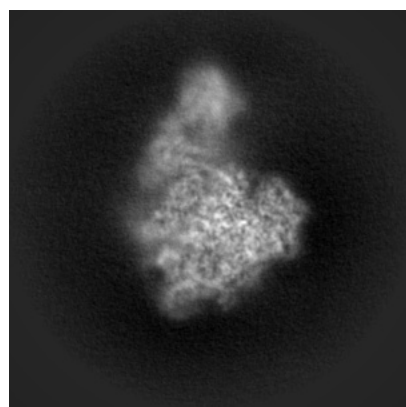


Y

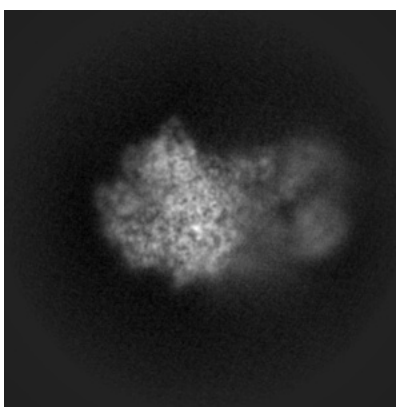


Z

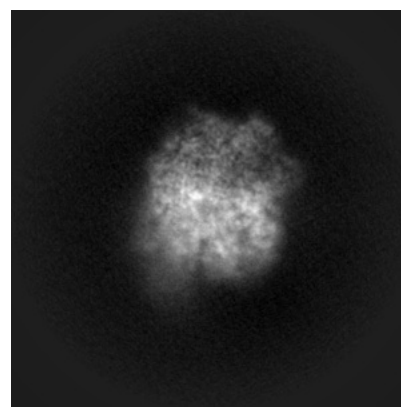
6.1.2 Raw map



X



Y

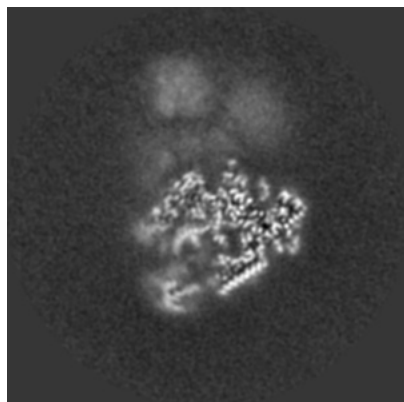


Z

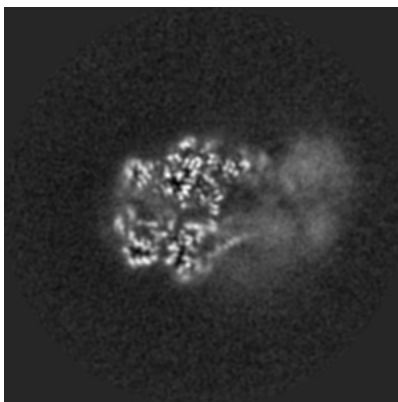
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

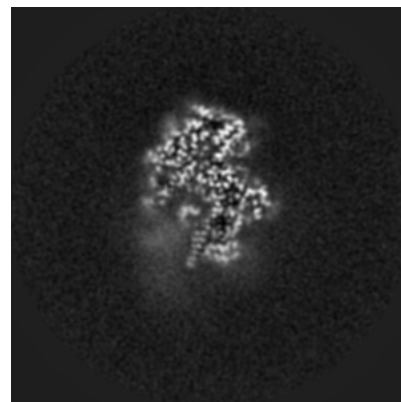
6.2.1 Primary map



X Index: 150

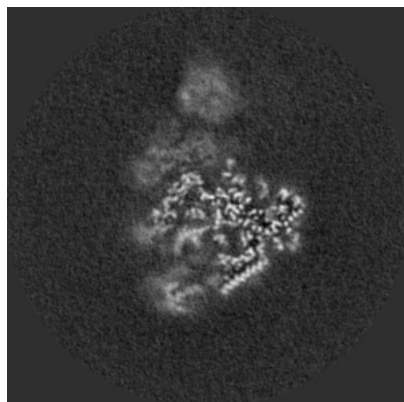


Y Index: 150

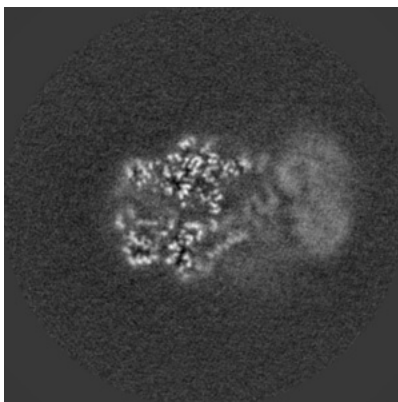


Z Index: 150

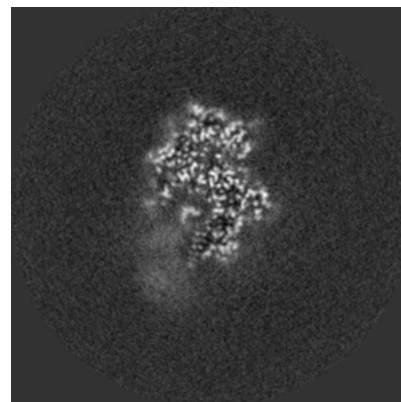
6.2.2 Raw map



X Index: 150



Y Index: 150

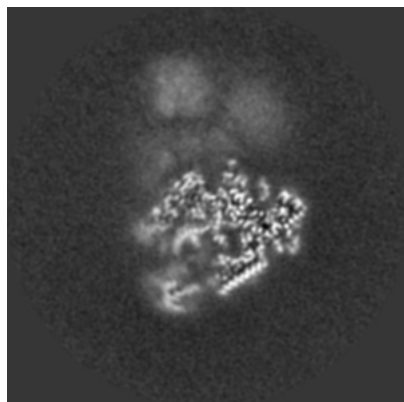


Z Index: 150

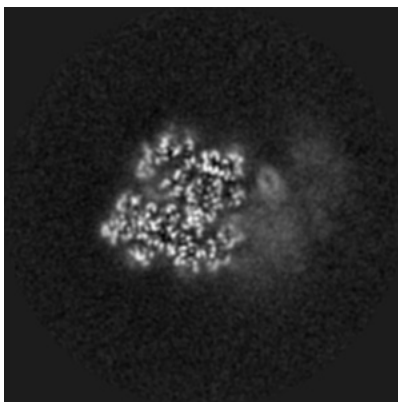
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

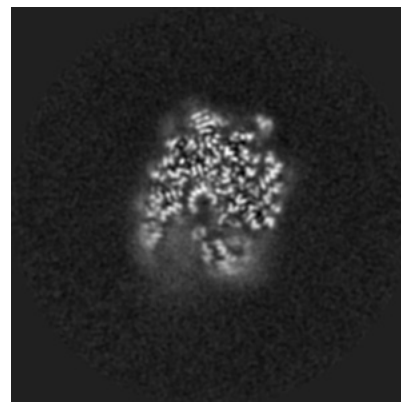
6.3.1 Primary map



X Index: 150

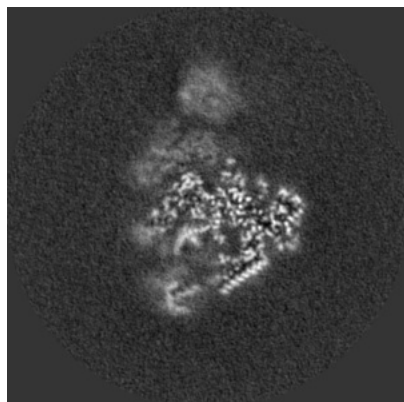


Y Index: 161

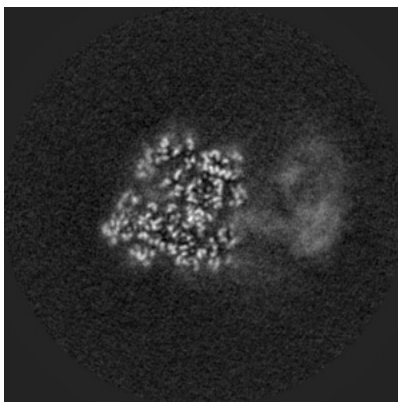


Z Index: 139

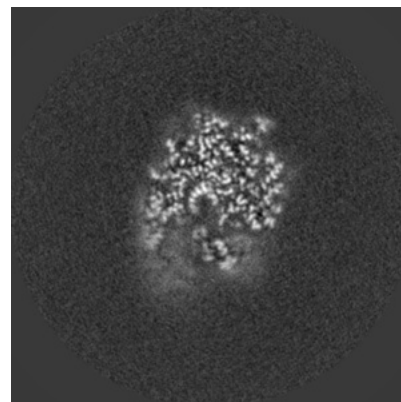
6.3.2 Raw map



X Index: 151



Y Index: 161

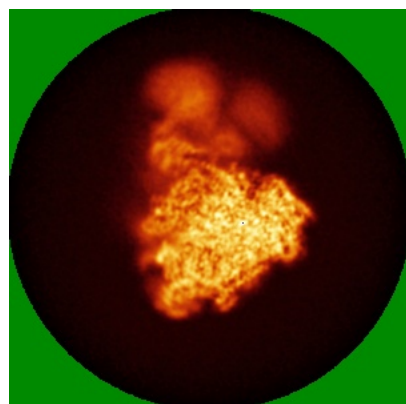


Z Index: 139

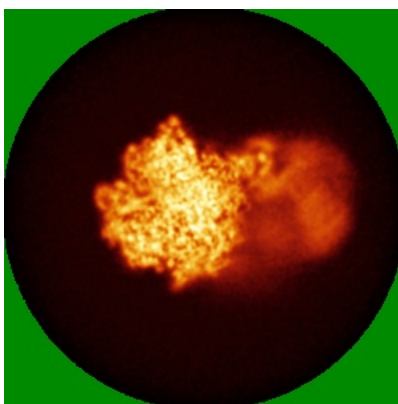
The images above show the largest variance slices of the map in three orthogonal directions.

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

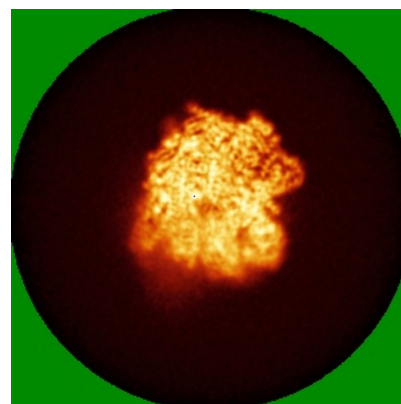
6.4.1 Primary map



X



Y

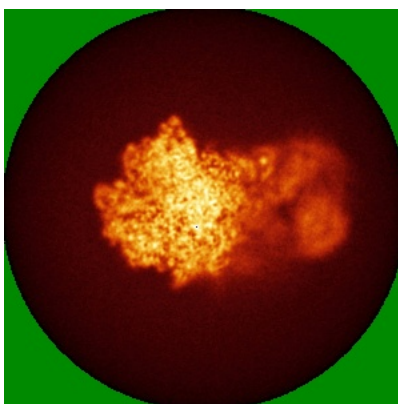


Z

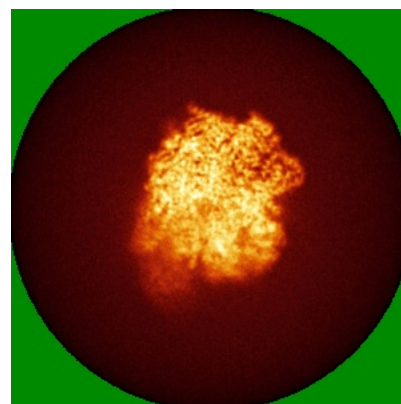
6.4.2 Raw map



X



Y

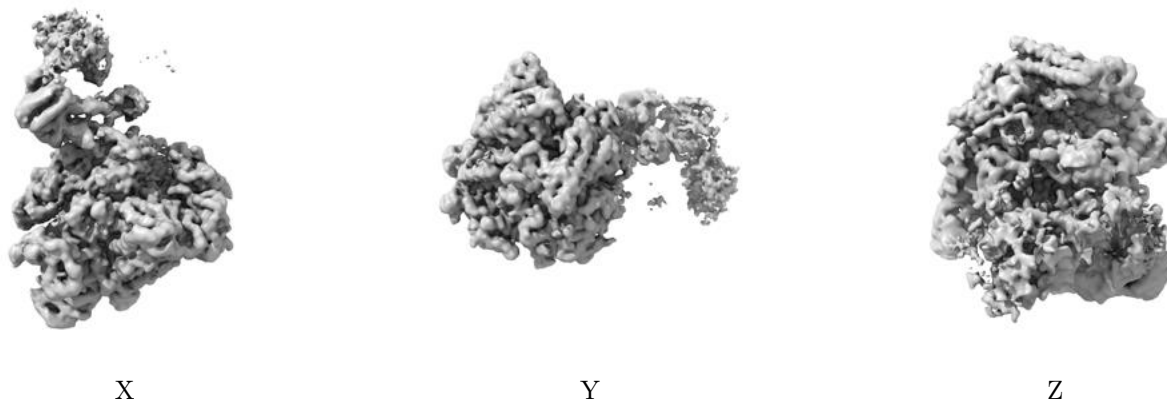


Z

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.

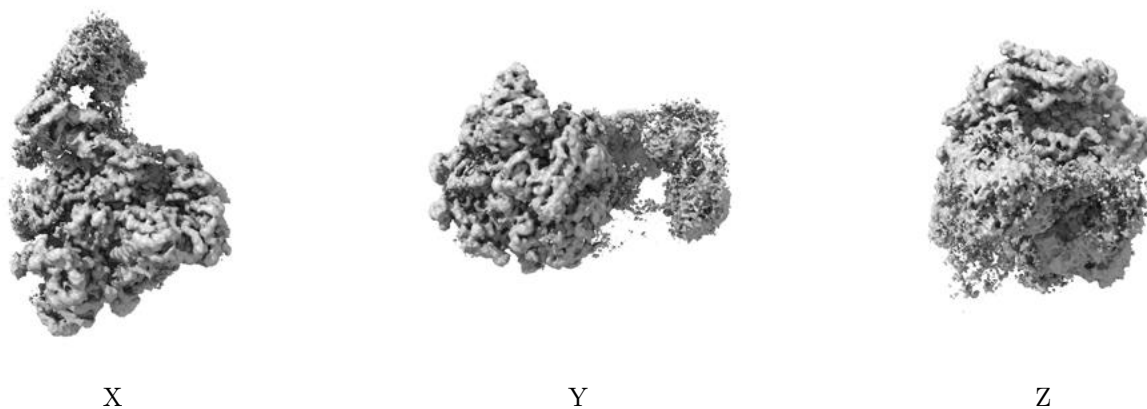
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0221. 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.

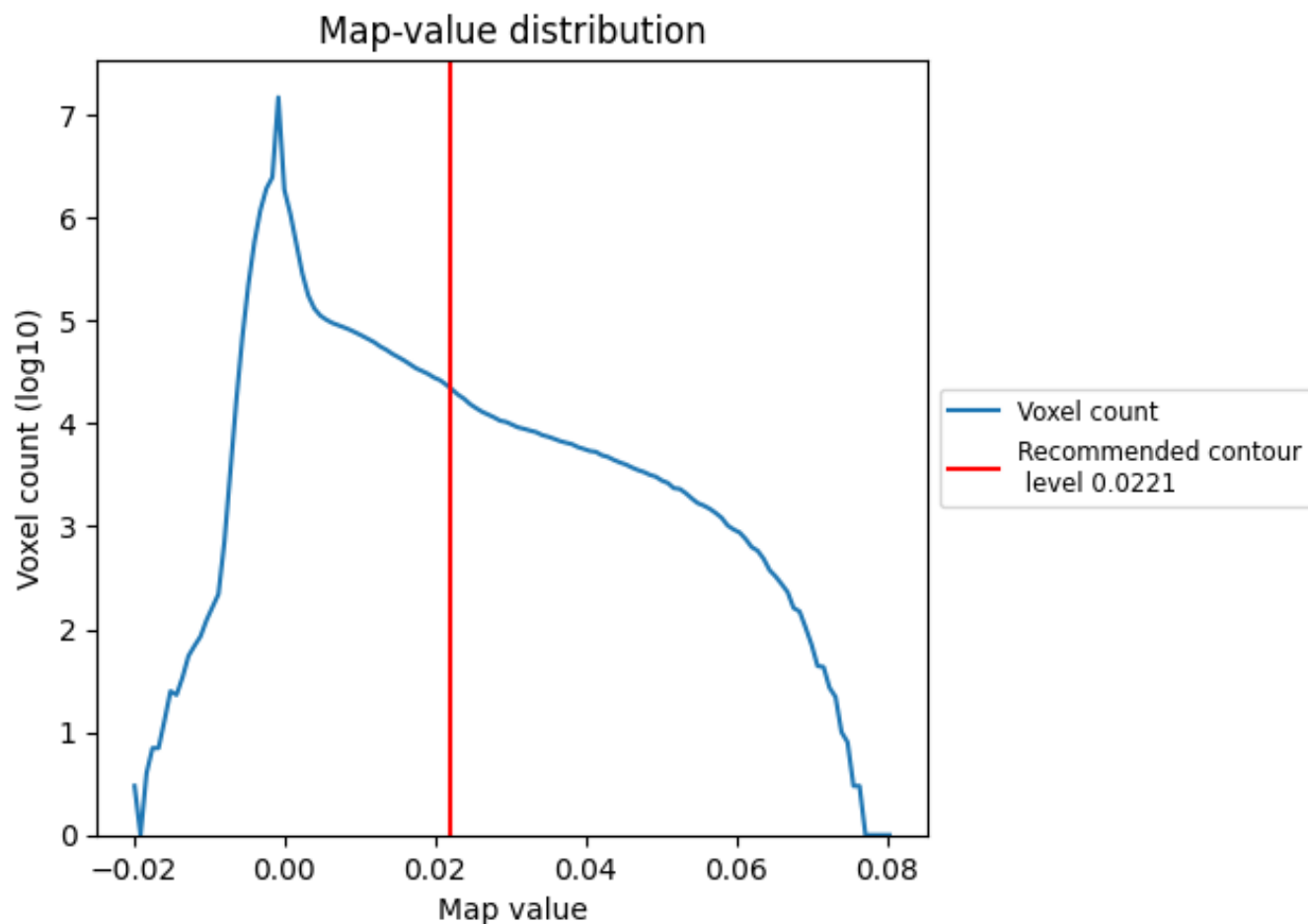
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

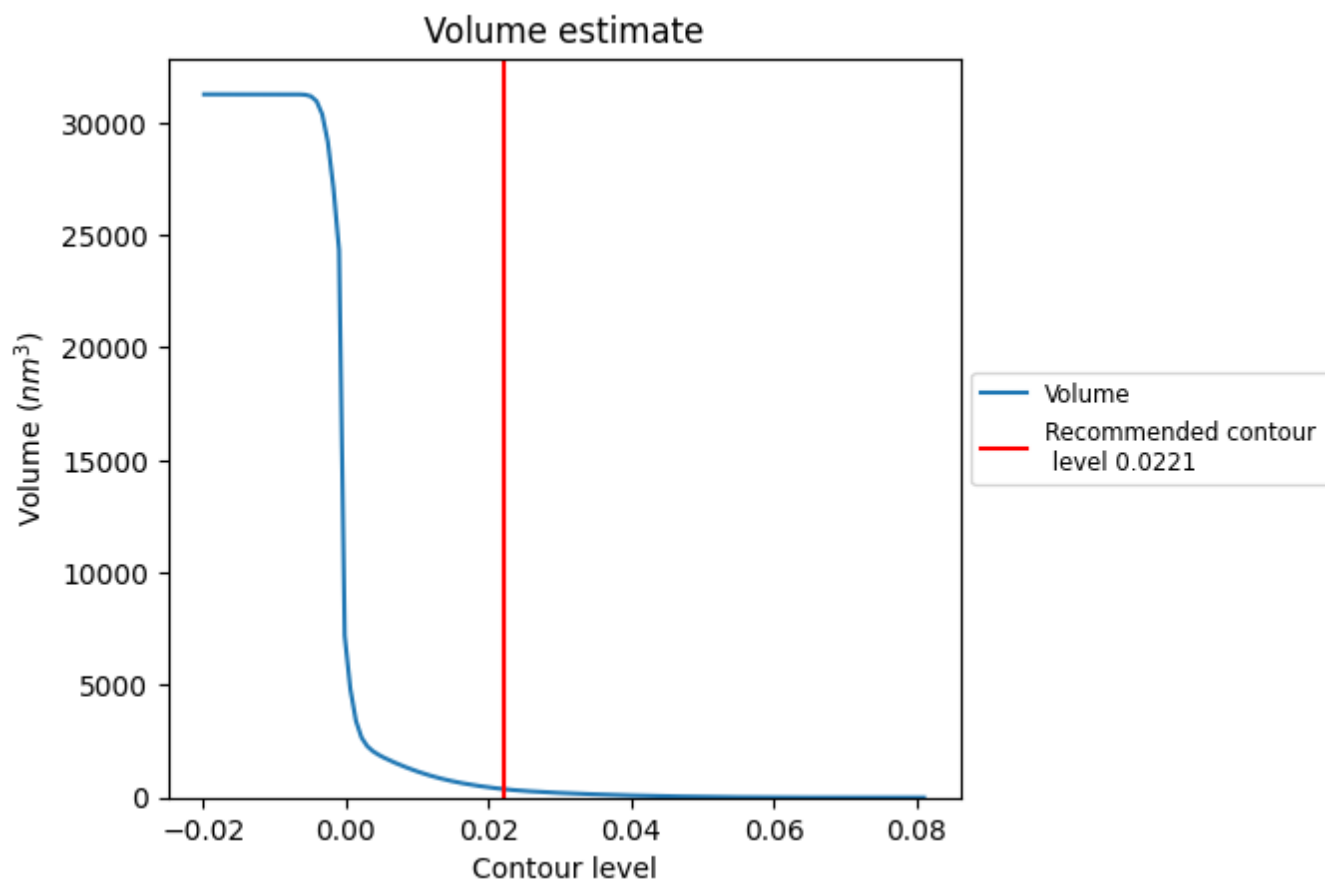
This section contains the results of statistical analysis of the map.

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.

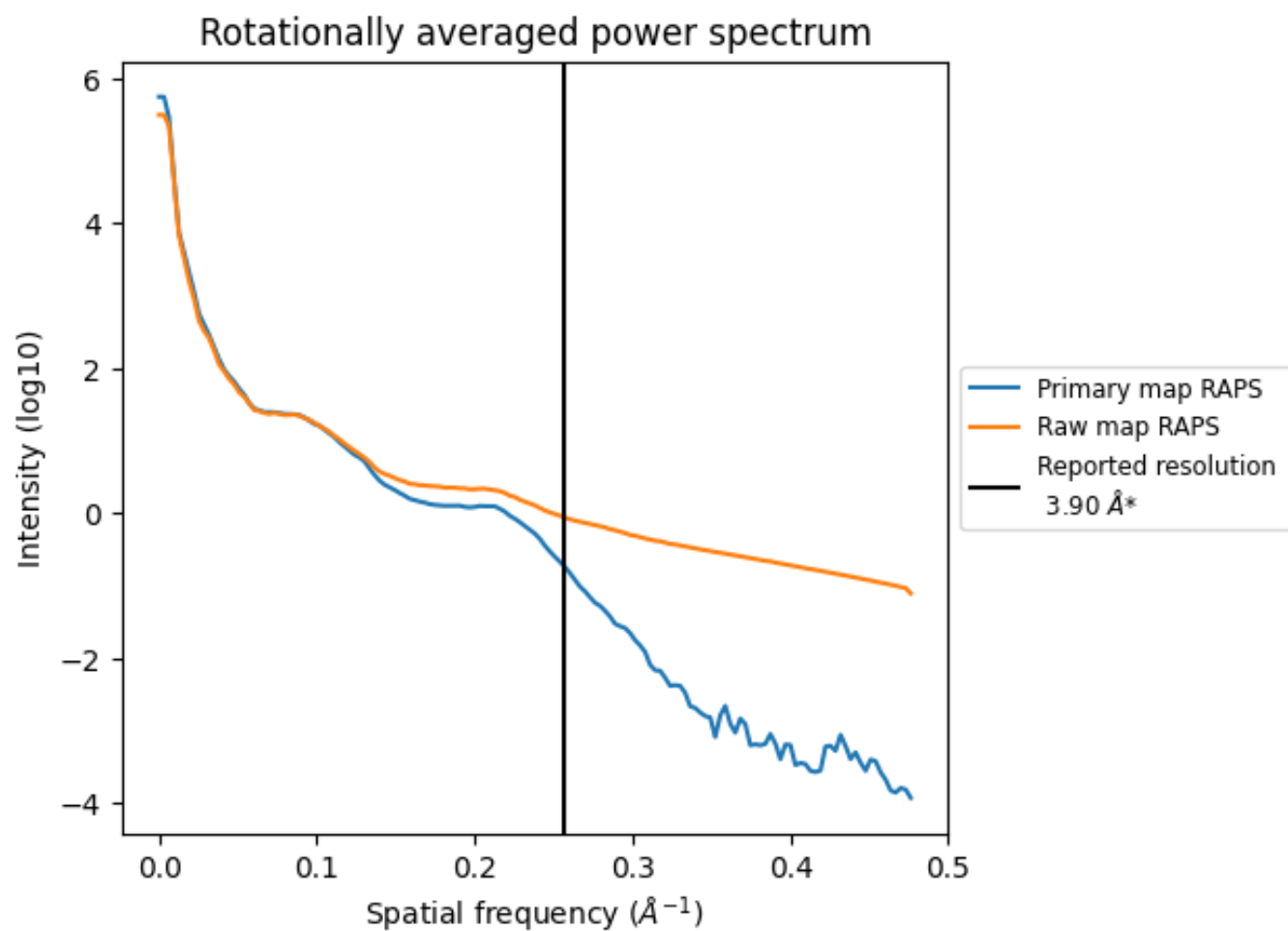
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 379 nm³; this corresponds to an approximate mass of 342 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 ⓘ

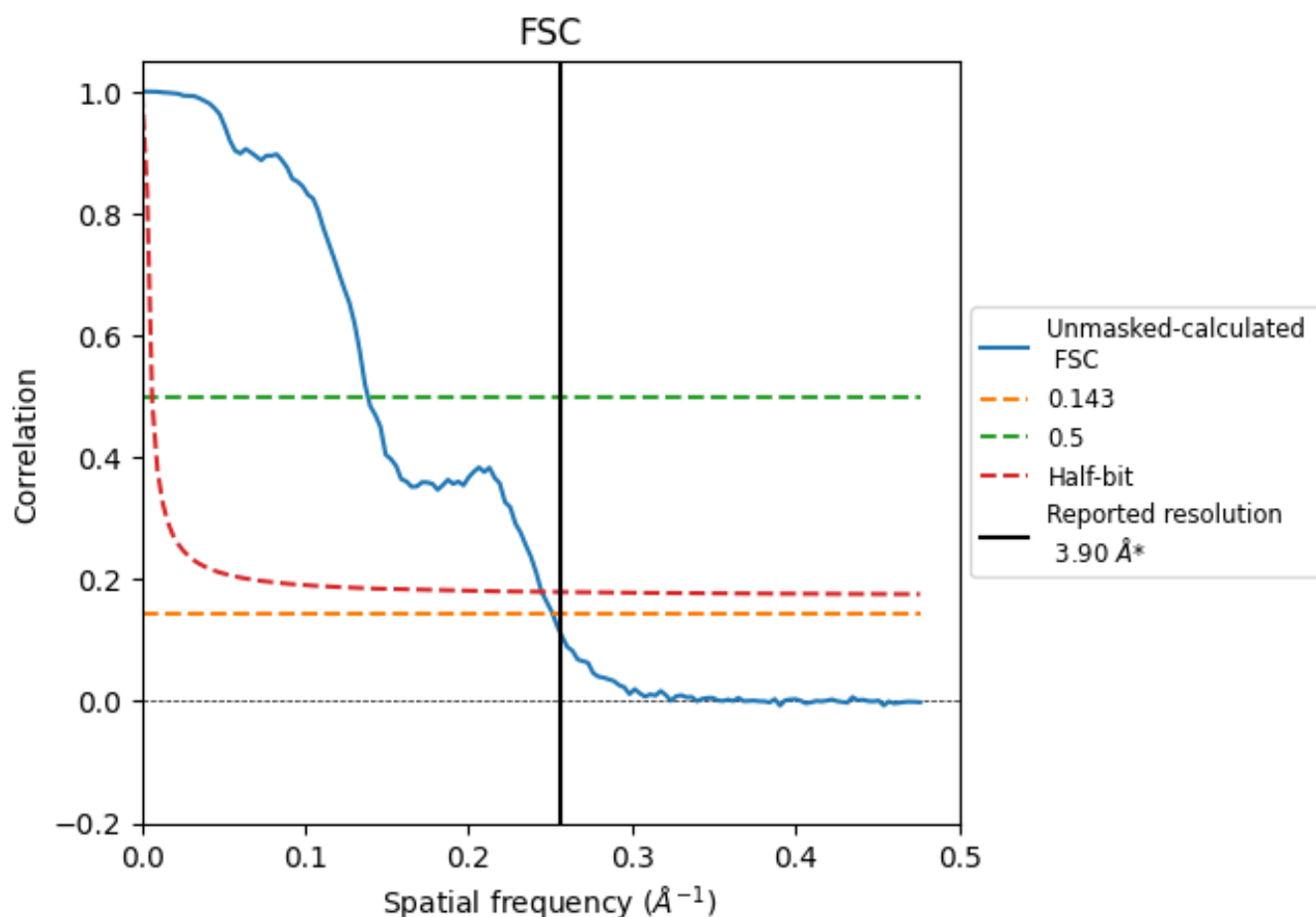


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 $0.256 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

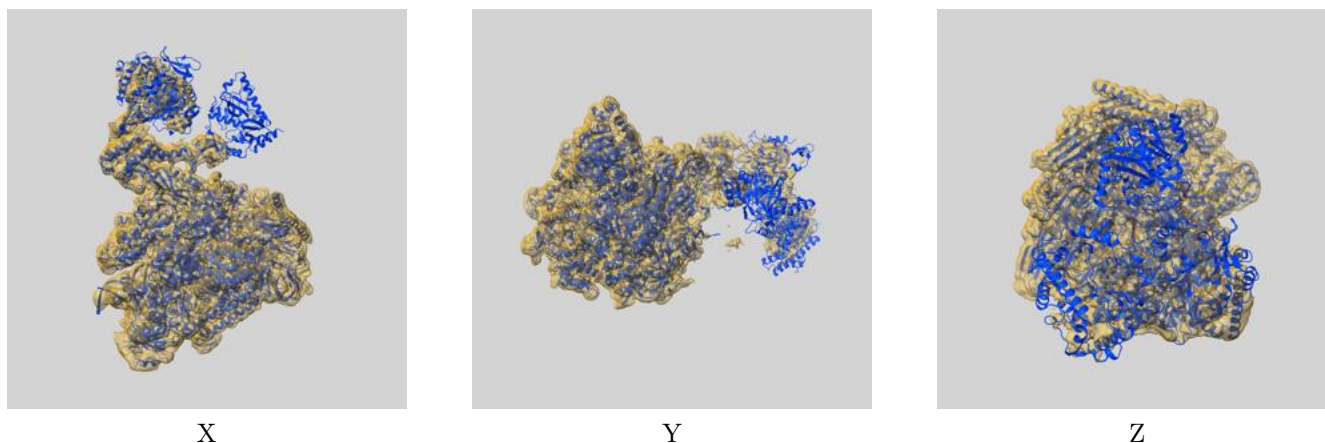
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.98	7.23	4.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

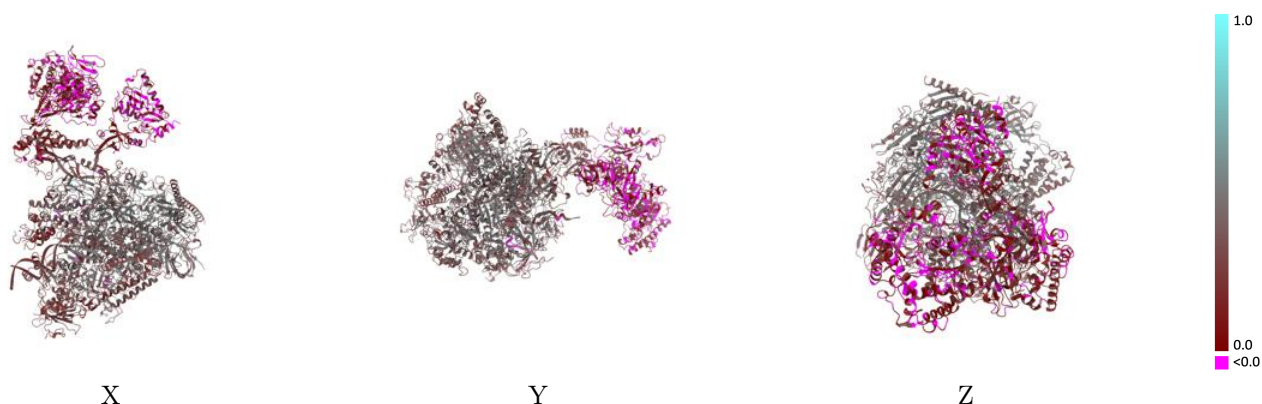
This section contains information regarding the fit between EMDB map EMD-17407 and PDB model 8P4E. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



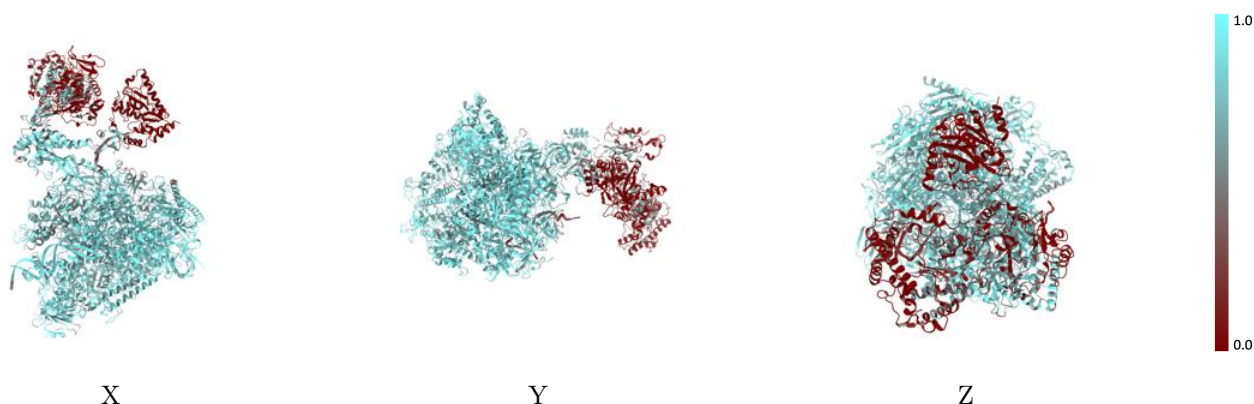
The images above show the 3D surface view of the map at the recommended contour level 0.0221 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



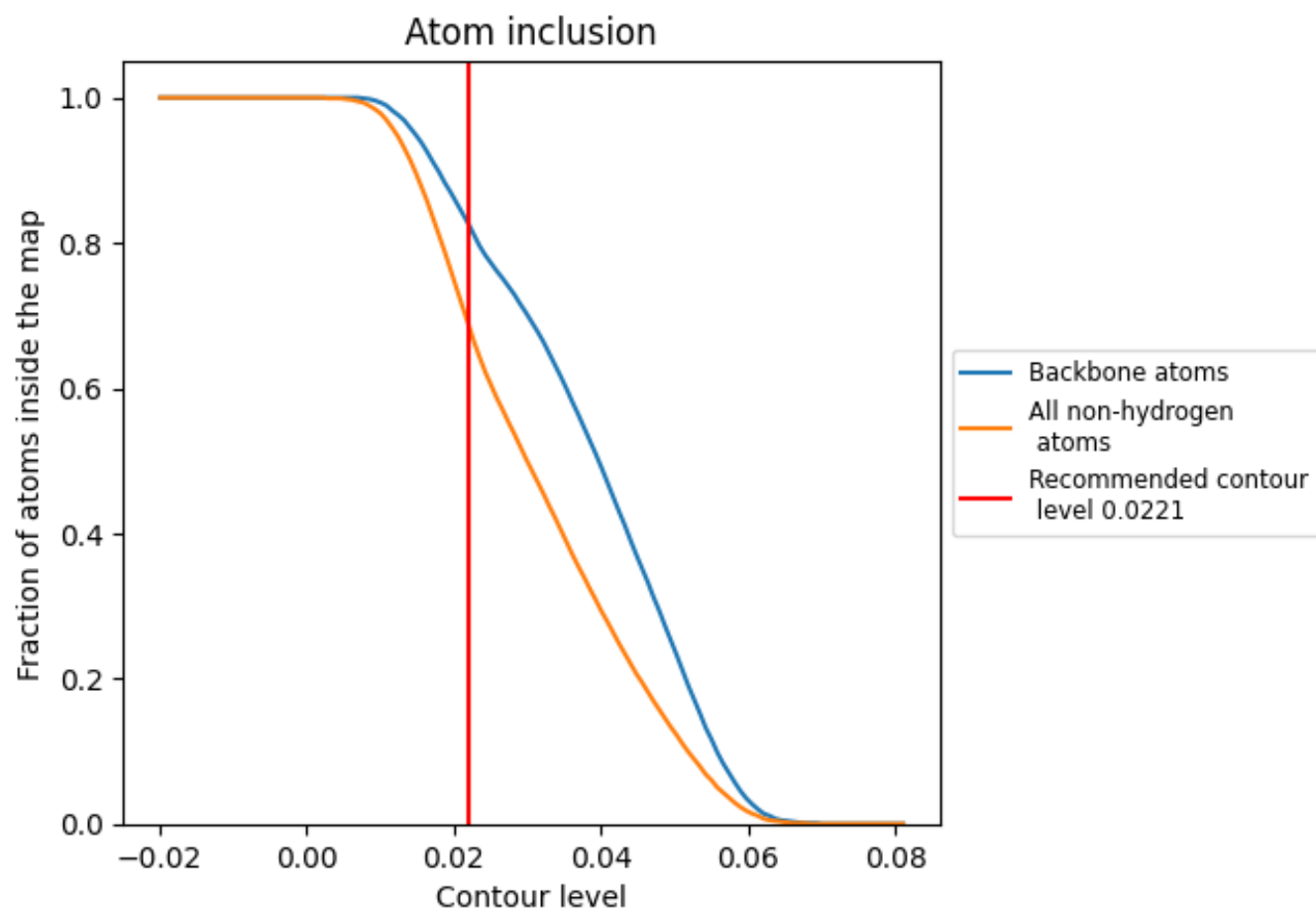
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0221).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 69% 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 (0.0221) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6860	 0.2970
A	 0.8160	 0.3630
B	 0.8340	 0.3820
C	 0.8530	 0.4020
D	 0.7220	 0.1970
E	 0.8360	 0.3340
F	 0.8190	 0.3890
G	 0.7440	 0.2530
H	 0.8340	 0.3920
I	 0.8280	 0.3200
J	 0.8580	 0.4020
K	 0.8490	 0.4020
L	 0.8100	 0.3500
M	 0.1100	 0.0650
N	 0.6130	 0.2020
O	 0.2200	 0.0600
P	 0.7040	 0.2650
T	 0.7590	 0.2700
Z	 0.5740	 0.4180

