



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:35 AM UTC

PDB ID : 9XGK / pdb_00009xgk
EMDB ID : EMD-66852
Title : Structure of mammalian RNA polymerase II stalled by Actinomycin D at the N-1 position.
Authors : Xu, J.; Zhao, W.
Deposited on : 2025-10-30
Resolution : 2.53 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

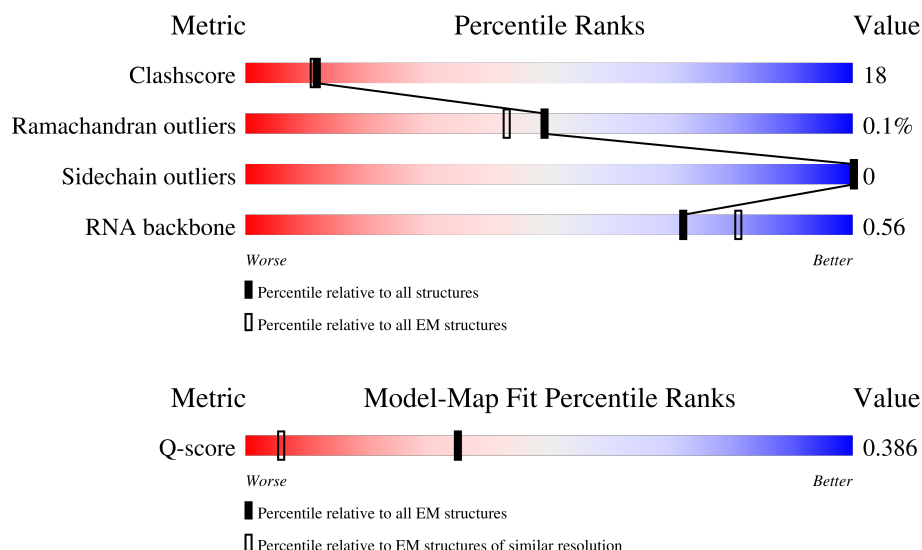
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.53 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	7309 (2.03 - 3.03)

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	1970	
2	B	1174	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	11	
14	N	48	
15	P	13	
16	T	49	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	MVA	M	11	-	-	X	-
13	DVA	M	2	-	-	X	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32455 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1427	Total	C	N	O	S	0	0
			11291	7102	2021	2096	72		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1711	1084	300	319	8		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			658	419	113	121	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

- 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	114	Total	C	N	O	S	0	0
			927	571	166	179	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.

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 DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 13 is a protein called Actinomycin D.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	11	Total	C	N	O	0	0
			90	62	12	16		

- Molecule 14 is a DNA chain called DNA (NTS, non-template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	20	Total	C	N	O	P	0	0
			414	198	81	115	20		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	11	Total	C	N	O	P	0	0
			234	105	43	75	11		

- Molecule 16 is a DNA chain called DNA (TS, template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	32	Total	C	N	O	P	0	0
			650	315	102	201	32		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total	Zn	0
			2	2	
17	B	1	Total	Zn	0
			1	1	
17	C	1	Total	Zn	0
			1	1	
17	I	2	Total	Zn	0
			2	2	
17	J	1	Total	Zn	0
			1	1	
17	L	1	Total	Zn	0
			1	1	

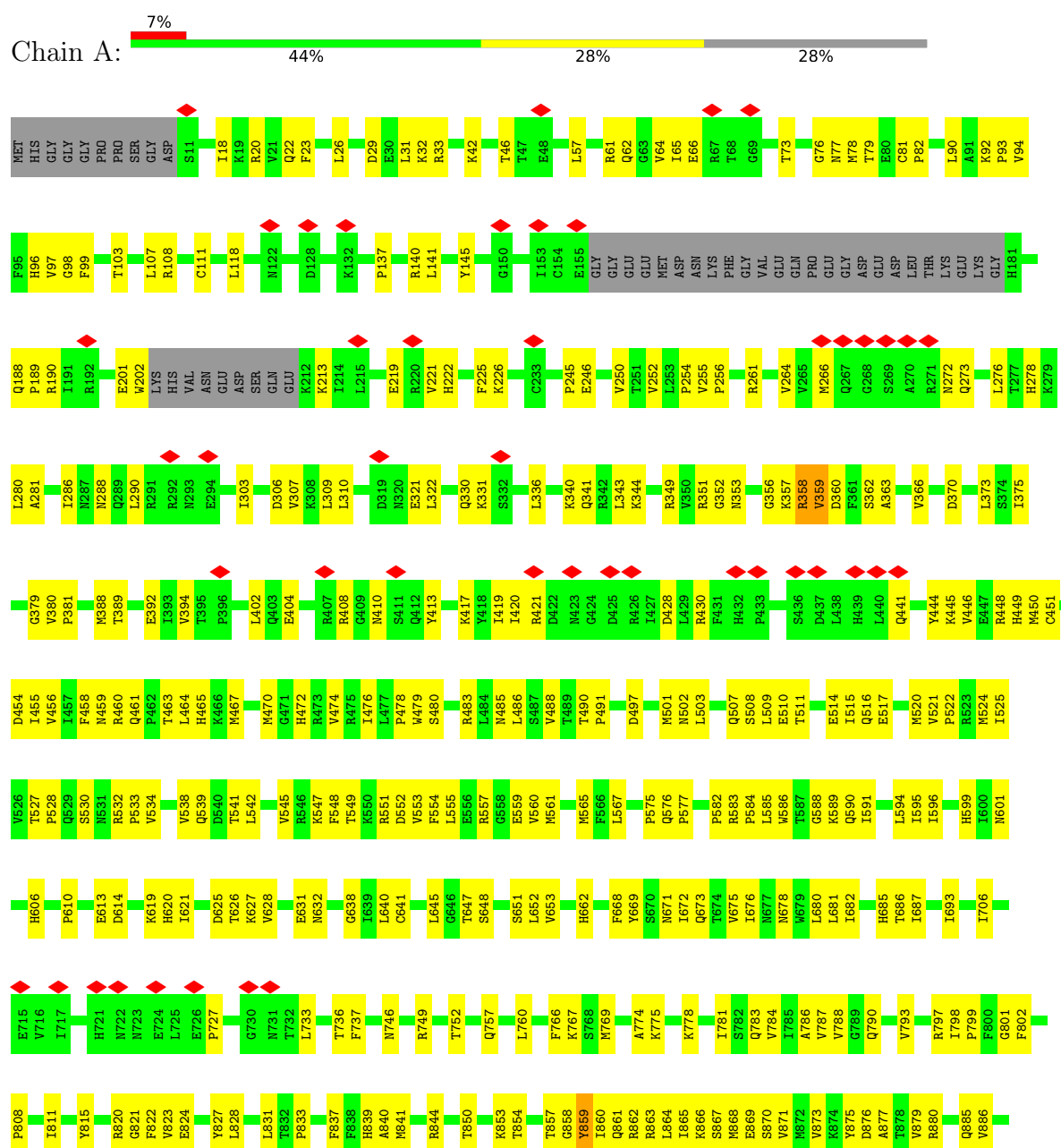
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots

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

• Molecule 1: DNA-directed RNA polymerase II subunit RPB1



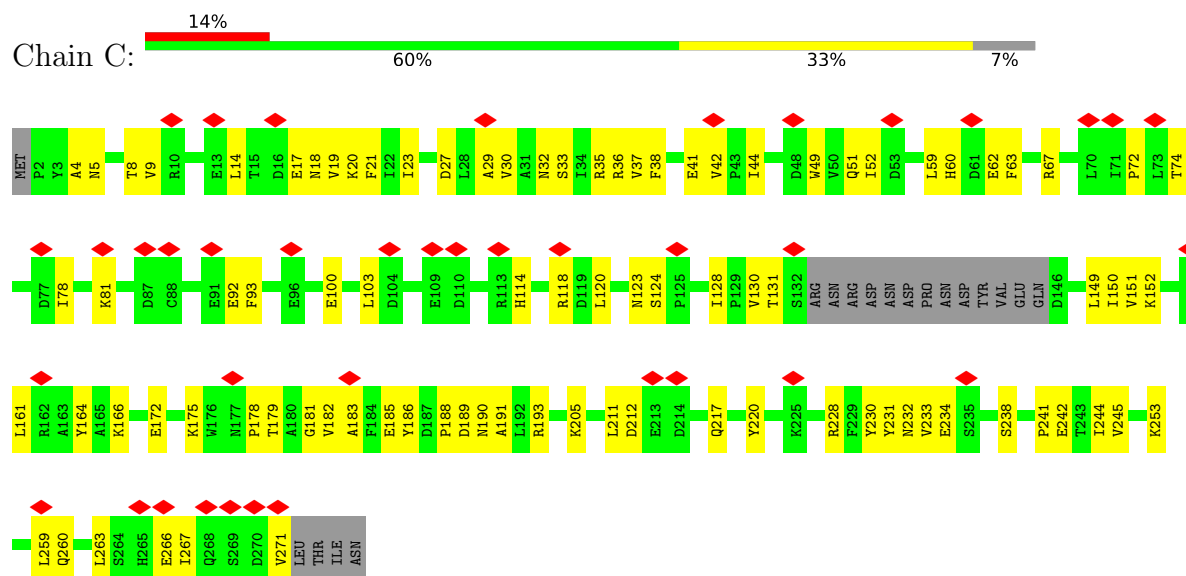


Chain B:

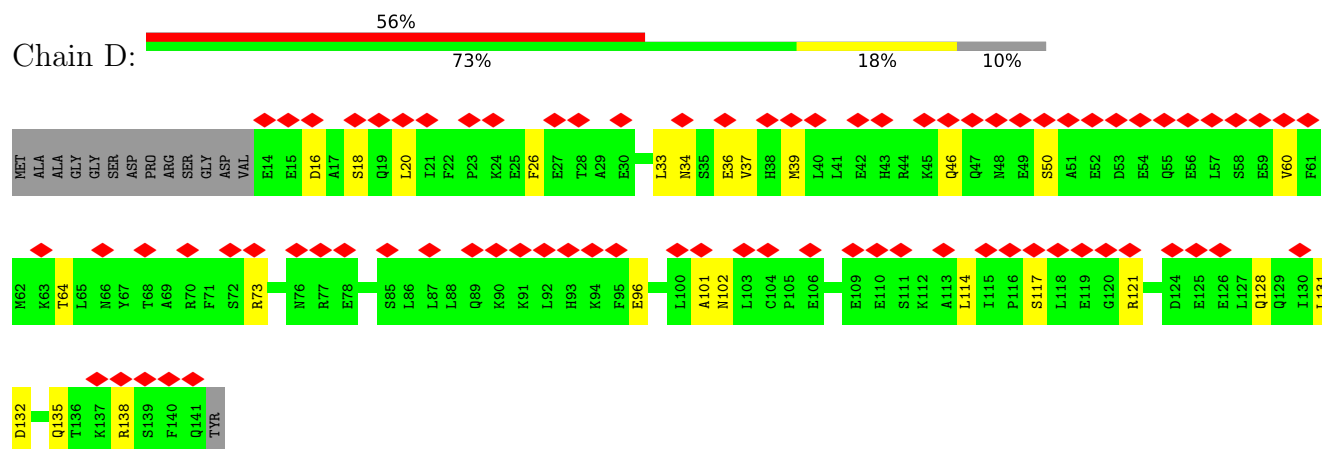




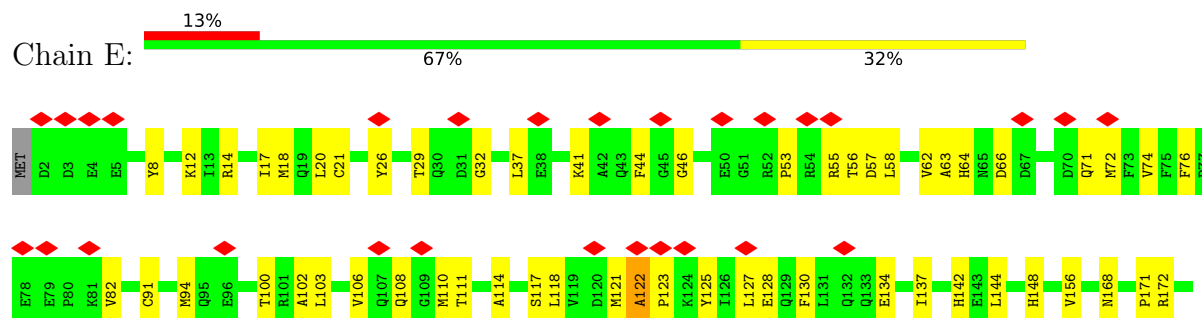
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

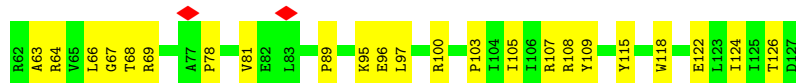
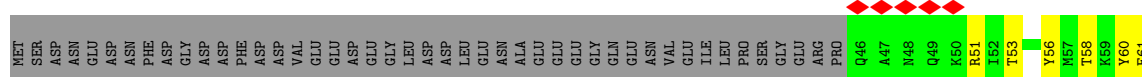
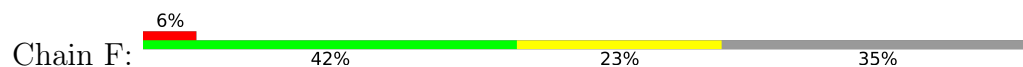


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

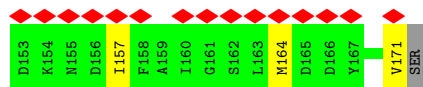
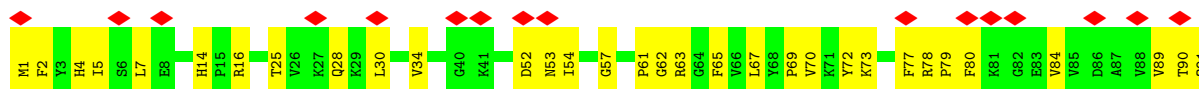




- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



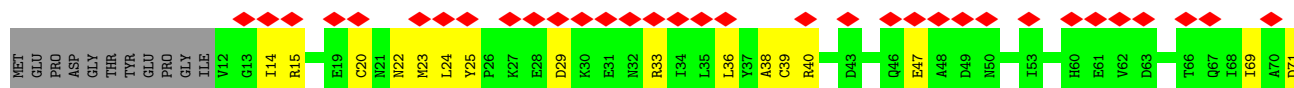
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

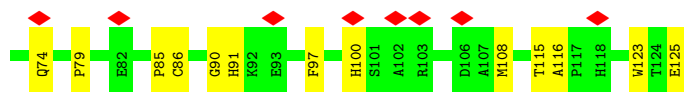


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

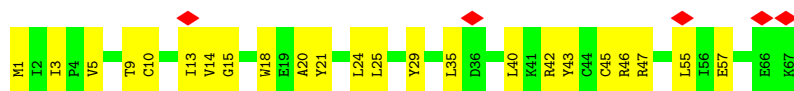


- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

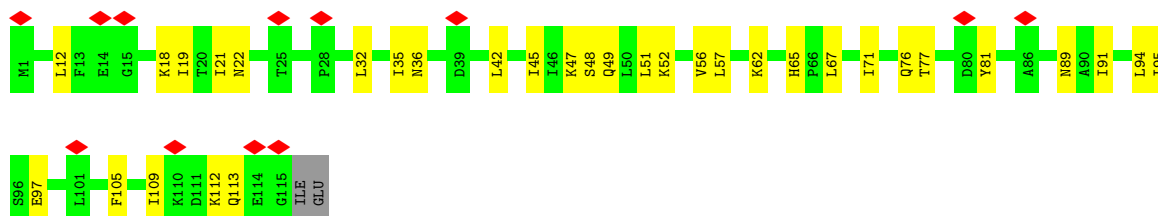




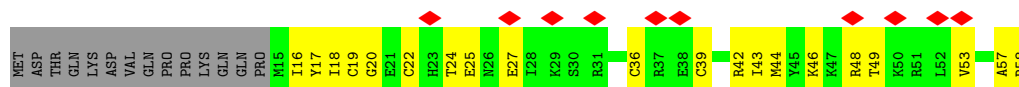
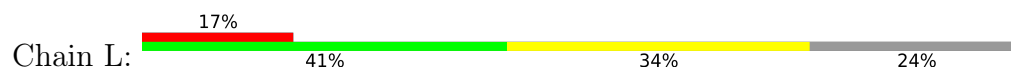
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



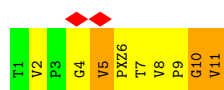
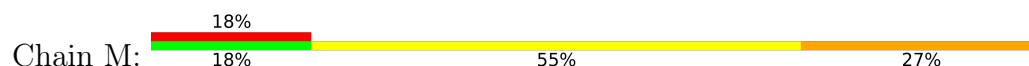
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



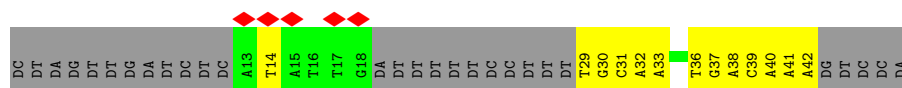
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 13: Actinomycin D

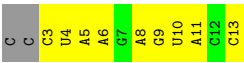


- Molecule 14: DNA (NTS, non-template strand)

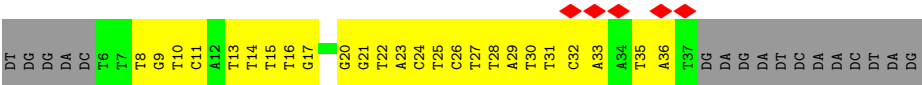
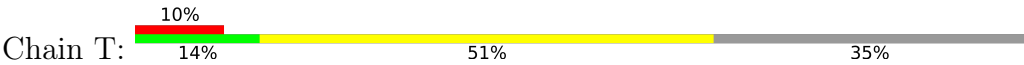


- Molecule 15: RNA





● Molecule 16: DNA (TS, template strand)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83354	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	297.6, 297.6, 297.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.20	1/11497 (0.0%)	0.41	6/15521 (0.0%)
2	B	0.14	0/9243	0.31	0/12475
3	C	0.11	0/2102	0.29	0/2857
4	D	0.09	0/1019	0.26	0/1374
5	E	0.11	0/1742	0.32	0/2353
6	F	0.12	0/668	0.30	0/903
7	G	0.09	0/1365	0.25	0/1853
8	H	0.12	0/1207	0.29	0/1628
9	I	0.10	0/948	0.30	0/1284
10	J	0.11	0/542	0.38	1/730 (0.1%)
11	K	0.12	0/939	0.26	0/1271
12	L	0.09	0/377	0.36	0/500
13	M	0.28	0/26	0.41	0/30
14	N	0.47	0/465	0.75	0/713
15	P	0.32	0/261	0.66	0/404
16	T	0.53	0/724	0.97	0/1115
All	All	0.18	1/33125 (0.0%)	0.39	7/45011 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	358	ARG	CA-C	-5.57	1.45	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	859	TYR	N-CA-CB	-7.63	98.87	110.16
1	A	359	VAL	N-CA-C	7.58	119.40	108.48
1	A	859	TYR	CA-CB-CG	-7.10	101.12	113.90
1	A	866	LYS	N-CA-C	-5.98	104.85	111.36
10	J	14	VAL	N-CA-C	-5.87	107.56	113.20
1	A	358	ARG	CA-C-N	-5.60	115.33	123.06
1	A	358	ARG	C-N-CA	-5.60	115.33	123.06

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	862	ARG	Sidechain
1	A	863	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11291	0	11402	474	0
2	B	9062	0	9107	389	0
3	C	2059	0	2007	78	0
4	D	1005	0	964	23	0
5	E	1711	0	1733	51	0
6	F	658	0	686	30	0
7	G	1334	0	1333	40	0
8	H	1186	0	1147	45	0
9	I	927	0	859	25	0
10	J	533	0	553	22	0
11	K	920	0	942	28	0
12	L	372	0	378	19	0
13	M	90	0	84	42	0
14	N	414	0	227	38	0
15	P	234	0	120	17	0
16	T	650	0	369	38	0
17	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	32455	0	31911	1132	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 18.

All (1132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1417:HIS:CE1	13:M:11:MVA:HG11	1.30	1.66
1:A:1417:HIS:CE1	13:M:11:MVA:CG1	1.90	1.53
1:A:1417:HIS:NE2	13:M:11:MVA:HG13	1.31	1.43
2:B:823:PHE:CE1	14:N:14:DT:H5''	1.78	1.18
1:A:859:TYR:HE2	13:M:2:DVA:CG1	1.59	1.16
2:B:436:LYS:HE2	16:T:33:DA:H5''	1.15	1.15
1:A:1417:HIS:NE2	13:M:11:MVA:CG1	2.03	1.08
13:M:9:PRO:HG2	14:N:32:DA:H5'	1.44	0.97
1:A:859:TYR:CE2	13:M:2:DVA:CG1	2.47	0.96
2:B:823:PHE:HE1	14:N:14:DT:H5''	1.13	0.94
1:A:859:TYR:CE2	13:M:2:DVA:HG13	2.03	0.93
1:A:865:ILE:HD13	2:B:1092:ASP:HB3	1.50	0.93
1:A:190:ARG:NH1	14:N:37:DG:O5'	2.03	0.92
2:B:897:ARG:NH1	16:T:26:DC:OP1	2.01	0.92
2:B:407:MET:HE1	2:B:444:LEU:HG	1.53	0.91
1:A:1417:HIS:HE2	13:M:11:MVA:HG13	0.98	0.90
1:A:1416:ARG:NE	13:M:11:MVA:HG12	1.88	0.89
2:B:495:LEU:HD22	14:N:29:DT:H4'	1.55	0.88
13:M:9:PRO:HG2	14:N:32:DA:C5'	2.03	0.88
13:M:9:PRO:CG	14:N:32:DA:H5'	2.04	0.85
13:M:9:PRO:HB2	14:N:32:DA:O4'	1.77	0.84
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.58	0.84
1:A:1087:VAL:HG12	1:A:1400:LEU:HD22	1.57	0.83
16:T:8:DT:H2''	16:T:9:DG:C8	2.14	0.82
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.44	0.81
1:A:1035:GLU:O	1:A:1039:LEU:HB2	1.80	0.81
2:B:897:ARG:HH12	16:T:26:DC:P	2.03	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.63	0.80
1:A:1173:THR:HG23	1:A:1214:VAL:HG12	1.64	0.80
1:A:1130:ILE:HD13	1:A:1411:LEU:HB3	1.62	0.79
13:M:6:PXZ:N2	14:N:31:DC:O4'	2.15	0.79
1:A:1292:MET:HA	1:A:1296:MET:HG2	1.63	0.78
15:P:4:U:H2'	15:P:5:A:C8	2.19	0.78
1:A:948:ILE:HG12	1:A:1007:ILE:HD11	1.65	0.78
2:B:159:THR:HA	2:B:164:ASN:HD22	1.48	0.78
2:B:260:LEU:HB2	2:B:263:ILE:HD12	1.66	0.78
2:B:423:ILE:HD11	2:B:429:PHE:HB2	1.65	0.78
1:A:621:ILE:HD11	8:H:124:ARG:HD2	1.66	0.77
2:B:357:CYS:SG	2:B:361:LYS:NZ	2.57	0.77
1:A:1371:ILE:HG12	5:E:207:ARG:HH12	1.50	0.76
1:A:1147:SER:HA	1:A:1153:ARG:HB2	1.68	0.76
13:M:11:MVA:HN3	16:T:16:DT:O2	1.85	0.76
1:A:841:MET:SD	2:B:503:ASN:ND2	2.58	0.76
1:A:680:LEU:HD11	1:A:685:HIS:HB2	1.68	0.75
1:A:1468:THR:HG23	6:F:64:ARG:HB2	1.68	0.75
1:A:857:THR:HB	1:A:1100:THR:HG22	1.66	0.75
1:A:1148:ALA:HB1	1:A:1333:GLU:HB2	1.66	0.75
1:A:1412:MET:SD	1:A:1422:GLN:NE2	2.60	0.75
2:B:236:TRP:HB2	2:B:259:THR:HB	1.67	0.74
1:A:1242:ASP:HA	1:A:1262:MET:HB2	1.68	0.74
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.19	0.74
1:A:538:VAL:HG12	1:A:539:GLN:HG2	1.70	0.74
2:B:580:PRO:HB2	2:B:605:ARG:HE	1.53	0.74
15:P:3:C:N4	16:T:30:DT:O4	2.20	0.74
8:H:32:SER:HB3	8:H:37:MET:H	1.51	0.73
2:B:363:TYR:HB3	2:B:573:TRP:HZ3	1.53	0.73
1:A:1143:LEU:HB2	1:A:1148:ALA:HB2	1.70	0.73
1:A:784:VAL:HG13	2:B:978:ILE:HD11	1.69	0.73
1:A:62:GLN:HE22	1:A:255:VAL:HG12	1.54	0.72
1:A:1416:ARG:HE	13:M:11:MVA:HG12	1.53	0.72
2:B:112:GLU:HG3	12:L:43:ILE:HD11	1.71	0.72
2:B:550:MET:HG2	2:B:551:GLU:H	1.54	0.72
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.63	0.72
2:B:274:ARG:NH1	2:B:311:ILE:O	2.23	0.72
1:A:190:ARG:NH1	14:N:37:DG:C5'	2.52	0.72
11:K:12:LEU:HD11	11:K:18:LYS:HD3	1.71	0.72
3:C:205:LYS:NZ	3:C:212:ASP:O	2.23	0.71
1:A:823:VAL:HG11	1:A:831:LEU:HD22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1358:THR:HG23	5:E:144:LEU:HD11	1.72	0.71
2:B:1028:LEU:HB2	2:B:1041:ILE:HD13	1.71	0.71
1:A:1208:SER:O	1:A:1260:ARG:NH1	2.24	0.71
2:B:157:ARG:NH2	2:B:177:CYS:O	2.24	0.71
2:B:507:GLY:HA2	2:B:703:ILE:HA	1.73	0.71
2:B:469:VAL:HG21	16:T:27:DT:H5"	1.71	0.70
2:B:1031:GLY:O	3:C:36:ARG:NH2	2.24	0.70
15:P:10:U:H2'	15:P:11:A:H8	1.56	0.70
1:A:107:LEU:HD21	1:A:221:VAL:HG13	1.73	0.70
3:C:29:ALA:HB3	11:K:48:SER:HB2	1.73	0.70
1:A:1417:HIS:HE1	13:M:11:MVA:HG11	0.91	0.70
1:A:98:GLY:HA3	1:A:1440:MET:HE2	1.74	0.70
9:I:97:PHE:HB2	9:I:100:HIS:HE2	1.56	0.70
2:B:626:LEU:HG	2:B:698:ILE:HD13	1.73	0.70
1:A:18:ILE:H	1:A:1462:GLN:HE22	1.39	0.69
1:A:118:LEU:HD21	1:A:188:GLN:HG3	1.74	0.69
1:A:1473:LEU:HD11	6:F:64:ARG:HG2	1.72	0.69
2:B:585:ASN:OD1	2:B:588:ARG:NH2	2.25	0.69
1:A:859:TYR:HE2	13:M:2:DVA:HG12	1.56	0.69
2:B:1129:ASN:ND2	2:B:1134:THR:OG1	2.25	0.69
2:B:713:PHE:HB3	2:B:716:HIS:HD2	1.57	0.69
2:B:115:LEU:HB3	2:B:908:MET:HE1	1.75	0.69
2:B:794:VAL:HG22	2:B:967:ILE:HG22	1.75	0.69
3:C:67:ARG:NH1	3:C:150:ILE:O	2.25	0.69
8:H:112:LEU:HB2	8:H:132:LEU:HD23	1.75	0.69
1:A:844:ARG:HG2	2:B:501:LEU:H	1.58	0.69
1:A:363:ALA:HB3	1:A:503:LEU:HB3	1.73	0.68
2:B:953:ASP:OD1	3:C:36:ARG:NH1	2.26	0.68
1:A:672:ILE:HG23	1:A:676:ILE:HD12	1.75	0.68
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.26	0.68
12:L:18:ILE:HG12	12:L:25:GLU:HG2	1.74	0.68
1:A:1085:GLU:HA	6:F:60:TYR:HE2	1.58	0.68
1:A:760:LEU:HD11	1:A:781:ILE:HG21	1.76	0.67
1:A:1093:GLN:HE22	2:B:1093:CYS:HA	1.59	0.67
2:B:823:PHE:CZ	14:N:14:DT:H5"	2.29	0.67
1:A:1180:ASN:HB2	1:A:1183:SER:HB3	1.77	0.67
1:A:1213:ARG:HG3	1:A:1256:VAL:HG13	1.75	0.67
8:H:7:GLU:HG2	8:H:59:VAL:HG22	1.76	0.67
1:A:790:GLN:NE2	1:A:820:ARG:O	2.26	0.66
10:J:3:ILE:HD13	10:J:18:TRP:HB2	1.76	0.66
2:B:505:LEU:HD22	2:B:509:VAL:HB	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:ALA:O	1:A:1059:ARG:NH1	2.29	0.66
1:A:141:LEU:HD13	1:A:1445:HIS:HE1	1.61	0.66
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.29	0.66
3:C:78:ILE:HG22	3:C:81:LYS:HD3	1.77	0.66
1:A:1417:HIS:HE1	13:M:11:MVA:CG1	1.65	0.66
2:B:474:THR:OG1	2:B:732:ALA:O	2.13	0.66
1:A:585:LEU:HD22	8:H:47:ILE:HD11	1.78	0.66
5:E:17:ILE:HA	5:E:20:LEU:HD12	1.78	0.65
1:A:727:PRO:HA	1:A:736:THR:HG21	1.78	0.65
2:B:249:LYS:HG3	2:B:255:ARG:HE	1.61	0.65
5:E:55:ARG:HH21	5:E:76:PHE:HD1	1.43	0.65
1:A:1474:LEU:HB2	6:F:105:ILE:HG13	1.76	0.65
2:B:46:SER:OG	2:B:397:GLY:N	2.26	0.65
4:D:26:PHE:HE1	7:G:5:ILE:HD13	1.60	0.65
5:E:55:ARG:HA	5:E:58:LEU:HD12	1.79	0.65
15:P:8:A:H2'	15:P:9:G:C8	2.32	0.65
2:B:109:MET:HE2	2:B:174:LEU:HD13	1.78	0.65
13:M:9:PRO:HG2	14:N:32:DA:C4'	2.26	0.65
14:N:38:DA:H2''	14:N:39:DC:H5'	1.79	0.65
1:A:20:ARG:NH2	2:B:1172:MET:SD	2.70	0.65
2:B:465:GLY:O	2:B:468:GLN:NE2	2.28	0.65
5:E:194:ILE:HG12	5:E:204:ILE:HG12	1.78	0.65
1:A:1205:ALA:HB3	1:A:1263:ASN:HB2	1.79	0.65
2:B:748:ALA:HB3	2:B:811:TYR:HB2	1.79	0.64
2:B:598:VAL:HG12	2:B:600:GLU:H	1.62	0.64
3:C:228:ARG:NH1	3:C:230:TYR:OH	2.30	0.64
13:M:9:PRO:HB3	14:N:31:DC:H1'	1.77	0.64
1:A:567:LEU:HD21	1:A:595:ILE:HG12	1.79	0.64
1:A:757:GLN:HE22	1:A:778:LYS:HB3	1.63	0.64
3:C:193:ARG:NH1	3:C:217:GLN:OE1	2.31	0.64
1:A:811:ILE:HG21	9:I:79:PRO:HB3	1.79	0.64
2:B:1028:LEU:HG	2:B:1043:ILE:HD11	1.79	0.64
7:G:152:VAL:HA	7:G:157:ILE:HA	1.80	0.64
1:A:420:ILE:HB	1:A:445:LYS:HB2	1.79	0.64
1:A:1212:LEU:HB3	1:A:1259:ILE:HB	1.79	0.64
2:B:310:VAL:HG23	2:B:311:ILE:HD12	1.78	0.64
1:A:1138:SER:OG	1:A:1360:ASN:ND2	2.30	0.64
1:A:478:PRO:O	1:A:483:ARG:NH2	2.31	0.64
2:B:258:ALA:HB2	2:B:269:ILE:HD13	1.80	0.64
1:A:860:ILE:O	1:A:864:LEU:HG	1.98	0.64
2:B:910:THR:HG22	12:L:43:ILE:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:HD11	1:A:281:ALA:HB2	1.79	0.63
1:A:46:THR:OG1	1:A:273:GLN:NE2	2.31	0.63
2:B:1115:GLN:HB3	2:B:1148:LEU:HD11	1.79	0.63
1:A:904:GLN:NE2	1:A:981:CYS:O	2.31	0.63
1:A:850:THR:O	1:A:854:THR:HG23	1.97	0.63
2:B:827:GLU:HG2	2:B:871:VAL:HG22	1.79	0.63
1:A:1125:LYS:NZ	13:M:5:MVA:HG12	2.13	0.63
2:B:506:TRP:NE1	2:B:697:GLU:OE2	2.27	0.63
2:B:777:ASN:O	10:J:47:ARG:NH1	2.31	0.63
2:B:1062:ARG:NH1	2:B:1081:ASP:O	2.29	0.63
10:J:5:VAL:HG22	10:J:15:GLY:HA3	1.80	0.62
1:A:1357:THR:O	5:E:142:HIS:NE2	2.29	0.62
4:D:46:GLN:O	4:D:50:SER:OG	2.14	0.62
7:G:144:ARG:HG3	7:G:171:VAL:HG22	1.82	0.62
1:A:541:THR:O	1:A:545:VAL:N	2.33	0.62
1:A:1347:LEU:HB3	5:E:137:ILE:HD13	1.80	0.62
3:C:172:GLU:OE1	12:L:58:ARG:NH2	2.32	0.62
5:E:103:LEU:HD22	5:E:128:GLU:HB2	1.81	0.62
2:B:177:CYS:SG	2:B:738:THR:OG1	2.57	0.62
1:A:370:ASP:OD1	11:K:65:HIS:NE2	2.33	0.62
8:H:59:VAL:HB	8:H:144:LEU:HB2	1.80	0.62
1:A:42:LYS:O	1:A:288:ASN:ND2	2.33	0.62
13:M:10:SAR:HN1	14:N:33:DA:H5'	1.82	0.62
1:A:349:ARG:O	1:A:353:ASN:HB2	2.00	0.62
1:A:1382:LEU:HB3	1:A:1398:LEU:HD22	1.80	0.62
5:E:63:ALA:HA	5:E:71:GLN:HA	1.82	0.62
5:E:106:VAL:HG12	5:E:108:GLN:H	1.65	0.62
8:H:14:ASP:HB2	8:H:29:HIS:HB2	1.82	0.62
1:A:201:GLU:OE2	1:A:213:LYS:NZ	2.33	0.61
1:A:532:ARG:NH1	1:A:647:THR:O	2.33	0.61
2:B:223:SER:HG	2:B:233:SER:HG	1.42	0.61
13:M:11:MVA:HG12	13:M:11:MVA:O	1.99	0.61
2:B:816:GLU:HG2	2:B:867:ILE:HG21	1.82	0.61
10:J:40:LEU:HD22	10:J:45:CYS:HB3	1.82	0.61
1:A:340:LYS:O	1:A:344:LYS:HB2	2.00	0.61
1:A:576:GLN:O	1:A:590:GLN:NE2	2.34	0.61
1:A:78:MET:O	2:B:1072:ARG:NH2	2.33	0.61
1:A:1315:ASP:HB3	1:A:1320:ILE:HD11	1.82	0.61
13:M:6:PXZ:N2	14:N:31:DC:O5'	2.33	0.61
5:E:17:ILE:HD13	5:E:74:VAL:HG11	1.81	0.61
16:T:16:DT:H2''	16:T:17:DG:C8	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:PRO:HG2	1:A:613:GLU:HG3	1.82	0.61
1:A:1319:LYS:HE2	1:A:1321:ILE:HD11	1.83	0.61
2:B:924:ARG:NH1	3:C:62:GLU:OE2	2.34	0.61
9:I:15:ARG:NH2	9:I:47:GLU:O	2.29	0.61
1:A:90:LEU:HD22	1:A:310:LEU:HD21	1.83	0.61
9:I:14:ILE:HG21	9:I:23:MET:HE2	1.82	0.61
2:B:1030:ASN:ND2	2:B:1033:THR:OG1	2.33	0.60
4:D:114:LEU:HD22	7:G:84:VAL:HG11	1.82	0.60
5:E:41:LYS:HG3	5:E:46:GLY:HA2	1.82	0.60
5:E:171:PRO:HB2	5:E:207:ARG:HD3	1.81	0.60
15:P:5:A:H2'	15:P:6:A:C8	2.36	0.60
1:A:392:GLU:OE1	1:A:448:ARG:NH1	2.33	0.60
2:B:34:PHE:HZ	2:B:528:LEU:HB3	1.66	0.60
7:G:89:VAL:HA	7:G:99:THR:HG22	1.82	0.60
1:A:510:GLU:OE2	2:B:1101:GLN:NE2	2.35	0.60
2:B:929:PRO:O	2:B:948:GLN:NE2	2.34	0.60
1:A:876:ASP:O	1:A:890:ARG:NH1	2.35	0.60
1:A:913:ASN:HB2	1:A:1326:GLY:HA3	1.82	0.60
1:A:1430:CYS:HB2	1:A:1435:THR:HA	1.82	0.60
2:B:760:THR:OG1	2:B:764:MET:SD	2.56	0.60
5:E:118:LEU:HD22	5:E:127:LEU:HB2	1.84	0.60
2:B:1026:GLU:HB3	2:B:1043:ILE:HD12	1.83	0.60
1:A:620:HIS:O	8:H:97:TYR:OH	2.18	0.60
1:A:458:PHE:HB3	1:A:472:HIS:HD2	1.66	0.60
2:B:961:ILE:HD11	10:J:42:ARG:HB2	1.84	0.60
13:M:6:PXZ:H163	14:N:30:DG:O6	2.01	0.60
2:B:871:VAL:O	2:B:890:ARG:N	2.35	0.59
1:A:1348:SER:O	5:E:12:LYS:NZ	2.33	0.59
8:H:30:CYS:HB2	8:H:39:LEU:HB3	1.82	0.59
1:A:757:GLN:HA	1:A:760:LEU:HG	1.83	0.59
2:B:907:VAL:HB	12:L:46:LYS:HB2	1.85	0.59
1:A:201:GLU:HG2	1:A:213:LYS:HG2	1.84	0.59
1:A:947:HIS:NE2	1:A:951:GLU:OE2	2.35	0.59
12:L:17:TYR:HB3	12:L:44:MET:HB3	1.83	0.59
1:A:1487:PRO:HD2	6:F:78:PRO:HB3	1.84	0.59
1:A:601:ASN:ND2	1:A:989:ASN:OD1	2.35	0.59
1:A:760:LEU:HD13	1:A:767:LYS:HB2	1.85	0.59
5:E:100:THR:HA	5:E:125:TYR:HD1	1.66	0.59
3:C:123:ASN:OD1	3:C:124:SER:N	2.35	0.59
8:H:58:LEU:HD11	8:H:143:LEU:HD11	1.85	0.59
1:A:1416:ARG:HE	13:M:11:MVA:CG1	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:29:THR:HG23	5:E:32:GLY:H	1.68	0.59
6:F:66:LEU:HD21	6:F:97:LEU:HB2	1.83	0.59
4:D:26:PHE:HE2	7:G:78:ARG:HB3	1.68	0.58
8:H:96:VAL:HG13	8:H:137:VAL:HA	1.85	0.58
13:M:6:PXZ:C2	14:N:30:DG:H2'	2.33	0.58
1:A:790:GLN:HA	1:A:822:PHE:HA	1.84	0.58
1:A:1258:ARG:HH22	1:A:1260:ARG:HH21	1.50	0.58
8:H:8:ASP:OD2	8:H:32:SER:OG	2.19	0.58
10:J:35:LEU:HD13	10:J:46:ARG:HB3	1.84	0.58
13:M:11:MVA:HN2	16:T:17:DG:C2	2.37	0.58
1:A:545:VAL:HG22	1:A:676:ILE:HD13	1.85	0.58
1:A:576:GLN:HA	8:H:75:TYR:HB2	1.85	0.58
2:B:268:PRO:HD2	2:B:271:ILE:HD12	1.85	0.58
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.84	0.58
3:C:266:GLU:OE2	11:K:21:ILE:N	2.36	0.58
2:B:384:ASP:OD2	2:B:502:HIS:NE2	2.35	0.58
1:A:1177:TYR:OH	9:I:29:ASP:O	2.22	0.58
2:B:866:ILE:HD11	2:B:896:LEU:HG	1.85	0.58
3:C:175:LYS:HZ2	12:L:57:ALA:HB3	1.69	0.58
13:M:6:PXZ:C3	14:N:30:DG:H2'	2.33	0.58
2:B:1036:LYS:NZ	3:C:186:TYR:O	2.34	0.58
3:C:67:ARG:NH2	10:J:3:ILE:O	2.37	0.58
4:D:33:LEU:HB2	4:D:36:GLU:H	1.68	0.58
5:E:185:ILE:HD13	5:E:191:VAL:HG11	1.86	0.58
11:K:18:LYS:NZ	11:K:36:ASN:O	2.29	0.58
1:A:844:ARG:HG2	2:B:501:LEU:N	2.18	0.58
1:A:1440:MET:SD	2:B:1167:ILE:HD11	2.43	0.58
1:A:555:LEU:HD12	1:A:591:ILE:HD12	1.85	0.58
1:A:1208:SER:HB3	1:A:1260:ARG:HB3	1.86	0.58
2:B:631:GLN:NE2	2:B:691:SER:O	2.35	0.58
2:B:852:GLY:O	2:B:868:GLY:N	2.37	0.58
4:D:102:ASN:ND2	7:G:1:MET:SD	2.77	0.58
12:L:19:CYS:HB2	12:L:36:CYS:SG	2.44	0.58
1:A:1416:ARG:CD	13:M:11:MVA:HG12	2.34	0.57
2:B:195:ILE:HD12	2:B:484:ARG:HB3	1.86	0.57
16:T:29:DA:H2'	16:T:30:DT:C6	2.39	0.57
1:A:357:LYS:HD2	2:B:1107:LEU:HA	1.85	0.57
1:A:528:PRO:HG2	1:A:1090:LEU:HD11	1.86	0.57
1:A:1139:LEU:HD13	1:A:1359:SER:HB3	1.86	0.57
2:B:935:PHE:HE1	2:B:1050:ARG:HG3	1.69	0.57
1:A:82:PRO:O	2:B:1160:GLN:NE2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ASN:OD1	1:A:460:ARG:N	2.38	0.57
2:B:817:GLN:NE2	2:B:818:GLU:O	2.36	0.57
2:B:934:LYS:HG2	2:B:1051:LEU:HD12	1.85	0.57
4:D:135:GLN:HE22	4:D:138:ARG:HH11	1.53	0.57
6:F:56:TYR:HD1	6:F:124:ILE:HB	1.69	0.57
1:A:1243:LEU:HD13	1:A:1288:ILE:HD13	1.87	0.57
2:B:628:VAL:HG22	2:B:633:LEU:HD23	1.85	0.57
2:B:775:GLY:HA2	2:B:806:PHE:HE1	1.69	0.57
3:C:92:GLU:HG3	3:C:93:PHE:H	1.68	0.57
3:C:179:THR:OG1	3:C:234:GLU:O	2.23	0.57
8:H:96:VAL:HA	8:H:116:VAL:HA	1.85	0.57
1:A:359:VAL:HG11	2:B:1106:ARG:HG3	1.87	0.57
1:A:766:PHE:CE2	1:A:784:VAL:HG11	2.39	0.57
4:D:96:GLU:OE1	4:D:121:ARG:NH1	2.38	0.57
1:A:1085:GLU:HA	6:F:60:TYR:CE2	2.40	0.57
1:A:1454:VAL:HA	1:A:1465:PRO:HD2	1.85	0.57
2:B:785:TYR:OH	2:B:953:ASP:O	2.20	0.57
2:B:196:ALA:HB1	2:B:393:LEU:HB3	1.86	0.57
2:B:873:LEU:HD12	2:B:874:PRO:HD2	1.86	0.57
16:T:30:DT:H5"	16:T:30:DT:H6	1.70	0.57
1:A:366:VAL:HG11	2:B:944:THR:HG21	1.87	0.57
1:A:381:PRO:HB3	1:A:480:SER:HA	1.86	0.57
1:A:793:VAL:HB	1:A:799:PRO:HD3	1.87	0.57
8:H:37:MET:HE1	8:H:132:LEU:HD13	1.87	0.56
1:A:901:VAL:HG11	1:A:1396:ARG:HH21	1.70	0.56
2:B:491:ARG:HB3	2:B:518:HIS:HB3	1.85	0.56
2:B:1142:ASN:HD21	2:B:1145:GLN:HG3	1.69	0.56
1:A:413:TYR:HE2	1:A:476:ILE:HD13	1.70	0.56
3:C:267:ILE:O	3:C:271:VAL:N	2.27	0.56
16:T:31:DT:H2"	16:T:32:DC:C5	2.41	0.56
1:A:802:PHE:HE2	1:A:808:PRO:HD3	1.70	0.56
2:B:67:LEU:HD21	2:B:420:GLN:HB2	1.88	0.56
2:B:1120:ASN:OD1	2:B:1147:SER:OG	2.16	0.56
1:A:464:LEU:HD13	1:A:1100:THR:HG21	1.86	0.56
1:A:839:HIS:HE2	2:B:718:GLN:HG3	1.70	0.56
3:C:30:VAL:HA	11:K:45:ILE:HG12	1.88	0.56
7:G:67:LEU:HD23	7:G:69:PRO:HD3	1.87	0.56
8:H:10:PHE:HB3	8:H:30:CYS:HB3	1.88	0.56
2:B:992:ASN:HD21	2:B:1020:TYR:HE2	1.54	0.56
5:E:111:THR:HG23	5:E:114:ALA:H	1.71	0.56
12:L:22:CYS:SG	12:L:24:THR:OG1	2.62	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:41:DA:H2''	14:N:42:DA:C8	2.40	0.56
2:B:636:LYS:H	2:B:639:HIS:HD2	1.54	0.56
1:A:865:ILE:O	1:A:869:GLU:N	2.39	0.56
2:B:1088:GLU:HA	2:B:1091:ARG:HG2	1.86	0.56
1:A:589:LYS:NZ	1:A:625:ASP:OD1	2.38	0.55
1:A:678:ASN:HA	1:A:681:LEU:HD13	1.88	0.55
1:A:1486:ILE:HG13	1:A:1487:PRO:HD3	1.87	0.55
12:L:36:CYS:HB2	12:L:44:MET:HE1	1.88	0.55
1:A:497:ASP:HA	2:B:943:GLY:HA2	1.88	0.55
9:I:115:THR:HG22	9:I:116:ALA:H	1.72	0.55
1:A:1125:LYS:HZ3	13:M:5:MVA:HG12	1.72	0.55
1:A:460:ARG:HH22	15:P:13:C:C4'	2.19	0.55
2:B:665:ILE:HG23	2:B:669:GLU:HB3	1.88	0.55
7:G:97:LEU:HB2	7:G:108:ILE:HB	1.87	0.55
1:A:906:LEU:HD13	1:A:966:LEU:HD13	1.87	0.55
1:A:1474:LEU:HD11	6:F:107:ARG:NE	2.21	0.55
1:A:20:ARG:NH1	1:A:22:GLN:OE1	2.39	0.55
1:A:1403:ASP:O	1:A:1407:CYS:HB2	2.07	0.55
14:N:40:DA:H2''	14:N:41:DA:C8	2.42	0.55
1:A:610:PRO:HD2	1:A:626:THR:HG21	1.88	0.55
1:A:1218:ARG:NH2	1:A:1252:ALA:O	2.39	0.55
1:A:1262:MET:HG2	1:A:1265:ASP:H	1.72	0.55
3:C:9:VAL:HG13	3:C:21:PHE:HB2	1.88	0.55
3:C:74:THR:N	3:C:128:ILE:O	2.40	0.55
5:E:122:ALA:H	5:E:123:PRO:HD2	1.71	0.55
11:K:81:TYR:OH	11:K:89:ASN:ND2	2.38	0.55
1:A:76:GLY:HA2	1:A:81:CYS:HB2	1.89	0.55
1:A:833:PRO:HG3	2:B:1002:PHE:CG	2.42	0.55
3:C:234:GLU:OE1	10:J:42:ARG:NH1	2.35	0.55
1:A:565:MET:HG3	11:K:62:LYS:HD3	1.89	0.54
1:A:833:PRO:HB2	2:B:677:MET:HE2	1.89	0.54
1:A:1179:PRO:HA	1:A:1209:PRO:HA	1.89	0.54
7:G:114:PRO:HG3	7:G:164:MET:HA	1.89	0.54
1:A:551:ARG:NH1	8:H:42:ASP:OD2	2.40	0.54
2:B:565:THR:HA	2:B:610:ARG:HG2	1.89	0.54
8:H:40:ILE:HD12	8:H:124:ARG:HD3	1.88	0.54
1:A:766:PHE:HB3	1:A:781:ILE:HG12	1.87	0.54
2:B:794:VAL:O	2:B:946:GLY:N	2.39	0.54
8:H:41:LEU:HD21	8:H:143:LEU:HD21	1.89	0.54
1:A:190:ARG:HH12	14:N:37:DG:H5'	1.72	0.54
1:A:1196:TYR:HE2	1:A:1248:ASN:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:580:PRO:HB3	2:B:612:ILE:HD11	1.89	0.54
2:B:710:ILE:HA	2:B:764:MET:HE2	1.89	0.54
2:B:803:ARG:NH2	10:J:10:CYS:O	2.41	0.54
2:B:955:PRO:HB2	2:B:1028:LEU:HD22	1.90	0.54
8:H:94:GLY:HA3	8:H:118:TYR:HA	1.89	0.54
1:A:873:VAL:HG22	1:A:879:VAL:HG22	1.90	0.54
9:I:85:PRO:HB2	9:I:90:GLY:HA2	1.90	0.54
13:M:11:MVA:HN2	16:T:17:DG:N3	2.22	0.54
2:B:625:LEU:HD13	2:B:675:LEU:HD21	1.90	0.54
3:C:44:ILE:HD11	3:C:238:SER:HB3	1.90	0.54
1:A:190:ARG:HH12	14:N:37:DG:C5'	2.18	0.54
1:A:1097:GLU:O	1:A:1100:THR:OG1	2.22	0.54
1:A:33:ARG:O	2:B:1138:ARG:HB3	2.08	0.54
1:A:1212:LEU:HB2	1:A:1285:LEU:HD21	1.90	0.54
2:B:205:VAL:O	2:B:371:ARG:NH1	2.41	0.54
2:B:485:LEU:HD21	2:B:526:LEU:HD21	1.88	0.54
2:B:776:ILE:HD12	2:B:806:PHE:H	1.72	0.54
8:H:17:PRO:HG3	8:H:29:HIS:CD2	2.43	0.54
2:B:553:LEU:HA	2:B:556:ILE:HD12	1.90	0.54
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.90	0.54
2:B:192:LYS:NZ	2:B:449:ALA:HA	2.23	0.53
1:A:467:MET:SD	1:A:524:MET:HE2	2.48	0.53
1:A:514:GLU:OE2	1:A:1468:THR:HG21	2.09	0.53
1:A:1258:ARG:NH2	1:A:1260:ARG:HH21	2.07	0.53
1:A:26:LEU:HD13	1:A:31:LEU:HD21	1.89	0.53
2:B:553:LEU:HD23	2:B:556:ILE:HD12	1.89	0.53
2:B:627:ILE:HD11	2:B:663:GLU:HB2	1.89	0.53
2:B:911:LEU:HD23	2:B:917:LYS:HA	1.90	0.53
8:H:37:MET:HG2	8:H:127:GLY:HA3	1.90	0.53
1:A:1354:PRO:HB3	5:E:137:ILE:HD11	1.88	0.53
2:B:159:THR:HA	2:B:164:ASN:ND2	2.20	0.53
2:B:570:ASN:OD1	2:B:616:THR:N	2.39	0.53
5:E:82:VAL:HB	5:E:110:MET:HE3	1.91	0.53
1:A:363:ALA:HB2	1:A:388:MET:SD	2.49	0.53
7:G:108:ILE:HD11	7:G:145:LEU:HD22	1.91	0.53
1:A:991:GLN:HA	1:A:996:ILE:HD12	1.91	0.53
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.91	0.53
13:M:9:PRO:HG3	14:N:32:DA:H5'	1.89	0.53
2:B:710:ILE:O	2:B:938:ARG:HD2	2.08	0.53
2:B:721:ARG:HD3	2:B:724:TYR:HD2	1.73	0.53
4:D:128:GLN:NE2	4:D:132:ASP:OD1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:HB2	1:A:73:THR:HG23	1.89	0.53
2:B:193:VAL:HG21	2:B:470:LEU:HD13	1.91	0.53
2:B:436:LYS:HD3	16:T:33:DA:OP1	2.08	0.53
2:B:533:SER:OG	2:B:620:ARG:N	2.41	0.53
2:B:764:MET:HE1	2:B:938:ARG:NH1	2.24	0.53
10:J:1:MET:HA	10:J:55:LEU:HB2	1.90	0.53
11:K:22:ASN:HB2	11:K:32:LEU:HB3	1.90	0.53
3:C:190:ASN:HD22	3:C:217:GLN:NE2	2.07	0.53
7:G:100:GLU:HA	7:G:105:SER:HA	1.90	0.53
2:B:728:MET:SD	2:B:934:LYS:NZ	2.82	0.52
2:B:823:PHE:HZ	14:N:14:DT:H3'	1.74	0.52
2:B:855:ALA:HB3	12:L:49:THR:HB	1.89	0.52
16:T:13:DT:H2''	16:T:14:DT:O5'	2.09	0.52
2:B:604:ILE:N	2:B:613:ARG:O	2.41	0.52
1:A:65:ILE:HG22	1:A:66:GLU:HG3	1.91	0.52
1:A:1457:ASN:HD22	1:A:1465:PRO:HD3	1.75	0.52
2:B:761:THR:H	2:B:764:MET:HE3	1.75	0.52
15:P:10:U:H2'	15:P:11:A:C8	2.39	0.52
1:A:93:PRO:HD2	1:A:219:GLU:HG2	1.90	0.52
1:A:811:ILE:HD11	2:B:690:CYS:HB2	1.91	0.52
1:A:977:VAL:HG12	1:A:979:LEU:HG	1.90	0.52
1:A:479:TRP:HB2	1:A:483:ARG:NH2	2.24	0.52
1:A:1180:ASN:OD1	9:I:33:ARG:NH1	2.42	0.52
3:C:42:VAL:HB	3:C:178:PRO:HG3	1.92	0.52
1:A:693:ILE:HG12	1:A:828:LEU:HD21	1.92	0.52
1:A:1171:ALA:HB2	1:A:1217:ASP:HB2	1.92	0.52
1:A:1228:MET:HE1	1:A:1257:LEU:HB2	1.91	0.52
2:B:713:PHE:HB3	2:B:716:HIS:CD2	2.41	0.52
7:G:4:HIS:CE1	7:G:73:LYS:HB3	2.44	0.52
8:H:79:ASP:O	8:H:82:PRO:HD2	2.10	0.52
1:A:428:ASP:OD2	1:A:430:ARG:NH1	2.43	0.52
1:A:769:MET:SD	2:B:973:PRO:HG3	2.50	0.52
2:B:285:LEU:HD11	2:B:305:LEU:HD11	1.92	0.52
2:B:733:MET:HE3	2:B:1052:LYS:HA	1.90	0.52
2:B:1118:VAL:HG21	2:B:1171:MET:SD	2.49	0.52
6:F:108:ARG:HD2	6:F:118:TRP:CD1	2.45	0.52
1:A:877:ALA:HB3	1:A:890:ARG:HH11	1.74	0.52
1:A:1213:ARG:HH22	1:A:1254:LYS:HD3	1.75	0.52
3:C:30:VAL:HG22	11:K:45:ILE:HG23	1.91	0.52
4:D:33:LEU:HD22	4:D:101:ALA:HB3	1.91	0.52
16:T:10:DT:H2''	16:T:11:DC:OP2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:918:PHE:CE2	2:B:920:LYS:HG3	2.45	0.52
7:G:30:LEU:HD22	7:G:70:VAL:HG11	1.92	0.52
8:H:88:PHE:CD2	8:H:144:LEU:HB3	2.44	0.52
1:A:22:GLN:NE2	1:A:1446:GLY:O	2.42	0.51
1:A:255:VAL:HG13	1:A:280:LEU:HD13	1.91	0.51
1:A:557:ARG:O	1:A:561:MET:HG2	2.09	0.51
1:A:861:GLN:HE22	1:A:1093:GLN:HA	1.75	0.51
1:A:1316:ASN:OD1	1:A:1317:LYS:N	2.42	0.51
8:H:26:SER:HB3	8:H:45:ILE:HD11	1.93	0.51
1:A:541:THR:HG23	1:A:676:ILE:HB	1.92	0.51
2:B:779:ILE:HB	2:B:963:PRO:HA	1.91	0.51
1:A:1248:ASN:ND2	1:A:1256:VAL:O	2.44	0.51
1:A:1386:ILE:HD12	1:A:1398:LEU:HD21	1.91	0.51
2:B:473:LEU:HD11	2:B:1052:LYS:HD3	1.92	0.51
2:B:495:LEU:CD2	14:N:29:DT:H4'	2.37	0.51
2:B:570:ASN:OD1	2:B:617:ASP:N	2.44	0.51
2:B:904:VAL:HG22	2:B:923:VAL:HG22	1.92	0.51
14:N:31:DC:H2''	14:N:32:DA:C8	2.45	0.51
16:T:35:DT:H2''	16:T:36:DA:N7	2.25	0.51
1:A:456:VAL:HG21	1:A:503:LEU:HD11	1.93	0.51
1:A:788:VAL:HB	1:A:823:VAL:HB	1.91	0.51
2:B:911:LEU:HD12	12:L:42:ARG:HD3	1.92	0.51
3:C:241:PRO:HA	3:C:244:ILE:HD12	1.91	0.51
1:A:542:LEU:HD23	1:A:774:ALA:HA	1.91	0.51
7:G:97:LEU:HD11	7:G:128:TYR:HE2	1.75	0.51
8:H:37:MET:HE3	8:H:127:GLY:HA3	1.92	0.51
16:T:25:DT:H2'	16:T:26:DC:C6	2.45	0.51
1:A:321:GLU:HG3	1:A:341:GLN:HE21	1.75	0.51
1:A:559:GLU:HG2	1:A:682:ILE:HD13	1.92	0.51
1:A:889:LEU:N	5:E:203:TYR:OH	2.39	0.51
2:B:633:LEU:HD11	2:B:679:PRO:HG3	1.92	0.51
2:B:731:GLN:NE2	15:P:10:U:O3'	2.44	0.51
3:C:5:ASN:HD22	11:K:52:LYS:NZ	2.08	0.51
3:C:253:LYS:HE3	11:K:95:ILE:HG23	1.93	0.51
7:G:52:ASP:H	7:G:72:TYR:HA	1.76	0.51
9:I:86:CYS:HA	9:I:123:TRP:CZ2	2.45	0.51
11:K:49:GLN:HG2	11:K:94:LEU:HG	1.93	0.51
2:B:117:ASN:OD1	2:B:815:LYS:NZ	2.44	0.51
2:B:252:ILE:HB	2:B:303:PRO:HA	1.92	0.51
1:A:567:LEU:HG	1:A:675:VAL:HG11	1.92	0.51
2:B:332:LYS:HA	2:B:335:ARG:HE	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:193:ARG:HG3	3:C:220:TYR:HD1	1.76	0.51
16:T:13:DT:H2'	16:T:14:DT:C6	2.46	0.51
1:A:254:PRO:HB2	2:B:1164:SER:HA	1.93	0.51
1:A:877:ALA:HB3	1:A:890:ARG:NH1	2.26	0.51
1:A:894:ASP:OD1	1:A:1396:ARG:NH1	2.42	0.51
1:A:1053:ARG:NH1	1:A:1057:GLU:OE1	2.44	0.51
10:J:10:CYS:SG	10:J:42:ARG:NH2	2.76	0.51
1:A:225:PHE:HB3	1:A:245:PRO:HB2	1.93	0.50
1:A:1082:HIS:HE1	6:F:126:THR:HG21	1.76	0.50
1:A:1168:LYS:NZ	1:A:1305:SER:O	2.42	0.50
4:D:131:LEU:O	4:D:135:GLN:HG2	2.11	0.50
14:N:29:DT:H5'	14:N:29:DT:C6	2.46	0.50
2:B:587:LEU:HB3	2:B:603:MET:SD	2.51	0.50
2:B:1104:ARG:NH1	7:G:61:PRO:HB2	2.26	0.50
3:C:72:PRO:HB2	3:C:130:VAL:HG21	1.92	0.50
8:H:40:ILE:HB	8:H:124:ARG:HB3	1.93	0.50
1:A:256:PRO:HD2	1:A:280:LEU:HD11	1.93	0.50
1:A:864:LEU:HD23	1:A:1414:ILE:HG21	1.93	0.50
1:A:890:ARG:HE	1:A:1023:VAL:HG22	1.75	0.50
1:A:1436:VAL:O	1:A:1440:MET:HG2	2.11	0.50
2:B:779:ILE:HD12	10:J:43:TYR:HE1	1.76	0.50
4:D:33:LEU:H	4:D:36:GLU:HB2	1.77	0.50
4:D:73:ARG:NE	4:D:102:ASN:O	2.33	0.50
1:A:485:ASN:OD1	1:A:486:LEU:N	2.45	0.50
1:A:839:HIS:HE2	2:B:718:GLN:HA	1.76	0.50
2:B:34:PHE:CZ	2:B:528:LEU:HB3	2.45	0.50
3:C:4:ALA:HB1	11:K:97:GLU:HB2	1.92	0.50
3:C:59:LEU:HD12	3:C:151:VAL:HG23	1.92	0.50
1:A:97:VAL:HG21	1:A:322:LEU:HD11	1.94	0.50
1:A:548:PHE:HE1	1:A:555:LEU:HD11	1.75	0.50
1:A:577:PRO:HG3	1:A:584:PRO:HB3	1.94	0.50
2:B:436:LYS:HE2	16:T:33:DA:C5'	2.11	0.50
1:A:1128:ILE:HG23	1:A:1414:ILE:HB	1.93	0.50
1:A:1476:ASP:HB2	6:F:105:ILE:HG23	1.92	0.50
7:G:101:ILE:N	7:G:104:MET:O	2.42	0.50
12:L:16:ILE:HG12	12:L:27:GLU:HG2	1.93	0.50
1:A:548:PHE:O	1:A:588:GLY:HA3	2.11	0.50
1:A:1457:ASN:HB2	1:A:1464:ALA:HA	1.94	0.50
2:B:419:ALA:O	2:B:423:ILE:HG12	2.11	0.50
2:B:761:THR:HG23	2:B:1000:THR:HA	1.93	0.50
2:B:826:GLU:H	2:B:872:THR:HG22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:9:DG:H2''	16:T:10:DT:O5'	2.11	0.50
2:B:403:LEU:HD21	2:B:447:SER:OG	2.12	0.50
11:K:49:GLN:HB2	11:K:94:LEU:HD21	1.93	0.50
1:A:356:GLY:O	2:B:1085:ARG:NH1	2.45	0.50
1:A:894:ASP:HB3	5:E:200:ALA:HB2	1.94	0.50
16:T:24:DC:H2'	16:T:25:DT:C6	2.46	0.50
1:A:64:VAL:HG12	1:A:78:MET:HE2	1.93	0.49
1:A:1355:VAL:HA	5:E:142:HIS:HA	1.93	0.49
2:B:706:VAL:HG13	2:B:767:LEU:HD22	1.94	0.49
3:C:74:THR:HB	3:C:128:ILE:HG13	1.94	0.49
1:A:548:PHE:CE1	1:A:555:LEU:HD11	2.47	0.49
1:A:867:SER:HB3	1:A:1414:ILE:HG23	1.93	0.49
2:B:534:VAL:N	2:B:600:GLU:OE2	2.45	0.49
3:C:259:LEU:HD11	11:K:42:LEU:HD21	1.94	0.49
5:E:156:VAL:HG22	5:E:190:VAL:HB	1.94	0.49
1:A:858:GLY:HA3	2:B:1089:MET:CE	2.42	0.49
1:A:1415:THR:HG21	13:M:8:DVA:HG11	1.94	0.49
1:A:18:ILE:N	1:A:1462:GLN:HE22	2.08	0.49
2:B:470:LEU:HD21	2:B:478:THR:HG23	1.95	0.49
2:B:483:ARG:NH2	2:B:527:ALA:O	2.29	0.49
2:B:792:ASP:OD1	2:B:975:ARG:NH2	2.45	0.49
1:A:685:HIS:CD2	1:A:769:MET:HE3	2.46	0.49
1:A:1196:TYR:OH	1:A:1249:ASP:OD1	2.28	0.49
1:A:1454:VAL:HA	1:A:1464:ALA:HB1	1.93	0.49
2:B:113:ALA:HA	2:B:118:LEU:HB2	1.95	0.49
1:A:1093:GLN:NE2	2:B:1093:CYS:HA	2.26	0.49
1:A:1429:LYS:HB2	1:A:1438:VAL:HG11	1.95	0.49
2:B:222:ARG:HG2	2:B:234:THR:HG22	1.93	0.49
5:E:102:ALA:HB3	5:E:127:LEU:HD22	1.94	0.49
1:A:525:ILE:O	1:A:534:VAL:N	2.32	0.49
1:A:552:ASP:OD1	8:H:22:PHE:HB3	2.13	0.49
1:A:871:VAL:HG11	1:A:1400:LEU:HD11	1.93	0.49
2:B:31:SER:HG	2:B:766:TYR:HH	1.61	0.49
9:I:24:LEU:HD23	9:I:39:CYS:HB2	1.95	0.49
1:A:490:THR:OG1	1:A:491:PRO:HD3	2.13	0.49
1:A:549:THR:HG21	1:A:640:LEU:HG	1.93	0.49
2:B:265:GLN:HE21	2:B:324:ARG:HE	1.60	0.49
2:B:810:PHE:HB2	2:B:927:ARG:HH12	1.78	0.49
3:C:18:ASN:OD1	3:C:19:VAL:N	2.46	0.49
16:T:20:DG:C2	16:T:21:DG:C5	3.01	0.49
1:A:554:PHE:HB3	1:A:585:LEU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1244:ASN:N	1:A:1260:ARG:O	2.46	0.49
2:B:50:PHE:HA	2:B:54:SER:HB2	1.95	0.49
2:B:255:ARG:HD2	2:B:307:GLU:HB2	1.95	0.49
2:B:677:MET:H	2:B:682:LEU:HD22	1.77	0.49
2:B:851:ASP:OD2	12:L:17:TYR:OH	2.30	0.49
2:B:1060:HIS:HE1	2:B:1081:ASP:HA	1.78	0.49
11:K:57:LEU:N	11:K:76:GLN:O	2.45	0.49
2:B:114:ARG:NH2	2:B:184:TYR:OH	2.46	0.49
2:B:348:LEU:HD23	2:B:351:VAL:HG21	1.93	0.49
2:B:474:THR:HG22	2:B:476:ALA:H	1.78	0.49
3:C:18:ASN:HD21	3:C:20:LYS:HE3	1.77	0.48
15:P:9:G:O5'	15:P:9:G:H8	1.95	0.48
1:A:96:HIS:NE2	2:B:1165:MET:O	2.45	0.48
2:B:83:ARG:HB2	2:B:133:ILE:HB	1.95	0.48
2:B:613:ARG:HB3	2:B:615:TYR:CE2	2.48	0.48
7:G:110:ARG:HA	7:G:113:ILE:HD12	1.95	0.48
1:A:1102:MET:HB3	1:A:1120:GLY:HA2	1.95	0.48
3:C:14:LEU:HD13	3:C:19:VAL:HG22	1.95	0.48
1:A:1005:HIS:CD2	1:A:1007:ILE:HB	2.48	0.48
2:B:96:PRO:HG2	2:B:120:TYR:CZ	2.48	0.48
2:B:549:SER:OG	2:B:550:MET:N	2.45	0.48
7:G:30:LEU:O	7:G:34:VAL:HG22	2.12	0.48
11:K:56:VAL:HA	11:K:77:THR:HG22	1.94	0.48
13:M:7:THR:CG2	16:T:17:DG:H2''	2.44	0.48
2:B:823:PHE:HZ	14:N:14:DT:C3'	2.27	0.48
3:C:149:LEU:HD21	3:C:152:LYS:HE3	1.96	0.48
1:A:648:SER:OG	1:A:651:SER:OG	2.29	0.48
1:A:801:GLY:HA3	2:B:503:ASN:HB2	1.94	0.48
1:A:1289:GLU:HA	1:A:1292:MET:HE2	1.96	0.48
3:C:33:SER:O	3:C:37:VAL:HG23	2.13	0.48
10:J:5:VAL:HG13	10:J:13:ILE:HG23	1.96	0.48
1:A:865:ILE:HD13	2:B:1092:ASP:CB	2.33	0.48
1:A:1246:ILE:HB	1:A:1258:ARG:HB2	1.95	0.48
2:B:363:TYR:HB3	2:B:573:TRP:CZ3	2.41	0.48
1:A:1141:VAL:HG13	1:A:1352:VAL:HG13	1.95	0.48
2:B:240:LEU:N	2:B:255:ARG:O	2.47	0.48
2:B:529:MET:HG2	2:B:702:MET:HB3	1.96	0.48
1:A:797:ARG:HH21	1:A:820:ARG:NH1	2.11	0.48
2:B:265:GLN:NE2	2:B:324:ARG:HE	2.11	0.48
2:B:1032:PHE:HA	3:C:36:ARG:NH2	2.29	0.48
2:B:1129:ASN:HD22	2:B:1132:THR:HB	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:VAL:HG12	3:C:21:PHE:HD1	1.79	0.48
16:T:13:DT:H2'	16:T:14:DT:H71	1.96	0.48
1:A:1082:HIS:HB3	6:F:58:THR:HB	1.96	0.48
1:A:1184:THR:OG1	1:A:1190:GLN:NE2	2.47	0.48
2:B:248:LYS:O	2:B:252:ILE:HG12	2.14	0.48
2:B:949:TYR:HB3	2:B:953:ASP:HB2	1.96	0.48
5:E:130:PHE:HE1	5:E:181:ARG:HB3	1.78	0.48
1:A:854:THR:HG21	15:P:13:C:C4	2.49	0.47
2:B:789:ASN:HB3	2:B:795:ILE:HG13	1.95	0.47
2:B:809:VAL:HG22	2:B:926:VAL:HG12	1.96	0.47
2:B:1072:ARG:HB2	2:B:1153:TYR:CD2	2.48	0.47
1:A:137:PRO:HA	1:A:140:ARG:HG2	1.96	0.47
2:B:192:LYS:HZ2	2:B:449:ALA:HA	1.79	0.47
2:B:910:THR:O	2:B:918:PHE:N	2.37	0.47
3:C:52:ILE:HA	3:C:161:LEU:HB3	1.96	0.47
16:T:27:DT:H2''	16:T:28:DT:O5'	2.14	0.47
1:A:389:THR:HG21	1:A:417:LYS:HD3	1.96	0.47
4:D:64:THR:HG23	7:G:2:PHE:CE1	2.50	0.47
5:E:55:ARG:HE	5:E:76:PHE:HB3	1.79	0.47
6:F:81:VAL:HG11	6:F:95:LYS:HG2	1.96	0.47
14:N:39:DC:C2	14:N:40:DA:C5	3.02	0.47
1:A:410:ASN:OD1	1:A:449:HIS:NE2	2.44	0.47
1:A:910:LYS:HG3	1:A:1328:PHE:HD2	1.79	0.47
1:A:1261:ILE:HG22	1:A:1262:MET:H	1.78	0.47
2:B:252:ILE:HD11	2:B:255:ARG:HD3	1.96	0.47
7:G:119:PHE:HB2	7:G:128:TYR:HE1	1.80	0.47
15:P:3:C:H42	16:T:30:DT:H3	1.62	0.47
1:A:32:LYS:HG3	1:A:252:VAL:HG21	1.96	0.47
1:A:370:ASP:OD2	1:A:373:LEU:HG	2.15	0.47
1:A:460:ARG:HB2	1:A:501:MET:HE2	1.94	0.47
1:A:1098:PRO:O	1:A:1102:MET:N	2.48	0.47
2:B:281:ASP:HB2	9:I:22:ASN:HA	1.96	0.47
2:B:728:MET:SD	2:B:942:LYS:HB3	2.54	0.47
1:A:190:ARG:NH1	14:N:37:DG:H5'	2.26	0.47
1:A:375:ILE:HG23	1:A:488:VAL:HG22	1.95	0.47
1:A:1189:ASP:HA	1:A:1192:TRP:CZ2	2.50	0.47
1:A:1464:ALA:O	1:A:1469:GLY:HA3	2.15	0.47
2:B:50:PHE:HB2	2:B:397:GLY:HA2	1.96	0.47
2:B:256:ILE:H	2:B:304:SER:HB2	1.80	0.47
2:B:565:THR:OG1	2:B:577:HIS:O	2.29	0.47
2:B:1085:ARG:NE	16:T:22:DT:OP1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:36:DT:H2"	14:N:37:DG:C8	2.49	0.47
1:A:76:GLY:CA	1:A:81:CYS:HB2	2.44	0.47
1:A:273:GLN:HB2	1:A:278:HIS:CE1	2.49	0.47
1:A:545:VAL:HG11	1:A:645:LEU:HD12	1.96	0.47
1:A:840:ALA:HA	2:B:719:SER:CB	2.44	0.47
2:B:65:ILE:HB	2:B:86:LEU:HB2	1.97	0.47
2:B:91:ILE:HG13	2:B:126:VAL:HG22	1.97	0.47
2:B:191:GLU:CD	2:B:743:ARG:HH22	2.20	0.47
2:B:535:GLY:N	2:B:600:GLU:OE2	2.26	0.47
2:B:872:THR:HA	2:B:889:LYS:HG2	1.97	0.47
7:G:62:GLY:O	7:G:63:ARG:HG2	2.15	0.47
7:G:63:ARG:HG3	7:G:65:PHE:HD2	1.80	0.47
8:H:17:PRO:HG3	8:H:29:HIS:NE2	2.29	0.47
9:I:123:TRP:CD1	9:I:125:GLU:HG3	2.50	0.47
1:A:353:ASN:ND2	2:B:1073:GLN:OE1	2.47	0.47
1:A:798:ILE:O	1:A:820:ARG:NE	2.47	0.47
3:C:263:LEU:HB2	11:K:19:ILE:HD12	1.97	0.47
5:E:94:MET:HE1	5:E:127:LEU:HD11	1.97	0.47
9:I:115:THR:HG22	9:I:116:ALA:N	2.29	0.47
1:A:798:ILE:HG13	1:A:821:GLY:HA3	1.97	0.47
2:B:567:ILE:HD11	2:B:577:HIS:HB2	1.97	0.47
2:B:751:LEU:HD11	2:B:806:PHE:HA	1.96	0.47
2:B:817:GLN:HE22	2:B:912:ASN:ND2	2.13	0.47
3:C:8:THR:O	3:C:23:ILE:HA	2.14	0.47
6:F:53:THR:OG1	6:F:118:TRP:NE1	2.48	0.47
8:H:90:TYR:HB3	8:H:145:MET:HB2	1.97	0.47
1:A:653:VAL:HG11	1:A:669:TYR:CZ	2.50	0.47
1:A:733:LEU:HA	1:A:736:THR:HG22	1.97	0.47
1:A:769:MET:HE2	2:B:970:HIS:CE1	2.50	0.47
2:B:1022:LEU:HD12	2:B:1023:ARG:HG2	1.97	0.47
5:E:21:CYS:HA	5:E:26:TYR:HD2	1.80	0.47
7:G:53:ASN:OD1	7:G:54:ILE:N	2.48	0.47
1:A:362:SER:HB2	2:B:1084:LEU:HD12	1.96	0.46
1:A:441:GLN:HG2	1:A:444:TYR:CE2	2.49	0.46
2:B:615:TYR:HB3	2:B:620:ARG:HD3	1.97	0.46
2:B:744:MET:HG3	2:B:908:MET:SD	2.56	0.46
2:B:1104:ARG:HH12	7:G:61:PRO:HB2	1.78	0.46
1:A:286:ILE:HD13	1:A:309:LEU:HG	1.96	0.46
1:A:419:ILE:HG12	1:A:446:VAL:HG22	1.96	0.46
1:A:885:GLN:HE22	1:A:1408:ARG:NH1	2.13	0.46
1:A:983:LEU:HD12	1:A:1044:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:GLN:HB3	2:B:83:ARG:HG2	1.97	0.46
2:B:131:THR:HG22	2:B:141:GLN:HB3	1.96	0.46
2:B:872:THR:HA	2:B:889:LYS:HA	1.95	0.46
2:B:1029:TYR:OH	3:C:185:GLU:HG3	2.15	0.46
3:C:114:HIS:ND1	3:C:152:LYS:HG2	2.30	0.46
1:A:379:GLY:HA3	1:A:483:ARG:HB2	1.96	0.46
1:A:583:ARG:HE	1:A:585:LEU:HD11	1.80	0.46
2:B:198:GLU:HB3	2:B:487:SER:HA	1.98	0.46
2:B:411:LEU:HD11	2:B:435:ILE:HG23	1.98	0.46
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.50	0.46
1:A:783:GLN:HA	1:A:787:VAL:O	2.15	0.46
1:A:1137:PRO:HB2	1:A:1341:VAL:HG23	1.97	0.46
4:D:34:ASN:HD22	4:D:102:ASN:HB3	1.81	0.46
1:A:1365:ILE:HG23	1:A:1369:LEU:HD12	1.97	0.46
3:C:38:PHE:CZ	3:C:245:VAL:HG22	2.50	0.46
1:A:1102:MET:HE2	1:A:1120:GLY:HA2	1.98	0.46
1:A:1480:CYS:SG	6:F:103:PRO:HB2	2.56	0.46
1:A:94:VAL:O	1:A:250:VAL:N	2.44	0.46
1:A:330:GLN:HG3	1:A:331:LYS:N	2.30	0.46
1:A:1176:TYR:CE2	1:A:1213:ARG:HD3	2.51	0.46
1:A:1284:PHE:CE2	1:A:1288:ILE:HD11	2.50	0.46
2:B:111:ASN:O	2:B:115:LEU:HG	2.16	0.46
2:B:242:ARG:N	2:B:254:GLN:HG2	2.31	0.46
2:B:792:ASP:O	2:B:943:GLY:HA3	2.15	0.46
7:G:79:PRO:HG3	7:G:104:MET:HE1	1.98	0.46
9:I:86:CYS:HB3	9:I:90:GLY:H	1.80	0.46
10:J:9:THR:OG1	10:J:47:ARG:NH2	2.44	0.46
15:P:3:C:H3'	15:P:4:U:C5	2.51	0.46
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.51	0.46
2:B:508:MET:HB3	2:B:621:ILE:HG12	1.98	0.46
12:L:36:CYS:HB3	12:L:39:CYS:SG	2.56	0.46
1:A:858:GLY:CA	2:B:1089:MET:HE2	2.46	0.46
1:A:1471:PHE:CE2	6:F:64:ARG:HD3	2.51	0.46
2:B:318:LEU:O	2:B:322:GLY:N	2.38	0.46
5:E:8:TYR:OH	5:E:12:LYS:HE3	2.16	0.46
5:E:195:ARG:NH1	5:E:205:THR:OG1	2.48	0.46
8:H:48:TYR:OH	8:H:147:LYS:HG3	2.16	0.46
1:A:92:LYS:HD3	1:A:307:VAL:HG21	1.97	0.45
1:A:380:VAL:HG11	1:A:450:MET:HE3	1.96	0.45
1:A:1082:HIS:CE1	6:F:126:THR:HG21	2.51	0.45
5:E:8:TYR:HD1	5:E:37:LEU:HD12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:THR:HA	2:B:1072:ARG:HH21	1.81	0.45
1:A:455:ILE:HD13	1:A:516:GLN:HB2	1.97	0.45
1:A:797:ARG:HH22	1:A:815:TYR:HB3	1.82	0.45
1:A:1013:VAL:HG11	1:A:1046:ARG:HG2	1.99	0.45
1:A:1344:MET:HE2	5:E:134:GLU:HA	1.98	0.45
2:B:577:HIS:HE1	2:B:579:ASP:HB3	1.81	0.45
2:B:581:GLU:OE2	9:I:74:GLN:NE2	2.40	0.45
2:B:733:MET:N	2:B:1050:ARG:O	2.49	0.45
8:H:32:SER:OG	8:H:33:GLU:O	2.34	0.45
1:A:483:ARG:HH21	2:B:931:ILE:HD11	1.80	0.45
1:A:549:THR:HG21	1:A:640:LEU:H	1.81	0.45
1:A:599:HIS:ND1	1:A:632:ASN:OD1	2.49	0.45
1:A:686:THR:HG21	2:B:1041:ILE:HA	1.98	0.45
2:B:198:GLU:O	2:B:488:PRO:HD3	2.16	0.45
2:B:653:TRP:CZ2	2:B:662:VAL:HG21	2.51	0.45
2:B:856:PRO:HG2	12:L:48:ARG:HA	1.97	0.45
2:B:866:ILE:HG22	2:B:867:ILE:HG13	1.97	0.45
1:A:1155:LYS:HD2	1:A:1158:LEU:HD23	1.99	0.45
1:A:1427:LEU:HB2	1:A:1456:GLU:HG2	1.98	0.45
1:A:1457:ASN:ND2	1:A:1465:PRO:HD3	2.31	0.45
2:B:907:VAL:HG13	2:B:921:ILE:HG12	1.98	0.45
1:A:330:GLN:HB3	1:A:336:LEU:HD21	1.98	0.45
1:A:394:VAL:HG22	1:A:402:LEU:HD13	1.99	0.45
1:A:510:GLU:OE2	6:F:68:THR:OG1	2.35	0.45
1:A:687:ILE:HD13	1:A:766:PHE:CE1	2.51	0.45
1:A:1375:ARG:HD2	1:A:1402:CYS:HB3	1.98	0.45
2:B:625:LEU:HD12	2:B:665:ILE:HD12	1.99	0.45
3:C:17:GLU:C	3:C:241:PRO:HG3	2.42	0.45
11:K:22:ASN:O	11:K:32:LEU:N	2.49	0.45
16:T:13:DT:H2'	16:T:14:DT:H6	1.81	0.45
1:A:802:PHE:CE1	2:B:504:THR:HG22	2.51	0.45
3:C:100:GLU:H	3:C:123:ASN:ND2	2.15	0.45
1:A:958:ARG:HH12	1:A:1014:LYS:HD2	1.81	0.45
1:A:1405:MET:HA	1:A:1412:MET:HB3	1.99	0.45
2:B:84:TYR:CE2	2:B:423:ILE:HD12	2.52	0.45
2:B:1072:ARG:O	2:B:1112:ASP:HB3	2.16	0.45
3:C:37:VAL:O	3:C:42:VAL:HG23	2.16	0.45
3:C:49:TRP:CZ3	3:C:51:GLN:HB2	2.51	0.45
4:D:39:MET:HE2	4:D:39:MET:HB3	1.90	0.45
9:I:25:TYR:HB2	9:I:40:ARG:HG3	1.99	0.45
9:I:69:ILE:HG22	9:I:71:ASP:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:VAL:O	1:A:272:ASN:N	2.49	0.45
1:A:461:GLN:HE22	1:A:502:ASN:HD22	1.63	0.45
1:A:552:ASP:OD2	8:H:23:ASP:N	2.50	0.45
2:B:468:GLN:HG2	15:P:8:A:O2'	2.17	0.45
2:B:959:GLU:OE1	2:B:1020:TYR:OH	2.23	0.45
1:A:330:GLN:HG3	1:A:331:LYS:H	1.82	0.45
1:A:360:ASP:OD1	2:B:1062:ARG:NE	2.37	0.45
1:A:601:ASN:HB3	1:A:988:TRP:CZ3	2.52	0.45
1:A:853:LYS:O	1:A:857:THR:HG23	2.17	0.45
1:A:1479:LYS:HD2	6:F:103:PRO:HA	1.98	0.45
2:B:110:PRO:HG3	2:B:120:TYR:CZ	2.52	0.45
2:B:603:MET:HG2	2:B:614:ILE:HG23	1.98	0.45
8:H:63:THR:HG21	8:H:70:LEU:HA	1.99	0.45
1:A:264:VAL:HB	1:A:272:ASN:HB2	1.98	0.45
1:A:542:LEU:HA	1:A:545:VAL:HB	1.98	0.45
2:B:191:GLU:OE2	2:B:743:ARG:NH2	2.35	0.45
2:B:298:MET:HB3	9:I:14:ILE:HD12	1.98	0.45
8:H:92:MET:HB2	8:H:143:LEU:HB3	1.99	0.45
9:I:97:PHE:HB2	9:I:100:HIS:NE2	2.30	0.45
13:M:7:THR:HG23	16:T:17:DG:H2''	1.99	0.45
1:A:467:MET:SD	1:A:524:MET:HB3	2.57	0.44
1:A:868:MET:HB3	1:A:1088:GLY:CA	2.46	0.44
1:A:1093:GLN:NE2	2:B:1093:CYS:SG	2.90	0.44
1:A:1196:TYR:CE2	1:A:1248:ASN:HA	2.52	0.44
2:B:992:ASN:OD1	10:J:43:TYR:HB3	2.16	0.44
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	1.98	0.44
1:A:508:SER:HB3	1:A:511:THR:HG22	1.99	0.44
1:A:514:GLU:CD	2:B:1101:GLN:HB2	2.42	0.44
1:A:517:GLU:OE1	6:F:63:ALA:HA	2.18	0.44
1:A:962:ASP:HB3	1:A:1043:ILE:HG23	1.98	0.44
2:B:85:LEU:HB2	2:B:131:THR:OG1	2.17	0.44
2:B:853:LEU:HD23	2:B:867:ILE:HA	2.00	0.44
2:B:865:VAL:HA	2:B:895:PHE:HD2	1.81	0.44
4:D:16:ASP:OD2	4:D:18:SER:OG	2.25	0.44
6:F:100:ARG:HH22	6:F:124:ILE:HG23	1.81	0.44
7:G:91:GLN:HB3	7:G:98:PHE:HB2	1.99	0.44
8:H:29:HIS:ND1	8:H:40:ILE:HG12	2.33	0.44
11:K:65:HIS:HE1	11:K:67:LEU:HD12	1.83	0.44
1:A:470:MET:HB3	1:A:521:VAL:HG22	1.99	0.44
2:B:1137:CYS:HB3	2:B:1142:ASN:HB3	1.98	0.44
6:F:51:ARG:NH1	6:F:122:GLU:OE1	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:LEU:HB2	1:A:1255:LEU:HD23	1.99	0.44
1:A:1226:LEU:HD13	1:A:1231:ILE:HD11	1.99	0.44
2:B:59:VAL:HG21	2:B:91:ILE:HD12	1.99	0.44
2:B:645:GLU:O	2:B:649:ASN:HB2	2.18	0.44
2:B:719:SER:OG	2:B:720:PRO:HD3	2.18	0.44
2:B:787:GLY:O	2:B:790:GLN:HG3	2.18	0.44
15:P:3:C:H2'	15:P:4:U:C6	2.52	0.44
1:A:486:LEU:HB2	1:A:673:GLN:NE2	2.33	0.44
1:A:533:PRO:HG2	1:A:647:THR:HA	1.98	0.44
1:A:1254:LYS:O	1:A:1256:VAL:HG23	2.18	0.44
1:A:1366:PHE:HE1	1:A:1371:ILE:HD13	1.82	0.44
1:A:1426:PRO:HD2	1:A:1449:ASP:HB2	2.00	0.44
2:B:39:LEU:HB3	2:B:483:ARG:HD2	1.98	0.44
2:B:216:ALA:HB2	2:B:241:ALA:HB2	2.00	0.44
2:B:617:ASP:OD1	2:B:618:ALA:N	2.49	0.44
2:B:747:LEU:HA	2:B:810:PHE:CE1	2.53	0.44
2:B:1062:ARG:NH2	2:B:1066:PRO:O	2.45	0.44
1:A:29:ASP:HB3	1:A:33:ARG:NH1	2.32	0.44
1:A:357:LYS:HB3	1:A:357:LYS:HE2	1.42	0.44
1:A:547:LYS:O	1:A:553:VAL:HG21	2.18	0.44
1:A:606:HIS:CE1	1:A:641:CYS:HB3	2.53	0.44
2:B:42:GLN:HE22	2:B:526:LEU:HD12	1.83	0.44
2:B:156:LEU:HD22	2:B:184:TYR:CE2	2.52	0.44
2:B:989:VAL:HG22	2:B:1015:LEU:HB2	1.99	0.44
8:H:17:PRO:HG3	8:H:29:HIS:HE2	1.82	0.44
1:A:77:ASN:C	1:A:79:THR:H	2.26	0.44
1:A:488:VAL:O	1:A:491:PRO:HD2	2.17	0.44
1:A:596:ILE:HG12	1:A:652:LEU:HD21	2.00	0.44
5:E:44:PHE:O	5:E:53:PRO:HD3	2.17	0.44
1:A:108:ARG:NH1	1:A:145:TYR:OH	2.48	0.44
1:A:1016:LEU:HD21	1:A:1072:ILE:HG21	2.00	0.44
5:E:117:SER:O	5:E:121:MET:HG2	2.16	0.44
12:L:43:ILE:O	12:L:44:MET:HE2	2.18	0.44
1:A:560:VAL:HG22	1:A:591:ILE:HD11	1.98	0.44
1:A:746:ASN:HA	1:A:749:ARG:HG2	2.00	0.44
1:A:916:PHE:HE2	1:A:960:ARG:HG2	1.83	0.44
3:C:42:VAL:HG21	3:C:244:ILE:HG23	1.98	0.44
3:C:118:ARG:HA	3:C:131:THR:HG21	2.00	0.44
4:D:34:ASN:HD22	4:D:102:ASN:CG	2.25	0.44
5:E:168:ASN:HA	5:E:172:ARG:HH21	1.82	0.44
11:K:35:ILE:HB	11:K:71:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LEU:HD11	1:A:303:ILE:HG23	1.99	0.43
1:A:541:THR:O	1:A:545:VAL:HG23	2.18	0.43
2:B:217:TYR:CE2	2:B:376:ALA:HA	2.53	0.43
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.98	0.43
2:B:918:PHE:HE2	2:B:920:LYS:HG3	1.83	0.43
3:C:18:ASN:HA	3:C:233:VAL:O	2.18	0.43
3:C:182:VAL:HG13	3:C:233:VAL:HG22	2.00	0.43
3:C:188:PRO:HD3	3:C:230:TYR:HE2	1.83	0.43
5:E:64:HIS:HD2	5:E:66:ASP:HB2	1.83	0.43
7:G:90:THR:O	7:G:139:GLN:NE2	2.51	0.43
1:A:222:HIS:ND1	1:A:246:GLU:HB2	2.33	0.43
1:A:582:PRO:HD2	8:H:47:ILE:HG23	2.00	0.43
1:A:631:GLU:HG2	1:A:988:TRP:CZ2	2.53	0.43
1:A:875:TYR:HA	1:A:1083:PRO:HB3	1.99	0.43
1:A:1230:GLN:HG2	1:A:1234:LYS:HE3	1.99	0.43
2:B:237:VAL:HG12	2:B:372:LEU:HD22	1.99	0.43
2:B:411:LEU:HA	2:B:439:ILE:HD13	2.00	0.43
2:B:470:LEU:HD11	2:B:478:THR:HG23	1.99	0.43
11:K:105:PHE:CE2	11:K:109:ILE:HD11	2.53	0.43
16:T:22:DT:H2'	16:T:23:DA:O4'	2.18	0.43
1:A:463:THR:OG1	2:B:1089:MET:HB3	2.19	0.43
1:A:1045:LEU:HD11	1:A:1072:ILE:HD13	1.99	0.43
1:A:1301:ILE:HG23	1:A:1345:ARG:HD2	2.00	0.43
2:B:388:TYR:CE2	2:B:524:LYS:HE3	2.53	0.43
9:I:36:LEU:HD23	9:I:47:GLU:HA	2.00	0.43
1:A:524:MET:HE1	2:B:1097:HIS:HE1	1.82	0.43
1:A:1128:ILE:CG2	1:A:1414:ILE:HB	2.49	0.43
2:B:818:GLU:HB2	2:B:829:PHE:CE2	2.53	0.43
5:E:130:PHE:CE1	5:E:181:ARG:HB3	2.53	0.43
8:H:39:LEU:HD22	8:H:58:LEU:HD22	2.00	0.43
9:I:25:TYR:O	9:I:38:ALA:N	2.38	0.43
12:L:19:CYS:SG	12:L:20:GLY:N	2.91	0.43
1:A:359:VAL:HG21	2:B:1106:ARG:HD2	2.00	0.43
1:A:831:LEU:HG	2:B:715:ASP:O	2.19	0.43
1:A:1175:ILE:HG23	1:A:1285:LEU:HD23	2.00	0.43
2:B:164:ASN:OD1	2:B:165:GLY:N	2.52	0.43
2:B:516:GLU:HA	2:B:520:VAL:HG12	2.00	0.43
2:B:527:ALA:HA	2:B:705:GLY:HA2	2.00	0.43
3:C:260:GLN:HB2	11:K:91:ILE:HG21	2.01	0.43
7:G:99:THR:O	7:G:106:CYS:N	2.43	0.43
7:G:104:MET:HG2	7:G:105:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:24:LEU:HD22	10:J:29:TYR:CD2	2.53	0.43
1:A:358:ARG:NH1	16:T:23:DA:OP1	2.46	0.43
1:A:837:PHE:HB2	2:B:506:TRP:HZ3	1.84	0.43
1:A:870:SER:HB3	1:A:1428:MET:HE1	2.00	0.43
1:A:1215:GLU:OE1	1:A:1254:LYS:HG2	2.18	0.43
1:A:1376:LYS:O	1:A:1379:GLU:HB3	2.19	0.43
2:B:274:ARG:NH1	2:B:308:ALA:O	2.52	0.43
2:B:388:TYR:CZ	2:B:505:LEU:HD21	2.54	0.43
2:B:816:GLU:HB2	2:B:867:ILE:HD13	2.00	0.43
2:B:1125:MET:HE1	2:B:1160:GLN:HG3	1.99	0.43
6:F:81:VAL:HG21	6:F:96:GLU:HA	1.99	0.43
1:A:351:ARG:HG3	2:B:1088:GLU:OE2	2.19	0.43
1:A:451:CYS:HA	1:A:476:ILE:HD11	2.00	0.43
1:A:451:CYS:N	1:A:454:ASP:OD2	2.48	0.43
1:A:908:THR:HG23	1:A:916:PHE:HE1	1.84	0.43
1:A:981:CYS:HB2	1:A:986:MET:SD	2.58	0.43
2:B:19:PRO:C	2:B:21:LEU:H	2.27	0.43
5:E:114:ALA:O	5:E:118:LEU:HG	2.18	0.43
7:G:7:LEU:HB2	7:G:72:TYR:CZ	2.53	0.43
13:M:7:THR:O	16:T:17:DG:N2	2.44	0.43
13:M:9:PRO:CB	14:N:31:DC:H1'	2.45	0.43
2:B:46:SER:HG	2:B:397:GLY:H	1.60	0.43
2:B:529:MET:HB3	2:B:624:PRO:HD2	2.01	0.43
2:B:758:LEU:HD11	10:J:47:ARG:HB3	2.00	0.43
16:T:20:DG:OP2	16:T:20:DG:H3'	2.18	0.43
1:A:858:GLY:HA3	2:B:1089:MET:HE2	2.01	0.43
1:A:1173:THR:HG21	1:A:1289:GLU:HG3	2.01	0.43
1:A:1176:TYR:HE2	1:A:1213:ARG:HD3	1.83	0.43
1:A:1181:PRO:HG3	1:A:1207:ILE:HD12	2.00	0.43
1:A:1216:LEU:HD12	1:A:1228:MET:SD	2.59	0.43
1:A:1471:PHE:CZ	6:F:61:GLU:HA	2.53	0.43
2:B:111:ASN:HD21	2:B:742:VAL:HG11	1.84	0.43
2:B:506:TRP:HZ2	2:B:677:MET:HE1	1.84	0.43
16:T:31:DT:H5'	16:T:31:DT:C6	2.54	0.43
1:A:626:THR:OG1	1:A:627:LYS:N	2.52	0.43
1:A:775:LYS:HE3	2:B:974:SER:OG	2.19	0.43
1:A:1229:GLU:HG2	1:A:1247:PHE:CD1	2.54	0.43
2:B:924:ARG:CZ	3:C:60:HIS:HB2	2.49	0.43
2:B:962:THR:O	10:J:9:THR:HG23	2.19	0.43
2:B:712:PRO:HG2	2:B:939:HIS:CE1	2.54	0.42
3:C:19:VAL:HG23	3:C:241:PRO:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:189:ASP:CG	3:C:211:LEU:HG	2.44	0.42
5:E:148:HIS:CD2	5:E:179:VAL:HG11	2.54	0.42
7:G:2:PHE:CD1	7:G:77:PHE:HB2	2.54	0.42
1:A:343:LEU:HD23	1:A:349:ARG:HB2	2.02	0.42
1:A:507:GLN:N	2:B:1105:GLU:OE2	2.39	0.42
1:A:737:PHE:CE2	9:I:108:MET:HE1	2.54	0.42
2:B:388:TYR:HE2	2:B:524:LYS:HE3	1.83	0.42
4:D:60:VAL:HG13	7:G:103:PRO:HB3	2.00	0.42
5:E:8:TYR:CD1	5:E:37:LEU:HD12	2.55	0.42
5:E:8:TYR:CZ	5:E:12:LYS:HE3	2.55	0.42
9:I:86:CYS:HB3	9:I:90:GLY:N	2.34	0.42
13:M:9:PRO:CB	14:N:32:DA:O4'	2.59	0.42
1:A:190:ARG:HH11	14:N:37:DG:C5'	2.32	0.42
1:A:1099:ALA:HA	1:A:1102:MET:HB2	2.01	0.42
1:A:1160:ARG:O	1:A:1300:GLY:HA2	2.19	0.42
1:A:1212:LEU:HD21	1:A:1292:MET:CE	2.49	0.42
3:C:35:ARG:HA	3:C:38:PHE:CD2	2.55	0.42
1:A:510:GLU:HG3	6:F:67:GLY:C	2.45	0.42
1:A:551:ARG:HD3	8:H:121:LEU:HD23	2.01	0.42
1:A:922:PHE:HD1	1:A:1052:ARG:HA	1.84	0.42
3:C:59:LEU:HD13	3:C:63:PHE:HE2	1.84	0.42
4:D:128:GLN:HE21	4:D:132:ASP:CG	2.27	0.42
1:A:522:PRO:O	1:A:662:HIS:HB2	2.20	0.42
1:A:706:ILE:HG21	1:A:824:GLU:HG3	2.01	0.42
1:A:752:THR:HB	1:A:786:ALA:HB1	2.00	0.42
1:A:869:GLU:OE1	1:A:1455:SER:OG	2.37	0.42
1:A:904:GLN:HE21	1:A:982:ASN:HA	1.83	0.42
3:C:103:LEU:HB2	3:C:120:LEU:HD23	2.01	0.42
3:C:152:LYS:NZ	10:J:57:GLU:OE2	2.34	0.42
8:H:43:VAL:HG13	8:H:90:TYR:CZ	2.54	0.42
1:A:675:VAL:HG23	1:A:676:ILE:HG13	2.02	0.42
1:A:1037:ALA:HA	5:E:200:ALA:HB1	2.00	0.42
2:B:91:ILE:HD11	2:B:124:LEU:HD21	2.02	0.42
7:G:14:HIS:HD2	7:G:16:ARG:HG2	1.84	0.42
16:T:20:DG:H2''	16:T:21:DG:H5'	2.02	0.42
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.54	0.42
1:A:509:LEU:HD13	6:F:89:PRO:HG3	2.01	0.42
2:B:556:ILE:HD13	2:B:576:ILE:HG12	2.01	0.42
2:B:763:SER:HA	2:B:766:TYR:CD2	2.54	0.42
3:C:20:LYS:HG2	3:C:231:TYR:O	2.20	0.42
8:H:98:ARG:HB3	8:H:115:TYR:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:91:HIS:CD2	9:I:115:THR:HB	2.55	0.42
1:A:575:PRO:HG3	1:A:594:LEU:HD11	2.02	0.42
1:A:840:ALA:HA	2:B:719:SER:HB2	2.02	0.42
1:A:1378:LEU:HD23	1:A:1402:CYS:HA	2.01	0.42
2:B:185:PHE:O	2:B:191:GLU:HA	2.20	0.42
2:B:712:PRO:O	2:B:939:HIS:HE1	2.03	0.42
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.52	0.42
10:J:20:ALA:O	10:J:24:LEU:HG	2.19	0.42
1:A:266:MET:SD	15:P:3:C:C2	3.13	0.42
1:A:1139:LEU:HD12	1:A:1358:THR:O	2.20	0.42
1:A:1261:ILE:HG22	1:A:1262:MET:N	2.35	0.42
1:A:1378:LEU:HG	1:A:1402:CYS:SG	2.60	0.42
2:B:17:ILE:HG22	2:B:18:THR:H	1.85	0.42
2:B:552:ASN:O	2:B:556:ILE:HG13	2.20	0.42
3:C:181:GLY:H	10:J:10:CYS:HB2	1.85	0.42
3:C:189:ASP:O	3:C:191:ALA:N	2.50	0.42
1:A:515:ILE:HD11	2:B:1102:PHE:CD1	2.55	0.42
1:A:1169:VAL:HG11	1:A:1226:LEU:HD12	2.02	0.42
1:A:1362:ILE:HG23	1:A:1374:VAL:HG13	2.01	0.42
1:A:1475:LEU:N	7:G:57:GLY:O	2.30	0.42
2:B:40:VAL:HG21	2:B:181:PRO:HB2	2.02	0.42
2:B:42:GLN:NE2	2:B:483:ARG:HA	2.35	0.42
2:B:235:ILE:HG21	2:B:368:MET:HE1	2.01	0.42
2:B:495:LEU:HG	2:B:498:PRO:HD3	2.02	0.42
2:B:751:LEU:HB3	2:B:754:PRO:HG3	2.02	0.42
2:B:1001:PRO:HB2	2:B:1002:PHE:CD2	2.55	0.42
16:T:14:DT:H2"	16:T:15:DT:OP2	2.20	0.42
1:A:23:PHE:O	1:A:1446:GLY:HA2	2.20	0.41
1:A:380:VAL:HG21	1:A:474:VAL:HG13	2.02	0.41
1:A:614:ASP:O	1:A:619:LYS:NZ	2.36	0.41
1:A:827:TYR:HB2	2:B:978:ILE:HD12	2.01	0.41
2:B:399:LEU:HB3	2:B:453:TRP:CZ2	2.54	0.41
2:B:794:VAL:HG13	2:B:965:ILE:HG23	2.01	0.41
2:B:927:ARG:HD2	2:B:1054:MET:SD	2.59	0.41
8:H:81:ARG:CG	8:H:82:PRO:HD3	2.49	0.41
1:A:189:PRO:HB3	1:A:202:TRP:CD2	2.55	0.41
2:B:36:GLU:OE2	2:B:654:GLN:HB2	2.20	0.41
2:B:42:GLN:HE22	2:B:483:ARG:HA	1.85	0.41
2:B:51:ILE:HG23	2:B:93:LEU:HD12	2.02	0.41
2:B:509:VAL:HG11	2:B:524:LYS:HD2	2.02	0.41
2:B:674:MET:HE2	2:B:690:CYS:SG	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1037:ILE:HG21	2:B:1041:ILE:HD11	2.02	0.41
1:A:18:ILE:H	1:A:1462:GLN:NE2	2.14	0.41
1:A:222:HIS:CD2	1:A:226:LYS:HE3	2.56	0.41
1:A:560:VAL:HG21	1:A:586:TRP:CD2	2.56	0.41
1:A:1443:ALA:HB2	2:B:1167:ILE:HG23	2.02	0.41
3:C:60:HIS:NE2	3:C:63:PHE:HB2	2.36	0.41
6:F:69:ARG:NH2	6:F:78:PRO:O	2.53	0.41
7:G:97:LEU:HD22	7:G:108:ILE:HD12	2.01	0.41
9:I:20:CYS:SG	9:I:22:ASN:ND2	2.93	0.41
1:A:352:GLY:HA2	2:B:1085:ARG:HH22	1.84	0.41
1:A:601:ASN:HB3	1:A:988:TRP:CE3	2.55	0.41
2:B:50:PHE:O	2:B:55:VAL:HG23	2.20	0.41
2:B:414:GLU:OE1	2:B:439:ILE:HD11	2.20	0.41
2:B:427:LYS:HG3	2:B:428:ASP:H	1.85	0.41
2:B:752:TYR:CE2	2:B:807:ARG:HD2	2.55	0.41
2:B:788:TYR:O	2:B:946:GLY:HA3	2.20	0.41
2:B:950:ARG:O	2:B:954:MET:HG2	2.20	0.41
1:A:404:GLU:O	1:A:408:ARG:HG3	2.20	0.41
1:A:880:ARG:HG2	1:A:886:VAL:HA	2.02	0.41
2:B:144:HIS:ND1	2:B:431:LEU:HD12	2.35	0.41
2:B:148:PHE:CD2	2:B:437:THR:HG21	2.55	0.41
2:B:419:ALA:O	2:B:423:ILE:N	2.54	0.41
2:B:796:MET:HE3	2:B:948:GLN:HE21	1.86	0.41
2:B:831:LYS:HD2	2:B:849:ASP:O	2.20	0.41
2:B:955:PRO:O	2:B:963:PRO:HD2	2.20	0.41
2:B:1086:PHE:CZ	2:B:1090:GLU:HB3	2.55	0.41
1:A:141:LEU:HD13	1:A:1445:HIS:CE1	2.47	0.41
1:A:190:ARG:NH1	14:N:37:DG:P	2.92	0.41
1:A:1049:LEU:HA	1:A:1054:MET:HE3	2.03	0.41
1:A:1417:HIS:O	1:A:1421:ARG:HG2	2.21	0.41
2:B:262:TYR:CD2	2:B:346:GLU:HG3	2.55	0.41
2:B:580:PRO:HB2	2:B:605:ARG:NE	2.27	0.41
2:B:592:ARG:NE	2:B:627:ILE:HD13	2.36	0.41
3:C:32:ASN:HA	3:C:35:ARG:HG2	2.03	0.41
4:D:26:PHE:HD2	7:G:80:PHE:HZ	1.67	0.41
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.56	0.41
1:A:857:THR:HG21	1:A:1100:THR:HA	2.03	0.41
1:A:857:THR:CB	1:A:1100:THR:HG22	2.43	0.41
1:A:890:ARG:HH21	1:A:1023:VAL:HG13	1.85	0.41
1:A:901:VAL:HA	1:A:980:PRO:HA	2.02	0.41
1:A:1197:TYR:OH	1:A:1258:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:TRP:CZ2	2:B:762:ARG:HB2	2.55	0.41
2:B:388:TYR:CE2	2:B:505:LEU:HD21	2.56	0.41
2:B:465:GLY:HA2	15:P:8:A:C5'	2.50	0.41
2:B:968:ASN:OD1	2:B:969:PRO:HD2	2.21	0.41
8:H:40:ILE:O	8:H:123:MET:HA	2.21	0.41
13:M:9:PRO:HA	13:M:10:SAR:HA3	1.70	0.41
1:A:261:ARG:HB3	1:A:276:LEU:HB2	2.03	0.41
1:A:1478:GLU:HG2	1:A:1482:TYR:HE2	1.86	0.41
2:B:125:TYR:HB3	2:B:146:LYS:HA	2.02	0.41
2:B:513:GLU:HG2	2:B:525:ASN:ND2	2.36	0.41
2:B:565:THR:HG21	2:B:580:PRO:HB3	2.02	0.41
2:B:1123:GLY:HA3	2:B:1171:MET:N	2.36	0.41
3:C:14:LEU:HB3	11:K:112:LYS:HG2	2.01	0.41
1:A:103:THR:HG23	1:A:225:PHE:CE2	2.56	0.41
1:A:441:GLN:HG2	1:A:444:TYR:CZ	2.56	0.41
1:A:757:GLN:NE2	1:A:778:LYS:HB3	2.33	0.41
1:A:934:LEU:HD11	1:A:938:LEU:HD22	2.03	0.41
1:A:1005:HIS:HD2	1:A:1007:ILE:HB	1.86	0.41
1:A:1016:LEU:O	1:A:1020:LEU:HG	2.21	0.41
1:A:1153:ARG:O	1:A:1157:ILE:HG12	2.20	0.41
1:A:1262:MET:SD	1:A:1265:ASP:HB2	2.61	0.41
2:B:524:LYS:HE2	2:B:524:LYS:HB2	1.93	0.41
2:B:591:ARG:HH12	2:B:603:MET:H	1.67	0.41
2:B:795:ILE:HB	2:B:966:ILE:HB	2.02	0.41
2:B:857:GLY:O	12:L:53:VAL:HG21	2.20	0.41
3:C:27:ASP:OD2	11:K:52:LYS:HE3	2.21	0.41
4:D:37:VAL:HG21	7:G:2:PHE:CB	2.50	0.41
5:E:56:THR:O	5:E:57:ASP:HB2	2.20	0.41
11:K:47:LYS:O	11:K:51:LEU:HG	2.21	0.41
14:N:39:DC:H2''	14:N:40:DA:C8	2.55	0.41
14:N:40:DA:H2''	14:N:41:DA:N7	2.36	0.41
15:P:4:U:H6	15:P:4:U:O5'	2.04	0.41
1:A:290:LEU:HD13	1:A:306:ASP:HB2	2.02	0.41
1:A:527:THR:HG23	1:A:530:SER:H	1.86	0.41
2:B:294:ASP:OD2	2:B:379:ARG:NH2	2.53	0.41
2:B:937:SER:OG	2:B:941:GLN:HB2	2.21	0.41
6:F:56:TYR:CD1	6:F:124:ILE:HB	2.54	0.41
8:H:95:LYS:HB2	8:H:140:ARG:HH11	1.86	0.41
2:B:33:TYR:HD1	2:B:653:TRP:CE2	2.39	0.40
2:B:924:ARG:HH12	3:C:62:GLU:CD	2.29	0.40
2:B:971:ALA:O	2:B:975:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1021:HIS:HB3	2:B:1025:ASN:O	2.21	0.40
5:E:21:CYS:SG	5:E:62:VAL:HG21	2.61	0.40
6:F:109:TYR:HD1	6:F:115:TYR:HB3	1.85	0.40
7:G:25:THR:HA	7:G:28:GLN:HG2	2.03	0.40
1:A:516:GLN:HA	1:A:520:MET:HG2	2.03	0.40
1:A:1239:PHE:HB3	1:A:1242:ASP:OD1	2.21	0.40
2:B:120:TYR:OH	2:B:161:CYS:SG	2.68	0.40
2:B:599:SER:HB3	2:B:664:TYR:HD2	1.86	0.40
2:B:1108:PHE:HD1	2:B:1152:PRO:HG3	1.86	0.40
3:C:242:GLU:OE1	11:K:113:GLN:NE2	2.54	0.40
1:A:460:ARG:HB2	1:A:501:MET:HG2	2.02	0.40
1:A:511:THR:HG21	2:B:1105:GLU:OE1	2.22	0.40
1:A:521:VAL:N	1:A:522:PRO:HD2	2.36	0.40
1:A:890:ARG:HH21	1:A:1023:VAL:HG22	1.87	0.40
1:A:916:PHE:CD1	1:A:963:ARG:HD2	2.56	0.40
1:A:1054:MET:HE2	1:A:1058:PHE:HD2	1.87	0.40
1:A:1417:HIS:CE1	13:M:11:MVA:CB	2.92	0.40
2:B:53:MET:HE2	2:B:57:ARG:HH21	1.86	0.40
2:B:826:GLU:H	2:B:872:THR:CG2	2.34	0.40
3:C:93:PHE:HE2	3:C:166:LYS:HG2	1.85	0.40
5:E:14:ARG:O	5:E:18:MET:HG2	2.22	0.40
5:E:71:GLN:HB3	5:E:72:MET:H	1.68	0.40
5:E:91:CYS:HA	5:E:94:MET:HE2	2.02	0.40
1:A:99:PHE:CE1	1:A:1440:MET:HE3	2.56	0.40
1:A:631:GLU:HG2	1:A:988:TRP:HZ2	1.87	0.40
1:A:671:ASN:O	1:A:675:VAL:HG22	2.22	0.40
1:A:987:ILE:HG23	1:A:1060:LEU:HD11	2.04	0.40
1:A:1167:ARG:NH1	1:A:1293:LEU:O	2.54	0.40
2:B:149:ILE:HA	2:B:437:THR:HG22	2.03	0.40
2:B:237:VAL:HG13	2:B:269:ILE:HD11	2.03	0.40
2:B:604:ILE:HG12	2:B:668:LEU:HD12	2.03	0.40
2:B:907:VAL:HG22	2:B:921:ILE:HG12	2.02	0.40
4:D:20:LEU:HG	4:D:117:SER:HB2	2.04	0.40
1:A:1065:PHE:O	1:A:1069:LEU:HG	2.22	0.40
1:A:1171:ALA:N	1:A:1215:GLU:O	2.52	0.40
2:B:486:ASN:OD1	2:B:491:ARG:NH2	2.51	0.40
2:B:757:PRO:HA	2:B:777:ASN:HD21	1.86	0.40
2:B:1116:VAL:O	2:B:1148:LEU:HD12	2.22	0.40
16:T:8:DT:H2"	16:T:9:DG:N7	2.31	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	1417/1970 (72%)	1337 (94%)	79 (6%)	1 (0%)	48	67
2	B	1128/1174 (96%)	1065 (94%)	63 (6%)	0	100	100
3	C	253/275 (92%)	241 (95%)	12 (5%)	0	100	100
4	D	126/142 (89%)	118 (94%)	8 (6%)	0	100	100
5	E	207/210 (99%)	196 (95%)	10 (5%)	1 (0%)	24	41
6	F	80/127 (63%)	77 (96%)	3 (4%)	0	100	100
7	G	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
8	H	146/150 (97%)	138 (94%)	7 (5%)	1 (1%)	18	32
9	I	112/125 (90%)	103 (92%)	9 (8%)	0	100	100
10	J	65/67 (97%)	59 (91%)	6 (9%)	0	100	100
11	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
12	L	42/58 (72%)	37 (88%)	5 (12%)	0	100	100
13	M	2/11 (18%)	2 (100%)	0	0	100	100
All	All	3860/4598 (84%)	3647 (94%)	210 (5%)	3 (0%)	49	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	122	ALA
1	A	1435	THR
8	H	34	SER

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	1252/1749 (72%)	1252 (100%)	0	100	100
2	B	993/1027 (97%)	993 (100%)	0	100	100
3	C	234/252 (93%)	234 (100%)	0	100	100
4	D	106/127 (84%)	106 (100%)	0	100	100
5	E	189/190 (100%)	189 (100%)	0	100	100
6	F	71/111 (64%)	71 (100%)	0	100	100
7	G	147/153 (96%)	147 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	103/112 (92%)	103 (100%)	0	100	100
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	104 (100%)	0	100	100
12	L	41/55 (74%)	41 (100%)	0	100	100
13	M	4/4 (100%)	4 (100%)	0	100	100
All	All	3429/4073 (84%)	3429 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	267	GLN
1	A	278	HIS
1	A	330	GLN
1	A	472	HIS
1	A	493	ASN
1	A	504	HIS
1	A	673	GLN
1	A	757	GLN
1	A	791	GLN
1	A	885	GLN
1	A	1032	GLN
1	A	1034	GLN
1	A	1082	HIS
1	A	1093	GLN

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Mol	Chain	Res	Type
1	A	1163	HIS
1	A	1190	GLN
1	A	1194	ASN
1	A	1310	HIS
1	A	1462	GLN
2	B	98	HIS
2	B	145	GLN
2	B	175	ASN
2	B	197	GLN
2	B	245	GLN
2	B	265	GLN
2	B	525	ASN
2	B	639	HIS
2	B	683	GLN
2	B	699	HIS
2	B	718	GLN
2	B	725	GLN
2	B	749	HIS
2	B	817	GLN
2	B	838	GLN
2	B	930	GLN
2	B	941	GLN
2	B	986	GLN
2	B	1097	HIS
2	B	1117	HIS
2	B	1129	ASN
3	C	108	ASN
3	C	177	ASN
3	C	190	ASN
3	C	265	HIS
4	D	34	ASN
4	D	48	ASN
4	D	129	GLN
5	E	107	GLN
5	E	189	GLN
6	F	46	GLN
7	G	4	HIS
7	G	14	HIS
8	H	46	GLN
9	I	41	ASN
9	I	91	HIS
11	K	49	GLN

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Mol	Chain	Res	Type
11	K	76	GLN
11	K	89	ASN
11	K	113	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	10/13 (76%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	MVA	M	11	13	6,7,8	1.13	1 (16%)	6,8,10	2.11	2 (33%)
13	DVA	M	8	13	4,6,7	0.49	0	6,7,9	0.66	0
13	MVA	M	5	13	6,7,8	0.82	0	6,8,10	1.41	2 (33%)
13	DVA	M	2	13	4,6,7	0.66	0	6,7,9	0.65	0
13	SAR	M	4	13	3,4,5	1.24	0	1,3,5	2.25	1 (100%)
13	SAR	M	10	13	3,4,5	1.11	0	1,3,5	2.20	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MVA	M	11	13	-	5/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	DVA	M	8	13	-	5/5/6/8	-
13	MVA	M	5	13	-	5/6/8/10	-
13	DVA	M	2	13	-	3/5/6/8	-
13	SAR	M	4	13	-	1/1/2/3	-
13	SAR	M	10	13	-	1/1/2/3	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	11	MVA	O-C	2.67	1.30	1.20

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	11	MVA	O-C-CA	-4.53	112.88	124.86
13	M	5	MVA	CB-CA-N	-2.39	108.06	111.17
13	M	4	SAR	O-C-CA	-2.25	117.42	125.17
13	M	10	SAR	O-C-CA	-2.20	117.61	125.17
13	M	5	MVA	CG1-CB-CA	2.10	114.39	111.18
13	M	11	MVA	CB-CA-C	-2.01	110.36	112.96

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	M	2	DVA	N-CA-CB-CG2
13	M	2	DVA	C-CA-CB-CG1
13	M	2	DVA	C-CA-CB-CG2
13	M	4	SAR	C-CA-N-CN
13	M	5	MVA	N-CA-CB-CG1
13	M	5	MVA	N-CA-CB-CG2
13	M	5	MVA	C-CA-CB-CG1
13	M	5	MVA	C-CA-CB-CG2
13	M	8	DVA	N-CA-CB-CG1
13	M	8	DVA	N-CA-CB-CG2
13	M	8	DVA	C-CA-CB-CG1
13	M	8	DVA	C-CA-CB-CG2
13	M	10	SAR	C-CA-N-CN
13	M	11	MVA	CB-CA-N-CN
13	M	11	MVA	N-CA-CB-CG1

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Mol	Chain	Res	Type	Atoms
13	M	11	MVA	N-CA-CB-CG2
13	M	11	MVA	C-CA-CB-CG1
13	M	11	MVA	C-CA-CB-CG2
13	M	8	DVA	O-C-CA-CB
13	M	5	MVA	CB-CA-N-CN

There are no ring outliers.

5 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	11	MVA	16	0
13	M	8	DVA	1	0
13	M	5	MVA	2	0
13	M	2	DVA	4	0
13	M	10	SAR	2	0

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 ⓘ

There are no chain breaks in this entry.

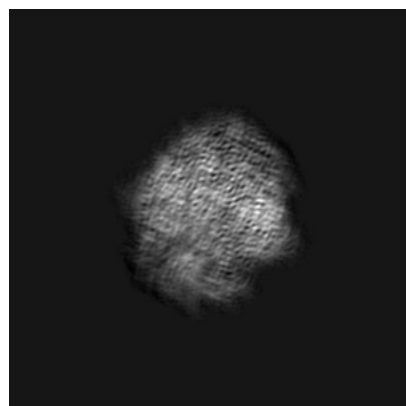
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66852. These allow visual inspection of the internal detail of the map and identification of artifacts.

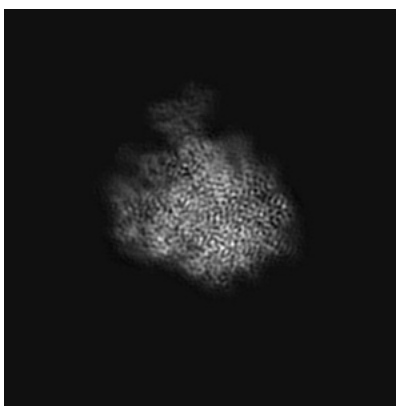
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

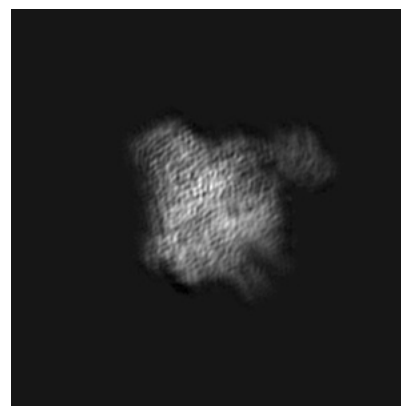
6.1.1 Primary map



X

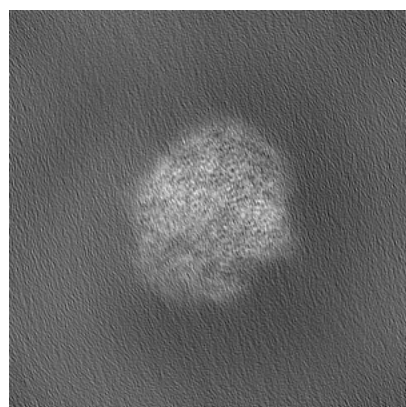


Y

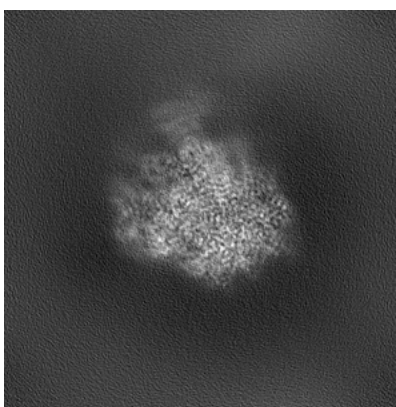


Z

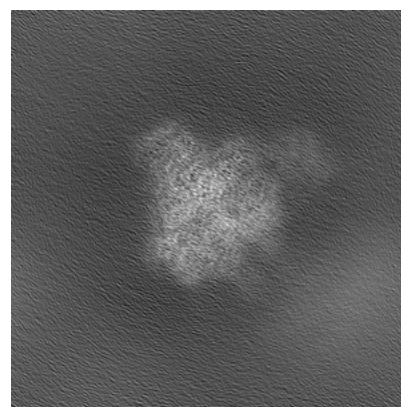
6.1.2 Raw map



X



Y

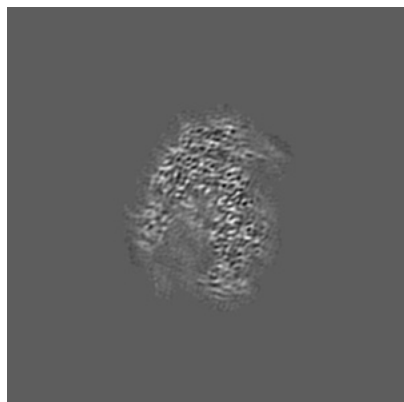


Z

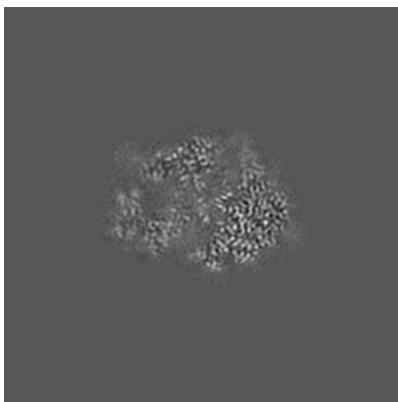
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

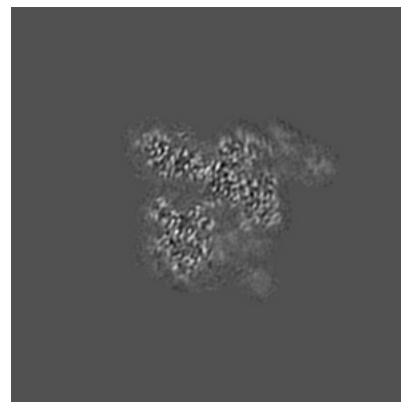
6.2.1 Primary map



X Index: 160

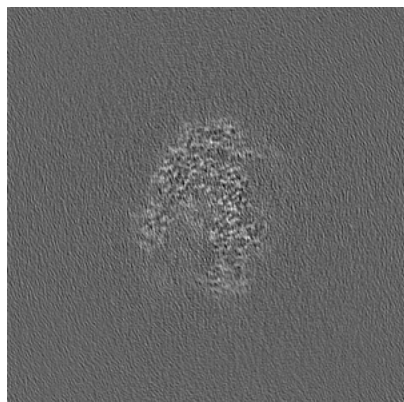


Y Index: 160

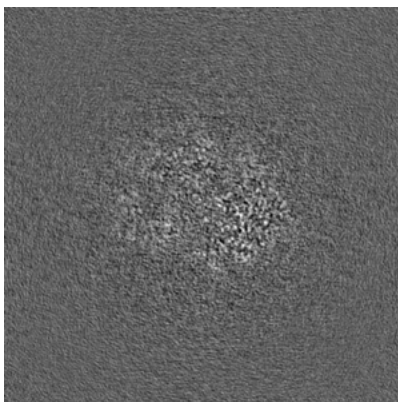


Z Index: 160

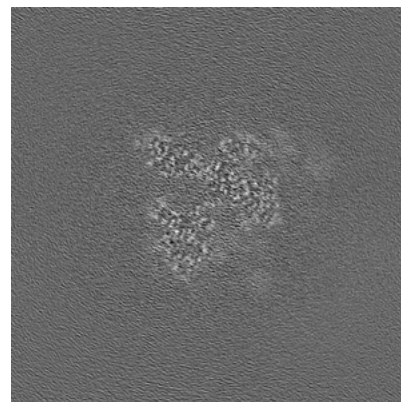
6.2.2 Raw map



X Index: 160



Y Index: 160

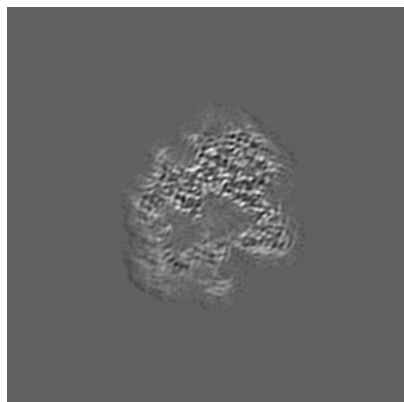


Z Index: 160

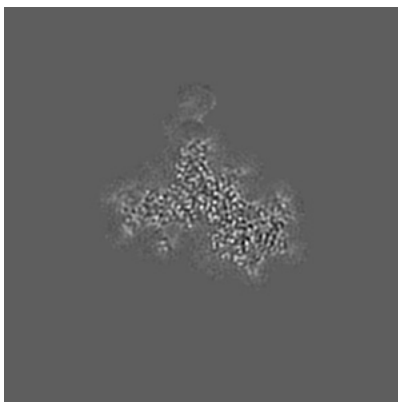
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

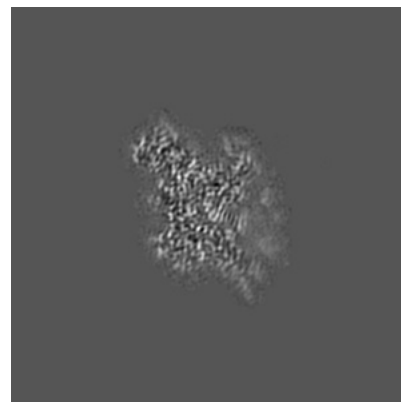
6.3.1 Primary map



X Index: 136

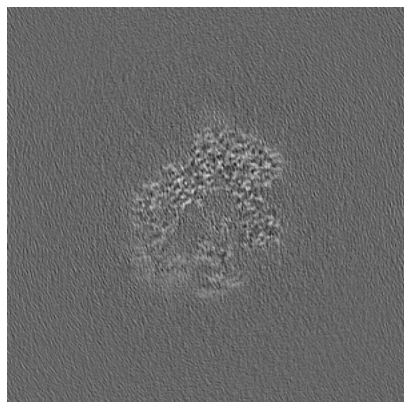


Y Index: 179

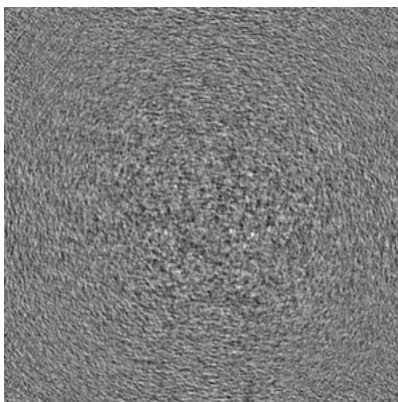


Z Index: 175

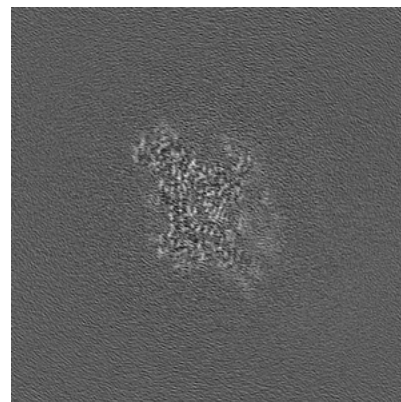
6.3.2 Raw map



X Index: 143



Y Index: 0

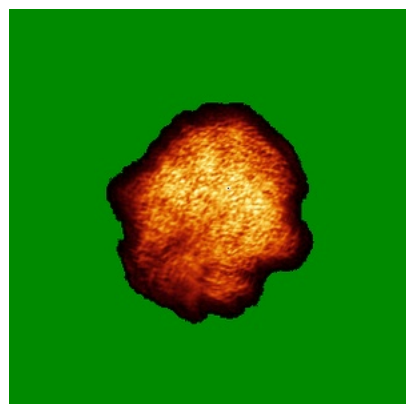


Z Index: 175

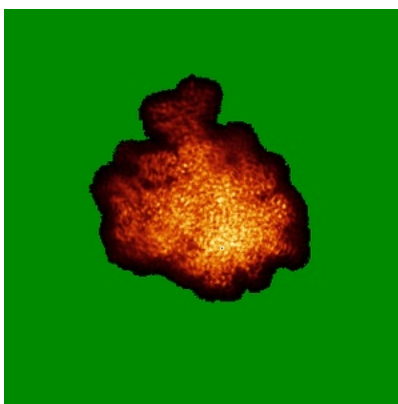
The images above show the largest variance slices of the map in three orthogonal directions.

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

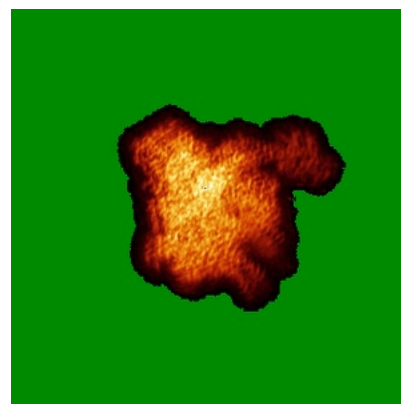
6.4.1 Primary map



X

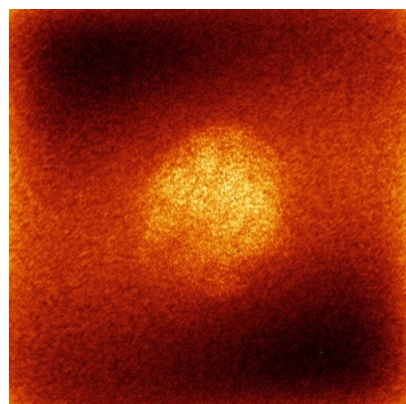


Y

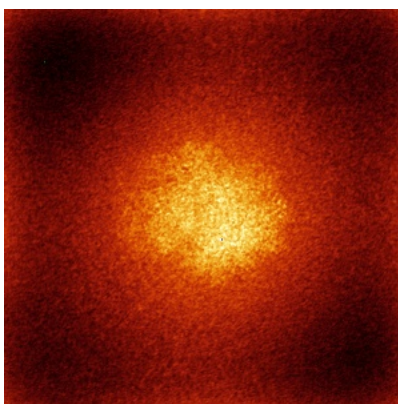


Z

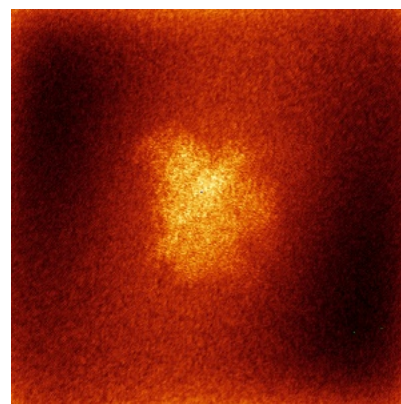
6.4.2 Raw map



X



Y

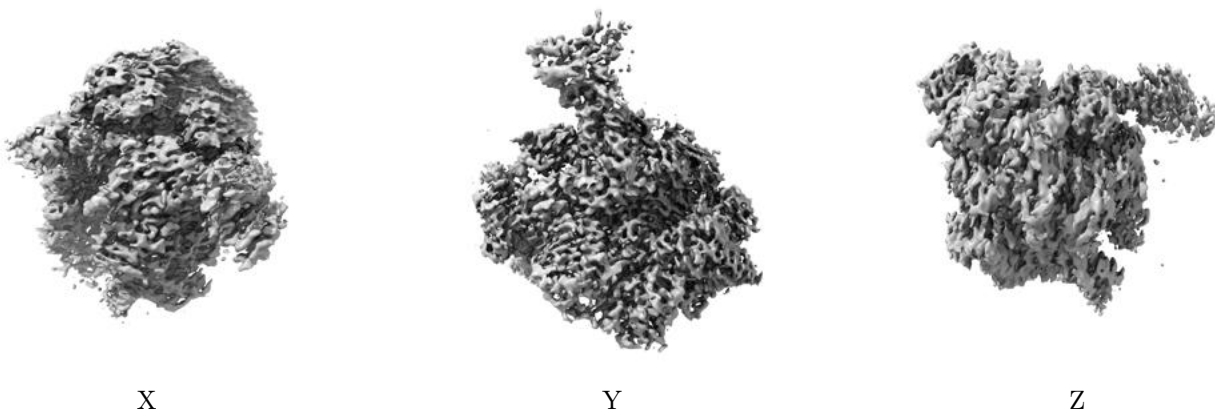


Z

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.

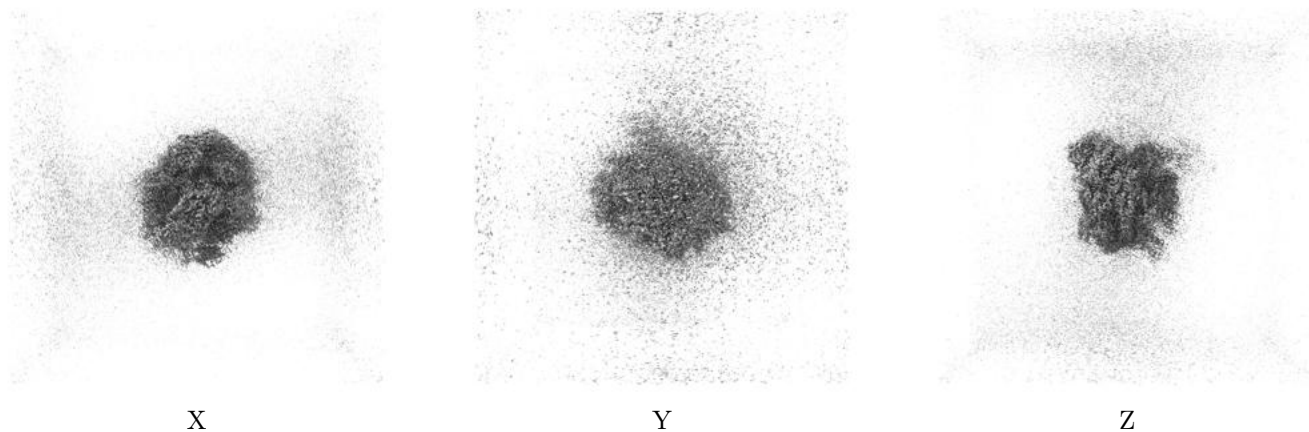
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

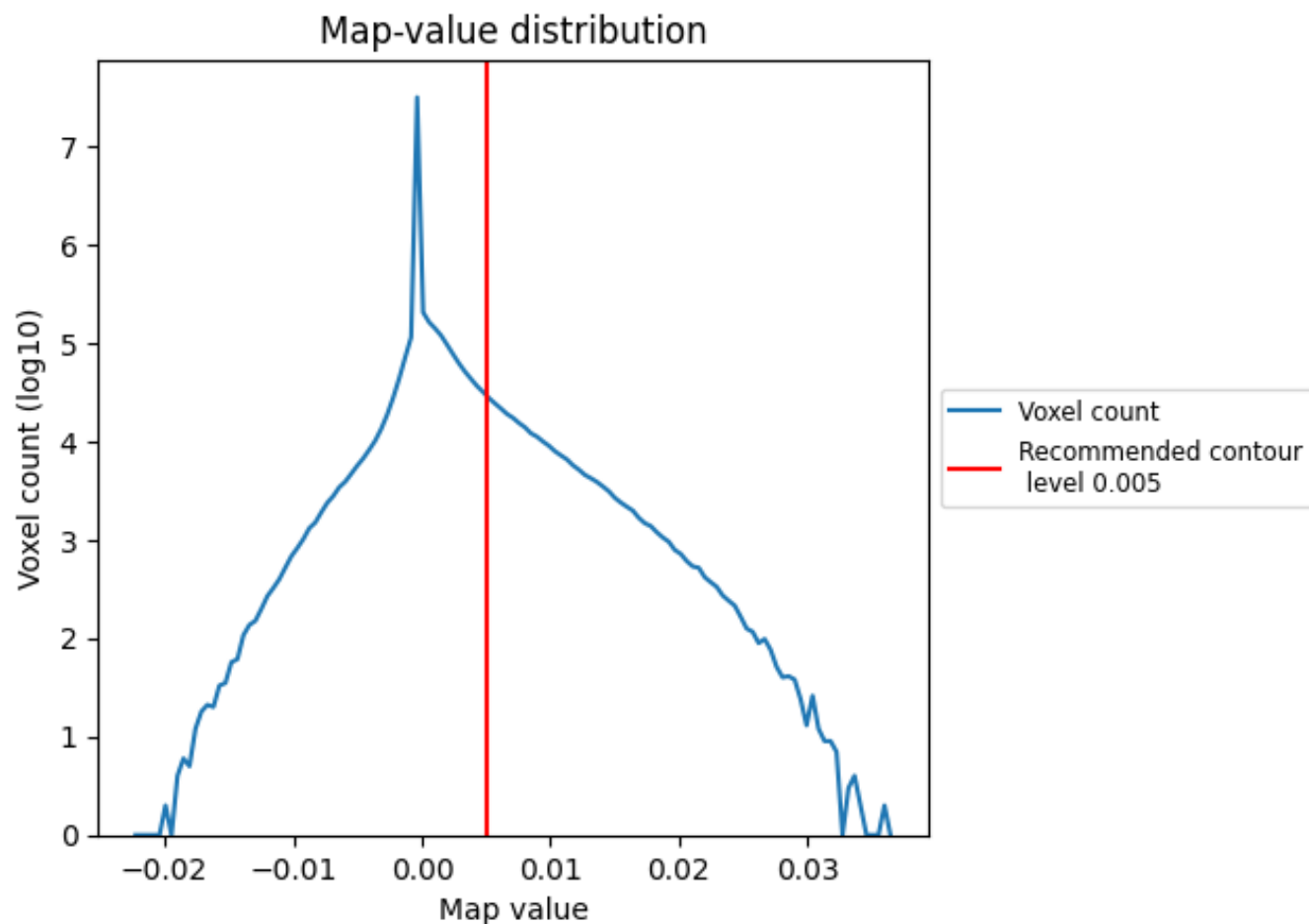
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

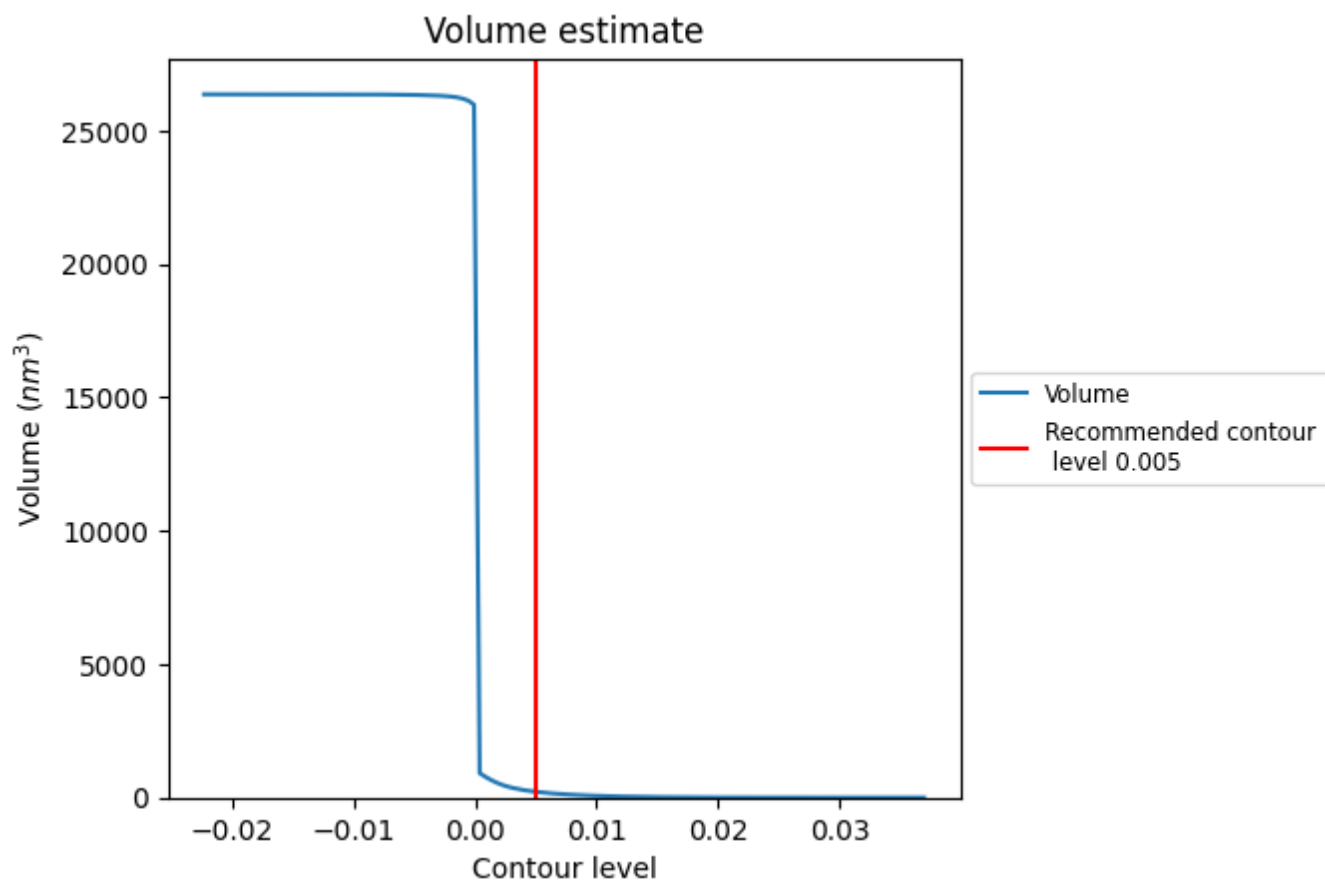
This section contains the results of statistical analysis of the map.

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.

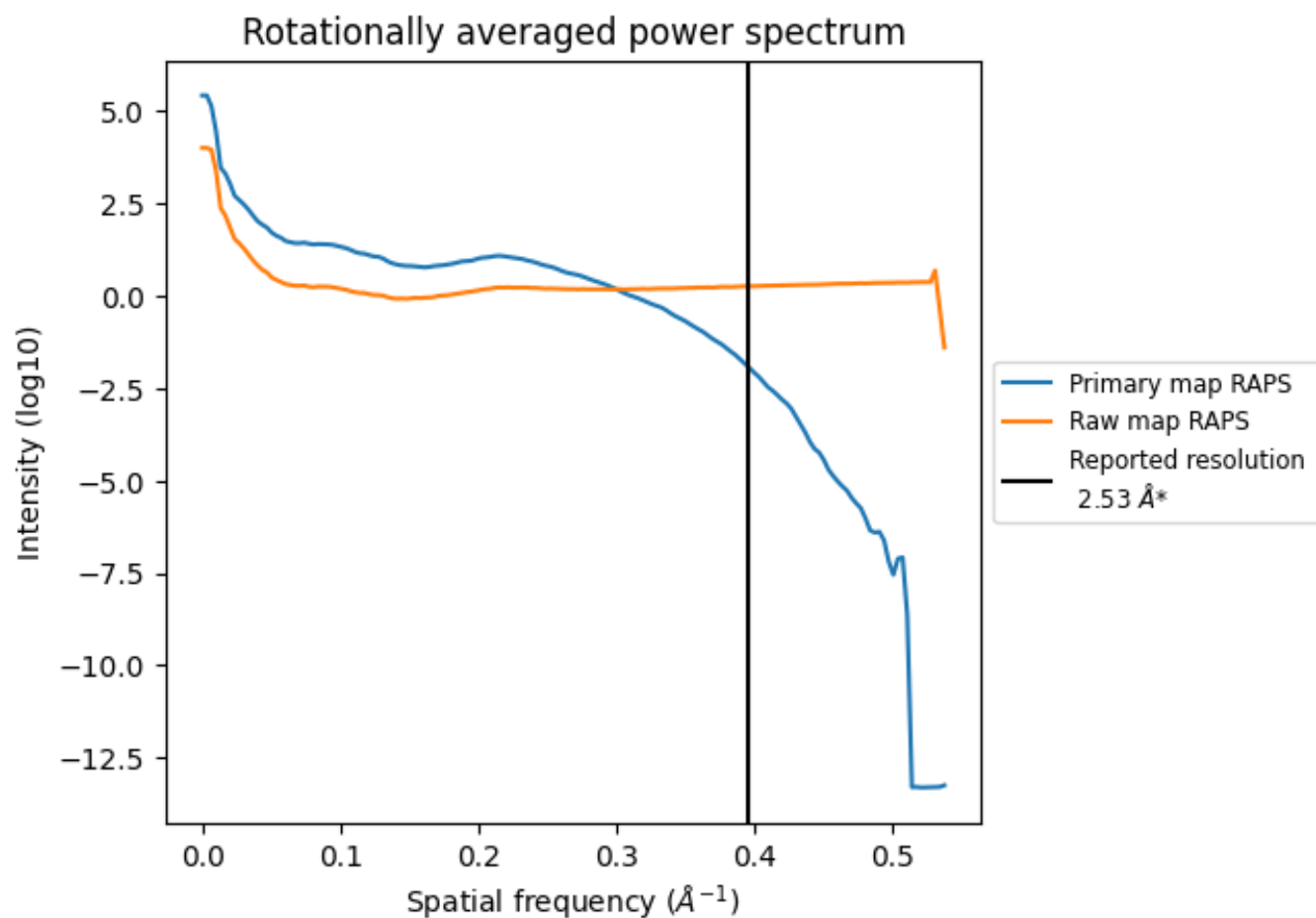
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 217 nm³; this corresponds to an approximate mass of 196 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 ⓘ

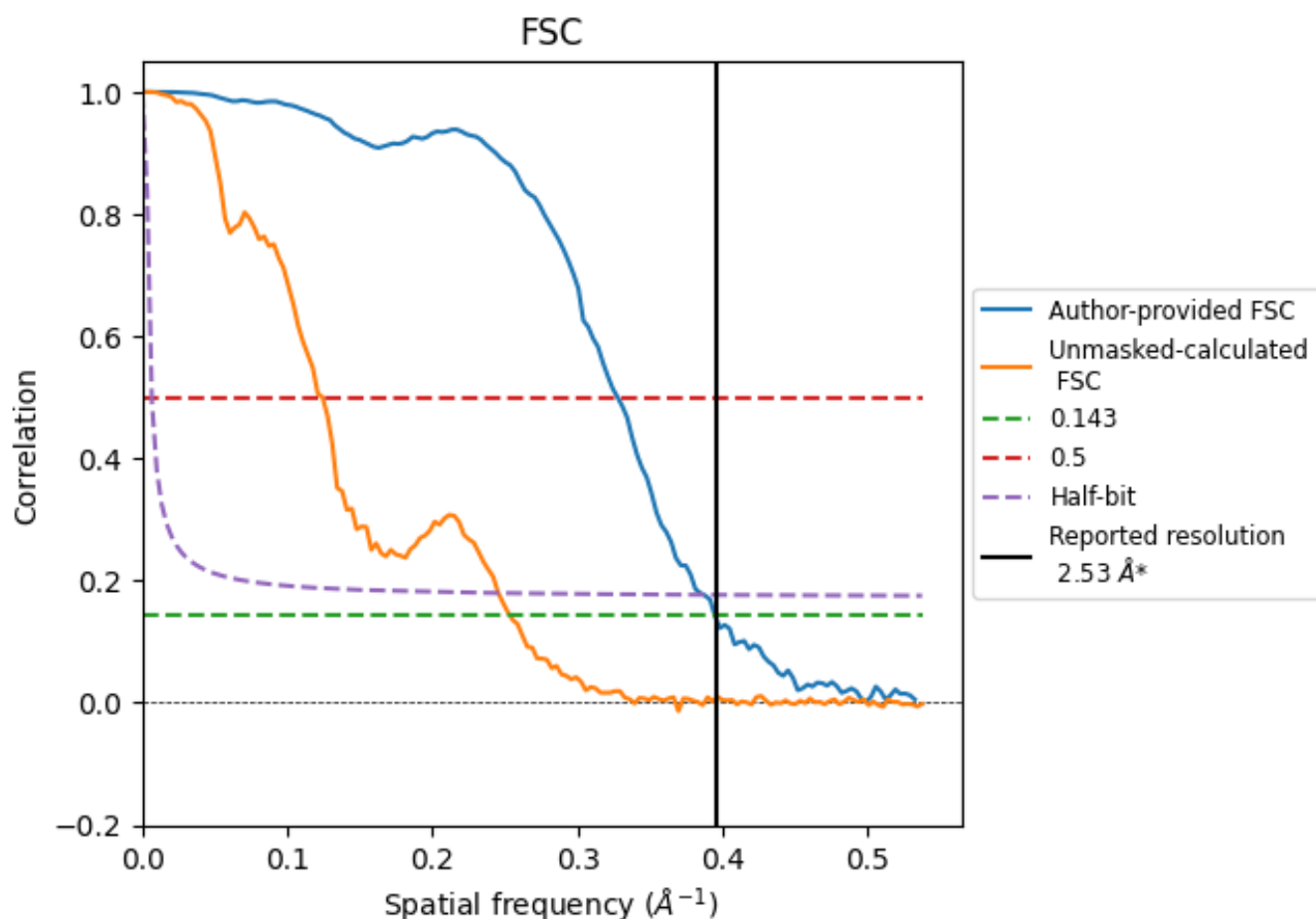


*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

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 0.395 Å⁻¹

8.2 Resolution estimates [i](#)

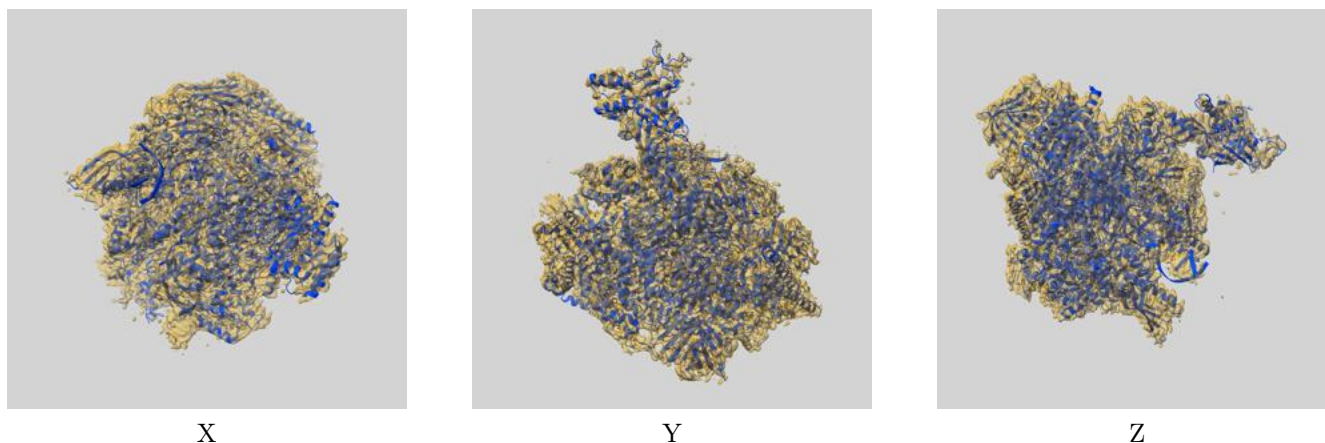
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	2.53	3.05	2.58
Unmasked-calculated*	3.95	8.05	4.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 2.53 by more than 10 %

9 Map-model fit [i](#)

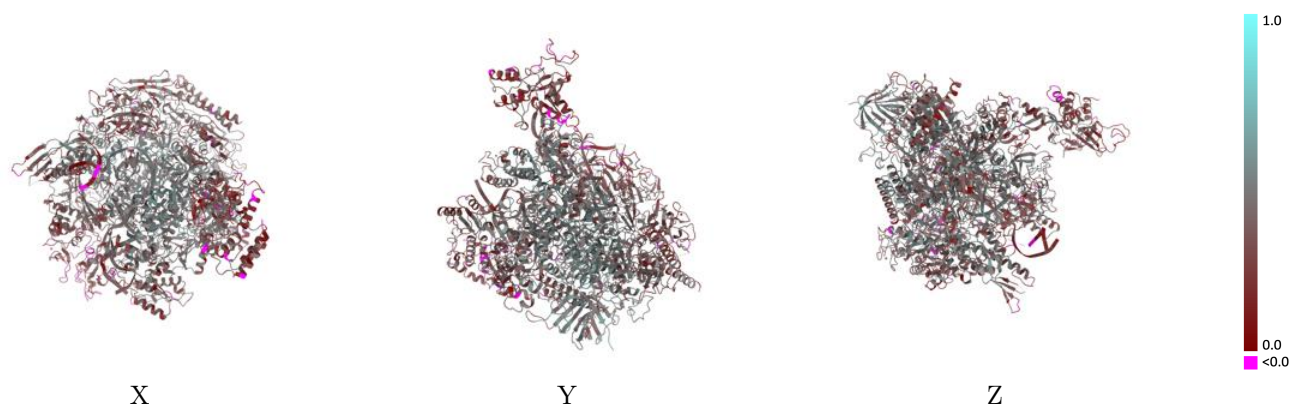
This section contains information regarding the fit between EMDB map EMD-66852 and PDB model 9XGK. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



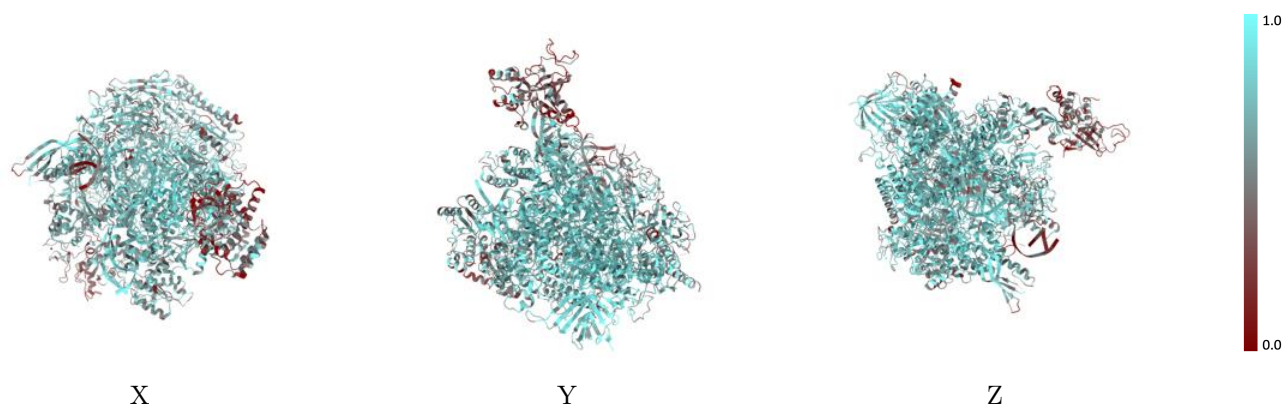
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



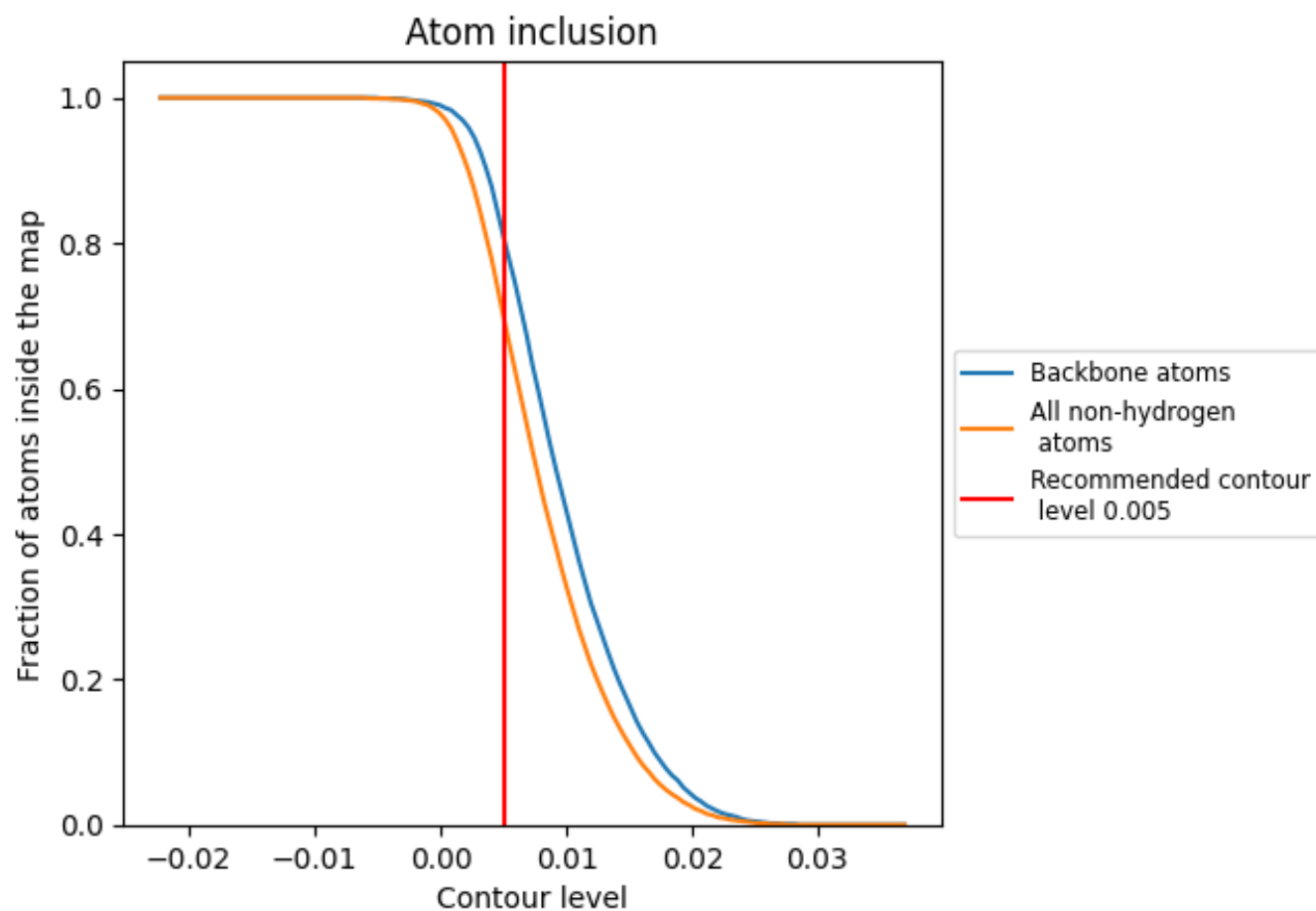
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 70% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7000	 0.3860
A	 0.7260	 0.4080
B	 0.7560	 0.4130
C	 0.6650	 0.3510
D	 0.3470	 0.2360
E	 0.6770	 0.3590
F	 0.7590	 0.4200
G	 0.4470	 0.3180
H	 0.7790	 0.4480
I	 0.5230	 0.2320
J	 0.7100	 0.3430
K	 0.6960	 0.3680
L	 0.6320	 0.3090
M	 0.7440	 0.3320
N	 0.6520	 0.2600
P	 0.9140	 0.5080
T	 0.7340	 0.3900

