Full wwPDB EM Validation Report ⓘ

Aug 8, 2023 – 07:37 pm BST

PDB ID	:	8P4A
EMDB ID	:	EMD-17403
Title	:	Structural insights into human co-transcriptional capping - structure 1
Authors	:	Garg, G.; Dienemann, C.; Farnung, L.; Schwarz, J.; Linden, A.; Urlaub, H.; Cramer, P.
Deposited on	:	2023-05-20
Resolution	:	3.60 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:

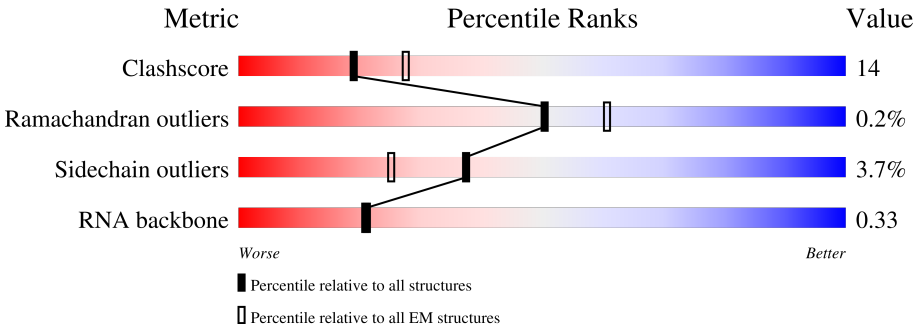
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	1984	51% 19% 29%
2	P	19	26% 32% 21% 47%
3	B	1174	68% 27% 5%
4	C	275	75% 19% 6%
5	D	142	43% 69% 22% 9%
6	E	210	74% 25%
7	F	127	5% 43% 21% 35%

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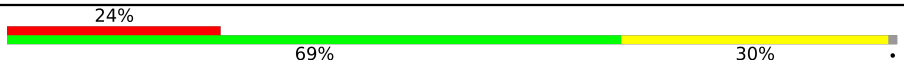
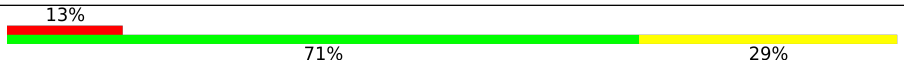
Mol	Chain	Length	Quality of chain
8	G	172	
9	H	150	
10	I	125	
11	J	67	
12	K	117	
13	L	58	
14	N	29	
15	T	38	
16	M	597	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 36673 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*CP*CP*CP*AP*GP*GP *GP*AP*AP*CP*CP*CP*AP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	P	19	405	182	78	126	19	0	0

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

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

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	258	2070	1301	352	411	6	0	0

- Molecule 5 is a protein called RNA polymerase II subunit D.

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

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

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

- 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 polymerase II subunit RPB7.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

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

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

- Molecule 14 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	29	Total	C	N	O	P	0	0
			591	283	107	172	29		

- Molecule 15 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	38	Total	C	N	O	P	0	0
			785	374	142	231	38		

- Molecule 16 is a protein called mRNA-capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	507	Total	C	N	O	S	0	0
			4083	2602	714	738	29		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	126	SER	CYS	conflict	UNP O60942

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

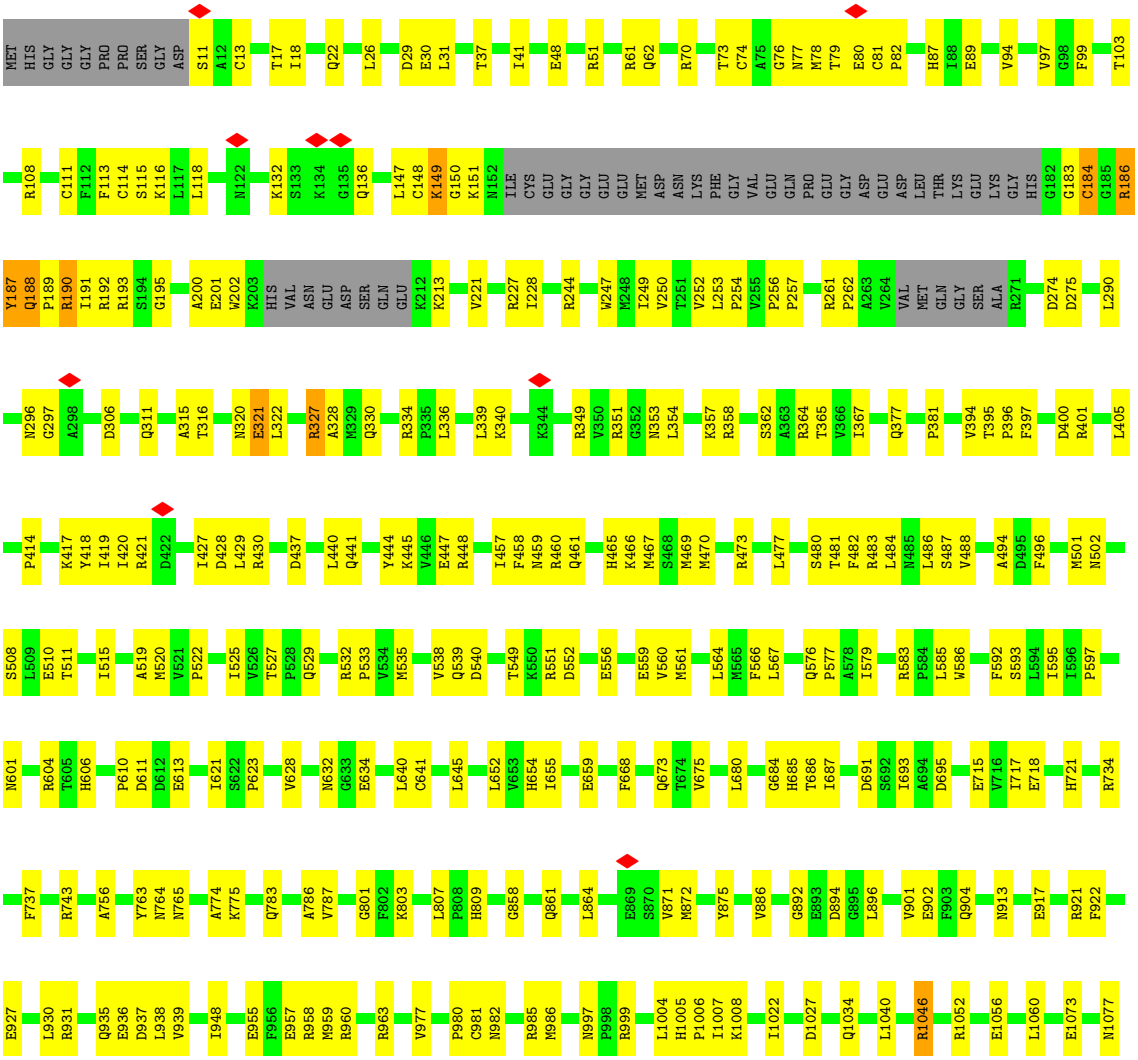
Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total	Zn	0
			2	2	
18	B	1	Total	Zn	0
			1	1	
18	C	1	Total	Zn	0
			1	1	
18	I	2	Total	Zn	0
			2	2	
18	J	1	Total	Zn	0
			1	1	
18	L	1	Total	Zn	0
			1	1	

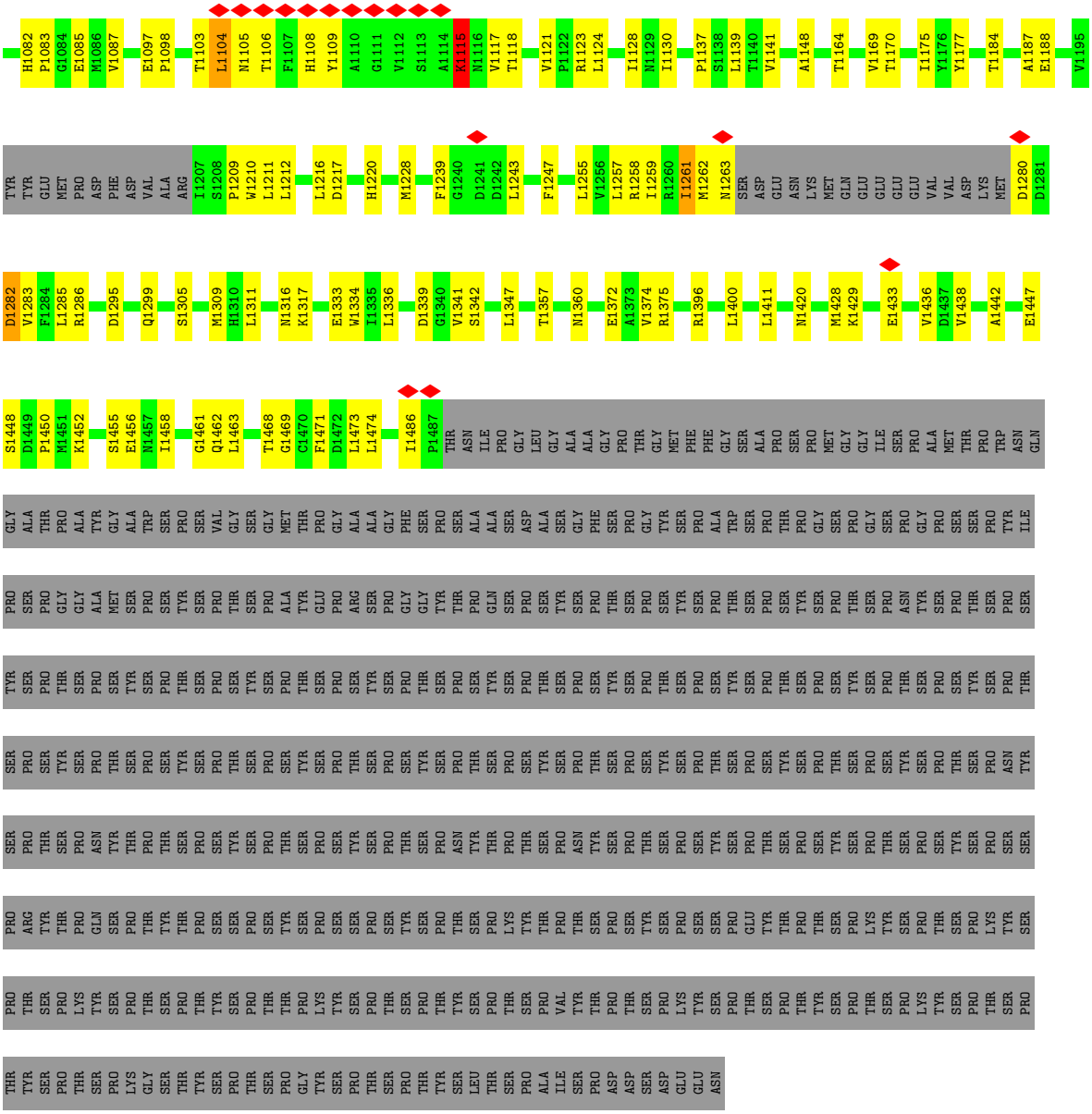
3 Residue-property plots (i)

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

- Molecule 1: DNA-directed RNA polymerase subunit

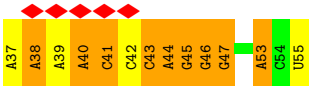
Chain A:





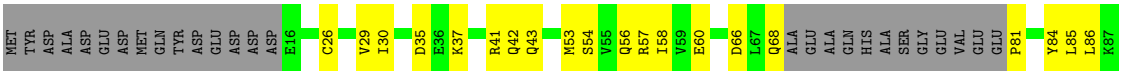
• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*CP*CP*CP*AP*GP*GP*GP*AP*AP*CP*CP*CP*AP*CP*U)-3')

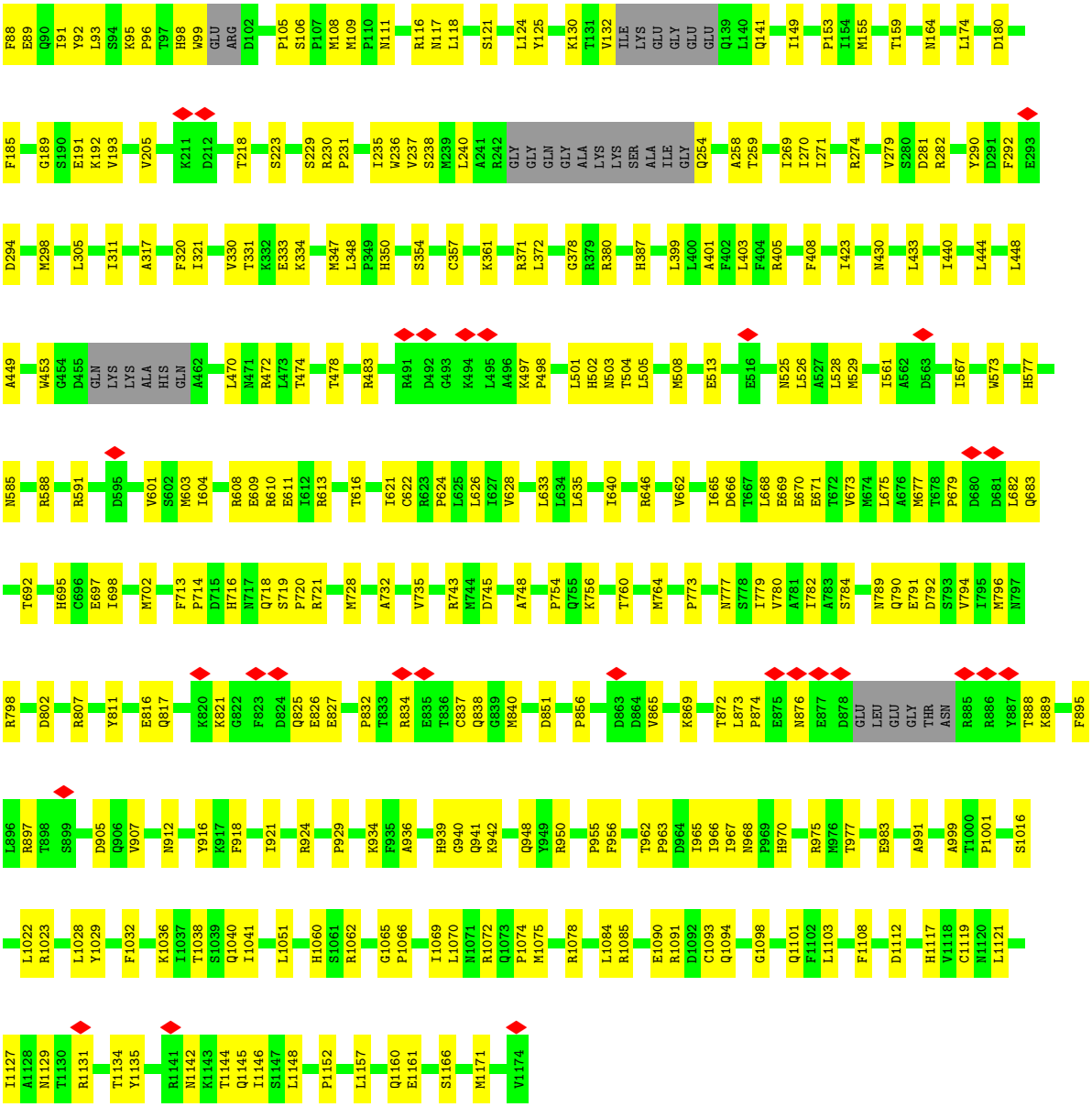
Chain P:



• Molecule 3: DNA-directed RNA polymerase subunit beta

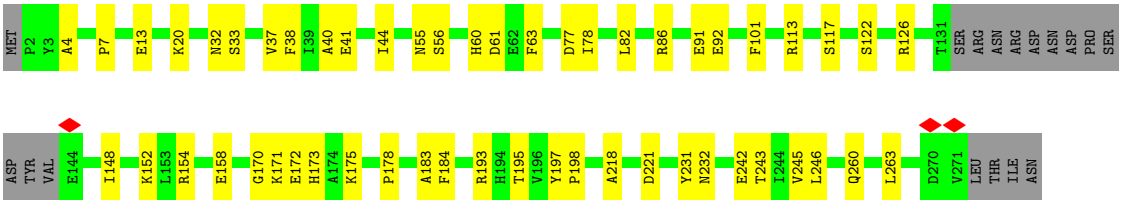
Chain B:





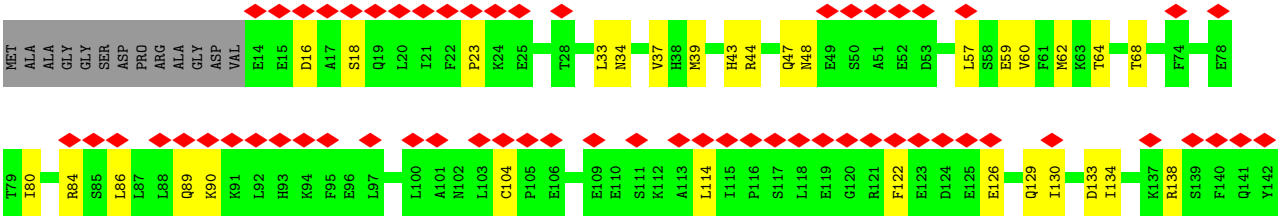
• Molecule 4: DNA-directed RNA polymerase II subunit RPB3

Chain C:

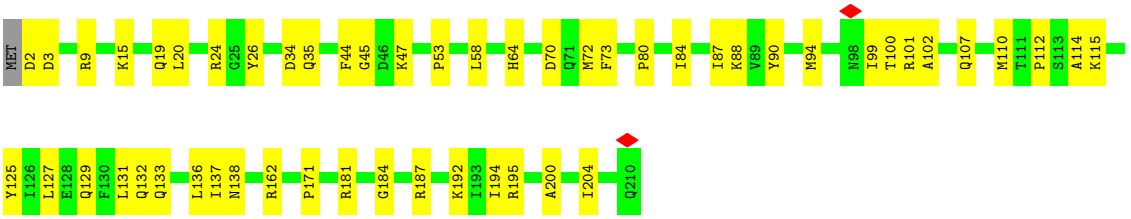


• Molecule 5: RNA polymerase II subunit D

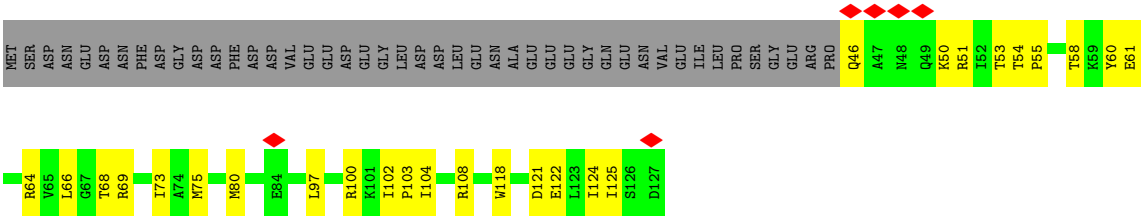
Chain D:



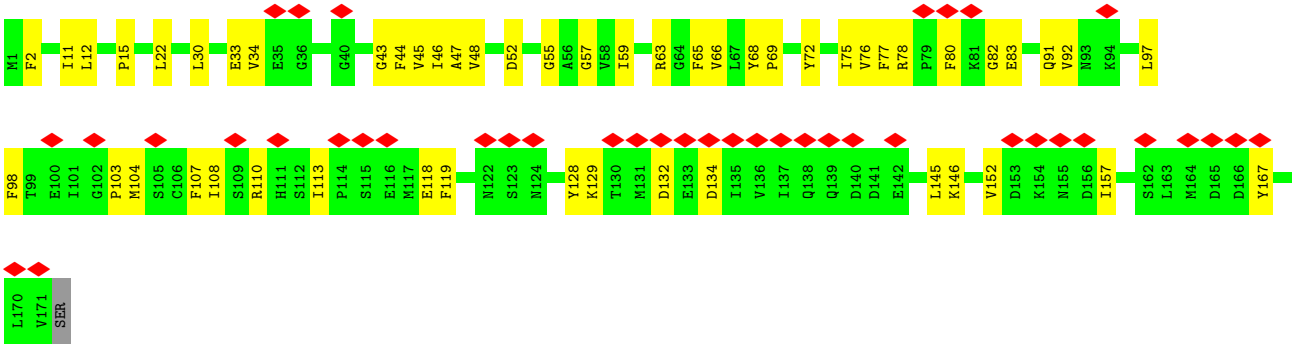
• Molecule 6: DNA-directed RNA polymerase II subunit E



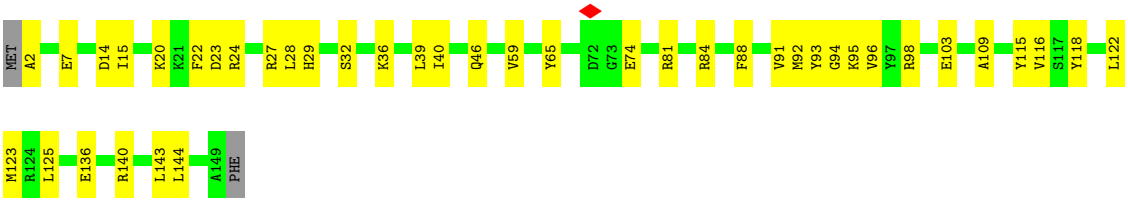
• Molecule 7: DNA-directed RNA polymerase II subunit F



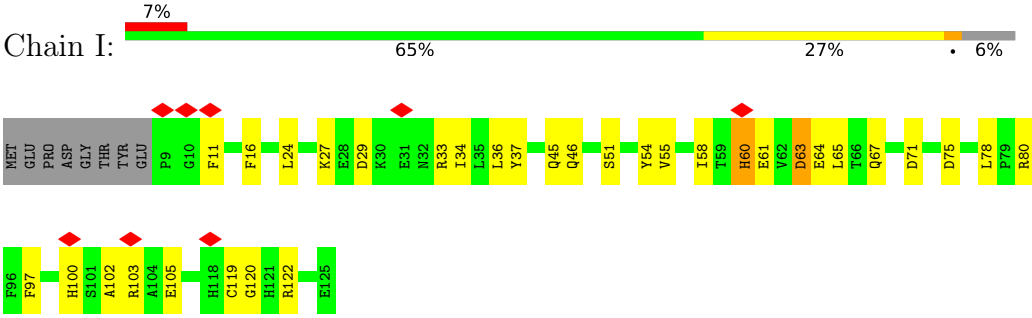
• Molecule 8: DNA-directed RNA polymerase II subunit RPB7



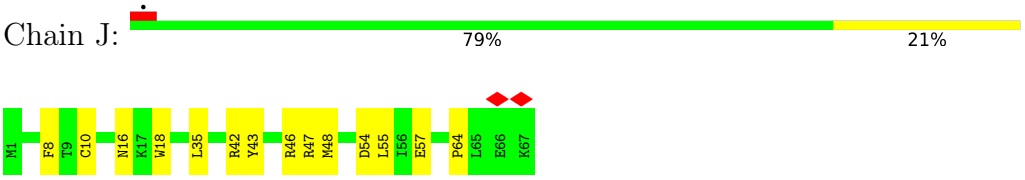
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



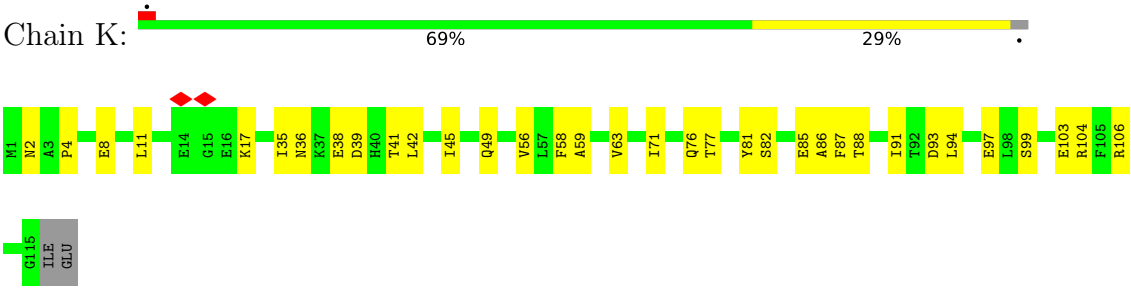
• Molecule 10: DNA-directed RNA polymerase II subunit RPB9



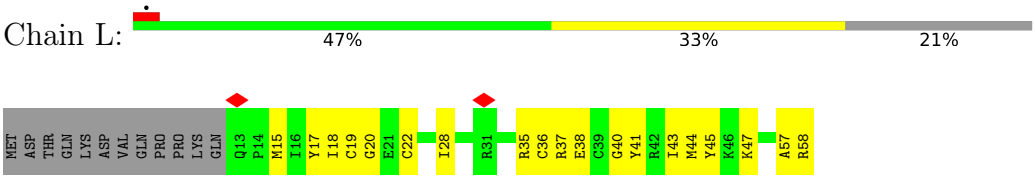
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



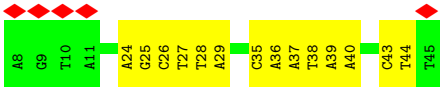
• Molecule 12: DNA-directed RNA polymerase II subunit RPB11-a



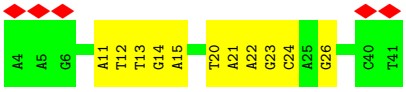
• Molecule 13: RNA polymerase II subunit K



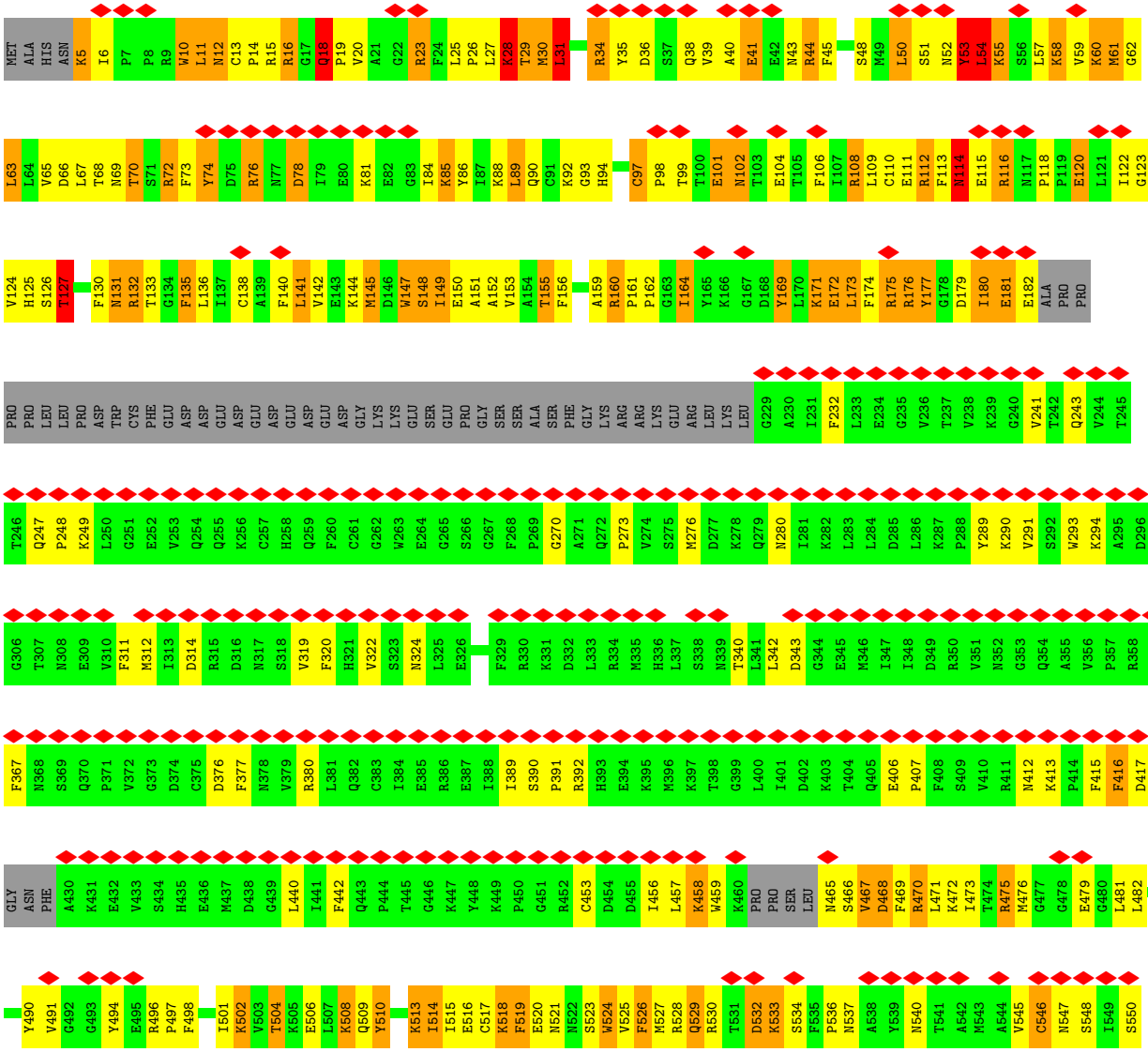
• Molecule 14: DNA (29-MER)

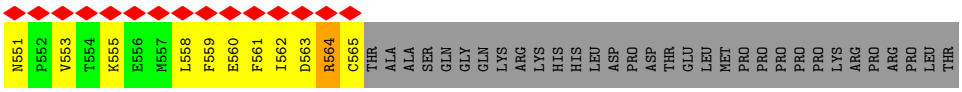


• Molecule 15: DNA (38-MER)



• Molecule 16: mRNA-capping enzyme




N551
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R564
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ALA
ALA
SER
GLN
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ASP
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THR
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LEU
MET
PRO
PRO
PRO
PRO
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LEU
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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34647	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 ($e^-/Å^2$)	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	0.082	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0257	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.28	0/11347	0.52	0/15321
2	P	0.28	0/453	0.73	0/703
3	B	0.28	0/9105	0.52	0/12290
4	C	0.27	0/2112	0.48	0/2869
5	D	0.24	0/1012	0.47	0/1366
6	E	0.27	0/1752	0.52	0/2366
7	F	0.26	0/668	0.53	0/901
8	G	0.28	0/1336	0.52	0/1820
9	H	0.30	0/1207	0.56	0/1628
10	I	0.29	0/973	0.55	0/1316
11	J	0.29	0/542	0.48	0/730
12	K	0.30	0/939	0.52	0/1271
13	L	0.31	0/395	0.66	0/524
14	N	0.44	0/661	0.89	0/1014
15	T	0.48	0/880	0.92	0/1358
16	M	0.57	1/4173 (0.0%)	0.80	9/5622 (0.2%)
All	All	0.33	1/37555 (0.0%)	0.58	9/51099 (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
16	M	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	18	GLN	C-N	20.80	1.73	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	M	28	LYS	N-CA-CB	-7.04	97.92	110.60
16	M	30	MET	N-CA-C	7.02	129.95	111.00
16	M	29	THR	N-CA-CB	-6.13	98.66	110.30
16	M	54	LEU	CB-CG-CD2	5.84	120.93	111.00
16	M	53	TYR	CB-CA-C	5.49	121.39	110.40
16	M	30	MET	CB-CA-C	-5.35	99.70	110.40
16	M	177	TYR	CB-CA-C	5.32	121.04	110.40
16	M	29	THR	N-CA-C	5.17	124.96	111.00
16	M	564	ARG	CB-CA-C	-5.03	100.35	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	M	30	MET	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	M	416	PHE	Peptide

5.2 Too-close contacts (i)

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	11142	0	11293	299	0
2	P	405	0	209	17	0
3	B	8928	0	8950	227	0
4	C	2070	0	2013	42	0
5	D	998	0	953	24	0
6	E	1721	0	1737	39	0
7	F	658	0	684	23	0
8	G	1305	0	1267	40	0
9	H	1186	0	1147	32	0
10	I	950	0	880	35	0
11	J	533	0	553	11	0
12	K	920	0	942	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	L	389	0	395	14	0
14	N	591	0	329	8	0
15	T	785	0	431	8	0
16	M	4083	0	4067	296	0
17	A	1	0	0	0	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	36673	0	35850	1027	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 14.

All (1027) 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)
16:M:18:GLN:C	16:M:19:PRO:N	1.73	1.42
16:M:153:VAL:HG13	16:M:173:LEU:HD13	1.33	1.07
5:D:86:LEU:O	5:D:90:LYS:NZ	1.96	0.98
3:B:230:ARG:HE	3:B:231:PRO:HD2	1.30	0.95
16:M:93:GLY:O	16:M:94:HIS:HB2	1.66	0.94
16:M:514:ILE:H	16:M:514:ILE:HD12	1.34	0.93
16:M:16:ARG:HH11	16:M:16:ARG:HB2	1.34	0.92
16:M:12:ASN:HD22	16:M:12:ASN:H	1.18	0.91
16:M:475:ARG:HA	16:M:485:ASN:HA	1.52	0.90
16:M:72:ARG:HH11	16:M:72:ARG:HG2	1.36	0.90
16:M:31:LEU:HD21	16:M:39:VAL:HG21	1.51	0.90
1:A:190:ARG:CZ	1:A:190:ARG:HA	2.04	0.87
16:M:293:TRP:HA	16:M:440:LEU:HD23	1.57	0.87
16:M:28:LYS:HA	16:M:125:HIS:HB2	1.58	0.85
16:M:132:ARG:HA	16:M:135:PHE:HB3	1.60	0.83
16:M:425:LEU:HD23	16:M:559:PHE:HB3	1.61	0.83
16:M:28:LYS:CA	16:M:125:HIS:HB2	2.10	0.82
16:M:419:CYS:H	16:M:564:ARG:CB	1.92	0.82
16:M:419:CYS:N	16:M:564:ARG:H	1.78	0.82
1:A:477:LEU:HB2	1:A:483:ARG:HH21	1.45	0.81
16:M:141:LEU:HA	16:M:145:MET:HB2	1.61	0.81
16:M:12:ASN:H	16:M:12:ASN:ND2	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:291:VAL:HG11	16:M:562:ILE:HB	1.62	0.81
16:M:530:ARG:HH11	16:M:530:ARG:HG3	1.44	0.81
16:M:421:SER:H	16:M:563:ASP:HB3	1.45	0.80
16:M:113:PHE:HA	16:M:116:ARG:HB2	1.63	0.80
16:M:149:ILE:HD13	16:M:149:ILE:H	1.45	0.79
16:M:20:VAL:HG22	16:M:159:ALA:HB3	1.66	0.78
16:M:67:LEU:HB2	16:M:126:SER:HA	1.65	0.78
16:M:421:SER:N	16:M:563:ASP:HB3	1.98	0.78
16:M:176:ARG:CZ	16:M:176:ARG:HA	2.14	0.77
16:M:171:LYS:HZ2	16:M:171:LYS:HA	1.48	0.77
3:B:1062:ARG:NH2	3:B:1066:PRO:O	2.17	0.77
1:A:1175:ILE:HG12	10:I:54:TYR:HB3	1.65	0.76
1:A:11:SER:N	3:B:1135:TYR:HH	1.84	0.76
16:M:30:MET:HA	16:M:73:PHE:HB3	1.67	0.76
1:A:256:PRO:O	1:A:261:ARG:NH1	2.19	0.76
16:M:10:TRP:CZ2	16:M:43:ASN:HB3	2.21	0.76
16:M:147:TRP:HB3	16:M:152:ALA:HB2	1.67	0.75
16:M:51:SER:HA	16:M:54:LEU:HB3	1.69	0.74
16:M:108:ARG:HH11	16:M:108:ARG:HB3	1.52	0.74
1:A:1433:GLU:HB2	15:T:23:DG:H4'	1.68	0.74
2:P:44:A:O3'	2:P:44:A:OP1	2.06	0.73
6:E:24:ARG:HH12	6:E:184:GLY:HA3	1.53	0.73
1:A:1261:ILE:HD12	1:A:1280:ASP:N	2.03	0.73
16:M:470:ARG:HD3	16:M:536:PRO:HD3	1.71	0.73
1:A:1261:ILE:HD12	1:A:1280:ASP:H	1.52	0.73
16:M:54:LEU:HG	16:M:60:LYS:HA	1.69	0.73
1:A:496:PHE:HD2	3:B:791:GLU:HB2	1.54	0.72
7:F:58:THR:OG1	7:F:61:GLU:OE1	2.07	0.72
10:I:82:GLU:O	10:I:92:LYS:NZ	2.22	0.72
3:B:567:ILE:HD11	3:B:577:HIS:HB2	1.71	0.72
10:I:65:LEU:HD12	10:I:122:ARG:HG3	1.72	0.72
16:M:34:ARG:HD2	16:M:34:ARG:O	1.90	0.72
1:A:188:GLN:HA	1:A:188:GLN:NE2	2.05	0.71
7:F:66:LEU:HD21	7:F:97:LEU:HD22	1.71	0.71
16:M:23:ARG:O	16:M:23:ARG:NH1	2.24	0.71
8:G:44:PHE:HE2	8:G:104:MET:HB2	1.55	0.71
16:M:14:PRO:O	16:M:28:LYS:NZ	2.23	0.71
16:M:276:MET:HA	16:M:280:ASN:HD22	1.56	0.71
1:A:188:GLN:HA	1:A:188:GLN:HE21	1.56	0.71
1:A:864:LEU:HD21	1:A:1128:ILE:HD12	1.71	0.71
7:F:46:GLN:HA	7:F:50:LYS:HE2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:O	1:A:244:ARG:NH2	2.24	0.70
3:B:109:MET:HE1	3:B:174:LEU:HD13	1.73	0.70
16:M:419:CYS:H	16:M:564:ARG:H	1.40	0.70
3:B:748:ALA:HB3	3:B:811:TYR:HB2	1.71	0.70
4:C:7:PRO:O	12:K:104:ARG:NH1	2.25	0.70
3:B:754:PRO:HB2	3:B:773:PRO:HG2	1.73	0.70
3:B:790:GLN:O	3:B:968:ASN:ND2	2.25	0.69
16:M:48:SER:O	16:M:52:ASN:N	2.19	0.69
1:A:132:LYS:HG2	6:E:187:ARG:HH12	1.57	0.69
3:B:84:TYR:HE1	3:B:423:ILE:HD12	1.58	0.69
3:B:794:VAL:HG12	3:B:967:ILE:HG22	1.74	0.69
16:M:515:ILE:HG22	16:M:529:GLN:HA	1.74	0.69
16:M:530:ARG:HG2	16:M:533:LYS:HB2	1.73	0.69
16:M:113:PHE:O	16:M:116:ARG:N	2.26	0.68
1:A:1261:ILE:CD1	1:A:1280:ASP:H	2.05	0.68
6:E:20:LEU:HD21	6:E:24:ARG:HH21	1.59	0.68
10:I:61:GLU:OE1	10:I:61:GLU:N	2.23	0.68
1:A:76:GLY:HA3	1:A:81:CYS:HB2	1.75	0.68
1:A:94:VAL:HG13	1:A:311:GLN:HG2	1.75	0.68
1:A:549:THR:HG21	1:A:640:LEU:H	1.59	0.68
8:G:107:PHE:HE2	16:M:118:PRO:HG2	1.58	0.68
1:A:420:ILE:HB	1:A:445:LYS:HB2	1.76	0.68
1:A:1083:PRO:HD2	7:F:58:THR:HG21	1.74	0.68
4:C:37:VAL:HG13	4:C:41:GLU:HB2	1.74	0.68
1:A:515:ILE:HG23	1:A:519:ALA:HB3	1.75	0.67
6:E:26:TYR:HD1	6:E:64:HIS:HA	1.59	0.67
6:E:131:LEU:HD23	6:E:133:GLN:H	1.59	0.67
1:A:111:CYS:HB3	1:A:116:LYS:H	1.58	0.67
16:M:304:ILE:HB	16:M:340:THR:HB	1.75	0.67
7:F:100:ARG:NH2	7:F:121:ASP:O	2.27	0.67
16:M:419:CYS:H	16:M:564:ARG:HB3	1.59	0.67
1:A:894:ASP:HB3	6:E:200:ALA:HB2	1.77	0.67
1:A:1087:VAL:HG12	1:A:1400:LEU:HD22	1.77	0.67
16:M:420:THR:N	16:M:564:ARG:HB2	2.10	0.67
1:A:1468:THR:HG23	7:F:64:ARG:HB2	1.77	0.67
1:A:894:ASP:OD2	1:A:1396:ARG:NH2	2.27	0.66
16:M:10:TRP:HZ2	16:M:43:ASN:HB3	1.58	0.66
16:M:290:LYS:HG2	16:M:415:PHE:HD2	1.60	0.66
16:M:417:ASP:N	16:M:562:ILE:O	2.28	0.66
16:M:273:PRO:HB2	16:M:458:LYS:HB2	1.75	0.66
16:M:468:ASP:OD1	16:M:468:ASP:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1119:CYS:HB2	3:B:1142:ASN:HD21	1.60	0.66
2:P:40:A:H3'	2:P:40:A:N3	2.10	0.66
1:A:1458:ILE:HD13	3:B:1091:ARG:HD3	1.77	0.65
4:C:152:LYS:NZ	11:J:57:GLU:OE2	2.29	0.65
16:M:513:LYS:NZ	16:M:513:LYS:HA	2.11	0.65
1:A:321:GLU:H	1:A:321:GLU:CD	1.99	0.65
16:M:175:ARG:HB2	16:M:180:ILE:HB	1.77	0.65
1:A:62:GLN:NE2	1:A:256:PRO:O	2.30	0.65
3:B:777:ASN:O	11:J:47:ARG:NH1	2.29	0.65
3:B:229:SER:HA	3:B:405:ARG:HD3	1.77	0.65
16:M:440:LEU:HD13	16:M:562:ILE:HD13	1.79	0.65
3:B:816:GLU:OE2	3:B:869:LYS:NZ	2.29	0.64
1:A:115:SER:HB3	1:A:227:ARG:HD3	1.79	0.64
16:M:10:TRP:CZ3	16:M:31:LEU:HG	2.32	0.64
16:M:10:TRP:CD1	16:M:10:TRP:N	2.61	0.64
16:M:16:ARG:HB2	16:M:16:ARG:NH1	2.09	0.64
3:B:796:MET:HB2	3:B:948:GLN:HG2	1.79	0.64
1:A:957:GLU:OE2	1:A:960:ARG:NH2	2.30	0.64
1:A:801:GLY:HA3	3:B:503:ASN:HB2	1.79	0.64
16:M:171:LYS:HA	16:M:171:LYS:NZ	2.13	0.64
16:M:470:ARG:HH11	16:M:470:ARG:HA	1.62	0.64
1:A:480:SER:HB3	12:K:2:ASN:HB2	1.79	0.64
16:M:72:ARG:HG2	16:M:72:ARG:NH1	2.10	0.63
16:M:515:ILE:HA	16:M:530:ARG:H	1.63	0.63
16:M:26:PRO:HB2	16:M:160:ARG:HB2	1.80	0.63
4:C:148:ILE:HD13	11:J:16:ASN:HB3	1.81	0.63
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.81	0.63
1:A:29:ASP:OD1	1:A:30:GLU:N	2.32	0.63
1:A:320:ASN:ND2	1:A:336:LEU:O	2.32	0.63
1:A:461:GLN:OE1	1:A:502:ASN:ND2	2.32	0.63
6:E:129:GLN:O	6:E:181:ARG:NH2	2.32	0.63
6:E:192:LYS:HE2	6:E:194:ILE:HD11	1.81	0.63
1:A:78:MET:O	3:B:1072:ARG:NH2	2.32	0.63
4:C:78:ILE:HD11	4:C:126:ARG:HD2	1.81	0.63
5:D:39:MET:O	5:D:43:HIS:ND1	2.27	0.63
12:K:45:ILE:HD12	12:K:45:ILE:H	1.63	0.63
16:M:418:ILE:HG22	16:M:419:CYS:SG	2.39	0.63
7:F:53:THR:OG1	7:F:118:TRP:NE1	2.32	0.63
16:M:502:LYS:O	16:M:502:LYS:NZ	2.22	0.63
3:B:601:VAL:HG22	3:B:616:THR:HG23	1.81	0.62
16:M:442:PHE:HZ	16:M:558:LEU:HD12	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLN:HG2	15:T:26:DG:H2"	1.82	0.62
3:B:817:GLN:HB3	3:B:918:PHE:HD1	1.64	0.62
12:K:63:VAL:HG12	12:K:71:ILE:HG22	1.82	0.62
16:M:164:ILE:O	16:M:164:ILE:HG13	1.99	0.62
9:H:94:GLY:HA3	9:H:118:TYR:HA	1.80	0.62
16:M:101:GLU:OE2	16:M:101:GLU:N	2.27	0.62
5:D:23:PRO:HG3	8:G:78:ARG:HH12	1.64	0.62
6:E:44:PHE:HB3	6:E:53:PRO:HB3	1.81	0.62
16:M:420:THR:O	16:M:422:ARG:N	2.32	0.62
1:A:428:ASP:OD1	1:A:430:ARG:N	2.31	0.61
1:A:458:PHE:CZ	1:A:501:MET:HG2	2.34	0.61
1:A:896:LEU:HB2	1:A:1396:ARG:HH21	1.65	0.61
1:A:108:ARG:HE	1:A:191:ILE:HB	1.65	0.61
3:B:236:TRP:HB2	3:B:259:THR:HB	1.81	0.61
16:M:417:ASP:HB3	16:M:565:CYS:N	2.16	0.61
16:M:78:ASP:N	16:M:78:ASP:OD1	2.32	0.61
1:A:1309:MET:HB3	1:A:1336:LEU:HD13	1.83	0.61
3:B:290:TYR:HB3	3:B:561:ILE:HG23	1.82	0.61
3:B:387:HIS:NE2	3:B:671:GLU:OE2	2.34	0.61
16:M:31:LEU:HD12	16:M:45:PHE:H	1.63	0.61
1:A:18:ILE:HD12	3:B:1171:MET:HB3	1.83	0.61
1:A:691:ASP:OD2	1:A:765:ASN:ND2	2.33	0.61
7:F:97:LEU:HA	7:F:102:ILE:HD11	1.83	0.61
6:E:80:PRO:HA	6:E:107:GLN:HB2	1.83	0.61
8:G:107:PHE:CE2	16:M:118:PRO:HG2	2.35	0.61
13:L:41:TYR:CE2	13:L:43:ILE:HB	2.36	0.61
16:M:524:TRP:N	16:M:524:TRP:CD1	2.67	0.61
1:A:1123:ARG:NH2	1:A:1360:ASN:OD1	2.34	0.61
4:C:172:GLU:OE2	13:L:58:ARG:NH2	2.34	0.60
3:B:274:ARG:NH2	3:B:281:ASP:OD1	2.34	0.60
5:D:64:THR:HG21	8:G:46:ILE:HD12	1.84	0.60
8:G:97:LEU:HB3	8:G:108:ILE:HB	1.82	0.60
10:I:37:TYR:HB2	10:I:46:GLN:HE21	1.66	0.60
1:A:1170:THR:HA	1:A:1216:LEU:HD13	1.84	0.60
1:A:1374:VAL:HG11	1:A:1411:LEU:HD21	1.83	0.60
2:P:45:G:H1'	3:B:1069:ILE:HG21	1.84	0.60
16:M:130:PHE:CD1	16:M:162:PRO:HA	2.37	0.60
1:A:17:THR:OG1	1:A:1462:GLN:OE1	2.20	0.60
1:A:680:LEU:HD21	3:B:784:SER:HB3	1.83	0.60
4:C:183:ALA:HB3	4:C:232:ASN:HB3	1.82	0.60
1:A:351:ARG:NH1	15:T:24:DC:OP1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:GLN:HG2	1:A:444:TYR:CE2	2.36	0.60
3:B:501:LEU:HD12	3:B:505:LEU:HD13	1.82	0.60
3:B:692:THR:HG21	10:I:80:ARG:HE	1.66	0.60
3:B:1119:CYS:HA	3:B:1146:ILE:HA	1.82	0.60
16:M:421:SER:OG	16:M:563:ASP:OD1	2.19	0.60
3:B:718:GLN:HG2	3:B:720:PRO:HD2	1.84	0.60
16:M:440:LEU:HD12	16:M:558:LEU:HD11	1.83	0.60
1:A:1217:ASP:OD2	1:A:1220:HIS:ND1	2.32	0.60
16:M:517:CYS:HA	16:M:527:MET:H	1.65	0.60
3:B:1062:ARG:HH12	3:B:1075:MET:H	1.50	0.60
1:A:31:LEU:HD11	1:A:254:PRO:HB3	1.83	0.59
16:M:31:LEU:HD13	16:M:31:LEU:O	2.02	0.59
3:B:99:TRP:HE1	3:B:105:PRO:HG3	1.67	0.59
1:A:1261:ILE:CD1	1:A:1280:ASP:N	2.65	0.59
1:A:913:ASN:OD1	1:A:963:ARG:NH1	2.35	0.59
16:M:29:THR:HG22	16:M:125:HIS:CD2	2.38	0.59
16:M:176:ARG:HA	16:M:176:ARG:NH1	2.16	0.59
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	1.85	0.59
3:B:378:GLY:HA3	10:I:102:ALA:HB3	1.85	0.59
16:M:131:ASN:OD1	16:M:131:ASN:N	2.35	0.59
3:B:192:LYS:HE3	3:B:449:ALA:HA	1.85	0.59
8:G:55:GLY:HA3	8:G:69:PRO:HG2	1.84	0.59
1:A:922:PHE:HA	1:A:1052:ARG:HD3	1.85	0.59
16:M:519:PHE:HA	16:M:524:TRP:HA	1.85	0.59
8:G:63:ARG:HE	8:G:65:PHE:HE1	1.51	0.58
1:A:481:THR:H	1:A:483:ARG:HH12	1.50	0.58
1:A:111:CYS:HA	1:A:118:LEU:HD12	1.85	0.58
16:M:169:TYR:N	16:M:169:TYR:CD1	2.71	0.58
3:B:223:SER:OG	3:B:350:HIS:ND1	2.26	0.58
3:B:474:THR:OG1	3:B:732:ALA:O	2.20	0.58
16:M:12:ASN:ND2	16:M:12:ASN:N	2.50	0.58
4:C:117:SER:HB3	4:C:148:ILE:HB	1.86	0.58
16:M:169:TYR:N	16:M:169:TYR:HD1	2.01	0.58
3:B:939:HIS:NE2	3:B:983:GLU:OE1	2.33	0.58
4:C:91:GLU:O	4:C:92:GLU:HG3	2.02	0.58
10:I:60:HIS:O	10:I:60:HIS:CG	2.57	0.58
16:M:419:CYS:H	16:M:564:ARG:N	2.00	0.58
1:A:79:THR:HA	3:B:1072:ARG:HH22	1.69	0.58
3:B:665:ILE:HG23	3:B:669:GLU:HB3	1.85	0.58
16:M:519:PHE:O	16:M:519:PHE:CD2	2.57	0.58
3:B:1144:THR:OG1	3:B:1145:GLN:OE1	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:260:GLN:HB2	12:K:91:ILE:HG21	1.85	0.58
6:E:112:PRO:HA	6:E:115:LYS:HD3	1.86	0.58
9:H:7:GLU:HG3	9:H:59:VAL:HG22	1.86	0.58
10:I:119:CYS:SG	10:I:120:GLY:N	2.77	0.58
3:B:149:ILE:HG22	3:B:440:ILE:HG21	1.85	0.57
3:B:851:ASP:OD2	13:L:17:TYR:OH	2.22	0.57
4:C:154:ARG:HD3	11:J:64:PRO:HD3	1.86	0.57
8:G:119:PHE:HB2	8:G:128:TYR:HE1	1.69	0.57
1:A:190:ARG:HA	1:A:190:ARG:NH1	2.19	0.57
16:M:160:ARG:CG	16:M:160:ARG:HH11	2.17	0.57
1:A:1139:LEU:HD11	1:A:1342:SER:H	1.69	0.57
1:A:1177:TYR:H	10:I:51:SER:HB3	1.69	0.57
1:A:362:SER:HB2	3:B:1084:LEU:HD12	1.85	0.57
1:A:460:ARG:NH2	2:P:55:U:O2'	2.37	0.57
1:A:465:HIS:CD2	1:A:467:MET:HB2	2.39	0.57
1:A:1005:HIS:HD2	1:A:1006:PRO:HD2	1.70	0.57
3:B:37:LYS:HB3	3:B:41:ARG:HG3	1.85	0.57
3:B:92:TYR:HB2	3:B:125:TYR:HB2	1.85	0.57
16:M:420:THR:H	16:M:564:ARG:CA	2.18	0.57
1:A:508:SER:HB3	1:A:511:THR:HG22	1.86	0.57
1:A:577:PRO:HG3	1:A:586:TRP:CZ2	2.39	0.57
16:M:324:ASN:HB2	16:M:407:PRO:HD3	1.86	0.57
8:G:110:ARG:HA	8:G:113:ILE:HD12	1.86	0.56
1:A:734:ARG:HH21	10:I:105:GLU:HB3	1.70	0.56
1:A:1184:THR:HG23	1:A:1187:ALA:H	1.71	0.56
8:G:78:ARG:HE	8:G:80:PHE:HE1	1.53	0.56
12:K:85:GLU:HA	12:K:88:THR:HG22	1.87	0.56
16:M:90:GLN:HA	16:M:90:GLN:NE2	2.20	0.56
1:A:1282:ASP:OD1	1:A:1282:ASP:N	2.38	0.56
3:B:721:ARG:HD2	3:B:975:ARG:HB3	1.86	0.56
12:K:17:LYS:O	12:K:36:ASN:ND2	2.30	0.56
16:M:29:THR:O	16:M:30:MET:HG3	2.06	0.56
1:A:593:SER:HB3	1:A:634:GLU:HG2	1.87	0.56
16:M:63:LEU:HD23	16:M:85:LYS:HB3	1.88	0.56
16:M:530:ARG:HH11	16:M:530:ARG:CG	2.17	0.56
3:B:626:LEU:HG	3:B:698:ILE:HG12	1.87	0.56
16:M:364:ILE:HD11	16:M:367:PHE:HB2	1.88	0.56
16:M:467:VAL:HA	16:M:537:ASN:HD21	1.71	0.56
16:M:518:LYS:HB3	16:M:527:MET:HB2	1.87	0.56
1:A:566:PHE:HB2	1:A:675:VAL:HG12	1.87	0.56
10:I:60:HIS:O	10:I:60:HIS:CD2	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:10:CYS:SG	11:J:42:ARG:NE	2.79	0.56
1:A:1473:LEU:HD22	7:F:68:THR:HG21	1.88	0.56
16:M:171:LYS:N	16:M:171:LYS:HD2	2.20	0.56
16:M:70:THR:HG23	16:M:73:PHE:HE2	1.71	0.56
1:A:539:GLN:HB3	3:B:970:HIS:CD2	2.41	0.55
1:A:561:MET:HE3	12:K:59:ALA:H	1.71	0.55
3:B:348:LEU:O	3:B:361:LYS:NZ	2.39	0.55
3:B:956:PHE:HB3	3:B:962:THR:HG22	1.87	0.55
11:J:18:TRP:NE1	11:J:54:ASP:OD2	2.39	0.55
3:B:792:ASP:OD2	3:B:975:ARG:NH2	2.37	0.55
5:D:33:LEU:HD11	5:D:84:ARG:HH12	1.69	0.55
6:E:19:GLN:OE1	6:E:138:ASN:ND2	2.39	0.55
16:M:10:TRP:CE3	16:M:11:LEU:HD23	2.41	0.55
16:M:40:ALA:O	16:M:44:ARG:N	2.38	0.55
1:A:82:PRO:O	3:B:1160:GLN:NE2	2.33	0.55
1:A:552:ASP:HB3	9:H:22:PHE:HB3	1.88	0.55
8:G:43:GLY:HA3	8:G:78:ARG:HB2	1.89	0.55
3:B:347:MET:SD	3:B:361:LYS:HD3	2.46	0.55
16:M:15:ARG:O	16:M:28:LYS:HE2	2.07	0.55
16:M:132:ARG:HH11	16:M:132:ARG:HG3	1.71	0.55
16:M:419:CYS:O	16:M:560:GLU:HB2	2.06	0.55
1:A:1141:VAL:HA	1:A:1357:THR:HG23	1.89	0.55
1:A:1473:LEU:HD23	7:F:104:ILE:HG21	1.88	0.55
3:B:230:ARG:NE	3:B:231:PRO:HD2	2.12	0.55
4:C:38:PHE:HE1	4:C:245:VAL:HA	1.72	0.55
4:C:246:LEU:HD22	12:K:106:ARG:HE	1.72	0.55
1:A:428:ASP:OD1	1:A:430:ARG:HG2	2.06	0.55
5:D:60:VAL:HG13	8:G:103:PRO:HG3	1.88	0.55
16:M:141:LEU:HB3	16:M:147:TRP:HB2	1.88	0.55
16:M:142:VAL:HG23	16:M:152:ALA:HB3	1.88	0.55
1:A:539:GLN:HA	1:A:774:ALA:HB1	1.89	0.55
6:E:9:ARG:HG3	6:E:136:LEU:HD21	1.88	0.55
16:M:10:TRP:HE3	16:M:11:LEU:HD23	1.72	0.55
16:M:176:ARG:HA	16:M:176:ARG:NE	2.19	0.55
16:M:291:VAL:N	16:M:416:PHE:O	2.36	0.55
1:A:428:ASP:OD1	1:A:429:LEU:N	2.40	0.55
5:D:16:ASP:OD2	5:D:18:SER:OG	2.22	0.55
9:H:20:LYS:HE2	9:H:23:ASP:HA	1.89	0.55
15:T:21:DA:H2"	15:T:22:DA:H5'	1.88	0.55
16:M:126:SER:H	16:M:133:THR:HG1	1.53	0.55
16:M:490:TYR:HB3	16:M:497:PRO:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ASN:HB3	1:A:469:MET:HG3	1.89	0.55
1:A:576:GLN:HB3	9:H:93:TYR:CE2	2.42	0.55
1:A:1073:GLU:OE2	1:A:1077:ASN:ND2	2.40	0.55
9:H:39:LEU:HD12	9:H:125:LEU:HD13	1.89	0.55
9:H:103:GLU:HB3	9:H:109:ALA:HB2	1.88	0.55
16:M:420:THR:H	16:M:564:ARG:N	2.05	0.55
3:B:1040:GLN:HE22	4:C:197:TYR:HA	1.71	0.54
9:H:92:MET:HB2	9:H:143:LEU:HD13	1.89	0.54
10:I:100:HIS:ND1	10:I:100:HIS:O	2.40	0.54
1:A:184:CYS:HB3	1:A:187:TYR:HD1	1.73	0.54
10:I:61:GLU:O	10:I:61:GLU:HG2	2.07	0.54
2:P:44:A:OP1	2:P:44:A:H4'	2.08	0.54
13:L:35:ARG:NH2	13:L:40:GLY:HA3	2.22	0.54
1:A:1169:VAL:HG12	1:A:1216:LEU:HD12	1.89	0.54
16:M:132:ARG:HG2	16:M:136:LEU:HG	1.90	0.54
16:M:270:GLY:HA2	16:M:301:MET:HE1	1.90	0.54
4:C:33:SER:HB2	12:K:45:ILE:HD11	1.89	0.54
12:K:56:VAL:HG22	12:K:77:THR:HG22	1.90	0.54
1:A:902:GLU:OE2	1:A:985:ARG:NH1	2.39	0.54
3:B:585:ASN:OD1	3:B:588:ARG:NH2	2.41	0.54
6:E:26:TYR:CD1	6:E:64:HIS:HA	2.41	0.54
7:F:51:ARG:NH1	7:F:122:GLU:OE1	2.40	0.54
16:M:153:VAL:CG1	16:M:173:LEU:HD13	2.23	0.54
16:M:424:LEU:HB2	16:M:559:PHE:CE2	2.43	0.54
3:B:1016:SER:HB2	3:B:1022:LEU:HD23	1.89	0.54
3:B:1142:ASN:HD22	3:B:1145:GLN:HG2	1.72	0.54
9:H:96:VAL:HA	9:H:116:VAL:HA	1.89	0.54
11:J:35:LEU:HD13	11:J:46:ARG:HB3	1.90	0.54
5:D:34:ASN:O	5:D:68:THR:OG1	2.25	0.54
16:M:18:GLN:O	16:M:159:ALA:HB1	2.08	0.54
16:M:98:PRO:HD3	16:M:132:ARG:HH11	1.73	0.54
16:M:132:ARG:HG2	16:M:132:ARG:O	2.08	0.53
1:A:892:GLY:HA3	1:A:1396:ARG:HG3	1.89	0.53
16:M:545:VAL:HA	16:M:548:SER:HB2	1.90	0.53
1:A:809:HIS:CD2	3:B:675:LEU:HD22	2.44	0.53
1:A:1022:ILE:N	1:A:1034:GLN:OE1	2.39	0.53
16:M:241:VAL:HG22	16:M:322:VAL:HG22	1.90	0.53
16:M:424:LEU:H	16:M:559:PHE:HE2	1.55	0.53
16:M:459:TRP:CG	16:M:558:LEU:HD13	2.42	0.53
3:B:26:CYS:O	3:B:30:ILE:HG12	2.09	0.53
16:M:59:VAL:HG12	16:M:59:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:66:ASP:HA	16:M:125:HIS:CD2	2.44	0.53
16:M:473:ILE:HA	16:M:487:GLY:HA2	1.90	0.53
1:A:1104:LEU:HA	1:A:1121:VAL:HG23	1.90	0.53
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.90	0.53
1:A:1212:LEU:HB2	1:A:1285:LEU:HD21	1.89	0.53
16:M:516:GLU:HB2	16:M:530:ARG:HB2	1.90	0.53
1:A:592:PHE:HA	1:A:595:ILE:HD12	1.91	0.53
3:B:270:ILE:HG13	3:B:305:LEU:HA	1.91	0.53
16:M:26:PRO:CB	16:M:160:ARG:HB2	2.38	0.53
16:M:424:LEU:HB2	16:M:559:PHE:CZ	2.44	0.53
1:A:189:PRO:HB2	1:A:200:ALA:HB1	1.91	0.53
1:A:606:HIS:CE1	1:A:641:CYS:HB3	2.44	0.53
1:A:1305:SER:OG	1:A:1339:ASP:HB3	2.09	0.53
2:P:38:A:H4'	2:P:38:A:OP2	2.09	0.53
16:M:532:ASP:OD1	16:M:532:ASP:N	2.36	0.53
16:M:551:ASN:O	16:M:553:VAL:HG23	2.09	0.53
3:B:635:LEU:HD21	3:B:640:ILE:HD11	1.91	0.53
1:A:469:MET:SD	3:B:1094:GLN:NE2	2.80	0.52
1:A:1052:ARG:NE	1:A:1056:GLU:OE1	2.37	0.52
2:P:37:A:H2'	2:P:37:A:N3	2.24	0.52
16:M:61:MET:HE1	16:M:84:ILE:HD13	1.90	0.52
16:M:148:SER:HB2	16:M:151:ALA:HB3	1.90	0.52
1:A:76:GLY:HA2	1:A:80:GLU:HG3	1.90	0.52
8:G:11:ILE:HD11	8:G:30:LEU:HD13	1.90	0.52
3:B:735:VAL:HG11	11:J:55:LEU:HD21	1.91	0.52
9:H:91:VAL:HG22	9:H:144:LEU:HD13	1.91	0.52
16:M:469:PHE:O	16:M:514:ILE:HA	2.09	0.52
1:A:349:ARG:HH22	3:B:1070:LEU:HD21	1.73	0.52
3:B:1062:ARG:HE	3:B:1065:GLY:H	1.58	0.52
12:K:38:GLU:OE2	12:K:42:LEU:HD23	2.10	0.52
16:M:422:ARG:HG3	16:M:425:LEU:HD21	1.91	0.52
10:I:80:ARG:HG3	10:I:95:VAL:HG12	1.90	0.52
3:B:240:LEU:O	3:B:254:GLN:NE2	2.42	0.52
1:A:743:ARG:HA	1:A:743:ARG:HH11	1.74	0.52
1:A:419:ILE:HG23	1:A:427:ILE:HB	1.91	0.52
1:A:1115:LYS:HD2	1:A:1115:LYS:O	2.10	0.52
16:M:174:PHE:HB3	16:M:180:ILE:HA	1.92	0.52
1:A:999:ARG:NH1	9:H:103:GLU:OE1	2.43	0.52
13:L:19:CYS:SG	13:L:44:MET:HE1	2.50	0.52
1:A:931:ARG:NH1	1:A:936:GLU:OE2	2.42	0.51
1:A:1115:LYS:HE2	1:A:1117:VAL:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:68:GLN:HE22	3:B:81:PRO:HD2	1.76	0.51
1:A:349:ARG:HE	3:B:1157:LEU:HD22	1.75	0.51
1:A:481:THR:H	1:A:483:ARG:NH1	2.08	0.51
3:B:912:ASN:OD1	3:B:916:TYR:N	2.41	0.51
8:G:108:ILE:HD11	8:G:145:LEU:HD22	1.91	0.51
1:A:875:TYR:HA	1:A:1083:PRO:HB3	1.92	0.51
3:B:1157:LEU:O	3:B:1161:GLU:OE1	2.29	0.51
8:G:82:GLY:HA2	8:G:146:LYS:HE2	1.91	0.51
1:A:576:GLN:NE2	9:H:74:GLU:O	2.42	0.51
1:A:1027:ASP:OD1	1:A:1027:ASP:N	2.43	0.51
8:G:47:ALA:O	8:G:75:ILE:N	2.43	0.51
16:M:459:TRP:CZ2	16:M:553:VAL:HG12	2.45	0.51
3:B:180:ASP:OD1	3:B:472:ARG:NH2	2.44	0.51
3:B:743:ARG:NE	3:B:745:ASP:OD2	2.34	0.51
3:B:821:LYS:HG3	3:B:825:GLN:NE2	2.26	0.51
4:C:263:LEU:HD22	12:K:87:PHE:HD2	1.75	0.51
16:M:459:TRP:CD1	16:M:558:LEU:HD13	2.45	0.51
1:A:1097:GLU:HB3	1:A:1098:PRO:HD3	1.93	0.51
16:M:299:ARG:NH2	16:M:343:ASP:OD2	2.43	0.51
16:M:418:ILE:H	16:M:565:CYS:H	1.59	0.51
1:A:187:TYR:HD2	1:A:187:TYR:C	2.13	0.51
1:A:358:ARG:HA	3:B:1085:ARG:HA	1.91	0.51
3:B:873:LEU:HD12	3:B:874:PRO:HD2	1.92	0.51
3:B:1038:THR:HA	4:C:195:THR:HA	1.93	0.51
8:G:12:LEU:HD22	8:G:65:PHE:CE2	2.45	0.51
1:A:381:PRO:HB3	1:A:480:SER:HA	1.93	0.51
3:B:274:ARG:NH1	3:B:311:ILE:O	2.42	0.51
3:B:782:ILE:HG12	3:B:967:ILE:HD11	1.91	0.51
4:C:60:HIS:CE1	4:C:63:PHE:HB2	2.46	0.51
7:F:46:GLN:HB3	7:F:50:LYS:HG3	1.93	0.51
16:M:98:PRO:HD3	16:M:132:ARG:NH1	2.26	0.51
10:I:75:ASP:HB3	10:I:78:LEU:HD23	1.93	0.51
16:M:559:PHE:HA	16:M:562:ILE:HG12	1.92	0.51
1:A:87:HIS:CD2	1:A:89:GLU:HG3	2.45	0.51
1:A:561:MET:CE	12:K:59:ALA:H	2.23	0.51
16:M:312:MET:O	16:M:319:VAL:HA	2.10	0.51
16:M:376:ASP:O	16:M:380:ARG:HG3	2.11	0.51
1:A:397:PHE:HZ	1:A:1486:ILE:HG12	1.75	0.50
1:A:510:GLU:OE2	3:B:1101:GLN:NE2	2.43	0.50
1:A:623:PRO:HA	9:H:27:ARG:HH21	1.76	0.50
1:A:691:ASP:O	1:A:764:ASN:ND2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:513:GLU:CD	3:B:525:ASN:HD22	2.14	0.50
3:B:826:GLU:H	3:B:872:THR:HG22	1.76	0.50
14:N:26:DC:H2'	14:N:27:DT:C6	2.46	0.50
1:A:693:ILE:HD12	3:B:1023:ARG:HE	1.76	0.50
1:A:917:GLU:OE2	1:A:921:ARG:NH1	2.44	0.50
8:G:45:VAL:HA	8:G:76:VAL:HG12	1.93	0.50
9:H:32:SER:OG	9:H:36:LYS:N	2.44	0.50
3:B:35:ASP:OD2	3:B:646:ARG:NH1	2.40	0.50
5:D:37:VAL:HG21	8:G:2:PHE:HD1	1.76	0.50
1:A:316:THR:HG21	1:A:328:ALA:HB2	1.93	0.50
16:M:342:LEU:HD13	16:M:361:ILE:HD13	1.94	0.50
1:A:187:TYR:C	1:A:187:TYR:CD2	2.84	0.50
3:B:760:THR:OG1	3:B:764:MET:HG3	2.12	0.50
8:G:33:GLU:OE2	8:G:34:VAL:HG13	2.11	0.50
16:M:113:PHE:O	16:M:115:GLU:N	2.45	0.50
16:M:476:MET:HE3	16:M:476:MET:O	2.11	0.50
1:A:189:PRO:HB3	1:A:202:TRP:CE2	2.47	0.50
1:A:201:GLU:HG3	1:A:213:LYS:HB3	1.93	0.50
1:A:421:ARG:HH21	1:A:437:ASP:HB2	1.77	0.50
16:M:418:ILE:O	16:M:561:PHE:HA	2.11	0.50
16:M:23:ARG:C	16:M:23:ARG:HH11	2.14	0.50
16:M:135:PHE:CG	16:M:173:LEU:HG	2.46	0.50
16:M:153:VAL:HG11	16:M:174:PHE:CD2	2.47	0.50
16:M:363:ASP:OD1	16:M:364:ILE:N	2.43	0.50
16:M:518:LYS:O	16:M:520:GLU:N	2.44	0.50
1:A:460:ARG:HD2	1:A:494:ALA:HB2	1.93	0.50
1:A:1474:LEU:HA	8:G:57:GLY:O	2.11	0.50
3:B:1091:ARG:HG2	3:B:1103:LEU:HD11	1.93	0.50
3:B:1040:GLN:NE2	4:C:197:TYR:HA	2.26	0.50
16:M:97:CYS:HB3	16:M:169:TYR:HA	1.94	0.50
16:M:135:PHE:C	16:M:135:PHE:CD1	2.85	0.50
16:M:294:LYS:H	16:M:440:LEU:HA	1.77	0.50
1:A:31:LEU:HD23	1:A:252:VAL:HG13	1.94	0.49
6:E:24:ARG:NH1	6:E:184:GLY:HA3	2.26	0.49
16:M:102:ASN:C	16:M:102:ASN:ND2	2.66	0.49
3:B:42:GLN:HG2	3:B:43:GLN:N	2.26	0.49
16:M:517:CYS:HA	16:M:526:PHE:HA	1.94	0.49
16:M:524:TRP:N	16:M:524:TRP:HD1	2.10	0.49
1:A:97:VAL:HG13	1:A:315:ALA:HB1	1.94	0.49
1:A:367:ILE:HG22	1:A:482:PHE:HB2	1.93	0.49
1:A:1209:PRO:HB3	10:I:33:ARG:HH21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:86:LEU:HD23	3:B:130:LYS:HB3	1.95	0.49
13:L:22:CYS:SG	13:L:38:GLU:HB2	2.52	0.49
14:N:43:DC:H2"	14:N:44:DT:H5'	1.94	0.49
16:M:417:ASP:HB2	16:M:563:ASP:O	2.12	0.49
1:A:1463:LEU:HD21	1:A:1469:GLY:HA3	1.94	0.49
10:I:11:PHE:HA	10:I:55:VAL:HG11	1.94	0.49
16:M:50:LEU:O	16:M:54:LEU:HB3	2.13	0.49
16:M:169:TYR:HD1	16:M:169:TYR:H	1.59	0.49
1:A:858:GLY:HA2	1:A:861:GLN:HE22	1.78	0.49
16:M:29:THR:C	16:M:30:MET:HG3	2.33	0.49
3:B:826:GLU:N	3:B:872:THR:HG22	2.28	0.49
7:F:80:MET:HG3	7:F:103:PRO:HD3	1.94	0.49
16:M:232:PHE:HE1	16:M:312:MET:HG3	1.78	0.49
1:A:114:CYS:O	1:A:227:ARG:NH1	2.46	0.49
3:B:626:LEU:HD23	3:B:662:VAL:HG12	1.93	0.49
5:D:44:ARG:NH1	8:G:48:VAL:H	2.10	0.49
9:H:98:ARG:HB3	9:H:115:TYR:HB2	1.93	0.49
16:M:142:VAL:HG22	16:M:149:ILE:HA	1.95	0.49
16:M:290:LYS:HG2	16:M:415:PHE:CD2	2.44	0.49
16:M:468:ASP:HB2	16:M:536:PRO:HA	1.94	0.49
1:A:461:GLN:NE2	3:B:1090:GLU:OE2	2.39	0.49
3:B:604:ILE:HG12	3:B:668:LEU:HB3	1.95	0.49
1:A:486:LEU:HB3	1:A:538:VAL:HG11	1.94	0.48
3:B:497:LYS:HG3	3:B:498:PRO:HD3	1.95	0.48
3:B:719:SER:OG	3:B:720:PRO:HD3	2.13	0.48
16:M:35:TYR:N	16:M:35:TYR:CD2	2.81	0.48
16:M:126:SER:N	16:M:133:THR:OG1	2.35	0.48
1:A:756:ALA:HB2	1:A:786:ALA:HB2	1.95	0.48
6:E:102:ALA:HB3	6:E:127:LEU:HD23	1.95	0.48
16:M:58:LYS:HZ2	16:M:58:LYS:HA	1.78	0.48
1:A:460:ARG:HB2	1:A:501:MET:SD	2.54	0.48
3:B:483:ARG:HH12	3:B:528:LEU:HA	1.77	0.48
3:B:934:LYS:HG2	3:B:1051:LEU:HD12	1.95	0.48
6:E:194:ILE:HG13	6:E:204:ILE:HG12	1.96	0.48
7:F:54:THR:O	7:F:108:ARG:NH1	2.40	0.48
1:A:457:ILE:HD11	1:A:515:ILE:HD12	1.96	0.48
3:B:780:VAL:HG12	3:B:965:ILE:HB	1.95	0.48
3:B:856:PRO:HD2	13:L:47:LYS:O	2.13	0.48
4:C:56:SER:HB2	4:C:158:GLU:H	1.78	0.48
1:A:520:MET:HB3	1:A:522:PRO:HD2	1.95	0.48
3:B:502:HIS:N	3:B:505:LEU:HD12	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:679:PRO:HA	3:B:683:GLN:OE1	2.13	0.48
3:B:798:ARG:HB2	3:B:950:ARG:HA	1.95	0.48
3:B:1112:ASP:OD1	3:B:1112:ASP:N	2.46	0.48
8:G:91:GLN:HB3	8:G:98:PHE:HB2	1.95	0.48
16:M:58:LYS:H	16:M:58:LYS:HZ3	1.62	0.48
1:A:1005:HIS:CD2	1:A:1006:PRO:HD2	2.47	0.48
1:A:1212:LEU:HB3	1:A:1259:ILE:HB	1.95	0.48
3:B:91:ILE:HD11	3:B:124:LEU:HD21	1.94	0.48
3:B:235:ILE:HD13	3:B:348:LEU:HD12	1.96	0.48
9:H:118:TYR:CZ	9:H:143:LEU:HD12	2.48	0.48
16:M:10:TRP:H	16:M:10:TRP:HD1	1.55	0.48
16:M:28:LYS:CD	16:M:28:LYS:H	2.27	0.48
1:A:1295:ASP:OD1	1:A:1295:ASP:N	2.47	0.48
3:B:807:ARG:HA	3:B:929:PRO:HD3	1.96	0.48
5:D:44:ARG:HH12	8:G:48:VAL:H	1.59	0.48
6:E:15:LYS:HE2	6:E:35:GLN:H	1.78	0.48
16:M:130:PHE:HE1	16:M:161:PRO:O	1.96	0.48
16:M:509:GLN:OE1	16:M:509:GLN:HA	2.12	0.48
1:A:74:CYS:HB3	3:B:1127:ILE:HG23	1.96	0.48
3:B:333:GLU:OE2	3:B:334:LYS:HE3	2.13	0.48
3:B:728:MET:HE1	3:B:940:GLY:HA2	1.95	0.48
4:C:4:ALA:HB1	12:K:97:GLU:OE1	2.13	0.48
16:M:508:LYS:HB2	16:M:508:LYS:HE3	1.49	0.48
1:A:743:ARG:HA	1:A:743:ARG:NH1	2.29	0.48
16:M:360:LEU:HD13	16:M:413:LYS:HG3	1.95	0.48
1:A:70:ARG:HE	3:B:1131:ARG:HH12	1.62	0.47
1:A:1130:ILE:HG13	1:A:1411:LEU:HB3	1.96	0.47
3:B:218:THR:HA	3:B:238:SER:HA	1.96	0.47
3:B:470:LEU:HD11	3:B:478:THR:HG23	1.95	0.47
3:B:1135:TYR:HB3	3:B:1146:ILE:HD13	1.96	0.47
8:G:107:PHE:HE2	16:M:118:PRO:CG	2.25	0.47
13:L:36:CYS:HB3	13:L:41:TYR:H	1.79	0.47
1:A:930:LEU:HB3	1:A:939:VAL:HG13	1.96	0.47
3:B:116:ARG:NH1	3:B:118:LEU:HD11	2.29	0.47
6:E:34:ASP:N	6:E:34:ASP:OD1	2.47	0.47
1:A:564:LEU:HA	1:A:567:LEU:HD13	1.95	0.47
3:B:205:VAL:O	3:B:371:ARG:NH1	2.47	0.47
4:C:55:ASN:ND2	4:C:61:ASP:OD1	2.39	0.47
4:C:184:PHE:CD1	4:C:231:TYR:HE1	2.32	0.47
8:G:91:GLN:NE2	8:G:92:VAL:O	2.47	0.47
16:M:113:PHE:O	16:M:114:ASN:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:HA	1:A:186:ARG:HD3	1.45	0.47
1:A:458:PHE:HE2	1:A:484:LEU:HD13	1.78	0.47
1:A:1170:THR:HG23	10:I:58:ILE:HG21	1.96	0.47
9:H:14:ASP:HB2	9:H:29:HIS:HB2	1.96	0.47
10:I:78:LEU:HD12	10:I:97:PHE:HB3	1.96	0.47
1:A:997:ASN:ND2	9:H:136:GLU:OE1	2.47	0.47
16:M:291:VAL:HG12	16:M:416:PHE:O	2.14	0.47
16:M:442:PHE:O	16:M:456:ILE:HG23	2.15	0.47
16:M:520:GLU:HB3	16:M:525:VAL:HG13	1.96	0.47
1:A:539:GLN:HG2	1:A:775:LYS:HB2	1.96	0.47
1:A:595:ILE:HD11	1:A:675:VAL:HG21	1.95	0.47
1:A:977:VAL:HG21	1:A:1040:LEU:HD21	1.95	0.47
12:K:4:PRO:HB2	12:K:8:GLU:OE2	2.14	0.47
1:A:1124:LEU:O	1:A:1128:ILE:HG12	2.15	0.47
3:B:237:VAL:HG12	3:B:372:LEU:HD22	1.95	0.47
3:B:294:ASP:OD1	3:B:294:ASP:N	2.43	0.47
3:B:610:ARG:NH1	10:I:71:ASP:OD2	2.48	0.47
3:B:1060:HIS:HB3	3:B:1078:ARG:HE	1.80	0.47
8:G:44:PHE:CE2	8:G:104:MET:HB2	2.43	0.47
1:A:459:ASN:OD1	1:A:502:ASN:HB2	2.15	0.47
1:A:560:VAL:HG21	1:A:586:TRP:HB2	1.96	0.47
3:B:865:VAL:HG12	3:B:895:PHE:CE1	2.50	0.47
16:M:416:PHE:HD2	16:M:563:ASP:HA	1.79	0.47
16:M:467:VAL:HG12	16:M:537:ASN:HD21	1.79	0.47
16:M:555:LYS:HA	16:M:558:LEU:CD2	2.45	0.47
3:B:779:ILE:HG23	3:B:963:PRO:HA	1.97	0.47
4:C:38:PHE:CE1	4:C:245:VAL:HA	2.49	0.47
4:C:221:ASP:OD1	4:C:221:ASP:N	2.48	0.47
5:D:44:ARG:O	5:D:47:GLN:HG3	2.15	0.47
7:F:75:MET:HE2	8:G:15:PRO:HD2	1.96	0.47
10:I:36:LEU:HD11	10:I:45:GLN:HB3	1.96	0.47
12:K:38:GLU:HG3	12:K:39:ASP:N	2.30	0.47
16:M:97:CYS:SG	16:M:172:GLU:OE1	2.72	0.47
16:M:540:ASN:H	16:M:540:ASN:ND2	2.13	0.47
3:B:292:PHE:HA	3:B:298:MET:HE1	1.97	0.47
2:P:43:C:OP1	2:P:43:C:H2'	2.14	0.46
3:B:677:MET:H	3:B:682:LEU:HD12	1.80	0.46
3:B:802:ASP:HB3	4:C:173:HIS:CE1	2.50	0.46
3:B:941:GLN:HE21	3:B:977:THR:HG21	1.81	0.46
16:M:76:ARG:NH1	16:M:76:ARG:HA	2.28	0.46
16:M:289:TYR:N	16:M:418:ILE:HD11	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:533:LYS:HD2	16:M:533:LYS:HA	1.55	0.46
1:A:1216:LEU:HB2	1:A:1255:LEU:HB2	1.97	0.46
3:B:924:ARG:NH1	4:C:60:HIS:HB2	2.30	0.46
12:K:81:TYR:CE2	12:K:86:ALA:HB2	2.51	0.46
16:M:97:CYS:HB3	16:M:169:TYR:CG	2.50	0.46
16:M:291:VAL:O	16:M:415:PHE:HA	2.15	0.46
1:A:364:ARG:HA	1:A:501:MET:O	2.15	0.46
1:A:1164:THR:HB	1:A:1299:GLN:HB2	1.97	0.46
3:B:88:PHE:HD2	3:B:408:PHE:HZ	1.62	0.46
6:E:58:LEU:HD23	6:E:58:LEU:H	1.81	0.46
10:I:27:LYS:N	10:I:36:LEU:O	2.48	0.46
16:M:53:TYR:HD1	16:M:54:LEU:N	2.14	0.46
16:M:62:GLY:N	16:M:120:GLU:HB3	2.30	0.46
7:F:97:LEU:HD11	7:F:125:ILE:HD13	1.97	0.46
16:M:232:PHE:CE1	16:M:312:MET:HG3	2.51	0.46
1:A:358:ARG:HD3	3:B:1085:ARG:HB2	1.96	0.46
1:A:623:PRO:HA	9:H:27:ARG:NH2	2.30	0.46
4:C:175:LYS:HZ2	13:L:57:ALA:HB3	1.80	0.46
6:E:110:MET:SD	6:E:114:ALA:HB3	2.55	0.46
9:H:24:ARG:HG2	9:H:46:GLN:HG3	1.97	0.46
12:K:38:GLU:HG3	12:K:39:ASP:H	1.80	0.46
16:M:20:VAL:HG11	16:M:155:THR:HG23	1.97	0.46
16:M:502:LYS:HB3	16:M:502:LYS:HE3	1.48	0.46
1:A:183:GLY:H	1:A:187:TYR:HE1	1.61	0.46
1:A:1347:LEU:HB3	6:E:137:ILE:HG12	1.96	0.46
1:A:1461:GLY:HA3	3:B:1152:PRO:HD3	1.98	0.46
3:B:54:SER:O	3:B:58:ILE:HG12	2.15	0.46
11:J:8:PHE:H	11:J:48:MET:HE2	1.80	0.46
16:M:6:ILE:HG22	16:M:72:ARG:HH22	1.80	0.46
16:M:63:LEU:HD12	16:M:113:PHE:CD2	2.51	0.46
1:A:62:GLN:HG2	1:A:257:PRO:HA	1.98	0.46
1:A:871:VAL:HG11	1:A:1400:LEU:HD11	1.97	0.46
1:A:1428:MET:HE1	1:A:1456:GLU:N	2.31	0.46
3:B:153:PRO:HG2	3:B:448:LEU:HD12	1.98	0.46
8:G:119:PHE:HB2	8:G:128:TYR:CE1	2.49	0.46
16:M:41:GLU:HA	16:M:44:ARG:HB2	1.98	0.46
3:B:84:TYR:CE1	3:B:423:ILE:HD12	2.43	0.46
3:B:675:LEU:HD21	3:B:697:GLU:HB2	1.97	0.46
3:B:1117:HIS:CE1	3:B:1148:LEU:HD13	2.51	0.46
3:B:1121:LEU:HD11	3:B:1145:GLN:HE21	1.80	0.46
16:M:419:CYS:N	16:M:564:ARG:HB3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:GLU:OE1	1:A:982:ASN:ND2	2.49	0.46
1:A:1311:LEU:HG	1:A:1334:TRP:CZ3	2.51	0.46
3:B:56:GLN:HE21	3:B:60:GLU:HG3	1.81	0.46
12:K:81:TYR:HE2	12:K:86:ALA:HB2	1.80	0.46
16:M:291:VAL:CG1	16:M:562:ILE:HB	2.40	0.46
1:A:108:ARG:NH2	1:A:191:ILE:O	2.42	0.46
1:A:244:ARG:HB3	1:A:247:TRP:CD2	2.51	0.46
1:A:886:VAL:HG23	6:E:171:PRO:HD3	1.98	0.46
3:B:403:LEU:HD23	3:B:444:LEU:HD13	1.98	0.46
3:B:834:ARG:HA	3:B:840:MET:CE	2.46	0.46
1:A:330:GLN:NE2	1:A:334:ARG:HB2	2.31	0.45
1:A:1211:LEU:HD22	1:A:1258:ARG:HH21	1.81	0.45
1:A:1372:GLU:OE2	6:E:195:ARG:NH1	2.50	0.45
3:B:26:CYS:O	3:B:29:VAL:HG12	2.16	0.45
3:B:56:GLN:NE2	3:B:89:GLU:O	2.44	0.45
3:B:93:LEU:HD12	3:B:124:LEU:HD13	1.97	0.45
3:B:714:PRO:HG2	3:B:1001:PRO:HB3	1.97	0.45
1:A:556:GLU:HB3	1:A:559:GLU:OE1	2.15	0.45
3:B:116:ARG:HG3	13:L:43:ILE:HD11	1.98	0.45
3:B:117:ASN:HA	3:B:189:GLY:HA3	1.98	0.45
5:D:126:GLU:O	5:D:130:ILE:HG12	2.16	0.45
8:G:59:ILE:HG13	8:G:66:VAL:HG23	1.98	0.45
12:K:35:ILE:HB	12:K:71:ILE:HG12	1.98	0.45
16:M:140:PHE:CD1	16:M:140:PHE:C	2.90	0.45
1:A:400:ASP:OD2	1:A:401:ARG:N	2.48	0.45
1:A:556:GLU:OE1	1:A:583:ARG:NH2	2.50	0.45
3:B:991:ALA:HB1	11:J:43:TYR:HB2	1.97	0.45
9:H:2:ALA:O	9:H:84:ARG:NH2	2.50	0.45
15:T:11:DA:H2"	15:T:12:DT:H5'	1.98	0.45
3:B:330:VAL:HG12	3:B:331:THR:HG23	1.98	0.45
12:K:99:SER:O	12:K:103:GLU:OE1	2.34	0.45
1:A:253:LEU:HD12	1:A:254:PRO:HD2	1.97	0.45
1:A:321:GLU:CD	1:A:321:GLU:N	2.69	0.45
1:A:901:VAL:HA	1:A:980:PRO:HA	1.99	0.45
3:B:760:THR:O	3:B:999:ALA:N	2.50	0.45
3:B:888:THR:OG1	3:B:889:LYS:N	2.48	0.45
9:H:88:PHE:CD2	9:H:144:LEU:HD12	2.52	0.45
14:N:24:DA:H2"	14:N:25:DG:H5"	1.97	0.45
16:M:27:LEU:H	16:M:27:LEU:HD23	1.81	0.45
16:M:31:LEU:O	16:M:31:LEU:CD1	2.64	0.45
16:M:392:ARG:NH2	16:M:406:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:TYR:HB2	1:A:447:GLU:HB2	1.99	0.45
1:A:695:ASP:N	1:A:695:ASP:OD1	2.48	0.45
1:A:981:CYS:HB3	1:A:986:MET:HE1	1.99	0.45
1:A:1118:THR:HG22	1:A:1118:THR:O	2.17	0.45
1:A:1429:LYS:HB2	1:A:1438:VAL:HG11	1.99	0.45
3:B:832:PRO:HB2	3:B:840:MET:SD	2.56	0.45
7:F:55:PRO:HB2	7:F:124:ILE:HD13	1.99	0.45
7:F:69:ARG:O	7:F:73:ILE:HG12	2.17	0.45
14:N:28:DT:H2"	14:N:29:DA:C8	2.52	0.45
16:M:30:MET:HB2	16:M:74:TYR:CD1	2.51	0.45
16:M:290:LYS:HA	16:M:416:PHE:O	2.17	0.45
2:P:41:C:H5'	2:P:41:C:C6	2.52	0.45
3:B:591:ARG:HD3	3:B:603:MET:SD	2.57	0.45
16:M:34:ARG:HD2	16:M:34:ARG:C	2.37	0.45
16:M:39:VAL:HG12	16:M:44:ARG:HG3	1.99	0.45
16:M:90:GLN:HA	16:M:90:GLN:HE21	1.78	0.45
16:M:419:CYS:N	16:M:564:ARG:CB	2.73	0.45
1:A:79:THR:HA	3:B:1072:ARG:NH2	2.32	0.45
1:A:1239:PHE:HB3	1:A:1243:LEU:HD23	1.98	0.45
3:B:155:MET:HB3	3:B:185:PHE:CD1	2.52	0.45
3:B:508:MET:HE3	3:B:621:ILE:HG12	1.98	0.45
8:G:44:PHE:N	8:G:77:PHE:O	2.48	0.45
11:J:43:TYR:HA	11:J:46:ARG:HD3	1.97	0.45
16:M:31:LEU:HA	16:M:31:LEU:HD22	1.21	0.45
16:M:302:MET:HA	16:M:311:PHE:O	2.17	0.45
16:M:418:ILE:N	16:M:564:ARG:N	2.65	0.45
1:A:459:ASN:HD22	1:A:469:MET:CE	2.30	0.45
1:A:763:TYR:HD2	4:C:198:PRO:HB3	1.82	0.45
3:B:561:ILE:HD11	3:B:573:TRP:CZ2	2.52	0.45
3:B:936:ALA:HA	3:B:942:LYS:HA	1.99	0.45
3:B:1032:PHE:O	4:C:32:ASN:ND2	2.49	0.45
1:A:339:LEU:HD22	3:B:1161:GLU:HB2	1.99	0.45
8:G:83:GLU:N	8:G:83:GLU:OE1	2.50	0.45
15:T:20:DT:H2"	15:T:21:DA:C8	2.52	0.45
16:M:54:LEU:HD23	16:M:55:LYS:N	2.32	0.45
16:M:112:ARG:HH11	16:M:112:ARG:HG2	1.82	0.45
1:A:680:LEU:O	1:A:684:GLY:N	2.48	0.44
1:A:1286:ARG:HH21	10:I:54:TYR:HB2	1.82	0.44
2:P:37:A:H2'	2:P:37:A:OP1	2.18	0.44
3:B:670:GLU:HA	3:B:673:VAL:HG12	1.99	0.44
6:E:45:GLY:HA3	6:E:53:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:93:TYR:OH	9:H:140:ARG:HD3	2.18	0.44
16:M:31:LEU:HD11	16:M:39:VAL:HG11	1.99	0.44
1:A:26:LEU:HD12	3:B:1166:SER:HA	1.98	0.44
1:A:99:PHE:O	1:A:103:THR:N	2.45	0.44
1:A:290:LEU:HD11	1:A:306:ASP:HB3	2.00	0.44
1:A:527:THR:HG22	1:A:532:ARG:O	2.17	0.44
1:A:613:GLU:OE2	1:A:623:PRO:HD2	2.17	0.44
1:A:1216:LEU:HD23	1:A:1257:LEU:HD23	1.99	0.44
3:B:789:ASN:ND2	3:B:966:ILE:HG22	2.32	0.44
3:B:1108:PHE:HD1	3:B:1152:PRO:HG3	1.82	0.44
12:K:82:SER:HB3	12:K:85:GLU:HG2	1.99	0.44
1:A:659:GLU:OE2	1:A:985:ARG:NE	2.50	0.44
1:A:686:THR:OG1	1:A:687:ILE:N	2.50	0.44
5:D:33:LEU:HD12	5:D:80:ILE:HD12	1.99	0.44
16:M:6:ILE:HB	16:M:10:TRP:HB3	1.99	0.44
16:M:115:GLU:HA	16:M:118:PRO:HG3	2.00	0.44
1:A:655:ILE:HG12	1:A:985:ARG:HH11	1.82	0.44
1:A:904:GLN:NE2	1:A:981:CYS:O	2.51	0.44
5:D:48:ASN:ND2	5:D:57:LEU:HG	2.33	0.44
12:K:49:GLN:HB2	12:K:94:LEU:HD21	2.00	0.44
16:M:112:ARG:HG2	16:M:112:ARG:NH1	2.33	0.44
16:M:160:ARG:HH11	16:M:160:ARG:HG3	1.82	0.44
1:A:274:ASP:OD1	1:A:275:ASP:N	2.51	0.44
16:M:89:LEU:HD12	16:M:89:LEU:HA	1.77	0.44
16:M:300:TYR:CE1	16:M:314:ASP:HB3	2.53	0.44
3:B:897:ARG:HB2	3:B:897:ARG:NH1	2.33	0.44
3:B:956:PHE:CE2	4:C:184:PHE:HB3	2.52	0.44
4:C:40:ALA:HB1	4:C:171:LYS:HG3	2.00	0.44
5:D:134:ILE:O	5:D:138:ARG:HG3	2.18	0.44
6:E:84:ILE:HA	6:E:87:ILE:HG12	2.00	0.44
16:M:101:GLU:OE2	16:M:101:GLU:O	2.36	0.44
1:A:927:GLU:O	1:A:931:ARG:HG2	2.17	0.44
3:B:483:ARG:HB3	3:B:526:LEU:HB3	2.00	0.44
3:B:692:THR:HG21	10:I:80:ARG:NE	2.31	0.44
4:C:40:ALA:O	4:C:170:GLY:N	2.46	0.44
6:E:84:ILE:O	6:E:88:LYS:HG2	2.18	0.44
9:H:91:VAL:HG13	9:H:144:LEU:HD22	2.00	0.44
16:M:67:LEU:HD11	16:M:124:VAL:HG12	2.00	0.44
16:M:420:THR:H	16:M:564:ARG:HB2	1.82	0.44
16:M:510:TYR:CD1	16:M:510:TYR:N	2.85	0.44
1:A:421:ARG:HA	1:A:444:TYR:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ASN:OD1	1:A:632:ASN:N	2.36	0.44
1:A:621:ILE:HA	9:H:122:LEU:HD13	2.00	0.44
1:A:872:MET:HB2	1:A:872:MET:HE3	1.68	0.44
3:B:1062:ARG:CZ	3:B:1074:PRO:HB3	2.48	0.44
4:C:13:GLU:HG2	4:C:20:LYS:HB3	1.99	0.44
6:E:72:MET:HA	6:E:101:ARG:O	2.17	0.44
10:I:24:LEU:HB3	10:I:37:TYR:HB3	1.99	0.44
16:M:418:ILE:H	16:M:565:CYS:N	2.15	0.44
16:M:442:PHE:CZ	16:M:558:LEU:HD12	2.46	0.44
16:M:530:ARG:HG3	16:M:530:ARG:NH1	2.21	0.44
1:A:1450:PRO:HB2	1:A:1452:LYS:HG2	2.00	0.44
3:B:66:ASP:OD1	3:B:85:LEU:HB3	2.17	0.44
3:B:905:ASP:HB2	3:B:924:ARG:HB2	1.99	0.44
6:E:112:PRO:HB3	15:T:15:DA:H5'	2.00	0.44
8:G:152:VAL:HB	8:G:157:ILE:HG12	1.99	0.44
16:M:176:ARG:NE	16:M:176:ARG:O	2.50	0.44
16:M:362:TYR:HB2	16:M:415:PHE:HZ	1.83	0.44
16:M:504:THR:HB	16:M:506:GLU:HG3	2.00	0.44
3:B:84:TYR:HB3	3:B:132:VAL:HG23	1.99	0.43
3:B:827:GLU:HB3	3:B:869:LYS:HD2	2.00	0.43
16:M:141:LEU:N	16:M:141:LEU:HD23	2.32	0.43
1:A:527:THR:OG1	1:A:529:GLN:HG2	2.17	0.43
1:A:783:GLN:HA	1:A:787:VAL:O	2.19	0.43
5:D:33:LEU:HD11	5:D:84:ARG:NH1	2.32	0.43
6:E:107:GLN:HA	6:E:132:GLN:HG3	2.00	0.43
16:M:101:GLU:O	16:M:101:GLU:CD	2.56	0.43
1:A:1188:GLU:OE2	1:A:1258:ARG:HD2	2.18	0.43
3:B:604:ILE:HB	3:B:613:ARG:HG3	2.00	0.43
3:B:728:MET:HE2	3:B:728:MET:HB2	1.85	0.43
16:M:291:VAL:HG12	16:M:416:PHE:C	2.38	0.43
3:B:317:ALA:O	3:B:321:ILE:HG12	2.19	0.43
16:M:135:PHE:C	16:M:135:PHE:HD1	2.21	0.43
16:M:160:ARG:CG	16:M:160:ARG:NH1	2.80	0.43
3:B:98:HIS:HB3	3:B:108:MET:SD	2.58	0.43
3:B:798:ARG:NH2	3:B:802:ASP:OD2	2.51	0.43
4:C:101:PHE:CE1	4:C:122:SER:HB2	2.52	0.43
5:D:37:VAL:HG21	8:G:2:PHE:CD1	2.53	0.43
6:E:94:MET:CE	6:E:99:ILE:HG13	2.49	0.43
16:M:135:PHE:CD2	16:M:173:LEU:HG	2.54	0.43
2:P:46:G:H5"	2:P:46:G:H8	1.83	0.43
3:B:430:ASN:ND2	3:B:433:LEU:HD23	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:779:ILE:HG23	3:B:779:ILE:O	2.18	0.43
3:B:955:PRO:HB2	3:B:1028:LEU:HD12	2.01	0.43
13:L:18:ILE:N	13:L:45:TYR:O	2.29	0.43
16:M:243:GLN:HA	16:M:320:PHE:HA	2.00	0.43
1:A:22:GLN:HA	1:A:1448:SER:HA	2.00	0.43
6:E:87:ILE:HA	6:E:90:TYR:HD2	1.83	0.43
16:M:18:GLN:C	16:M:19:PRO:CD	2.76	0.43
1:A:551:ARG:HH12	9:H:27:ARG:HH21	1.66	0.43
1:A:955:GLU:HA	1:A:958:ARG:HE	1.83	0.43
3:B:193:VAL:HG21	3:B:470:LEU:HD13	2.00	0.43
3:B:282:ARG:HH11	10:I:16:PHE:HD2	1.66	0.43
3:B:1028:LEU:HD23	3:B:1041:ILE:HB	2.01	0.43
3:B:1098:GLY:HA3	7:F:60:TYR:HE1	1.84	0.43
16:M:289:TYR:H	16:M:418:ILE:HD11	1.84	0.43
16:M:362:TYR:HB2	16:M:415:PHE:CZ	2.53	0.43
1:A:221:VAL:HG12	1:A:249:ILE:HD11	2.00	0.43
1:A:1468:THR:H	7:F:60:TYR:HB3	1.83	0.43
3:B:271:ILE:HG21	3:B:320:PHE:HD2	1.83	0.43
3:B:622:CYS:HA	3:B:666:ASP:HA	2.01	0.43
12:K:41:THR:O	12:K:42:LEU:HD22	2.19	0.43
16:M:131:ASN:O	16:M:132:ARG:NE	2.51	0.43
16:M:181:GLU:N	16:M:181:GLU:CD	2.72	0.43
16:M:521:ASN:OD1	16:M:521:ASN:N	2.51	0.43
1:A:394:VAL:HG21	1:A:440:LEU:HD22	2.00	0.43
1:A:937:ASP:OD1	1:A:938:LEU:N	2.51	0.43
3:B:98:HIS:NE2	3:B:106:SER:OG	2.51	0.43
3:B:159:THR:HA	3:B:164:ASN:ND2	2.34	0.43
16:M:30:MET:HB3	16:M:31:LEU:H	1.18	0.43
16:M:419:CYS:H	16:M:564:ARG:CA	2.31	0.43
1:A:61:ARG:O	1:A:73:THR:OG1	2.36	0.42
3:B:756:LYS:O	3:B:777:ASN:ND2	2.52	0.42
10:I:64:GLU:HA	10:I:64:GLU:OE2	2.18	0.42
16:M:516:GLU:HG3	16:M:527:MET:HB3	2.00	0.42
1:A:132:LYS:O	1:A:136:GLN:NE2	2.52	0.42
1:A:349:ARG:O	1:A:354:LEU:N	2.49	0.42
1:A:533:PRO:HD3	1:A:654:HIS:HB2	2.01	0.42
2:P:44:A:N3	2:P:44:A:H3'	2.34	0.42
3:B:191:GLU:OE2	3:B:743:ARG:NH1	2.40	0.42
3:B:628:VAL:HG22	3:B:633:LEU:HD23	2.01	0.42
16:M:138:CYS:SG	16:M:152:ALA:O	2.74	0.42
16:M:513:LYS:HA	16:M:513:LYS:HZ3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:116:ARG:HH11	3:B:118:LEU:HD11	1.84	0.42
3:B:258:ALA:HB2	3:B:269:ILE:HD13	2.01	0.42
3:B:380:ARG:NH2	3:B:609:GLU:HG2	2.34	0.42
3:B:907:VAL:HG22	3:B:921:ILE:HG12	2.01	0.42
3:B:968:ASN:ND2	3:B:970:HIS:HB2	2.34	0.42
16:M:519:PHE:O	16:M:519:PHE:HD2	2.02	0.42
1:A:1442:ALA:HB1	1:A:1447:GLU:HB2	2.00	0.42
3:B:380:ARG:HH22	3:B:611:GLU:CD	2.23	0.42
10:I:29:ASP:HB3	10:I:34:ILE:H	1.84	0.42
13:L:35:ARG:HH22	13:L:40:GLY:HA3	1.85	0.42
16:M:6:ILE:HG23	16:M:35:TYR:CD1	2.55	0.42
16:M:290:LYS:HD2	16:M:377:PHE:CE2	2.54	0.42
16:M:312:MET:HB2	16:M:320:PHE:HB2	2.01	0.42
1:A:187:TYR:HD2	1:A:187:TYR:O	2.02	0.42
3:B:380:ARG:HH21	3:B:609:GLU:HG2	1.84	0.42
5:D:59:GLU:HA	5:D:62:MET:SD	2.59	0.42
6:E:73:PHE:CE1	6:E:99:ILE:HD11	2.54	0.42
16:M:51:SER:O	16:M:54:LEU:HD22	2.20	0.42
16:M:132:ARG:CZ	16:M:132:ARG:HB3	2.48	0.42
1:A:1004:LEU:HD22	1:A:1060:LEU:O	2.19	0.42
3:B:401:ALA:O	3:B:405:ARG:HG3	2.20	0.42
4:C:77:ASP:OD1	4:C:77:ASP:N	2.52	0.42
10:I:37:TYR:HD2	10:I:46:GLN:NE2	2.18	0.42
16:M:25:LEU:HB3	16:M:27:LEU:HD22	2.01	0.42
16:M:99:THR:H	16:M:101:GLU:CD	2.23	0.42
1:A:261:ARG:HA	1:A:262:PRO:HD3	1.93	0.42
1:A:922:PHE:HB2	1:A:1052:ARG:HB2	2.01	0.42
3:B:42:GLN:HE22	3:B:483:ARG:HG2	1.84	0.42
3:B:130:LYS:O	3:B:141:GLN:HA	2.19	0.42
4:C:78:ILE:HG22	4:C:82:LEU:HG	2.01	0.42
4:C:193:ARG:NH2	4:C:218:ALA:O	2.46	0.42
16:M:61:MET:HE2	16:M:84:ILE:HG21	2.01	0.42
16:M:126:SER:O	16:M:127:THR:C	2.58	0.42
1:A:37:THR:HG21	1:A:41:ILE:HD13	2.01	0.42
1:A:250:VAL:HG13	1:A:250:VAL:O	2.20	0.42
1:A:467:MET:HA	1:A:470:MET:SD	2.60	0.42
1:A:685:HIS:HB3	3:B:784:SER:HB2	2.00	0.42
5:D:129:GLN:NE2	5:D:133:ASP:OD2	2.52	0.42
16:M:31:LEU:HB3	16:M:45:PHE:O	2.20	0.42
16:M:58:LYS:HD2	16:M:58:LYS:N	2.34	0.42
16:M:270:GLY:CA	16:M:301:MET:HE1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:442:PHE:CE2	16:M:562:ILE:HG22	2.55	0.42
1:A:377:GLN:HE21	1:A:473:ARG:HH12	1.68	0.42
1:A:484:LEU:HD23	1:A:484:LEU:H	1.85	0.42
1:A:1082:HIS:O	1:A:1085:GLU:HG3	2.19	0.42
4:C:44:ILE:HG21	4:C:178:PRO:HB3	2.01	0.42
10:I:36:LEU:HG	10:I:46:GLN:O	2.20	0.42
1:A:610:PRO:HD2	1:A:613:GLU:OE1	2.20	0.42
1:A:1420:ASN:HA	1:A:1429:LYS:HG2	2.01	0.42
4:C:4:ALA:HB2	12:K:93:ASP:HB3	2.02	0.42
9:H:65:TYR:CE2	9:H:81:ARG:HD2	2.55	0.42
15:T:13:DT:H2"	15:T:14:DG:C8	2.55	0.42
16:M:440:LEU:HD13	16:M:562:ILE:CD1	2.50	0.42
16:M:560:GLU:HA	16:M:563:ASP:HB2	2.01	0.42
1:A:13:CYS:HB2	3:B:1148:LEU:HB2	2.02	0.41
1:A:296:ASN:OD1	1:A:297:GLY:N	2.53	0.41
3:B:121:SER:HA	3:B:153:PRO:HA	2.02	0.41
4:C:242:GLU:HG2	4:C:243:THR:N	2.34	0.41
5:D:90:LYS:HB3	5:D:122:PHE:CZ	2.55	0.41
8:G:118:GLU:HG3	8:G:129:LYS:O	2.19	0.41
16:M:15:ARG:HB3	16:M:45:PHE:CE1	2.56	0.41
16:M:28:LYS:CD	16:M:28:LYS:N	2.81	0.41
16:M:558:LEU:O	16:M:562:ILE:HG23	2.20	0.41
2:P:37:A:N3	2:P:37:A:C2'	2.83	0.41
13:L:20:GLY:HA3	13:L:41:TYR:CD2	2.55	0.41
16:M:152:ALA:O	16:M:155:THR:HG22	2.19	0.41
16:M:160:ARG:HA	16:M:160:ARG:HD3	1.56	0.41
16:M:416:PHE:CD2	16:M:562:ILE:O	2.73	0.41
1:A:48:GLU:O	1:A:51:ARG:HG2	2.20	0.41
1:A:421:ARG:NH2	1:A:437:ASP:HB2	2.35	0.41
1:A:466:LYS:HA	3:B:1093:CYS:SG	2.61	0.41
1:A:935:GLN:O	1:A:939:VAL:HG23	2.20	0.41
1:A:1428:MET:CE	1:A:1455:SER:HB3	2.50	0.41
2:P:53:A:H2'	2:P:53:A:N3	2.34	0.41
3:B:728:MET:SD	3:B:942:LYS:HB3	2.60	0.41
9:H:95:LYS:C	9:H:116:VAL:HG23	2.40	0.41
14:N:36:DA:H2"	14:N:37:DA:C8	2.55	0.41
1:A:417:LYS:HA	1:A:429:LEU:HB2	2.01	0.41
1:A:579:ILE:HB	1:A:585:LEU:HB3	2.03	0.41
1:A:1471:PHE:CZ	7:F:61:GLU:HA	2.56	0.41
1:A:1471:PHE:CE2	7:F:64:ARG:HD3	2.56	0.41
10:I:63:ASP:O	10:I:67:GLN:NE2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:15:MET:HB2	13:L:28:ILE:HG22	2.03	0.41
16:M:249:LYS:HA	16:M:249:LYS:HD2	1.87	0.41
16:M:389:ILE:HG13	16:M:412:ASN:ND2	2.36	0.41
1:A:193:ARG:NH1	1:A:195:GLY:O	2.53	0.41
1:A:405:LEU:HD22	1:A:414:PRO:O	2.21	0.41
1:A:717:ILE:CG2	1:A:721:HIS:CE1	3.04	0.41
10:I:61:GLU:H	10:I:61:GLU:CD	2.13	0.41
14:N:39:DA:H2"	14:N:40:DA:C8	2.56	0.41
1:A:365:THR:HG22	1:A:482:PHE:CE2	2.56	0.41
3:B:274:ARG:HD3	3:B:279:VAL:HA	2.03	0.41
3:B:713:PHE:HB3	3:B:716:HIS:ND1	2.36	0.41
3:B:1040:GLN:OE1	3:B:1040:GLN:N	2.54	0.41
9:H:94:GLY:O	9:H:140:ARG:NH2	2.54	0.41
14:N:37:DA:H2"	14:N:38:DT:H5'	2.01	0.41
16:M:65:VAL:N	16:M:123:GLY:O	2.46	0.41
16:M:126:SER:N	16:M:133:THR:HG1	2.15	0.41
16:M:290:LYS:HG2	16:M:415:PHE:HB3	2.01	0.41
16:M:390:SER:HB3	16:M:391:PRO:HD3	2.02	0.41
16:M:530:ARG:CG	16:M:530:ARG:NH1	2.78	0.41
1:A:540:ASP:HA	3:B:970:HIS:CE1	2.56	0.41
1:A:803:LYS:NZ	3:B:671:GLU:HB3	2.35	0.41
2:P:40:A:N3	2:P:40:A:H5"	2.35	0.41
3:B:837:CYS:SG	3:B:838:GLN:N	2.93	0.41
3:B:1161:GLU:OE1	3:B:1161:GLU:N	2.47	0.41
10:I:60:HIS:HA	10:I:103:ARG:NH2	2.35	0.41
16:M:513:LYS:HA	16:M:513:LYS:HZ2	1.83	0.41
16:M:555:LYS:HA	16:M:558:LEU:HD23	2.03	0.41
16:M:559:PHE:CD1	16:M:562:ILE:HD11	2.55	0.41
1:A:113:PHE:HD2	1:A:187:TYR:HB2	1.86	0.41
1:A:190:ARG:HA	1:A:190:ARG:NE	2.33	0.41
1:A:488:VAL:HG22	1:A:535:MET:HE1	2.03	0.41
1:A:611:ASP:OD1	1:A:611:ASP:N	2.51	0.41
1:A:807:LEU:HB3	1:A:809:HIS:ND1	2.35	0.41
1:A:948:ILE:HG23	1:A:1007:ILE:HD13	2.03	0.41
1:A:1137:PRO:HB2	1:A:1341:VAL:HB	2.03	0.41
1:A:1210:TRP:HD1	1:A:1285:LEU:HD13	1.86	0.41
1:A:1228:MET:HG2	1:A:1247:PHE:HB2	2.03	0.41
3:B:53:MET:O	3:B:57:ARG:HG2	2.20	0.41
3:B:354:SER:OG	3:B:357:CYS:SG	2.69	0.41
5:D:104:CYS:HB3	5:D:138:ARG:HD2	2.03	0.41
6:E:70:ASP:OD1	6:E:70:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:247:GLN:N	16:M:248:PRO:HD2	2.36	0.41
1:A:37:THR:HG23	1:A:61:ARG:NH2	2.36	0.41
1:A:395:THR:OG1	1:A:396:PRO:HD2	2.21	0.41
1:A:487:SER:OG	1:A:673:GLN:NE2	2.54	0.41
1:A:604:ARG:HB2	1:A:628:VAL:HB	2.02	0.41
1:A:1148:ALA:HB1	1:A:1333:GLU:HB2	2.02	0.41
2:P:47:G:C8	2:P:47:G:H5"	2.55	0.41
3:B:1029:TYR:HA	3:B:1036:LYS:HA	2.03	0.41
5:D:114:LEU:HD21	8:G:167:TYR:HD2	1.86	0.41
6:E:94:MET:HE3	6:E:99:ILE:O	2.21	0.41
6:E:100:THR:O	6:E:125:TYR:HB2	2.20	0.41
10:I:78:LEU:O	10:I:80:ARG:NH1	2.54	0.41
14:N:35:DC:H2"	14:N:36:DA:C8	2.56	0.41
16:M:30:MET:HB2	16:M:74:TYR:CG	2.56	0.41
16:M:176:ARG:HB3	16:M:177:TYR:CE2	2.56	0.41
16:M:453:CYS:SG	16:M:456:ILE:HD12	2.61	0.41
16:M:491:VAL:HB	16:M:537:ASN:O	2.20	0.41
1:A:353:ASN:O	1:A:357:LYS:HE2	2.21	0.41
1:A:1316:ASN:OD1	1:A:1317:LYS:N	2.54	0.41
3:B:95:LYS:HD3	3:B:96:PRO:HD2	2.03	0.41
3:B:561:ILE:HD11	3:B:573:TRP:HZ2	1.86	0.41
4:C:86:ARG:HD2	12:K:11:LEU:HD11	2.03	0.41
8:G:22:LEU:HD21	8:G:68:TYR:OH	2.21	0.41
9:H:40:ILE:O	9:H:123:MET:HA	2.21	0.41
16:M:5:LYS:HA	16:M:35:TYR:HE1	1.85	0.41
16:M:518:LYS:HZ2	16:M:527:MET:HA	1.85	0.41
1:A:190:ARG:NE	1:A:190:ARG:CA	2.83	0.40
1:A:448:ARG:H	1:A:448:ARG:HG3	1.75	0.40
1:A:525:ILE:O	1:A:533:PRO:HA	2.21	0.40
1:A:533:PRO:HD3	1:A:654:HIS:ND1	2.35	0.40
1:A:645:LEU:HD21	1:A:652:LEU:HD23	2.03	0.40
1:A:959:MET:HE1	1:A:1046:ARG:O	2.22	0.40
3:B:873:LEU:HB3	3:B:876:ASN:OD1	2.21	0.40
6:E:47:LYS:H	6:E:53:PRO:HG3	1.86	0.40
6:E:94:MET:HE3	6:E:99:ILE:HG13	2.03	0.40
16:M:138:CYS:HB2	16:M:173:LEU:HD21	2.04	0.40
1:A:1082:HIS:CD2	7:F:58:THR:HB	2.56	0.40
2:P:46:G:H8	2:P:46:G:C5'	2.34	0.40
6:E:2:ASP:OD1	6:E:3:ASP:N	2.52	0.40
8:G:52:ASP:H	8:G:72:TYR:HA	1.86	0.40
1:A:327:ARG:HA	1:A:327:ARG:NH1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ILE:HD11	9:H:27:ARG:HH12	1.85	0.40
1:A:1005:HIS:HB3	1:A:1008:LYS:HG2	2.04	0.40
3:B:399:LEU:HB3	3:B:453:TRP:CZ2	2.57	0.40
3:B:529:MET:HE1	3:B:624:PRO:HG2	2.03	0.40
3:B:1129:ASN:HB2	3:B:1134:THR:OG1	2.21	0.40
1:A:228:ILE:H	1:A:228:ILE:HD12	1.87	0.40
1:A:540:ASP:HB3	3:B:790:GLN:HE22	1.86	0.40
1:A:597:PRO:HD3	1:A:668:PHE:CD1	2.56	0.40
3:B:387:HIS:CD2	3:B:504:THR:HG21	2.57	0.40
3:B:529:MET:SD	3:B:702:MET:HG3	2.61	0.40
3:B:1075:MET:HE3	3:B:1075:MET:HA	2.04	0.40
8:G:132:ASP:HB3	8:G:134:ASP:OD1	2.22	0.40
16:M:51:SER:HA	16:M:54:LEU:CB	2.44	0.40
1:A:77:ASN:C	1:A:79:THR:H	2.24	0.40
1:A:149:LYS:HB3	1:A:150:GLY:H	1.61	0.40
1:A:715:GLU:HA	1:A:718:GLU:HG2	2.03	0.40
1:A:717:ILE:HG12	1:A:737:PHE:CZ	2.57	0.40
3:B:675:LEU:HA	3:B:695:HIS:O	2.21	0.40
5:D:86:LEU:HA	5:D:89:GLN:HE22	1.87	0.40
9:H:15:ILE:HG12	9:H:28:LEU:HD22	2.04	0.40
16:M:546:CYS:O	16:M:550:SER:OG	2.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1399/1984 (70%)	1323 (95%)	74 (5%)	2 (0%)	51 83
3	B	1102/1174 (94%)	1047 (95%)	55 (5%)	0	100 100
4	C	254/275 (92%)	248 (98%)	6 (2%)	0	100 100
5	D	127/142 (89%)	123 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	E	207/210 (99%)	201 (97%)	6 (3%)	0	100 100
7	F	80/127 (63%)	79 (99%)	1 (1%)	0	100 100
8	G	169/172 (98%)	164 (97%)	5 (3%)	0	100 100
9	H	146/150 (97%)	139 (95%)	7 (5%)	0	100 100
10	I	115/125 (92%)	110 (96%)	5 (4%)	0	100 100
11	J	65/67 (97%)	63 (97%)	2 (3%)	0	100 100
12	K	113/117 (97%)	108 (96%)	5 (4%)	0	100 100
13	L	44/58 (76%)	43 (98%)	1 (2%)	0	100 100
16	M	499/597 (84%)	466 (93%)	27 (5%)	6 (1%)	13 51
All	All	4320/5198 (83%)	4114 (95%)	198 (5%)	8 (0%)	50 79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1115	LYS
16	M	13	CYS
16	M	31	LEU
1	A	1263	ASN
16	M	519	PHE
16	M	114	ASN
16	M	28	LYS
16	M	127	THR

5.3.2 Protein sidechains (i)

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	1238/1763 (70%)	1212 (98%)	26 (2%)	53 78
3	B	979/1027 (95%)	977 (100%)	2 (0%)	93 98
4	C	234/252 (93%)	233 (100%)	1 (0%)	91 97
5	D	104/126 (82%)	104 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	E	191/192 (100%)	190 (100%)	1 (0%)	88 95
7	F	71/111 (64%)	71 (100%)	0	100 100
8	G	138/153 (90%)	138 (100%)	0	100 100
9	H	129/131 (98%)	129 (100%)	0	100 100
10	I	105/112 (94%)	103 (98%)	2 (2%)	57 80
11	J	56/56 (100%)	56 (100%)	0	100 100
12	K	104/106 (98%)	104 (100%)	0	100 100
13	L	43/55 (78%)	42 (98%)	1 (2%)	50 76
16	M	447/534 (84%)	337 (75%)	110 (25%)	0 4
All	All	3839/4618 (83%)	3696 (96%)	143 (4%)	37 66

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	A	148	CYS
1	A	149	LYS
1	A	151	LYS
1	A	184	CYS
1	A	186	ARG
1	A	187	TYR
1	A	188	GLN
1	A	190	ARG
1	A	192	ARG
1	A	321	GLU
1	A	322	LEU
1	A	327	ARG
1	A	1046	ARG
1	A	1103	THR
1	A	1104	LEU
1	A	1105	ASN
1	A	1106	THR
1	A	1108	HIS
1	A	1109	TYR
1	A	1115	LYS
1	A	1261	ILE
1	A	1262	MET
1	A	1282	ASP
1	A	1283	VAL

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Mol	Chain	Res	Type
1	A	1375	ARG
3	B	111	ASN
3	B	608	ARG
4	C	113	ARG
6	E	162	ARG
10	I	60	HIS
10	I	63	ASP
13	L	37	ARG
16	M	5	LYS
16	M	10	TRP
16	M	11	LEU
16	M	12	ASN
16	M	16	ARG
16	M	18	GLN
16	M	23	ARG
16	M	28	LYS
16	M	31	LEU
16	M	34	ARG
16	M	36	ASP
16	M	38	GLN
16	M	41	GLU
16	M	44	ARG
16	M	50	LEU
16	M	53	TYR
16	M	54	LEU
16	M	55	LYS
16	M	57	LEU
16	M	58	LYS
16	M	60	LYS
16	M	61	MET
16	M	63	LEU
16	M	68	THR
16	M	69	ASN
16	M	70	THR
16	M	72	ARG
16	M	74	TYR
16	M	76	ARG
16	M	78	ASP
16	M	81	LYS
16	M	85	LYS
16	M	86	TYR
16	M	88	LYS

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Mol	Chain	Res	Type
16	M	89	LEU
16	M	92	LYS
16	M	97	CYS
16	M	101	GLU
16	M	102	ASN
16	M	104	GLU
16	M	106	PHE
16	M	108	ARG
16	M	109	LEU
16	M	110	CYS
16	M	111	GLU
16	M	112	ARG
16	M	114	ASN
16	M	116	ARG
16	M	120	GLU
16	M	122	ILE
16	M	127	THR
16	M	131	ASN
16	M	132	ARG
16	M	135	PHE
16	M	141	LEU
16	M	144	LYS
16	M	145	MET
16	M	147	TRP
16	M	148	SER
16	M	149	ILE
16	M	150	GLU
16	M	155	THR
16	M	156	PHE
16	M	160	ARG
16	M	164	ILE
16	M	169	TYR
16	M	171	LYS
16	M	172	GLU
16	M	173	LEU
16	M	175	ARG
16	M	176	ARG
16	M	179	ASP
16	M	180	ILE
16	M	181	GLU
16	M	182	GLU
16	M	423	LYS

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Mol	Chain	Res	Type
16	M	457	LEU
16	M	458	LYS
16	M	465	ASN
16	M	466	SER
16	M	467	VAL
16	M	468	ASP
16	M	470	ARG
16	M	471	LEU
16	M	472	LYS
16	M	475	ARG
16	M	479	GLU
16	M	481	LEU
16	M	482	LEU
16	M	494	TYR
16	M	496	ARG
16	M	498	PHE
16	M	501	ILE
16	M	502	LYS
16	M	504	THR
16	M	508	LYS
16	M	510	TYR
16	M	513	LYS
16	M	514	ILE
16	M	518	LYS
16	M	523	SER
16	M	524	TRP
16	M	526	PHE
16	M	528	ARG
16	M	529	GLN
16	M	532	ASP
16	M	533	LYS
16	M	534	SER
16	M	546	CYS
16	M	547	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	62	GLN
1	A	330	GLN
1	A	459	ASN

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Mol	Chain	Res	Type
1	A	465	HIS
1	A	504	HIS
1	A	606	HIS
1	A	721	HIS
1	A	791	GLN
1	A	1005	HIS
1	A	1105	ASN
1	A	1116	ASN
3	B	68	GLN
10	I	46	GLN
10	I	60	HIS
13	L	23	HIS
16	M	12	ASN
16	M	69	ASN
16	M	90	GLN
16	M	114	ASN
16	M	125	HIS
16	M	128	HIS
16	M	280	ASN
16	M	465	ASN
16	M	537	ASN
16	M	540	ASN
16	M	547	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	P	18/19 (94%)	11 (61%)	2 (11%)

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	P	38	A
2	P	39	A
2	P	40	A
2	P	41	C
2	P	42	C
2	P	43	C
2	P	44	A
2	P	45	G
2	P	46	G

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Mol	Chain	Res	Type
2	P	47	G
2	P	53	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	P	40	A
2	P	41	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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
14	N	1
16	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	14:DT	O3'	24:DA	P	38.36
1	M	18:GLN	C	19:PRO	N	1.73

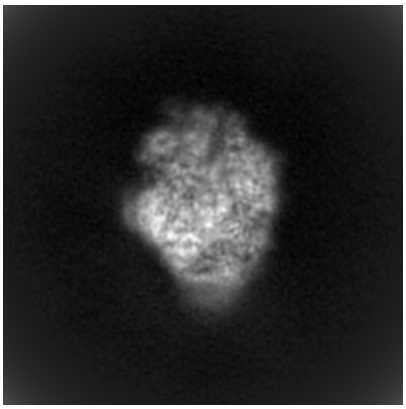
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17403. These allow visual inspection of the internal detail of the map and identification of artifacts.

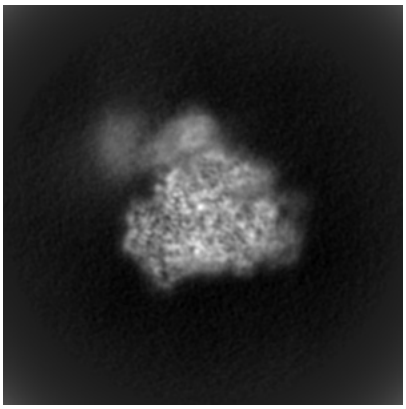
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

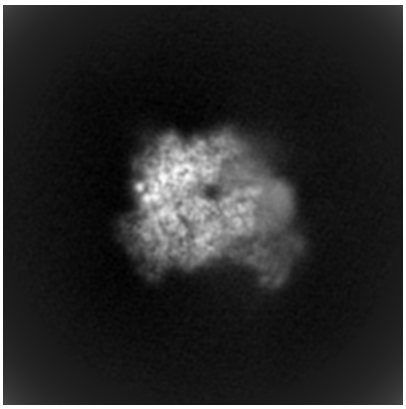
6.1.1 Primary map



X

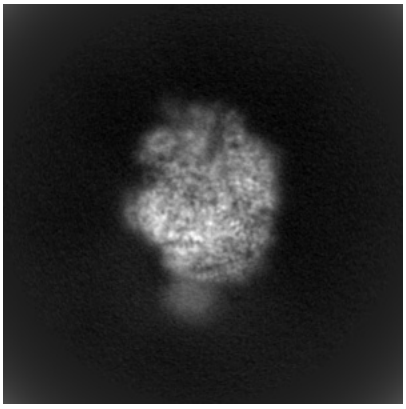


Y

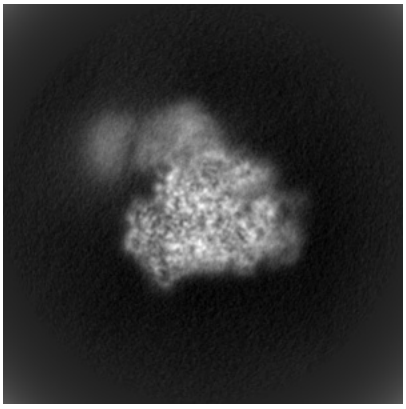


Z

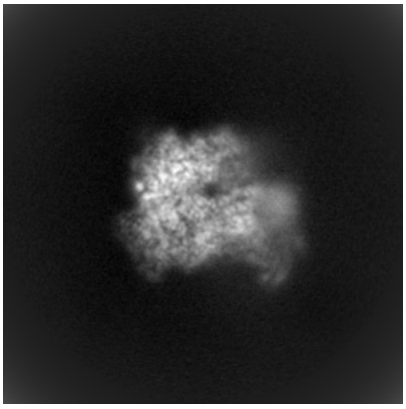
6.1.2 Raw map



X



Y

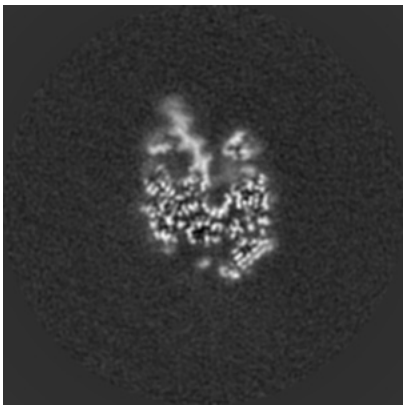


Z

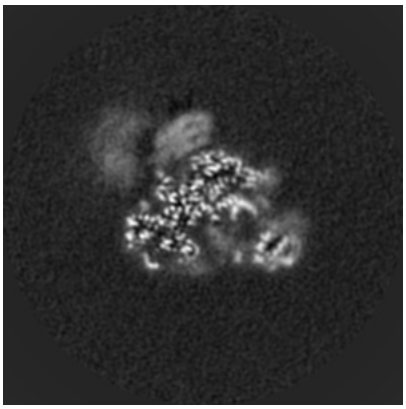
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

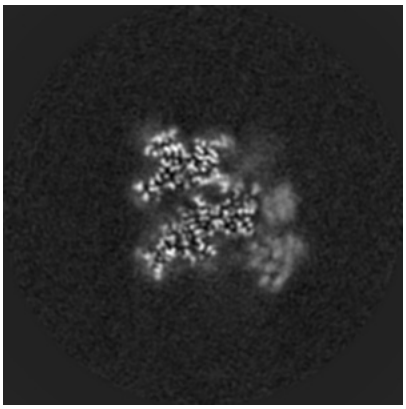
6.2.1 Primary map



X Index: 150

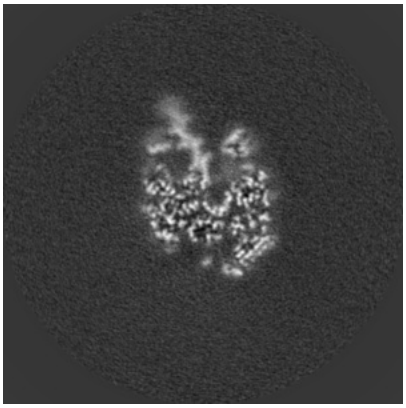


Y Index: 150

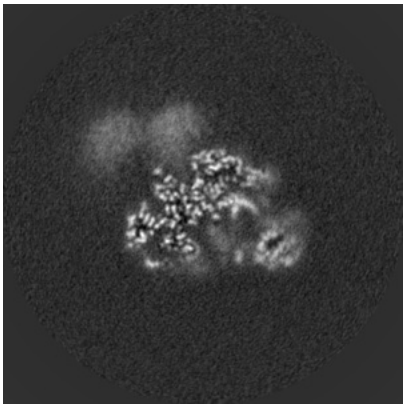


Z Index: 150

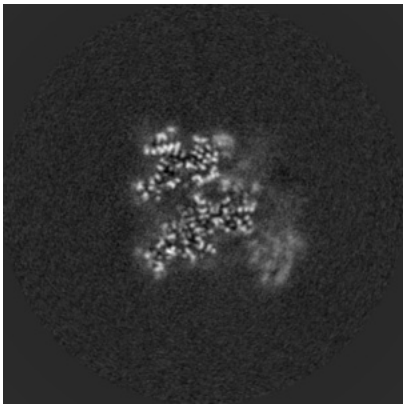
6.2.2 Raw map



X Index: 150



Y Index: 150

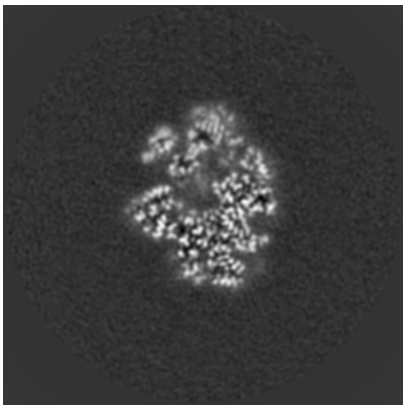


Z Index: 150

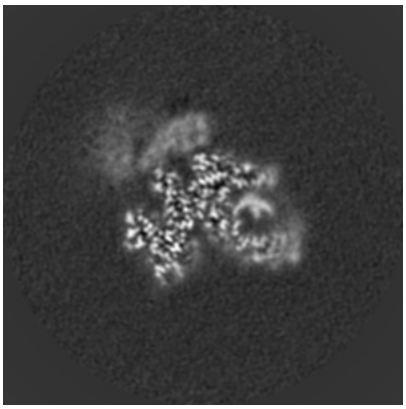
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

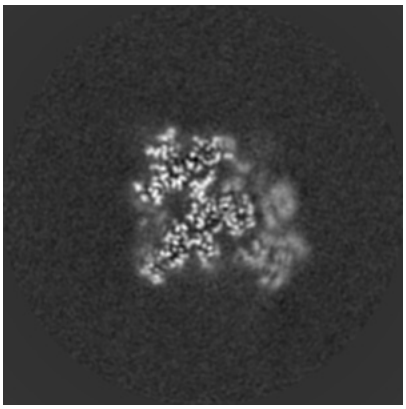
6.3.1 Primary map



X Index: 120

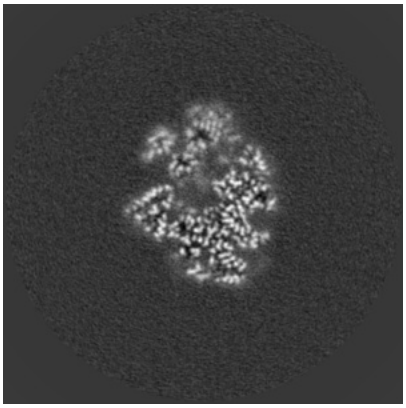


Y Index: 144

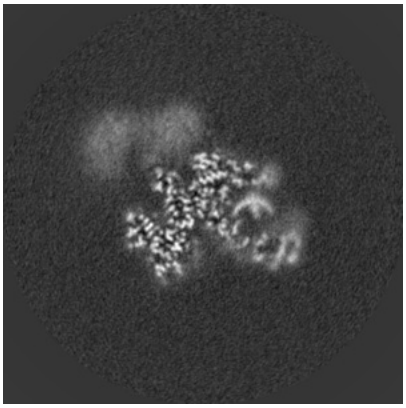


Z Index: 146

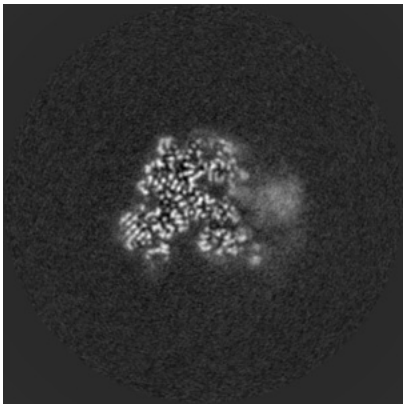
6.3.2 Raw map



X Index: 119



Y Index: 145

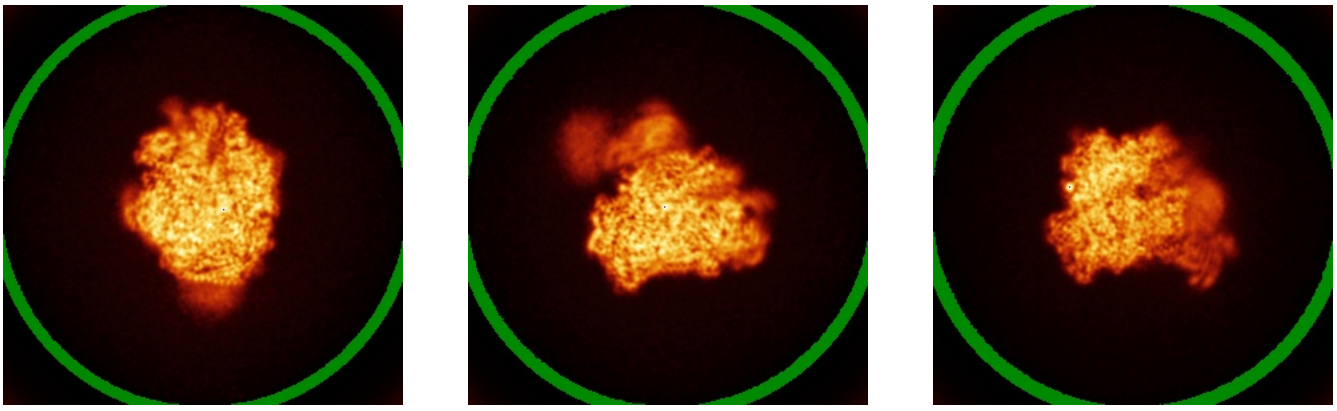


Z Index: 127

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

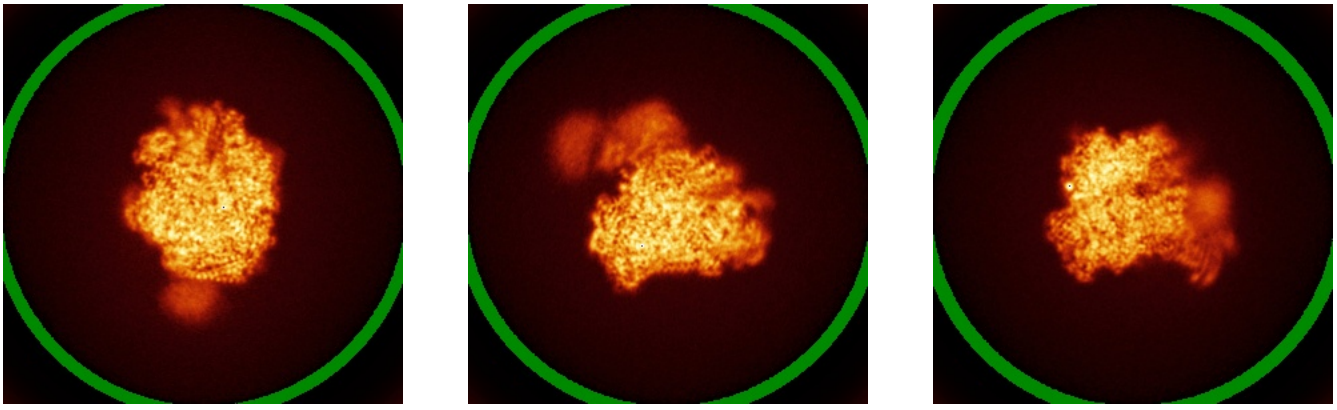
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

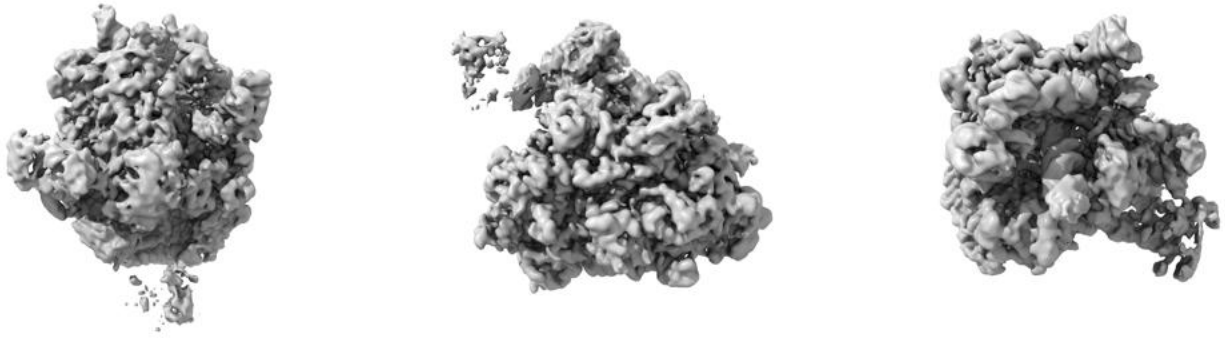


X Y Z

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

6.5 Orthogonal surface views (i)

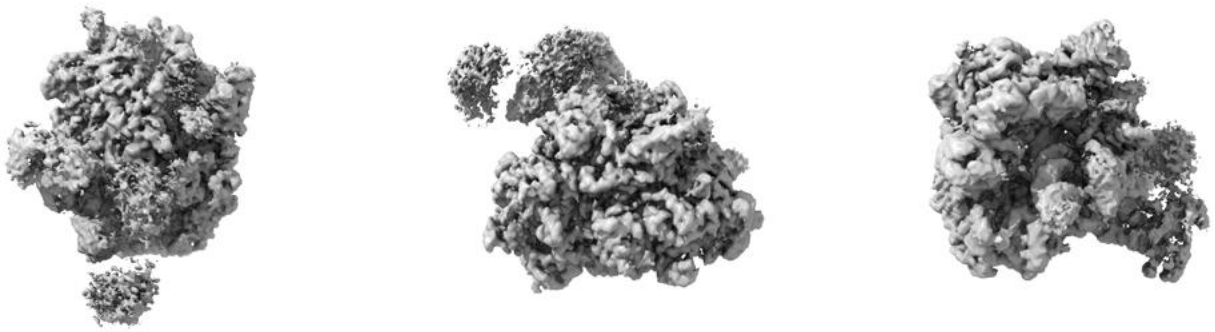
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0257. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

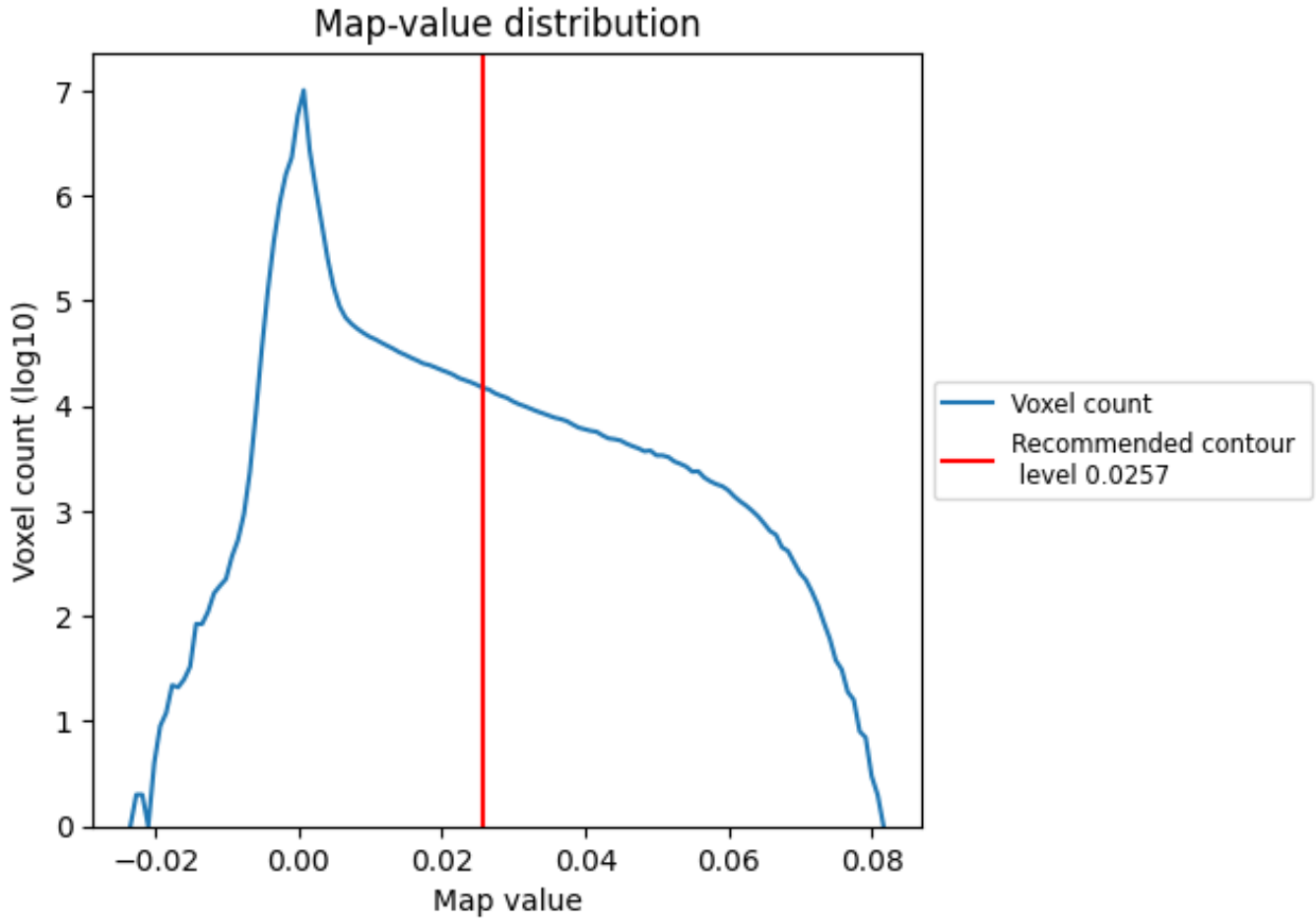
6.6 Mask visualisation (i)

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

7 Map analysis

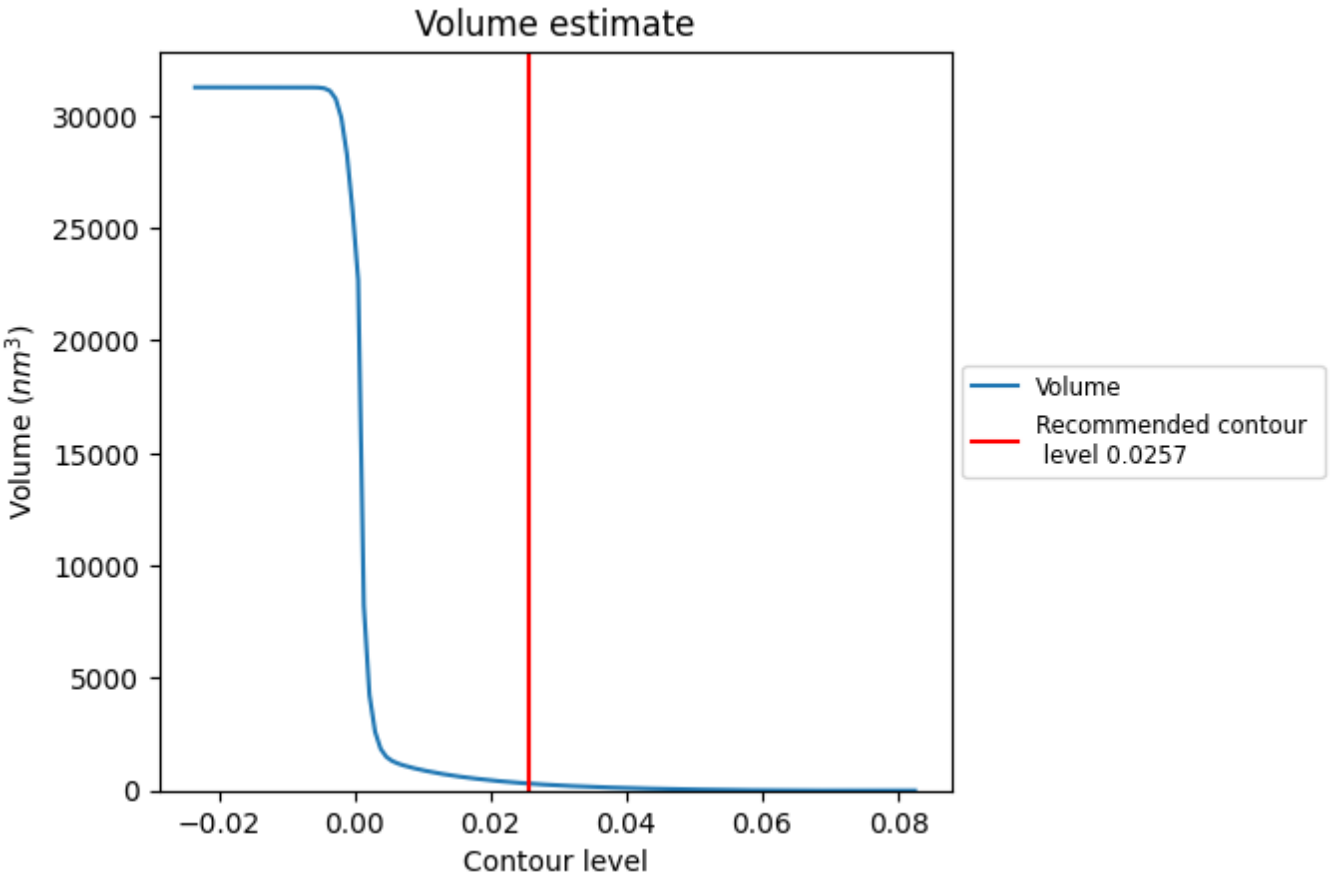
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

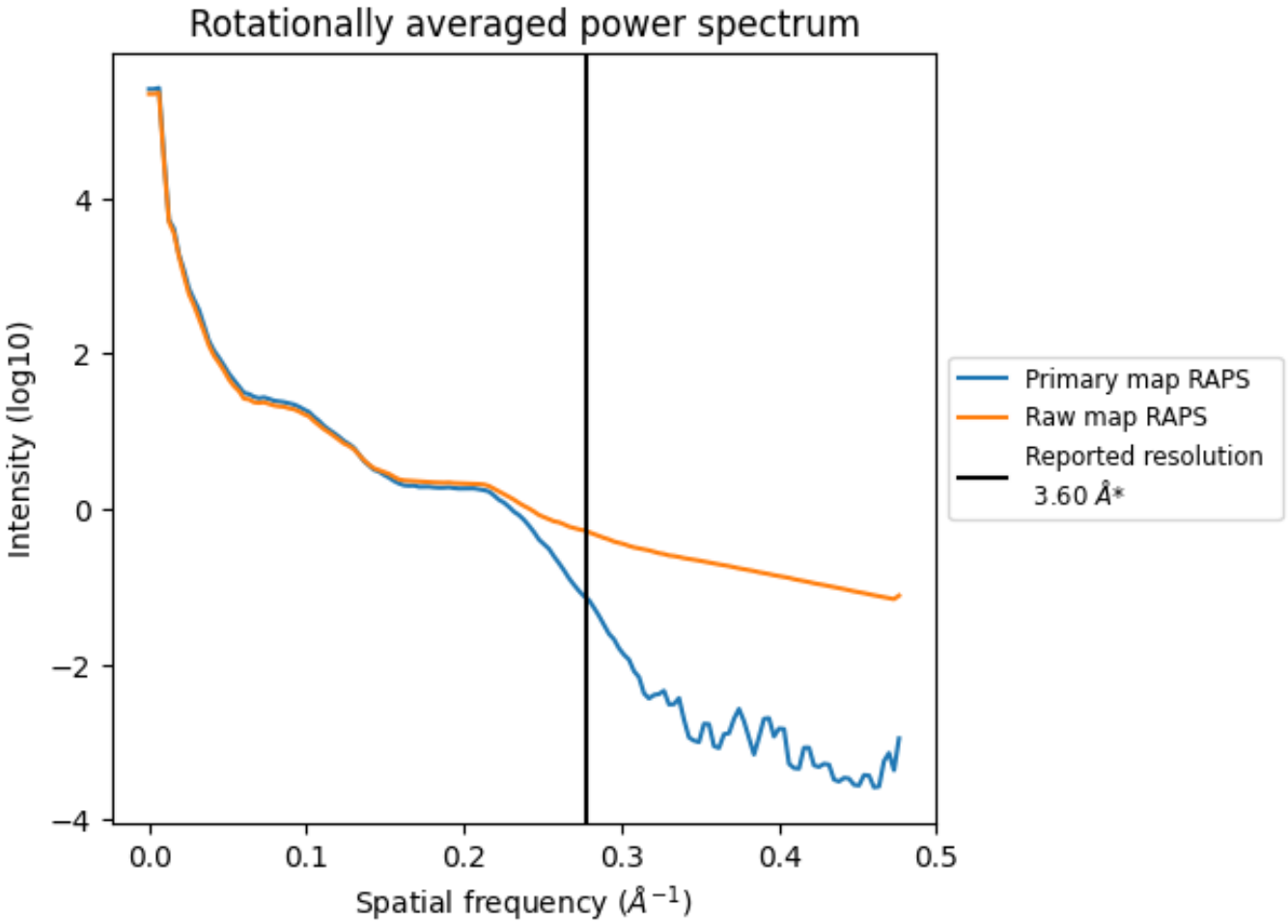
7.2 Volume estimate



The volume at the recommended contour level is 310 nm^3; this corresponds to an approximate mass of 280 kDa.

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

7.3 Rotationally averaged power spectrum (i)

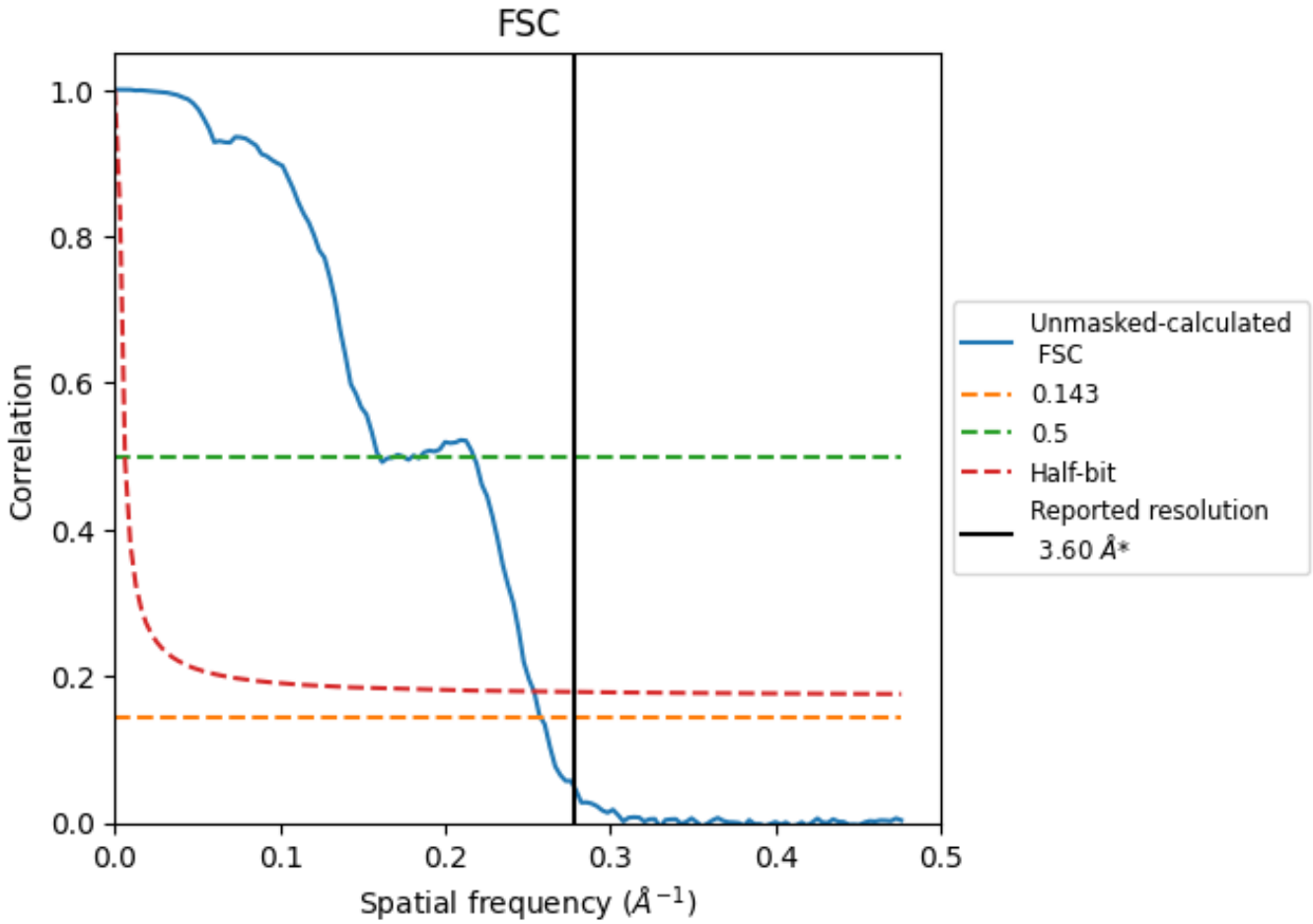


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

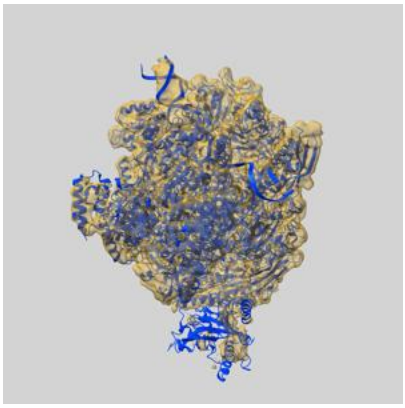
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	6.25	3.94

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

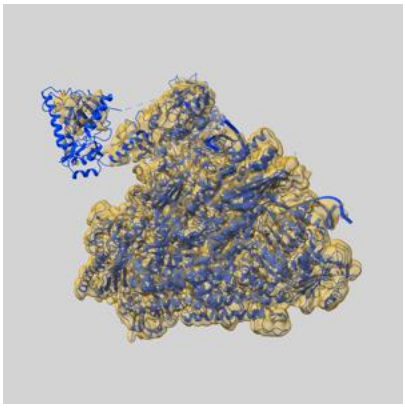
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17403 and PDB model 8P4A. Per-residue inclusion information can be found in section 3 on page 7.

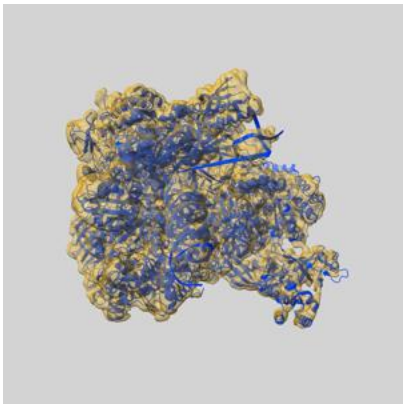
9.1 Map-model overlay



X



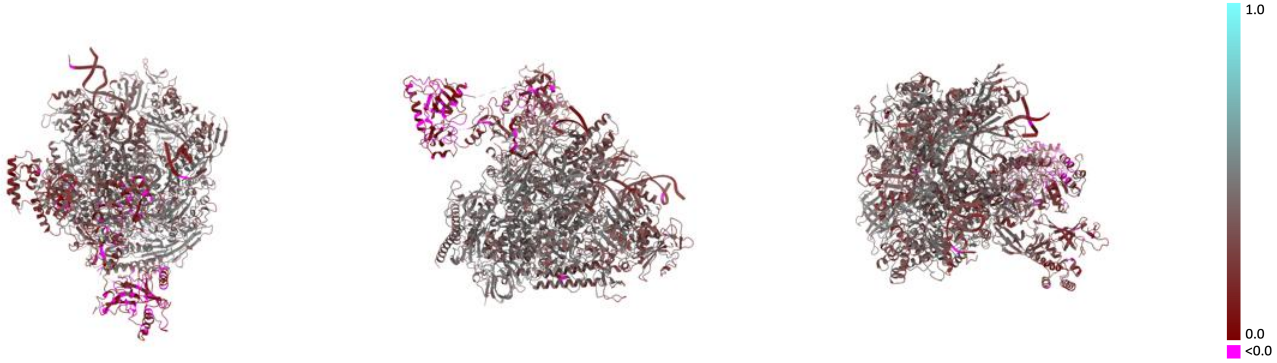
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0257 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.

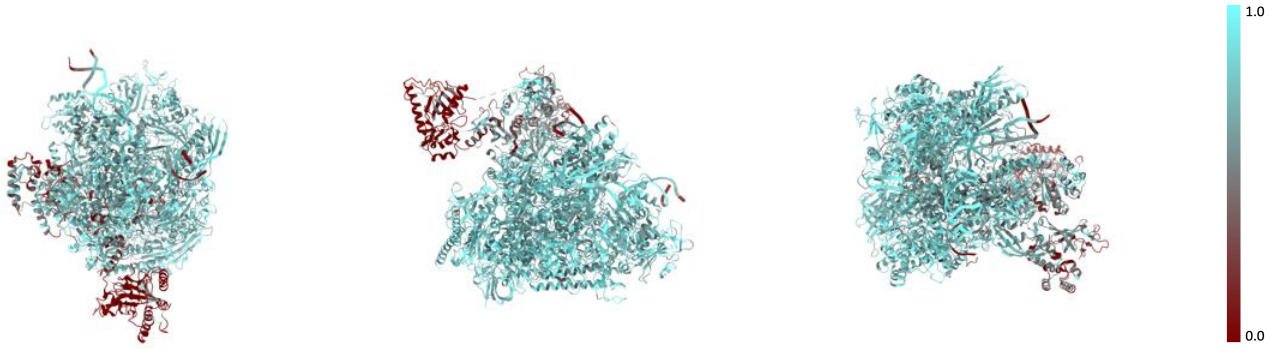
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

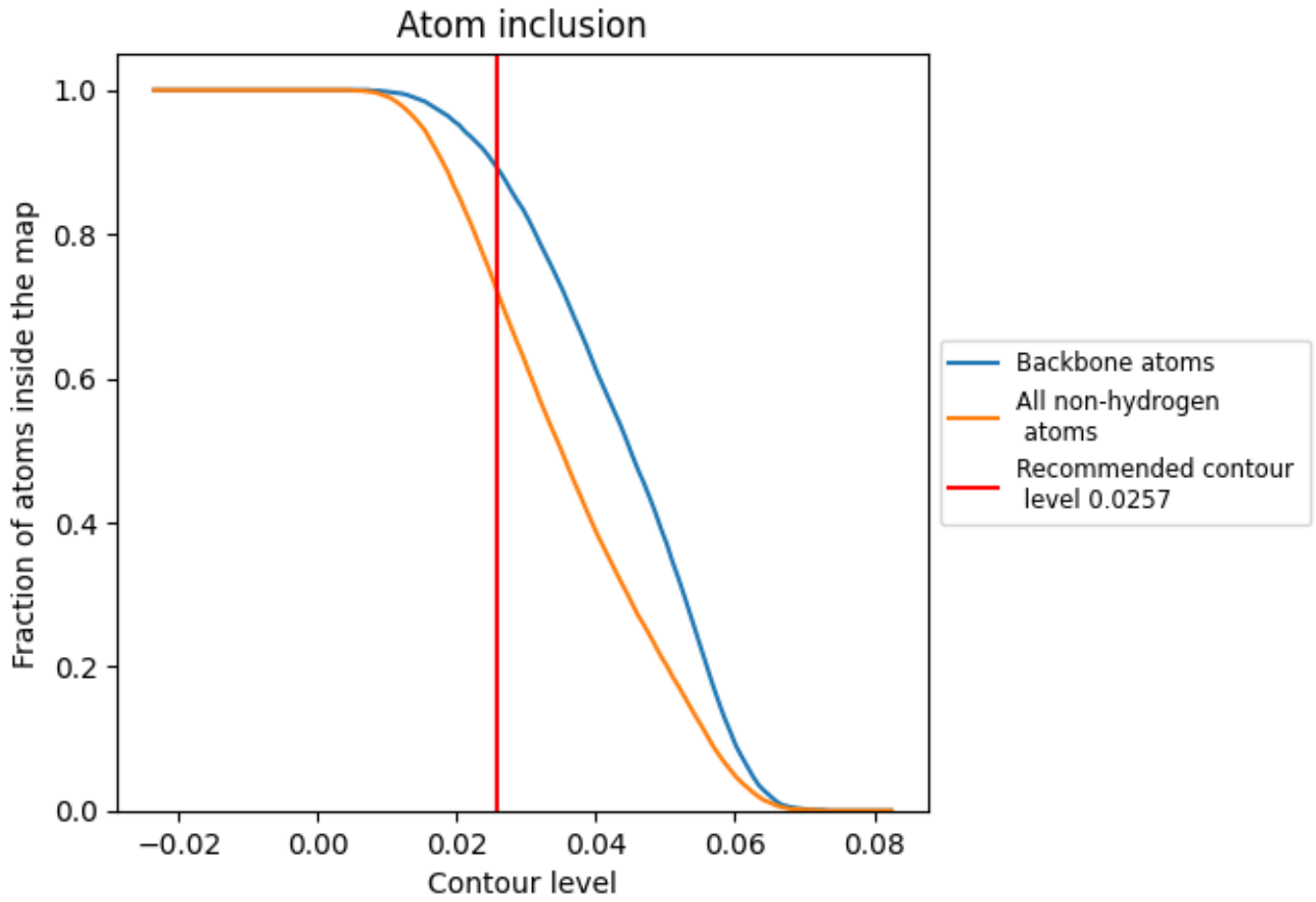
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0257).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 72% 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 (0.0257) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7230	0.3440
A	0.7820	0.3810
B	0.7930	0.3990
C	0.8180	0.4160
D	0.4140	0.2180
E	0.8070	0.3700
F	0.7890	0.4070
G	0.5750	0.2580
H	0.8240	0.4100
I	0.7900	0.3390
J	0.8270	0.4050
K	0.8150	0.4060
L	0.7610	0.3770
M	0.3490	0.1220
N	0.6920	0.2340
P	0.6640	0.2430
T	0.7880	0.2720