Full wwPDB EM Validation Report (i)

May 15, 2023 – 10:21 am BST

PDB ID	:	7QXI
EMDB ID	:	EMD-14200
Title	:	Cryo-EM structure of RNA polymerase-sigma54 holo enzyme with promoter DNA closed complex
Authors	:	Ye, F.Z.; Zhang, X.D.
Deposited on	:	2022-01-26
Resolution	:	3.40 Å(reported)
Based on initial model	:	5NSR

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

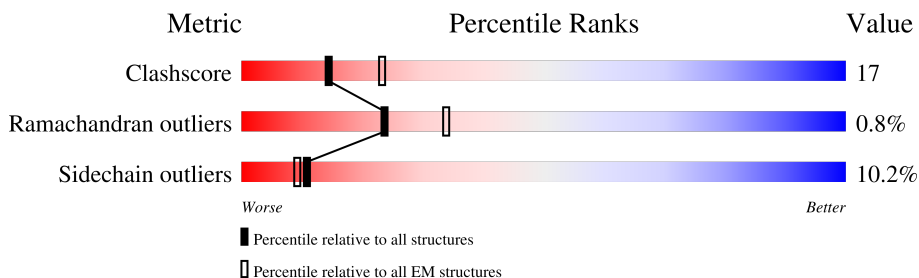|		
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.40 Å.

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

Metric	Percentile Ranks	Value
Clashscore		17
Ramachandran outliers		0.8%
Sidechain outliers		10.2%

Worse   *Better*

▮ Percentile relative to all structures
⬚ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	329	8% / 75% · 18% · 6%
1	B	329	· / 50% · 15% · 33%
2	C	1342	· / 74% · 21% · 5%
3	D	1407	5% / 80% · 14% · 5%
4	E	91	74% · 8% · 19%
5	M	497	6% / 35% · 28% · 16% · 19%
6	N	63	5% / 35% · 19% · 43%
7	T	63	10% / 22% · 32% · 43%

WORLDWIDE PDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 28928 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	309	Total 2316	C 1450	N 404	O 455	S 7	0	0
1	B	222	Total 1671	C 1042	N 293	O 331	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1341	Total 10125	C 6360	N 1761	O 1964	S 40	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1334	Total 9632	C 6049	N 1730	O 1814	S 39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	74	Total 546	C 335	N 109	O 101	S 1	0	0

- Molecule 5 is a protein called RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	403	Total 3162	C 1974	N 551	O 626	S 11	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-19	MET	-	initiating methionine	UNP A0A0N9UTC1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-18	GLY	-	expression tag	UNP A0A0N9UTC1
M	-17	SER	-	expression tag	UNP A0A0N9UTC1
M	-16	SER	-	expression tag	UNP A0A0N9UTC1
M	-15	HIS	-	expression tag	UNP A0A0N9UTC1
M	-14	HIS	-	expression tag	UNP A0A0N9UTC1
M	-13	HIS	-	expression tag	UNP A0A0N9UTC1
M	-12	HIS	-	expression tag	UNP A0A0N9UTC1
M	-11	HIS	-	expression tag	UNP A0A0N9UTC1
M	-10	HIS	-	expression tag	UNP A0A0N9UTC1
M	-9	SER	-	expression tag	UNP A0A0N9UTC1
M	-8	SER	-	expression tag	UNP A0A0N9UTC1
M	-7	GLY	-	expression tag	UNP A0A0N9UTC1
M	-6	LEU	-	expression tag	UNP A0A0N9UTC1
M	-5	VAL	-	expression tag	UNP A0A0N9UTC1
M	-4	PRO	-	expression tag	UNP A0A0N9UTC1
M	-3	ARG	-	expression tag	UNP A0A0N9UTC1
M	-2	GLY	-	expression tag	UNP A0A0N9UTC1
M	-1	SER	-	expression tag	UNP A0A0N9UTC1
M	0	HIS	-	expression tag	UNP A0A0N9UTC1
M	49	GLU	GLN	conflict	UNP A0A0N9UTC1
M	80	GLU	ASP	conflict	UNP A0A0N9UTC1

- Molecule 6 is a DNA chain called Non-Template promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	N	36	738	349	137	216	36	0	0

- Molecule 7 is a DNA chain called Template DNA promoter.

| Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	T	36	738	349	137	216	36	0	0

3 Residue-property plots ⓘ

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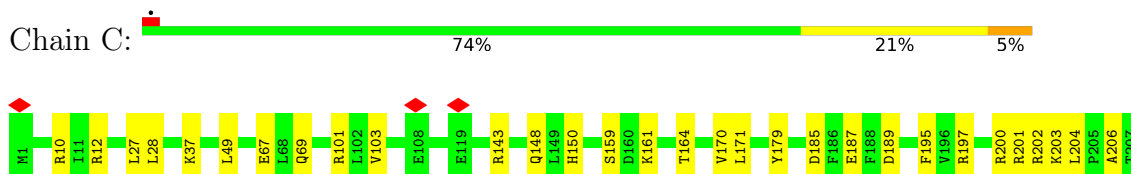
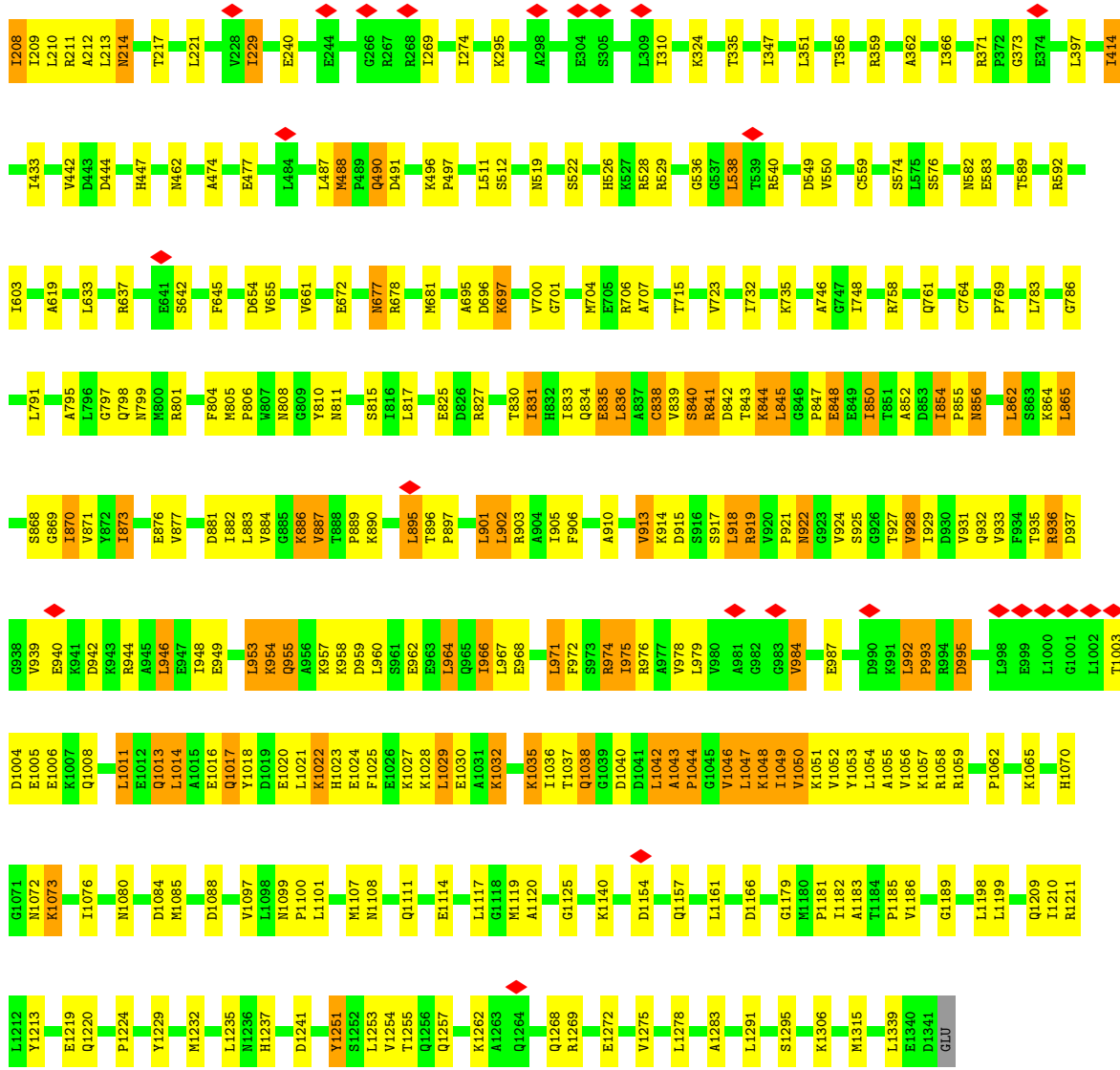- Molecule 1: DNA-directed RNA polymerase subunit alpha
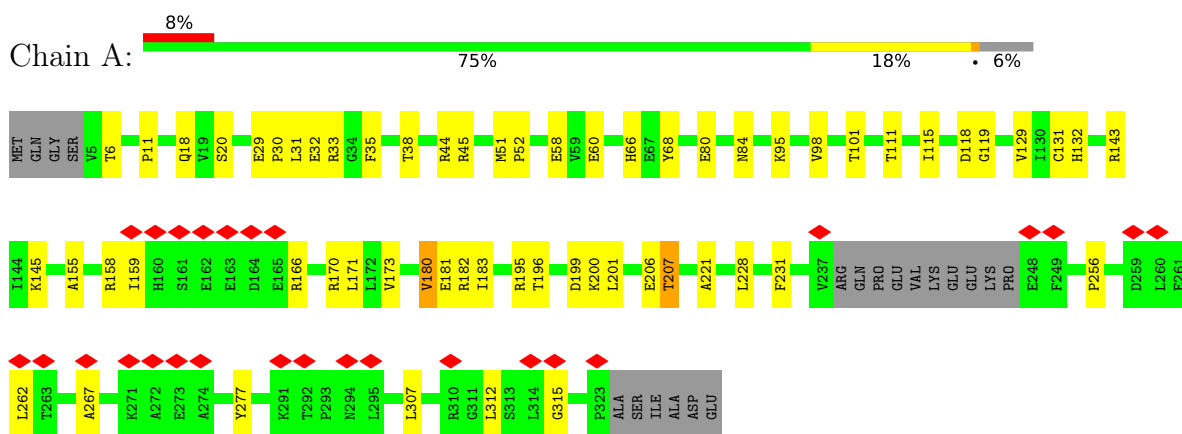
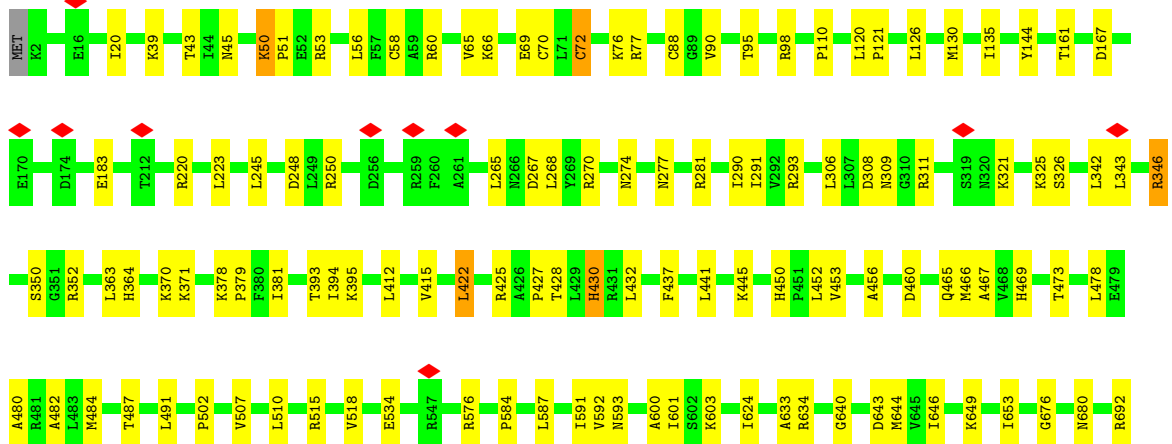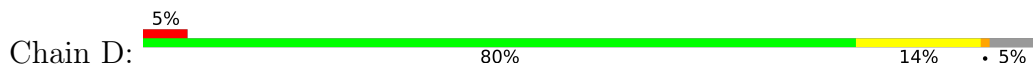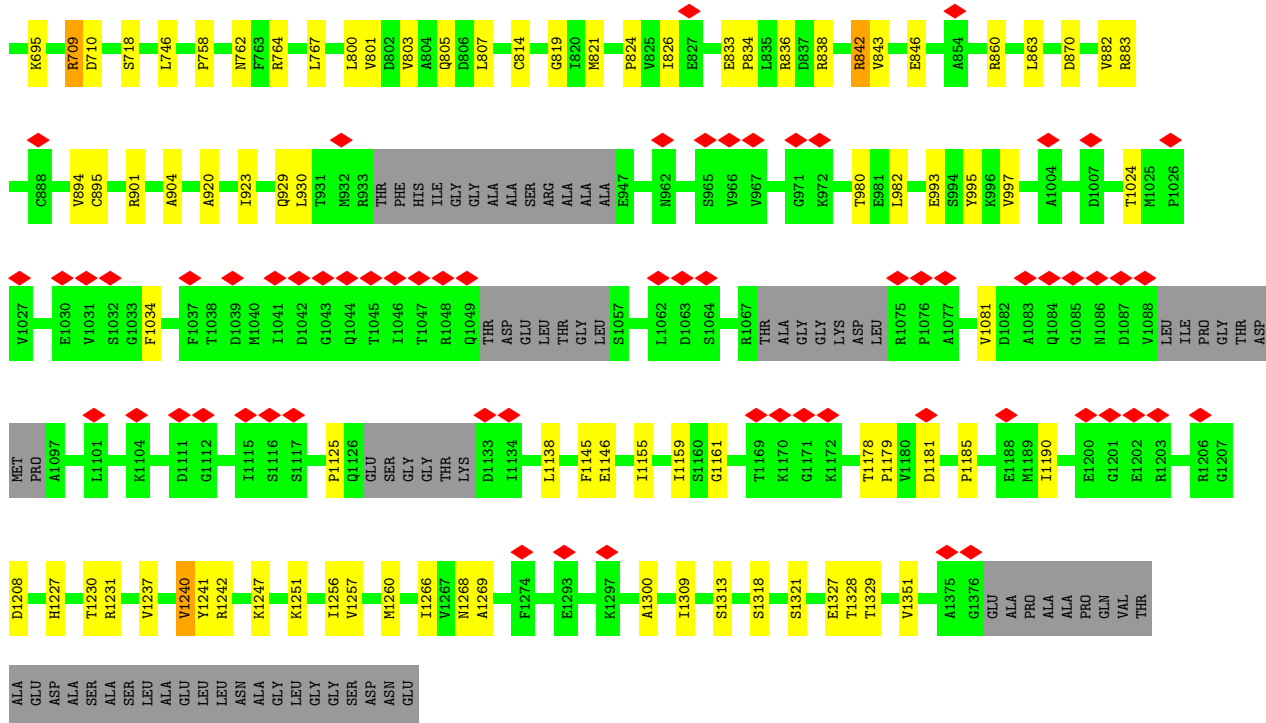- Molecule 1: DNA-directed RNA polymerase subunit alpha
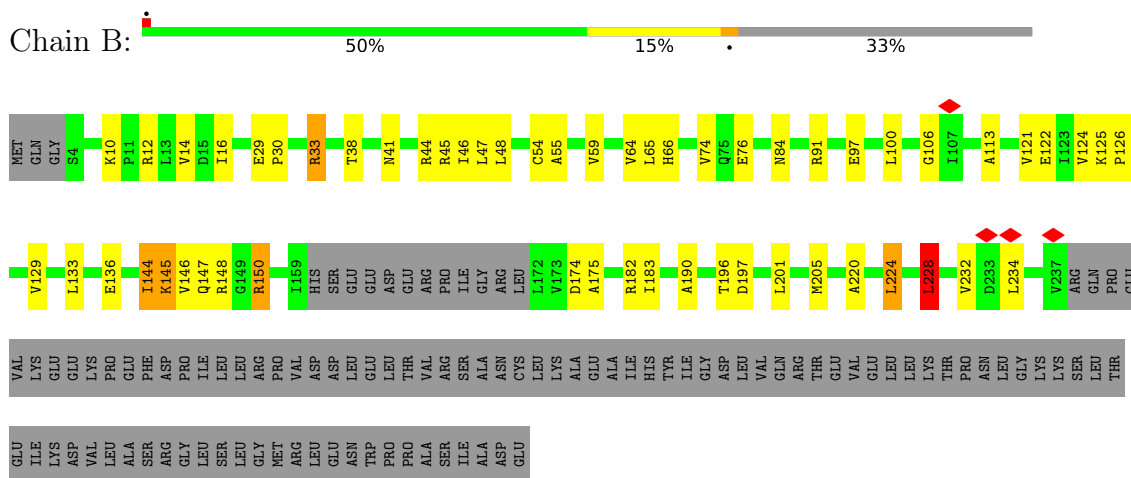
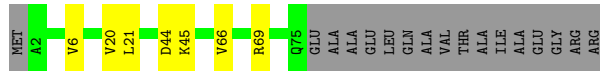- Molecule 2: DNA-directed RNA polymerase subunit beta
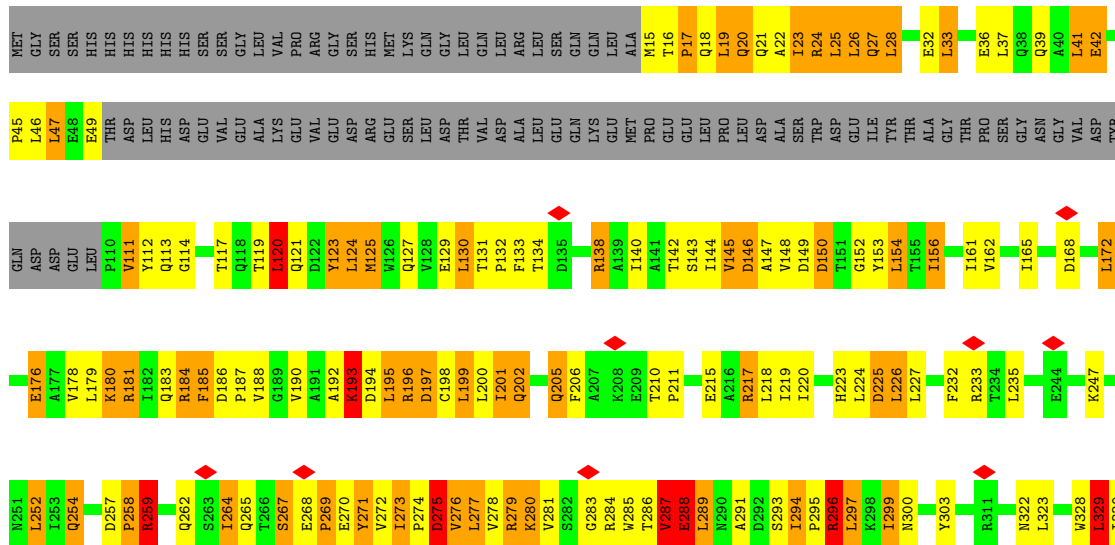
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:

• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 74%   8%   19%

• Molecule 5: RNA polymerase sigma-54 factor

Chain M: 6%   35%   28%   16%   19%

S332 L333 E334 S335 R336 N337 D338 T339 L340 L341 R342 V343 S344 R345 C346 I347 V348 E349 Q350 Q351 Q352 A353 F354 E359 M362 V366 L367 A368 D369 I370 A371 Q372 M376 H377 E378 S379 T380 R383 V384 T385 T386 Q387 K388 Y389 L390 H391 S392 P393 R394 G395 I396 F397 E398 L399 K400

Y401 F402 F403 S404 S405 H406 V407 N408 T409 E410 A415 S416 S417 T418 A419 I420 R421 A422 L423 V424 K425 K426 A429 A430 E431 K435 P436 L437 S438 D439 L442 I451 M452 V453 A454 R455 R456 T457 K460 Y461 R462 E463 S464 L465 S466 P469 S470 N471 Q472 R473 K474 Q475 L476

V477

• Molecule 6: Non-Template promoter DNA

Chain N:

5%

35% 19% • 43%

DG A-34 G-33 A-32 G-26 T-18 T-17 T-16 C-13 A-12 C-11 G-10 A-9 T-8 C-7 A-6 G0 G1 DG DC DG DC DG DC DA DT DG DC DT DG DT DT DG DC DG DC DA DT DT DC DA DT DG DT
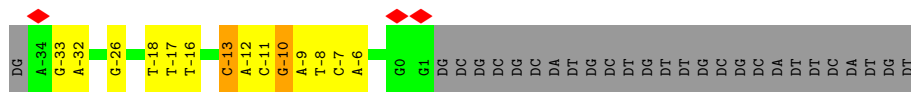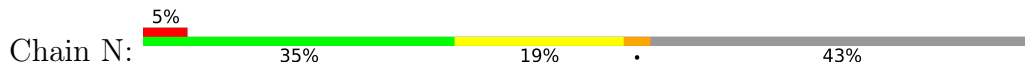
• Molecule 7: Template DNA promoter

Chain T:

10%

22% 32% • 43%

DA DC DA DT DG DA DA DT DG DC DG DC DA DA DC DA DG DC DA DT DG DC DG DC DG DC C-1 C0 A1 T6 G7 A8 T9 C10 G11 T12 G13 C14 A15 T20 C21 G22 T23 G24 C29 C30 G31 T32 C33 T34 DC
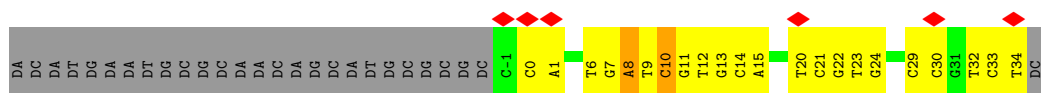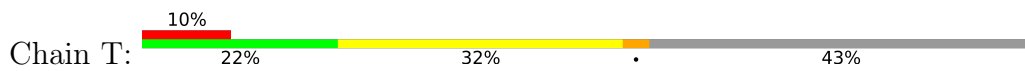
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29321	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.216	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.23	0/2345	0.42	0/3195
1	B	0.23	0/1688	0.45	1/2293 (0.0%)
2	C	0.23	0/10283	0.40	0/13940
3	D	0.23	0/9766	0.41	1/13267 (0.0%)
4	E	0.22	0/547	0.37	0/740
5	M	0.72	3/3204 (0.1%)	0.88	7/4339 (0.2%)
6	N	0.73	2/827 (0.2%)	0.92	5/1274 (0.4%)
7	T	0.52	1/827 (0.1%)	0.95	3/1274 (0.2%)
All	All	0.35	6/29487 (0.0%)	0.53	17/40322 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	-10	DG	C4'-O4'	15.90	1.60	1.45
6	N	-13	DC	C4'-O4'	-9.66	1.35	1.45
7	T	10	DC	C4'-O4'	9.52	1.54	1.45
5	M	402	PHE	CG-CD1	5.91	1.47	1.38
5	M	285	TRP	CG-CD1	-5.87	1.28	1.36
5	M	258	PRO	CA-C	-5.85	1.41	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	10	DC	O4'-C4'-C3'	-16.10	96.34	106.00
6	N	-10	DG	O3'-P-O5'	-11.20	82.72	104.00
6	N	-10	DG	C1'-O4'-C4'	-8.37	101.73	110.10
6	N	-10	DG	C5'-C4'-O4'	-6.74	96.49	109.30
5	M	287	VAL	CG1-CB-CG2	-5.72	101.75	110.90
5	M	417	SER	N-CA-CB	5.70	119.05	110.50
5	M	252	LEU	CA-CB-CG	-5.58	102.46	115.30
3	D	870	ASP	CB-CG-OD2	5.21	122.99	118.30
6	N	-13	DC	C5'-C4'-O4'	5.20	119.17	109.30
5	M	47	LEU	CB-CA-C	-5.19	100.33	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	252	LEU	CB-CG-CD2	5.18	119.81	111.00
7	T	8	DA	O5'-P-OP2	-5.13	101.08	105.70
1	B	228	LEU	CA-CB-CG	5.08	126.99	115.30
7	T	10	DC	C1'-O4'-C4'	-5.08	105.02	110.10
6	N	-10	DG	OP1-P-O3'	5.07	116.36	105.20
5	M	329	LEU	CB-CG-CD2	5.03	119.56	111.00
5	M	205	GLN	N-CA-CB	5.02	119.64	110.60

There are no chirality outliers.

There are no planarity outliers.

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	2316	0	2297	55	0
1	B	1671	0	1674	32	0
2	C	10125	0	9829	279	0
3	D	9632	0	9238	112	0
4	E	546	0	548	5	0
5	M	3162	0	3169	510	0
6	N	738	0	404	39	0
7	T	738	0	404	61	0
All	All	28928	0	27563	965	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 17.

All (965) 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)
5:M:226:LEU:CD1	5:M:235:LEU:HB2	1.31	1.57
5:M:144:ILE:CD1	5:M:161:ILE:HG21	1.42	1.45
5:M:226:LEU:HD12	5:M:235:LEU:CB	1.50	1.39
5:M:17:PRO:HB3	6:N:-12:DA:C2	1.57	1.36
5:M:23:ILE:HG21	7:T:12:DT:C6	1.66	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:366:VAL:CG1	6:N:-18:DT:H3'	1.64	1.26
5:M:16:THR:CG2	5:M:19:LEU:HD12	1.69	1.23
2:C:1043:ALA:HB1	2:C:1044:PRO:CD	1.68	1.22
5:M:16:THR:HG21	5:M:19:LEU:CB	1.70	1.21
5:M:144:ILE:HD11	5:M:161:ILE:CG2	1.71	1.19
5:M:16:THR:HG21	5:M:19:LEU:CD1	1.78	1.14
5:M:144:ILE:HD11	5:M:161:ILE:HD13	1.29	1.13
5:M:144:ILE:CD1	5:M:161:ILE:HD13	1.77	1.13
2:C:906:PHE:CZ	5:M:258:PRO:HG3	1.83	1.12
5:M:23:ILE:HG23	7:T:12:DT:H71	1.23	1.12
5:M:366:VAL:HG13	6:N:-18:DT:H3'	1.13	1.11
5:M:47:LEU:HD11	5:M:297:LEU:HD12	1.22	1.11
5:M:16:THR:CG2	5:M:19:LEU:CD1	2.29	1.10
5:M:144:ILE:CD1	5:M:161:ILE:CG2	2.25	1.09
5:M:16:THR:HG21	5:M:19:LEU:HB3	1.12	1.09
2:C:854:ILE:HG22	2:C:855:PRO:CD	1.82	1.08
5:M:438:SER:O	5:M:442:LEU:HG	1.49	1.08
5:M:278:VAL:CG1	5:M:392:SER:HA	1.83	1.08
5:M:186:ASP:HB3	5:M:187:PRO:HD3	1.25	1.08
5:M:421:ARG:HG3	5:M:465:LEU:HD11	1.21	1.07
5:M:16:THR:CG2	5:M:19:LEU:HB3	1.84	1.07
5:M:287:VAL:CG1	5:M:342:ARG:HA	1.84	1.06
5:M:154:LEU:HD11	5:M:193:LYS:HB2	1.34	1.05
5:M:278:VAL:HG13	5:M:392:SER:HA	1.39	1.05
5:M:17:PRO:CB	6:N:-12:DA:C2	2.39	1.05
2:C:854:ILE:HD12	2:C:854:ILE:H	1.22	1.04
7:T:12:DT:H5"	7:T:13:DG:H5'	1.37	1.04
5:M:184:ARG:NH2	5:M:201:ILE:HD13	1.72	1.04
5:M:27:GLN:HB3	5:M:383:ARG:HG2	1.34	1.04
2:C:1043:ALA:HB1	2:C:1044:PRO:HD3	1.07	1.02
5:M:16:THR:HG22	5:M:19:LEU:HD12	1.38	1.02
5:M:144:ILE:CG1	5:M:161:ILE:HD13	1.89	1.01
5:M:26:LEU:CB	5:M:336:ARG:CD	2.37	1.01
5:M:469:PRO:HG3	6:N:-26:DG:OP1	1.60	1.01
5:M:366:VAL:HG13	6:N:-17:DT:OP2	1.61	1.01
5:M:23:ILE:HG21	7:T:12:DT:H6	1.04	1.00
5:M:26:LEU:HB2	5:M:336:ARG:CD	1.91	1.00
5:M:287:VAL:HG13	5:M:342:ARG:HA	1.05	1.00
5:M:418:THR:HG22	5:M:421:ARG:HH21	1.22	1.00
2:C:1043:ALA:CB	2:C:1044:PRO:CD	2.38	0.99
2:C:854:ILE:CG2	2:C:855:PRO:HD2	1.91	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:23:ILE:CG2	7:T:12:DT:C6	2.46	0.99
6:N:-9:DA:H1'	6:N:-8:DT:H5'	1.45	0.98
5:M:391:HIS:HB2	5:M:396:ILE:CG1	1.93	0.98
5:M:217:ARG:HH21	5:M:217:ARG:HB2	1.29	0.98
2:C:955:GLN:HE21	2:C:955:GLN:HA	1.25	0.97
5:M:16:THR:HG21	5:M:19:LEU:HD12	1.38	0.97
5:M:275:ASP:HB2	5:M:389:TYR:O	1.64	0.97
5:M:162:VAL:HG21	5:M:172:LEU:HD22	1.44	0.97
5:M:340:LEU:HB2	5:M:384:VAL:HG13	1.47	0.96
2:C:936:ARG:HD3	5:M:393:PRO:O	1.64	0.96
5:M:390:LEU:O	5:M:396:ILE:HG23	1.65	0.96
2:C:906:PHE:CE1	5:M:258:PRO:HG3	1.99	0.96
2:C:838:CYS:HB3	2:C:918:LEU:HD22	1.48	0.95
5:M:26:LEU:HB3	5:M:336:ARG:CG	1.97	0.95
5:M:17:PRO:HB3	6:N:-12:DA:N1	1.81	0.94
2:C:854:ILE:HG22	2:C:855:PRO:HD2	0.97	0.94
5:M:26:LEU:HB3	5:M:336:ARG:HG3	1.46	0.94
5:M:16:THR:HG21	5:M:19:LEU:CG	1.98	0.93
5:M:386:THR:HG23	5:M:400:LYS:NZ	1.83	0.93
5:M:184:ARG:NH2	5:M:201:ILE:CD1	2.31	0.93
5:M:20:GLN:C	5:M:23:ILE:HD11	1.88	0.93
5:M:195:LEU:CD1	5:M:199:LEU:HD11	1.98	0.93
5:M:391:HIS:HA	5:M:396:ILE:HG13	1.47	0.93
2:C:836:LEU:H	2:C:836:LEU:HD22	1.33	0.92
5:M:16:THR:HG23	5:M:20:GLN:N	1.83	0.92
5:M:144:ILE:HG21	5:M:179:LEU:HD23	1.49	0.92
5:M:421:ARG:CG	5:M:465:LEU:HD11	2.00	0.92
2:C:906:PHE:CZ	5:M:258:PRO:CG	2.52	0.91
5:M:28:LEU:HD12	5:M:28:LEU:H	1.35	0.91
5:M:456:ARG:HD3	7:T:24:DG:N7	1.85	0.91
5:M:391:HIS:HB2	5:M:396:ILE:HG12	1.52	0.91
5:M:366:VAL:HG13	6:N:-18:DT:C3'	1.98	0.91
5:M:23:ILE:CG2	7:T:12:DT:H71	2.01	0.91
5:M:46:LEU:O	5:M:299:ILE:HD12	1.70	0.91
5:M:16:THR:O	5:M:20:GLN:HB2	1.71	0.90
5:M:386:THR:HG23	5:M:400:LYS:HZ3	1.34	0.90
5:M:349:GLU:HA	5:M:352:GLN:OE1	1.72	0.90
5:M:186:ASP:HB3	5:M:187:PRO:CD	2.00	0.90
5:M:20:GLN:O	5:M:23:ILE:CD1	2.20	0.89
5:M:278:VAL:HG21	5:M:393:PRO:CD	2.01	0.89
5:M:226:LEU:CD1	5:M:235:LEU:CB	2.26	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:278:VAL:HG21	5:M:393:PRO:HD3	1.52	0.89
5:M:140:ILE:HG22	5:M:178:VAL:HG11	1.53	0.89
2:C:835:GLU:HB2	2:C:1053:TYR:HA	1.55	0.88
5:M:26:LEU:CB	5:M:336:ARG:HD3	2.04	0.88
2:C:1306:LYS:HD2	5:M:129:GLU:OE1	1.74	0.88
5:M:23:ILE:HD12	5:M:23:ILE:H	1.38	0.88
5:M:297:LEU:O	5:M:330:ILE:HD12	1.71	0.87
5:M:456:ARG:HH11	7:T:24:DG:H8	1.22	0.87
5:M:144:ILE:HD11	5:M:161:ILE:CD1	2.04	0.87
5:M:144:ILE:HD11	5:M:161:ILE:HG21	0.87	0.87
2:C:871:VAL:HG21	2:C:883:LEU:HD12	1.54	0.87
2:C:902:LEU:HD23	2:C:910:ALA:CB	2.05	0.87
5:M:181:ARG:O	5:M:181:ARG:HD3	1.74	0.87
5:M:386:THR:CG2	5:M:400:LYS:NZ	2.38	0.87
5:M:26:LEU:HB2	5:M:336:ARG:HD2	1.54	0.86
5:M:400:LYS:HE3	6:N:-16:DT:OP2	1.75	0.86
5:M:20:GLN:O	5:M:23:ILE:HD11	1.75	0.86
5:M:287:VAL:HG13	5:M:342:ARG:CA	2.00	0.86
6:N:-10:DG:H1	7:T:10:DC:H42	1.19	0.86
5:M:39:GLN:O	5:M:39:GLN:NE2	2.08	0.86
5:M:26:LEU:HD13	5:M:26:LEU:H	1.41	0.86
5:M:49:GLU:HA	5:M:296:ARG:O	1.75	0.86
5:M:279:ARG:NH2	5:M:279:ARG:O	2.09	0.85
5:M:277:LEU:HD12	5:M:277:LEU:H	1.40	0.85
1:A:315:GLY:HA3	5:M:132:PRO:HG3	1.58	0.85
5:M:26:LEU:HB3	5:M:336:ARG:CD	2.04	0.85
6:N:-11:DC:H42	7:T:11:DG:H1	1.24	0.84
5:M:366:VAL:HG11	6:N:-18:DT:H3'	1.57	0.84
5:M:431:GLU:OE1	5:M:437:LEU:HG	1.76	0.84
2:C:1022:LYS:HA	2:C:1022:LYS:CE	2.07	0.83
5:M:400:LYS:HE3	6:N:-16:DT:P	2.18	0.83
5:M:278:VAL:CG2	5:M:393:PRO:HD3	2.08	0.83
2:C:1042:LEU:HD12	2:C:1042:LEU:H	1.43	0.83
5:M:297:LEU:HB3	5:M:330:ILE:CD1	2.09	0.83
5:M:456:ARG:NH1	7:T:24:DG:C8	2.46	0.83
5:M:123:TYR:CZ	5:M:186:ASP:OD2	2.32	0.83
5:M:217:ARG:HB2	5:M:217:ARG:NH2	1.95	0.82
2:C:1032:LYS:O	2:C:1032:LYS:HD3	1.79	0.82
2:C:964:LEU:O	2:C:964:LEU:HD12	1.80	0.82
2:C:1254:VAL:HG21	5:M:112:TYR:CB	2.10	0.82
5:M:280:LYS:HE2	5:M:280:LYS:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:197:ASP:OD1	5:M:197:ASP:N	2.14	0.81
5:M:294:ILE:HD12	5:M:295:PRO:HD2	1.62	0.81
2:C:974:ARG:HH21	2:C:974:ARG:HB2	1.42	0.80
2:C:1011:LEU:HD22	2:C:1011:LEU:O	1.81	0.80
5:M:144:ILE:HG13	5:M:161:ILE:HD13	1.61	0.80
5:M:259:ARG:HG3	5:M:259:ARG:HH11	1.45	0.80
5:M:17:PRO:HG3	6:N:-12:DA:C4	2.17	0.80
5:M:193:LYS:HD2	5:M:193:LYS:O	1.81	0.80
6:N:-13:DC:H42	7:T:13:DG:H1	1.29	0.80
2:C:1032:LYS:CE	2:C:1032:LYS:HA	2.11	0.80
5:M:386:THR:HG22	5:M:400:LYS:HE2	1.64	0.79
5:M:349:GLU:O	5:M:352:GLN:HG2	1.82	0.79
5:M:391:HIS:CA	5:M:396:ILE:HG13	2.11	0.79
2:C:1032:LYS:HA	2:C:1032:LYS:HZ2	1.45	0.79
5:M:400:LYS:CE	6:N:-16:DT:OP2	2.30	0.79
5:M:22:ALA:HA	5:M:25:LEU:HD13	1.65	0.78
5:M:15:MET:CE	6:N:-11:DC:H5"	2.13	0.78
5:M:154:LEU:CD1	5:M:193:LYS:HB2	2.11	0.78
5:M:278:VAL:HG11	5:M:392:SER:CB	2.13	0.78
5:M:19:LEU:O	5:M:19:LEU:HD22	1.84	0.78
5:M:386:THR:CG2	5:M:400:LYS:CE	2.62	0.78
5:M:287:VAL:HG21	5:M:345:ARG:NH1	1.99	0.77
5:M:456:ARG:HD2	7:T:23:DT:H2'	1.65	0.77
5:M:16:THR:HG23	5:M:20:GLN:H	1.47	0.77
2:C:992:LEU:HD22	2:C:993:PRO:HD2	1.66	0.77
5:M:26:LEU:CB	5:M:336:ARG:CG	2.63	0.77
7:T:9:DT:H2"	7:T:10:DC:H5"	1.67	0.77
5:M:278:VAL:CG1	5:M:392:SER:CB	2.63	0.77
5:M:278:VAL:HG11	5:M:392:SER:HA	1.65	0.77
5:M:456:ARG:HG3	7:T:23:DT:C5	2.20	0.77
2:C:906:PHE:CE1	5:M:258:PRO:CG	2.68	0.77
5:M:26:LEU:HB2	5:M:336:ARG:HD3	1.64	0.77
5:M:336:ARG:C	5:M:336:ARG:HE	1.89	0.77
1:A:68:TYR:HB3	2:C:929:ILE:CD1	2.15	0.76
5:M:456:ARG:NH1	7:T:24:DG:H8	1.82	0.76
5:M:19:LEU:O	5:M:23:ILE:HG13	1.84	0.76
5:M:278:VAL:CG1	5:M:392:SER:CA	2.61	0.76
2:C:953:LEU:HD12	2:C:953:LEU:O	1.84	0.76
5:M:295:PRO:HD2	5:M:333:LEU:HD21	1.66	0.76
2:C:955:GLN:HA	2:C:955:GLN:NE2	1.96	0.76
5:M:456:ARG:HD2	7:T:23:DT:C2'	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:144:ILE:HD13	5:M:161:ILE:HG21	1.61	0.76
5:M:294:ILE:HD12	5:M:295:PRO:CD	2.16	0.76
2:C:1022:LYS:HA	2:C:1022:LYS:HZ3	1.50	0.76
5:M:225:ASP:OD1	5:M:225:ASP:N	2.17	0.76
5:M:217:ARG:HH21	5:M:217:ARG:CB	1.99	0.75
5:M:391:HIS:HB2	5:M:396:ILE:HG13	1.67	0.75
5:M:277:LEU:HD12	5:M:277:LEU:N	2.01	0.75
2:C:902:LEU:HD23	2:C:910:ALA:HB1	1.68	0.75
5:M:340:LEU:HB2	5:M:384:VAL:CG1	2.17	0.75
5:M:46:LEU:O	5:M:299:ILE:CD1	2.34	0.74
5:M:184:ARG:HH11	5:M:205:GLN:HE22	1.35	0.74
5:M:27:GLN:CB	5:M:383:ARG:HG2	2.16	0.74
5:M:16:THR:CG2	5:M:19:LEU:CB	2.55	0.74
5:M:421:ARG:HG3	5:M:465:LEU:CD1	2.10	0.74
5:M:273:ILE:H	5:M:273:ILE:HD12	1.53	0.74
5:M:20:GLN:C	5:M:23:ILE:CD1	2.57	0.73
5:M:47:LEU:CD1	5:M:297:LEU:HD12	2.11	0.73
5:M:278:VAL:HG11	5:M:392:SER:HB2	1.69	0.73
2:C:1032:LYS:HA	2:C:1032:LYS:NZ	2.04	0.73
5:M:226:LEU:HD12	5:M:235:LEU:HB2	0.73	0.73
2:C:1043:ALA:CB	2:C:1044:PRO:HD3	1.96	0.73
5:M:26:LEU:HB3	5:M:336:ARG:HD3	1.69	0.73
5:M:150:ASP:N	5:M:150:ASP:OD1	2.22	0.73
5:M:456:ARG:HG3	7:T:23:DT:H73	1.70	0.73
7:T:33:DC:H2"	7:T:34:DT:C6	2.24	0.73
5:M:226:LEU:HD13	5:M:235:LEU:HB2	1.62	0.72
1:A:312:LEU:HD22	5:M:181:ARG:NH1	2.03	0.72
5:M:340:LEU:CD1	5:M:388:LYS:HD2	2.20	0.72
2:C:1022:LYS:HZ3	2:C:1022:LYS:CA	2.02	0.72
5:M:400:LYS:NZ	6:N:-16:DT:OP2	2.22	0.72
7:T:32:DT:H2"	7:T:33:DC:C5	2.25	0.72
1:A:45:ARG:NH1	1:B:38:THR:OG1	2.22	0.71
5:M:121:GLN:OE1	5:M:121:GLN:HA	1.90	0.71
5:M:343:VAL:HG11	5:M:384:VAL:HG11	1.70	0.71
5:M:456:ARG:HH11	7:T:23:DT:H2"	1.55	0.71
5:M:339:THR:O	5:M:343:VAL:HB	1.90	0.71
2:C:856:ASN:ND2	5:M:257:ASP:OD2	2.23	0.71
3:D:43:THR:HG22	3:D:56:LEU:HB2	1.73	0.71
5:M:179:LEU:HD22	5:M:179:LEU:O	1.90	0.71
2:C:1032:LYS:HZ2	2:C:1032:LYS:CA	2.03	0.71
2:C:1029:LEU:HD12	2:C:1029:LEU:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:138:ARG:HB2	5:M:138:ARG:CZ	2.21	0.71
5:M:184:ARG:HH21	5:M:201:ILE:CD1	2.03	0.71
1:A:11:PRO:HA	1:A:30:PRO:HG2	1.73	0.70
5:M:140:ILE:HG12	5:M:165:ILE:HD13	1.72	0.70
5:M:130:LEU:HD23	5:M:130:LEU:N	2.05	0.70
5:M:297:LEU:O	5:M:330:ILE:CD1	2.38	0.70
5:M:456:ARG:HG3	7:T:23:DT:C7	2.21	0.70
5:M:16:THR:O	5:M:20:GLN:CB	2.38	0.70
5:M:23:ILE:HD12	5:M:23:ILE:N	2.03	0.70
5:M:390:LEU:HB3	5:M:399:LEU:HD21	1.73	0.70
5:M:388:LYS:O	5:M:399:LEU:HD23	1.92	0.70
5:M:15:MET:HE3	6:N:-11:DC:H5"	1.71	0.70
5:M:366:VAL:CG1	6:N:-17:DT:OP2	2.39	0.69
1:B:46:ILE:HG13	1:B:224:LEU:HG	1.73	0.69
5:M:421:ARG:HD2	5:M:465:LEU:HD21	1.74	0.69
2:C:1022:LYS:HA	2:C:1022:LYS:NZ	2.06	0.69
5:M:366:VAL:HG21	6:N:-18:DT:H5"	1.73	0.69
5:M:456:ARG:HG3	7:T:23:DT:C6	2.28	0.69
5:M:140:ILE:HG12	5:M:165:ILE:CD1	2.23	0.69
5:M:273:ILE:HD12	5:M:273:ILE:N	2.07	0.69
5:M:278:VAL:HG11	5:M:393:PRO:CD	2.23	0.69
5:M:391:HIS:CB	5:M:396:ILE:HG13	2.23	0.69
5:M:23:ILE:HG23	7:T:12:DT:C7	2.13	0.69
5:M:336:ARG:HH21	5:M:337:ASN:HA	1.57	0.69
5:M:125:MET:CE	5:M:142:THR:HG22	2.22	0.68
5:M:227:LEU:HD13	5:M:227:LEU:C	2.14	0.68
2:C:979:LEU:C	2:C:979:LEU:HD12	2.14	0.68
5:M:41:LEU:HG	5:M:41:LEU:O	1.92	0.68
5:M:140:ILE:CG2	5:M:178:VAL:HG11	2.24	0.68
5:M:226:LEU:HD12	5:M:235:LEU:CG	2.23	0.68
5:M:438:SER:OG	5:M:439:ASP:N	2.27	0.68
5:M:289:LEU:C	5:M:289:LEU:HD23	2.15	0.68
5:M:295:PRO:O	5:M:297:LEU:HD23	1.94	0.68
5:M:28:LEU:CD2	5:M:32:GLU:HB3	2.24	0.67
2:C:213:LEU:O	2:C:214:ASN:ND2	2.27	0.67
5:M:127:GLN:HE22	5:M:186:ASP:N	1.93	0.67
5:M:278:VAL:HG11	5:M:392:SER:CA	2.23	0.67
1:A:312:LEU:HB3	5:M:181:ARG:HH11	1.59	0.67
2:C:979:LEU:HD12	2:C:979:LEU:O	1.95	0.67
2:C:1253:LEU:HG	5:M:114:GLY:O	1.95	0.67
2:C:932:GLN:HA	2:C:932:GLN:NE2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:19:LEU:HD13	5:M:19:LEU:C	2.15	0.67
5:M:386:THR:CG2	5:M:400:LYS:HE2	2.24	0.67
5:M:349:GLU:HG2	5:M:352:GLN:OE1	1.94	0.66
5:M:421:ARG:CD	5:M:465:LEU:HD21	2.25	0.66
2:C:700:VAL:HG21	2:C:1114:GLU:HG3	1.78	0.66
2:C:1032:LYS:HD3	2:C:1032:LYS:C	2.15	0.66
5:M:187:PRO:HG2	5:M:190:VAL:HB	1.76	0.66
5:M:295:PRO:O	5:M:297:LEU:CD2	2.43	0.66
2:C:918:LEU:C	2:C:918:LEU:HD12	2.15	0.66
5:M:26:LEU:HG	5:M:336:ARG:HG2	1.78	0.66
5:M:195:LEU:CG	5:M:199:LEU:HD11	2.26	0.66
2:C:836:LEU:HD22	2:C:836:LEU:N	2.02	0.66
5:M:406:HIS:CE1	7:T:22:DG:H4'	2.31	0.66
5:M:287:VAL:HG21	5:M:345:ARG:HH12	1.59	0.66
5:M:405:SER:OG	7:T:21:DC:H5'	1.96	0.65
3:D:920:ALA:HB2	3:D:1256:ILE:HD11	1.78	0.65
2:C:1011:LEU:HD22	2:C:1011:LEU:C	2.14	0.65
2:C:906:PHE:CZ	5:M:258:PRO:CD	2.79	0.65
2:C:960:LEU:C	2:C:960:LEU:HD12	2.17	0.65
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.78	0.65
3:D:45:ASN:ND2	3:D:50:LYS:O	2.30	0.65
1:A:68:TYR:HB3	2:C:929:ILE:HD13	1.78	0.65
2:C:953:LEU:HD12	2:C:953:LEU:C	2.17	0.65
5:M:20:GLN:CA	5:M:23:ILE:HD11	2.26	0.65
5:M:124:LEU:HD12	5:M:145:VAL:HG21	1.79	0.65
1:B:47:LEU:HD13	1:B:220:ALA:HB2	1.78	0.65
2:C:954:LYS:HD2	2:C:954:LYS:O	1.96	0.65
3:D:803:VAL:HG22	3:D:1313:SER:HB3	1.78	0.65
5:M:173:GLU:OE1	5:M:173:GLU:N	2.29	0.65
3:D:98:ARG:HG2	3:D:248:ASP:HB2	1.79	0.64
5:M:120:LEU:HD13	5:M:120:LEU:O	1.97	0.64
5:M:20:GLN:O	5:M:20:GLN:NE2	2.29	0.64
5:M:120:LEU:O	5:M:120:LEU:HD22	1.97	0.64
5:M:172:LEU:N	5:M:172:LEU:HD23	2.11	0.64
5:M:23:ILE:CG2	7:T:12:DT:C5	2.79	0.64
5:M:195:LEU:O	5:M:199:LEU:HD12	1.98	0.64
5:M:287:VAL:CG1	5:M:342:ARG:CA	2.71	0.64
2:C:974:ARG:HH21	2:C:974:ARG:CB	2.11	0.64
5:M:186:ASP:CB	5:M:187:PRO:HD3	2.17	0.64
5:M:195:LEU:HD11	5:M:199:LEU:HD11	1.80	0.64
5:M:384:VAL:O	5:M:388:LYS:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:NH2	2:C:1084:ASP:OD1	2.31	0.64
5:M:181:ARG:HD3	5:M:181:ARG:C	2.16	0.64
5:M:376:MET:CE	5:M:380:THR:HG21	2.27	0.64
2:C:817:LEU:HB3	2:C:1097:VAL:HB	1.80	0.63
2:C:848:GLU:OE1	2:C:848:GLU:N	2.30	0.63
5:M:297:LEU:HB3	5:M:330:ILE:HD13	1.79	0.63
1:A:68:TYR:CB	2:C:929:ILE:HD13	2.28	0.63
1:A:315:GLY:HA3	5:M:132:PRO:CG	2.26	0.63
1:B:74:VAL:HG13	1:B:76:GLU:H	1.62	0.63
2:C:918:LEU:HD12	2:C:918:LEU:O	1.98	0.63
2:C:987:GLU:H	2:C:987:GLU:CD	2.01	0.63
2:C:706:ARG:NH2	2:C:791:LEU:O	2.32	0.63
5:M:390:LEU:HD22	5:M:397:PHE:H	1.63	0.63
5:M:455:ARG:NH2	6:N:-26:DG:O6	2.27	0.63
2:C:1070:HIS:NE2	2:C:1114:GLU:OE1	2.32	0.63
5:M:154:LEU:HD12	5:M:154:LEU:O	1.98	0.63
5:M:195:LEU:HG	5:M:199:LEU:HD11	1.78	0.63
5:M:366:VAL:HG12	5:M:368:ALA:H	1.64	0.63
5:M:289:LEU:HD23	5:M:289:LEU:O	1.98	0.63
2:C:854:ILE:CG2	2:C:855:PRO:CD	2.64	0.63
1:B:97:GLU:OE2	1:B:145:LYS:NZ	2.31	0.62
2:C:229:ILE:HD12	2:C:240:GLU:H	1.63	0.62
2:C:490:GLN:O	2:C:490:GLN:NE2	2.33	0.62
3:D:1145:PHE:HB3	3:D:1309:ILE:HD12	1.81	0.62
5:M:16:THR:HG22	5:M:19:LEU:CD1	2.14	0.62
2:C:987:GLU:OE1	2:C:987:GLU:N	2.19	0.62
5:M:23:ILE:CG2	7:T:12:DT:C7	2.74	0.62
5:M:15:MET:HE1	6:N:-11:DC:H5"	1.80	0.62
5:M:144:ILE:HD12	5:M:161:ILE:CG2	2.28	0.62
5:M:347:ILE:HD11	5:M:402:PHE:HD2	1.64	0.62
5:M:376:MET:HE3	5:M:380:THR:HG21	1.80	0.62
2:C:949:GLU:HA	2:C:949:GLU:OE1	2.00	0.62
5:M:179:LEU:O	5:M:179:LEU:HD13	1.99	0.62
5:M:386:THR:HG22	5:M:400:LYS:HG3	1.81	0.62
2:C:808:ASN:H	3:D:633:ALA:HB2	1.65	0.62
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.33	0.62
1:B:29:GLU:HG3	1:B:30:PRO:HD2	1.82	0.62
2:C:804:PHE:HB3	2:C:1100:PRO:HB3	1.82	0.62
3:D:819:GLY:HA2	3:D:883:ARG:HA	1.82	0.62
5:M:17:PRO:O	5:M:19:LEU:N	2.32	0.62
5:M:125:MET:HE3	5:M:142:THR:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:345:ARG:HG2	5:M:345:ARG:O	1.99	0.62
5:M:386:THR:HG22	5:M:400:LYS:CE	2.28	0.62
3:D:1268:ASN:HB3	3:D:1300:ALA:HA	1.82	0.61
5:M:19:LEU:HD23	7:T:12:DT:H72	1.82	0.61
2:C:975:ILE:HD11	2:C:1014:LEU:HB3	1.83	0.61
3:D:482:ALA:HA	4:E:6:VAL:HG21	1.82	0.61
5:M:144:ILE:HG13	5:M:161:ILE:CD1	2.30	0.61
5:M:281:VAL:O	5:M:281:VAL:HG13	2.01	0.61
5:M:366:VAL:HG13	6:N:-17:DT:P	2.40	0.61
5:M:418:THR:HG22	5:M:421:ARG:NH2	2.05	0.61
1:B:100:LEU:HD21	1:B:121:VAL:HG21	1.83	0.61
3:D:576:ARG:NH1	3:D:593:ASN:OD1	2.33	0.61
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.83	0.61
3:D:800:LEU:HB3	3:D:920:ALA:HB1	1.82	0.61
5:M:196:ARG:HH21	5:M:196:ARG:CG	2.14	0.61
5:M:262:GLN:O	5:M:262:GLN:HG2	2.00	0.61
5:M:340:LEU:HD13	5:M:388:LYS:HD2	1.82	0.61
2:C:1043:ALA:HB3	2:C:1046:VAL:HG23	1.83	0.61
1:A:312:LEU:HD22	5:M:181:ARG:HH12	1.66	0.60
5:M:111:VAL:HG22	5:M:111:VAL:O	2.00	0.60
2:C:12:ARG:HG3	2:C:1181:PRO:HB2	1.82	0.60
2:C:1241:ASP:O	2:C:1262:LYS:NZ	2.31	0.60
7:T:12:DT:H5”	7:T:13:DG:C5’	2.24	0.60
2:C:371:ARG:NH1	2:C:373:GLY:O	2.34	0.60
2:C:526:HIS:CE1	2:C:529:ARG:HH21	2.18	0.60
3:D:281:ARG:HG2	5:M:42:GLU:OE2	2.00	0.60
5:M:180:LYS:HZ3	5:M:180:LYS:C	2.04	0.60
3:D:1161:GLY:HA2	3:D:1179:PRO:HB3	1.82	0.60
2:C:896:THR:HG23	2:C:896:THR:O	2.00	0.60
5:M:294:ILE:O	5:M:294:ILE:HG23	2.01	0.60
5:M:28:LEU:C	5:M:28:LEU:HD13	2.22	0.60
5:M:287:VAL:CG2	5:M:345:ARG:NH1	2.63	0.60
1:A:101:THR:HG22	1:A:143:ARG:HG2	1.82	0.60
5:M:288:GLU:OE1	5:M:288:GLU:HA	2.02	0.60
1:A:262:LEU:HG	1:A:267:ALA:HB2	1.84	0.60
5:M:26:LEU:HD13	5:M:26:LEU:N	2.14	0.60
5:M:37:LEU:HD11	5:M:297:LEU:HD21	1.84	0.60
5:M:226:LEU:HD11	5:M:235:LEU:HB2	1.66	0.60
2:C:212:ALA:O	2:C:359:ARG:NH1	2.35	0.60
2:C:1062:PRO:HA	2:C:1076:ILE:HB	1.83	0.59
5:M:366:VAL:CG1	6:N:-18:DT:C3’	2.60	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:O	1:A:84:ASN:ND2	2.35	0.59
2:C:1050:VAL:HG22	2:C:1050:VAL:O	2.02	0.59
3:D:826:ILE:HB	3:D:993:GLU:HA	1.84	0.59
5:M:16:THR:HG23	5:M:16:THR:O	2.02	0.59
2:C:884:VAL:O	2:C:884:VAL:HG12	2.01	0.59
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.85	0.59
5:M:45:PRO:HD2	5:M:322:ASN:HD22	1.67	0.59
2:C:928:VAL:HG22	2:C:928:VAL:O	2.00	0.59
2:C:939:VAL:HG21	2:C:1047:LEU:HD11	1.85	0.59
5:M:28:LEU:HD22	5:M:32:GLU:HB3	1.83	0.59
2:C:1339:LEU:HD23	3:D:20:ILE:HD13	1.85	0.59
5:M:17:PRO:C	5:M:19:LEU:H	2.05	0.59
1:B:124:VAL:HG13	1:B:125:LYS:HG2	1.85	0.59
2:C:1020:GLU:HA	2:C:1020:GLU:OE2	2.03	0.59
5:M:456:ARG:HG2	5:M:457:THR:H	1.67	0.59
1:A:307:LEU:O	1:A:312:LEU:N	2.35	0.58
2:C:211:ARG:NH1	2:C:356:THR:O	2.36	0.58
5:M:259:ARG:HG2	5:M:259:ARG:O	2.02	0.58
5:M:275:ASP:CB	5:M:389:TYR:O	2.45	0.58
5:M:340:LEU:HD11	5:M:388:LYS:HD2	1.84	0.58
1:A:312:LEU:HB3	5:M:181:ARG:NH1	2.18	0.58
3:D:676:GLY:O	3:D:680:ASN:ND2	2.33	0.58
5:M:226:LEU:HD12	5:M:235:LEU:CA	2.28	0.58
5:M:406:HIS:O	7:T:22:DG:H5"	2.03	0.58
5:M:28:LEU:HD12	5:M:28:LEU:N	2.09	0.58
5:M:184:ARG:HH21	5:M:201:ILE:HD11	1.68	0.58
5:M:49:GLU:CA	5:M:296:ARG:O	2.50	0.58
1:A:312:LEU:CB	5:M:181:ARG:HH11	2.17	0.58
5:M:279:ARG:HB2	5:M:286:THR:HG22	1.85	0.58
2:C:902:LEU:CD2	2:C:910:ALA:CB	2.81	0.57
2:C:833:ILE:O	2:C:833:ILE:HG22	2.03	0.57
5:M:21:GLN:C	5:M:23:ILE:H	2.07	0.57
3:D:653:ILE:HG23	3:D:692:ARG:HH11	1.69	0.57
5:M:386:THR:HG23	5:M:400:LYS:CE	2.32	0.57
5:M:16:THR:CG2	5:M:19:LEU:HD13	2.30	0.57
5:M:438:SER:O	5:M:442:LEU:CG	2.40	0.57
6:N:-7:DC:H2"	6:N:-6:DA:C8	2.39	0.57
1:A:68:TYR:CB	2:C:929:ILE:CD1	2.83	0.57
1:B:84:ASN:ND2	1:B:129:VAL:O	2.36	0.57
2:C:197:ARG:HA	2:C:204:LEU:HD13	1.85	0.57
7:T:11:DG:OP2	7:T:11:DG:C8	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1251:TYR:N	2:C:1251:TYR:CD1	2.73	0.57
5:M:19:LEU:HD22	5:M:23:ILE:HG13	1.87	0.57
5:M:28:LEU:H	5:M:28:LEU:CD1	2.13	0.57
2:C:902:LEU:CD2	2:C:910:ALA:HB1	2.34	0.57
5:M:47:LEU:HD11	5:M:297:LEU:CD1	2.16	0.57
1:A:315:GLY:CA	5:M:132:PRO:HG3	2.34	0.57
2:C:1022:LYS:HZ3	2:C:1022:LYS:CB	2.18	0.56
2:C:1043:ALA:CB	2:C:1044:PRO:HD2	2.33	0.56
2:C:914:LYS:HD3	5:M:267:SER:OG	2.05	0.56
2:C:960:LEU:HD21	2:C:1029:LEU:HB2	1.86	0.56
2:C:1154:ASP:OD1	2:C:1157:GLN:NE2	2.38	0.56
5:M:125:MET:HE1	5:M:142:THR:HG22	1.86	0.56
2:C:906:PHE:HZ	5:M:258:PRO:HG3	1.58	0.56
3:D:807:LEU:HD11	3:D:894:VAL:HG23	1.87	0.56
5:M:278:VAL:HG11	5:M:393:PRO:HD2	1.88	0.56
5:M:386:THR:CG2	5:M:400:LYS:HZ1	2.16	0.56
2:C:954:LYS:HD2	2:C:954:LYS:C	2.25	0.56
5:M:19:LEU:CD2	7:T:12:DT:C7	2.82	0.56
5:M:156:ILE:HD13	5:M:156:ILE:N	2.20	0.56
5:M:19:LEU:O	5:M:23:ILE:CG1	2.54	0.56
2:C:873:ILE:N	2:C:873:ILE:HD13	2.20	0.56
5:M:127:GLN:NE2	5:M:186:ASP:N	2.54	0.56
3:D:352:ARG:HE	3:D:465:GLN:HB3	1.71	0.56
5:M:15:MET:HE3	6:N:-11:DC:C5'	2.35	0.56
5:M:386:THR:HA	5:M:400:LYS:HG2	1.87	0.56
5:M:127:GLN:NE2	5:M:186:ASP:HB2	2.21	0.56
3:D:110:PRO:HG2	3:D:183:GLU:HB3	1.88	0.56
1:A:33:ARG:NH1	1:A:199:ASP:OD2	2.39	0.55
2:C:488:MET:SD	2:C:488:MET:N	2.75	0.55
2:C:582:ASN:OD1	2:C:583:GLU:N	2.39	0.55
2:C:955:GLN:HE21	2:C:955:GLN:CA	2.08	0.55
3:D:126:LEU:O	3:D:220:ARG:NH1	2.40	0.55
3:D:507:VAL:HG22	3:D:601:ILE:HD11	1.88	0.55
1:A:312:LEU:HD13	3:D:393:THR:HG23	1.88	0.55
2:C:528:ARG:NH1	2:C:576:SER:O	2.39	0.55
2:C:1275:VAL:HB	3:D:343:LEU:HG	1.88	0.55
5:M:192:ALA:CB	5:M:198:CYS:HB2	2.35	0.55
3:D:309:ASN:OD1	3:D:326:SER:OG	2.24	0.55
5:M:398:GLU:HG2	5:M:401:TYR:H	1.71	0.55
5:M:123:TYR:CE1	5:M:186:ASP:OD2	2.59	0.55
1:A:18:GLN:NE2	1:A:20:SER:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.78	0.55
5:M:27:GLN:O	5:M:27:GLN:NE2	2.40	0.55
5:M:287:VAL:HG11	5:M:342:ARG:HB3	1.87	0.55
2:C:889:PRO:HA	2:C:913:VAL:HG12	1.88	0.55
1:A:80:GLU:HG2	1:A:84:ASN:HD21	1.71	0.55
1:A:131:CYS:SG	1:A:132:HIS:N	2.80	0.55
3:D:480:ALA:HA	3:D:484:MET:HB2	1.89	0.55
5:M:156:ILE:H	5:M:156:ILE:CD1	2.19	0.55
1:B:106:GLY:HA3	1:B:136:GLU:HA	1.88	0.55
5:M:340:LEU:HG	5:M:340:LEU:O	2.07	0.55
2:C:873:ILE:HD13	2:C:873:ILE:O	2.06	0.55
5:M:154:LEU:HD12	5:M:154:LEU:C	2.27	0.55
5:M:390:LEU:CD1	5:M:399:LEU:HD22	2.36	0.55
2:C:764:CYS:SG	2:C:831:ILE:HB	2.47	0.54
2:C:873:ILE:H	2:C:873:ILE:CD1	2.20	0.54
5:M:196:ARG:NH2	5:M:196:ARG:HG3	2.21	0.54
2:C:185:ASP:OD2	2:C:200:ARG:NH2	2.41	0.54
2:C:1013:GLN:HA	2:C:1013:GLN:OE1	2.07	0.54
3:D:838:ARG:HE	3:D:1231:ARG:HH12	1.54	0.54
2:C:964:LEU:HD12	2:C:964:LEU:C	2.26	0.54
2:C:1107:MET:SD	2:C:1107:MET:N	2.81	0.54
5:M:19:LEU:O	5:M:23:ILE:CD1	2.56	0.54
5:M:26:LEU:H	5:M:26:LEU:CD1	2.17	0.54
5:M:195:LEU:HD12	5:M:199:LEU:HD11	1.84	0.54
2:C:902:LEU:HD23	2:C:910:ALA:HB2	1.87	0.54
3:D:77:ARG:NH1	5:M:146:ASP:O	2.40	0.54
5:M:184:ARG:CZ	5:M:201:ILE:HD13	2.35	0.54
5:M:194:ASP:O	5:M:197:ASP:OD1	2.25	0.54
2:C:839:VAL:HA	2:C:1049:ILE:HG23	1.90	0.54
3:D:510:LEU:HD11	3:D:624:ILE:HG23	1.90	0.54
5:M:16:THR:CB	5:M:19:LEU:HB3	2.37	0.54
5:M:193:LYS:HD2	5:M:193:LYS:C	2.28	0.54
1:A:256:PRO:HA	1:A:277:TYR:HB3	1.90	0.54
5:M:271:TYR:CD1	5:M:271:TYR:N	2.74	0.54
2:C:1211:ARG:NH2	2:C:1220:GLN:OE1	2.36	0.54
2:C:841:ARG:O	2:C:841:ARG:HG3	2.08	0.54
2:C:975:ILE:HG13	2:C:1014:LEU:HD12	1.90	0.54
3:D:576:ARG:HD3	3:D:593:ASN:HA	1.89	0.53
5:M:124:LEU:HD12	5:M:145:VAL:CG2	2.38	0.53
2:C:1080:ASN:ND2	2:C:1085:MET:SD	2.81	0.53
7:T:12:DT:C5'	7:T:13:DG:H5'	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:19:LEU:CD2	7:T:12:DT:H72	2.37	0.53
5:M:354:PHE:CD1	5:M:359:GLU:HA	2.43	0.53
5:M:377:HIS:HB2	7:T:13:DG:OP2	2.08	0.53
3:D:644:MET:HG2	3:D:764:ARG:HD2	1.90	0.53
5:M:22:ALA:HB2	5:M:328:TRP:HZ2	1.74	0.53
1:B:64:VAL:HG12	1:B:66:HIS:H	1.74	0.53
2:C:1022:LYS:HA	2:C:1022:LYS:HE2	1.89	0.53
5:M:47:LEU:HD21	5:M:297:LEU:HD11	1.90	0.53
5:M:259:ARG:HH11	5:M:259:ARG:CG	2.14	0.53
5:M:278:VAL:CG1	5:M:393:PRO:HD3	2.38	0.53
7:T:29:DC:H2”	7:T:30:DC:C6	2.44	0.53
5:M:421:ARG:CD	5:M:465:LEU:HD11	2.38	0.53
2:C:850:ILE:HG22	2:C:886:LYS:HB2	1.91	0.53
2:C:979:LEU:HD13	2:C:984:VAL:HB	1.90	0.53
3:D:1024:THR:HA	3:D:1125:PRO:HB3	1.91	0.53
5:M:28:LEU:HD13	5:M:28:LEU:O	2.08	0.53
5:M:28:LEU:HD23	5:M:32:GLU:HB3	1.91	0.53
5:M:133:PHE:HZ	5:M:181:ARG:HG3	1.74	0.53
2:C:1032:LYS:HZ2	2:C:1032:LYS:CB	2.21	0.53
5:M:431:GLU:CB	5:M:437:LEU:HG	2.39	0.53
2:C:1027:LYS:HA	2:C:1030:GLU:HB3	1.92	0.52
3:D:346:ARG:H	3:D:346:ARG:HD2	1.74	0.52
3:D:1327:GLU:OE1	3:D:1329:THR:OG1	2.26	0.52
4:E:44:ASP:OD1	4:E:45:LYS:N	2.42	0.52
2:C:825:GLU:HB3	2:C:827:ARG:HG2	1.91	0.52
3:D:833:GLU:OE1	3:D:1242:ARG:NH1	2.43	0.52
2:C:840:SER:HB2	2:C:1048:LYS:H	1.74	0.52
5:M:25:LEU:HD23	5:M:26:LEU:HD12	1.91	0.52
5:M:259:ARG:HG3	5:M:259:ARG:NH1	2.21	0.52
5:M:26:LEU:N	5:M:26:LEU:CD1	2.73	0.52
5:M:127:GLN:NE2	5:M:186:ASP:H	2.07	0.52
5:M:200:LEU:HD13	5:M:200:LEU:C	2.29	0.52
5:M:278:VAL:HG21	5:M:393:PRO:CG	2.39	0.52
2:C:161:LYS:HA	2:C:170:VAL:HG12	1.92	0.52
5:M:405:SER:HB2	7:T:21:DC:H4’	1.92	0.52
2:C:150:HIS:HE1	2:C:536:GLY:HA3	1.74	0.52
2:C:798:GLN:HB3	2:C:827:ARG:HH21	1.74	0.52
2:C:148:GLN:HB2	2:C:511:LEU:HD21	1.92	0.52
2:C:836:LEU:N	2:C:836:LEU:CD2	2.73	0.52
2:C:902:LEU:HA	2:C:905:ILE:HD12	1.92	0.52
2:C:935:THR:HG22	2:C:1048:LYS:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1268:ASN:OD1	3:D:1269:ALA:N	2.42	0.52
5:M:400:LYS:HE3	6:N:-16:DT:OP1	2.10	0.52
1:A:58:GLU:HG2	1:A:145:LYS:HE2	1.91	0.52
1:A:182:ARG:HB3	1:A:206:GLU:HB3	1.91	0.52
2:C:873:ILE:N	2:C:873:ILE:CD1	2.73	0.52
2:C:1023:HIS:CE1	2:C:1027:LYS:HE3	2.45	0.52
5:M:20:GLN:HA	5:M:23:ILE:HD11	1.91	0.52
5:M:343:VAL:HG11	5:M:384:VAL:CG1	2.38	0.52
5:M:399:LEU:CD2	5:M:399:LEU:N	2.73	0.52
6:N:-11:DC:N4	7:T:11:DG:H1	2.02	0.52
2:C:797:GLY:HA3	2:C:1232:MET:O	2.10	0.51
5:M:268:GLU:O	5:M:268:GLU:HG3	2.09	0.51
5:M:287:VAL:CG2	5:M:345:ARG:HH11	2.22	0.51
2:C:295:LYS:HE2	2:C:335:THR:HG21	1.91	0.51
5:M:144:ILE:HD11	5:M:161:ILE:CB	2.37	0.51
5:M:172:LEU:N	5:M:172:LEU:CD2	2.73	0.51
5:M:278:VAL:HG11	5:M:393:PRO:HD3	1.91	0.51
5:M:279:ARG:C	5:M:279:ARG:HH21	2.13	0.51
3:D:51:PRO:HB2	3:D:58:CYS:HA	1.92	0.51
5:M:120:LEU:HD13	5:M:120:LEU:C	2.31	0.51
2:C:758:ARG:HD2	2:C:835:GLU:HB3	1.92	0.51
5:M:277:LEU:CD1	5:M:288:GLU:HB3	2.41	0.51
5:M:17:PRO:CA	6:N:-12:DA:C2	2.94	0.51
2:C:1022:LYS:NZ	2:C:1022:LYS:CB	2.73	0.51
5:M:200:LEU:HD22	5:M:200:LEU:O	2.11	0.51
5:M:431:GLU:HB2	5:M:437:LEU:HG	1.92	0.51
2:C:697:LYS:O	2:C:799:ASN:ND2	2.43	0.51
5:M:259:ARG:CG	5:M:259:ARG:NH1	2.73	0.51
5:M:277:LEU:HD11	5:M:288:GLU:HB3	1.93	0.51
2:C:592:ARG:NH1	2:C:654:ASP:O	2.43	0.51
5:M:423:LEU:HA	5:M:426:LYS:HG2	1.93	0.51
5:M:456:ARG:NH1	7:T:23:DT:H2"	2.23	0.51
2:C:1219:GLU:OE1	3:D:634:ARG:NH1	2.44	0.51
5:M:26:LEU:HG	5:M:336:ARG:CG	2.41	0.51
5:M:49:GLU:CB	5:M:296:ARG:O	2.58	0.51
5:M:377:HIS:CB	7:T:13:DG:OP2	2.59	0.51
2:C:10:ARG:HH21	2:C:1181:PRO:HG2	1.76	0.50
1:A:166:ARG:NH1	2:C:876:GLU:OE1	2.44	0.50
1:B:97:GLU:HA	1:B:146:VAL:O	2.11	0.50
2:C:1022:LYS:N	2:C:1022:LYS:HD2	2.26	0.50
5:M:28:LEU:N	5:M:28:LEU:CD1	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:409:THR:HG23	5:M:451:ILE:HA	1.92	0.50
2:C:1291:LEU:O	2:C:1295:SER:OG	2.28	0.50
3:D:291:ILE:HG23	5:M:303:TYR:CE1	2.47	0.50
5:M:227:LEU:HD22	5:M:232:PHE:HE1	1.76	0.50
1:A:118:ASP:OD1	1:A:119:GLY:N	2.42	0.50
2:C:1032:LYS:NZ	2:C:1032:LYS:CB	2.73	0.50
3:D:982:LEU:HB2	3:D:995:TYR:HB2	1.92	0.50
2:C:1017:GLN:HA	2:C:1017:GLN:OE1	2.12	0.50
5:M:19:LEU:HD21	7:T:12:DT:C7	2.40	0.50
5:M:247:LYS:O	5:M:250:VAL:HB	2.11	0.50
5:M:392:SER:C	5:M:394:ARG:H	2.15	0.50
2:C:877:VAL:O	2:C:877:VAL:HG13	2.12	0.50
5:M:142:THR:O	5:M:146:ASP:HB3	2.12	0.50
7:T:11:DG:OP2	7:T:11:DG:H8	1.94	0.50
2:C:976:ARG:HA	2:C:979:LEU:HD23	1.92	0.50
3:D:415:VAL:O	4:E:45:LYS:NZ	2.40	0.50
5:M:156:ILE:N	5:M:156:ILE:CD1	2.73	0.50
5:M:279:ARG:CB	5:M:286:THR:HG22	2.42	0.50
3:D:709:ARG:HG3	3:D:710:ASP:H	1.77	0.50
5:M:123:TYR:CD1	5:M:123:TYR:C	2.85	0.50
3:D:437:PHE:HZ	3:D:453:VAL:HG21	1.77	0.50
5:M:273:ILE:HG22	5:M:274:PRO:HD2	1.94	0.50
2:C:704:MET:HB2	2:C:707:ALA:HB3	1.94	0.49
5:M:340:LEU:HA	5:M:384:VAL:HG11	1.94	0.49
2:C:1209:GLN:HB3	2:C:1224:PRO:HB2	1.94	0.49
3:D:842:ARG:HH21	3:D:1251:LYS:HG2	1.77	0.49
5:M:456:ARG:NH1	7:T:24:DG:OP2	2.46	0.49
2:C:723:VAL:O	2:C:735:LYS:N	2.41	0.49
2:C:1032:LYS:HA	2:C:1032:LYS:HE3	1.93	0.49
2:C:1018:TYR:CD1	2:C:1018:TYR:C	2.86	0.49
2:C:995:ASP:OD1	2:C:995:ASP:N	2.46	0.49
5:M:16:THR:CG2	5:M:20:GLN:N	2.69	0.49
2:C:1037:THR:HG23	2:C:1037:THR:O	2.13	0.49
5:M:386:THR:HG21	5:M:400:LYS:HZ1	1.78	0.49
5:M:456:ARG:H	5:M:456:ARG:HE	1.61	0.49
1:A:231:PHE:HZ	1:B:201:LEU:HD11	1.77	0.49
1:B:54:CYS:HB3	1:B:148:ARG:HD2	1.95	0.49
2:C:677:ASN:N	2:C:677:ASN:OD1	2.45	0.49
5:M:387:GLN:N	5:M:387:GLN:NE2	2.60	0.49
1:A:95:LYS:HE2	1:A:98:VAL:HG12	1.95	0.49
2:C:942:ASP:HB3	2:C:946:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:976:ARG:HA	2:C:979:LEU:CD2	2.43	0.49
2:C:1315:MET:HB2	3:D:473:THR:HG21	1.95	0.49
5:M:25:LEU:HD23	5:M:25:LEU:C	2.33	0.49
3:D:290:ILE:HG12	3:D:293:ARG:HH22	1.77	0.48
3:D:646:ILE:HD11	3:D:762:ASN:HD21	1.78	0.48
5:M:184:ARG:HH11	5:M:205:GLN:NE2	2.08	0.48
6:N:-10:DG:H1'	6:N:-9:DA:H5'	1.95	0.48
1:A:68:TYR:HB3	2:C:929:ILE:HD11	1.93	0.48
3:D:45:ASN:HD21	3:D:50:LYS:HG3	1.78	0.48
5:M:405:SER:CB	7:T:21:DC:H4'	2.42	0.48
2:C:269:ILE:HD11	2:C:274:ILE:HD11	1.95	0.48
3:D:929:GLN:HB2	3:D:1138:LEU:HD13	1.95	0.48
5:M:268:GLU:N	5:M:269:PRO:HD3	2.28	0.48
5:M:295:PRO:O	5:M:297:LEU:HD22	2.13	0.48
5:M:390:LEU:HB3	5:M:399:LEU:CD2	2.42	0.48
5:M:391:HIS:CB	5:M:396:ILE:CG1	2.76	0.48
5:M:399:LEU:HD23	5:M:399:LEU:N	2.28	0.48
2:C:208:ILE:HD11	2:C:362:ALA:HB1	1.95	0.48
2:C:833:ILE:HD13	2:C:1055:ALA:HB2	1.95	0.48
3:D:460:ASP:OD1	3:D:460:ASP:N	2.46	0.48
2:C:444:ASP:HB3	2:C:447:HIS:HB2	1.94	0.48
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	1.95	0.48
5:M:276:VAL:O	5:M:276:VAL:HG12	2.14	0.48
2:C:672:GLU:HB2	3:D:767:LEU:HB2	1.96	0.48
3:D:1318:SER:OG	3:D:1321:SER:OG	2.32	0.48
5:M:133:PHE:CZ	5:M:181:ARG:HG3	2.47	0.48
2:C:870:ILE:HG22	2:C:870:ILE:O	2.13	0.48
3:D:923:ILE:O	3:D:1241:TYR:OH	2.31	0.48
2:C:1108:ASN:O	2:C:1111:GLN:HG2	2.14	0.48
5:M:279:ARG:CZ	5:M:281:VAL:HB	2.44	0.48
2:C:844:LYS:O	2:C:844:LYS:HG2	2.07	0.48
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.95	0.48
3:D:394:ILE:HG21	5:M:130:LEU:HD12	1.95	0.48
6:N:-9:DA:C1'	6:N:-8:DT:H5'	2.32	0.48
2:C:633:LEU:HA	2:C:645:PHE:O	2.13	0.47
5:M:176:GLU:O	5:M:180:LYS:HB2	2.13	0.47
5:M:297:LEU:HB3	5:M:330:ILE:HD12	1.92	0.47
5:M:390:LEU:HD13	5:M:397:PHE:O	2.14	0.47
2:C:549:ASP:OD1	2:C:550:VAL:N	2.45	0.47
2:C:841:ARG:HH22	2:C:1046:VAL:HG22	1.79	0.47
5:M:387:GLN:NE2	5:M:387:GLN:H	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:371:LYS:HD2	3:D:445:LYS:HE3	1.97	0.47
5:M:390:LEU:HD13	5:M:399:LEU:HD22	1.95	0.47
2:C:810:TYR:O	2:C:815:SER:OG	2.23	0.47
3:D:515:ARG:NH1	3:D:718:SER:O	2.46	0.47
3:D:980:THR:OG1	3:D:997:VAL:O	2.33	0.47
5:M:399:LEU:HD23	5:M:399:LEU:H	1.79	0.47
2:C:835:GLU:HG3	2:C:1053:TYR:CE1	2.50	0.47
5:M:26:LEU:CB	5:M:336:ARG:HD2	2.23	0.47
1:B:30:PRO:HB3	1:B:190:ALA:HB3	1.96	0.47
2:C:844:LYS:CE	5:M:271:TYR:HB3	2.44	0.47
2:C:852:ALA:HB2	2:C:869:GLY:N	2.30	0.47
2:C:932:GLN:NE2	2:C:932:GLN:CA	2.73	0.47
2:C:971:LEU:HD12	2:C:971:LEU:HA	1.72	0.47
2:C:1043:ALA:HB3	2:C:1046:VAL:CG2	2.45	0.47
3:D:1034:PHE:N	3:D:1081:VAL:O	2.48	0.47
5:M:125:MET:CE	5:M:142:THR:CG2	2.93	0.47
2:C:197:ARG:HH21	2:C:203:LYS:HG2	1.79	0.47
2:C:1030:GLU:OE1	2:C:1030:GLU:HA	2.15	0.47
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.96	0.47
5:M:196:ARG:HH21	5:M:196:ARG:CB	2.27	0.47
5:M:278:VAL:CG1	5:M:392:SER:HB3	2.45	0.47
2:C:845:LEU:HD11	5:M:271:TYR:CE2	2.50	0.47
5:M:180:LYS:HB3	5:M:180:LYS:HZ2	1.79	0.47
5:M:390:LEU:HD11	5:M:402:PHE:CZ	2.50	0.47
7:T:0:DC:H2"	7:T:1:DA:C8	2.50	0.47
1:A:32:GLU:OE2	1:B:150:ARG:NH2	2.37	0.46
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.96	0.46
2:C:836:LEU:HD23	2:C:836:LEU:C	2.35	0.46
1:A:66:HIS:HD2	1:A:68:TYR:HB2	1.80	0.46
1:A:158:ARG:NH2	1:A:173:VAL:O	2.45	0.46
2:C:1291:LEU:HD11	3:D:1351:VAL:HG13	1.97	0.46
5:M:377:HIS:ND1	5:M:379:SER:OG	2.47	0.46
5:M:406:HIS:O	7:T:22:DG:C5'	2.63	0.46
5:M:421:ARG:HD3	5:M:465:LEU:HD21	1.97	0.46
1:B:33:ARG:O	1:B:33:ARG:NH1	2.47	0.46
5:M:180:LYS:O	5:M:180:LYS:NZ	2.43	0.46
5:M:436:PRO:HB2	5:M:470:SER:HB3	1.97	0.46
2:C:715:THR:HG22	2:C:786:GLY:H	1.79	0.46
3:D:591:ILE:HG23	3:D:592:VAL:HG13	1.98	0.46
5:M:264:ILE:HG23	5:M:264:ILE:O	2.14	0.46
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:250:ARG:HB3	3:D:265:LEU:HD23	1.97	0.46
3:D:308:ASP:OD2	3:D:311:ARG:NH1	2.49	0.46
3:D:846:GLU:HA	3:D:860:ARG:HA	1.96	0.46
2:C:143:ARG:NH2	2:C:512:SER:O	2.43	0.46
2:C:187:GLU:HB2	2:C:195:PHE:HB2	1.98	0.46
3:D:60:ARG:H	3:D:90:VAL:HG22	1.80	0.46
5:M:142:THR:HA	5:M:145:VAL:HG12	1.98	0.46
1:B:174:ASP:OD1	1:B:174:ASP:N	2.49	0.46
2:C:538:LEU:HD13	2:C:538:LEU:H	1.81	0.46
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.97	0.46
2:C:746:ALA:HB2	2:C:967:LEU:HD21	1.97	0.46
2:C:1254:VAL:HG12	2:C:1255:THR:HG23	1.97	0.46
5:M:386:THR:HA	5:M:400:LYS:CG	2.45	0.46
7:T:20:DT:H2"	7:T:21:DC:C6	2.51	0.46
2:C:414:ILE:HD13	2:C:414:ILE:H	1.81	0.46
1:A:312:LEU:CD2	5:M:181:ARG:NH1	2.75	0.46
1:B:197:ASP:OD1	1:B:197:ASP:N	2.49	0.46
2:C:921:PRO:HB2	2:C:924:VAL:CG2	2.46	0.46
5:M:390:LEU:C	5:M:390:LEU:CD2	2.85	0.46
2:C:854:ILE:H	2:C:854:ILE:CD1	1.96	0.45
5:M:46:LEU:HD11	5:M:322:ASN:HB3	1.98	0.45
2:C:179:TYR:OH	2:C:462:ASN:OD1	2.28	0.45
2:C:1048:LYS:HE2	2:C:1048:LYS:HB2	1.78	0.45
5:M:17:PRO:C	5:M:19:LEU:N	2.70	0.45
7:T:6:DT:H2"	7:T:7:DG:C8	2.51	0.45
3:D:352:ARG:NE	3:D:465:GLN:HB3	2.31	0.45
5:M:176:GLU:OE1	5:M:176:GLU:HA	2.16	0.45
7:T:8:DA:H1'	7:T:9:DT:H5'	1.97	0.45
5:M:341:LEU:HD23	5:M:342:ARG:HG2	1.99	0.45
1:A:180:VAL:O	1:A:207:THR:HA	2.16	0.45
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.81	0.45
2:C:1042:LEU:HD12	2:C:1042:LEU:N	2.22	0.45
2:C:1253:LEU:HD12	5:M:114:GLY:HA3	1.98	0.45
3:D:70:CYS:CB	3:D:72:CYS:SG	3.05	0.45
5:M:184:ARG:NH1	5:M:205:GLN:HE22	2.10	0.45
1:A:155:ALA:O	1:A:159:ILE:HG12	2.17	0.45
2:C:206:ALA:O	2:C:208:ILE:N	2.46	0.45
3:D:814:CYS:CB	3:D:895:CYS:SG	3.05	0.45
3:D:1155:ILE:HG21	3:D:1190:ILE:HG12	1.98	0.45
5:M:144:ILE:HD11	5:M:161:ILE:CG1	2.46	0.45
5:M:350:GLN:OE1	5:M:370:ILE:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:VAL:HG13	1:B:234:LEU:H	1.82	0.45
5:M:299:ILE:HD12	5:M:300:ASN:H	1.81	0.45
2:C:1269:ARG:HA	3:D:346:ARG:HA	1.98	0.45
5:M:345:ARG:HD3	5:M:346:CYS:SG	2.57	0.45
5:M:349:GLU:O	5:M:352:GLN:CG	2.58	0.45
2:C:27:LEU:O	2:C:528:ARG:NH2	2.50	0.45
2:C:496:LYS:HB2	2:C:497:PRO:HD3	1.99	0.45
2:C:836:LEU:CD2	2:C:836:LEU:C	2.86	0.45
5:M:196:ARG:C	5:M:196:ARG:HD2	2.37	0.45
5:M:392:SER:C	5:M:394:ARG:N	2.70	0.45
6:N:-33:DG:H2”	6:N:-32:DA:N7	2.31	0.45
1:B:91:ARG:HB3	1:B:122:GLU:HB2	1.99	0.45
2:C:805:MET:O	2:C:811:ASN:ND2	2.50	0.45
3:D:453:VAL:O	3:D:456:ALA:HB3	2.17	0.45
3:D:842:ARG:HG3	3:D:882:VAL:HG21	1.99	0.45
5:M:180:LYS:HA	5:M:180:LYS:HD2	1.61	0.45
5:M:196:ARG:C	5:M:196:ARG:CD	2.86	0.45
2:C:854:ILE:HD12	2:C:854:ILE:N	2.07	0.44
3:D:1181:ASP:HA	3:D:1185:PRO:HB3	1.99	0.44
5:M:123:TYR:CD1	5:M:123:TYR:O	2.70	0.44
5:M:154:LEU:CD1	5:M:154:LEU:C	2.85	0.44
5:M:376:MET:HE2	5:M:380:THR:HG21	1.99	0.44
2:C:661:VAL:HG21	2:C:1186:VAL:HG11	1.99	0.44
3:D:65:VAL:HG13	3:D:66:LYS:HG2	1.99	0.44
5:M:25:LEU:HD23	5:M:26:LEU:N	2.33	0.44
5:M:385:THR:O	5:M:399:LEU:HB2	2.17	0.44
2:C:877:VAL:HG21	2:C:883:LEU:HD13	2.00	0.44
3:D:600:ALA:HA	3:D:603:LYS:HE3	1.99	0.44
5:M:33:LEU:O	5:M:33:LEU:HD23	2.17	0.44
5:M:454:ALA:HB1	5:M:456:ARG:NE	2.32	0.44
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.99	0.44
3:D:640:GLY:N	3:D:643:ASP:OD2	2.43	0.44
5:M:23:ILE:CD1	5:M:23:ILE:C	2.86	0.44
5:M:24:ARG:NH1	5:M:25:LEU:HA	2.33	0.44
5:M:349:GLU:C	5:M:351:GLN:N	2.68	0.44
5:M:390:LEU:HD12	5:M:399:LEU:HD22	1.99	0.44
2:C:310:ILE:H	2:C:310:ILE:HG13	1.59	0.44
3:D:824:PRO:HB3	3:D:834:PRO:HA	1.99	0.44
2:C:637:ARG:HG2	2:C:642:SER:HB3	2.00	0.44
2:C:1038:GLN:O	2:C:1038:GLN:HG3	2.13	0.44
3:D:478:LEU:HB2	4:E:20:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:147:ALA:HB1	5:M:156:ILE:HD12	1.99	0.44
5:M:202:GLN:O	5:M:206:PHE:CD1	2.71	0.44
2:C:1088:ASP:HA	2:C:1213:TYR:HD1	1.83	0.44
2:C:519:ASN:OD1	2:C:522:SER:N	2.51	0.44
3:D:95:THR:HG23	3:D:98:ARG:HH22	1.83	0.44
3:D:430:HIS:CE1	3:D:432:LEU:HB2	2.52	0.44
5:M:17:PRO:HG3	6:N:-12:DA:C5	2.52	0.44
5:M:26:LEU:C	5:M:28:LEU:H	2.21	0.44
6:N:-13:DC:N3	7:T:13:DG:N2	2.50	0.44
5:M:28:LEU:C	5:M:28:LEU:CD1	2.85	0.44
2:C:964:LEU:HD22	2:C:1025:PHE:CB	2.48	0.43
2:C:1050:VAL:O	2:C:1050:VAL:HG13	2.18	0.43
3:D:378:LYS:HB3	3:D:379:PRO:HD3	1.99	0.43
3:D:466:MET:HG3	3:D:467:ALA:H	1.83	0.43
4:E:66:VAL:HG22	4:E:69:ARG:HH12	1.83	0.43
5:M:140:ILE:CG1	5:M:165:ILE:HD13	2.44	0.43
1:A:180:VAL:HG23	1:A:181:GLU:H	1.83	0.43
1:A:228:LEU:HD13	1:B:224:LEU:HB3	2.00	0.43
2:C:559:CYS:N	2:C:574:SER:O	2.51	0.43
2:C:921:PRO:HB2	2:C:924:VAL:HG23	2.00	0.43
3:D:267:ASP:HA	3:D:270:ARG:HG2	1.99	0.43
2:C:159:SER:HB2	2:C:442:VAL:HG11	2.00	0.43
2:C:918:LEU:C	2:C:918:LEU:CD1	2.86	0.43
2:C:1073:LYS:H	2:C:1073:LYS:HD3	1.84	0.43
5:M:223:HIS:HB3	5:M:235:LEU:HD21	2.00	0.43
5:M:329:LEU:HD13	5:M:329:LEU:O	2.18	0.43
5:M:406:HIS:HE1	7:T:22:DG:H4'	1.81	0.43
1:B:48:LEU:HD11	3:D:534:GLU:HG3	2.00	0.43
2:C:1047:LEU:O	2:C:1047:LEU:HD12	2.18	0.43
3:D:1227:HIS:O	3:D:1230:THR:OG1	2.32	0.43
5:M:26:LEU:CG	5:M:336:ARG:CG	2.97	0.43
7:T:32:DT:H2"	7:T:33:DC:C6	2.54	0.43
1:B:55:ALA:HB3	1:B:175:ALA:HB1	2.00	0.43
2:C:801:ARG:HB2	2:C:1229:TYR:CE2	2.54	0.43
3:D:72:CYS:SG	3:D:88:CYS:CB	3.07	0.43
5:M:19:LEU:CD2	7:T:12:DT:H71	2.48	0.43
2:C:960:LEU:C	2:C:960:LEU:CD1	2.85	0.43
2:C:966:ILE:HA	2:C:966:ILE:HD12	1.72	0.43
2:C:979:LEU:HD13	2:C:984:VAL:CB	2.48	0.43
3:D:1208:ASP:N	3:D:1208:ASP:OD1	2.52	0.43
5:M:22:ALA:HB2	5:M:328:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:39:LYS:O	3:D:277:ASN:ND2	2.31	0.43
3:D:843:VAL:HG22	3:D:863:LEU:HD13	2.00	0.43
5:M:19:LEU:HA	5:M:22:ALA:HB3	1.99	0.43
1:A:60:GLU:HB3	1:A:170:ARG:HG3	1.99	0.43
2:C:347:ILE:HD11	2:C:433:ILE:HD13	2.00	0.43
1:B:144:ILE:HD13	1:B:144:ILE:H	1.84	0.43
2:C:474:ALA:HA	2:C:477:GLU:HG2	2.00	0.43
2:C:877:VAL:HG21	2:C:883:LEU:CD1	2.48	0.43
2:C:1268:GLN:HG2	3:D:350:SER:HB2	2.00	0.43
5:M:21:GLN:NE2	5:M:328:TRP:CZ2	2.87	0.43
5:M:131:THR:HB	5:M:132:PRO:HD2	2.01	0.43
1:A:195:ARG:HG2	1:A:196:THR:H	1.84	0.42
1:A:221:ALA:HB1	1:B:228:LEU:HD23	2.00	0.42
2:C:1004:ASP:HA	2:C:1008:GLN:NE2	2.33	0.42
5:M:277:LEU:HD11	5:M:289:LEU:CD2	2.49	0.42
5:M:456:ARG:HG2	5:M:457:THR:N	2.33	0.42
2:C:758:ARG:CD	2:C:1053:TYR:CE2	3.02	0.42
2:C:841:ARG:NH2	2:C:1046:VAL:HG22	2.34	0.42
5:M:180:LYS:HZ2	5:M:180:LYS:CB	2.31	0.42
5:M:280:LYS:O	5:M:280:LYS:HG2	2.18	0.42
7:T:7:DG:H4'	7:T:8:DA:OP1	2.19	0.42
1:A:51:MET:SD	1:A:52:PRO:HD2	2.59	0.42
1:A:98:VAL:O	1:A:145:LYS:HA	2.19	0.42
2:C:1182:ILE:HG22	2:C:1183:ALA:H	1.84	0.42
5:M:36:GLU:HA	5:M:39:GLN:HB3	2.01	0.42
5:M:144:ILE:CD1	5:M:161:ILE:CD1	2.68	0.42
5:M:386:THR:O	5:M:388:LYS:NZ	2.53	0.42
3:D:801:VAL:O	3:D:805:GLN:HB2	2.19	0.42
5:M:456:ARG:HD2	7:T:23:DT:H2"	1.99	0.42
1:A:80:GLU:HG2	1:A:84:ASN:ND2	2.33	0.42
5:M:140:ILE:HG12	5:M:165:ILE:HD11	1.99	0.42
5:M:180:LYS:HD2	5:M:183:GLN:HG3	2.00	0.42
6:N:-10:DG:C2	6:N:-9:DA:C4	3.07	0.42
1:A:166:ARG:HH22	2:C:876:GLU:CD	2.21	0.42
2:C:619:ALA:HB2	2:C:654:ASP:HB2	2.02	0.42
3:D:746:LEU:HD23	3:D:758:PRO:HB3	2.00	0.42
3:D:1237:VAL:O	3:D:1240:VAL:HG12	2.19	0.42
5:M:27:GLN:NE2	5:M:27:GLN:C	2.73	0.42
5:M:362:MET:SD	5:M:418:THR:OG1	2.75	0.42
1:A:35:PHE:HA	1:A:38:THR:HG22	2.00	0.42
2:C:678:ARG:HA	2:C:681:MET:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:865:LEU:N	2:C:865:LEU:CD2	2.82	0.42
2:C:992:LEU:HA	2:C:993:PRO:HD2	1.91	0.42
2:C:1099:ASN:OD1	2:C:1101:LEU:HB2	2.19	0.42
2:C:1278:LEU:HB3	2:C:1283:ALA:HB3	2.02	0.42
5:M:277:LEU:HD11	5:M:289:LEU:HD22	2.01	0.42
2:C:848:GLU:N	2:C:848:GLU:CD	2.72	0.42
3:D:69:GLU:HB3	3:D:76:LYS:HA	2.01	0.42
3:D:1146:GLU:OE1	3:D:1309:ILE:N	2.53	0.42
3:D:1257:VAL:HA	3:D:1260:MET:HE2	2.01	0.42
5:M:26:LEU:C	5:M:26:LEU:HD22	2.40	0.42
5:M:210:THR:HA	5:M:211:PRO:HD3	1.90	0.42
5:M:338:ASP:OD1	5:M:342:ARG:NE	2.53	0.42
5:M:354:PHE:HD1	5:M:359:GLU:HA	1.84	0.42
2:C:972:PHE:CE1	2:C:993:PRO:HB3	2.55	0.42
5:M:19:LEU:CD2	5:M:23:ILE:HG13	2.49	0.42
5:M:425:LYS:HD2	5:M:465:LEU:HD13	2.02	0.42
2:C:559:CYS:HB3	2:C:574:SER:HB3	2.02	0.41
2:C:1272:GLU:HA	2:C:1275:VAL:HG12	2.02	0.41
3:D:364:HIS:HB3	3:D:487:THR:HG23	2.02	0.41
5:M:124:LEU:CD1	5:M:145:VAL:CG2	2.98	0.41
2:C:217:THR:HG23	2:C:351:LEU:HD11	2.02	0.41
3:D:491:LEU:HB2	3:D:904:ALA:HA	2.01	0.41
1:A:111:THR:HA	1:A:129:VAL:HA	2.02	0.41
2:C:189:ASP:HB2	2:C:195:PHE:CE2	2.55	0.41
2:C:701:GLY:HA3	2:C:1182:ILE:O	2.21	0.41
2:C:1035:LYS:HE3	2:C:1035:LYS:HB2	1.22	0.41
3:D:1178:THR:HB	3:D:1179:PRO:HD3	2.02	0.41
3:D:1328:THR:O	3:D:1329:THR:C	2.59	0.41
5:M:20:GLN:C	5:M:20:GLN:NE2	2.73	0.41
2:C:67:GLU:HB2	2:C:103:VAL:HB	2.02	0.41
2:C:758:ARG:HD3	2:C:1053:TYR:CE2	2.56	0.41
5:M:162:VAL:HG21	5:M:172:LEU:CD2	2.33	0.41
2:C:862:LEU:HD12	2:C:862:LEU:HA	1.82	0.41
2:C:1251:TYR:HB3	2:C:1257:GLN:C	2.41	0.41
5:M:21:GLN:C	5:M:23:ILE:N	2.70	0.41
5:M:173:GLU:N	5:M:173:GLU:CD	2.73	0.41
5:M:456:ARG:CG	7:T:23:DT:C6	3.02	0.41
1:A:29:GLU:HB3	1:A:30:PRO:HD3	2.03	0.41
1:A:38:THR:HB	1:B:45:ARG:HG2	2.02	0.41
5:M:250:VAL:O	5:M:254:GLN:N	2.50	0.41
1:B:59:VAL:HG12	1:B:144:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ALA:HB2	1:B:126:PRO:HB2	2.02	0.41
2:C:69:GLN:HB2	2:C:101:ARG:HB3	2.03	0.41
2:C:887:VAL:HB	2:C:913:VAL:HB	2.02	0.41
5:M:123:TYR:CE1	5:M:186:ASP:HB2	2.56	0.41
5:M:294:ILE:HD12	5:M:295:PRO:N	2.36	0.41
5:M:391:HIS:O	5:M:391:HIS:CG	2.70	0.41
2:C:592:ARG:NH2	2:C:655:VAL:O	2.51	0.41
2:C:936:ARG:O	2:C:936:ARG:HG2	2.20	0.41
5:M:180:LYS:C	5:M:180:LYS:NZ	2.73	0.41
5:M:283:GLY:O	5:M:284:ARG:HG3	2.20	0.41
5:M:294:ILE:HA	5:M:295:PRO:HD3	1.90	0.41
5:M:420:ILE:O	5:M:424:VAL:HG23	2.20	0.41
1:A:68:TYR:HB2	2:C:929:ILE:HD13	1.99	0.41
2:C:366:ILE:H	2:C:366:ILE:HG13	1.65	0.41
2:C:490:GLN:HE21	2:C:490:GLN:HB2	1.65	0.41
2:C:696:ASP:OD2	2:C:799:ASN:ND2	2.33	0.41
3:D:422:LEU:HG	3:D:469:HIS:HB2	2.02	0.41
5:M:17:PRO:HG3	6:N:-12:DA:N3	2.34	0.41
5:M:28:LEU:HD23	5:M:32:GLU:HG2	2.02	0.41
5:M:215:GLU:H	5:M:215:GLU:HG2	1.63	0.41
7:T:7:DG:H1'	7:T:8:DA:H5"	2.02	0.41
2:C:886:LYS:HZ3	2:C:886:LYS:HG2	1.68	0.41
2:C:1022:LYS:CA	2:C:1022:LYS:NZ	2.73	0.41
3:D:502:PRO:HG2	3:D:601:ILE:HD12	2.03	0.41
5:M:24:ARG:O	5:M:27:GLN:HG3	2.21	0.41
5:M:196:ARG:HH21	5:M:196:ARG:HG3	1.79	0.41
1:A:312:LEU:CA	5:M:181:ARG:HH11	2.34	0.40
1:B:183:ILE:HD13	1:B:205:MET:HE2	2.03	0.40
2:C:884:VAL:HG11	2:C:1050:VAL:HG11	2.02	0.40
2:C:1120:ALA:HB2	2:C:1199:LEU:HD23	2.03	0.40
3:D:130:MET:HB3	3:D:135:ILE:HD11	2.03	0.40
5:M:125:MET:HE3	5:M:142:THR:CG2	2.51	0.40
5:M:168:ASP:OD1	5:M:168:ASP:N	2.55	0.40
5:M:196:ARG:HH21	5:M:196:ARG:HB3	1.86	0.40
5:M:219:ILE:O	5:M:219:ILE:HG22	2.21	0.40
7:T:14:DC:H2"	7:T:15:DA:C8	2.56	0.40
1:B:97:GLU:HB2	1:B:147:GLN:HG3	2.04	0.40
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.51	0.40
3:D:343:LEU:HD13	3:D:343:LEU:HA	1.87	0.40
5:M:147:ALA:HB1	5:M:156:ILE:CD1	2.51	0.40
5:M:185:PHE:HB3	5:M:186:ASP:H	1.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:277:LEU:HB2	5:M:278:VAL:H	1.76	0.40
2:C:695:ALA:HB1	2:C:795:ALA:HB3	2.03	0.40
2:C:901:LEU:HD11	2:C:905:ILE:HD11	2.02	0.40
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.87	0.40
5:M:279:ARG:NH2	5:M:281:VAL:HB	2.37	0.40
7:T:6:DT:H2"	7:T:7:DG:N7	2.37	0.40
2:C:491:ASP:OD1	2:C:491:ASP:N	2.55	0.40
2:C:700:VAL:HG13	2:C:1117:LEU:HD23	2.04	0.40
2:C:902:LEU:CD2	2:C:910:ALA:HB2	2.48	0.40
3:D:1328:THR:OG1	3:D:1329:THR:N	2.55	0.40
5:M:46:LEU:H	5:M:46:LEU:HG	1.65	0.40
5:M:227:LEU:HD13	5:M:227:LEU:O	2.19	0.40
6:N:-13:DC:N4	7:T:13:DG:H1	2.06	0.40
1:A:31:LEU:HD21	1:A:200:LYS:HA	2.03	0.40
2:C:201:ARG:HG2	2:C:202:ARG:H	1.86	0.40
2:C:1120:ALA:HB1	2:C:1198:LEU:HG	2.02	0.40
3:D:370:LYS:HG2	3:D:441:LEU:HD23	2.04	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	305/329 (93%)	283 (93%)	22 (7%)	0	100	100
1	B	218/329 (66%)	207 (95%)	11 (5%)	0	100	100
2	C	1339/1342 (100%)	1239 (92%)	89 (7%)	11 (1%)	19	51
3	D	1322/1407 (94%)	1228 (93%)	94 (7%)	0	100	100
4	E	72/91 (79%)	71 (99%)	1 (1%)	0	100	100
5	M	399/497 (80%)	330 (83%)	52 (13%)	17 (4%)	2	17
All	All	3655/3995 (92%)	3358 (92%)	269 (7%)	28 (1%)	24	51

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1043	ALA
2	C	1044	PRO
5	M	18	GLN
5	M	120	LEU
5	M	195	LEU
5	M	287	VAL
5	M	288	GLU
2	C	922	ASN
2	C	1050	VAL
5	M	111	VAL
5	M	275	ASP
5	M	296	ARG
5	M	405	SER
5	M	407	VAL
2	C	897	PRO
2	C	1005	GLU
5	M	17	PRO
2	C	895	LEU
2	C	1003	THR
5	M	291	ALA
2	C	847	PRO
2	C	919	ARG
5	M	119	THR
5	M	193	LYS
2	C	993	PRO
5	M	152	GLY
5	M	259	ARG
5	M	269	PRO

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	248/286 (87%)	242 (98%)	6 (2%)	49	74
1	B	180/286 (63%)	166 (92%)	14 (8%)	12	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	1047/1157 (90%)	920 (88%)	127 (12%)	5	18
3	D	913/1168 (78%)	882 (97%)	31 (3%)	37	65
4	E	53/75 (71%)	52 (98%)	1 (2%)	57	78
5	M	350/440 (80%)	243 (69%)	107 (31%)	0	1
All	All	2791/3412 (82%)	2505 (90%)	286 (10%)	11	26

All (286) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	115	ILE
1	A	171	LEU
1	A	180	VAL
1	A	201	LEU
1	A	207	THR
1	B	10	LYS
1	B	12	ARG
1	B	14	VAL
1	B	16	ILE
1	B	33	ARG
1	B	65	LEU
1	B	133	LEU
1	B	144	ILE
1	B	145	LYS
1	B	150	ARG
1	B	182	ARG
1	B	196	THR
1	B	224	LEU
1	B	228	LEU
2	C	28	LEU
2	C	37	LYS
2	C	49	LEU
2	C	164	THR
2	C	171	LEU
2	C	208	ILE
2	C	209	ILE
2	C	210	LEU
2	C	214	ASN
2	C	221	LEU
2	C	229	ILE
2	C	324	LYS

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Mol	Chain	Res	Type
2	C	397	LEU
2	C	414	ILE
2	C	487	LEU
2	C	488	MET
2	C	490	GLN
2	C	538	LEU
2	C	540	ARG
2	C	589	THR
2	C	603	ILE
2	C	677	ASN
2	C	697	LYS
2	C	748	ILE
2	C	761	GLN
2	C	783	LEU
2	C	830	THR
2	C	831	ILE
2	C	834	GLN
2	C	835	GLU
2	C	836	LEU
2	C	838	CYS
2	C	840	SER
2	C	841	ARG
2	C	842	ASP
2	C	843	THR
2	C	844	LYS
2	C	845	LEU
2	C	848	GLU
2	C	850	ILE
2	C	854	ILE
2	C	856	ASN
2	C	862	LEU
2	C	864	LYS
2	C	865	LEU
2	C	868	SER
2	C	870	ILE
2	C	873	ILE
2	C	881	ASP
2	C	882	ILE
2	C	886	LYS
2	C	887	VAL
2	C	890	LYS
2	C	895	LEU

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Mol	Chain	Res	Type
2	C	901	LEU
2	C	902	LEU
2	C	903	ARG
2	C	913	VAL
2	C	915	ASP
2	C	917	SER
2	C	918	LEU
2	C	919	ARG
2	C	922	ASN
2	C	925	SER
2	C	927	THR
2	C	928	VAL
2	C	931	VAL
2	C	933	VAL
2	C	936	ARG
2	C	937	ASP
2	C	940	GLU
2	C	944	ARG
2	C	946	LEU
2	C	948	ILE
2	C	953	LEU
2	C	954	LYS
2	C	955	GLN
2	C	957	LYS
2	C	958	LYS
2	C	959	ASP
2	C	962	GLU
2	C	964	LEU
2	C	966	ILE
2	C	968	GLU
2	C	971	LEU
2	C	974	ARG
2	C	975	ILE
2	C	978	VAL
2	C	984	VAL
2	C	992	LEU
2	C	995	ASP
2	C	1006	GLU
2	C	1011	LEU
2	C	1013	GLN
2	C	1014	LEU
2	C	1016	GLU

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Mol	Chain	Res	Type
2	C	1017	GLN
2	C	1021	LEU
2	C	1022	LYS
2	C	1024	GLU
2	C	1028	LYS
2	C	1029	LEU
2	C	1032	LYS
2	C	1035	LYS
2	C	1036	ILE
2	C	1038	GLN
2	C	1040	ASP
2	C	1042	LEU
2	C	1046	VAL
2	C	1047	LEU
2	C	1048	LYS
2	C	1049	ILE
2	C	1051	LYS
2	C	1052	VAL
2	C	1054	LEU
2	C	1056	VAL
2	C	1057	LYS
2	C	1058	ARG
2	C	1059	ARG
2	C	1073	LYS
2	C	1119	MET
2	C	1140	LYS
2	C	1161	LEU
2	C	1166	ASP
2	C	1210	ILE
2	C	1237	HIS
2	C	1251	TYR
3	D	50	LYS
3	D	53	ARG
3	D	72	CYS
3	D	144	TYR
3	D	161	THR
3	D	167	ASP
3	D	223	LEU
3	D	245	LEU
3	D	274	ASN
3	D	321	LYS
3	D	325	LYS

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Mol	Chain	Res	Type
3	D	342	LEU
3	D	346	ARG
3	D	363	LEU
3	D	395	LYS
3	D	422	LEU
3	D	428	THR
3	D	430	HIS
3	D	518	VAL
3	D	649	LYS
3	D	695	LYS
3	D	709	ARG
3	D	821	MET
3	D	836	ARG
3	D	842	ARG
3	D	901	ARG
3	D	930	LEU
3	D	1159	ILE
3	D	1240	VAL
3	D	1247	LYS
3	D	1266	ILE
4	E	21	LEU
5	M	19	LEU
5	M	20	GLN
5	M	23	ILE
5	M	24	ARG
5	M	25	LEU
5	M	26	LEU
5	M	27	GLN
5	M	28	LEU
5	M	33	LEU
5	M	41	LEU
5	M	42	GLU
5	M	113	GLN
5	M	117	THR
5	M	120	LEU
5	M	123	TYR
5	M	124	LEU
5	M	125	MET
5	M	130	LEU
5	M	134	THR
5	M	138	ARG
5	M	143	SER

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Mol	Chain	Res	Type
5	M	145	VAL
5	M	146	ASP
5	M	148	VAL
5	M	149	ASP
5	M	150	ASP
5	M	153	TYR
5	M	154	LEU
5	M	156	ILE
5	M	172	LEU
5	M	173	GLU
5	M	176	GLU
5	M	180	LYS
5	M	181	ARG
5	M	184	ARG
5	M	185	PHE
5	M	188	VAL
5	M	193	LYS
5	M	196	ARG
5	M	197	ASP
5	M	199	LEU
5	M	201	ILE
5	M	202	GLN
5	M	217	ARG
5	M	218	LEU
5	M	220	ILE
5	M	224	LEU
5	M	225	ASP
5	M	226	LEU
5	M	233	ARG
5	M	252	LEU
5	M	254	GLN
5	M	259	ARG
5	M	264	ILE
5	M	265	GLN
5	M	267	SER
5	M	270	GLU
5	M	271	TYR
5	M	272	VAL
5	M	273	ILE
5	M	275	ASP
5	M	276	VAL
5	M	277	LEU

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Mol	Chain	Res	Type
5	M	279	ARG
5	M	280	LYS
5	M	287	VAL
5	M	288	GLU
5	M	289	LEU
5	M	293	SER
5	M	294	ILE
5	M	296	ARG
5	M	297	LEU
5	M	299	ILE
5	M	323	LEU
5	M	329	LEU
5	M	331	LYS
5	M	335	SER
5	M	336	ARG
5	M	338	ASP
5	M	340	LEU
5	M	341	LEU
5	M	342	ARG
5	M	343	VAL
5	M	344	SER
5	M	345	ARG
5	M	347	ILE
5	M	350	GLN
5	M	378	GLU
5	M	379	SER
5	M	383	ARG
5	M	386	THR
5	M	387	GLN
5	M	390	LEU
5	M	391	HIS
5	M	394	ARG
5	M	398	GLU
5	M	399	LEU
5	M	400	LYS
5	M	405	SER
5	M	408	ASN
5	M	426	LYS
5	M	435	LYS
5	M	452	MET
5	M	455	ARG
5	M	456	ARG

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Mol	Chain	Res	Type
5	M	460	LYS
5	M	474	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
2	C	490	GLN
2	C	526	HIS
2	C	834	GLN
2	C	932	GLN
2	C	955	GLN
2	C	1038	GLN
3	D	45	ASN
3	D	450	HIS
5	M	27	GLN
5	M	34	GLN
5	M	39	GLN
5	M	127	GLN
5	M	205	GLN
5	M	322	ASN
5	M	387	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-14200. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

| X | Y | Z |
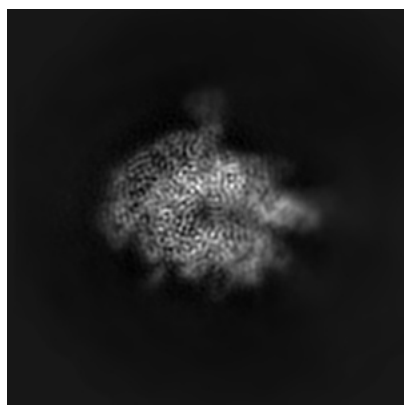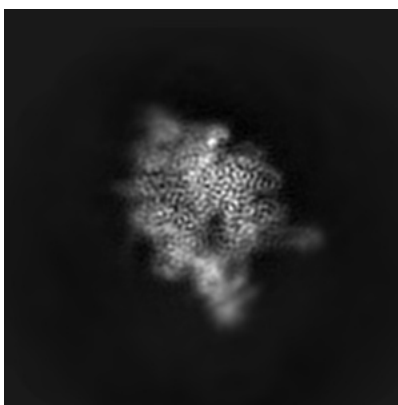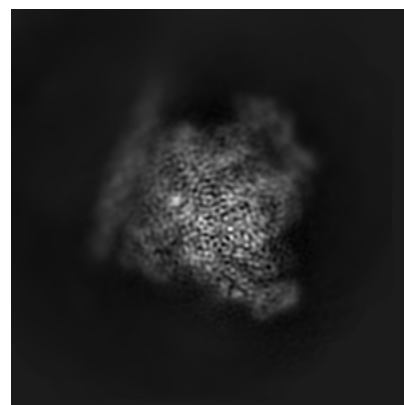
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
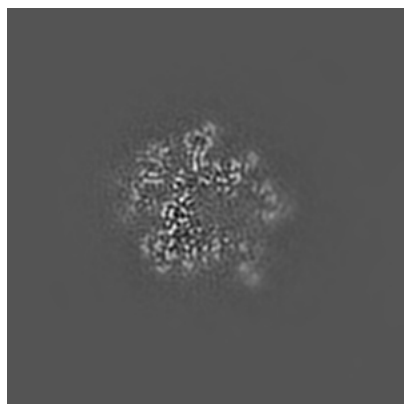
6.2.1 Primary map
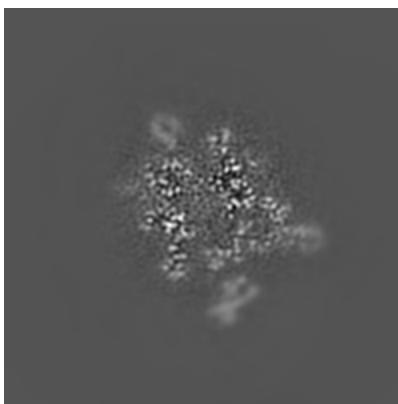
| X Index: 128 | Y Index: 128 | Z Index: 128 |
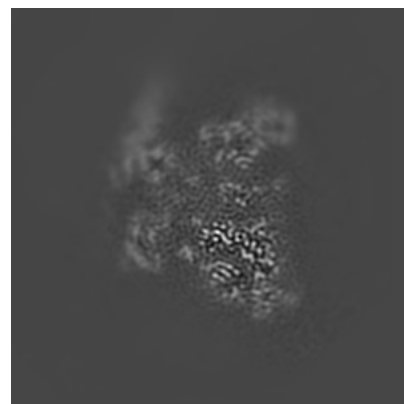
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
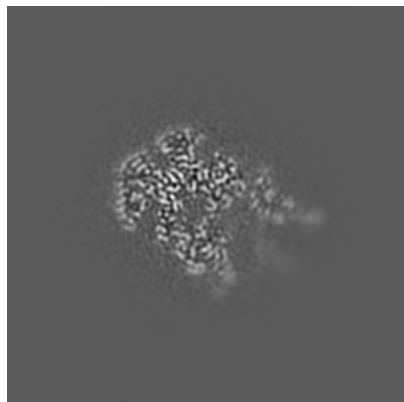
6.3.1 Primary map
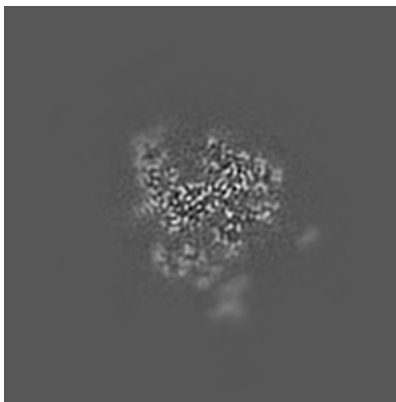
| X Index: 145 | Y Index: 115 | Z Index: 144 |
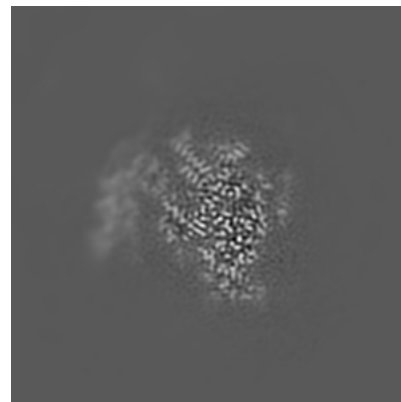
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

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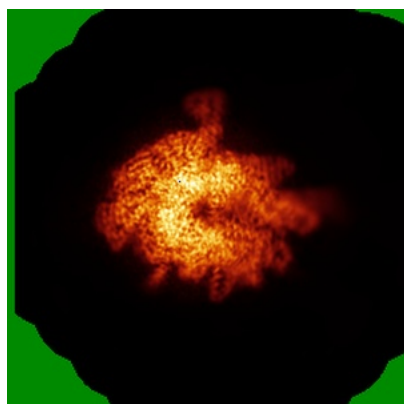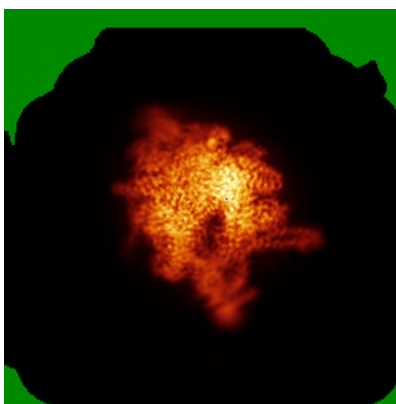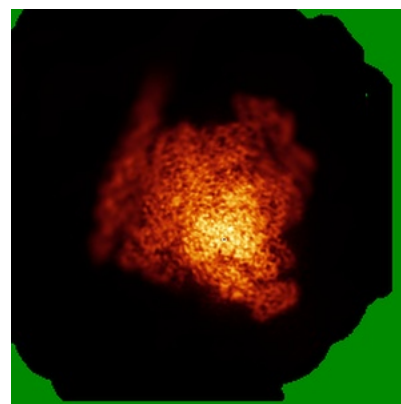
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X   Y   Z
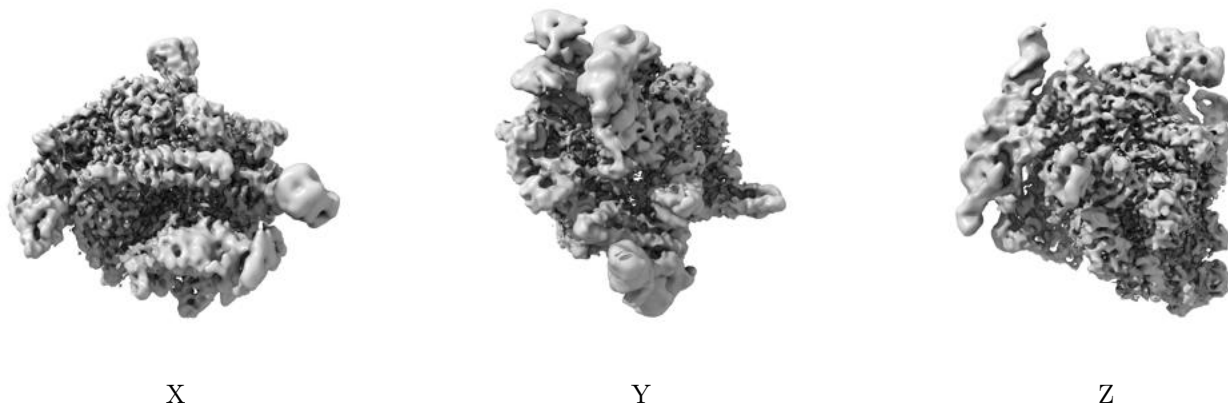
The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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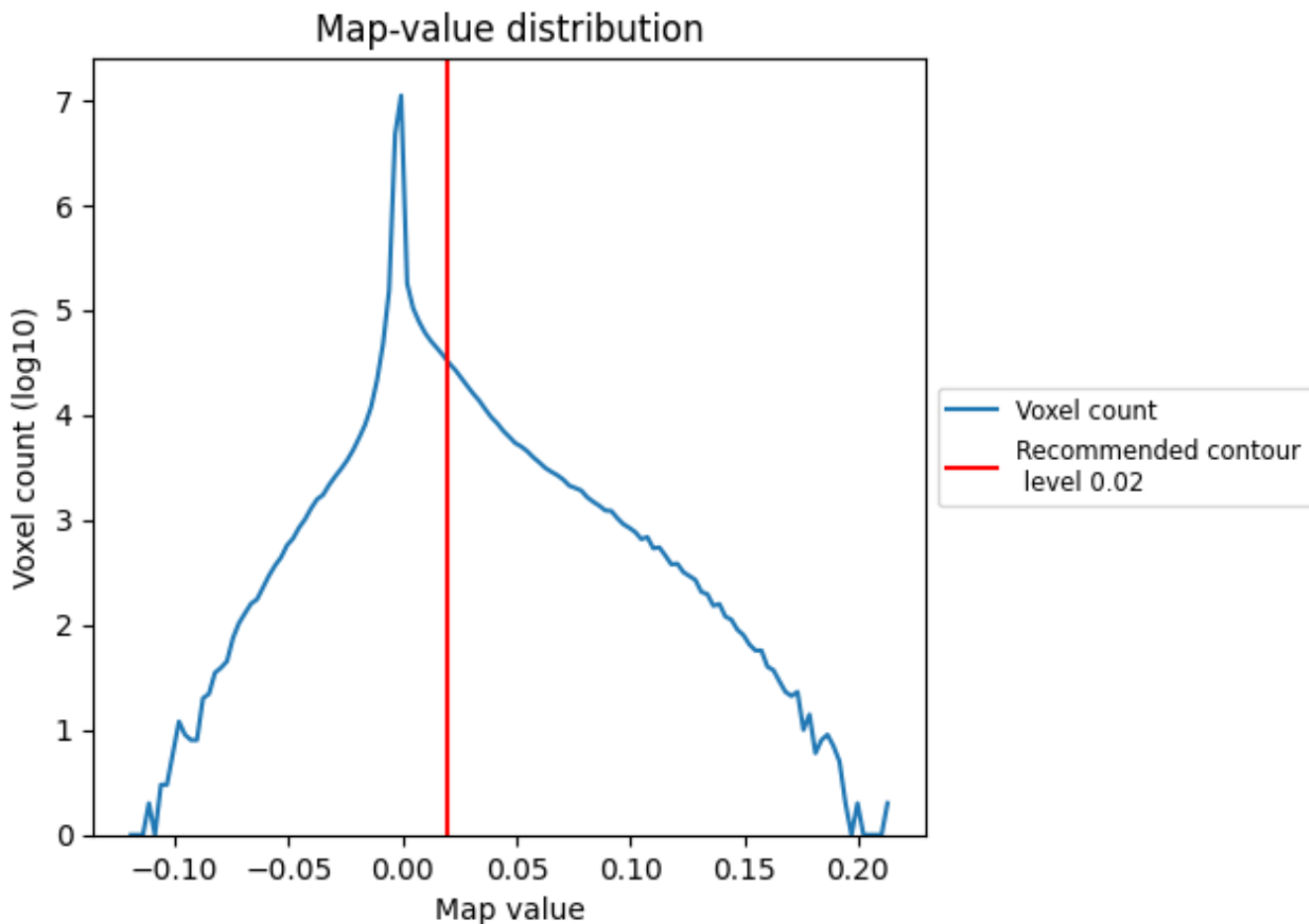
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
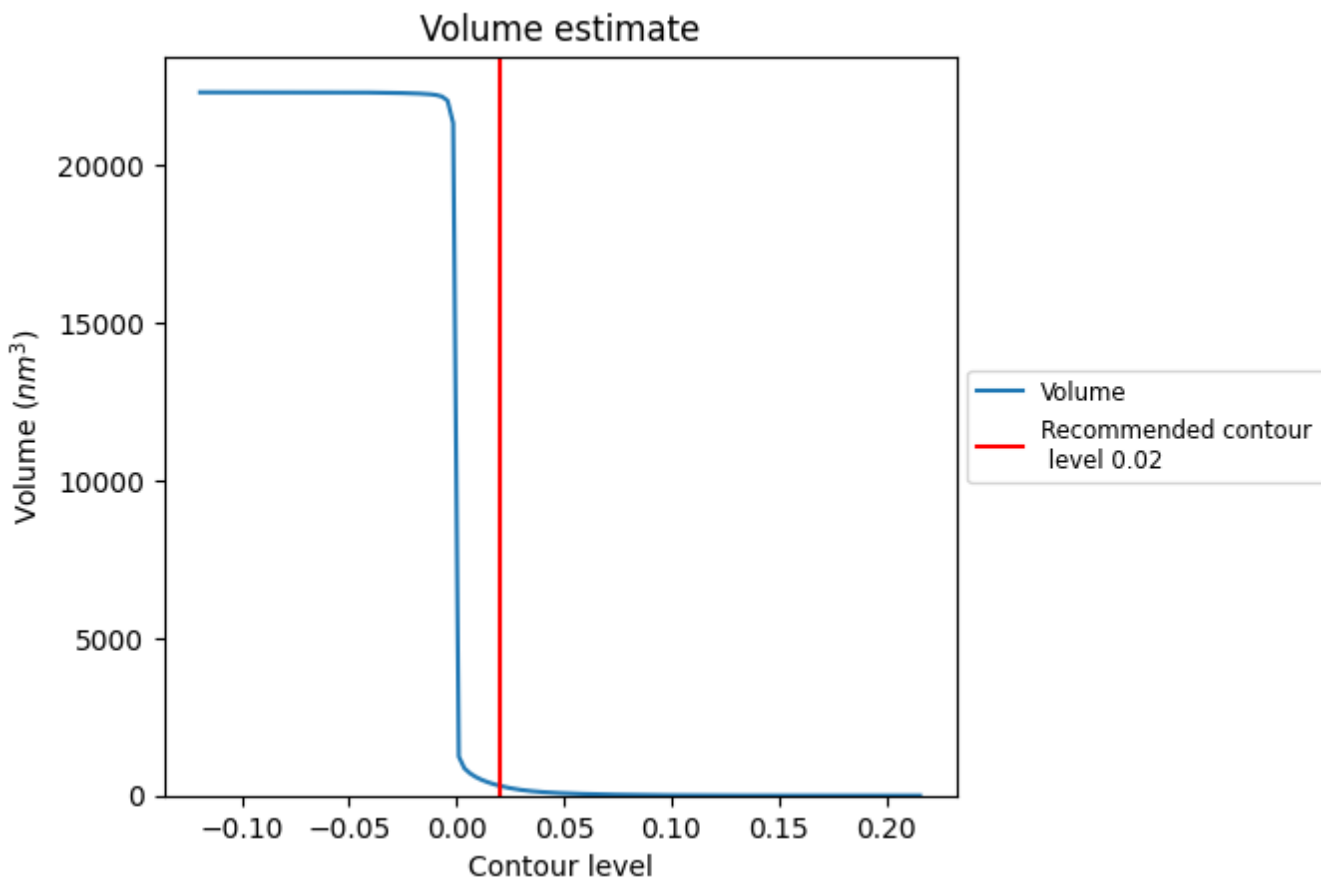
The volume at the recommended contour level is 312 nm^3; this corresponds to an approximate mass of 281 kDa.

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 ⓘ
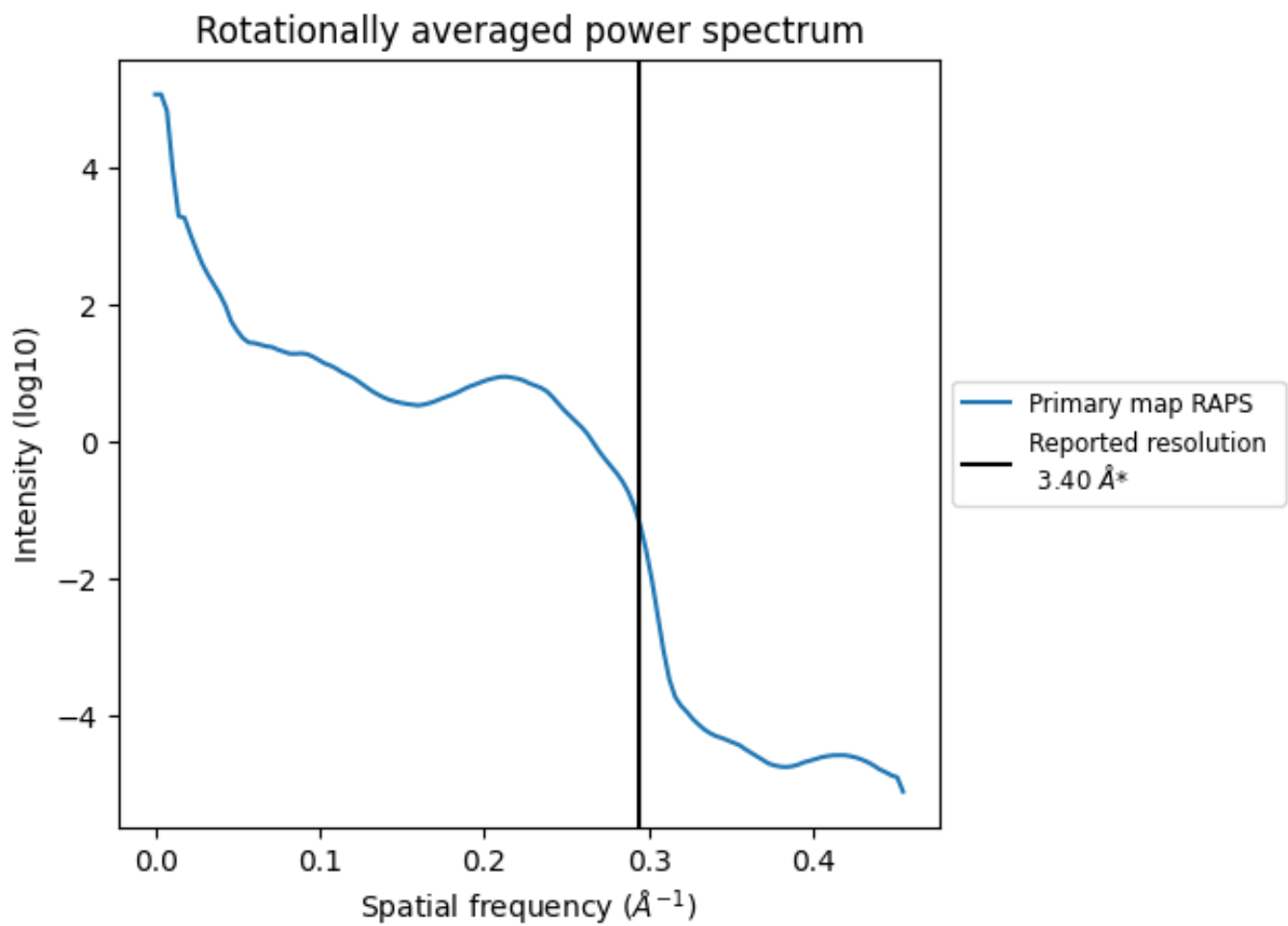
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14200 and PDB model 7QXI. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay (i)

X   Y   Z
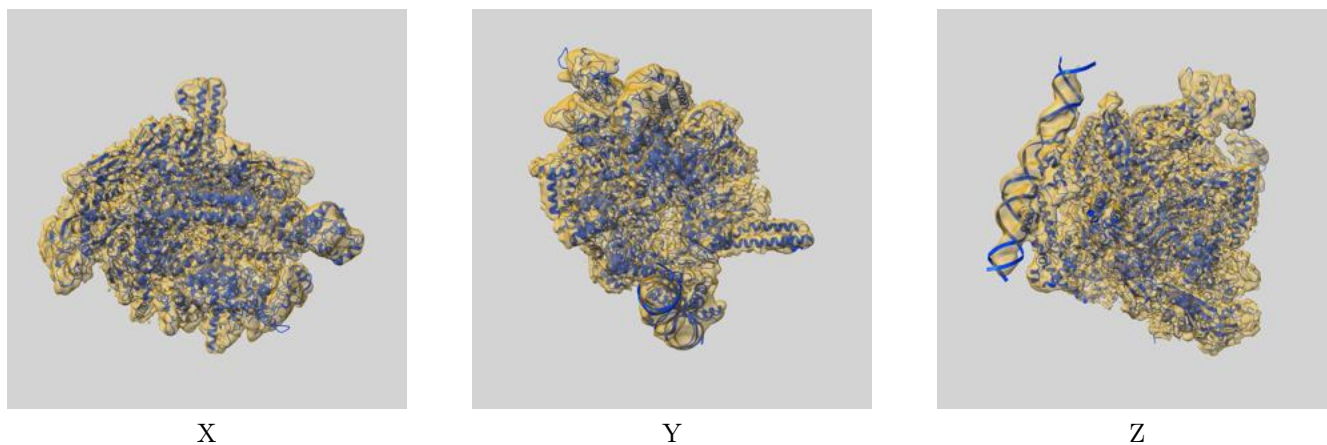
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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 ⓘ

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 (0.02).

9.4 Atom inclusion ⓘ
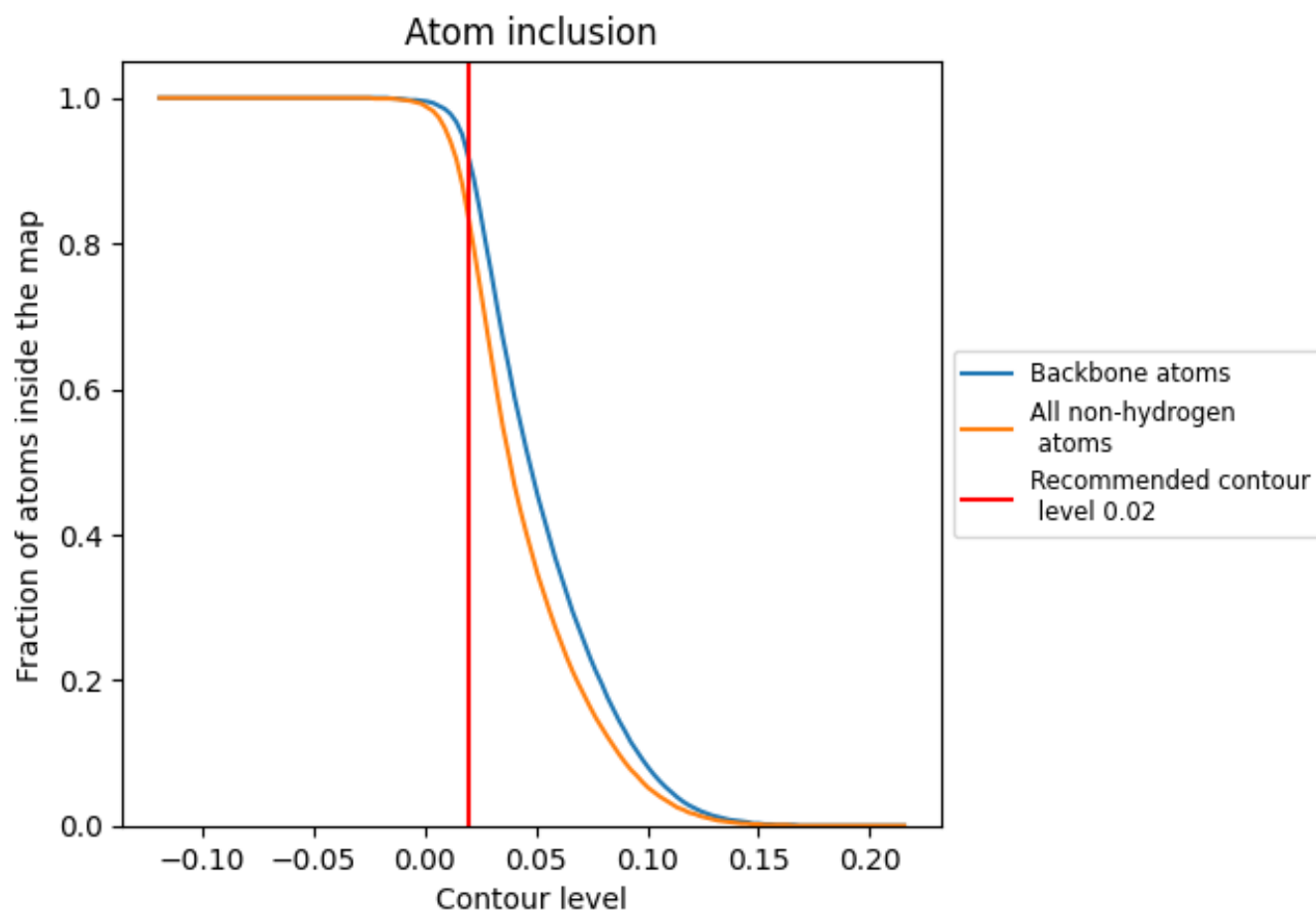
At the recommended contour level, 91% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8290	0.3640
A	0.7870	0.3820
B	0.8450	0.3680
C	0.8610	0.4040
D	0.8310	0.3630
E	0.8770	0.4130
M	0.7920	0.3010
N	0.7470	0.1710
T	0.6800	0.1780

1.0

0.0
<0.0