Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 04:35 am GMT

PDB ID	:	6GYS
EMDB ID	:	EMD-0096
Title	:	Cryo-EM structure of the CBF3-CEN3 complex of the budding yeast kinetochore
Authors	:	Yan, K.; Zhang, Z.; Yang, J.; McLaughlin, S.H.; Barford, D.
Deposited on	:	2018-07-01
Resolution	:	4.40 Å(reported)
Based on initial model	:	6GYP

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 (i) 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 (i)) were used in the production of this report:

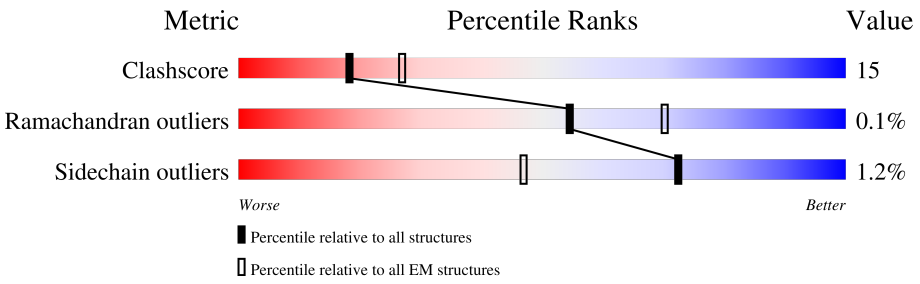
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	478	53% 33% • 12%
1	H	478	• 54% 32% • 12%
2	B	608	• 66% 29% • 5%
2	C	608	6% 68% 26% • 6%
2	I	608	13% 60% 35% 5%
2	J	608	18% 63% 28% 9%
3	D	194	46% 31% • 22%
3	K	194	• 45% 31% • 22%

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Mol	Chain	Length	Quality of chain
4	E	956	35% 17% 47%
4	L	956	32% 21% 47%
5	F	52	29% 62% 37%
6	G	52	27% 65% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	ZN	J	701	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 38890 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 Centromere DNA-binding protein complex CBF3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	421	3517	2294	592	619	12	0	0
1	H	421	3517	2294	592	619	12	0	0

- Molecule 2 is a protein called Centromere DNA-binding protein complex CBF3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	579	4775	3084	786	876	29	0	0
2	C	573	4691	3029	773	860	29	0	0
2	I	579	4775	3084	786	876	29	0	0
2	J	554	4575	2958	751	837	29	0	0

- Molecule 3 is a protein called Suppressor of kinetochore protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	151	1226	767	214	241	4	0	0
3	K	151	1226	767	214	241	4	0	0

- Molecule 4 is a protein called Centromere DNA-binding protein complex CBF3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	506	4224	2731	698	785	10	0	0
4	L	506	4224	2731	698	785	10	0	0

- Molecule 5 is a DNA chain called DNA (52-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	F	52	1079	518	205	304	52	0	0

- Molecule 6 is a DNA chain called DNA (52-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	G	52	1053	512	169	320	52	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

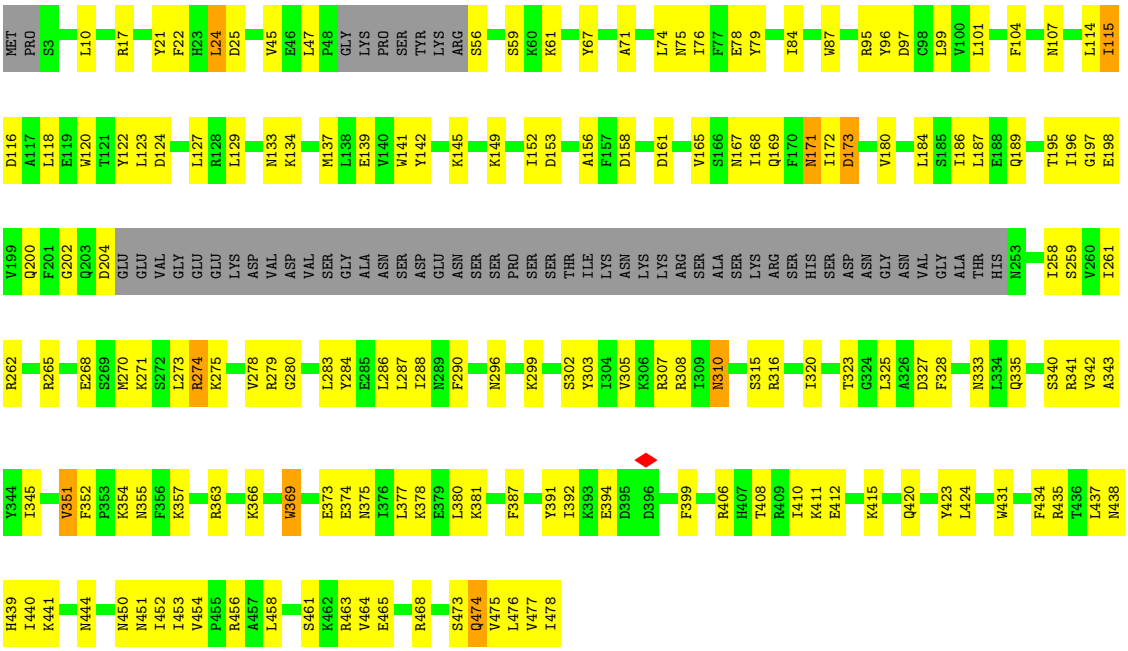
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
7	B	2	2	2	0
7	C	2	2	2	0
7	I	2	2	2	0
7	J	2	2	2	0

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.

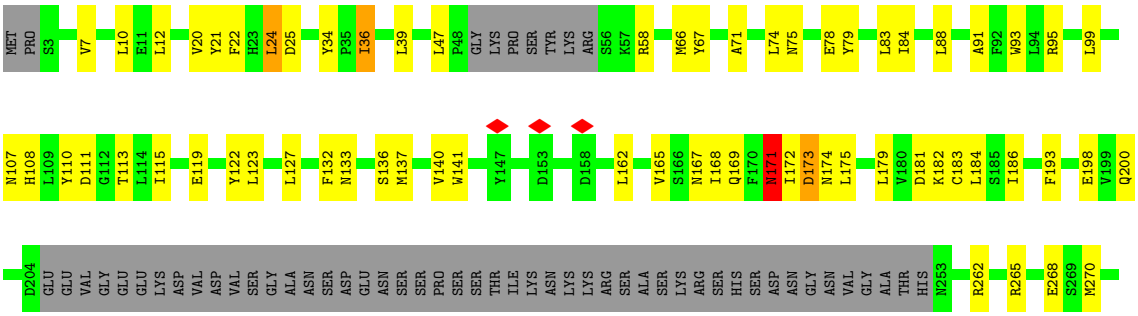
• Molecule 1: Centromere DNA-binding protein complex CBF3 subunit C

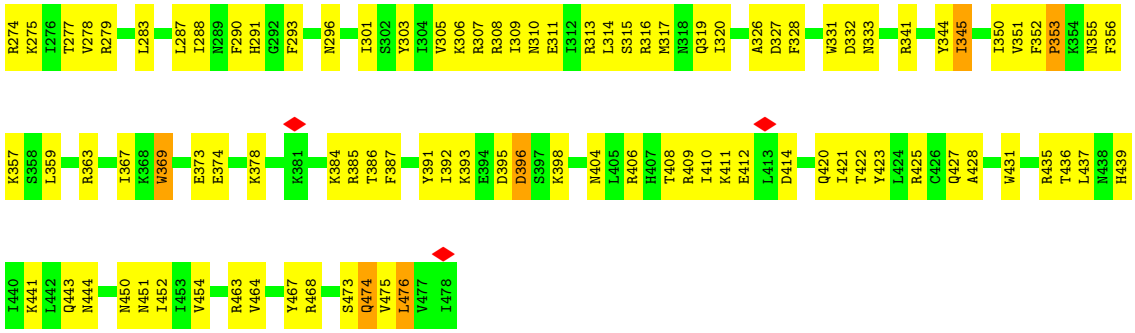
Chain A: 53% 33% • 12%



• Molecule 1: Centromere DNA-binding protein complex CBF3 subunit C

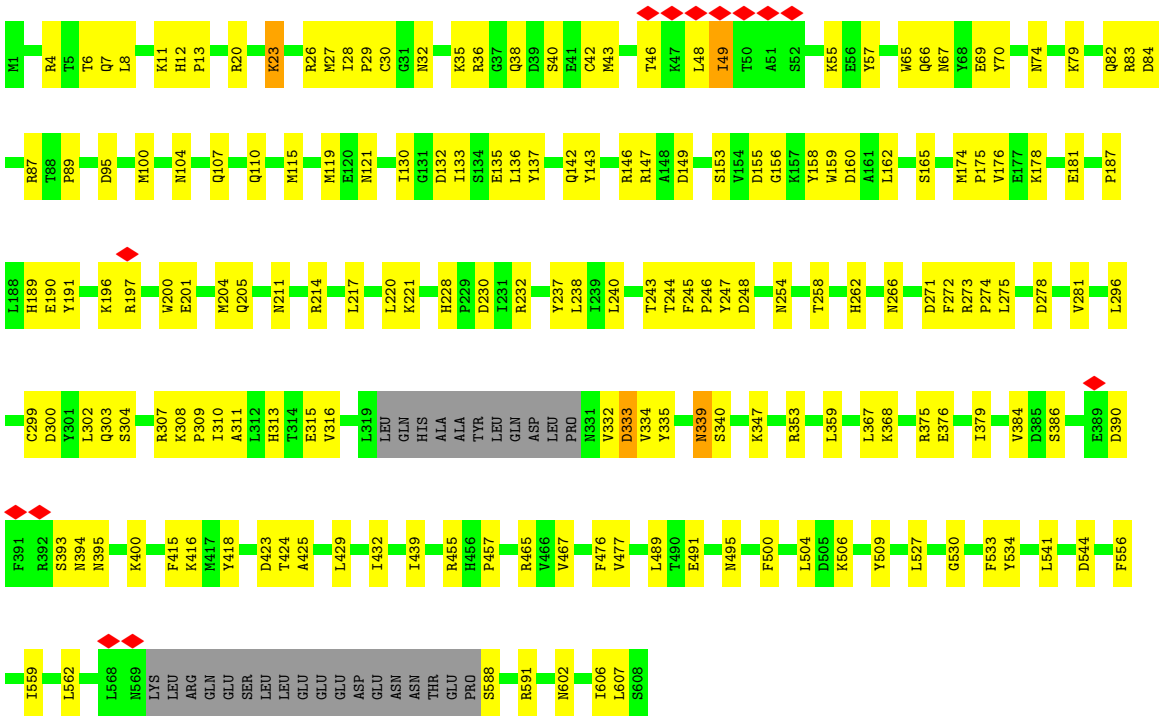
Chain H: • 54% 32% • 12%





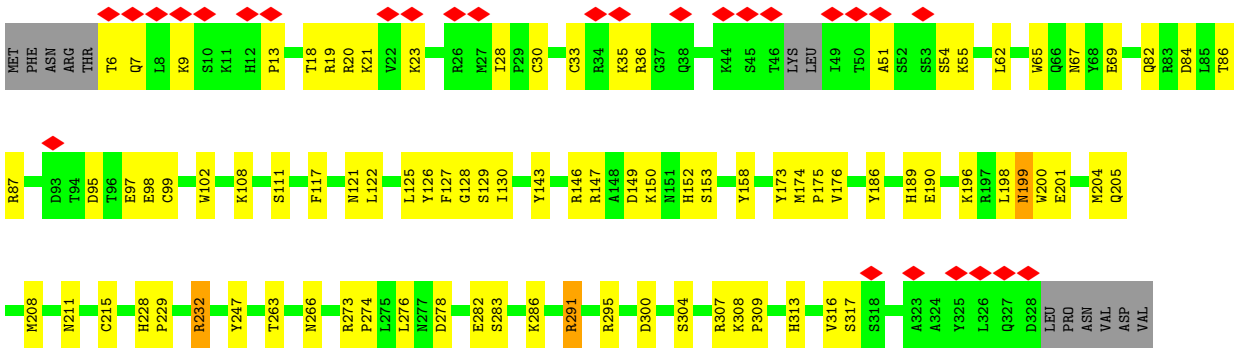
• Molecule 2: Centromere DNA-binding protein complex CBF3 subunit B

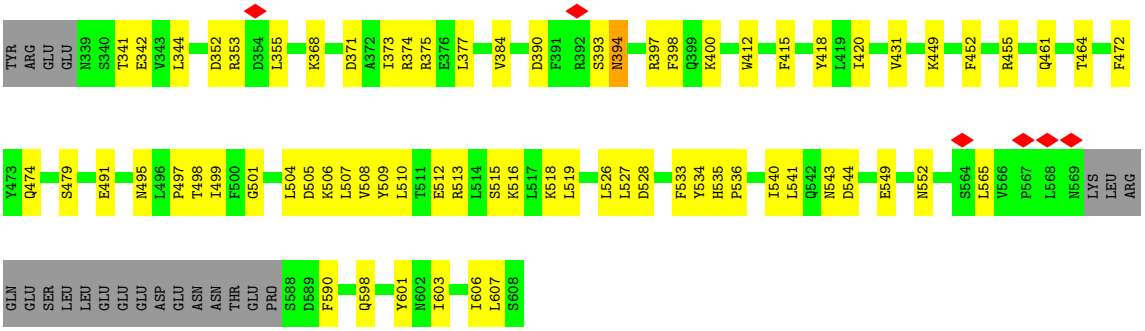
Chain B:



• Molecule 2: Centromere DNA-binding protein complex CBF3 subunit B

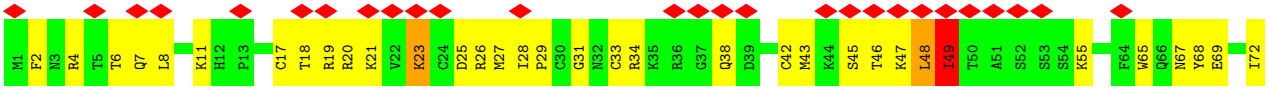
Chain C:

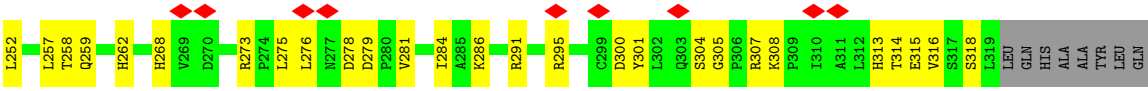


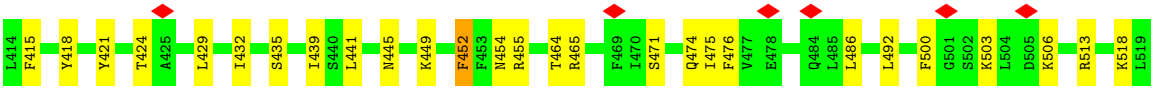


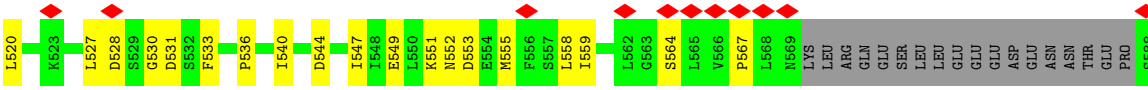
• Molecule 2: Centromere DNA-binding protein complex CBF3 subunit B

Chain I:



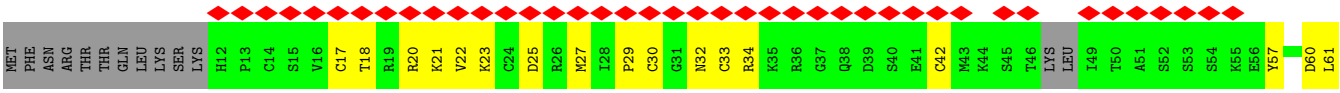


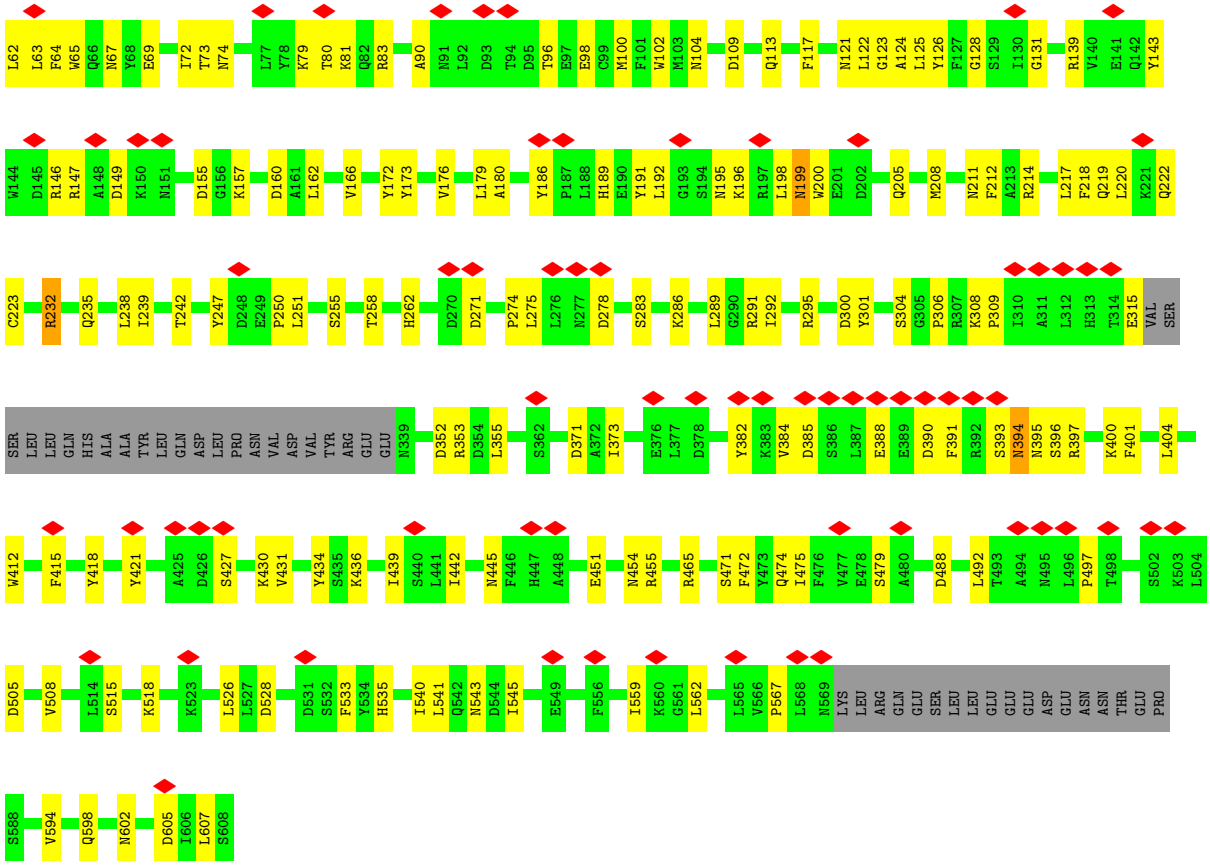




• Molecule 2: Centromere DNA-binding protein complex CBF3 subunit B

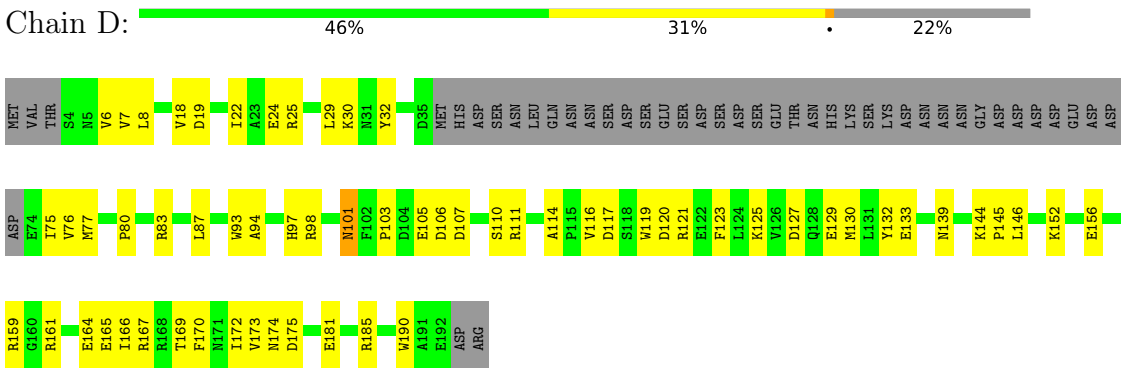
Chain J:





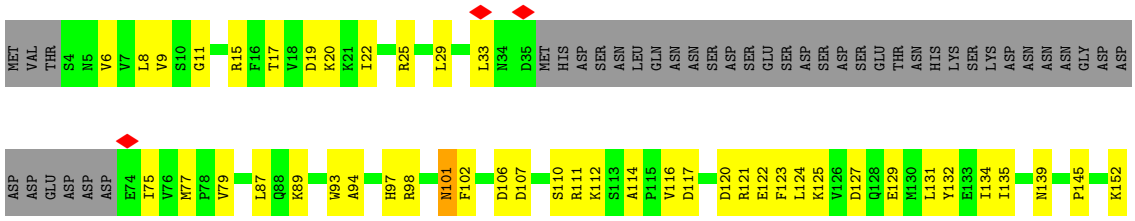
- Molecule 3: Suppressor of kinetochore protein 1

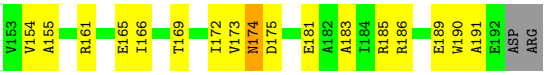
Chain D:



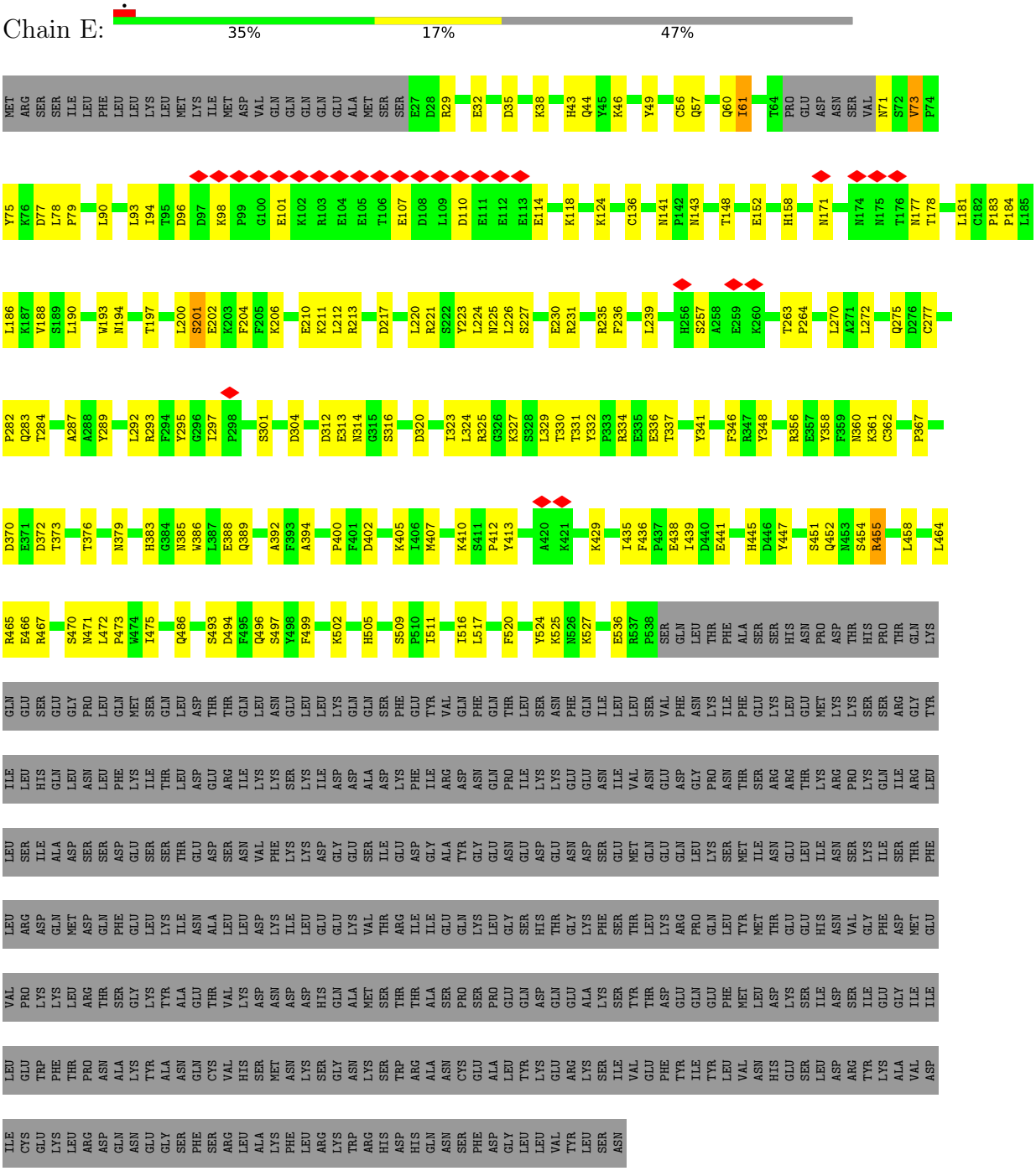
- Molecule 3: Suppressor of kinetochore protein 1

Chain K:

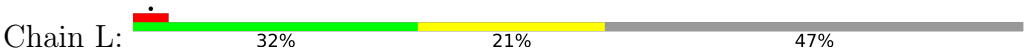


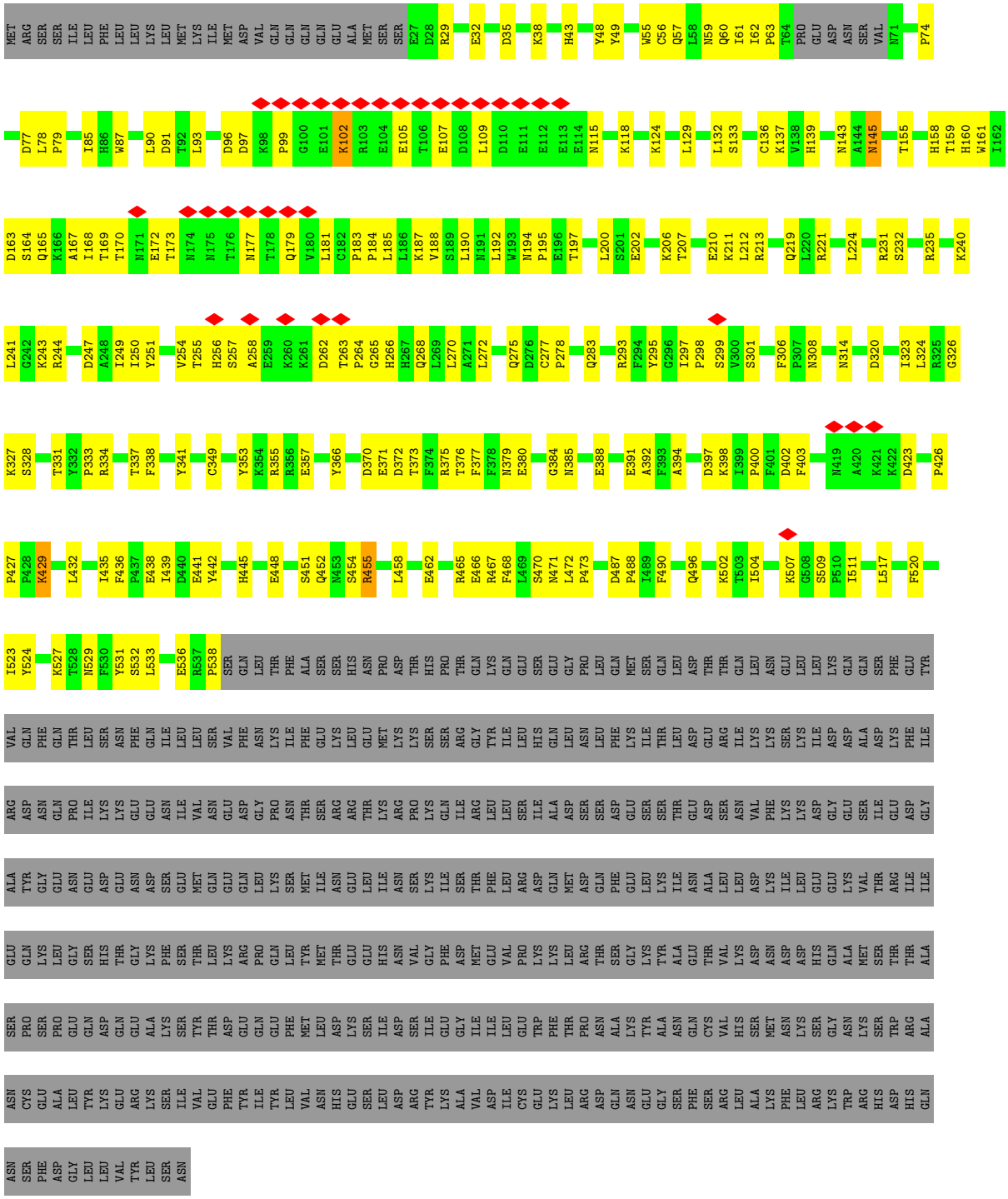


• Molecule 4: Centromere DNA-binding protein complex CBF3 subunit A



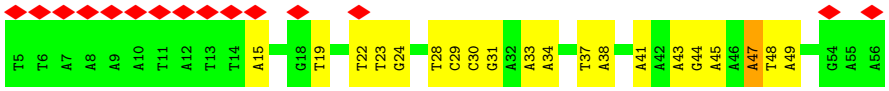
• Molecule 4: Centromere DNA-binding protein complex CBF3 subunit A





• Molecule 5: DNA (52-MER)

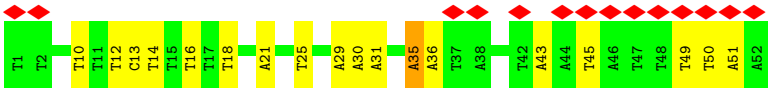
Chain F:



• Molecule 6: DNA (52-MER)

Chain G:

27%
65%
33%


T1
T2
T10
T11
T12
C13
T14
T15
T16
T17
T18
A21
T25
A29
A30
A31
A35
A36
T37
A38
T42
A43
A44
T45
A46
T47
T48
T49
T50
A51
A52

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22668	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 ($e^-/Å^2$)	27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.128	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.55	0/3595	0.73	4/4857 (0.1%)
1	H	0.44	0/3595	0.70	4/4857 (0.1%)
2	B	0.47	0/4885	0.61	0/6606
2	C	0.41	0/4798	0.56	1/6490 (0.0%)
2	I	0.35	0/4885	0.57	1/6606 (0.0%)
2	J	0.33	0/4682	0.52	0/6332
3	D	0.49	0/1247	0.58	0/1687
3	K	0.36	0/1247	0.55	0/1687
4	E	0.45	0/4348	0.59	0/5898
4	L	0.44	0/4348	0.58	0/5898
5	F	0.96	1/1215 (0.1%)	1.11	0/1875
6	G	0.91	0/1175	1.21	2/1809 (0.1%)
All	All	0.47	1/40020 (0.0%)	0.66	12/54602 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	H	0	6
2	B	0	1
2	I	0	1
2	J	0	2
3	K	0	1
4	E	0	3
4	L	0	6
All	All	0	24

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	47	DA	N9-C4	-5.55	1.34	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	24	LEU	CA-CB-CG	8.84	135.62	115.30
1	H	173	ASP	CB-CG-OD1	8.39	125.85	118.30
1	A	173	ASP	CB-CG-OD1	8.03	125.53	118.30
1	A	24	LEU	CA-CB-CG	6.94	131.25	115.30
6	G	35	DA	C3'-C2'-C1'	-6.49	94.72	102.50
6	G	49	DT	O4'-C4'-C3'	-5.51	102.30	104.50
1	H	476	LEU	CA-CB-CG	5.30	127.49	115.30
2	C	198	LEU	CA-CB-CG	5.23	127.33	115.30
1	H	172	ILE	C-N-CA	5.23	134.78	121.70
2	I	114	LEU	CA-CB-CG	5.15	127.15	115.30
1	A	172	ILE	C-N-CA	5.06	134.35	121.70
1	A	286	LEU	C-N-CA	-5.01	109.17	121.70

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ILE	Peptide
1	A	116	ASP	Peptide
1	A	274	ARG	Peptide
1	A	420	GLN	Peptide
2	B	333	ASP	Peptide
4	E	201	SER	Peptide
4	E	263	THR	Peptide
4	E	61	ILE	Peptide
1	H	171	ASN	Peptide
1	H	274	ARG	Peptide
1	H	345	ILE	Peptide
1	H	353	PRO	Peptide
1	H	36	ILE	Peptide
1	H	396	ASP	Peptide
2	I	452	PHE	Peptide
2	J	198	LEU	Peptide
2	J	61	LEU	Peptide
3	K	174	ASN	Peptide
4	L	102	LYS	Peptide
4	L	145	ASN	Peptide

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Mol	Chain	Res	Type	Group
4	L	254	VAL	Peptide
4	L	258	ALA	Peptide
4	L	263	THR	Peptide
4	L	97	ASP	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	3517	0	3553	123	0
1	H	3517	0	3553	120	0
2	B	4775	0	4754	126	0
2	C	4691	0	4647	121	0
2	I	4775	0	4755	175	0
2	J	4575	0	4550	118	0
3	D	1226	0	1194	48	0
3	K	1226	0	1194	62	0
4	E	4224	0	4114	119	0
4	L	4224	0	4114	138	0
5	F	1079	0	590	31	0
6	G	1053	0	598	16	0
7	B	2	0	0	0	0
7	C	2	0	0	1	0
7	I	2	0	0	1	0
7	J	2	0	0	3	0
All	All	38890	0	37616	1103	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 15.

All (1103) 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)
2:J:42:CYS:SG	7:J:702:ZN:ZN	0.87	1.58
5:F:34:DA:OP2	4:L:334:ARG:NH1	1.81	1.14
2:I:43:MET:O	2:I:48:LEU:CD2	2.01	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASP:OD2	3:D:161:ARG:NH1	1.86	1.07
3:D:156:GLU:OE2	3:D:159:ARG:NH1	1.93	1.00
2:I:43:MET:O	2:I:48:LEU:HD23	1.57	1.00
2:J:436:LYS:NZ	2:J:488:ASP:OD2	1.96	0.98
3:K:94:ALA:O	3:K:98:ARG:HB2	1.64	0.98
2:I:28:ILE:HG21	2:I:49:ILE:CB	1.87	0.97
4:E:230:GLU:OE2	4:E:361:LYS:NZ	1.98	0.95
2:C:33:CYS:SG	7:C:702:ZN:ZN	1.57	0.94
2:I:45:SER:O	2:I:46:THR:HG23	1.69	0.92
2:C:127:PHE:O	2:C:291:ARG:NH1	2.03	0.91
2:I:43:MET:HB3	2:I:48:LEU:HD22	1.47	0.91
3:D:114:ALA:O	3:D:152:LYS:NZ	2.07	0.86
2:I:211:ASN:OD1	2:I:214:ARG:NH1	2.08	0.86
1:H:374:GLU:OE2	1:H:378:LYS:NZ	2.09	0.86
1:H:95:ARG:NH1	1:H:141:TRP:O	2.09	0.86
3:K:89:LYS:NZ	3:K:123:PHE:O	2.07	0.86
4:E:327:LYS:NZ	6:G:10:DT:O5'	2.09	0.84
1:H:122:TYR:OH	1:H:182:LYS:NZ	2.10	0.84
2:B:55:LYS:NZ	2:B:476:PHE:O	2.11	0.83
1:H:22:PHE:O	3:K:112:LYS:NZ	2.12	0.83
2:J:74:ASN:OD1	2:J:79:LYS:NZ	2.11	0.83
4:L:511:ILE:O	4:L:527:LYS:NZ	2.10	0.83
2:B:79:LYS:NZ	2:B:304:SER:O	2.11	0.82
1:A:363:ARG:NH1	4:E:35:ASP:OD2	2.12	0.82
2:B:28:ILE:HG21	2:B:49:ILE:HB	1.61	0.82
4:L:179:GLN:OE1	4:L:187:LYS:NZ	2.12	0.82
2:C:18:THR:O	2:C:21:LYS:NZ	2.11	0.82
3:D:119:TRP:O	3:D:123:PHE:HB2	1.79	0.82
2:I:342:GLU:OE2	2:I:399:GLN:NE2	2.13	0.81
4:L:195:PRO:O	4:L:211:LYS:NZ	2.14	0.81
1:A:415:LYS:NZ	1:A:423:TYR:OH	2.12	0.81
4:E:194:ASN:O	4:E:211:LYS:NZ	2.13	0.80
4:L:241:LEU:H	4:L:243:LYS:HZ1	1.29	0.80
2:B:132:ASP:OD2	2:B:135:GLU:N	2.11	0.80
2:C:278:ASP:OD2	2:C:286:LYS:NZ	2.12	0.80
2:I:45:SER:O	2:I:46:THR:CG2	2.29	0.80
2:C:509:TYR:O	2:C:512:GLU:HB3	1.82	0.80
4:E:466:GLU:OE1	4:E:467:ARG:NH1	2.13	0.79
2:I:474:GLN:O	2:I:518:LYS:NZ	2.15	0.79
2:I:18:THR:O	2:I:21:LYS:NZ	2.15	0.79
2:I:79:LYS:NZ	2:I:304:SER:O	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:23:LYS:NZ	2:J:25:ASP:OD2	2.16	0.78
4:L:470:SER:O	4:L:502:LYS:NZ	2.17	0.78
2:B:384:VAL:O	2:B:400:LYS:NZ	2.16	0.78
1:A:352:PHE:O	1:A:435:ARG:NH1	2.17	0.77
2:C:316:VAL:HB	2:C:353:ARG:HH12	1.50	0.77
2:C:368:LYS:NZ	5:F:24:DG:OP1	2.17	0.77
2:I:34:ARG:NH1	2:I:530:GLY:O	2.18	0.77
3:D:181:GLU:OE2	3:D:185:ARG:NE	2.15	0.77
3:K:114:ALA:O	3:K:152:LYS:NZ	2.18	0.76
4:E:435:ILE:O	4:E:465:ARG:NH1	2.18	0.76
1:A:316:ARG:HH22	1:A:341:ARG:HH11	1.31	0.76
1:A:145:LYS:O	1:A:149:LYS:HB2	1.86	0.76
2:C:474:GLN:O	2:C:518:LYS:NZ	2.19	0.76
3:K:181:GLU:OE2	3:K:185:ARG:NE	2.10	0.76
2:J:515:SER:O	2:J:518:LYS:HB3	1.85	0.76
4:E:221:ARG:HD3	4:E:231:ARG:NH1	2.02	0.75
2:I:43:MET:O	2:I:48:LEU:HD21	1.86	0.75
2:I:301:TYR:OH	2:I:356:ASP:OD2	2.05	0.75
2:I:275:LEU:N	2:I:278:ASP:OD2	2.18	0.75
2:C:300:ASP:OD2	2:C:313:HIS:ND1	2.20	0.74
2:I:17:CYS:SG	7:I:701:ZN:ZN	1.76	0.74
1:A:461:SER:OG	2:B:347:LYS:NZ	2.19	0.74
2:B:211:ASN:OD1	2:B:214:ARG:NH1	2.20	0.74
1:H:352:PHE:O	1:H:435:ARG:NH1	2.21	0.72
2:I:314:THR:OG1	2:I:333:ASP:OD2	2.06	0.72
3:K:120:ASP:HA	3:K:123:PHE:HB3	1.71	0.72
2:C:501:GLY:O	2:C:504:LEU:HB3	1.90	0.72
4:E:511:ILE:O	4:E:527:LYS:NZ	2.22	0.72
1:A:262:ARG:NH1	1:A:265:ARG:NH1	2.39	0.71
2:C:176:VAL:HG23	2:C:200:TRP:HB2	1.73	0.71
2:I:47:LYS:HZ1	3:K:173:VAL:CA	2.04	0.71
4:E:235:ARG:NH1	4:E:320:ASP:O	2.24	0.70
4:E:470:SER:O	4:E:502:LYS:NZ	2.23	0.70
2:C:515:SER:O	2:C:518:LYS:HB3	1.92	0.69
2:I:273:ARG:O	2:I:286:LYS:NZ	2.23	0.69
4:E:158:HIS:NE2	4:E:402:ASP:OD2	2.25	0.69
2:J:300:ASP:O	2:J:308:LYS:NZ	2.18	0.69
2:J:30:CYS:SG	7:J:701:ZN:ZN	1.81	0.68
1:H:316:ARG:HH12	1:H:341:ARG:HH11	1.42	0.68
2:J:474:GLN:O	2:J:518:LYS:NZ	2.26	0.68
1:A:456:ARG:HD2	1:A:477:VAL:HG12	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:543:ASN:HD22	2:C:598:GLN:HE22	1.41	0.68
2:I:20:ARG:NH1	2:I:33:CYS:SG	2.67	0.68
2:J:18:THR:O	2:J:21:LYS:NZ	2.24	0.67
5:F:33:DA:O5'	4:L:327:LYS:NZ	2.25	0.67
4:E:297:ILE:HB	4:E:301:SER:H	1.59	0.67
2:B:48:LEU:C	2:B:48:LEU:HD13	2.15	0.67
3:D:94:ALA:O	3:D:98:ARG:HB2	1.95	0.67
2:I:93:ASP:OD2	2:I:96:THR:OG1	2.11	0.67
2:C:51:ALA:HA	2:C:527:LEU:HA	1.77	0.67
2:C:307:ARG:NH1	2:C:552:ASN:O	2.28	0.66
4:E:312:ASP:OD2	4:E:451:SER:OG	2.12	0.66
4:E:293:ARG:NH1	4:E:323:ILE:O	2.27	0.66
2:J:72:ILE:HD11	2:J:545:ILE:HA	1.77	0.66
1:A:61:LYS:NZ	3:D:190:TRP:O	2.22	0.66
2:B:315:GLU:HB2	2:B:335:TYR:HB2	1.77	0.66
2:J:17:CYS:SG	7:J:701:ZN:ZN	1.85	0.66
1:H:268:GLU:O	1:H:308:ARG:NH2	2.28	0.66
2:J:391:PHE:HA	2:J:397:ARG:HD2	1.77	0.65
1:A:316:ARG:HH22	1:A:341:ARG:NH1	1.95	0.65
2:C:84:ASP:HB3	2:C:87:ARG:HB2	1.79	0.65
2:C:186:TYR:O	2:C:196:LYS:NZ	2.30	0.65
1:H:409:ARG:H	1:H:474:GLN:H	1.46	0.64
3:D:83:ARG:NH1	3:D:133:GLU:OE1	2.18	0.64
4:L:241:LEU:H	4:L:243:LYS:NZ	1.94	0.64
1:H:387:PHE:HA	1:H:391:TYR:HB2	1.78	0.64
2:I:47:LYS:HZ1	3:K:173:VAL:N	1.95	0.64
4:E:297:ILE:H	4:E:301:SER:HB2	1.61	0.64
1:A:47:LEU:HD11	4:E:57:GLN:HE22	1.63	0.64
2:B:84:ASP:OD2	2:B:87:ARG:NH1	2.31	0.64
2:C:62:LEU:HD22	2:C:420:ILE:HG12	1.80	0.64
4:E:202:GLU:OE2	4:E:206:LYS:NZ	2.28	0.63
1:H:316:ARG:HH22	1:H:341:ARG:NH1	1.96	0.63
4:L:297:ILE:HG22	4:L:299:SER:H	1.63	0.63
2:B:155:ASP:O	2:B:232:ARG:NH1	2.31	0.63
2:C:526:LEU:HD11	2:C:533:PHE:HB3	1.80	0.63
1:A:204:ASP:OD2	4:E:38:LYS:NZ	2.28	0.63
1:H:398:LYS:HB3	2:I:386:SER:HA	1.81	0.63
2:I:121:ASN:HA	2:I:394:ASN:HB3	1.81	0.63
2:I:474:GLN:HG2	2:I:486:LEU:HD22	1.78	0.63
4:L:257:SER:HB2	4:L:264:PRO:HG3	1.78	0.63
2:J:180:ALA:HB2	2:J:199:ASN:HD21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:137:LYS:NZ	4:L:145:ASN:OD1	2.32	0.63
4:E:60:GLN:NE2	4:E:385:ASN:O	2.32	0.63
2:J:125:LEU:HA	2:J:295:ARG:HH12	1.62	0.63
3:D:19:ASP:H	3:D:22:ILE:HD12	1.64	0.63
2:B:200:TRP:HA	2:B:204:MET:HB2	1.81	0.62
4:E:323:ILE:HG23	4:E:324:LEU:HD23	1.80	0.62
2:I:307:ARG:NH1	2:I:552:ASN:OD1	2.32	0.62
2:I:273:ARG:C	2:I:286:LYS:HZ2	2.03	0.62
1:A:278:VAL:HG11	1:A:287:LEU:HD21	1.82	0.62
1:H:99:LEU:HD23	3:K:161:ARG:HH12	1.65	0.62
2:I:45:SER:C	2:I:46:THR:HG23	2.18	0.62
1:A:373:GLU:OE1	1:A:451:ASN:ND2	2.33	0.62
2:C:540:ILE:HA	2:C:598:GLN:HE21	1.64	0.62
2:C:143:TYR:O	2:C:147:ARG:N	2.33	0.61
2:I:43:MET:C	2:I:48:LEU:CD2	2.67	0.61
2:I:103:MET:O	2:I:147:ARG:NH2	2.34	0.61
2:I:445:ASN:O	2:I:454:ASN:ND2	2.32	0.61
2:J:74:ASN:HB2	2:J:465:ARG:HH21	1.66	0.61
2:I:47:LYS:HE3	3:K:172:ILE:O	2.01	0.61
4:L:435:ILE:HG13	4:L:465:ARG:HD2	1.82	0.61
2:B:65:TRP:NE1	2:B:69:GLU:OE1	2.34	0.61
1:H:182:LYS:HE2	1:H:186:ILE:HD11	1.82	0.61
4:L:370:ASP:OD2	4:L:373:THR:N	2.26	0.61
3:K:122:GLU:OE2	3:K:125:LYS:NZ	2.24	0.61
1:H:452:ILE:HB	1:H:475:VAL:HA	1.83	0.61
4:L:243:LYS:N	4:L:397:ASP:OD2	2.34	0.61
4:L:99:PRO:HA	4:L:102:LYS:HB2	1.82	0.61
2:C:158:TYR:OH	2:C:228:HIS:O	2.19	0.61
2:C:373:ILE:O	2:C:377:LEU:HB2	2.01	0.61
2:I:106:LEU:HB3	2:I:147:ARG:HH22	1.66	0.61
1:H:171:ASN:HA	1:H:200:GLN:HB2	1.83	0.60
1:A:452:ILE:HB	1:A:475:VAL:HA	1.82	0.60
2:I:47:LYS:HE3	3:K:173:VAL:HA	1.82	0.60
1:A:107:ASN:ND2	1:A:115:ILE:O	2.30	0.60
2:B:46:THR:OG1	3:D:174:ASN:ND2	2.35	0.60
2:B:189:HIS:HB3	2:B:196:LYS:NZ	2.17	0.60
2:J:57:TYR:HA	2:J:60:ASP:HB3	1.81	0.60
4:L:295:TYR:OH	4:L:438:GLU:OE1	2.19	0.60
2:C:98:GLU:OE2	2:C:102:TRP:NE1	2.35	0.60
2:I:143:TYR:OH	2:I:147:ARG:NH1	2.35	0.60
1:A:374:GLU:CD	1:A:378:LYS:HZ2	2.06	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:GLN:HG3	2:B:8:LEU:HG	1.84	0.60
2:B:275:LEU:N	2:B:278:ASP:OD2	2.35	0.60
4:E:136:CYS:HB3	4:E:141:ASN:HB3	1.83	0.60
1:H:79:TYR:OH	4:L:43:HIS:ND1	2.33	0.60
4:L:504:ILE:O	4:L:507:LYS:NZ	2.29	0.60
2:B:28:ILE:CG2	2:B:49:ILE:HB	2.31	0.59
2:C:62:LEU:HB3	2:C:420:ILE:HG23	1.84	0.59
4:L:232:SER:O	4:L:235:ARG:NH2	2.35	0.59
2:C:374:ARG:HD3	2:C:375:ARG:NH1	2.17	0.59
3:D:25:ARG:HH12	3:D:145:PRO:HG2	1.66	0.59
1:A:287:LEU:HG	1:A:288:ILE:HG23	1.84	0.59
2:C:273:ARG:HH12	5:F:15:DA:H5"	1.66	0.59
2:C:505:ASP:O	2:C:508:VAL:HB	2.02	0.59
4:L:373:THR:HA	4:L:376:THR:HB	1.84	0.59
4:L:509:SER:HB2	4:L:527:LYS:HZ1	1.66	0.59
4:E:293:ARG:HH12	4:E:323:ILE:C	2.05	0.59
3:K:116:VAL:HG21	3:K:121:ARG:HH11	1.67	0.59
3:K:117:ASP:HB3	3:K:120:ASP:HB2	1.84	0.59
4:L:436:PHE:O	4:L:465:ARG:NH1	2.35	0.59
2:C:175:PRO:HA	2:C:455:ARG:HH22	1.67	0.59
1:H:169:GLN:OE1	1:H:200:GLN:NE2	2.35	0.59
4:L:490:PHE:O	4:L:496:GLN:NE2	2.35	0.59
1:A:273:LEU:O	1:A:274:ARG:NH1	2.35	0.59
2:I:157:LYS:HZ2	2:I:219:GLN:HG2	1.68	0.59
4:L:170:THR:HG22	4:L:172:GLU:H	1.68	0.59
1:A:394:GLU:HA	1:A:411:LYS:HA	1.84	0.59
2:B:187:PRO:O	2:B:191:TYR:HB2	2.02	0.59
1:A:412:GLU:OE2	1:A:456:ARG:NH1	2.36	0.58
4:L:167:ALA:HA	4:L:173:THR:HG21	1.84	0.58
4:L:297:ILE:HB	4:L:301:SER:H	1.66	0.58
2:C:304:SER:HA	2:C:308:LYS:HD2	1.85	0.58
1:H:107:ASN:ND2	1:H:115:ILE:O	2.35	0.58
1:A:279:ARG:HH11	4:E:38:LYS:HE2	1.68	0.58
2:C:368:LYS:HZ1	5:F:24:DG:P	2.26	0.58
4:E:221:ARG:NH2	4:E:362:CYS:SG	2.77	0.58
1:H:451:ASN:HD22	1:H:476:LEU:HD21	1.67	0.58
3:K:25:ARG:HH11	3:K:93:TRP:HH2	1.51	0.58
3:K:25:ARG:HH12	3:K:145:PRO:HG2	1.68	0.58
4:L:462:GLU:OE2	4:L:465:ARG:NH2	2.36	0.58
1:H:198:GLU:HB3	1:H:275:LYS:HB3	1.85	0.58
1:H:420:GLN:HE22	2:I:284:ILE:HG12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:TYR:OH	1:A:307:ARG:NH2	2.37	0.58
4:E:334:ARG:NH2	4:E:336:GLU:OE2	2.37	0.58
2:I:155:ASP:OD1	2:I:232:ARG:NH2	2.37	0.58
2:I:316:VAL:H	2:I:332:VAL:HG12	1.69	0.58
3:K:19:ASP:H	3:K:22:ILE:HD12	1.68	0.58
4:E:171:ASN:HA	4:E:181:LEU:HD11	1.84	0.58
1:H:278:VAL:HG11	1:H:287:LEU:HD21	1.85	0.58
2:J:155:ASP:OD1	2:J:232:ARG:NH2	2.37	0.58
2:J:62:LEU:O	2:J:65:TRP:HB3	2.04	0.58
3:K:20:LYS:NZ	3:K:33:LEU:HD13	2.18	0.58
2:J:162:LEU:HD22	2:J:232:ARG:HG3	1.86	0.58
1:H:293:PHE:HB3	1:H:296:ASN:HD21	1.67	0.57
1:A:468:ARG:NH1	3:D:110:SER:OG	2.33	0.57
4:E:517:LEU:HB2	4:E:520:PHE:HB2	1.86	0.57
2:I:564:SER:OG	2:J:139:ARG:NH2	2.37	0.57
2:B:4:ARG:NH1	2:B:28:ILE:O	2.27	0.57
2:I:117:PHE:O	2:I:121:ASN:ND2	2.37	0.57
2:B:20:ARG:NH2	2:B:32:ASN:O	2.34	0.57
2:B:20:ARG:NH1	2:B:36:ARG:HD2	2.19	0.57
3:D:119:TRP:O	3:D:123:PHE:CB	2.51	0.57
1:H:78:GLU:HA	1:H:84:ILE:HD11	1.85	0.57
2:C:126:TYR:HA	2:C:129:SER:HB3	1.85	0.57
2:I:200:TRP:HB3	2:I:205:GLN:HB2	1.86	0.57
4:L:333:PRO:HB2	4:L:338:PHE:HE2	1.70	0.57
1:A:378:LYS:HA	1:A:381:LYS:NZ	2.19	0.57
2:C:384:VAL:O	2:C:400:LYS:NZ	2.37	0.57
1:H:71:ALA:O	1:H:75:ASN:ND2	2.37	0.57
1:A:173:ASP:HB3	1:A:202:GLY:HA3	1.87	0.57
4:E:334:ARG:NH1	6:G:12:DT:OP2	2.38	0.57
1:H:58:ARG:NH2	3:K:191:ALA:O	2.37	0.57
2:I:157:LYS:NZ	2:I:219:GLN:HG2	2.19	0.57
4:L:272:LEU:O	4:L:283:GLN:NE2	2.36	0.57
1:H:328:PHE:HB2	1:H:353:PRO:HG3	1.87	0.57
2:I:413:LYS:HE2	2:I:465:ARG:HG3	1.87	0.57
4:L:115:ASN:HA	4:L:118:LYS:HB2	1.87	0.57
1:A:171:ASN:ND2	1:A:173:ASP:OD1	2.37	0.57
1:A:363:ARG:N	1:A:444:ASN:O	2.36	0.57
2:B:104:ASN:OD1	2:B:147:ARG:NH2	2.37	0.57
2:J:69:GLU:O	2:J:73:THR:OG1	2.21	0.57
2:B:299:CYS:HA	2:B:302:LEU:HB2	1.87	0.57
2:I:257:LEU:HD21	2:I:300:ASP:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:20:ARG:NH1	2:J:33:CYS:SG	2.78	0.57
1:A:354:LYS:HA	1:A:435:ARG:HH22	1.69	0.56
1:H:268:GLU:OE2	1:H:308:ARG:NH1	2.38	0.56
1:H:404:ASN:ND2	3:K:102:PHE:O	2.38	0.56
2:J:81:LYS:HD2	2:J:250:PRO:HD2	1.86	0.56
4:L:466:GLU:OE1	4:L:467:ARG:NH1	2.38	0.56
2:C:282:GLU:HG2	2:C:286:LYS:HE2	1.86	0.56
4:E:441:GLU:O	4:E:445:HIS:N	2.37	0.56
1:H:181:ASP:HA	1:H:262:ARG:HE	1.69	0.56
2:I:19:ARG:NH2	2:I:38:GLN:OE1	2.38	0.56
2:I:244:THR:HG21	2:I:500:PHE:HA	1.86	0.56
4:L:442:TYR:HA	4:L:445:HIS:HB3	1.87	0.56
2:B:40:SER:HA	2:B:43:MET:HB2	1.87	0.56
1:H:287:LEU:HG	1:H:288:ILE:HG23	1.86	0.56
2:I:222:GLN:HB3	2:J:90:ALA:HB1	1.86	0.56
2:I:316:VAL:HG12	2:I:318:SER:H	1.71	0.56
4:L:213:ARG:NH2	4:L:341:TYR:OH	2.36	0.56
2:B:11:LYS:O	2:B:26:ARG:NH2	2.39	0.56
1:H:291:HIS:N	1:H:327:ASP:OD2	2.37	0.56
2:C:474:GLN:HG3	2:C:518:LYS:NZ	2.21	0.56
4:E:197:THR:HB	4:E:200:LEU:HB3	1.87	0.56
1:H:373:GLU:OE1	1:H:451:ASN:ND2	2.39	0.56
2:I:82:GLN:HG2	2:I:551:LYS:HD2	1.86	0.56
4:L:441:GLU:O	4:L:445:HIS:N	2.38	0.56
1:A:118:LEU:O	1:A:169:GLN:N	2.37	0.56
2:B:115:MET:HB3	2:B:137:TYR:HE1	1.71	0.56
2:C:189:HIS:NE2	2:C:204:MET:SD	2.79	0.56
1:H:127:LEU:HD13	1:H:186:ILE:HB	1.88	0.56
2:C:368:LYS:NZ	5:F:24:DG:H5'	2.21	0.55
1:A:95:ARG:HB2	1:A:142:TYR:HE1	1.72	0.55
1:H:133:ASN:OD1	1:H:137:MET:N	2.39	0.55
2:I:384:VAL:O	2:I:400:LYS:NZ	2.38	0.55
4:E:284:THR:OG1	4:E:471:ASN:ND2	2.37	0.55
2:I:173:TYR:HD1	2:I:452:PHE:HB2	1.71	0.55
1:A:270:MET:HG3	1:A:273:LEU:HD13	1.89	0.55
1:A:406:ARG:NH2	3:D:101:ASN:OD1	2.39	0.55
1:A:75:ASN:HA	1:A:78:GLU:OE2	2.06	0.55
1:A:87:TRP:HH2	1:A:139:GLU:HA	1.71	0.55
3:D:103:PRO:HB3	3:D:110:SER:HB3	1.88	0.55
1:H:277:THR:HB	1:H:313:ARG:HB3	1.87	0.55
2:B:588:SER:HB3	2:B:591:ARG:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:LEU:HD13	2:C:420:ILE:HA	1.87	0.55
2:J:126:TYR:O	2:J:131:GLY:N	2.40	0.55
4:L:158:HIS:NE2	4:L:402:ASP:OD2	2.40	0.55
4:L:165:GLN:HA	4:L:168:ILE:HG22	1.88	0.55
2:B:30:CYS:HB3	2:B:32:ASN:H	1.71	0.55
2:B:142:GLN:HB3	2:B:146:ARG:HH12	1.72	0.55
2:C:128:GLY:HA3	2:C:295:ARG:NH1	2.20	0.55
4:E:201:SER:HB3	4:E:204:PHE:H	1.72	0.55
2:J:559:ILE:HB	2:J:567:PRO:HB3	1.89	0.55
2:B:247:TYR:HE2	2:B:457:PRO:HB3	1.72	0.55
2:C:352:ASP:HA	2:C:355:LEU:HD12	1.89	0.55
2:I:82:GLN:HE21	2:I:551:LYS:HB3	1.71	0.55
2:I:176:VAL:HG23	2:I:200:TRP:HB2	1.89	0.55
2:I:412:TRP:NE1	2:I:435:SER:OG	2.38	0.55
2:C:247:TYR:OH	2:C:461:GLN:NE2	2.40	0.54
4:E:313:GLU:HB3	4:E:316:SER:HB3	1.89	0.54
2:C:205:GLN:HE22	2:C:455:ARG:NH1	2.05	0.54
1:H:91:ALA:HB1	1:H:141:TRP:HH2	1.73	0.54
1:H:406:ARG:NH1	3:K:101:ASN:OD1	2.39	0.54
4:L:90:LEU:HD13	4:L:394:ALA:HB1	1.89	0.54
1:A:76:ILE:HG23	4:E:44:GLN:HG3	1.89	0.54
1:H:391:TYR:HA	1:H:414:ASP:OD2	2.08	0.54
3:K:121:ARG:HG2	3:K:125:LYS:HE3	1.88	0.54
4:E:295:TYR:HE2	4:E:436:PHE:H	1.55	0.54
1:H:357:LYS:NZ	1:H:436:THR:HB	2.23	0.54
2:I:175:PRO:HA	2:I:455:ARG:HH22	1.72	0.54
2:J:121:ASN:HA	2:J:394:ASN:HB3	1.89	0.54
2:J:172:TYR:O	2:J:455:ARG:NH1	2.40	0.54
2:J:543:ASN:HD22	2:J:598:GLN:HE22	1.55	0.54
4:L:455:ARG:HA	4:L:458:LEU:HD12	1.89	0.54
2:C:317:SER:O	2:C:353:ARG:NH2	2.39	0.54
1:A:180:VAL:HG21	1:A:259:SER:HB2	1.88	0.54
1:A:279:ARG:HG2	1:A:315:SER:HB3	1.89	0.54
2:J:29:PRO:HB2	2:J:42:CYS:HB3	1.90	0.54
3:K:8:LEU:HD13	3:K:87:LEU:HD11	1.89	0.54
1:A:323:THR:HG23	1:A:325:LEU:H	1.72	0.54
2:B:281:VAL:HG13	2:C:565:LEU:HD22	1.90	0.54
5:F:41:DA:OP2	5:F:41:DA:H2'	2.08	0.54
2:I:7:GLN:HG3	2:I:8:LEU:HG	1.89	0.54
2:J:472:PHE:HA	2:J:475:ILE:HD12	1.90	0.54
2:B:66:GLN:OE1	2:B:416:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:GLU:O	2:B:353:ARG:NH2	2.41	0.54
2:I:34:ARG:NH2	2:I:528:ASP:OD2	2.41	0.54
2:I:102:TRP:HH2	2:I:188:LEU:HD12	1.73	0.54
4:L:93:LEU:O	4:L:118:LYS:NZ	2.40	0.54
2:J:20:ARG:NH1	2:J:32:ASN:O	2.39	0.54
2:J:235:GLN:HE21	2:J:292:ILE:HD11	1.72	0.54
4:L:334:ARG:O	4:L:337:THR:OG1	2.23	0.54
2:B:316:VAL:HG23	2:B:332:VAL:HG11	1.90	0.54
3:K:11:GLY:N	3:K:79:VAL:O	2.41	0.54
4:L:221:ARG:NH2	4:L:357:GLU:O	2.41	0.54
4:E:213:ARG:NH2	4:E:341:TYR:OH	2.41	0.53
3:K:161:ARG:HG3	3:K:166:ILE:HD11	1.89	0.53
3:K:127:ASP:OD2	3:K:129:GLU:HB3	2.08	0.53
1:A:310:ASN:O	1:A:335:GLN:N	2.40	0.53
1:A:392:ILE:HD12	1:A:411:LYS:HD3	1.91	0.53
4:E:200:LEU:HD13	4:E:348:TYR:HB2	1.91	0.53
2:C:526:LEU:HA	2:C:535:HIS:HD2	1.73	0.53
1:H:443:GLN:HA	1:H:467:TYR:HB2	1.90	0.53
2:J:505:ASP:O	2:J:508:VAL:HB	2.08	0.53
4:L:448:GLU:CD	4:L:455:ARG:HH12	2.12	0.53
1:A:296:ASN:HB3	1:A:299:LYS:HZ3	1.74	0.53
1:H:386:THR:O	1:H:391:TYR:N	2.39	0.53
2:J:29:PRO:HD2	2:J:34:ARG:HD2	1.90	0.53
3:K:107:ASP:OD2	3:K:110:SER:HB2	2.09	0.53
1:A:374:GLU:OE1	1:A:378:LYS:NZ	2.41	0.53
2:B:74:ASN:HB2	2:B:465:ARG:HH21	1.73	0.53
2:C:516:LYS:HA	2:C:519:LEU:HD13	1.90	0.53
2:B:390:ASP:HB3	2:B:393:SER:HB3	1.90	0.53
3:K:116:VAL:HG21	3:K:121:ARG:NH1	2.24	0.53
3:K:131:LEU:HA	3:K:134:ILE:HD12	1.90	0.53
2:C:84:ASP:OD2	2:C:87:ARG:NH1	2.42	0.53
4:L:115:ASN:ND2	4:L:165:GLN:OE1	2.38	0.53
4:L:251:TYR:HB3	4:L:270:LEU:HB2	1.90	0.53
4:E:225:ASN:ND2	4:E:407:MET:SD	2.81	0.53
2:I:55:LYS:NZ	2:I:476:PHE:O	2.42	0.53
6:G:21:DA:H8	6:G:21:DA:OP2	1.92	0.53
2:J:186:TYR:O	2:J:196:LYS:NZ	2.37	0.53
2:J:278:ASP:HB2	2:J:283:SER:HB3	1.89	0.53
2:J:445:ASN:O	2:J:454:ASN:ND2	2.42	0.53
2:J:526:LEU:HA	2:J:535:HIS:HD2	1.73	0.53
2:J:528:ASP:HB3	2:J:533:PHE:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ALA:O	1:A:75:ASN:ND2	2.42	0.52
2:C:497:PRO:HB2	2:C:499:ILE:HG22	1.90	0.52
1:H:301:ILE:HG23	1:H:306:LYS:HE2	1.91	0.52
1:A:78:GLU:HA	1:A:84:ILE:HD11	1.90	0.52
2:B:155:ASP:OD1	2:B:232:ARG:NH2	2.43	0.52
4:E:356:ARG:HG2	4:E:360:ASN:HB2	1.91	0.52
1:H:363:ARG:N	1:H:444:ASN:O	2.39	0.52
4:L:194:ASN:ND2	4:L:536:GLU:OE1	2.43	0.52
4:E:312:ASP:OD2	4:E:454:SER:OG	2.27	0.52
1:H:24:LEU:HB3	3:K:155:ALA:HB1	1.90	0.52
1:H:320:ILE:HB	1:H:326:ALA:HB2	1.92	0.52
2:J:301:TYR:O	2:J:304:SER:OG	2.24	0.52
2:I:11:LYS:HB2	3:K:175:ASP:H	1.74	0.52
1:A:369:TRP:HB3	1:A:450:ASN:HD22	1.75	0.52
2:B:89:PRO:HA	2:C:153:SER:HA	1.90	0.52
2:C:513:ARG:HE	2:C:601:TYR:HB3	1.74	0.52
4:L:32:GLU:HA	4:L:35:ASP:HB2	1.91	0.52
2:B:23:LYS:O	2:B:32:ASN:ND2	2.42	0.52
2:B:158:TYR:OH	2:B:228:HIS:O	2.26	0.52
1:H:319:GLN:HG2	1:H:344:TYR:HB3	1.92	0.52
4:E:436:PHE:HB2	4:E:465:ARG:HH11	1.75	0.52
2:I:291:ARG:NH2	2:I:341:THR:OG1	2.43	0.52
5:F:33:DA:C5'	4:L:327:LYS:HZ3	2.22	0.51
2:I:248:ASP:HA	2:I:503:LYS:NZ	2.24	0.51
2:I:313:HIS:HB2	2:I:353:ARG:HH11	1.75	0.51
2:I:351:LEU:HD11	2:I:373:ILE:HG23	1.92	0.51
2:J:301:TYR:OH	2:J:352:ASP:O	2.27	0.51
2:B:189:HIS:HB3	2:B:196:LYS:HZ3	1.73	0.51
3:D:107:ASP:HB2	3:D:111:ARG:HG3	1.92	0.51
4:E:370:ASP:OD2	4:E:372:ASP:HB3	2.10	0.51
6:G:43:DA:OP2	6:G:43:DA:H8	1.94	0.51
2:J:124:ALA:O	2:J:295:ARG:NH2	2.40	0.51
1:A:79:TYR:OH	4:E:43:HIS:ND1	2.38	0.51
4:E:29:ARG:HA	4:E:32:GLU:OE2	2.10	0.51
1:H:279:ARG:HA	1:H:315:SER:HB3	1.92	0.51
1:H:326:ALA:HB3	1:H:350:ILE:HA	1.92	0.51
2:I:47:LYS:CE	3:K:173:VAL:HA	2.40	0.51
2:J:474:GLN:NE2	2:J:479:SER:O	2.36	0.51
4:L:436:PHE:HB2	4:L:465:ARG:HD3	1.93	0.51
2:I:47:LYS:NZ	3:K:173:VAL:CA	2.74	0.51
2:I:65:TRP:NE1	2:I:69:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:219:GLN:O	2:J:223:CYS:N	2.43	0.51
2:J:384:VAL:O	2:J:400:LYS:NZ	2.44	0.51
3:D:25:ARG:HH12	3:D:145:PRO:CG	2.23	0.51
2:I:95:ASP:HA	2:I:98:GLU:HB3	1.92	0.51
3:K:20:LYS:HE2	3:K:33:LEU:HD22	1.92	0.51
2:C:412:TRP:HE1	2:C:431:VAL:HG13	1.74	0.51
1:H:314:LEU:HD13	1:H:317:MET:HE1	1.93	0.51
2:I:2:PHE:HB2	2:I:533:PHE:H	1.75	0.51
2:J:109:ASP:O	2:J:113:GLN:HB2	2.11	0.51
4:E:435:ILE:HG13	4:E:465:ARG:HD2	1.93	0.51
2:I:120:GLU:O	2:I:395:ASN:N	2.44	0.51
2:I:356:ASP:HA	2:I:359:LEU:HG	1.91	0.51
2:I:513:ARG:HG3	2:I:601:TYR:HB3	1.92	0.51
3:K:132:TYR:HA	3:K:135:ILE:HD12	1.92	0.51
4:L:314:ASN:HD21	4:L:452:GLN:H	1.58	0.51
2:C:7:GLN:OE1	2:C:9:LYS:NZ	2.43	0.51
4:E:96:ASP:HA	4:E:98:LYS:HE2	1.93	0.51
6:G:13:DC:OP2	6:G:13:DC:H2'	2.11	0.51
2:J:79:LYS:HZ1	2:J:247:TYR:HE1	1.59	0.51
3:K:106:ASP:HA	3:K:111:ARG:NH1	2.26	0.51
4:L:435:ILE:O	4:L:465:ARG:NH1	2.44	0.51
4:L:531:TYR:HB3	4:L:538:PRO:HB3	1.94	0.51
2:C:174:MET:C	2:C:455:ARG:HH12	2.14	0.50
4:E:511:ILE:HD12	4:E:525:LYS:HE3	1.92	0.50
4:E:93:LEU:HD11	4:E:118:LYS:HB3	1.92	0.50
4:E:194:ASN:ND2	4:E:536:GLU:OE1	2.45	0.50
1:H:34:TYR:HD2	1:H:39:LEU:HD21	1.77	0.50
1:H:409:ARG:HB3	1:H:474:GLN:HA	1.93	0.50
2:B:107:GLN:N	2:B:110:GLN:OE1	2.42	0.50
2:C:504:LEU:O	2:C:507:LEU:HB3	2.10	0.50
1:H:468:ARG:NH1	3:K:110:SER:OG	2.44	0.50
2:J:275:LEU:HB2	2:J:278:ASP:OD2	2.11	0.50
4:L:293:ARG:NH1	4:L:323:ILE:O	2.45	0.50
4:L:373:THR:O	4:L:377:PHE:N	2.43	0.50
1:A:67:TYR:OH	1:A:78:GLU:OE2	2.19	0.50
2:B:28:ILE:CG2	2:B:49:ILE:CB	2.89	0.50
1:H:332:ASP:OD1	1:H:332:ASP:N	2.44	0.50
2:I:105:TYR:OH	2:I:184:SER:O	2.26	0.50
2:I:394:ASN:O	2:I:398:PHE:HB2	2.12	0.50
2:J:401:PHE:HA	2:J:404:LEU:HB3	1.93	0.50
4:L:29:ARG:HA	4:L:32:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:218:PHE:O	2:J:222:GLN:N	2.40	0.50
2:B:79:LYS:HZ3	2:B:304:SER:N	2.10	0.50
2:B:155:ASP:OD2	2:B:159:TRP:NE1	2.43	0.50
2:C:208:MET:HA	2:C:211:ASN:HD22	1.77	0.50
4:E:114:GLU:HG3	4:E:118:LYS:NZ	2.27	0.50
4:E:439:ILE:HG23	4:E:458:LEU:HB3	1.92	0.50
2:I:69:GLU:O	2:I:73:THR:OG1	2.27	0.50
2:I:77:LEU:HD11	2:I:506:LYS:HB3	1.94	0.50
4:L:74:PRO:HD2	4:L:77:ASP:OD2	2.12	0.50
1:H:171:ASN:ND2	1:H:173:ASP:OD1	2.44	0.50
2:I:315:GLU:O	2:I:353:ARG:NH2	2.45	0.50
2:I:536:PRO:HA	2:I:594:VAL:HG22	1.94	0.50
1:A:357:LYS:O	1:A:438:ASN:N	2.42	0.49
2:B:467:VAL:HG23	2:B:489:LEU:HD23	1.94	0.49
2:B:509:TYR:OH	2:B:602:ASN:O	2.25	0.49
2:C:30:CYS:HB2	2:C:33:CYS:H	1.76	0.49
2:I:146:ARG:NE	2:I:160:ASP:OD1	2.39	0.49
2:B:309:PRO:HG2	2:B:310:ILE:HG13	1.93	0.49
2:C:371:ASP:OD1	2:C:418:TYR:OH	2.24	0.49
2:C:415:PHE:HA	2:C:418:TYR:HD2	1.77	0.49
4:E:272:LEU:O	4:E:283:GLN:NE2	2.40	0.49
1:H:283:LEU:HD23	1:H:287:LEU:HD22	1.94	0.49
1:A:268:GLU:O	1:A:308:ARG:NH2	2.39	0.49
1:A:438:ASN:HB2	1:A:463:ARG:HG2	1.94	0.49
2:C:173:TYR:HD1	2:C:452:PHE:HB2	1.77	0.49
3:D:29:LEU:HD13	3:D:77:MET:HG2	1.95	0.49
4:E:452:GLN:OE1	4:E:455:ARG:NH2	2.41	0.49
4:E:493:SER:HA	4:E:496:GLN:HB2	1.93	0.49
5:F:43:DA:OP2	5:F:43:DA:H2'	2.13	0.49
1:H:12:LEU:HD13	3:K:132:TYR:HB3	1.94	0.49
2:C:397:ARG:HD3	2:C:449:LYS:HE2	1.94	0.49
4:E:455:ARG:HA	4:E:458:LEU:HD12	1.94	0.49
4:L:436:PHE:HB2	4:L:465:ARG:HH11	1.77	0.49
1:A:122:TYR:HD1	1:A:127:LEU:HB2	1.77	0.49
1:A:377:LEU:HD23	1:A:380:LEU:HD21	1.95	0.49
2:B:146:ARG:NH2	2:B:160:ASP:OD1	2.40	0.49
2:C:200:TRP:HA	2:C:204:MET:HB3	1.93	0.49
5:F:38:DA:OP2	5:F:38:DA:H8	1.96	0.49
1:H:107:ASN:O	1:H:111:ASP:N	2.46	0.49
2:I:158:TYR:OH	2:I:228:HIS:O	2.28	0.49
2:J:57:TYR:HB3	2:J:533:PHE:HD2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:78:LEU:HD12	4:L:79:PRO:HD2	1.93	0.49
4:L:188:VAL:O	4:L:192:LEU:HB2	2.11	0.49
2:C:158:TYR:HB3	2:C:232:ARG:HG2	1.93	0.49
3:D:105:GLU:OE2	3:D:144:LYS:HB3	2.11	0.49
1:H:122:TYR:HB3	1:H:179:LEU:HD21	1.94	0.49
2:I:268:HIS:NE2	2:J:306:PRO:O	2.35	0.49
2:I:475:ILE:HG23	2:I:518:LYS:HA	1.94	0.49
2:I:559:ILE:HG21	2:I:567:PRO:HD3	1.95	0.49
2:J:30:CYS:HB2	2:J:33:CYS:HB2	1.93	0.49
1:A:21:TYR:HA	1:A:24:LEU:HD23	1.94	0.49
2:B:189:HIS:HD2	2:B:196:LYS:HA	1.78	0.49
4:E:183:PRO:HG2	4:E:186:LEU:HB3	1.94	0.49
1:H:315:SER:O	1:H:341:ARG:N	2.45	0.49
4:L:60:GLN:NE2	4:L:385:ASN:O	2.44	0.49
4:L:308:ASN:O	4:L:442:TYR:OH	2.27	0.49
1:A:325:LEU:HD13	2:C:9:LYS:HZ1	1.78	0.49
1:A:328:PHE:H	1:A:351:VAL:HG12	1.77	0.49
4:E:388:GLU:OE2	4:E:392:ALA:HB3	2.12	0.49
6:G:16:DT:H2'	6:G:16:DT:OP2	2.13	0.49
1:H:290:PHE:N	1:H:327:ASP:OD1	2.45	0.49
1:H:303:TYR:OH	1:H:307:ARG:NH2	2.46	0.49
2:I:307:ARG:HH12	2:I:552:ASN:HA	1.78	0.49
2:J:289:LEU:HG	2:J:292:ILE:HD12	1.95	0.49
2:J:427:SER:O	2:J:431:VAL:N	2.42	0.49
3:K:117:ASP:O	3:K:121:ARG:N	2.45	0.49
1:A:316:ARG:NH1	4:E:35:ASP:O	2.42	0.49
2:B:217:LEU:HD23	2:B:220:LEU:HD12	1.95	0.49
2:B:415:PHE:HA	2:B:418:TYR:HD2	1.77	0.49
1:H:431:TRP:HB3	2:I:273:ARG:NH1	2.28	0.49
2:I:11:LYS:O	2:I:26:ARG:NH2	2.45	0.49
2:I:81:LYS:HE2	2:I:249:GLU:OE2	2.13	0.49
3:K:6:VAL:O	3:K:17:THR:HA	2.13	0.49
5:F:44:DG:OP2	5:F:44:DG:H2'	2.13	0.49
1:H:108:HIS:HE1	1:H:162:LEU:HA	1.77	0.49
1:H:356:PHE:HE2	1:H:359:LEU:HD22	1.76	0.49
2:I:604:SER:HA	2:I:607:LEU:HD13	1.94	0.49
4:L:523:ILE:O	4:L:529:ASN:ND2	2.46	0.49
1:A:123:LEU:HD12	1:A:124:ASP:HB2	1.95	0.48
5:F:33:DA:H3'	4:L:327:LYS:HZ2	1.76	0.48
2:I:401:PHE:HE1	2:I:441:LEU:HB3	1.78	0.48
4:L:207:THR:OG1	4:L:210:GLU:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:375:ARG:HH21	4:L:398:LYS:HZ3	1.61	0.48
4:L:429:LYS:HA	4:L:432:LEU:HD12	1.95	0.48
1:A:168:ILE:O	1:A:197:GLY:N	2.42	0.48
4:E:314:ASN:HD21	4:E:452:GLN:H	1.60	0.48
1:H:384:LYS:HD3	1:H:385:ARG:HH12	1.77	0.48
2:I:139:ARG:O	2:I:143:TYR:HB2	2.13	0.48
2:I:527:LEU:HD13	2:I:590:PHE:HE2	1.79	0.48
2:I:597:PHE:HA	2:I:600:GLU:HB3	1.94	0.48
4:L:298:PRO:HG2	4:L:488:PRO:HD2	1.94	0.48
2:C:122:LEU:HB3	2:C:125:LEU:HD12	1.95	0.48
2:C:506:LYS:HZ2	2:C:606:ILE:HA	1.78	0.48
1:H:384:LYS:HE2	1:H:385:ARG:HH22	1.78	0.48
2:I:47:LYS:HZ1	3:K:173:VAL:CB	2.26	0.48
2:I:348:ILE:HD11	2:I:407:ILE:HB	1.94	0.48
5:F:34:DA:H2'	4:L:334:ARG:HH22	1.78	0.48
1:H:275:LYS:HA	1:H:311:GLU:HG3	1.94	0.48
2:J:412:TRP:HE1	2:J:431:VAL:HG13	1.79	0.48
4:L:221:ARG:HD3	4:L:231:ARG:NH1	2.28	0.48
1:H:327:ASP:HA	1:H:351:VAL:HB	1.95	0.48
1:H:422:THR:HA	1:H:425:ARG:HB2	1.95	0.48
2:I:346:TRP:HZ2	2:I:353:ARG:NH1	2.11	0.48
3:K:97:HIS:HB3	3:K:102:PHE:HZ	1.79	0.48
1:A:408:THR:HG22	1:A:473:SER:HA	1.94	0.48
2:B:55:LYS:NZ	2:B:477:VAL:HA	2.29	0.48
2:B:429:LEU:HD13	3:D:80:PRO:HB2	1.96	0.48
2:I:228:HIS:HD2	2:J:83:ARG:HD2	1.79	0.48
2:J:23:LYS:HG3	2:J:25:ASP:HB2	1.95	0.48
4:L:517:LEU:HB2	4:L:520:PHE:HB2	1.96	0.48
2:B:246:PRO:HG3	2:B:303:GLN:HE21	1.79	0.48
4:E:257:SER:HB2	4:E:264:PRO:HG3	1.95	0.48
4:L:85:ILE:HG12	4:L:129:LEU:HD13	1.95	0.48
1:A:171:ASN:HA	1:A:200:GLN:HB2	1.95	0.48
1:H:179:LEU:O	1:H:183:CYS:HB2	2.13	0.48
1:H:305:VAL:HG23	1:H:308:ARG:HD2	1.95	0.48
2:I:126:TYR:O	2:I:130:ILE:N	2.36	0.48
2:J:394:ASN:HD22	2:J:397:ARG:HB2	1.78	0.48
2:C:190:GLU:N	2:C:196:LYS:HZ1	2.12	0.48
4:E:210:GLU:HA	4:E:213:ARG:HG2	1.96	0.48
5:F:34:DA:H8	4:L:334:ARG:HH12	1.60	0.48
1:H:93:TRP:HH2	3:K:185:ARG:HG2	1.79	0.48
1:H:193:PHE:HB3	1:H:270:MET:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:439:HIS:HD2	1:H:463:ARG:HH21	1.61	0.48
2:I:126:TYR:HA	2:I:129:SER:HB3	1.96	0.48
2:I:364:LYS:HG2	2:I:421:TYR:HD1	1.78	0.48
2:J:80:THR:HG22	2:J:607:LEU:HD21	1.96	0.48
4:L:353:TYR:CZ	4:L:355:ARG:HA	2.49	0.48
2:B:266:ASN:OD1	2:C:307:ARG:NE	2.38	0.48
2:C:84:ASP:OD2	2:C:87:ARG:HD3	2.13	0.48
2:C:368:LYS:HZ3	5:F:24:DG:H5'	1.79	0.48
1:H:21:TYR:HA	1:H:24:LEU:HD23	1.94	0.48
2:I:4:ARG:HD3	2:I:27:MET:HG3	1.95	0.48
2:I:475:ILE:HA	2:I:518:LYS:HG3	1.96	0.48
4:L:197:THR:HB	4:L:200:LEU:HB3	1.95	0.48
2:C:390:ASP:HB3	2:C:393:SER:HB3	1.97	0.47
2:J:176:VAL:HG23	2:J:200:TRP:HB2	1.96	0.47
2:J:300:ASP:CG	2:J:308:LYS:HZ1	2.17	0.47
4:L:265:GLY:H	4:L:371:GLU:HB2	1.80	0.47
4:L:268:GLN:HE21	4:L:366:TYR:HB2	1.78	0.47
1:A:45:VAL:HG22	4:E:75:TYR:CZ	2.49	0.47
2:I:47:LYS:HZ1	3:K:173:VAL:HB	1.79	0.47
4:L:96:ASP:HB3	4:L:105:GLU:OE2	2.14	0.47
1:A:104:PHE:HE1	1:A:118:LEU:HD21	1.79	0.47
2:B:119:MET:HB2	2:B:133:ILE:HD13	1.95	0.47
2:B:244:THR:O	2:B:248:ASP:N	2.47	0.47
2:I:258:THR:HG21	2:J:262:HIS:HB2	1.95	0.47
2:I:376:GLU:HG3	2:I:379:ILE:HD12	1.95	0.47
4:L:249:ILE:HB	4:L:272:LEU:HD12	1.96	0.47
2:C:19:ARG:NH1	2:C:20:ARG:HD3	2.29	0.47
2:J:191:TYR:HD2	2:J:192:LEU:HD12	1.79	0.47
2:B:35:LYS:HA	2:B:530:GLY:HA3	1.96	0.47
2:C:117:PHE:O	2:C:121:ASN:ND2	2.47	0.47
2:C:316:VAL:HB	2:C:353:ARG:NH1	2.25	0.47
2:C:516:LYS:O	2:C:519:LEU:HB2	2.14	0.47
2:C:528:ASP:HA	2:C:534:TYR:H	1.80	0.47
5:F:19:DT:OP2	5:F:19:DT:H2'	2.15	0.47
5:F:23:DT:H2"	5:F:24:DG:C8	2.50	0.47
5:F:49:DA:H2'	5:F:49:DA:OP2	2.14	0.47
6:G:18:DT:OP2	4:L:355:ARG:HB3	2.13	0.47
1:H:410:ILE:HA	1:H:475:VAL:HG13	1.97	0.47
2:I:68:TYR:O	2:I:72:ILE:N	2.46	0.47
2:I:558:LEU:HD11	2:J:289:LEU:HD21	1.95	0.47
2:J:271:ASP:HB3	2:J:286:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:513:ARG:NH1	2:C:603:ILE:HD13	2.29	0.47
3:D:164:GLU:OE2	3:D:167:ARG:NH2	2.43	0.47
4:E:190:LEU:HA	4:E:193:TRP:HD1	1.79	0.47
2:I:186:TYR:HD1	2:I:196:LYS:HD3	1.80	0.47
2:I:378:ASP:HA	2:I:381:GLN:HB2	1.95	0.47
2:J:81:LYS:HD3	2:J:251:LEU:HD13	1.97	0.47
4:L:451:SER:OG	4:L:454:SER:N	2.47	0.47
1:A:47:LEU:HD12	4:E:71:ASN:HA	1.96	0.47
1:A:153:ASP:HA	1:A:156:ALA:HB3	1.96	0.47
2:B:29:PRO:HB2	2:B:42:CYS:HB3	1.97	0.47
2:B:245:PHE:HA	2:B:248:ASP:OD2	2.14	0.47
2:C:150:LYS:O	2:C:152:HIS:ND1	2.48	0.47
4:E:78:LEU:HD12	4:E:79:PRO:HD2	1.97	0.47
4:E:325:ARG:HE	4:E:329:LEU:HA	1.79	0.47
6:G:25:DT:OP2	6:G:25:DT:H71	2.14	0.47
1:H:25:ASP:HA	1:H:115:ILE:HG21	1.95	0.47
1:H:369:TRP:HB3	1:H:450:ASN:HD22	1.79	0.47
2:I:146:ARG:HA	2:I:149:ASP:OD2	2.14	0.47
2:J:20:ARG:HH11	2:J:22:VAL:HG11	1.80	0.47
4:L:295:TYR:HE1	4:L:306:PHE:HB2	1.80	0.47
4:L:297:ILE:H	4:L:301:SER:HB2	1.79	0.47
1:A:129:LEU:N	1:A:142:TYR:O	2.41	0.47
2:C:229:PRO:HB2	2:C:263:THR:HG23	1.97	0.47
1:A:133:ASN:OD1	1:A:137:MET:N	2.48	0.47
1:A:198:GLU:HG2	1:A:275:LYS:HB3	1.97	0.47
2:I:393:SER:OG	2:I:395:ASN:OD1	2.30	0.47
2:I:559:ILE:HD13	2:I:567:PRO:HG3	1.95	0.47
2:J:63:LEU:HD21	2:J:421:TYR:HA	1.97	0.47
2:J:122:LEU:HB3	2:J:125:LEU:HD12	1.96	0.47
2:J:415:PHE:HA	2:J:418:TYR:HD2	1.79	0.47
4:L:136:CYS:HA	4:L:139:HIS:HB2	1.97	0.47
2:C:464:THR:HG23	2:C:507:LEU:HD13	1.97	0.46
3:D:8:LEU:HB3	3:D:87:LEU:HD21	1.97	0.46
4:E:509:SER:C	4:E:527:LYS:HZ3	2.18	0.46
1:H:279:ARG:HB3	4:L:38:LYS:HZ1	1.80	0.46
2:J:283:SER:HA	2:J:286:LYS:HE2	1.97	0.46
3:K:135:ILE:HD11	3:K:154:VAL:HG21	1.96	0.46
4:L:375:ARG:HH21	4:L:398:LYS:NZ	2.12	0.46
2:B:368:LYS:HE2	2:B:368:LYS:HB3	1.81	0.46
4:E:383:HIS:O	4:E:389:GLN:NE2	2.45	0.46
4:L:240:LYS:HB2	4:L:250:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:541:LEU:HD23	2:B:544:ASP:OD2	2.16	0.46
2:I:174:MET:C	2:I:455:ARG:HH12	2.18	0.46
2:I:259:GLN:HE22	2:J:255:SER:HB3	1.80	0.46
2:J:189:HIS:HB2	2:J:196:LYS:HG2	1.97	0.46
4:L:247:ASP:O	4:L:283:GLN:NE2	2.40	0.46
2:B:237:TYR:HA	2:B:240:LEU:HD12	1.97	0.46
2:B:429:LEU:HA	2:B:432:ILE:HD12	1.97	0.46
2:I:418:TYR:HB3	2:I:424:THR:HG22	1.97	0.46
4:L:326:GLY:N	4:L:331:THR:O	2.46	0.46
1:H:345:ILE:HD11	1:H:367:ILE:HG12	1.97	0.46
1:H:393:LYS:HE3	1:H:395:ASP:HB2	1.96	0.46
2:J:173:TYR:OH	2:J:242:THR:O	2.33	0.46
2:B:13:PRO:HG3	2:B:26:ARG:NH1	2.31	0.46
2:B:308:LYS:NZ	2:B:311:ALA:HA	2.31	0.46
2:C:276:LEU:N	6:G:45:DT:OP1	2.46	0.46
4:E:235:ARG:NH1	4:E:330:THR:O	2.40	0.46
5:F:45:DA:OP2	5:F:45:DA:H2'	2.16	0.46
5:F:49:DA:OP2	5:F:49:DA:H8	1.98	0.46
1:H:123:LEU:HD11	1:H:141:TRP:CG	2.50	0.46
3:K:25:ARG:NH1	3:K:145:PRO:HG2	2.31	0.46
3:K:183:ALA:CA	3:K:186:ARG:HH11	2.29	0.46
4:L:251:TYR:HD2	4:L:270:LEU:HD13	1.80	0.46
4:L:372:ASP:O	4:L:376:THR:OG1	2.25	0.46
2:B:156:GLY:HA2	2:B:159:TRP:HD1	1.80	0.46
2:B:333:ASP:HB3	2:B:334:VAL:HG13	1.98	0.46
3:D:173:VAL:HG13	3:D:175:ASP:HB2	1.97	0.46
1:H:428:ALA:HB1	2:I:275:LEU:HD23	1.98	0.46
4:L:190:LEU:HD23	4:L:533:LEU:HB2	1.98	0.46
4:L:473:PRO:HD2	4:L:502:LYS:NZ	2.31	0.46
4:L:487:ASP:HB3	4:L:490:PHE:HD2	1.81	0.46
1:A:25:ASP:OD2	1:A:134:LYS:NZ	2.47	0.46
1:A:283:LEU:HD23	1:A:287:LEU:HD22	1.97	0.46
2:B:376:GLU:HA	2:B:379:ILE:HD12	1.98	0.46
3:D:127:ASP:HB3	3:D:130:MET:HB3	1.97	0.46
4:E:46:LYS:HA	4:E:49:TYR:CZ	2.51	0.46
2:J:104:ASN:OD1	2:J:147:ARG:NH2	2.49	0.46
4:E:61:ILE:HG12	4:E:386:TRP:CE2	2.50	0.46
6:G:29:DA:OP2	6:G:29:DA:H2'	2.16	0.46
1:H:7:VAL:HA	1:H:10:LEU:HB2	1.98	0.46
2:I:429:LEU:HD23	2:I:432:ILE:HD12	1.98	0.46
2:I:520:LEU:HD21	2:I:536:PRO:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:371:ASP:OD1	2:J:418:TYR:OH	2.34	0.46
4:L:56:CYS:HA	4:L:61:ILE:HD12	1.98	0.46
4:L:255:THR:HB	4:L:266:HIS:H	1.81	0.46
1:A:127:LEU:HD13	1:A:186:ILE:HB	1.98	0.46
2:B:155:ASP:HA	2:B:232:ARG:HH22	1.80	0.46
1:H:66:MET:HB2	1:H:88:LEU:HD13	1.98	0.46
1:H:119:GLU:OE2	1:H:174:ASN:ND2	2.49	0.46
1:A:95:ARG:NH2	1:A:96:TYR:OH	2.49	0.45
2:B:176:VAL:HG11	2:B:201:GLU:HB3	1.98	0.45
4:E:221:ARG:NE	4:E:226:LEU:O	2.48	0.45
2:I:313:HIS:HB2	2:I:353:ARG:NH1	2.31	0.45
4:L:87:TRP:NE1	4:L:91:ASP:OD2	2.49	0.45
1:A:161:ASP:N	1:A:161:ASP:OD1	2.48	0.45
1:A:315:SER:O	1:A:341:ARG:N	2.41	0.45
1:A:453:ILE:HG12	1:A:476:LEU:HD11	1.96	0.45
2:B:70:TYR:HB2	2:B:359:LEU:HB3	1.97	0.45
2:C:274:PRO:HG2	2:C:283:SER:HB2	1.97	0.45
1:H:439:HIS:CE1	1:H:441:LYS:HB2	2.51	0.45
2:I:81:LYS:HB2	2:I:250:PRO:HD2	1.98	0.45
4:L:427:PRO:HG3	4:L:470:SER:HB2	1.98	0.45
1:A:186:ILE:HG23	1:A:189:GLN:HE21	1.81	0.45
2:C:127:PHE:HE2	2:C:342:GLU:HB2	1.81	0.45
4:E:293:ARG:NH1	4:E:324:LEU:HA	2.32	0.45
1:A:355:ASN:OD1	1:A:355:ASN:N	2.50	0.45
2:B:556:PHE:HA	2:B:559:ILE:HD12	1.97	0.45
2:J:355:LEU:HD23	2:J:373:ILE:HD13	1.98	0.45
2:B:174:MET:C	2:B:455:ARG:HH12	2.17	0.45
2:C:108:LYS:O	2:C:111:SER:OG	2.24	0.45
3:D:105:GLU:OE2	3:D:145:PRO:HD3	2.17	0.45
4:L:293:ARG:NH1	4:L:324:LEU:HA	2.32	0.45
1:A:95:ARG:NH1	1:A:141:TRP:O	2.48	0.45
1:A:258:ILE:HA	1:A:261:ILE:HD12	1.98	0.45
1:A:302:SER:O	1:A:305:VAL:N	2.50	0.45
2:B:159:TRP:CD1	2:B:232:ARG:NH1	2.85	0.45
2:B:217:LEU:HA	2:B:220:LEU:HD12	1.99	0.45
2:B:500:PHE:HB2	2:B:504:LEU:HB2	1.97	0.45
2:C:541:LEU:HD23	2:C:544:ASP:OD2	2.16	0.45
1:H:20:VAL:O	1:H:24:LEU:N	2.46	0.45
1:H:454:VAL:HG11	1:H:464:VAL:HG11	1.97	0.45
4:L:328:SER:HB3	4:L:331:THR:HG22	1.99	0.45
1:A:343:ALA:O	1:A:366:LYS:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LEU:HB3	2:B:274:PRO:HG2	1.99	0.45
2:C:146:ARG:HA	2:C:149:ASP:OD2	2.15	0.45
3:D:93:TRP:CG	3:D:146:LEU:HD13	2.52	0.45
4:E:331:THR:OG1	4:E:332:TYR:N	2.50	0.45
4:E:472:LEU:HA	4:E:475:ILE:HD12	1.97	0.45
2:I:239:ILE:O	2:I:242:THR:OG1	2.26	0.45
4:E:473:PRO:HB3	4:E:499:PHE:HA	1.99	0.45
2:I:549:GLU:O	2:I:553:ASP:N	2.46	0.45
4:L:275:GLN:HG3	4:L:277:CYS:H	1.82	0.45
2:B:82:GLN:HB2	2:B:607:LEU:HD23	1.99	0.45
2:B:95:ASP:OD2	2:B:221:LYS:NZ	2.44	0.45
2:B:429:LEU:HD23	2:B:432:ILE:HD12	1.98	0.45
2:C:62:LEU:HD23	2:C:472:PHE:HE2	1.82	0.45
4:E:275:GLN:HG3	4:E:277:CYS:H	1.82	0.45
2:I:238:LEU:HD22	2:I:295:ARG:HG3	1.98	0.45
2:J:79:LYS:NZ	2:J:247:TYR:HE1	2.14	0.45
4:L:87:TRP:HA	4:L:90:LEU:HD12	1.99	0.45
4:L:388:GLU:OE2	4:L:392:ALA:HB3	2.16	0.45
2:J:602:ASN:HB3	2:J:605:ASP:OD2	2.17	0.45
4:L:256:HIS:HA	4:L:264:PRO:HB3	1.98	0.45
2:B:230:ASP:OD2	2:B:232:ARG:HB2	2.17	0.44
4:E:217:ASP:HA	4:E:220:LEU:HD12	1.98	0.44
4:E:231:ARG:NH2	4:E:358:TYR:O	2.48	0.44
4:E:289:TYR:CZ	4:E:293:ARG:HD2	2.51	0.44
4:E:493:SER:O	4:E:497:SER:OG	2.26	0.44
1:H:392:ILE:HD12	1:H:411:LYS:HB3	1.99	0.44
4:L:187:LYS:HG3	4:L:349:CYS:HB3	1.97	0.44
2:B:429:LEU:HB3	3:D:80:PRO:HG2	1.99	0.44
2:B:562:LEU:HD23	2:B:562:LEU:HA	1.85	0.44
2:C:35:LYS:HG3	2:C:36:ARG:HG3	1.98	0.44
2:C:82:GLN:HB2	2:C:607:LEU:HD13	1.99	0.44
2:C:201:GLU:O	2:C:498:THR:OG1	2.35	0.44
2:C:394:ASN:O	2:C:398:PHE:HB2	2.17	0.44
3:D:7:VAL:HB	3:D:76:VAL:HG12	1.98	0.44
3:D:105:GLU:HA	3:D:111:ARG:HH11	1.83	0.44
4:E:56:CYS:O	4:E:61:ILE:N	2.43	0.44
4:E:297:ILE:HG12	4:E:486:GLN:HB2	1.99	0.44
4:E:505:HIS:ND1	4:E:509:SER:OG	2.38	0.44
3:K:173:VAL:HG13	3:K:175:ASP:HB2	2.00	0.44
4:L:224:LEU:HD22	4:L:270:LEU:HD23	1.98	0.44
1:H:357:LYS:HA	1:H:437:LEU:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:47:LYS:NZ	3:K:173:VAL:HB	2.31	0.44
2:I:439:ILE:HG23	2:I:492:LEU:HD13	1.99	0.44
2:J:388:GLU:O	2:J:396:SER:OG	2.35	0.44
2:B:262:HIS:CE1	2:C:309:PRO:HD2	2.52	0.44
2:C:19:ARG:HH12	2:C:20:ARG:HD3	1.82	0.44
3:D:24:GLU:HA	3:D:30:LYS:HB2	1.98	0.44
4:E:188:VAL:HG21	4:E:346:PHE:HE1	1.82	0.44
4:E:367:PRO:HG3	4:E:400:PRO:HG2	2.00	0.44
6:G:31:DA:H8	6:G:31:DA:OP2	2.00	0.44
1:H:411:LYS:HB2	1:H:476:LEU:HA	1.99	0.44
2:I:262:HIS:HB2	2:J:258:THR:HG21	2.00	0.44
2:I:555:MET:O	2:I:559:ILE:N	2.41	0.44
2:J:275:LEU:HG	2:J:286:LYS:HZ1	1.81	0.44
3:K:101:ASN:HD22	3:K:102:PHE:H	1.65	0.44
1:A:378:LYS:HA	1:A:381:LYS:HZ3	1.83	0.44
1:A:438:ASN:OD1	1:A:439:HIS:N	2.51	0.44
2:B:238:LEU:HD21	2:B:296:LEU:HA	2.00	0.44
2:C:199:ASN:HB3	2:C:201:GLU:HG3	2.00	0.44
2:C:397:ARG:NH1	2:C:449:LYS:HG3	2.33	0.44
1:H:36:ILE:HG23	1:H:39:LEU:HB2	1.99	0.44
2:J:102:TRP:HB3	2:J:212:PHE:HE1	1.82	0.44
2:J:117:PHE:O	2:J:121:ASN:HB2	2.17	0.44
2:J:436:LYS:HG2	2:J:439:ILE:HD12	1.98	0.44
1:A:357:LYS:HA	1:A:437:LEU:HA	2.00	0.44
2:B:424:THR:OG1	2:B:425:ALA:N	2.50	0.44
3:D:116:VAL:HG12	3:D:152:LYS:HE3	1.99	0.44
4:E:370:ASP:OD2	4:E:373:THR:HG23	2.17	0.44
5:F:33:DA:H3'	4:L:327:LYS:NZ	2.32	0.44
6:G:30:DA:H2"	6:G:31:DA:C8	2.53	0.44
1:H:99:LEU:CD2	3:K:161:ARG:HH12	2.31	0.44
2:I:208:MET:HA	2:I:211:ASN:HD22	1.83	0.44
2:J:98:GLU:HG2	2:J:214:ARG:HD2	1.98	0.44
1:A:375:ASN:HD22	1:A:378:LYS:NZ	2.16	0.44
2:C:21:LYS:HD2	5:F:29:DC:H41	1.81	0.44
2:I:43:MET:C	2:I:48:LEU:HD21	2.35	0.44
2:I:81:LYS:HB3	2:I:251:LEU:HD13	1.99	0.44
2:J:64:PHE:HE2	2:J:541:LEU:HB3	1.82	0.44
5:F:34:DA:OP2	5:F:34:DA:H8	2.00	0.44
1:H:393:LYS:N	1:H:412:GLU:O	2.50	0.44
2:I:385:ASP:HA	2:I:400:LYS:NZ	2.33	0.44
2:J:157:LYS:HD2	2:J:160:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:6:VAL:HA	3:K:75:ILE:HB	1.99	0.44
4:L:165:GLN:O	4:L:169:THR:N	2.50	0.44
1:A:87:TRP:CH2	1:A:139:GLU:HA	2.51	0.44
1:A:97:ASP:OD2	1:A:99:LEU:HB2	2.18	0.44
2:B:100:MET:HG2	2:B:104:ASN:HD21	1.82	0.44
2:C:95:ASP:N	2:C:97:GLU:OE1	2.50	0.44
6:G:50:DT:H2"	6:G:51:DA:C6	2.53	0.44
1:H:341:ARG:HH21	1:H:363:ARG:HH12	1.66	0.44
2:I:23:LYS:NZ	2:I:25:ASP:HB2	2.33	0.44
1:A:158:ASP:OD1	1:A:158:ASP:N	2.48	0.43
1:A:165:VAL:HG12	1:A:168:ILE:HD11	2.00	0.43
2:B:375:ARG:NE	3:D:106:ASP:OD1	2.51	0.43
2:B:506:LYS:HZ3	2:B:606:ILE:HA	1.83	0.43
3:D:129:GLU:HA	3:D:132:TYR:HD2	1.81	0.43
2:I:415:PHE:HA	2:I:418:TYR:HD2	1.83	0.43
2:C:341:THR:HA	2:C:344:LEU:HB3	2.00	0.43
2:C:541:LEU:HA	2:C:544:ASP:OD2	2.18	0.43
4:E:447:TYR:CZ	4:E:455:ARG:HG3	2.53	0.43
4:E:494:ASP:OD1	4:E:494:ASP:N	2.51	0.43
1:H:47:LEU:HD13	4:L:57:GLN:HE22	1.82	0.43
2:J:382:TYR:HA	2:J:385:ASP:HB2	2.00	0.43
2:J:451:GLU:OE2	2:J:497:PRO:HG2	2.18	0.43
4:L:160:HIS:HA	4:L:163:ASP:OD2	2.18	0.43
2:B:130:ILE:HD11	2:B:136:LEU:HD22	1.99	0.43
2:C:536:PRO:HG3	2:C:590:PHE:HA	1.98	0.43
1:H:408:THR:HA	1:H:473:SER:HA	2.01	0.43
2:I:28:ILE:HA	2:I:29:PRO:HA	1.86	0.43
2:J:143:TYR:O	2:J:147:ARG:N	2.37	0.43
2:J:540:ILE:HD11	2:J:594:VAL:HA	2.00	0.43
4:L:244:ARG:NH1	4:L:392:ALA:HA	2.33	0.43
1:A:168:ILE:HD13	1:A:195:THR:HG22	2.00	0.43
1:A:431:TRP:CD2	2:B:273:ARG:NH1	2.85	0.43
2:B:12:HIS:HE1	3:D:174:ASN:HB3	1.83	0.43
2:B:55:LYS:HB3	2:B:57:TYR:CZ	2.53	0.43
2:B:146:ARG:HA	2:B:149:ASP:OD2	2.18	0.43
2:B:175:PRO:HA	2:B:455:ARG:HH22	1.83	0.43
3:D:117:ASP:OD2	3:D:119:TRP:HB3	2.18	0.43
4:E:447:TYR:O	4:E:455:ARG:NH1	2.51	0.43
5:F:45:DA:OP2	5:F:45:DA:H8	2.01	0.43
2:I:4:ARG:NH1	2:I:29:PRO:HD2	2.33	0.43
2:J:528:ASP:HB3	2:J:533:PHE:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:165:GLU:O	3:K:169:THR:N	2.36	0.43
2:B:20:ARG:NH1	2:B:38:GLN:OE1	2.51	0.43
2:C:273:ARG:HH12	5:F:15:DA:C5'	2.31	0.43
2:J:390:ASP:HB3	2:J:393:SER:HB3	2.00	0.43
2:B:121:ASN:OD1	2:B:394:ASN:ND2	2.52	0.43
3:D:165:GLU:OE2	3:D:166:ILE:HG13	2.19	0.43
4:E:94:ILE:O	4:E:96:ASP:N	2.51	0.43
2:I:214:ARG:HA	2:I:217:LEU:HD12	2.00	0.43
1:A:120:TRP:HE1	1:A:196:ILE:HG22	1.84	0.43
1:A:305:VAL:HG23	1:A:308:ARG:HD2	2.00	0.43
1:A:387:PHE:HA	1:A:391:TYR:HB2	2.01	0.43
2:B:439:ILE:HD11	2:B:489:LEU:HD12	2.00	0.43
2:C:126:TYR:O	2:C:130:ILE:N	2.45	0.43
4:E:334:ARG:O	4:E:337:THR:OG1	2.34	0.43
2:I:115:MET:HB3	2:I:137:TYR:CE1	2.53	0.43
4:L:161:TRP:O	4:L:164:SER:OG	2.30	0.43
1:A:169:GLN:OE1	1:A:200:GLN:NE2	2.51	0.43
2:C:6:THR:OG1	2:C:7:GLN:N	2.50	0.43
2:C:126:TYR:HB2	2:C:130:ILE:HG12	2.00	0.43
5:F:30:DC:H2"	5:F:31:DG:OP2	2.18	0.43
1:H:132:PHE:HB3	1:H:136:SER:HA	2.00	0.43
1:H:423:TYR:O	1:H:427:GLN:N	2.50	0.43
4:L:380:GLU:O	4:L:384:GLY:N	2.52	0.43
1:A:152:ILE:O	1:A:156:ALA:N	2.51	0.43
2:C:54:SER:OG	2:C:55:LYS:N	2.51	0.43
2:C:491:GLU:HG2	2:C:495:ASN:HD21	1.84	0.43
3:D:18:VAL:HB	3:D:22:ILE:HD12	2.01	0.43
3:D:170:PHE:HE2	3:D:181:GLU:HG2	1.83	0.43
2:I:101:PHE:HA	2:I:104:ASN:HD22	1.82	0.43
4:L:62:ILE:HA	4:L:63:PRO:HD3	1.89	0.43
1:A:410:ILE:HA	1:A:475:VAL:HG13	2.01	0.43
1:H:184:LEU:HD12	1:H:262:ARG:HG3	2.00	0.43
2:I:305:GLY:H	2:I:308:LYS:HB3	1.84	0.43
2:J:208:MET:HA	2:J:211:ASN:HD22	1.84	0.43
2:J:217:LEU:HD23	2:J:220:LEU:HD12	2.00	0.43
1:A:438:ASN:HA	1:A:458:LEU:HD11	1.99	0.42
2:B:55:LYS:NZ	2:B:477:VAL:HG22	2.35	0.42
2:C:506:LYS:O	2:C:509:TYR:HB3	2.19	0.42
2:I:75:ILE:HA	2:I:79:LYS:HB2	2.00	0.42
3:K:9:VAL:HG22	3:K:15:ARG:HG2	1.99	0.42
1:A:271:LYS:H	1:A:308:ARG:NH2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:TYR:O	2:B:147:ARG:N	2.52	0.42
2:B:178:LYS:HA	2:B:181:GLU:HB2	2.01	0.42
2:B:313:HIS:HB2	2:B:353:ARG:NH1	2.35	0.42
4:E:98:LYS:HD2	4:E:101:GLU:OE2	2.20	0.42
4:E:402:ASP:N	4:E:402:ASP:OD1	2.51	0.42
2:I:248:ASP:HA	2:I:503:LYS:HZ3	1.81	0.42
2:I:394:ASN:O	2:I:398:PHE:CB	2.67	0.42
2:J:315:GLU:CD	2:J:353:ARG:HH12	2.22	0.42
4:L:49:TYR:HB2	4:L:132:LEU:HD22	2.00	0.42
4:L:235:ARG:NH1	4:L:320:ASP:O	2.52	0.42
1:A:381:LYS:HD3	1:A:381:LYS:HA	1.85	0.42
2:B:11:LYS:HB2	3:D:175:ASP:HA	2.01	0.42
2:B:82:GLN:O	2:B:83:ARG:NE	2.52	0.42
2:C:549:GLU:HA	2:C:552:ASN:HD22	1.85	0.42
1:H:67:TYR:HE1	1:H:74:LEU:HB3	1.83	0.42
1:H:95:ARG:HE	1:H:140:VAL:HA	1.83	0.42
1:H:268:GLU:HG2	1:H:305:VAL:HB	2.01	0.42
2:I:6:THR:HG22	2:I:27:MET:HB3	2.01	0.42
2:I:47:LYS:NZ	3:K:173:VAL:HA	2.34	0.42
4:L:468:PHE:O	4:L:472:LEU:HB2	2.19	0.42
1:A:399:PHE:HB2	2:B:386:SER:HB2	2.01	0.42
1:A:473:SER:OG	1:A:474:GLN:N	2.52	0.42
4:E:516:ILE:HG21	4:E:524:TYR:HB2	2.01	0.42
1:H:58:ARG:HH21	3:K:191:ALA:HB1	1.84	0.42
1:H:309:ILE:HG12	1:H:331:TRP:HZ3	1.84	0.42
2:I:46:THR:OG1	3:K:174:ASN:HA	2.20	0.42
2:J:439:ILE:HG12	2:J:492:LEU:HD13	2.01	0.42
4:L:212:LEU:HA	4:L:212:LEU:HD23	1.83	0.42
1:A:22:PHE:HA	1:A:114:LEU:HD11	2.01	0.42
2:B:162:LEU:O	2:B:165:SER:OG	2.26	0.42
2:B:418:TYR:O	2:B:423:ASP:N	2.47	0.42
2:C:474:GLN:HG3	2:C:518:LYS:HZ3	1.84	0.42
3:D:97:HIS:NE2	3:D:120:ASP:OD1	2.50	0.42
4:E:223:TYR:CZ	4:E:282:PRO:HD3	2.55	0.42
1:H:421:ILE:HD12	1:H:421:ILE:HA	1.88	0.42
2:J:123:GLY:H	2:J:395:ASN:HA	1.83	0.42
4:L:185:LEU:HD11	4:L:219:GLN:HG2	2.02	0.42
2:B:189:HIS:CD2	2:B:196:LYS:HA	2.55	0.42
2:C:474:GLN:NE2	2:C:479:SER:O	2.53	0.42
4:E:77:ASP:OD1	4:E:77:ASP:N	2.49	0.42
4:E:107:GLU:HB3	4:E:110:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:195:ASN:N	2:J:195:ASN:OD1	2.53	0.42
3:K:29:LEU:HD13	3:K:77:MET:HG2	2.01	0.42
4:L:59:ASN:OD1	4:L:388:GLU:N	2.42	0.42
4:L:202:GLU:OE2	4:L:206:LYS:HA	2.20	0.42
4:E:202:GLU:OE2	4:E:206:LYS:HG2	2.20	0.42
4:E:212:LEU:HD12	4:E:292:LEU:HD12	2.01	0.42
4:E:224:LEU:HD22	4:E:270:LEU:HD23	2.02	0.42
4:L:107:GLU:HG3	4:L:109:LEU:H	1.84	0.42
2:B:393:SER:OG	2:B:395:ASN:OD1	2.24	0.42
1:H:110:TYR:HB3	1:H:113:THR:HB	2.01	0.42
2:I:117:PHE:HE1	2:I:178:LYS:HZ2	1.64	0.42
2:I:279:ASP:OD2	2:I:281:VAL:HB	2.20	0.42
2:I:281:VAL:HG12	2:J:559:ILE:HD13	2.02	0.42
2:B:240:LEU:O	2:B:243:THR:OG1	2.33	0.42
2:B:339:ASN:HD22	2:B:340:SER:H	1.68	0.42
2:B:527:LEU:HB3	2:B:534:TYR:HB2	2.01	0.42
1:H:262:ARG:HH11	1:H:265:ARG:NH1	2.17	0.42
2:I:29:PRO:HB2	2:I:42:CYS:HB3	2.01	0.42
2:J:27:MET:HB2	2:J:30:CYS:HA	2.02	0.42
4:L:55:TRP:HZ2	4:L:91:ASP:OD2	2.03	0.42
2:B:57:TYR:HB3	2:B:533:PHE:HD2	1.85	0.42
3:D:8:LEU:HD13	3:D:87:LEU:HD11	2.01	0.42
4:E:56:CYS:HB3	4:E:61:ILE:HB	2.02	0.42
1:H:167:ASN:H	1:H:168:ILE:HD12	1.85	0.42
2:I:395:ASN:HA	2:I:398:PHE:HB3	2.02	0.42
2:J:146:ARG:HA	2:J:149:ASP:OD2	2.20	0.42
4:L:129:LEU:HD23	4:L:129:LEU:HA	1.90	0.42
1:A:45:VAL:HG23	4:E:73:VAL:HB	2.01	0.41
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.88	0.41
3:D:6:VAL:HG12	3:D:75:ILE:HB	2.02	0.41
4:E:114:GLU:HG3	4:E:118:LYS:HZ1	1.85	0.41
2:I:262:HIS:CE1	2:J:309:PRO:HD2	2.55	0.41
2:J:238:LEU:HD13	2:J:295:ARG:HB2	2.01	0.41
2:B:491:GLU:O	2:B:495:ASN:ND2	2.52	0.41
1:H:425:ARG:NH2	2:I:276:LEU:O	2.53	0.41
2:I:167:PHE:O	2:I:171:ILE:HG12	2.20	0.41
4:L:244:ARG:NH1	4:L:391:GLU:HG2	2.35	0.41
2:C:13:PRO:HG2	5:F:28:DT:H3'	2.02	0.41
3:D:165:GLU:O	3:D:169:THR:N	2.42	0.41
4:E:90:LEU:HD13	4:E:394:ALA:HB1	2.02	0.41
4:E:178:THR:HA	4:E:181:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:307:ARG:NH1	2:I:552:ASN:HA	2.35	0.41
4:L:48:TYR:HE2	4:L:124:LYS:HB3	1.86	0.41
4:L:181:LEU:O	4:L:524:TYR:OH	2.32	0.41
1:A:67:TYR:O	1:A:71:ALA:N	2.54	0.41
1:A:290:PHE:N	1:A:327:ASP:OD1	2.54	0.41
1:A:431:TRP:HA	1:A:434:PHE:HD2	1.85	0.41
2:B:200:TRP:HB3	2:B:205:GLN:HB2	2.02	0.41
1:H:122:TYR:HA	1:H:127:LEU:HA	2.02	0.41
1:H:355:ASN:OD1	1:H:355:ASN:N	2.54	0.41
1:H:422:THR:H	1:H:425:ARG:HD3	1.86	0.41
2:J:96:THR:O	2:J:100:MET:N	2.41	0.41
2:J:128:GLY:HA3	2:J:295:ARG:CZ	2.51	0.41
4:L:400:PRO:HB2	4:L:403:PHE:HB2	2.02	0.41
4:L:529:ASN:O	4:L:532:SER:OG	2.30	0.41
1:A:320:ILE:HG23	1:A:342:VAL:HG21	2.02	0.41
2:B:11:LYS:HE2	3:D:173:VAL:HG21	2.02	0.41
2:B:300:ASP:O	2:B:304:SER:OG	2.29	0.41
3:D:161:ARG:HG3	3:D:166:ILE:HD11	2.02	0.41
4:E:183:PRO:HA	4:E:184:PRO:HD3	1.96	0.41
2:I:162:LEU:O	2:I:165:SER:OG	2.28	0.41
2:I:307:ARG:HH12	2:I:552:ASN:CB	2.33	0.41
2:I:540:ILE:HG13	2:I:594:VAL:HG13	2.01	0.41
3:K:20:LYS:HZ3	3:K:33:LEU:HD13	1.84	0.41
4:L:155:THR:O	4:L:159:THR:OG1	2.28	0.41
4:L:423:ASP:OD2	4:L:426:PRO:HA	2.21	0.41
1:A:184:LEU:HA	1:A:184:LEU:HD23	1.87	0.41
1:A:315:SER:HA	1:A:340:SER:HB3	2.01	0.41
2:B:271:ASP:OD1	2:B:272:PHE:N	2.53	0.41
2:C:121:ASN:HA	2:C:394:ASN:HB3	2.03	0.41
1:H:66:MET:HG2	3:K:190:TRP:HZ2	1.85	0.41
1:H:392:ILE:HG13	1:H:411:LYS:HD3	2.02	0.41
2:I:159:TRP:CD2	2:I:232:ARG:NH1	2.88	0.41
2:I:346:TRP:CE2	2:I:350:SER:HB3	2.55	0.41
2:I:392:ARG:HA	2:I:449:LYS:NZ	2.34	0.41
4:L:249:ILE:HB	4:L:272:LEU:HB2	2.03	0.41
1:A:439:HIS:CE1	1:A:441:LYS:HB2	2.55	0.41
3:D:169:THR:HA	3:D:172:ILE:HD11	2.03	0.41
2:I:159:TRP:CD1	2:I:232:ARG:NH1	2.89	0.41
2:J:442:ILE:HG21	2:J:492:LEU:HD21	2.03	0.41
3:K:124:LEU:HD22	3:K:134:ILE:HD13	2.03	0.41
3:K:186:ARG:HA	3:K:189:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:133:SER:O	4:L:137:LYS:HG2	2.21	0.41
4:L:278:PRO:HB3	4:L:471:ASN:HB3	2.01	0.41
4:L:487:ASP:HB3	4:L:490:PHE:CD2	2.56	0.41
1:A:56:SER:O	1:A:59:SER:OG	2.28	0.41
2:C:6:THR:HG21	2:C:28:ILE:H	1.85	0.41
2:C:313:HIS:O	2:C:353:ARG:NH1	2.53	0.41
4:E:412:PRO:HD2	4:E:413:TYR:CE2	2.55	0.41
5:F:23:DT:H2"	5:F:24:DG:N7	2.36	0.41
2:I:503:LYS:HD3	2:I:506:LYS:HD2	2.03	0.41
2:I:544:ASP:HA	2:I:547:ILE:HD12	2.02	0.41
4:L:473:PRO:HB2	4:L:502:LYS:HD2	2.02	0.41
1:A:265:ARG:HG3	1:A:265:ARG:HH11	1.86	0.41
2:B:153:SER:HB2	2:C:86:THR:HA	2.01	0.41
2:B:254:ASN:O	2:B:258:THR:OG1	2.30	0.41
3:D:32:TYR:CE2	3:D:77:MET:HB3	2.56	0.41
4:E:295:TYR:OH	4:E:438:GLU:OE1	2.38	0.41
4:E:373:THR:HA	4:E:376:THR:HB	2.02	0.41
4:E:386:TRP:HB2	4:E:389:GLN:NE2	2.36	0.41
4:E:405:LYS:HB3	4:E:410:LYS:HB2	2.02	0.41
5:F:22:DT:H1'	5:F:23:DT:H5'	2.02	0.41
5:F:47:DA:H1'	5:F:48:DT:H5'	2.03	0.41
6:G:13:DC:H2"	6:G:14:DT:OP2	2.20	0.41
6:G:35:DA:H2"	6:G:36:DA:H5'	2.03	0.41
1:H:108:HIS:CE1	1:H:162:LEU:HG	2.56	0.41
2:I:73:THR:HB	2:I:464:THR:HG22	2.02	0.41
2:I:75:ILE:HD13	2:I:79:LYS:HD2	2.03	0.41
2:I:245:PHE:HZ	2:I:252:LEU:HD23	1.86	0.41
2:I:384:VAL:HG22	2:I:400:LYS:HD2	2.02	0.41
2:J:143:TYR:HA	2:J:146:ARG:HB3	2.01	0.41
4:L:262:ASP:OD1	4:L:262:ASP:N	2.54	0.41
4:L:326:GLY:HA2	4:L:333:PRO:HG3	2.03	0.41
4:L:439:ILE:HD12	4:L:465:ARG:NH1	2.36	0.41
1:A:167:ASN:OD1	1:A:167:ASN:N	2.54	0.41
1:A:320:ILE:HG12	1:A:345:ILE:HG22	2.01	0.41
1:H:165:VAL:HG12	1:H:168:ILE:HD11	2.03	0.41
2:J:274:PRO:HA	2:J:286:LYS:HE3	2.03	0.41
1:A:280:GLY:O	1:A:284:TYR:N	2.42	0.40
1:A:454:VAL:O	1:A:478:ILE:N	2.49	0.40
2:C:527:LEU:O	2:C:534:TYR:N	2.53	0.40
6:G:14:DT:OP2	6:G:14:DT:H6	2.04	0.40
2:I:204:MET:HA	2:I:207:VAL:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:397:ARG:HH12	2:I:449:LYS:HD3	1.86	0.40
2:B:6:THR:N	2:B:27:MET:SD	2.90	0.40
2:B:190:GLU:OE2	2:B:196:LYS:NZ	2.52	0.40
2:C:65:TRP:NE1	2:C:69:GLU:OE1	2.54	0.40
4:E:304:ASP:OD2	4:E:325:ARG:HD3	2.20	0.40
2:I:31:GLY:HA3	2:I:531:ASP:OD2	2.20	0.40
2:I:115:MET:HB3	2:I:137:TYR:HE1	1.86	0.40
2:I:471:SER:O	2:I:475:ILE:HG13	2.21	0.40
2:J:200:TRP:HB3	2:J:205:GLN:HB2	2.03	0.40
4:L:183:PRO:HA	4:L:184:PRO:HD3	1.91	0.40
1:A:10:LEU:HA	1:A:17:ARG:HD3	2.03	0.40
2:B:307:ARG:NH2	2:C:266:ASN:O	2.41	0.40
2:C:99:CYS:HA	2:C:215:CYS:SG	2.61	0.40
4:E:236:PHE:HA	4:E:239:LEU:HD12	2.03	0.40
2:I:102:TRP:CH2	2:I:188:LEU:HD12	2.53	0.40
2:J:166:VAL:HG22	2:J:239:ILE:HG21	2.03	0.40
2:J:430:LYS:HD2	2:J:434:TYR:HE2	1.86	0.40
2:J:471:SER:O	2:J:475:ILE:HG13	2.21	0.40
1:A:440:ILE:HB	1:A:464:VAL:HG23	2.04	0.40
2:C:274:PRO:HB3	2:C:278:ASP:OD2	2.22	0.40
3:D:121:ARG:HG2	3:D:125:LYS:HE3	2.03	0.40
4:E:124:LYS:HB3	4:E:124:LYS:HE2	1.87	0.40
4:E:221:ARG:NH1	4:E:225:ASN:HA	2.36	0.40
4:E:227:SER:H	4:E:230:GLU:HB2	1.85	0.40
4:E:287:ALA:HB2	4:E:464:LEU:HB3	2.04	0.40
2:I:157:LYS:HG3	2:J:90:ALA:HB2	2.04	0.40
2:J:559:ILE:HG23	2:J:562:LEU:HD12	2.03	0.40
1:A:441:LYS:HG3	1:A:465:GLU:OE2	2.21	0.40
2:C:273:ARG:HA	2:C:274:PRO:HD3	1.79	0.40
2:C:506:LYS:O	2:C:510:LEU:N	2.48	0.40
4:E:148:THR:O	4:E:152:GLU:N	2.46	0.40
5:F:37:DT:OP2	5:F:37:DT:H6	2.05	0.40
1:H:396:ASP:OD1	1:H:396:ASP:N	2.53	0.40
2:I:159:TRP:CG	2:I:232:ARG:NH1	2.90	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	415/478 (87%)	343 (83%)	71 (17%)	1 (0%)	47	81
1	H	415/478 (87%)	338 (81%)	76 (18%)	1 (0%)	47	81
2	B	573/608 (94%)	519 (91%)	54 (9%)	0	100	100
2	C	565/608 (93%)	528 (94%)	37 (6%)	0	100	100
2	I	573/608 (94%)	514 (90%)	57 (10%)	2 (0%)	41	76
2	J	546/608 (90%)	505 (92%)	41 (8%)	0	100	100
3	D	147/194 (76%)	138 (94%)	9 (6%)	0	100	100
3	K	147/194 (76%)	137 (93%)	10 (7%)	0	100	100
4	E	502/956 (52%)	436 (87%)	66 (13%)	0	100	100
4	L	502/956 (52%)	449 (89%)	53 (11%)	0	100	100
All	All	4385/5688 (77%)	3907 (89%)	474 (11%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	48	LEU
1	A	369	TRP
2	I	49	ILE
1	H	369	TRP

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	388/449 (86%)	381 (98%)	7 (2%)	59	77
1	H	388/449 (86%)	382 (98%)	6 (2%)	65	80
2	B	539/569 (95%)	533 (99%)	6 (1%)	73	85
2	C	524/569 (92%)	518 (99%)	6 (1%)	73	85
2	I	539/569 (95%)	535 (99%)	4 (1%)	84	90
2	J	516/569 (91%)	510 (99%)	6 (1%)	71	84
3	D	136/179 (76%)	134 (98%)	2 (2%)	65	80
3	K	136/179 (76%)	134 (98%)	2 (2%)	65	80
4	E	476/897 (53%)	470 (99%)	6 (1%)	69	82
4	L	476/897 (53%)	471 (99%)	5 (1%)	73	85
All	All	4118/5326 (77%)	4068 (99%)	50 (1%)	72	84

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LEU
1	A	171	ASN
1	A	187	LEU
1	A	310	ASN
1	A	333	ASN
1	A	351	VAL
1	A	474	GLN
2	B	23	LYS
2	B	49	ILE
2	B	67	ASN
2	B	197	ARG
2	B	339	ASN
2	B	367	LEU
2	C	23	LYS
2	C	67	ASN
2	C	199	ASN
2	C	232	ARG
2	C	291	ARG
2	C	394	ASN
3	D	101	ASN
3	D	139	ASN
4	E	73	VAL
4	E	143	ASN
4	E	177	ASN

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Mol	Chain	Res	Type
4	E	379	ASN
4	E	429	LYS
4	E	455	ARG
1	H	83	LEU
1	H	171	ASN
1	H	175	LEU
1	H	310	ASN
1	H	333	ASN
1	H	474	GLN
2	I	23	LYS
2	I	49	ILE
2	I	67	ASN
2	I	339	ASN
2	J	67	ASN
2	J	179	LEU
2	J	199	ASN
2	J	232	ARG
2	J	291	ARG
2	J	394	ASN
3	K	101	ASN
3	K	139	ASN
4	L	143	ASN
4	L	177	ASN
4	L	379	ASN
4	L	429	LYS
4	L	455	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	189	GLN
1	A	310	ASN
1	A	333	ASN
1	A	375	ASN
1	A	404	ASN
1	A	439	HIS
1	A	450	ASN
2	B	67	ASN
2	B	82	GLN
2	B	303	GLN
2	B	339	ASN

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Mol	Chain	Res	Type
2	B	445	ASN
2	B	454	ASN
2	B	495	ASN
2	B	543	ASN
2	C	66	GLN
2	C	67	ASN
2	C	199	ASN
2	C	211	ASN
2	C	259	GLN
2	C	445	ASN
2	C	461	GLN
2	C	495	ASN
2	C	552	ASN
2	C	598	GLN
3	D	128	GLN
3	D	174	ASN
4	E	57	GLN
4	E	86	HIS
4	E	143	ASN
4	E	177	ASN
4	E	225	ASN
4	E	340	ASN
4	E	379	ASN
4	E	453	ASN
1	H	108	HIS
1	H	289	ASN
1	H	296	ASN
1	H	310	ASN
1	H	333	ASN
1	H	420	GLN
1	H	439	HIS
1	H	444	ASN
1	H	450	ASN
2	I	67	ASN
2	I	82	GLN
2	I	104	ASN
2	I	152	HIS
2	I	254	ASN
2	I	259	GLN
2	I	339	ASN
2	I	543	ASN
2	J	67	ASN

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Mol	Chain	Res	Type
2	J	199	ASN
2	J	211	ASN
2	J	235	GLN
2	J	394	ASN
2	J	598	GLN
3	K	101	ASN
3	K	139	ASN
4	L	57	GLN
4	L	86	HIS
4	L	143	ASN
4	L	177	ASN
4	L	268	GLN
4	L	340	ASN
4	L	379	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

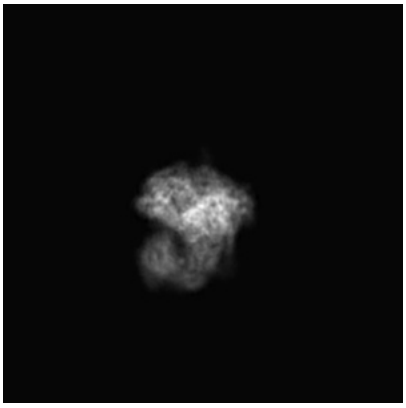
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0096. These allow visual inspection of the internal detail of the map and identification of artifacts.

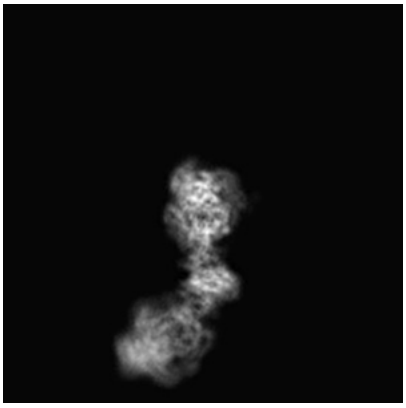
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

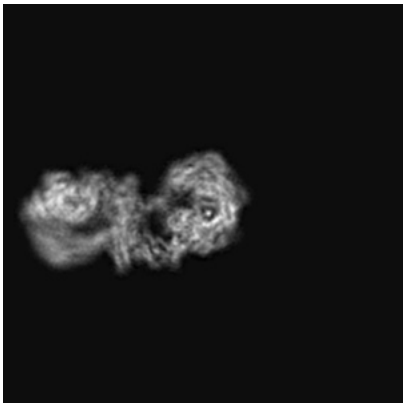
6.1.1 Primary map



X



Y



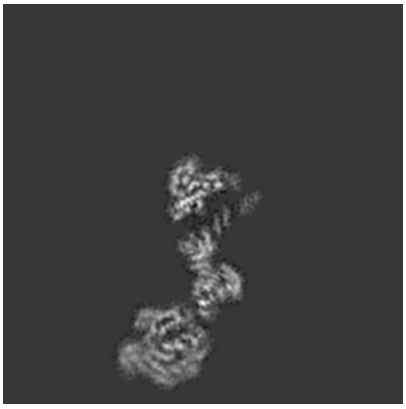
Z

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

6.2 Central slices (i)

6.2.1 Primary map

X Index: 200



Y Index: 200

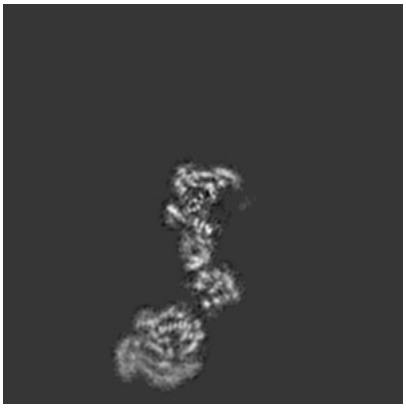
Z Index: 200

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: 205



Y Index: 194

Z Index: 203

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

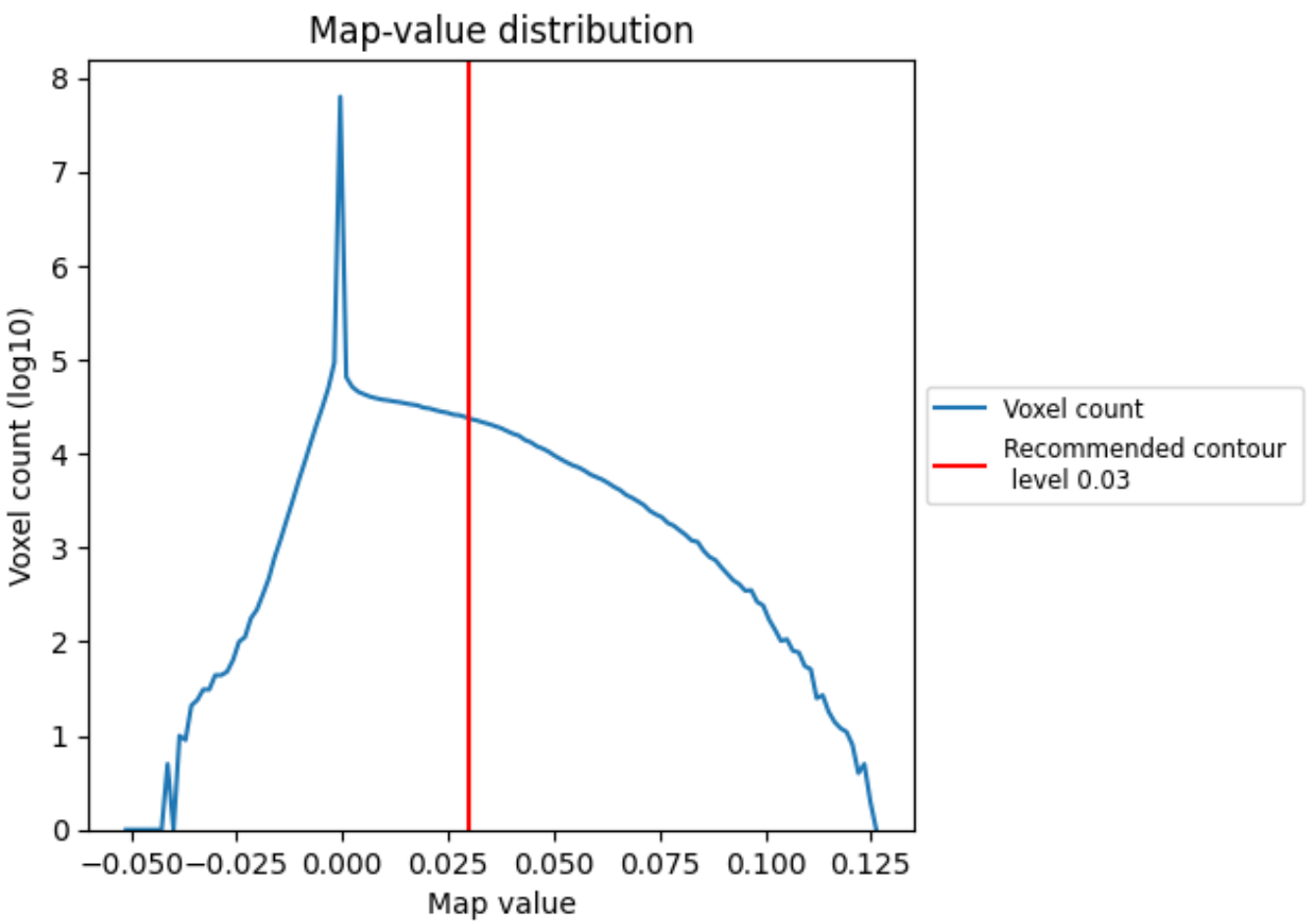
6.5 Mask visualisation (i)

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

7 Map analysis (i)

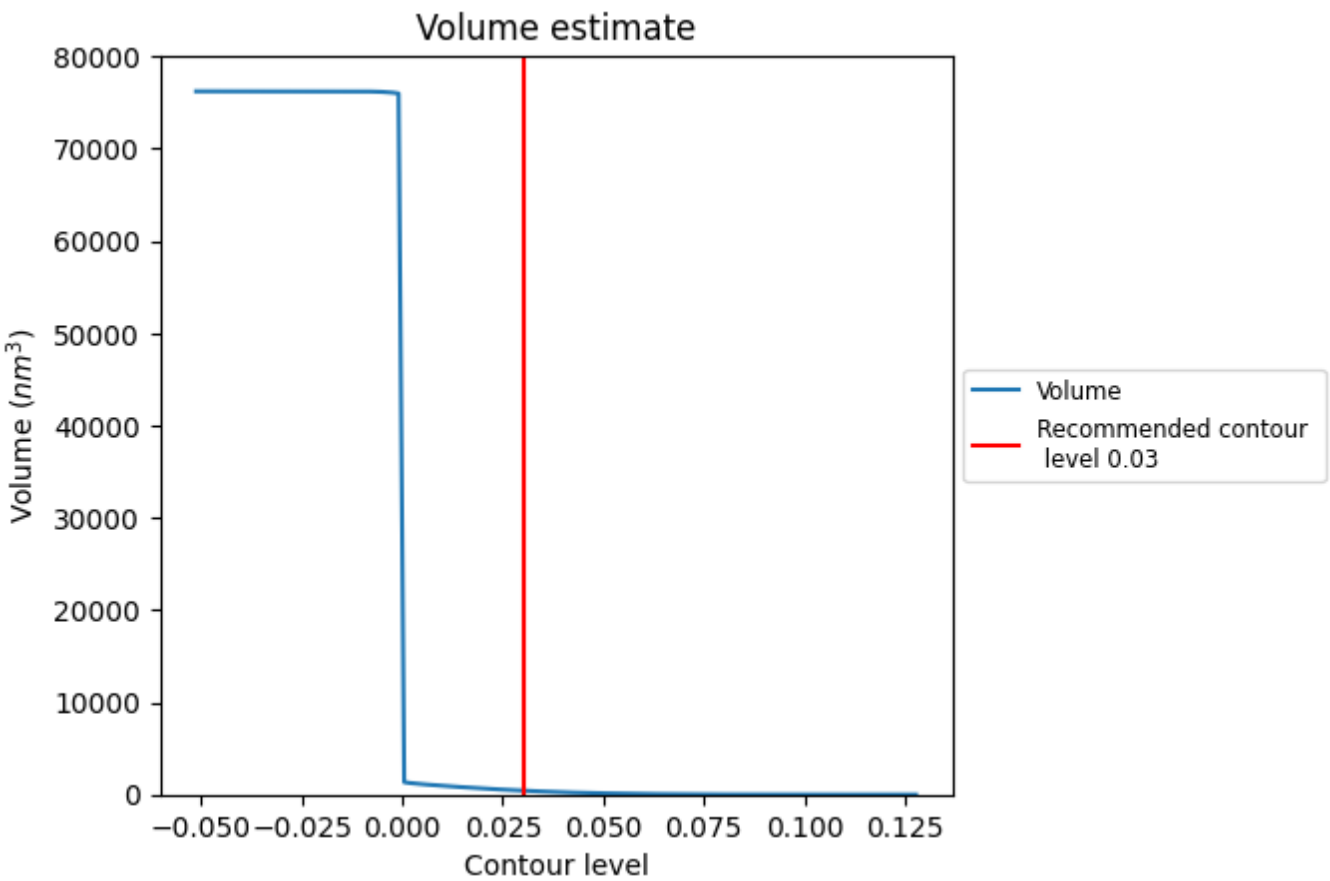
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

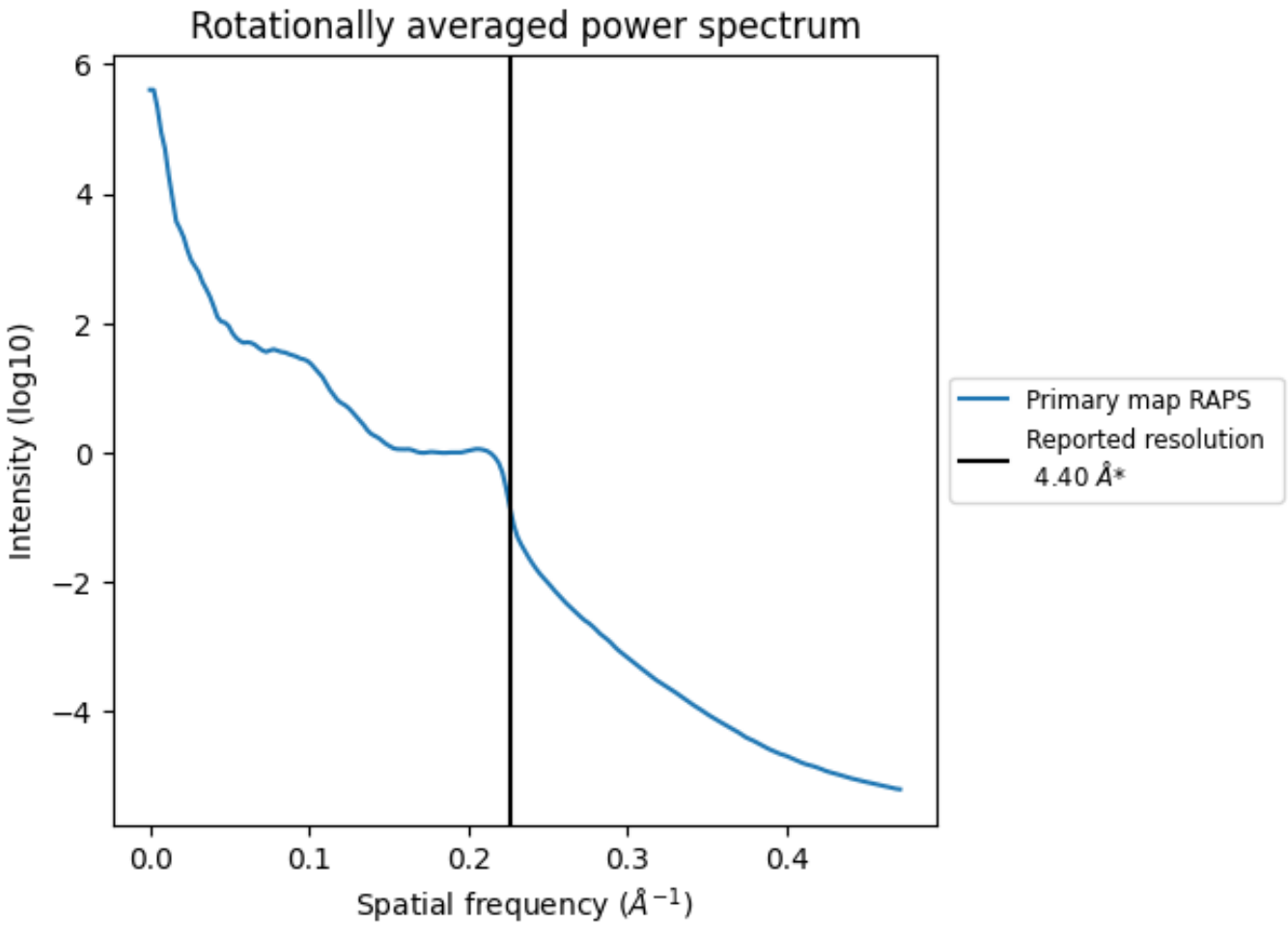
7.2 Volume estimate (i)



The volume at the recommended contour level is 426 nm^3; this corresponds to an approximate mass of 385 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 0.227 Å^{-1}

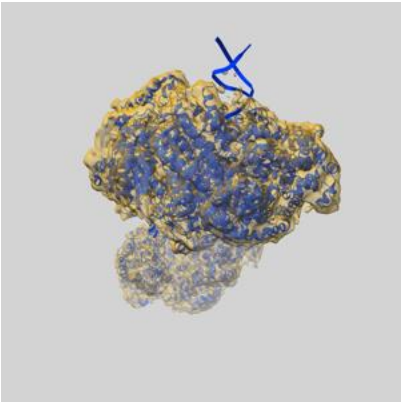
8 Fourier-Shell correlation (i)

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

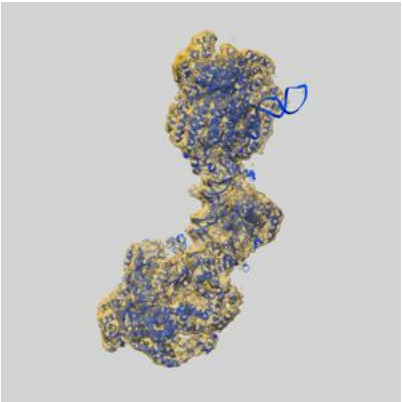
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0096 and PDB model 6GYS. Per-residue inclusion information can be found in section 3 on page 6.

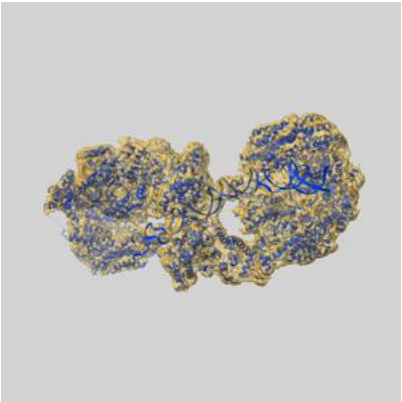
9.1 Map-model overlay (i)



X



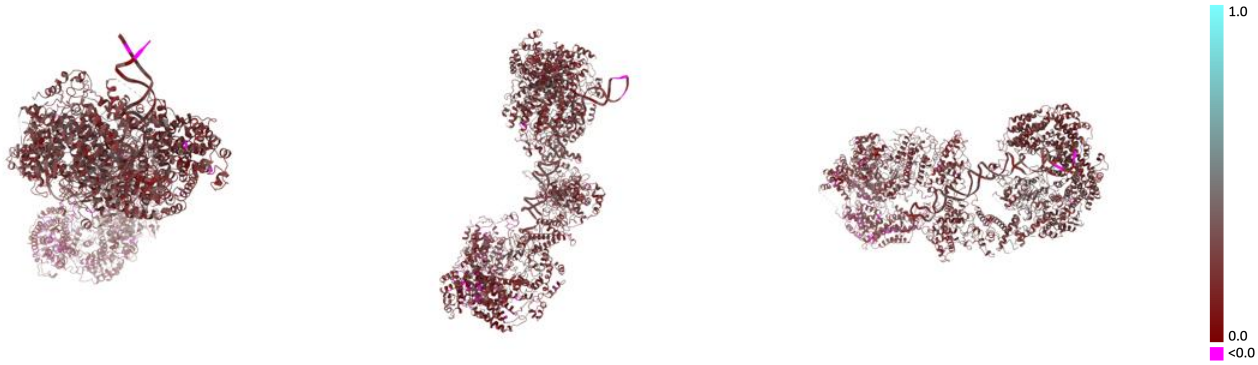
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

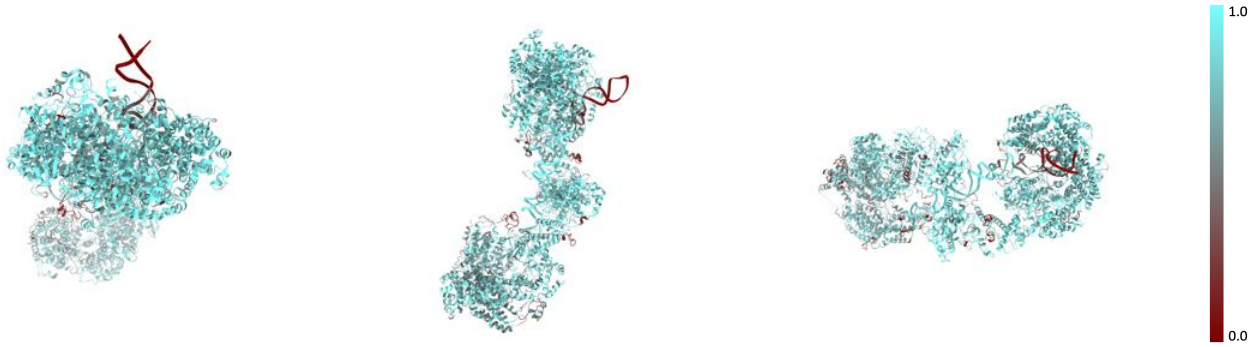
9.2 Q-score mapped to coordinate model (i)



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.

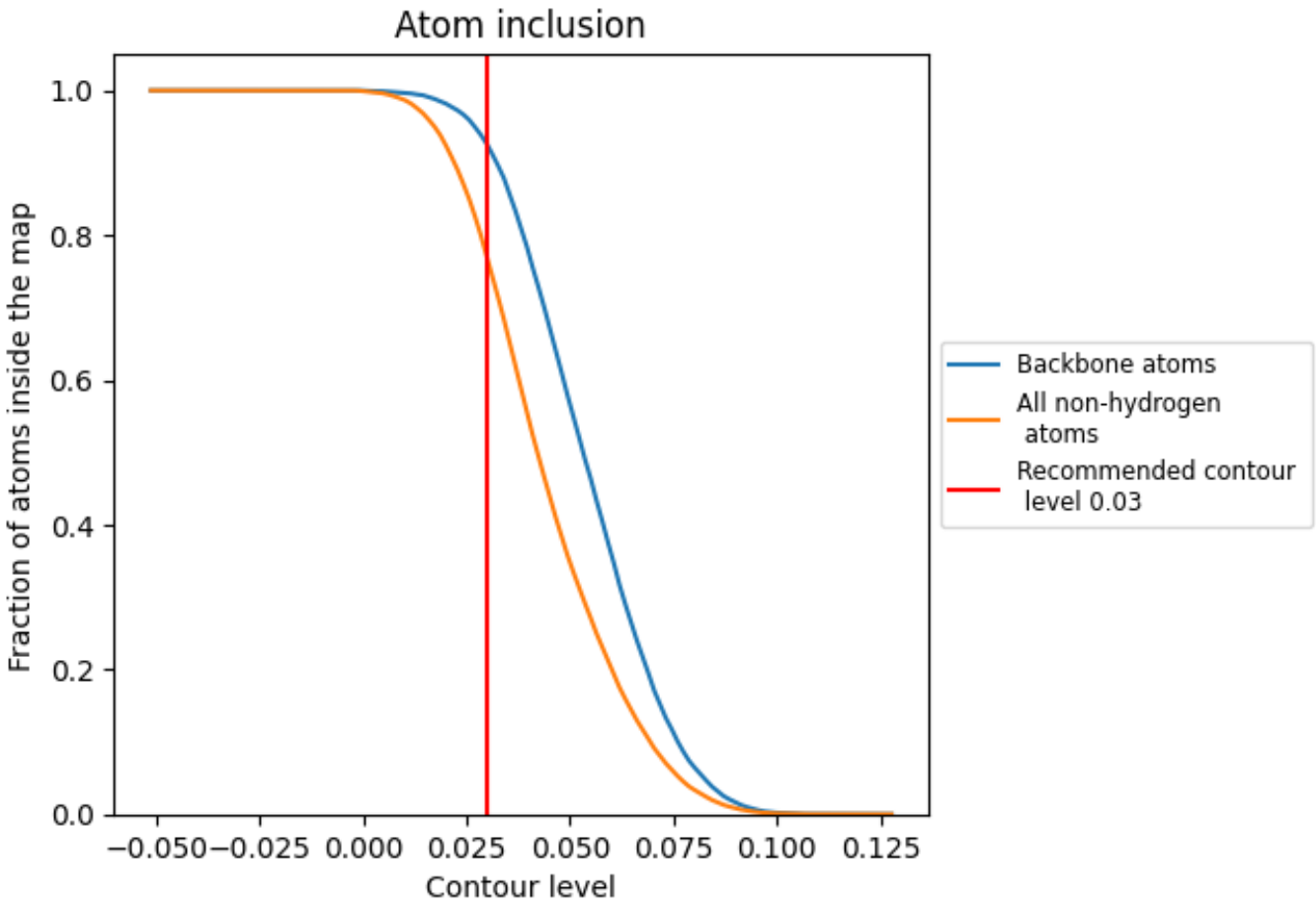
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 77% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7688	0.2450
A	0.8522	0.3210
B	0.8238	0.2740
C	0.7967	0.2440
D	0.8570	0.2790
E	0.8028	0.2720
F	0.6645	0.2450
G	0.6676	0.2630
H	0.7966	0.2560
I	0.6905	0.1960
J	0.6499	0.1630
K	0.7851	0.2140
L	0.7898	0.2560