Full wwPDB EM Validation Report

Jan 15, 2023 – 10:18 PM JST

PDB ID	:	7XHN
EMDB ID	:	EMD-33196
Title	:	Structure of human inner kinetochore CCAN-DNA complex
Authors	:	Sun, L.F.; Tian, T.; Wang, C.L.; Yang, Z.S.; Zang, J.Y.
Deposited on	:	2022-04-09
Resolution	:	3.71 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

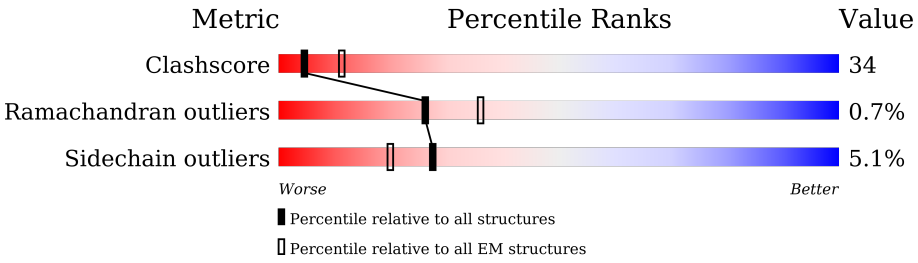
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.71 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	O	300	29% 37% 31%
1	o	300	96%
2	H	253	34% 40% 23%
3	I	756	31% 35% 32%
4	K	269	39% 38% 7% 14%
5	L	344	51% 35% 12%
6	M	180	43% 46% 7%
7	N	345	48% 37% 12%

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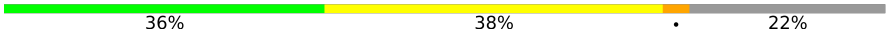
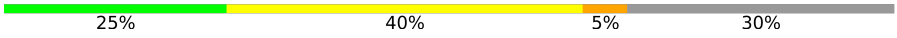
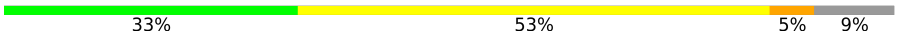
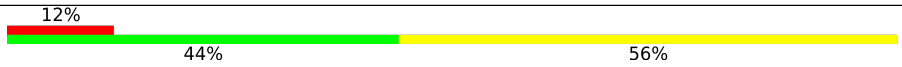
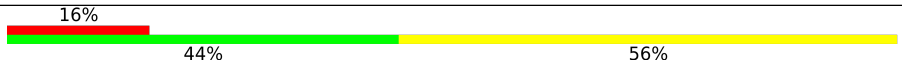
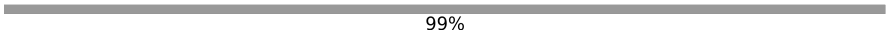
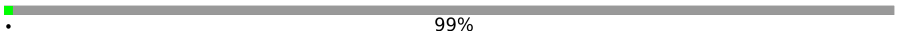
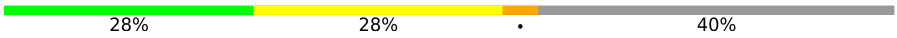
Mol	Chain	Length	Quality of chain
8	P	288	
9	S	138	
10	T	561	
11	W	88	
12	X	81	
13	G	25	
14	J	25	
15	C	943	
15	c	943	
16	Q	274	
17	U	418	
18	R	177	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 23364 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 protein O.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	o	12	Total C N O 95 59 18 18	0	0
1	O	206	Total C N O S 1588 1017 269 294 8	0	0

- Molecule 2 is a protein called Centromere protein H.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	H	195	Total C N O S 1560 980 273 299 8	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	248	HIS	-	expression tag	UNP Q9H3R5
H	249	HIS	-	expression tag	UNP Q9H3R5
H	250	HIS	-	expression tag	UNP Q9H3R5
H	251	HIS	-	expression tag	UNP Q9H3R5
H	252	HIS	-	expression tag	UNP Q9H3R5
H	253	HIS	-	expression tag	UNP Q9H3R5

- Molecule 3 is a protein called Centromere protein I.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	I	517	Total C N O S 4111 2700 661 724 26	0	0

- Molecule 4 is a protein called Centromere protein K.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	K	230	Total C N O S 1869 1183 312 364 10	0	0

- Molecule 5 is a protein called Centromere protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	302	Total	C	N	O	S	0	0
			2422	1576	396	436	14		

- Molecule 6 is a protein called Centromere protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	168	Total	C	N	O	S	0	0
			1298	825	232	234	7		

- Molecule 7 is a protein called Centromere protein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	305	Total	C	N	O	S	0	0
			2493	1601	434	448	10		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	340	HIS	-	expression tag	UNP Q96H22
N	341	HIS	-	expression tag	UNP Q96H22
N	342	HIS	-	expression tag	UNP Q96H22
N	343	HIS	-	expression tag	UNP Q96H22
N	344	HIS	-	expression tag	UNP Q96H22
N	345	HIS	-	expression tag	UNP Q96H22

- Molecule 8 is a protein called Centromere protein P.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	224	Total	C	N	O	S	0	0
			1808	1144	311	344	9		

- Molecule 9 is a protein called Centromere protein S.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	97	Total	C	N	O	S	0	0
			790	494	141	150	5		

- Molecule 10 is a protein called Centromere protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	99	Total	C	N	O	S	0	0
			804	516	139	142	7		

- Molecule 11 is a protein called CENP-W.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	75	Total	C	N	O	S	0	0
			584	367	119	95	3		

- Molecule 12 is a protein called Centromere protein X.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	74	Total	C	N	O	S	0	0
			590	378	104	107	1		

- Molecule 13 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	25	Total	C	N	O	P	0	0
			513	241	98	149	25		

- Molecule 14 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	25	Total	C	N	O	P	0	0
			512	241	95	151	25		

- Molecule 15 is a protein called Centromere protein C.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	C	5	Total	C	N	O	0	0
			40	28	5	7		
15	c	13	Total	C	N	O	0	0
			105	69	17	19		

- Molecule 16 is a protein called Centromere protein Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	164	Total	C	N	O	S	0	0
			1175	718	207	242	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	269	HIS	-	expression tag	UNP Q7L2Z9
Q	270	HIS	-	expression tag	UNP Q7L2Z9
Q	271	HIS	-	expression tag	UNP Q7L2Z9
Q	272	HIS	-	expression tag	UNP Q7L2Z9
Q	273	HIS	-	expression tag	UNP Q7L2Z9
Q	274	HIS	-	expression tag	UNP Q7L2Z9

- Molecule 17 is a protein called Centromere protein U.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	U	140	Total	C	N	O	0	0
			699	419	140	140		

- Molecule 18 is a protein called Centromere protein R.

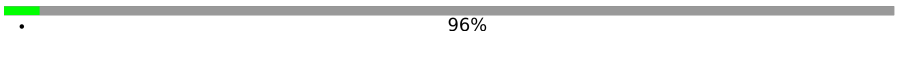
Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	62	Total	C	N	O	0	0
			308	184	62	62		

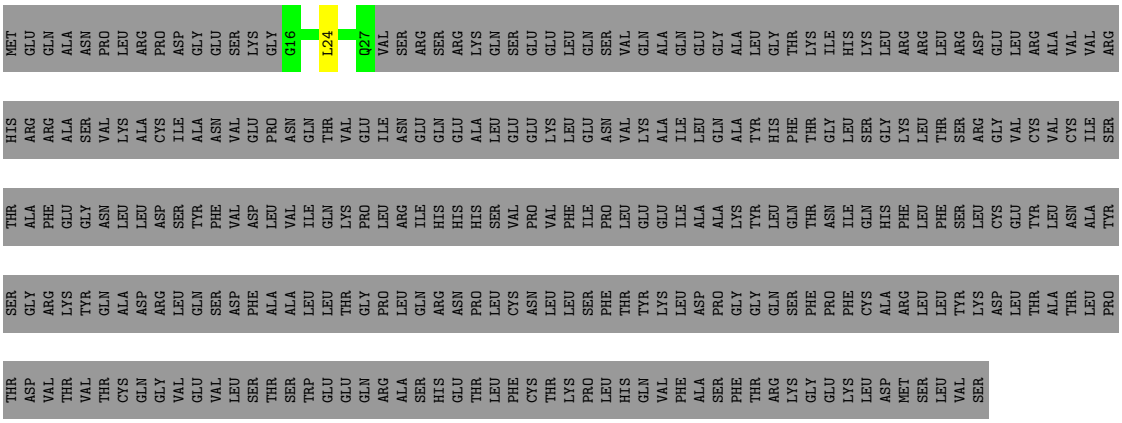
3 Residue-property plots (i)

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 protein O

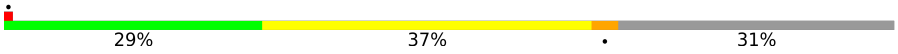
Chain o:

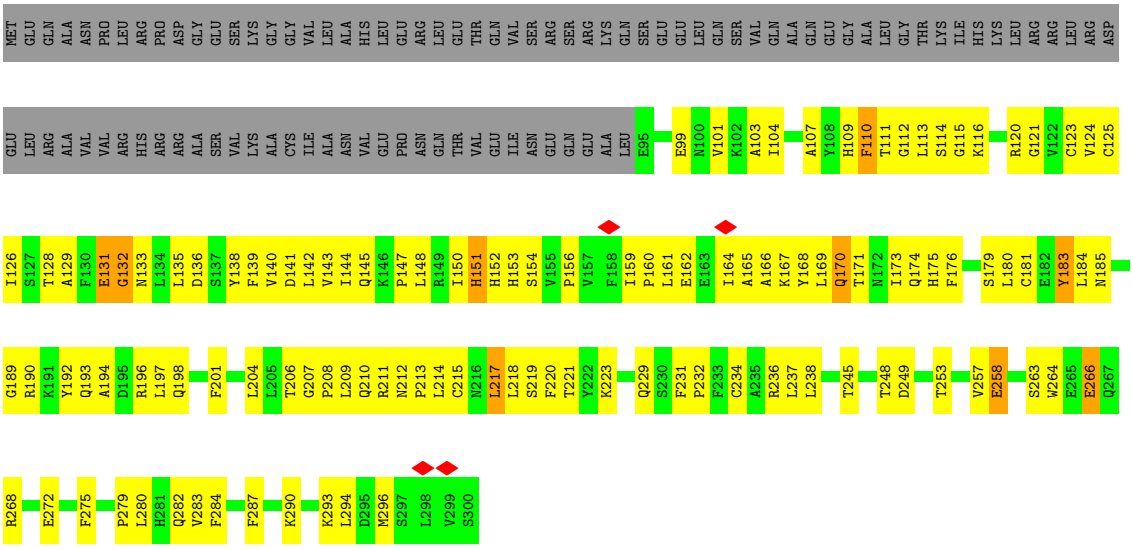




• Molecule 1: Centromere protein O

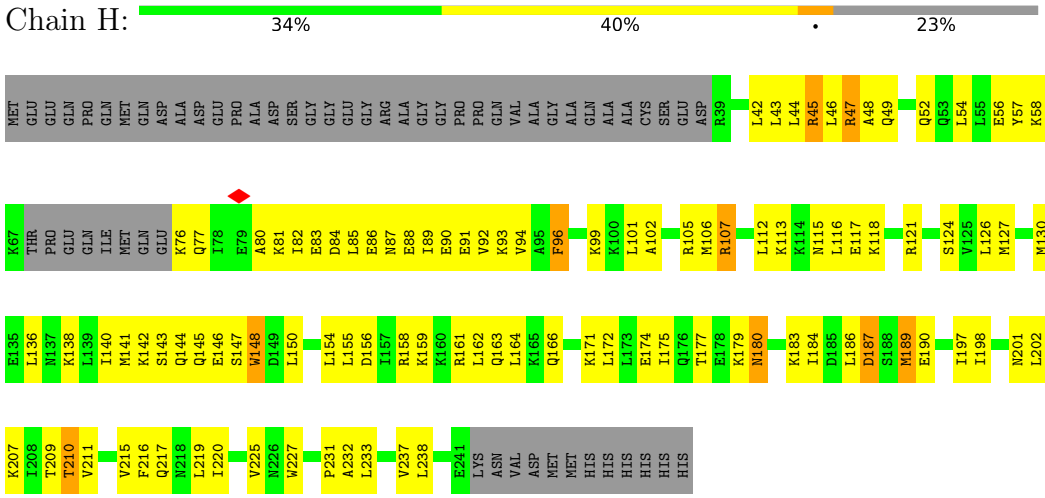
Chain O:





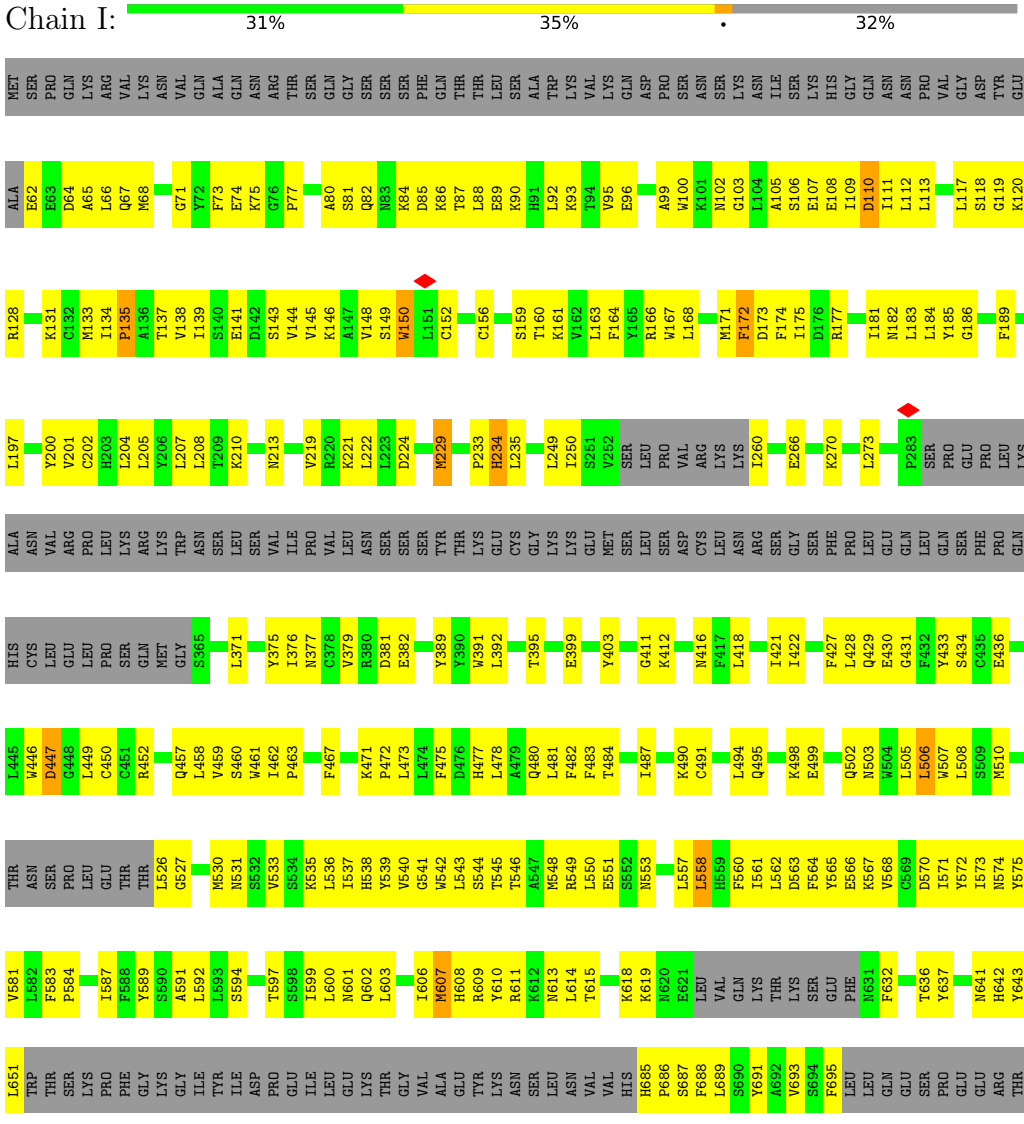
• Molecule 2: Centromere protein H

Chain H:



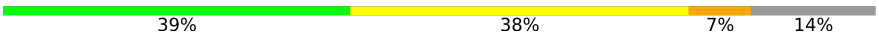
• Molecule 3: Centromere protein I

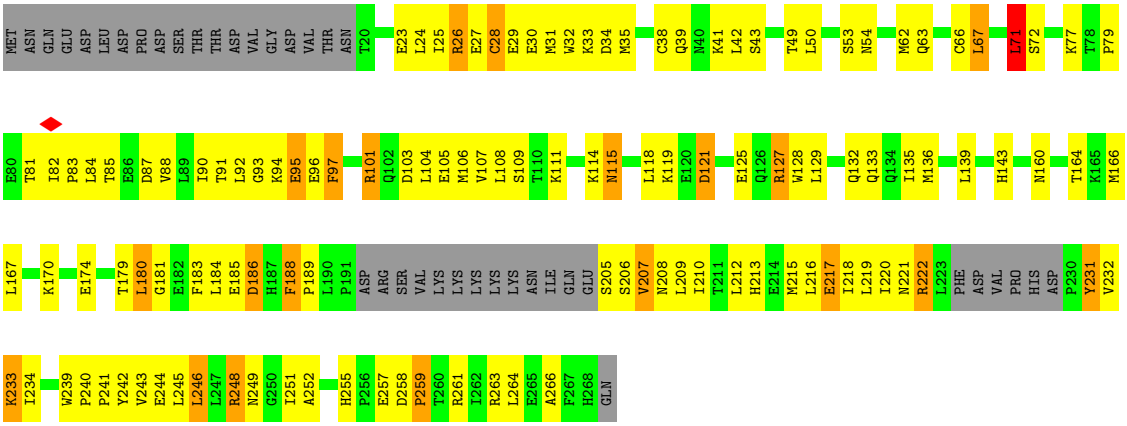
Chain I:



• Molecule 4: Centromere protein K

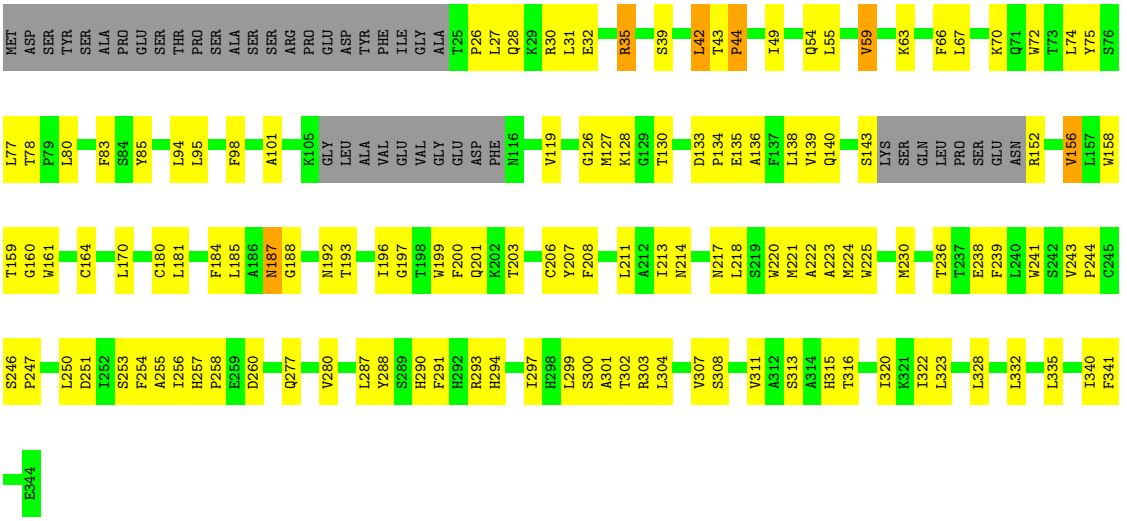
Chain K:





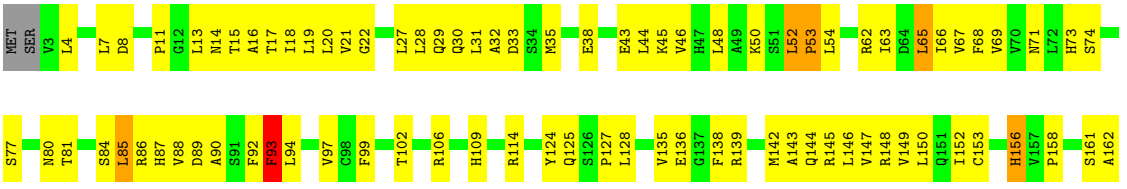
• Molecule 5: Centromere protein L

Chain L:



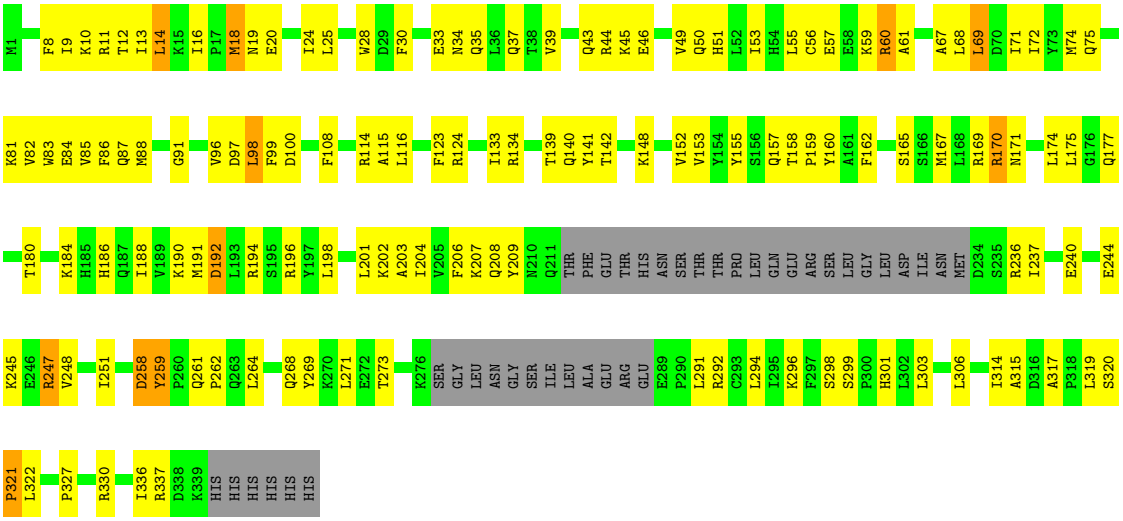
• Molecule 6: Centromere protein M

Chain M:



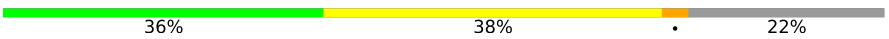
• Molecule 7: Centromere protein N

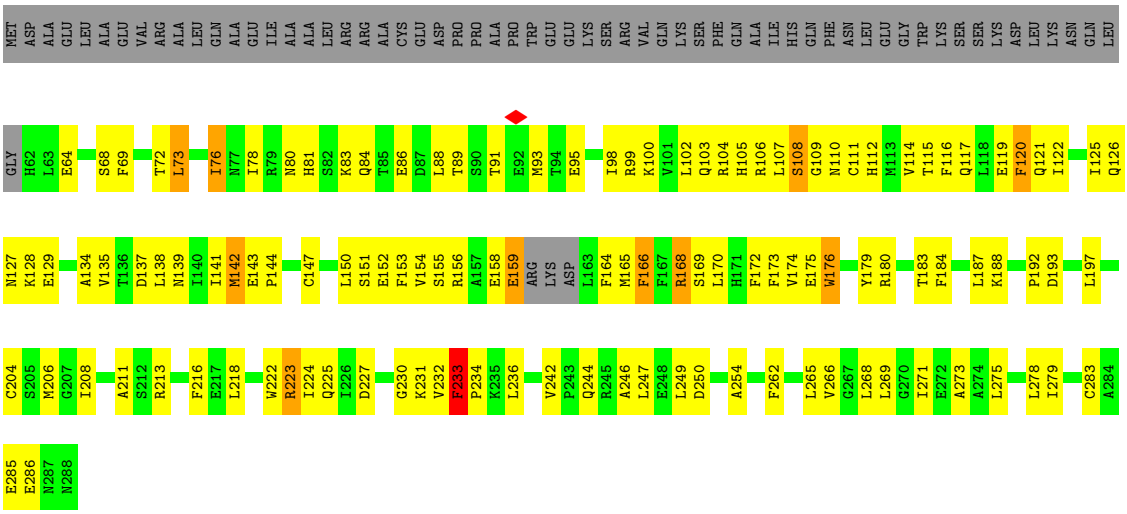
Chain N:



• Molecule 8: Centromere protein P

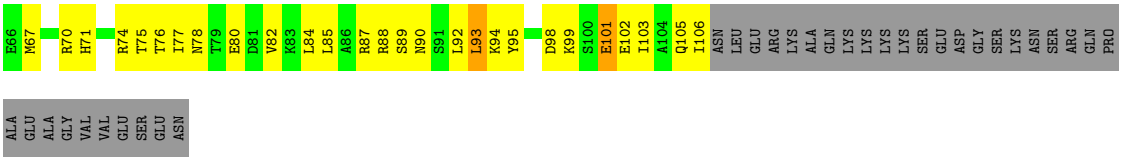
Chain P:





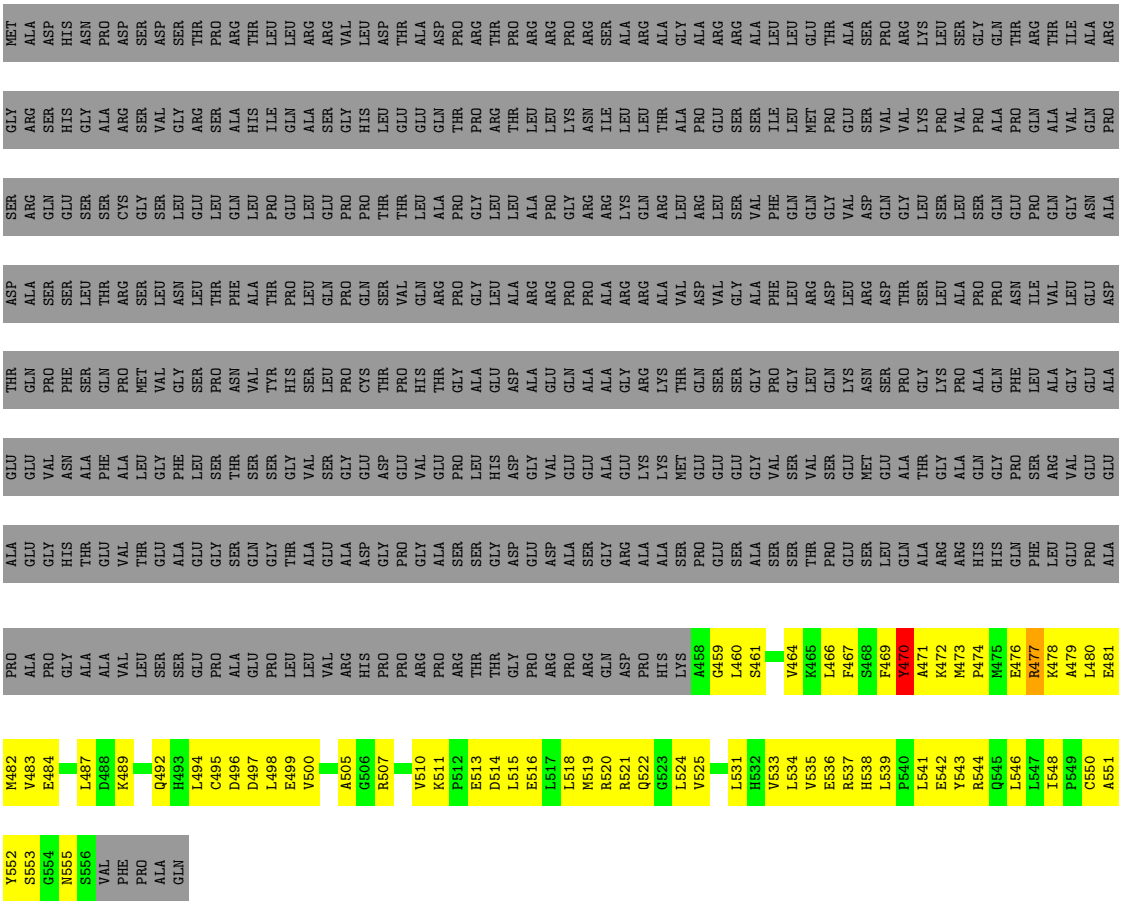
• Molecule 9: Centromere protein S

Chain S:



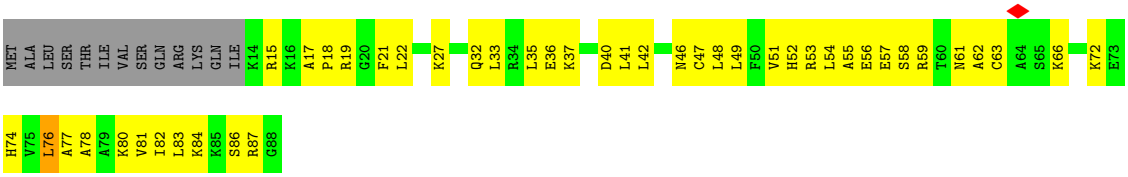
• Molecule 10: Centromere protein T

Chain T: 6% 11% 82%



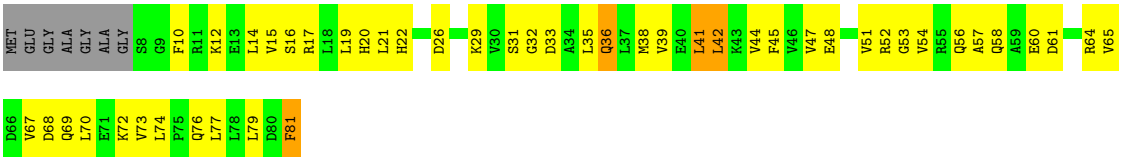
• Molecule 11: CENP-W

Chain W: 35% 49% 15%

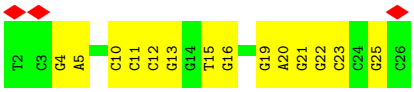


• Molecule 12: Centromere protein X

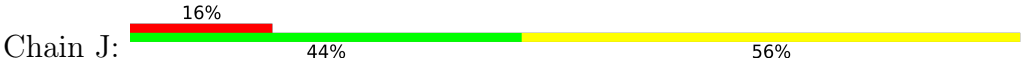
Chain X: 33% 53% 5% 9%

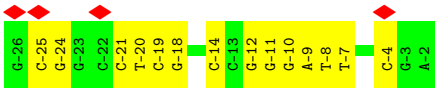


• Molecule 13: DNA (25-MER)

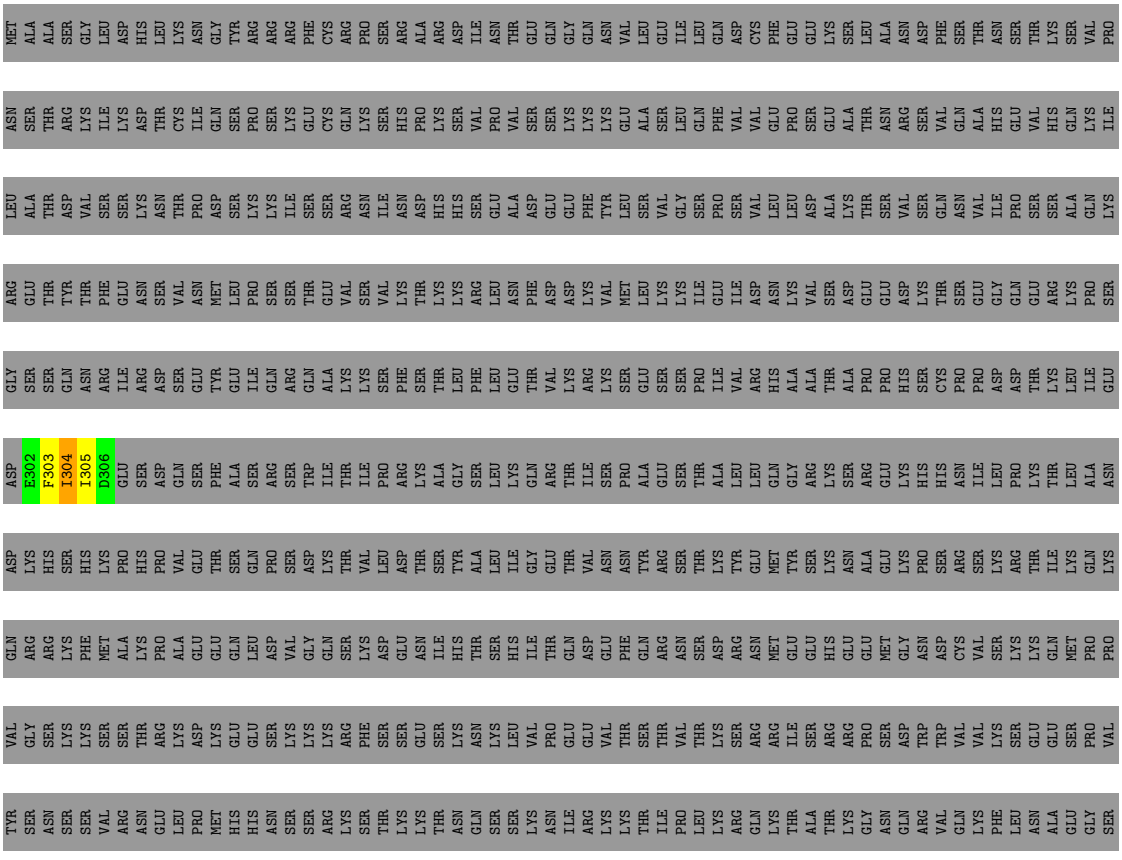


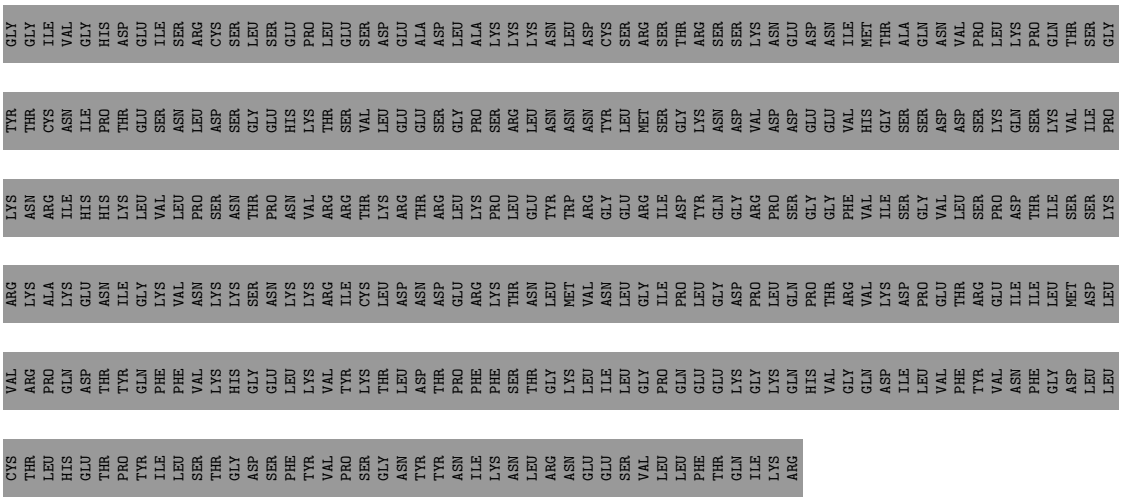
• Molecule 14: DNA (25-MER)





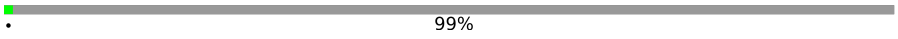
• Molecule 15: Centromere protein C

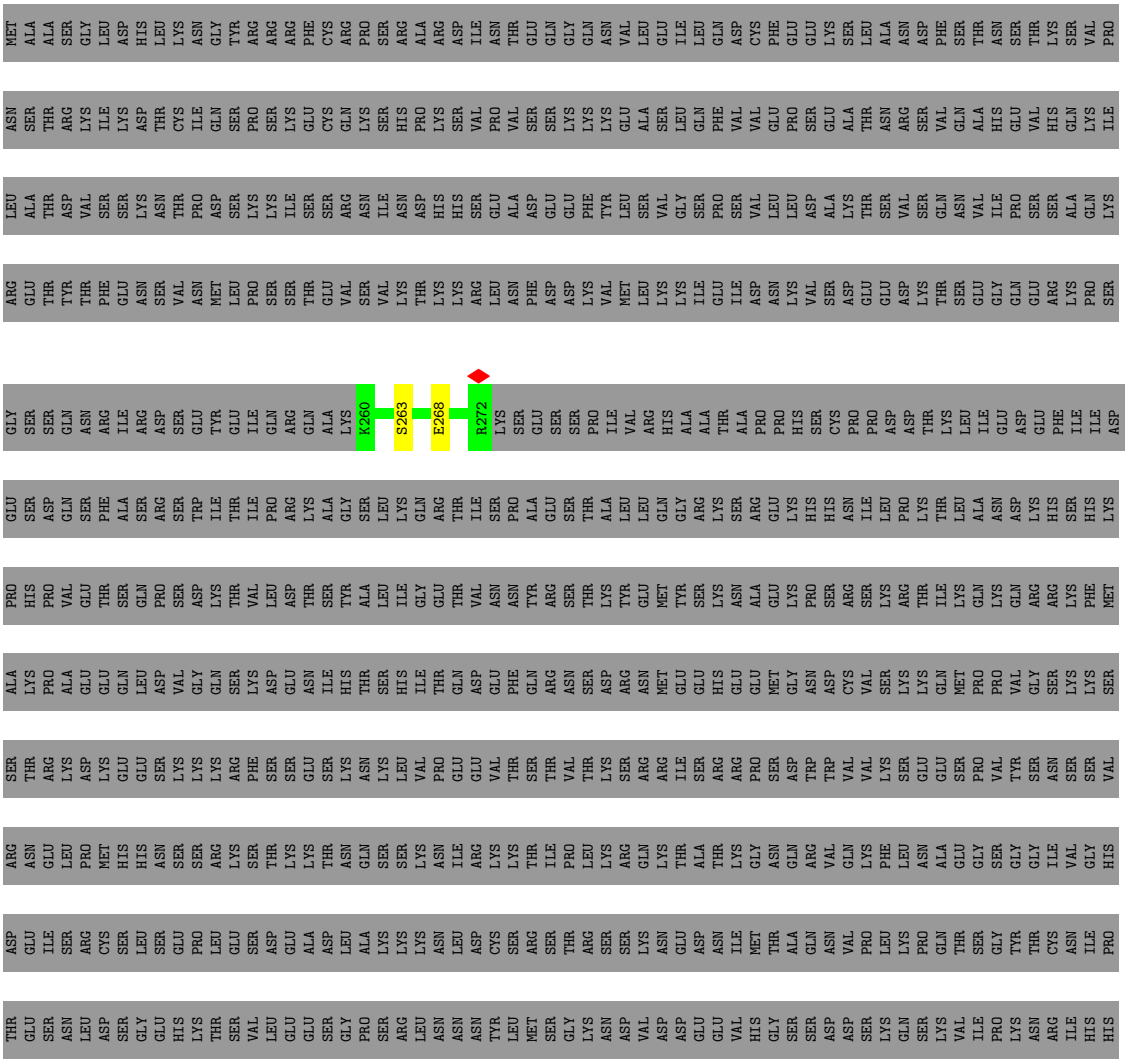


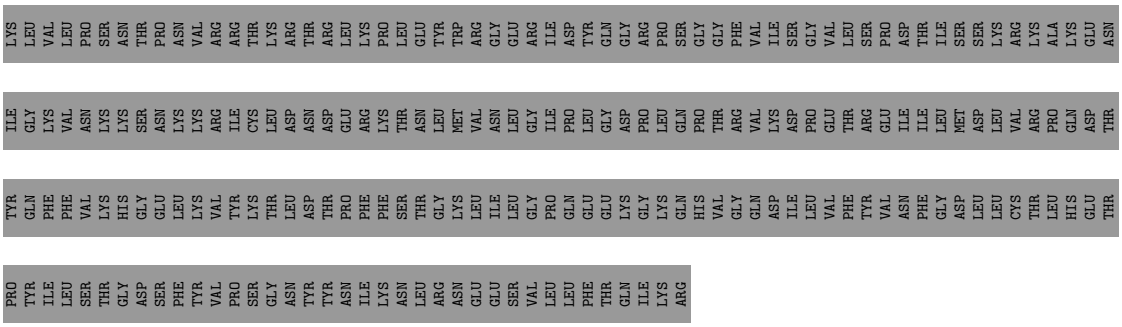


• Molecule 15: Centromere protein C

Chain c:

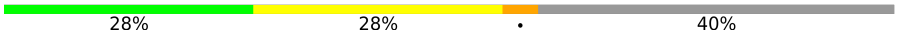


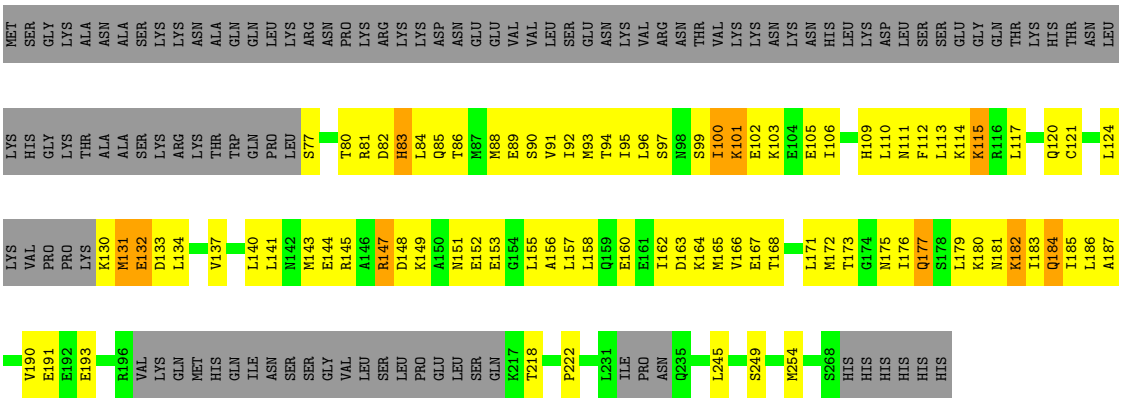




• Molecule 16: Centromere protein Q

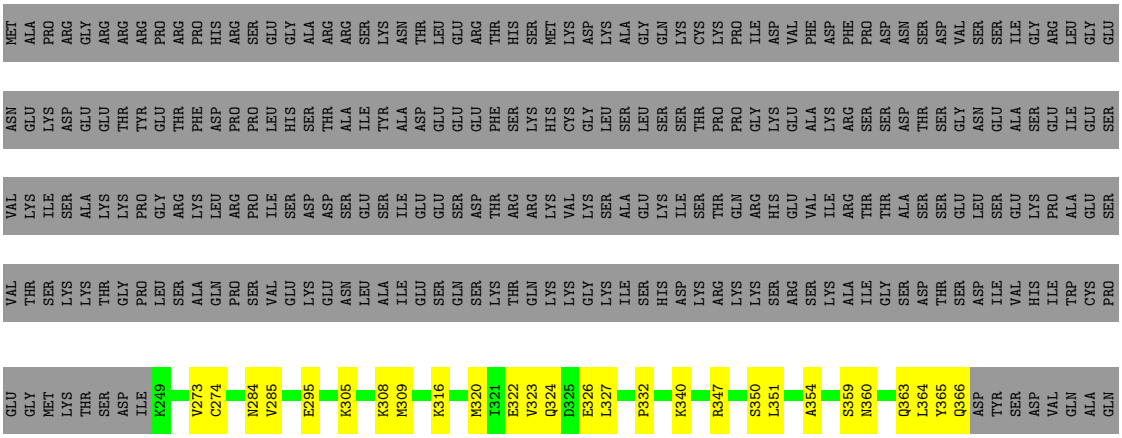
Chain Q:





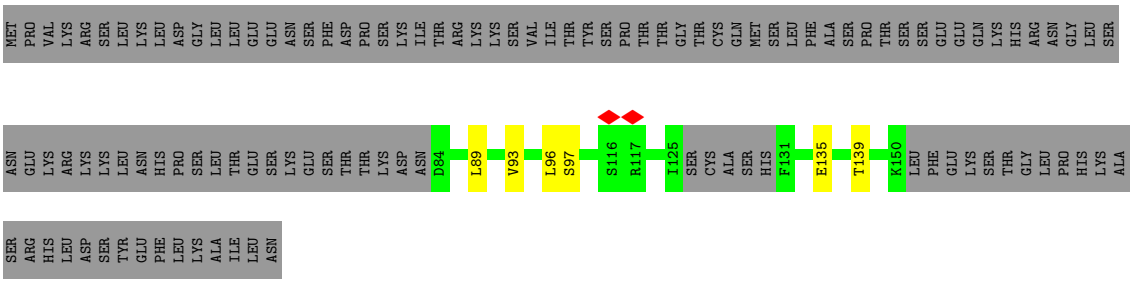
• Molecule 17: Centromere protein U

Chain U:



• Molecule 18: Centromere protein R

Chain R:


MET PRO VAL LYS ARG SER LEU LYS LEU ASP GLY LEU LEU GLU GLU ASN SER PHE ASP PRO SER LYS ILE THR ARG LYS LYS SER VAL ILE THR TYR SER PRO THR THR GLY THR CYS GLN MET SER LEU PHE ALA SER PRO THR SER SER GLU GLU GLN LYS HIS ARG ASN GLY LEU SER
ASN GLU LYS ARG LYS LYS LEU ASN HIS PRO SER LEU THR GLU SER LYS GLU SER THR THR LYS ASP ASN D84 L89 V93 L96 S97 S116 R117 I125 SER CYS ALA SER HIS F131 E135 T139 K150 LEU PHE GLU LYS SER THR GLY LEU PRO HIS LYS ALA
SER ARG HIS LEU ASP SER TYR GLU PHE LEU LYS ALA ILE LEU ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79777	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.924	Depositor
Minimum map value	-2.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	380.64, 380.64, 380.64	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	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	O	0.82	6/1624 (0.4%)	1.14	8/2208 (0.4%)
1	o	0.31	0/95	0.62	0/127
2	H	0.35	0/1566	0.64	0/2093
3	I	0.51	7/4210 (0.2%)	0.63	5/5704 (0.1%)
4	K	0.38	2/1897 (0.1%)	0.66	5/2558 (0.2%)
5	L	0.40	1/2487 (0.0%)	0.56	1/3379 (0.0%)
6	M	0.60	4/1320 (0.3%)	0.75	3/1791 (0.2%)
7	N	0.32	0/2547	0.58	3/3440 (0.1%)
8	P	0.58	7/1839 (0.4%)	0.68	2/2474 (0.1%)
9	S	0.39	1/799 (0.1%)	0.74	2/1070 (0.2%)
10	T	0.71	3/821 (0.4%)	0.74	1/1105 (0.1%)
11	W	0.34	0/590	0.69	0/785
12	X	0.38	0/596	0.72	1/801 (0.1%)
13	G	0.53	0/575	0.83	0/885
14	J	0.55	0/573	0.89	0/882
15	C	0.24	0/40	0.67	0/53
15	c	0.24	0/106	0.55	0/141
16	Q	0.39	1/1175 (0.1%)	0.65	1/1580 (0.1%)
17	U	0.25	0/697	0.39	1/972 (0.1%)
18	R	0.22	0/306	0.36	0/424
All	All	0.49	32/23863 (0.1%)	0.70	33/32472 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1
8	P	0	1
All	All	0	2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	208	PRO	CB-CG	18.91	2.44	1.50
1	O	208	PRO	CG-CD	-14.15	1.03	1.50
3	I	724	PHE	CE1-CZ	-12.82	1.12	1.37
6	M	52	LEU	CG-CD2	-11.77	1.08	1.51
8	P	159	GLU	CD-OE2	-11.29	1.13	1.25
5	L	156	VAL	CB-CG1	-11.05	1.29	1.52
10	T	470	TYR	CG-CD2	-10.88	1.25	1.39
3	I	724	PHE	CG-CD2	-10.31	1.23	1.38
10	T	470	TYR	CE1-CZ	-9.70	1.25	1.38
3	I	734	PHE	CG-CD2	-8.97	1.25	1.38
10	T	470	TYR	CD2-CE2	-8.96	1.25	1.39
3	I	734	PHE	CE2-CZ	-8.66	1.20	1.37
1	O	208	PRO	N-CD	7.70	1.58	1.47
8	P	233	PHE	CE2-CZ	-7.67	1.22	1.37
8	P	233	PHE	CD1-CE1	-7.62	1.24	1.39
3	I	724	PHE	CD2-CE2	-6.90	1.25	1.39
8	P	176	TRP	CZ3-CH2	-6.89	1.29	1.40
8	P	159	GLU	CD-OE1	-6.43	1.18	1.25
1	O	208	PRO	N-CA	-6.16	1.36	1.47
6	M	85	LEU	CG-CD2	-5.86	1.30	1.51
6	M	93	PHE	CD2-CE2	-5.82	1.27	1.39
16	Q	132	GLU	CD-OE2	-5.81	1.19	1.25
9	S	23	VAL	CB-CG1	-5.79	1.40	1.52
4	K	67	LEU	CG-CD2	-5.78	1.30	1.51
8	P	176	TRP	CD2-CE2	-5.69	1.34	1.41
3	I	506	LEU	CG-CD2	-5.58	1.31	1.51
1	O	206	THR	C-N	5.50	1.43	1.33
8	P	176	TRP	CE2-CZ2	-5.46	1.30	1.39
4	K	95	GLU	CD-OE1	-5.44	1.19	1.25
6	M	93	PHE	CE1-CZ	-5.17	1.27	1.37
3	I	734	PHE	CE1-CZ	-5.13	1.27	1.37
1	O	207	GLY	C-N	5.11	1.44	1.34

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	208	PRO	CB-CG-CD	-27.30	0.05	106.50
1	O	208	PRO	CA-N-CD	-21.06	82.02	111.50
1	O	207	GLY	C-N-CD	17.51	165.16	128.40
6	M	53	PRO	CA-N-CD	-12.48	94.02	111.50
1	O	208	PRO	N-CD-CG	-12.45	84.53	103.20
1	O	208	PRO	CA-CB-CG	-12.36	80.52	104.00
10	T	470	TYR	CZ-CE2-CD2	12.31	130.88	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	607	MET	CG-SD-CE	-11.90	81.16	100.20
8	P	159	GLU	OE1-CD-OE2	-10.41	110.81	123.30
9	S	93	LEU	CA-CB-CG	8.96	135.91	115.30
4	K	259	PRO	CA-N-CD	-8.04	100.25	111.50
6	M	52	LEU	CB-CG-CD2	7.27	123.36	111.00
6	M	52	LEU	CD1-CG-CD2	-7.25	88.76	110.50
5	L	42	LEU	CA-CB-CG	6.95	131.28	115.30
3	I	724	PHE	CZ-CE2-CD2	6.65	128.08	120.10
7	N	98	LEU	CA-CB-CG	6.64	130.57	115.30
4	K	95	GLU	OE1-CD-OE2	-6.04	116.05	123.30
7	N	319	LEU	CA-CB-CG	6.02	129.14	115.30
1	O	207	GLY	O-C-N	-5.86	109.96	121.10
3	I	720	LEU	CA-CB-CG	5.76	128.55	115.30
1	O	183	TYR	CZ-CE2-CD2	5.74	124.97	119.80
17	U	332	PRO	N-CA-CB	5.74	110.18	103.30
9	S	38	LYS	CA-CB-CG	5.73	126.02	113.40
4	K	71	LEU	CA-CB-CG	5.66	128.32	115.30
16	Q	222	PRO	N-CA-CB	5.60	110.02	103.30
4	K	246	LEU	CA-CB-CG	5.45	127.84	115.30
4	K	67	LEU	CB-CG-CD2	5.31	120.03	111.00
7	N	97	ASP	CB-CG-OD1	5.29	123.06	118.30
12	X	41	LEU	CA-CB-CG	5.29	127.46	115.30
3	I	734	PHE	CB-CG-CD1	5.20	124.44	120.80
1	O	208	PRO	N-CA-CB	-5.20	96.89	102.60
8	P	73	LEU	CA-CB-CG	5.09	127.01	115.30
3	I	558	LEU	CB-CG-CD2	5.00	119.50	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	47	ARG	Sidechain
8	P	168	ARG	Sidechain

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	O	1588	0	1540	135	0
1	o	95	0	96	0	0
2	H	1560	0	1633	158	0
3	I	4111	0	4032	308	0
4	K	1869	0	1857	147	0
5	L	2422	0	2398	120	0
6	M	1298	0	1349	117	0
7	N	2493	0	2511	136	0
8	P	1808	0	1810	147	0
9	S	790	0	798	77	0
10	T	804	0	814	87	0
11	W	584	0	631	57	0
12	X	590	0	620	75	0
13	G	513	0	279	19	0
14	J	512	0	280	23	0
15	C	40	0	36	3	0
15	c	105	0	106	0	0
16	Q	1175	0	1058	144	0
17	U	699	0	303	46	0
18	R	308	0	127	4	0
All	All	23364	0	22278	1545	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 34.

All (1545) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:145:ARG:HH12	17:U:308:LYS:CB	1.13	1.56
8:P:165:MET:CE	8:P:168:ARG:HD2	1.10	1.54
8:P:165:MET:CE	8:P:168:ARG:CD	1.93	1.45
8:P:165:MET:HE2	8:P:168:ARG:CD	1.47	1.38
16:Q:145:ARG:NH1	17:U:308:LYS:CB	1.93	1.30
16:Q:254:MET:CB	18:R:96:LEU:CB	2.13	1.27
8:P:165:MET:SD	8:P:168:ARG:HD2	1.83	1.16
3:I:720:LEU:HB3	3:I:724:PHE:CE2	1.81	1.14
7:N:158:THR:HG22	7:N:160:TYR:H	1.16	1.06
3:I:558:LEU:HD22	3:I:599:ILE:HD11	1.36	1.06
1:O:135:LEU:HB2	1:O:192:TYR:OH	1.57	1.05
8:P:156:ARG:HA	8:P:159:GLU:OE2	1.55	1.04
16:Q:181:ASN:O	16:Q:184:GLN:NE2	1.91	1.04
8:P:165:MET:HE1	8:P:168:ARG:CZ	1.89	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:179:SER:HB3	1:O:183:TYR:HE2	1.21	1.02
16:Q:83:HIS:HB3	16:Q:131:MET:HE1	1.39	1.02
12:X:33:ASP:HA	12:X:36:GLN:HE21	1.25	1.00
2:H:112:LEU:HD23	2:H:116:LEU:HD21	1.41	0.99
1:O:179:SER:HB3	1:O:183:TYR:CE2	1.97	0.99
12:X:15:VAL:HB	12:X:38:MET:HE1	1.45	0.99
2:H:186:LEU:HA	2:H:189:MET:SD	2.03	0.99
8:P:165:MET:HE1	8:P:168:ARG:CD	1.93	0.98
7:N:98:LEU:HA	1:O:217:LEU:HD11	1.45	0.97
16:Q:179:LEU:HD12	16:Q:182:LYS:HE3	1.45	0.97
16:Q:102:GLU:HG2	16:Q:105:GLU:HB2	1.47	0.96
3:I:195:ASP:OD1	11:W:15:ARG:HD3	1.65	0.95
8:P:165:MET:HE1	8:P:168:ARG:HD2	1.48	0.94
1:O:210:GLN:OE1	1:O:219:SER:OG	1.83	0.94
6:M:85:LEU:CD2	6:M:93:PHE:HZ	1.83	0.92
1:O:126:ILE:HD11	1:O:185:ASN:HD22	1.31	0.92
4:K:39:GLN:NE2	6:M:7:LEU:O	2.02	0.92
1:O:141:ASP:OD2	1:O:151:HIS:ND1	2.02	0.91
3:I:720:LEU:HB3	3:I:724:PHE:CZ	2.05	0.91
1:O:159:ILE:HA	1:O:213:PRO:HB3	1.53	0.91
2:H:113:LYS:HD3	2:H:116:LEU:HD12	1.50	0.90
8:P:170:LEU:O	8:P:174:VAL:HG12	1.70	0.90
3:I:723:LEU:HD23	3:I:724:PHE:CE1	2.07	0.89
8:P:250:ASP:CG	17:U:364:LEU:HA	1.92	0.89
3:I:548:MET:CE	3:I:553:ASN:HA	2.03	0.89
5:L:74:LEU:HD21	5:L:335:LEU:HD13	1.55	0.89
2:H:215:VAL:HG11	4:K:213:HIS:NE2	1.87	0.88
3:I:720:LEU:HB3	3:I:724:PHE:HE2	1.38	0.88
9:S:88:ARG:HD3	10:T:521:ARG:HH21	1.37	0.88
6:M:52:LEU:HD21	6:M:68:PHE:HE1	1.34	0.88
8:P:165:MET:CE	8:P:168:ARG:NE	2.37	0.87
7:N:96:VAL:HG22	7:N:184:LYS:HB2	1.54	0.87
3:I:632:PHE:O	3:I:636:THR:HB	1.74	0.87
12:X:15:VAL:HG11	12:X:39:VAL:HG22	1.54	0.87
3:I:558:LEU:HD22	3:I:599:ILE:CD1	2.04	0.87
8:P:165:MET:HE2	8:P:168:ARG:HD2	0.88	0.87
8:P:176:TRP:HE1	8:P:234:PRO:HB3	1.39	0.87
9:S:70:ARG:HH12	9:S:75:THR:HA	1.38	0.87
16:Q:85:GLN:HG2	16:Q:117:LEU:HD21	1.56	0.87
2:H:88:GLU:HG3	4:K:67:LEU:HB3	1.55	0.87
6:M:85:LEU:HD21	6:M:93:PHE:HZ	1.36	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:74:LEU:HD12	5:L:320:ILE:HB	1.57	0.86
8:P:155:SER:O	8:P:159:GLU:HG3	1.75	0.86
8:P:165:MET:HE2	8:P:168:ARG:NE	1.90	0.86
9:S:65:LEU:HD21	9:S:85:LEU:HD22	1.58	0.86
8:P:176:TRP:CZ3	8:P:224:ILE:HB	2.12	0.85
8:P:164:PHE:O	8:P:168:ARG:HG3	1.77	0.85
16:Q:145:ARG:HD3	17:U:305:LYS:CB	2.06	0.85
12:X:33:ASP:HA	12:X:36:GLN:NE2	1.92	0.84
8:P:216:PHE:HA	8:P:242:VAL:HG13	1.58	0.84
3:I:526:LEU:HG	3:I:530:MET:HG2	1.59	0.84
10:T:470:TYR:HE2	11:W:52:HIS:CB	1.89	0.84
4:K:63:GLN:NE2	6:M:166:LEU:HD11	1.91	0.84
9:S:15:TYR:HD1	12:X:17:ARG:HH12	1.25	0.84
9:S:65:LEU:CD2	9:S:85:LEU:HD22	2.08	0.84
1:O:193:GLN:NE2	1:O:197:LEU:HD22	1.92	0.83
8:P:165:MET:CE	8:P:168:ARG:CZ	2.55	0.83
7:N:167:MET:SD	7:N:169:ARG:HD3	2.17	0.83
1:O:170:GLN:HA	1:O:174:GLN:HB2	1.58	0.83
3:I:502:GLN:O	3:I:506:LEU:HD23	1.76	0.83
16:Q:173:THR:O	16:Q:177:GLN:HB2	1.78	0.83
8:P:176:TRP:CZ2	8:P:223:ARG:O	2.32	0.83
5:L:161:TRP:HB3	5:L:185:LEU:HB2	1.61	0.82
3:I:723:LEU:O	3:I:725:SER:N	2.12	0.82
3:I:172:PHE:CD2	3:I:207:LEU:HB3	2.14	0.82
7:N:158:THR:HG22	7:N:160:TYR:N	1.95	0.82
16:Q:83:HIS:CE1	16:Q:131:MET:HG3	2.15	0.82
1:O:126:ILE:HD11	1:O:185:ASN:ND2	1.95	0.81
16:Q:149:LYS:O	16:Q:149:LYS:HD3	1.78	0.81
1:O:193:GLN:HE21	1:O:197:LEU:HD13	1.43	0.81
10:T:470:TYR:CE2	11:W:52:HIS:ND1	2.48	0.81
8:P:227:ASP:H	8:P:233:PHE:HE1	1.29	0.81
4:K:232:VAL:HG13	4:K:233:LYS:H	1.45	0.81
2:H:88:GLU:HG3	4:K:67:LEU:CB	2.11	0.81
6:M:167:SER:HA	6:M:170:ARG:HH12	1.44	0.80
12:X:32:GLY:O	12:X:36:GLN:HG3	1.81	0.80
2:H:145:GLN:HA	2:H:148:TRP:CZ3	2.16	0.80
8:P:176:TRP:NE1	8:P:234:PRO:HB3	1.96	0.80
12:X:33:ASP:O	12:X:36:GLN:NE2	2.13	0.80
8:P:176:TRP:CH2	8:P:224:ILE:HB	2.16	0.80
3:I:510:MET:HA	3:I:513:HIS:HB3	1.63	0.80
6:M:52:LEU:HD23	6:M:84:SER:CB	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:570:ASP:HB3	3:I:609:ARG:HE	1.45	0.80
5:L:328:LEU:O	5:L:332:LEU:HB2	1.80	0.80
6:M:52:LEU:HD23	6:M:84:SER:HB2	1.64	0.80
1:O:185:ASN:O	8:P:168:ARG:NH2	2.14	0.80
16:Q:145:ARG:NH1	17:U:305:LYS:HA	1.97	0.80
16:Q:106:ILE:HA	16:Q:109:HIS:CD2	2.17	0.79
8:P:111:CYS:SG	8:P:112:HIS:N	2.56	0.78
12:X:68:ASP:O	12:X:72:LYS:HE2	1.83	0.78
3:I:720:LEU:CB	3:I:724:PHE:CE2	2.65	0.78
16:Q:149:LYS:HE2	16:Q:149:LYS:HA	1.65	0.78
1:O:176:PHE:HB2	1:O:179:SER:HB2	1.64	0.78
1:O:143:VAL:HG13	1:O:151:HIS:HB2	1.66	0.78
9:S:70:ARG:NH1	9:S:75:THR:HA	1.99	0.78
3:I:537:ILE:HD13	3:I:568:VAL:HG13	1.67	0.77
12:X:48:GLU:OE2	12:X:52:ARG:NH1	2.17	0.77
6:M:167:SER:HA	6:M:170:ARG:HH22	1.50	0.77
7:N:158:THR:CG2	7:N:160:TYR:H	1.98	0.77
16:Q:83:HIS:HB3	16:Q:131:MET:CE	2.15	0.77
4:K:25:ILE:HA	4:K:28:CYS:HB3	1.66	0.77
3:I:573:ILE:HG21	3:I:609:ARG:HH21	1.46	0.77
4:K:53:SER:O	4:K:54:ASN:ND2	2.18	0.77
6:M:52:LEU:CD2	6:M:84:SER:HB2	2.15	0.77
2:H:138:LYS:HE2	3:I:726:GLN:HG3	1.68	0.76
6:M:19:LEU:HB2	6:M:63:ILE:HD11	1.67	0.76
3:I:477:HIS:O	3:I:481:LEU:HD12	1.86	0.76
3:I:597:THR:HG21	3:I:691:TYR:HE2	1.50	0.76
2:H:112:LEU:CD2	2:H:116:LEU:HD21	2.14	0.76
1:O:193:GLN:HG3	1:O:245:THR:CG2	2.14	0.76
9:S:16:GLN:NE2	9:S:17:GLN:OE1	2.19	0.76
2:H:237:VAL:HG13	2:H:238:LEU:HD12	1.68	0.76
16:Q:144:GLU:HB3	16:Q:147:ARG:NH2	2.01	0.76
8:P:213:ARG:NE	17:U:364:LEU:O	2.16	0.75
1:O:151:HIS:O	1:O:152:HIS:ND1	2.19	0.75
9:S:19:LEU:O	9:S:23:VAL:HG12	1.87	0.75
11:W:37:LYS:HE3	11:W:37:LYS:HA	1.69	0.75
7:N:87:GLN:HB2	7:N:191:MET:HE1	1.69	0.75
8:P:106:ARG:HB3	8:P:117:GLN:HE22	1.50	0.75
3:I:510:MET:HB2	3:I:514:MET:CE	2.16	0.74
1:O:294:LEU:O	1:O:296:MET:CE	2.35	0.74
3:I:573:ILE:HG22	3:I:613:ASN:OD1	1.86	0.74
2:H:215:VAL:HG11	4:K:213:HIS:CE1	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:63:GLN:HE22	6:M:166:LEU:HD21	1.51	0.74
6:M:65:LEU:HD12	6:M:150:LEU:HD13	1.69	0.74
10:T:495:CYS:O	10:T:499:GLU:HG3	1.88	0.74
10:T:522:GLN:HB3	11:W:53:ARG:HH22	1.52	0.74
4:K:245:LEU:HD12	10:T:551:ALA:HB3	1.68	0.74
8:P:120:PHE:CE1	8:P:122:ILE:HG23	2.23	0.74
16:Q:102:GLU:HG2	16:Q:105:GLU:CB	2.18	0.74
6:M:85:LEU:HD13	6:M:124:TYR:CZ	2.22	0.74
10:T:470:TYR:CD2	11:W:52:HIS:HA	2.22	0.74
3:I:175:ILE:HG21	3:I:181:ILE:HD11	1.70	0.73
3:I:597:THR:HG21	3:I:691:TYR:CE2	2.22	0.73
3:I:530:MET:HE3	3:I:530:MET:HA	1.68	0.73
6:M:85:LEU:CD2	6:M:93:PHE:CZ	2.70	0.73
9:S:45:GLN:HG3	12:X:67:VAL:HG22	1.68	0.73
6:M:85:LEU:HD21	6:M:93:PHE:CZ	2.22	0.73
12:X:33:ASP:CA	12:X:36:GLN:HE21	2.00	0.73
7:N:84:GLU:HG3	7:N:165:SER:HB3	1.69	0.73
8:P:156:ARG:CA	8:P:159:GLU:OE2	2.35	0.73
3:I:482:PHE:HD2	3:I:543:LEU:HD22	1.53	0.73
3:I:482:PHE:CD2	3:I:543:LEU:HD22	2.24	0.73
10:T:470:TYR:HE2	11:W:52:HIS:HB2	1.52	0.73
4:K:31:MET:HA	4:K:34:ASP:OD2	1.88	0.73
9:S:24:HIS:HB2	16:Q:93:MET:HE3	1.71	0.73
2:H:57:TYR:OH	6:M:11:PRO:HD3	1.89	0.73
8:P:165:MET:SD	8:P:168:ARG:CD	2.65	0.73
16:Q:131:MET:HG2	16:Q:132:GLU:OE2	1.88	0.73
16:Q:163:ASP:HA	16:Q:166:VAL:HB	1.71	0.72
3:I:127:THR:OG1	3:I:131:LYS:NZ	2.22	0.72
3:I:591:ALA:HB3	3:I:603:LEU:HD12	1.71	0.72
2:H:61:VAL:HG11	4:K:38:CYS:HB3	1.71	0.72
2:H:96:PHE:HA	2:H:99:LYS:HB3	1.72	0.72
2:H:206:ILE:O	2:H:210:THR:HG22	1.88	0.72
1:O:126:ILE:CD1	1:O:185:ASN:HD22	2.03	0.72
2:H:85:LEU:HA	2:H:88:GLU:OE1	1.89	0.72
2:H:113:LYS:HA	2:H:116:LEU:HG	1.69	0.72
16:Q:131:MET:HA	16:Q:134:LEU:HB3	1.71	0.72
2:H:83:GLU:O	2:H:87:ASN:ND2	2.23	0.71
16:Q:102:GLU:OE1	16:Q:105:GLU:HB3	1.90	0.71
3:I:647:MET:HG2	3:I:651:LEU:CD2	2.20	0.71
8:P:73:LEU:HD12	8:P:73:LEU:O	1.89	0.71
8:P:213:ARG:HB2	17:U:365:TYR:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:602:GLN:O	3:I:606:ILE:HG13	1.90	0.71
1:O:126:ILE:HG22	1:O:138:TYR:O	1.90	0.71
10:T:466:LEU:HD21	11:W:48:LEU:CD2	2.20	0.71
7:N:13:ILE:HG22	7:N:49:VAL:HG12	1.71	0.71
1:O:179:SER:CB	1:O:183:TYR:CE2	2.74	0.71
12:X:15:VAL:HB	12:X:38:MET:CE	2.19	0.71
8:P:227:ASP:OD2	8:P:233:PHE:HZ	1.73	0.71
2:H:52:GLN:NE2	6:M:161:SER:OG	2.24	0.71
3:I:589:TYR:OH	3:I:642:HIS:CE1	2.44	0.70
2:H:112:LEU:HD23	2:H:116:LEU:CD2	2.19	0.70
3:I:433:TYR:HB3	5:L:31:LEU:HD11	1.72	0.70
10:T:470:TYR:CE2	11:W:52:HIS:HA	2.26	0.70
4:K:91:THR:O	4:K:95:GLU:OE1	2.10	0.70
3:I:597:THR:CG2	3:I:691:TYR:HE2	2.04	0.70
1:O:193:GLN:HG3	1:O:245:THR:HG23	1.72	0.70
12:X:38:MET:HA	12:X:41:LEU:HG	1.72	0.70
9:S:99:LYS:O	9:S:103:ILE:HG12	1.91	0.70
3:I:565:TYR:HA	3:I:568:VAL:HG23	1.74	0.70
8:P:176:TRP:CD2	8:P:224:ILE:HD13	2.27	0.70
2:H:158:ARG:HG2	3:I:429:GLN:HE21	1.56	0.69
16:Q:180:LYS:HA	16:Q:183:ILE:HB	1.73	0.69
1:O:179:SER:O	1:O:183:TYR:CD2	2.45	0.69
8:P:69:PHE:O	8:P:73:LEU:HG	1.92	0.69
2:H:140:ILE:HG22	2:H:144:GLN:OE1	1.92	0.69
7:N:204:ILE:HG12	7:N:261:GLN:HE21	1.57	0.69
8:P:110:ASN:HA	8:P:115:THR:HA	1.74	0.69
1:O:139:PHE:HB3	1:O:154:SER:HB3	1.74	0.69
9:S:87:ARG:O	9:S:87:ARG:NH1	2.24	0.69
16:Q:100:ILE:O	16:Q:103:LYS:HD3	1.92	0.69
16:Q:134:LEU:HD11	17:U:295:GLU:HA	1.74	0.69
2:H:112:LEU:O	2:H:116:LEU:HG	1.93	0.69
1:O:229:GLN:HG2	1:O:264:TRP:HE1	1.58	0.69
3:I:530:MET:HA	3:I:530:MET:CE	2.22	0.69
12:X:26:ASP:O	12:X:29:LYS:NZ	2.25	0.69
4:K:232:VAL:HA	4:K:261:ARG:HB3	1.73	0.69
8:P:88:LEU:HD22	8:P:102:LEU:HD13	1.75	0.69
1:O:237:LEU:HD11	1:O:275:PHE:HD2	1.58	0.69
8:P:213:ARG:NH2	17:U:366:GLN:C	2.47	0.69
2:H:146:GLU:O	2:H:150:LEU:N	2.18	0.68
6:M:167:SER:HA	6:M:170:ARG:NH1	2.08	0.68
1:O:126:ILE:HG23	1:O:138:TYR:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:466:LEU:HD21	11:W:48:LEU:HD23	1.75	0.68
7:N:83:TRP:CD2	7:N:198:LEU:HD12	2.28	0.68
10:T:535:VAL:HG13	10:T:539:LEU:HD12	1.75	0.68
3:I:73:PHE:HE1	3:I:81:SER:HB2	1.58	0.68
3:I:505:LEU:HD21	3:I:533:VAL:HG11	1.75	0.68
6:M:19:LEU:HD22	6:M:66:ILE:HG12	1.76	0.68
1:O:282:GLN:N	1:O:282:GLN:OE1	2.27	0.68
16:Q:112:PHE:HA	16:Q:115:LYS:HE2	1.75	0.68
16:Q:179:LEU:CD1	16:Q:182:LYS:HE3	2.23	0.68
16:Q:102:GLU:OE2	17:U:274:CYS:N	2.26	0.68
16:Q:172:MET:O	16:Q:176:ILE:HG12	1.93	0.68
3:I:182:ASN:ND2	3:I:208:LEU:O	2.27	0.68
8:P:176:TRP:HZ2	8:P:223:ARG:O	1.75	0.68
3:I:494:LEU:HD22	3:I:561:ILE:HG12	1.76	0.68
7:N:56:CYS:HA	7:N:59:LYS:HB2	1.75	0.67
7:N:261:GLN:OE1	7:N:261:GLN:N	2.18	0.67
10:T:543:TYR:CE2	11:W:17:ALA:HB3	2.29	0.67
16:Q:130:LYS:HZ1	16:Q:132:GLU:HG2	1.58	0.67
2:H:112:LEU:O	2:H:116:LEU:N	2.26	0.67
4:K:39:GLN:O	4:K:43:SER:N	2.26	0.67
7:N:116:LEU:HD23	7:N:174:LEU:HD23	1.77	0.67
13:G:13:DG:O6	14:J:-14:DC:N4	2.27	0.67
3:I:138:VAL:HG12	3:I:141:GLU:HG3	1.77	0.67
5:L:156:VAL:CG1	5:L:159:THR:OG1	2.43	0.67
1:O:121:GLY:HA2	1:O:144:ILE:HG12	1.77	0.67
10:T:470:TYR:CE2	11:W:52:HIS:CB	2.74	0.67
2:H:99:LYS:HE3	4:K:77:LYS:HE3	1.76	0.67
7:N:171:ASN:O	7:N:175:LEU:N	2.25	0.67
8:P:165:MET:HE1	8:P:168:ARG:NE	2.07	0.67
3:I:510:MET:HB2	3:I:514:MET:HE2	1.77	0.67
3:I:573:ILE:HG21	3:I:609:ARG:NH2	2.10	0.67
16:Q:82:ASP:O	16:Q:85:GLN:NE2	2.27	0.67
8:P:165:MET:HA	8:P:168:ARG:HB2	1.77	0.67
12:X:57:ALA:O	12:X:61:ASP:N	2.27	0.67
3:I:548:MET:HE1	3:I:553:ASN:HA	1.77	0.67
1:O:132:GLY:O	8:P:135:VAL:N	2.28	0.67
10:T:496:ASP:HA	10:T:499:GLU:HB2	1.77	0.67
16:Q:83:HIS:ND1	16:Q:131:MET:HE2	2.09	0.67
12:X:32:GLY:HA2	12:X:35:LEU:HB2	1.77	0.66
3:I:647:MET:SD	3:I:651:LEU:HD23	2.35	0.66
9:S:95:TYR:O	9:S:99:LYS:HG2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:520:ARG:HD3	10:T:525:VAL:O	1.95	0.66
8:P:78:ILE:HG23	8:P:107:LEU:HD21	1.76	0.66
8:P:236:LEU:HD21	8:P:271:ILE:HG23	1.77	0.66
5:L:254:PHE:HE2	5:L:287:LEU:HD22	1.60	0.66
1:O:131:GLU:O	1:O:133:ASN:N	2.27	0.66
16:Q:181:ASN:CA	16:Q:184:GLN:HE21	2.08	0.66
16:Q:99:SER:O	16:Q:101:LYS:N	2.28	0.66
16:Q:109:HIS:HA	16:Q:112:PHE:CD2	2.31	0.66
3:I:74:GLU:HB3	3:I:117:LEU:HB3	1.78	0.66
7:N:321:PRO:HG2	15:C:304:ILE:HD13	1.77	0.66
8:P:176:TRP:CE3	8:P:224:ILE:HD13	2.31	0.66
16:Q:83:HIS:CB	16:Q:131:MET:HE1	2.22	0.66
2:H:77:GLN:O	2:H:81:LYS:N	2.27	0.66
4:K:63:GLN:HG3	4:K:67:LEU:HD21	1.78	0.66
5:L:143:SER:O	5:L:152:ARG:N	2.30	0.65
16:Q:133:ASP:O	16:Q:137:VAL:HB	1.97	0.65
3:I:102:ASN:OD1	3:I:103:GLY:N	2.29	0.65
3:I:172:PHE:CD1	3:I:172:PHE:O	2.49	0.65
7:N:194:ARG:NH1	7:N:194:ARG:HB3	2.11	0.65
1:O:162:GLU:O	1:O:166:ALA:N	2.29	0.65
3:I:480:GLN:NE2	6:M:128:LEU:O	2.29	0.65
12:X:60:GLU:OE2	12:X:69:GLN:NE2	2.22	0.65
2:H:101:LEU:HD21	3:I:589:TYR:CD2	2.31	0.65
2:H:150:LEU:HD11	4:K:119:LYS:HG3	1.79	0.65
10:T:520:ARG:HG2	10:T:520:ARG:HH11	1.62	0.65
16:Q:83:HIS:CD2	16:Q:132:GLU:OE2	2.49	0.65
1:O:283:VAL:O	1:O:287:PHE:N	2.30	0.64
2:H:106:MET:SD	2:H:106:MET:N	2.70	0.64
5:L:257:HIS:HB3	5:L:260:ASP:HB2	1.79	0.64
1:O:194:ALA:HB1	1:O:215:CYS:HB2	1.79	0.64
7:N:190:LYS:NZ	7:N:194:ARG:HD2	2.12	0.64
2:H:127:MET:HA	2:H:130:MET:HG2	1.79	0.64
3:I:111:ILE:HD12	3:I:144:VAL:HB	1.78	0.64
1:O:136:ASP:HB3	1:O:192:TYR:CE2	2.32	0.64
1:O:180:LEU:O	1:O:184:LEU:N	2.29	0.64
9:S:15:TYR:CD1	12:X:17:ARG:NH1	2.66	0.64
3:I:571:ILE:HG21	3:I:579:LEU:HB3	1.79	0.64
4:K:67:LEU:HD13	6:M:163:LEU:HD21	1.78	0.64
8:P:227:ASP:OD1	8:P:230:GLY:N	2.30	0.64
10:T:470:TYR:HE2	11:W:52:HIS:CA	2.09	0.64
2:H:154:LEU:HD12	4:K:118:LEU:HD13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:65:LEU:HD11	6:M:149:VAL:HG12	1.79	0.64
16:Q:106:ILE:HA	16:Q:109:HIS:HD2	1.62	0.64
2:H:101:LEU:HD21	3:I:589:TYR:HB2	1.79	0.64
5:L:139:VAL:O	5:L:160:GLY:N	2.27	0.64
5:L:156:VAL:HG11	5:L:159:THR:OG1	1.97	0.64
8:P:99:ARG:HB2	8:P:126:GLN:HG2	1.79	0.64
1:O:238:LEU:HB2	1:O:249:ASP:HB3	1.80	0.64
8:P:227:ASP:HB3	8:P:233:PHE:CZ	2.32	0.64
10:T:507:ARG:NH1	10:T:514:ASP:OD2	2.27	0.64
3:I:64:ASP:O	3:I:68:MET:HG2	1.98	0.64
4:K:35:MET:O	4:K:39:GLN:HB2	1.98	0.64
8:P:176:TRP:CD1	8:P:234:PRO:HB3	2.33	0.64
6:M:85:LEU:HD13	6:M:124:TYR:CE1	2.33	0.63
9:S:98:ASP:O	9:S:101:GLU:OE1	2.16	0.63
3:I:637:TYR:O	3:I:641:ASN:ND2	2.31	0.63
2:H:101:LEU:HD21	3:I:589:TYR:CG	2.33	0.63
5:L:313:SER:HB3	5:L:322:ILE:HB	1.80	0.63
4:K:66:CYS:HB3	6:M:163:LEU:HD11	1.79	0.63
8:P:254:ALA:HB2	17:U:360:ASN:CB	2.28	0.63
16:Q:181:ASN:C	16:Q:184:GLN:HE21	2.00	0.63
7:N:13:ILE:HD13	7:N:16:ILE:HD11	1.81	0.63
9:S:102:GLU:HA	9:S:105:GLN:HG2	1.80	0.63
16:Q:130:LYS:NZ	16:Q:132:GLU:HG2	2.12	0.63
6:M:38:GLU:N	6:M:38:GLU:OE2	2.30	0.63
3:I:120:LYS:O	3:I:124:ALA:N	2.31	0.63
3:I:250:ILE:HG21	5:L:98:PHE:HA	1.80	0.63
3:I:510:MET:CB	3:I:514:MET:HE2	2.29	0.63
3:I:551:GLU:OE2	6:M:148:ARG:NH2	2.31	0.63
7:N:75:GLN:HE22	7:N:124:ARG:HH11	1.47	0.63
16:Q:101:LYS:NZ	17:U:273:VAL:CB	2.62	0.63
16:Q:130:LYS:HB3	16:Q:133:ASP:HB3	1.80	0.63
6:M:85:LEU:HD22	6:M:93:PHE:HZ	1.64	0.63
9:S:23:VAL:O	9:S:27:VAL:HB	1.98	0.63
3:I:201:VAL:O	3:I:205:LEU:HG	1.99	0.63
4:K:82:ILE:HG13	4:K:83:PRO:HD3	1.81	0.63
4:K:248:ARG:HD2	10:T:548:ILE:HD11	1.80	0.63
6:M:30:GLN:OE1	6:M:139:ARG:NH2	2.32	0.63
8:P:188:LYS:HD2	8:P:197:LEU:HB3	1.81	0.63
8:P:227:ASP:N	8:P:233:PHE:HE1	1.97	0.63
3:I:66:LEU:HD11	3:I:88:LEU:HB3	1.81	0.62
3:I:490:LYS:O	3:I:494:LEU:HD12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:502:GLN:HG3	3:I:575:TYR:OH	1.98	0.62
8:P:111:CYS:N	8:P:114:VAL:O	2.25	0.62
3:I:210:LYS:H	3:I:213:ASN:HD22	1.45	0.62
3:I:601:ASN:HB3	3:I:728:LEU:HD13	1.79	0.62
9:S:19:LEU:HD21	12:X:17:ARG:CZ	2.29	0.62
6:M:167:SER:HA	6:M:170:ARG:NH2	2.12	0.62
3:I:644:LEU:HA	3:I:647:MET:HE3	1.80	0.62
10:T:470:TYR:CE2	11:W:52:HIS:CG	2.87	0.62
16:Q:144:GLU:HB3	16:Q:147:ARG:HH21	1.63	0.62
12:X:48:GLU:CD	12:X:52:ARG:HH12	2.03	0.62
2:H:102:ALA:HA	2:H:105:ARG:HG2	1.80	0.62
2:H:161:ARG:NH1	3:I:427:PHE:O	2.31	0.62
5:L:158:TRP:HE1	5:L:193:THR:HG1	1.47	0.62
1:O:198:GLN:HG3	1:O:209:LEU:HD13	1.81	0.62
3:I:86:LYS:O	3:I:90:LYS:CB	2.48	0.62
3:I:721:ASP:O	3:I:725:SER:HB3	1.99	0.62
12:X:60:GLU:CD	12:X:69:GLN:HE21	2.03	0.62
2:H:88:GLU:O	2:H:91:GLU:N	2.33	0.62
3:I:597:THR:HA	3:I:600:LEU:HB3	1.82	0.62
2:H:145:GLN:HA	2:H:148:TRP:CE3	2.34	0.62
4:K:248:ARG:HE	4:K:248:ARG:HA	1.65	0.62
8:P:86:GLU:OE2	8:P:104:ARG:NH1	2.33	0.62
6:M:167:SER:CA	6:M:170:ARG:HH22	2.13	0.61
17:U:305:LYS:O	17:U:309:MET:N	2.33	0.61
2:H:49:GLN:HG2	6:M:156:HIS:HA	1.82	0.61
10:T:489:LYS:HA	10:T:492:GLN:HB3	1.81	0.61
2:H:88:GLU:N	2:H:88:GLU:OE2	2.31	0.61
16:Q:156:ALA:O	16:Q:160:GLU:HG2	2.00	0.61
16:Q:181:ASN:HA	16:Q:184:GLN:HE21	1.64	0.61
3:I:597:THR:HG23	3:I:687:SER:HB2	1.83	0.61
5:L:70:LYS:HE3	5:L:187:ASN:HD22	1.66	0.61
5:L:220:TRP:NE1	5:L:277:GLN:OE1	2.32	0.61
3:I:510:MET:O	3:I:514:MET:HG2	2.00	0.61
3:I:723:LEU:HG	3:I:724:PHE:H	1.65	0.61
6:M:15:THR:HA	6:M:43:GLU:HB2	1.83	0.61
12:X:76:GLN:OE1	12:X:76:GLN:N	2.32	0.61
5:L:55:LEU:HB3	5:L:59:VAL:HG21	1.82	0.61
5:L:250:LEU:HA	7:N:299:SER:HB2	1.83	0.61
8:P:250:ASP:CB	17:U:364:LEU:HA	2.31	0.61
6:M:18:ILE:HB	6:M:150:LEU:HD11	1.82	0.61
8:P:147:CYS:O	8:P:151:SER:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:-10:DG:H5'	14:J:-10:DG:C8	2.35	0.61
4:K:63:GLN:O	4:K:67:LEU:HD22	2.01	0.61
12:X:69:GLN:HA	12:X:72:LYS:CE	2.31	0.61
2:H:101:LEU:HD11	3:I:589:TYR:HB3	1.81	0.61
7:N:99:PHE:O	1:O:212:ASN:ND2	2.34	0.61
16:Q:145:ARG:CZ	17:U:305:LYS:HA	2.31	0.61
2:H:162:LEU:HD23	3:I:510:MET:CE	2.31	0.60
1:O:280:LEU:HA	1:O:283:VAL:HB	1.83	0.60
16:Q:164:LYS:HD3	16:Q:165:MET:N	2.16	0.60
4:K:246:LEU:O	4:K:252:ALA:N	2.34	0.60
1:O:150:ILE:HD11	1:O:153:HIS:HB3	1.83	0.60
3:I:482:PHE:O	3:I:490:LYS:NZ	2.27	0.60
7:N:88:MET:N	7:N:159:PRO:O	2.25	0.60
10:T:534:LEU:HD22	11:W:49:LEU:HD11	1.83	0.60
3:I:562:LEU:O	3:I:566:GLU:N	2.33	0.60
4:K:104:LEU:HA	4:K:107:VAL:HG12	1.83	0.60
11:W:62:ALA:HA	11:W:74:HIS:CE1	2.37	0.60
3:I:111:ILE:CD1	3:I:144:VAL:HB	2.31	0.60
3:I:720:LEU:O	3:I:724:PHE:CD2	2.55	0.60
5:L:260:ASP:HB3	7:N:291:LEU:HD12	1.83	0.60
6:M:74:SER:OG	6:M:77:SER:OG	2.20	0.60
8:P:250:ASP:CG	17:U:364:LEU:CA	2.66	0.60
2:H:202:LEU:HG	4:K:166:MET:HE2	1.83	0.60
8:P:142:MET:HG3	8:P:147:CYS:SG	2.42	0.60
8:P:164:PHE:HB3	8:P:168:ARG:HH11	1.66	0.60
1:O:223:LYS:HD3	1:O:232:PRO:HB3	1.83	0.60
11:W:54:LEU:HD13	11:W:82:ILE:HD12	1.83	0.60
3:I:603:LEU:HA	3:I:606:ILE:HD12	1.84	0.60
4:K:212:LEU:O	4:K:215:MET:HG2	2.02	0.60
5:L:217:ASN:O	5:L:221:MET:HG2	2.01	0.60
6:M:35:MET:HA	6:M:143:ALA:HB1	1.84	0.60
9:S:89:SER:O	9:S:93:LEU:HG	2.02	0.60
16:Q:80:THR:HA	16:Q:131:MET:HE3	1.82	0.60
2:H:42:LEU:O	2:H:46:LEU:HG	2.02	0.60
3:I:723:LEU:HD23	3:I:724:PHE:CZ	2.37	0.60
4:K:63:GLN:O	4:K:67:LEU:CD2	2.50	0.60
1:O:193:GLN:HG2	1:O:197:LEU:HD13	1.84	0.60
4:K:216:LEU:HD12	4:K:246:LEU:HD11	1.82	0.59
1:O:193:GLN:HE21	1:O:197:LEU:CD1	2.14	0.59
9:S:41:GLN:NE2	12:X:64:ARG:HG2	2.17	0.59
7:N:155:TYR:OH	7:N:202:LYS:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:112:GLY:O	1:O:126:ILE:HG13	2.02	0.59
3:I:487:ILE:HG13	3:I:551:GLU:HG3	1.84	0.59
9:S:71:HIS:HE1	10:T:514:ASP:HA	1.67	0.59
3:I:558:LEU:O	3:I:558:LEU:HD23	2.03	0.59
7:N:203:ALA:HB1	7:N:209:TYR:HB3	1.85	0.59
9:S:65:LEU:HD12	9:S:77:ILE:HG21	1.83	0.59
1:O:103:ALA:HB2	8:P:81:HIS:CE1	2.38	0.59
8:P:250:ASP:OD2	17:U:364:LEU:CB	2.50	0.59
10:T:494:LEU:HD23	10:T:495:CYS:N	2.17	0.59
12:X:45:PHE:HE1	12:X:81:PHE:HB3	1.65	0.59
2:H:84:ASP:HA	2:H:87:ASN:HD21	1.67	0.59
3:I:685:HIS:O	3:I:689:LEU:N	2.33	0.59
7:N:44:ARG:HE	7:N:45:LYS:HZ3	1.49	0.59
7:N:303:LEU:HD13	7:N:306:LEU:HD12	1.85	0.59
1:O:114:SER:O	1:O:125:CYS:N	2.36	0.59
1:O:279:PRO:HG2	1:O:282:GLN:OE1	2.02	0.59
3:I:150:TRP:CE2	3:I:152:CYS:HB2	2.37	0.59
12:X:56:GLN:O	12:X:60:GLU:OE1	2.20	0.59
3:I:510:MET:SD	3:I:510:MET:N	2.76	0.59
4:K:245:LEU:O	4:K:249:ASN:ND2	2.36	0.59
6:M:85:LEU:HD22	6:M:93:PHE:CZ	2.37	0.59
10:T:470:TYR:CE2	11:W:52:HIS:CA	2.86	0.59
3:I:508:LEU:HB3	3:I:577:LEU:HD11	1.84	0.58
1:O:126:ILE:CD1	1:O:185:ASN:ND2	2.65	0.58
2:H:233:LEU:O	2:H:237:VAL:N	2.30	0.58
6:M:52:LEU:HD21	6:M:68:PHE:CE1	2.26	0.58
1:O:160:PRO:O	1:O:164:ILE:N	2.24	0.58
8:P:244:GLN:HA	8:P:247:LEU:HB2	1.85	0.58
3:I:607:MET:CE	3:I:734:PHE:CE2	2.86	0.58
8:P:119:GLU:O	8:P:139:ASN:N	2.33	0.58
5:L:200:PHE:HB3	5:L:206:CYS:SG	2.43	0.58
1:O:193:GLN:HE22	1:O:197:LEU:HD22	1.65	0.58
16:Q:143:MET:HE1	16:Q:144:GLU:HG3	1.85	0.58
2:H:105:ARG:HG3	2:H:106:MET:SD	2.43	0.58
3:I:502:GLN:O	3:I:506:LEU:CD2	2.49	0.58
3:I:558:LEU:HD22	3:I:599:ILE:CG1	2.34	0.58
9:S:53:LEU:HD12	12:X:74:LEU:HD11	1.85	0.58
3:I:96:GLU:HA	3:I:100:TRP:HA	1.84	0.58
1:O:294:LEU:O	1:O:296:MET:HE2	2.02	0.58
2:H:101:LEU:HD21	3:I:589:TYR:CB	2.33	0.58
4:K:85:THR:HG22	4:K:87:ASP:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:516:GLU:HB2	10:T:531:LEU:HD22	1.84	0.58
12:X:10:PHE:HE1	12:X:14:LEU:HB3	1.69	0.58
16:Q:99:SER:C	16:Q:101:LYS:H	2.06	0.58
3:I:591:ALA:HA	3:I:594:SER:HB2	1.84	0.58
4:K:108:LEU:HD12	4:K:109:SER:N	2.18	0.58
4:K:219:LEU:HG	4:K:233:LYS:HA	1.85	0.58
6:M:50:LYS:O	6:M:80:ASN:ND2	2.37	0.58
16:Q:89:GLU:HA	16:Q:92:ILE:HD12	1.86	0.58
16:Q:180:LYS:HE3	17:U:340:LYS:CB	2.34	0.58
2:H:45:ARG:HE	6:M:14:ASN:HD21	1.52	0.58
3:I:538:HIS:O	3:I:542:TRP:N	2.36	0.58
6:M:29:GLN:NE2	6:M:33:ASP:OD2	2.37	0.58
16:Q:102:GLU:CG	16:Q:105:GLU:HB2	2.29	0.58
16:Q:140:LEU:O	16:Q:143:MET:HE3	2.04	0.58
3:I:568:VAL:HA	3:I:571:ILE:HD11	1.86	0.57
2:H:88:GLU:O	2:H:92:VAL:HG12	2.04	0.57
2:H:144:GLN:HA	2:H:147:SER:HB3	1.86	0.57
4:K:84:LEU:HG	4:K:85:THR:H	1.69	0.57
7:N:68:LEU:HA	7:N:71:ILE:HD12	1.85	0.57
12:X:68:ASP:C	12:X:72:LYS:HE2	2.24	0.57
6:M:53:PRO:HD2	6:M:87:HIS:ND1	2.20	0.57
7:N:46:GLU:HA	7:N:49:VAL:HG22	1.85	0.57
1:O:124:VAL:HB	1:O:140:VAL:HG13	1.85	0.57
1:O:126:ILE:CG2	1:O:138:TYR:HB2	2.33	0.57
3:I:86:LYS:O	3:I:86:LYS:HD2	2.03	0.57
4:K:240:PRO:HA	4:K:243:VAL:HG12	1.87	0.57
8:P:169:SER:O	8:P:173:PHE:N	2.35	0.57
12:X:33:ASP:CA	12:X:36:GLN:NE2	2.64	0.57
7:N:18:MET:CE	7:N:18:MET:H	2.17	0.57
16:Q:85:GLN:HA	16:Q:88:MET:HB2	1.86	0.57
3:I:389:TYR:HE2	5:L:30:ARG:HH11	1.52	0.57
2:H:101:LEU:HD11	3:I:589:TYR:CB	2.35	0.57
2:H:180:ASN:O	2:H:184:ILE:HD12	2.04	0.57
4:K:170:LYS:O	4:K:174:GLU:HG2	2.03	0.57
7:N:157:GLN:HB3	1:O:161:LEU:HD21	1.85	0.57
16:Q:82:ASP:CA	16:Q:85:GLN:HE21	2.17	0.57
16:Q:102:GLU:OE1	16:Q:109:HIS:NE2	2.27	0.57
16:Q:131:MET:CG	16:Q:132:GLU:OE2	2.53	0.57
7:N:244:GLU:OE2	7:N:247:ARG:NH1	2.36	0.56
7:N:34:ASN:OD1	7:N:35:GLN:N	2.38	0.56
10:T:543:TYR:HD2	11:W:41:LEU:HD11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:53:GLY:O	12:X:56:GLN:NE2	2.33	0.56
2:H:156:ASP:HA	2:H:159:LYS:HE3	1.87	0.56
1:O:165:ALA:O	1:O:169:LEU:HB3	2.05	0.56
8:P:91:THR:HG22	8:P:95:GLU:HG2	1.87	0.56
8:P:236:LEU:HD23	8:P:266:VAL:HG11	1.87	0.56
10:T:459:GLY:HA3	11:W:21:PHE:CD2	2.39	0.56
3:I:391:TRP:HD1	5:L:207:TYR:CE2	2.23	0.56
3:I:607:MET:SD	3:I:734:PHE:HD2	2.29	0.56
4:K:232:VAL:O	4:K:234:ILE:N	2.37	0.56
5:L:301:ALA:HA	6:M:74:SER:HB2	1.86	0.56
1:O:234:CYS:SG	1:O:253:THR:OG1	2.63	0.56
8:P:151:SER:HA	8:P:154:VAL:HG22	1.86	0.56
8:P:176:TRP:CZ2	8:P:223:ARG:C	2.79	0.56
13:G:21:DG:C6	13:G:22:DG:C6	2.94	0.56
3:I:120:LYS:HD3	3:I:121:PHE:H	1.71	0.56
6:M:153:CYS:HA	6:M:162:ALA:HB2	1.87	0.56
2:H:88:GLU:O	2:H:92:VAL:N	2.35	0.56
8:P:129:GLU:N	8:P:129:GLU:OE2	2.38	0.56
8:P:231:LYS:O	8:P:233:PHE:CE1	2.59	0.56
10:T:477:ARG:HA	10:T:480:LEU:HG	1.88	0.56
12:X:12:LYS:HA	12:X:15:VAL:HG22	1.88	0.56
5:L:158:TRP:CD1	5:L:188:GLY:HA3	2.41	0.56
10:T:543:TYR:HA	10:T:546:LEU:CD1	2.35	0.56
12:X:48:GLU:OE2	12:X:48:GLU:O	2.24	0.56
16:Q:173:THR:O	16:Q:177:GLN:CB	2.53	0.56
4:K:50:LEU:HG	6:M:86:ARG:O	2.04	0.56
5:L:238:GLU:HA	5:L:255:ALA:HA	1.87	0.56
9:S:38:LYS:O	9:S:38:LYS:HD3	2.05	0.56
9:S:40:MET:HE1	9:S:41:GLN:OE1	2.05	0.56
9:S:98:ASP:HA	9:S:101:GLU:HG3	1.88	0.56
3:I:93:LYS:HA	3:I:96:GLU:CD	2.26	0.56
3:I:498:LYS:HG3	3:I:564:PHE:HA	1.87	0.56
5:L:156:VAL:HG12	5:L:156:VAL:O	2.04	0.56
1:O:193:GLN:CG	1:O:245:THR:HG23	2.35	0.56
9:S:65:LEU:HD23	9:S:85:LEU:HD22	1.85	0.56
3:I:96:GLU:HB3	3:I:100:TRP:HB3	1.87	0.56
3:I:548:MET:HE3	3:I:553:ASN:HA	1.84	0.56
4:K:206:SER:OG	4:K:207:VAL:N	2.39	0.56
6:M:142:MET:HE2	6:M:145:ARG:HD3	1.88	0.56
7:N:139:THR:HG23	7:N:141:TYR:H	1.71	0.56
8:P:153:PHE:HA	8:P:156:ARG:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:233:PRO:HB3	3:I:260:ILE:HD13	1.88	0.55
3:I:572:TYR:HD1	3:I:578:PRO:HA	1.71	0.55
7:N:56:CYS:HB3	7:N:61:ALA:HB2	1.88	0.55
12:X:31:SER:O	12:X:35:LEU:N	2.37	0.55
3:I:102:ASN:O	3:I:106:SER:N	2.22	0.55
3:I:152:CYS:HG	10:T:552:TYR:HE2	1.53	0.55
3:I:156:CYS:SG	3:I:160:THR:OG1	2.60	0.55
6:M:89:ASP:OD1	6:M:90:ALA:N	2.40	0.55
10:T:469:PHE:O	10:T:472:LYS:HE2	2.06	0.55
2:H:46:LEU:O	2:H:47:ARG:C	2.43	0.55
3:I:71:GLY:O	3:I:75:LYS:HG2	2.07	0.55
4:K:63:GLN:HG3	4:K:67:LEU:CD2	2.35	0.55
4:K:103:ASP:O	4:K:107:VAL:N	2.39	0.55
5:L:70:LYS:HE3	5:L:187:ASN:ND2	2.21	0.55
7:N:152:VAL:HG21	7:N:175:LEU:HD11	1.88	0.55
11:W:21:PHE:HD2	11:W:22:LEU:HD22	1.70	0.55
12:X:69:GLN:HA	12:X:72:LYS:HE3	1.89	0.55
13:G:10:DC:H1'	13:G:11:DC:H5'	1.88	0.55
2:H:84:ASP:HA	2:H:87:ASN:ND2	2.21	0.55
13:G:22:DG:N2	14:J:-21:DC:O2	2.40	0.55
2:H:171:LYS:O	2:H:175:ILE:HG12	2.06	0.55
2:H:215:VAL:HG13	4:K:251:ILE:HG12	1.88	0.55
3:I:716:TRP:O	3:I:720:LEU:HG	2.07	0.55
4:K:27:GLU:OE2	4:K:27:GLU:N	2.29	0.55
2:H:140:ILE:HA	2:H:143:SER:HB3	1.89	0.55
5:L:95:LEU:HD11	5:L:196:ILE:HG12	1.89	0.55
6:M:125:GLN:HE22	6:M:170:ARG:HE	1.54	0.55
5:L:59:VAL:HG12	5:L:127:MET:CE	2.37	0.55
7:N:268:GLN:HG2	7:N:296:LYS:HG2	1.88	0.55
10:T:518:LEU:HD12	10:T:518:LEU:O	2.07	0.55
2:H:43:LEU:HD13	2:H:46:LEU:HD12	1.89	0.55
6:M:144:GLN:OE1	6:M:144:GLN:N	2.40	0.55
1:O:103:ALA:O	1:O:107:ALA:N	2.30	0.55
8:P:227:ASP:HB3	8:P:233:PHE:CE1	2.42	0.55
4:K:93:GLY:O	4:K:96:GLU:HG3	2.07	0.55
10:T:470:TYR:CE2	11:W:52:HIS:HB2	2.37	0.55
2:H:187:ASP:HA	2:H:190:GLU:HG2	1.89	0.54
5:L:54:GLN:N	5:L:54:GLN:OE1	2.39	0.54
8:P:246:ALA:HA	8:P:249:LEU:HD13	1.88	0.54
12:X:70:LEU:HA	12:X:73:VAL:HG22	1.89	0.54
16:Q:157:LEU:O	16:Q:157:LEU:HD12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:211:VAL:O	2:H:215:VAL:HG23	2.07	0.54
3:I:490:LYS:HZ1	3:I:550:LEU:HD12	1.73	0.54
3:I:647:MET:HA	3:I:650:CYS:HB2	1.90	0.54
4:K:246:LEU:HB2	4:K:251:ILE:HB	1.88	0.54
9:S:20:LYS:HA	9:S:23:VAL:CG1	2.37	0.54
14:J:-9:DA:H2"	14:J:-8:DT:C7	2.37	0.54
3:I:159:SER:O	3:I:163:LEU:HD22	2.08	0.54
2:H:77:GLN:HG3	2:H:80:ALA:HB3	1.88	0.54
2:H:132:HIS:HB3	4:K:101:ARG:NH2	2.22	0.54
2:H:132:HIS:NE2	2:H:136:LEU:HD21	2.22	0.54
3:I:537:ILE:HD13	3:I:568:VAL:CG1	2.36	0.54
9:S:24:HIS:HB2	16:Q:93:MET:CE	2.36	0.54
3:I:164:PHE:O	3:I:168:LEU:HD22	2.07	0.54
3:I:195:ASP:CG	11:W:15:ARG:HD3	2.28	0.54
3:I:475:PHE:HB3	3:I:539:TYR:CZ	2.42	0.54
4:K:28:CYS:O	4:K:32:TRP:HD1	1.91	0.54
10:T:538:HIS:CE1	11:W:49:LEU:HD21	2.43	0.54
3:I:73:PHE:CE1	3:I:81:SER:HB2	2.41	0.54
4:K:121:ASP:O	4:K:125:GLU:HG3	2.08	0.54
6:M:4:LEU:HD11	6:M:54:LEU:HD22	1.90	0.54
6:M:94:LEU:O	6:M:166:LEU:HD22	2.08	0.54
11:W:78:ALA:O	11:W:82:ILE:HG13	2.07	0.54
13:G:22:DG:H22	14:J:-21:DC:H1'	1.73	0.54
3:I:720:LEU:C	3:I:724:PHE:CD2	2.81	0.54
4:K:231:TYR:HA	4:K:263:ARG:HB3	1.90	0.54
5:L:294:HIS:O	7:N:320:SER:OG	2.24	0.54
1:O:113:LEU:HD23	1:O:126:ILE:HD12	1.89	0.54
9:S:19:LEU:HD12	12:X:21:LEU:HD22	1.90	0.54
9:S:28:GLY:O	9:S:32:GLU:HG2	2.08	0.54
10:T:546:LEU:H	10:T:546:LEU:HD12	1.73	0.54
3:I:139:ILE:HD11	3:I:177:ARG:HB2	1.90	0.54
5:L:95:LEU:HD23	5:L:119:VAL:HG11	1.90	0.54
6:M:170:ARG:NH1	6:M:170:ARG:HB2	2.23	0.54
7:N:33:GLU:OE1	7:N:37:GLN:NE2	2.40	0.54
9:S:54:THR:HG22	12:X:45:PHE:HD2	1.71	0.54
11:W:66:LYS:HE2	11:W:66:LYS:HA	1.90	0.54
12:X:35:LEU:O	12:X:39:VAL:HG23	2.08	0.54
2:H:54:LEU:HG	4:K:31:MET:HB3	1.88	0.54
3:I:563:ASP:OD2	4:K:111:LYS:NZ	2.41	0.54
7:N:86:PHE:HB3	7:N:188:ILE:HD11	1.89	0.54
7:N:114:ARG:HG3	16:Q:158:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:470:TYR:CZ	11:W:52:HIS:ND1	2.76	0.54
13:G:4:DG:N1	14:J:-4:DC:O2	2.41	0.54
3:I:607:MET:SD	3:I:734:PHE:CD2	3.01	0.54
9:S:67:MET:HA	9:S:70:ARG:HG2	1.89	0.54
16:Q:145:ARG:CD	17:U:305:LYS:CB	2.82	0.54
2:H:154:LEU:CD1	4:K:118:LEU:HD13	2.39	0.53
7:N:96:VAL:CG2	7:N:184:LYS:HB2	2.34	0.53
12:X:44:VAL:HA	12:X:47:VAL:HB	1.90	0.53
3:I:392:LEU:HD22	3:I:421:ILE:HD11	1.90	0.53
8:P:156:ARG:HG3	8:P:159:GLU:OE2	2.07	0.53
9:S:19:LEU:HD12	12:X:21:LEU:CD2	2.38	0.53
5:L:78:THR:HG1	5:L:207:TYR:H	1.54	0.53
16:Q:82:ASP:HA	16:Q:85:GLN:HE21	1.74	0.53
2:H:175:ILE:HD11	4:K:143:HIS:HB2	1.90	0.53
3:I:266:GLU:O	3:I:270:LYS:N	2.42	0.53
4:K:63:GLN:OE1	6:M:94:LEU:HD22	2.08	0.53
7:N:45:LYS:HZ2	14:J:-20:DT:H5"	1.73	0.53
1:O:110:PHE:O	1:O:111:THR:OG1	2.21	0.53
3:I:376:ILE:HG12	3:I:428:LEU:HD11	1.91	0.53
1:O:113:LEU:HD22	1:O:181:CYS:HB3	1.90	0.53
10:T:461:SER:HA	10:T:464:VAL:HG22	1.90	0.53
2:H:46:LEU:CD1	6:M:13:LEU:HD13	2.38	0.53
2:H:86:GLU:HA	2:H:89:ILE:HG12	1.90	0.53
5:L:70:LYS:HB3	5:L:187:ASN:ND2	2.24	0.53
7:N:271:LEU:HD22	7:N:336:ILE:HD11	1.90	0.53
16:Q:92:ILE:HD11	16:Q:113:LEU:HD13	1.91	0.53
16:Q:163:ASP:O	16:Q:167:GLU:HG2	2.09	0.53
7:N:67:ALA:HB1	7:N:134:ARG:HD3	1.90	0.53
7:N:157:GLN:HE21	1:O:212:ASN:HB3	1.74	0.53
8:P:89:THR:C	8:P:93:MET:HE2	2.29	0.53
10:T:478:LYS:O	10:T:482:MET:HG2	2.09	0.53
3:I:502:GLN:HE22	3:I:567:LYS:HG3	1.73	0.53
16:Q:179:LEU:HG	16:Q:180:LYS:HZ3	1.74	0.53
3:I:505:LEU:HD22	3:I:577:LEU:HD12	1.91	0.52
3:I:527:GLY:H	3:I:530:MET:HG2	1.75	0.52
10:T:519:MET:HB3	10:T:525:VAL:HG23	1.90	0.52
3:I:558:LEU:HD11	3:I:591:ALA:HB2	1.91	0.52
7:N:139:THR:HG22	7:N:142:THR:HG22	1.91	0.52
5:L:223:ALA:HB3	5:L:280:VAL:HG22	1.91	0.52
10:T:520:ARG:HG2	10:T:520:ARG:NH1	2.23	0.52
16:Q:100:ILE:HG12	16:Q:103:LYS:HZ2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:190:VAL:HG11	17:U:347:ARG:HA	1.91	0.52
2:H:183:LYS:HA	2:H:186:LEU:HG	1.91	0.52
3:I:583:PHE:HB2	3:I:643:TYR:HE2	1.74	0.52
1:O:121:GLY:HA3	1:O:143:VAL:HA	1.92	0.52
8:P:120:PHE:CZ	8:P:122:ILE:HG23	2.44	0.52
4:K:67:LEU:HD13	6:M:163:LEU:CD2	2.38	0.52
5:L:158:TRP:HA	5:L:188:GLY:HA3	1.92	0.52
7:N:208:GLN:HE22	1:O:154:SER:HA	1.73	0.52
9:S:56:ARG:CZ	9:S:56:ARG:HA	2.39	0.52
16:Q:193:GLU:OE1	17:U:351:LEU:CB	2.56	0.52
2:H:118:LYS:HA	2:H:121:ARG:HD3	1.91	0.52
3:I:580:VAL:O	3:I:580:VAL:HG13	2.10	0.52
1:O:185:ASN:OD1	8:P:168:ARG:NE	2.42	0.52
9:S:53:LEU:CD1	12:X:74:LEU:HD11	2.40	0.52
4:K:103:ASP:HA	4:K:106:MET:HB3	1.92	0.52
4:K:115:ASN:HA	4:K:118:LEU:HB2	1.92	0.52
8:P:271:ILE:HD11	16:Q:218:THR:CB	2.40	0.52
9:S:92:LEU:HA	9:S:95:TYR:HB3	1.90	0.52
3:I:156:CYS:O	3:I:160:THR:OG1	2.28	0.52
9:S:67:MET:SD	9:S:67:MET:N	2.82	0.52
10:T:515:LEU:HD21	11:W:46:ASN:OD1	2.10	0.52
13:G:13:DG:N2	14:J:-12:DG:C2	2.78	0.52
8:P:80:ASN:O	8:P:108:SER:N	2.43	0.52
8:P:84:GLN:HE22	8:P:106:ARG:HG3	1.75	0.52
12:X:69:GLN:O	12:X:73:VAL:HG13	2.09	0.52
3:I:375:TYR:O	3:I:379:VAL:HG22	2.10	0.52
3:I:541:GLY:O	3:I:545:THR:HG23	2.09	0.52
4:K:39:GLN:HE22	6:M:8:ASP:HA	1.75	0.52
9:S:24:HIS:HE1	9:S:48:ALA:HA	1.75	0.52
10:T:466:LEU:HD21	11:W:48:LEU:HD21	1.91	0.52
16:Q:102:GLU:CD	16:Q:105:GLU:HB3	2.31	0.52
16:Q:109:HIS:CE1	17:U:274:CYS:CB	2.93	0.52
3:I:167:TRP:CD1	3:I:171:MET:HG2	2.44	0.51
3:I:219:VAL:HG13	3:I:249:LEU:HD23	1.90	0.51
1:O:126:ILE:CG1	1:O:185:ASN:ND2	2.73	0.51
1:O:128:THR:HG21	1:O:138:TYR:HE1	1.74	0.51
1:O:263:SER:O	1:O:266:GLU:OE1	2.28	0.51
16:Q:141:LEU:HD12	16:Q:141:LEU:O	2.10	0.51
4:K:248:ARG:NH1	10:T:536:GLU:HG3	2.25	0.51
5:L:243:VAL:HB	7:N:314:ILE:HD13	1.93	0.51
6:M:21:VAL:O	6:M:69:VAL:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:73:HIS:CE1	6:M:109:HIS:HB2	2.45	0.51
1:O:161:LEU:HB2	1:O:214:LEU:CD2	2.41	0.51
9:S:88:ARG:NH1	9:S:88:ARG:O	2.43	0.51
3:I:558:LEU:HD21	3:I:591:ALA:HB2	1.92	0.51
5:L:236:THR:HA	5:L:258:PRO:HD3	1.91	0.51
6:M:81:THR:O	6:M:85:LEU:N	2.44	0.51
7:N:157:GLN:HG3	1:O:213:PRO:HD2	1.93	0.51
7:N:177:GLN:OE1	17:U:324:GLN:N	2.44	0.51
1:O:258:GLU:CD	1:O:258:GLU:H	2.13	0.51
8:P:227:ASP:OD2	8:P:233:PHE:CZ	2.58	0.51
9:S:15:TYR:HD1	12:X:17:ARG:NH1	1.96	0.51
9:S:21:ALA:HB2	16:Q:96:LEU:HD13	1.93	0.51
16:Q:141:LEU:O	16:Q:145:ARG:HG2	2.11	0.51
4:K:32:TRP:CE3	4:K:35:MET:HE3	2.45	0.51
4:K:63:GLN:CD	6:M:166:LEU:HD11	2.30	0.51
1:O:126:ILE:O	1:O:138:TYR:N	2.29	0.51
8:P:165:MET:HE2	8:P:168:ARG:CG	2.34	0.51
16:Q:147:ARG:HD2	16:Q:151:ASN:OD1	2.10	0.51
2:H:46:LEU:HD13	6:M:13:LEU:HD13	1.92	0.51
2:H:57:TYR:CD1	6:M:7:LEU:HD13	2.45	0.51
5:L:66:PHE:CD2	5:L:67:LEU:HD12	2.44	0.51
6:M:152:ILE:HG21	6:M:165:LEU:HD13	1.91	0.51
1:O:133:ASN:HA	8:P:134:ALA:HA	1.93	0.51
3:I:412:LYS:O	3:I:416:ASN:ND2	2.36	0.51
7:N:99:PHE:O	7:N:99:PHE:CD1	2.64	0.51
1:O:169:LEU:O	1:O:173:ILE:N	2.40	0.51
3:I:65:ALA:HA	3:I:68:MET:SD	2.51	0.51
3:I:92:LEU:O	3:I:96:GLU:HG3	2.11	0.51
5:L:164:CYS:HB2	5:L:181:LEU:HA	1.93	0.51
5:L:213:ILE:HG13	5:L:320:ILE:HD13	1.92	0.51
6:M:20:LEU:HB3	6:M:28:LEU:HD22	1.93	0.51
4:K:84:LEU:HG	4:K:85:THR:N	2.26	0.51
7:N:194:ARG:HB3	7:N:194:ARG:HH11	1.75	0.51
1:O:159:ILE:HG22	1:O:213:PRO:HA	1.93	0.51
1:O:162:GLU:HA	1:O:165:ALA:HB3	1.93	0.51
8:P:250:ASP:HB2	17:U:364:LEU:HA	1.92	0.51
2:H:60:MET:HG3	6:M:7:LEU:HD11	1.93	0.50
3:I:436:GLU:HB2	3:I:440:TYR:CE2	2.46	0.50
3:I:643:TYR:O	3:I:647:MET:HB3	2.12	0.50
4:K:136:MET:HA	4:K:136:MET:CE	2.40	0.50
7:N:28:TRP:CD2	7:N:69:LEU:HG	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:98:LEU:HD12	7:N:98:LEU:O	2.11	0.50
7:N:155:TYR:CE2	7:N:206:PHE:HE2	2.29	0.50
3:I:540:VAL:HA	3:I:543:LEU:HB2	1.92	0.50
6:M:81:THR:HA	6:M:84:SER:OG	2.12	0.50
7:N:96:VAL:O	7:N:96:VAL:HG12	2.11	0.50
9:S:94:LYS:HA	9:S:94:LYS:HE2	1.92	0.50
10:T:470:TYR:HD2	11:W:52:HIS:HA	1.71	0.50
10:T:552:TYR:O	10:T:553:SER:OG	2.24	0.50
5:L:27:LEU:HG	5:L:31:LEU:CD2	2.42	0.50
5:L:49:ILE:HD12	5:L:49:ILE:H	1.76	0.50
7:N:87:GLN:HB2	7:N:191:MET:CE	2.41	0.50
1:O:237:LEU:HD11	1:O:275:PHE:CD2	2.44	0.50
8:P:262:PHE:HA	8:P:265:LEU:HD12	1.94	0.50
16:Q:121:CYS:HA	16:Q:124:LEU:HG	1.94	0.50
3:I:440:TYR:CD1	3:I:473:LEU:HB3	2.47	0.50
4:K:259:PRO:HB2	10:T:533:VAL:HG21	1.94	0.50
5:L:85:TYR:CE2	5:L:135:GLU:O	2.65	0.50
6:M:18:ILE:HB	6:M:150:LEU:CD1	2.41	0.50
2:H:58:LYS:HA	2:H:61:VAL:HG22	1.93	0.50
5:L:315:HIS:H	5:L:320:ILE:HA	1.77	0.50
6:M:93:PHE:CE1	6:M:97:VAL:HG11	2.47	0.50
7:N:115:ALA:O	7:N:140:GLN:NE2	2.45	0.50
13:G:22:DG:N2	14:J:-21:DC:H1'	2.26	0.50
16:Q:83:HIS:HA	16:Q:86:THR:OG1	2.12	0.50
3:I:105:ALA:O	3:I:109:ILE:HG12	2.11	0.50
3:I:389:TYR:CD1	3:I:434:SER:HB2	2.46	0.50
3:I:461:TRP:NE1	3:I:503:ASN:OD1	2.44	0.50
5:L:74:LEU:HD22	5:L:211:LEU:HD23	1.92	0.50
6:M:71:ASN:HA	6:M:102:THR:HG23	1.92	0.50
6:M:167:SER:HA	6:M:170:ARG:CZ	2.42	0.50
7:N:85:VAL:HG22	7:N:162:PHE:CD1	2.46	0.50
1:O:116:LYS:HB3	1:O:123:CYS:HB2	1.92	0.50
2:H:56:GLU:OE2	6:M:7:LEU:HD21	2.11	0.50
3:I:149:SER:HA	3:I:161:LYS:NZ	2.27	0.50
8:P:117:GLN:HB3	8:P:141:ILE:HD13	1.93	0.50
9:S:20:LYS:HA	9:S:23:VAL:HG12	1.93	0.50
16:Q:101:LYS:HZ1	17:U:273:VAL:CB	2.24	0.50
16:Q:120:GLN:HA	16:Q:120:GLN:OE1	2.12	0.50
2:H:136:LEU:O	2:H:140:ILE:HG13	2.11	0.50
2:H:184:ILE:HA	2:H:187:ASP:OD1	2.12	0.50
3:I:427:PHE:HB2	4:K:128:TRP:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:248:ARG:CZ	10:T:536:GLU:HG3	2.42	0.50
8:P:204:CYS:HB3	8:P:222:TRP:H	1.77	0.50
11:W:19:ARG:HD3	11:W:40:ASP:OD2	2.11	0.50
16:Q:102:GLU:HB3	16:Q:106:ILE:HG13	1.94	0.50
2:H:87:ASN:O	2:H:91:GLU:HB2	2.12	0.50
2:H:202:LEU:HD23	4:K:166:MET:HE1	1.94	0.50
3:I:614:LEU:O	3:I:618:LYS:HG2	2.12	0.50
6:M:52:LEU:HD22	6:M:84:SER:HB2	1.93	0.50
7:N:262:PRO:HB3	7:N:301:HIS:CD2	2.47	0.50
12:X:38:MET:O	12:X:42:LEU:HG	2.12	0.50
7:N:251:ILE:HD12	7:N:317:ALA:HB1	1.94	0.49
8:P:216:PHE:HA	8:P:242:VAL:CG1	2.38	0.49
10:T:494:LEU:HG	10:T:498:LEU:CD2	2.42	0.49
10:T:515:LEU:HD22	11:W:42:LEU:HB3	1.94	0.49
2:H:130:MET:O	2:H:134:LEU:HG	2.12	0.49
3:I:164:PHE:O	3:I:167:TRP:HB3	2.12	0.49
5:L:67:LEU:HD11	5:L:138:LEU:HD11	1.93	0.49
6:M:52:LEU:H	6:M:84:SER:HB2	1.77	0.49
6:M:94:LEU:C	6:M:166:LEU:HD22	2.32	0.49
16:Q:149:LYS:HD3	16:Q:149:LYS:C	2.32	0.49
1:O:115:GLY:HA2	1:O:124:VAL:HA	1.95	0.49
1:O:159:ILE:O	1:O:159:ILE:HG13	2.12	0.49
8:P:72:THR:HG23	8:P:73:LEU:H	1.77	0.49
9:S:11:GLN:OE1	9:S:12:ARG:NH1	2.45	0.49
13:G:15:DT:H2'	13:G:16:DG:H8	1.75	0.49
3:I:173:ASP:OD1	3:I:173:ASP:N	2.45	0.49
4:K:231:TYR:CE1	4:K:263:ARG:HD2	2.47	0.49
1:O:99:GLU:O	8:P:81:HIS:NE2	2.44	0.49
12:X:45:PHE:HD1	12:X:81:PHE:CD2	2.31	0.49
2:H:140:ILE:O	2:H:144:GLN:N	2.45	0.49
2:H:158:ARG:HG2	3:I:429:GLN:NE2	2.26	0.49
2:H:162:LEU:HD21	3:I:510:MET:HG2	1.94	0.49
4:K:50:LEU:CD2	6:M:86:ARG:O	2.60	0.49
5:L:75:TYR:HA	5:L:211:LEU:H	1.77	0.49
2:H:162:LEU:HD23	3:I:510:MET:HE2	1.94	0.49
2:H:231:PRO:HD2	2:H:232:ALA:H	1.78	0.49
3:I:471:LYS:HB3	3:I:472:PRO:HD3	1.93	0.49
4:K:129:LEU:O	4:K:133:GLN:HG2	2.13	0.49
5:L:77:LEU:HD13	5:L:208:PHE:CE2	2.48	0.49
6:M:32:ALA:HB1	7:N:237:ILE:HG12	1.93	0.49
7:N:44:ARG:NE	7:N:45:LYS:HZ3	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:49:ALA:O	9:S:53:LEU:HD22	2.12	0.49
9:S:74:ARG:NH1	9:S:76:THR:O	2.45	0.49
12:X:48:GLU:CD	12:X:52:ARG:NH1	2.65	0.49
16:Q:168:THR:HA	16:Q:171:LEU:HD12	1.93	0.49
3:I:62:GLU:O	3:I:66:LEU:N	2.40	0.49
7:N:25:LEU:HD23	7:N:28:TRP:HE1	1.77	0.49
7:N:59:LYS:O	7:N:60:ARG:HG2	2.13	0.49
7:N:153:VAL:CG1	7:N:155:TYR:HE1	2.25	0.49
14:J:-10:DG:H2"	14:J:-9:DA:N7	2.27	0.49
1:O:126:ILE:CG1	1:O:185:ASN:HD22	2.25	0.49
16:Q:181:ASN:O	16:Q:185:ILE:HG12	2.12	0.49
18:R:135:GLU:O	18:R:139:THR:N	2.39	0.49
3:I:531:ASN:OD1	3:I:531:ASN:O	2.30	0.49
5:L:213:ILE:HD12	5:L:320:ILE:HG21	1.94	0.49
8:P:211:ALA:HB3	8:P:286:GLU:HG2	1.94	0.49
2:H:225:VAL:HG23	2:H:227:TRP:H	1.78	0.49
3:I:95:VAL:O	3:I:99:ALA:N	2.32	0.49
3:I:583:PHE:HB2	3:I:643:TYR:CE2	2.47	0.49
3:I:607:MET:HE1	3:I:734:PHE:CE2	2.48	0.49
4:K:248:ARG:HH12	10:T:536:GLU:HA	1.78	0.49
9:S:65:LEU:HD12	9:S:77:ILE:CG2	2.43	0.49
16:Q:82:ASP:HA	16:Q:85:GLN:HG3	1.95	0.49
2:H:93:LYS:HA	2:H:96:PHE:CE1	2.47	0.48
2:H:116:LEU:HD23	3:I:689:LEU:HD11	1.94	0.48
2:H:207:LYS:HA	2:H:210:THR:CG2	2.43	0.48
3:I:181:ILE:HG22	3:I:208:LEU:HD11	1.94	0.48
8:P:184:PHE:HD1	8:P:187:LEU:HD21	1.78	0.48
8:P:227:ASP:N	8:P:233:PHE:CE1	2.81	0.48
13:G:12:DC:H2"	13:G:13:DG:C8	2.48	0.48
16:Q:83:HIS:CG	16:Q:131:MET:HE2	2.48	0.48
16:Q:102:GLU:CG	16:Q:105:GLU:CB	2.88	0.48
2:H:61:VAL:HG12	4:K:42:LEU:HG	1.95	0.48
4:K:239:TRP:CH2	4:K:241:PRO:HG2	2.48	0.48
7:N:269:TYR:OH	7:N:322:LEU:O	2.29	0.48
8:P:213:ARG:CZ	17:U:366:GLN:C	2.82	0.48
14:J:-10:DG:H2"	14:J:-9:DA:C8	2.47	0.48
4:K:216:LEU:HD13	4:K:264:LEU:HD13	1.95	0.48
5:L:253:SER:HB2	7:N:296:LYS:HB2	1.94	0.48
1:O:161:LEU:HG	1:O:214:LEU:HD13	1.95	0.48
3:I:145:VAL:HA	3:I:148:VAL:HG23	1.94	0.48
5:L:223:ALA:CB	5:L:280:VAL:HG22	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:190:LYS:HZ3	7:N:194:ARG:HD2	1.77	0.48
8:P:109:GLY:O	8:P:116:PHE:N	2.35	0.48
17:U:360:ASN:O	17:U:364:LEU:N	2.45	0.48
2:H:162:LEU:HD23	3:I:510:MET:HE3	1.96	0.48
3:I:172:PHE:CE2	3:I:207:LEU:HB3	2.48	0.48
3:I:422:ILE:HD13	3:I:457:GLN:OE1	2.13	0.48
6:M:65:LEU:HD12	6:M:150:LEU:CD1	2.42	0.48
1:O:189:GLY:HA3	8:P:168:ARG:HH22	1.78	0.48
9:S:24:HIS:CD2	16:Q:93:MET:HB3	2.49	0.48
12:X:48:GLU:HA	12:X:51:VAL:HG12	1.95	0.48
7:N:20:GLU:O	7:N:24:ILE:HD12	2.13	0.48
1:O:209:LEU:HG	1:O:220:PHE:HB3	1.96	0.48
10:T:510:VAL:HB	11:W:35:LEU:HD23	1.95	0.48
12:X:74:LEU:HA	12:X:77:LEU:HB3	1.95	0.48
13:G:19:DG:H2"	13:G:20:DA:H8	1.78	0.48
2:H:113:LYS:HA	2:H:116:LEU:CG	2.40	0.48
2:H:130:MET:SD	2:H:130:MET:N	2.87	0.48
2:H:164:LEU:HD22	4:K:136:MET:HG2	1.95	0.48
9:S:30:LEU:O	9:S:34:VAL:HG13	2.14	0.48
11:W:15:ARG:O	11:W:15:ARG:HG3	2.13	0.48
12:X:51:VAL:HA	12:X:54:VAL:HG22	1.96	0.48
16:Q:88:MET:HE1	17:U:285:VAL:N	2.29	0.48
5:L:67:LEU:HD23	5:L:161:TRP:CE3	2.49	0.48
7:N:53:ILE:O	7:N:57:GLU:HG2	2.14	0.48
7:N:167:MET:CE	14:J:-10:DG:H4'	2.43	0.48
1:O:287:PHE:HA	1:O:290:LYS:HG2	1.96	0.48
9:S:46:THR:HG23	12:X:70:LEU:HD11	1.96	0.48
10:T:515:LEU:HD22	11:W:42:LEU:HD13	1.94	0.48
10:T:524:LEU:HB3	10:T:534:LEU:HD11	1.95	0.48
12:X:10:PHE:HB3	12:X:39:VAL:HG13	1.95	0.48
16:Q:171:LEU:O	16:Q:175:ASN:HB3	2.14	0.48
17:U:350:SER:O	17:U:354:ALA:N	2.23	0.48
3:I:99:ALA:HB1	3:I:134:ILE:HD13	1.96	0.48
5:L:27:LEU:HG	5:L:31:LEU:HD21	1.95	0.48
5:L:28:GLN:O	5:L:32:GLU:HG2	2.13	0.48
5:L:43:THR:O	5:L:44:PRO:C	2.52	0.48
5:L:67:LEU:HD21	5:L:138:LEU:HD21	1.95	0.48
7:N:56:CYS:O	7:N:60:ARG:N	2.47	0.48
16:Q:109:HIS:HE1	17:U:274:CYS:CB	2.27	0.48
3:I:106:SER:OG	3:I:141:GLU:OE2	2.31	0.48
3:I:181:ILE:HD12	3:I:181:ILE:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:24:ILE:HG23	7:N:72:ILE:HG22	1.96	0.48
7:N:123:PHE:HD1	7:N:133:ILE:HG12	1.79	0.48
10:T:480:LEU:HA	10:T:483:VAL:HG22	1.96	0.48
10:T:515:LEU:HD13	11:W:42:LEU:HB3	1.96	0.48
2:H:102:ALA:O	2:H:106:MET:HG2	2.14	0.47
3:I:431:GLY:HA2	3:I:461:TRP:HB3	1.96	0.47
3:I:446:TRP:HZ2	3:I:452:ARG:HA	1.79	0.47
5:L:75:TYR:HB2	5:L:184:PHE:HD2	1.79	0.47
8:P:227:ASP:CB	8:P:233:PHE:CE1	2.97	0.47
13:G:19:DG:H2"	13:G:20:DA:C8	2.49	0.47
16:Q:83:HIS:CG	16:Q:131:MET:CE	2.98	0.47
2:H:112:LEU:C	2:H:116:LEU:HG	2.35	0.47
2:H:197:ILE:O	2:H:201:ASN:ND2	2.47	0.47
3:I:607:MET:SD	3:I:608:HIS:N	2.87	0.47
5:L:77:LEU:HD11	5:L:206:CYS:SG	2.55	0.47
5:L:297:ILE:HG22	7:N:315:ALA:HB2	1.94	0.47
7:N:82:VAL:O	7:N:165:SER:OG	2.28	0.47
16:Q:77:SER:O	16:Q:81:ARG:HG2	2.15	0.47
2:H:91:GLU:HA	2:H:94:VAL:HG22	1.95	0.47
3:I:166:ARG:HB2	3:I:200:TYR:CE2	2.49	0.47
7:N:45:LYS:HB2	7:N:45:LYS:HE2	1.62	0.47
12:X:33:ASP:C	12:X:36:GLN:NE2	2.67	0.47
4:K:180:LEU:O	4:K:184:LEU:HB2	2.14	0.47
6:M:85:LEU:HD13	6:M:124:TYR:CE2	2.49	0.47
1:O:294:LEU:O	1:O:296:MET:SD	2.72	0.47
2:H:101:LEU:CD2	3:I:589:TYR:HB2	2.44	0.47
4:K:91:THR:HA	4:K:94:LYS:NZ	2.29	0.47
5:L:80:LEU:HD11	5:L:181:LEU:HD12	1.97	0.47
7:N:140:GLN:HB3	16:Q:151:ASN:CG	2.34	0.47
10:T:483:VAL:O	10:T:487:LEU:HG	2.13	0.47
2:H:82:ILE:HA	2:H:85:LEU:HB3	1.96	0.47
3:I:382:GLU:OE2	5:L:26:PRO:CG	2.63	0.47
3:I:565:TYR:HA	3:I:568:VAL:CG2	2.41	0.47
3:I:589:TYR:HA	3:I:592:LEU:HB3	1.97	0.47
7:N:18:MET:SD	7:N:19:ASN:N	2.88	0.47
1:O:101:VAL:O	1:O:104:ILE:HG12	2.15	0.47
12:X:60:GLU:CD	12:X:69:GLN:NE2	2.67	0.47
2:H:117:GLU:O	2:H:121:ARG:HG3	2.15	0.47
3:I:128:ARG:HA	3:I:131:LYS:HB2	1.95	0.47
3:I:558:LEU:HD23	3:I:562:LEU:HG	1.97	0.47
3:I:723:LEU:HD23	3:I:724:PHE:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:734:PHE:CD1	3:I:734:PHE:C	2.88	0.47
4:K:127:ARG:HH21	4:K:128:TRP:HE1	1.63	0.47
5:L:28:GLN:CD	5:L:28:GLN:H	2.18	0.47
5:L:127:MET:HB2	5:L:136:ALA:HB3	1.97	0.47
8:P:285:GLU:HB3	17:U:366:GLN:CB	2.45	0.47
9:S:95:TYR:HE2	12:X:44:VAL:HG11	1.78	0.47
10:T:482:MET:SD	10:T:482:MET:N	2.88	0.47
10:T:497:ASP:HA	10:T:500:VAL:HG12	1.97	0.47
12:X:52:ARG:HD3	12:X:73:VAL:HB	1.97	0.47
16:Q:187:ALA:O	16:Q:191:GLU:HG3	2.15	0.47
7:N:9:ILE:HA	7:N:12:THR:HG22	1.97	0.47
1:O:218:LEU:HB3	1:O:220:PHE:HE2	1.80	0.47
12:X:35:LEU:HD22	12:X:38:MET:HE1	1.96	0.47
3:I:530:MET:CE	3:I:530:MET:CA	2.93	0.47
3:I:644:LEU:HA	3:I:647:MET:CE	2.44	0.47
4:K:23:GLU:O	4:K:26:ARG:HB3	2.15	0.47
4:K:216:LEU:CD1	4:K:246:LEU:HD11	2.45	0.47
8:P:68:SER:O	8:P:72:THR:HG22	2.15	0.47
16:Q:111:ASN:O	16:Q:115:LYS:HG2	2.14	0.47
2:H:136:LEU:HD12	4:K:104:LEU:HB3	1.97	0.47
2:H:172:LEU:HD12	2:H:172:LEU:O	2.15	0.47
3:I:644:LEU:HD23	3:I:647:MET:HE1	1.97	0.47
9:S:19:LEU:CD1	12:X:21:LEU:HD22	2.45	0.47
9:S:90:ASN:HA	9:S:93:LEU:CD1	2.45	0.47
10:T:494:LEU:O	10:T:497:ASP:N	2.48	0.47
13:G:25:DG:C5	14:J:-24:DG:C2	3.03	0.47
16:Q:155:LEU:HD11	17:U:316:LYS:CB	2.44	0.47
3:I:611:ARG:NE	3:I:737:SER:OG	2.46	0.46
5:L:291:PHE:HE1	5:L:297:ILE:HD11	1.80	0.46
11:W:56:GLU:HG3	11:W:57:GLU:N	2.30	0.46
4:K:259:PRO:HB3	10:T:537:ARG:HH21	1.80	0.46
5:L:218:LEU:HG	5:L:307:VAL:HG22	1.97	0.46
2:H:44:LEU:HD11	4:K:92:LEU:HD21	1.97	0.46
3:I:377:ASN:HA	3:I:428:LEU:HG	1.97	0.46
6:M:88:VAL:HG12	6:M:92:PHE:HB3	1.96	0.46
7:N:202:LYS:HG2	7:N:206:PHE:CE2	2.50	0.46
8:P:100:LYS:HG2	8:P:125:ILE:HG23	1.97	0.46
2:H:238:LEU:HB3	3:I:183:LEU:HD21	1.97	0.46
3:I:548:MET:SD	3:I:558:LEU:HB2	2.55	0.46
3:I:562:LEU:HB3	3:I:606:ILE:HD11	1.98	0.46
3:I:647:MET:HG2	3:I:651:LEU:HD23	1.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:188:PHE:CE1	4:K:189:PRO:O	2.68	0.46
5:L:221:MET:HB2	5:L:225:TRP:CH2	2.51	0.46
7:N:86:PHE:HD1	7:N:190:LYS:HA	1.80	0.46
7:N:159:PRO:HD3	1:O:164:ILE:HD11	1.97	0.46
10:T:498:LEU:HD11	10:T:515:LEU:HD12	1.97	0.46
2:H:163:GLN:O	2:H:166:GLN:NE2	2.49	0.46
3:I:189:PHE:HE2	3:I:221:LYS:HD2	1.81	0.46
3:I:270:LYS:HA	3:I:273:LEU:CB	2.45	0.46
3:I:442:SER:O	3:I:446:TRP:HB2	2.15	0.46
4:K:30:GLU:HA	4:K:33:LYS:HG3	1.98	0.46
8:P:120:PHE:HB2	8:P:138:LEU:HD13	1.97	0.46
16:Q:106:ILE:O	16:Q:110:LEU:HG	2.16	0.46
3:I:647:MET:O	3:I:651:LEU:N	2.49	0.46
6:M:144:GLN:HA	6:M:147:VAL:HG12	1.98	0.46
7:N:74:MET:HE1	7:N:81:LYS:HD2	1.98	0.46
1:O:209:LEU:HD21	1:O:218:LEU:HD23	1.98	0.46
12:X:39:VAL:O	12:X:42:LEU:HD12	2.16	0.46
12:X:41:LEU:HD12	12:X:42:LEU:N	2.29	0.46
2:H:215:VAL:HG12	2:H:215:VAL:O	2.16	0.46
3:I:106:SER:O	3:I:110:ASP:HB2	2.16	0.46
3:I:446:TRP:CZ2	3:I:452:ARG:HA	2.51	0.46
4:K:93:GLY:O	4:K:97:PHE:CD1	2.69	0.46
8:P:147:CYS:HA	8:P:150:LEU:HB2	1.96	0.46
9:S:38:LYS:HD2	12:X:58:GLN:HE21	1.81	0.46
11:W:32:GLN:O	11:W:33:LEU:HD22	2.16	0.46
14:J:-25:DC:H2"	14:J:-24:DG:C8	2.50	0.46
3:I:395:THR:O	3:I:399:GLU:HB3	2.15	0.46
3:I:542:TRP:HZ2	6:M:168:LEU:HA	1.81	0.46
5:L:170:LEU:HB2	5:L:340:ILE:HD12	1.97	0.46
5:L:199:TRP:O	5:L:203:THR:HG23	2.16	0.46
7:N:209:TYR:OH	7:N:327:PRO:HB2	2.16	0.46
16:Q:81:ARG:HA	16:Q:84:LEU:HB2	1.98	0.46
16:Q:101:LYS:HZ2	17:U:273:VAL:CB	2.28	0.46
16:Q:145:ARG:CZ	17:U:308:LYS:CB	2.85	0.46
3:I:539:TYR:O	3:I:543:LEU:N	2.46	0.46
4:K:248:ARG:HH11	10:T:548:ILE:HD11	1.81	0.46
5:L:297:ILE:HA	7:N:315:ALA:HA	1.98	0.46
7:N:45:LYS:NZ	14:J:-20:DT:H5"	2.31	0.46
7:N:100:ASP:OD1	1:O:210:GLN:NE2	2.48	0.46
7:N:167:MET:HE2	14:J:-10:DG:H4'	1.98	0.46
8:P:108:SER:HB2	8:P:117:GLN:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:-9:DA:H2"	14:J:-8:DT:C5	2.51	0.46
4:K:181:GLY:O	4:K:185:GLU:HG2	2.16	0.46
5:L:59:VAL:HG12	5:L:127:MET:HE3	1.97	0.46
16:Q:91:VAL:HG11	17:U:284:ASN:CB	2.45	0.46
18:R:89:LEU:O	18:R:93:VAL:N	2.37	0.46
2:H:225:VAL:HG23	2:H:227:TRP:N	2.31	0.45
3:I:128:ARG:CZ	3:I:164:PHE:HB2	2.45	0.45
5:L:130:THR:N	5:L:133:ASP:OD2	2.35	0.45
6:M:20:LEU:HD13	6:M:67:VAL:CG2	2.46	0.45
7:N:68:LEU:O	7:N:72:ILE:HG13	2.16	0.45
10:T:543:TYR:CD2	11:W:41:LEU:HD11	2.51	0.45
11:W:41:LEU:HD12	11:W:41:LEU:HA	1.64	0.45
12:X:64:ARG:HD2	12:X:65:VAL:N	2.30	0.45
16:Q:94:THR:O	16:Q:97:SER:OG	2.21	0.45
2:H:85:LEU:O	2:H:89:ILE:HG23	2.16	0.45
2:H:102:ALA:HA	2:H:105:ARG:CG	2.47	0.45
2:H:113:LYS:CA	2:H:116:LEU:HG	2.41	0.45
3:I:134:ILE:HB	3:I:135:PRO:HD3	1.98	0.45
4:K:88:VAL:HG13	4:K:90:ILE:HG22	1.99	0.45
5:L:222:ALA:HB1	5:L:239:PHE:HE2	1.81	0.45
7:N:39:VAL:HG22	7:N:51:HIS:ND1	2.32	0.45
7:N:82:VAL:HA	7:N:196:ARG:HA	1.98	0.45
10:T:541:LEU:HA	10:T:544:ARG:NE	2.32	0.45
2:H:183:LYS:O	2:H:186:LEU:HB2	2.16	0.45
3:I:118:SER:OG	3:I:119:GLY:N	2.49	0.45
3:I:537:ILE:CD1	3:I:568:VAL:HG13	2.41	0.45
3:I:607:MET:HE3	3:I:734:PHE:HE2	1.82	0.45
3:I:720:LEU:CB	3:I:724:PHE:HE2	2.13	0.45
4:K:26:ARG:HB3	4:K:26:ARG:HE	1.60	0.45
5:L:67:LEU:HD23	5:L:161:TRP:CZ3	2.52	0.45
8:P:156:ARG:HA	8:P:159:GLU:CD	2.30	0.45
10:T:555:ASN:N	10:T:555:ASN:OD1	2.50	0.45
16:Q:90:SER:O	16:Q:94:THR:HG23	2.16	0.45
2:H:138:LYS:HD3	2:H:142:LYS:HZ2	1.81	0.45
4:K:255:HIS:CE1	4:K:257:GLU:HB3	2.52	0.45
7:N:140:GLN:HB3	16:Q:151:ASN:OD1	2.16	0.45
1:O:196:ARG:O	1:O:196:ARG:HD3	2.16	0.45
10:T:478:LYS:HA	10:T:481:GLU:OE2	2.16	0.45
16:Q:88:MET:HE1	17:U:285:VAL:CA	2.46	0.45
3:I:607:MET:HA	3:I:610:TYR:HB2	1.98	0.45
4:K:239:TRP:CD1	4:K:242:TYR:CD1	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:35:GLN:HG2	7:N:55:LEU:HD22	1.99	0.45
7:N:114:ARG:NH1	16:Q:162:ILE:HD11	2.32	0.45
8:P:179:TYR:O	8:P:183:THR:OG1	2.26	0.45
12:X:35:LEU:HD23	12:X:35:LEU:HA	1.79	0.45
16:Q:81:ARG:HD2	16:Q:84:LEU:HD12	1.98	0.45
16:Q:100:ILE:HG12	16:Q:103:LYS:NZ	2.32	0.45
3:I:444:PRO:HG3	3:I:477:HIS:CD2	2.51	0.45
3:I:471:LYS:HA	3:I:475:PHE:HD2	1.80	0.45
2:H:115:ASN:HA	2:H:118:LYS:HB2	1.98	0.45
2:H:140:ILE:HD13	4:K:107:VAL:HG13	1.99	0.45
2:H:207:LYS:HA	2:H:210:THR:HG22	1.98	0.45
3:I:483:PHE:CZ	3:I:543:LEU:HD23	2.51	0.45
6:M:85:LEU:HA	6:M:85:LEU:HD23	1.53	0.45
7:N:8:PHE:HA	7:N:11:ARG:HE	1.82	0.45
7:N:204:ILE:HA	7:N:209:TYR:HE2	1.81	0.45
1:O:161:LEU:HA	1:O:164:ILE:HB	1.97	0.45
10:T:471:ALA:HA	11:W:59:ARG:HH21	1.82	0.45
13:G:15:DT:H2'	13:G:16:DG:C8	2.52	0.45
3:I:172:PHE:CD1	3:I:172:PHE:C	2.89	0.45
4:K:24:LEU:HD12	4:K:24:LEU:HA	1.80	0.45
4:K:218:ILE:O	4:K:222:ARG:NH1	2.48	0.45
4:K:255:HIS:HB3	4:K:258:ASP:O	2.17	0.45
4:K:255:HIS:HE1	4:K:257:GLU:HB3	1.81	0.45
5:L:214:ASN:OD1	5:L:214:ASN:N	2.50	0.45
2:H:126:LEU:O	2:H:130:MET:SD	2.74	0.45
5:L:63:LYS:HA	5:L:63:LYS:HD3	1.70	0.45
1:O:168:TYR:O	1:O:171:THR:OG1	2.28	0.45
8:P:83:LYS:NZ	8:P:105:HIS:HB2	2.32	0.45
16:Q:83:HIS:ND1	16:Q:131:MET:HG3	2.29	0.45
16:Q:102:GLU:OE2	17:U:274:CYS:CA	2.64	0.45
2:H:138:LYS:NZ	2:H:142:LYS:NZ	2.65	0.45
2:H:179:LYS:O	2:H:183:LYS:HG2	2.17	0.45
3:I:192:LEU:HD11	3:I:202:CYS:SG	2.57	0.45
3:I:428:LEU:HD22	3:I:430:GLU:HG2	1.99	0.45
3:I:546:THR:HG22	3:I:549:ARG:HH22	1.82	0.45
3:I:647:MET:O	3:I:651:LEU:HD22	2.17	0.45
5:L:161:TRP:HH2	5:L:328:LEU:HD12	1.82	0.45
8:P:233:PHE:N	8:P:233:PHE:CD1	2.85	0.45
14:J:-7:DT:H5'	14:J:-7:DT:C6	2.52	0.45
16:Q:80:THR:HA	16:Q:131:MET:CE	2.47	0.45
16:Q:158:LEU:HD23	16:Q:158:LEU:HA	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:130:MET:CE	4:K:97:PHE:HB3	2.47	0.44
2:H:180:ASN:O	2:H:183:LYS:HB2	2.16	0.44
3:I:90:LYS:HA	3:I:93:LYS:HB2	1.99	0.44
3:I:128:ARG:HB2	3:I:131:LYS:HZ1	1.82	0.44
3:I:430:GLU:HB3	3:I:507:TRP:CZ2	2.52	0.44
3:I:467:PHE:CZ	3:I:536:LEU:HA	2.52	0.44
3:I:608:HIS:CE1	3:I:733:LEU:HB3	2.52	0.44
4:K:183:PHE:O	4:K:186:ASP:HB3	2.17	0.44
7:N:245:LYS:HA	7:N:248:VAL:HG12	1.98	0.44
1:O:136:ASP:HB3	1:O:192:TYR:CD2	2.52	0.44
14:J:-25:DC:H2"	14:J:-24:DG:N7	2.32	0.44
2:H:48:ALA:HB1	6:M:158:PRO:HB3	1.99	0.44
3:I:371:LEU:HD22	3:I:371:LEU:H	1.82	0.44
3:I:459:VAL:HG21	3:I:478:LEU:HD11	1.99	0.44
4:K:231:TYR:CZ	4:K:263:ARG:HD2	2.52	0.44
8:P:98:ILE:HG22	8:P:127:ASN:OD1	2.17	0.44
9:S:51:SER:O	9:S:54:THR:OG1	2.29	0.44
2:H:90:GLU:O	2:H:94:VAL:HG22	2.16	0.44
2:H:217:GLN:OE1	3:I:186:GLY:HA3	2.18	0.44
3:I:581:VAL:O	3:I:610:TYR:OH	2.19	0.44
3:I:607:MET:HE3	3:I:734:PHE:CE2	2.52	0.44
5:L:254:PHE:CZ	5:L:256:ILE:HD11	2.53	0.44
5:L:297:ILE:HG22	7:N:315:ALA:CB	2.48	0.44
6:M:17:THR:HG22	6:M:45:LYS:HB2	2.00	0.44
1:O:184:LEU:HD12	1:O:184:LEU:O	2.17	0.44
8:P:170:LEU:HA	8:P:173:PHE:HB3	1.99	0.44
9:S:61:PHE:CD1	9:S:85:LEU:HD21	2.53	0.44
9:S:71:HIS:NE2	10:T:505:ALA:HB2	2.32	0.44
9:S:90:ASN:HA	9:S:93:LEU:HD12	1.99	0.44
11:W:18:PRO:O	11:W:22:LEU:HD23	2.17	0.44
3:I:427:PHE:HB2	4:K:128:TRP:CZ2	2.53	0.44
1:O:161:LEU:HB2	1:O:214:LEU:HD22	1.99	0.44
10:T:479:ALA:O	10:T:483:VAL:HG13	2.17	0.44
2:H:93:LYS:HE2	2:H:93:LYS:HB2	1.85	0.44
2:H:154:LEU:HD12	4:K:118:LEU:CD1	2.47	0.44
3:I:156:CYS:O	3:I:161:LYS:HG2	2.18	0.44
3:I:161:LYS:HB3	3:I:161:LYS:HE3	1.61	0.44
4:K:101:ARG:O	4:K:105:GLU:HG2	2.18	0.44
4:K:244:GLU:OE2	10:T:550:CYS:HA	2.18	0.44
7:N:85:VAL:HG23	7:N:201:LEU:HD13	1.99	0.44
8:P:119:GLU:HB2	8:P:139:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:24:HIS:CE1	9:S:48:ALA:HA	2.51	0.44
17:U:323:VAL:O	17:U:327:LEU:N	2.39	0.44
2:H:174:GLU:HA	2:H:177:THR:HG22	2.00	0.44
3:I:689:LEU:O	3:I:693:VAL:HG23	2.17	0.44
4:K:29:GLU:O	4:K:33:LYS:HG3	2.18	0.44
4:K:50:LEU:CG	6:M:86:ARG:O	2.65	0.44
4:K:94:LYS:HA	4:K:97:PHE:HD1	1.83	0.44
1:O:219:SER:HB2	1:O:236:ARG:HG2	1.99	0.44
8:P:158:GLU:OE1	8:P:158:GLU:N	2.50	0.44
16:Q:89:GLU:HA	16:Q:92:ILE:HB	2.00	0.44
2:H:56:GLU:OE2	6:M:62:ARG:NH2	2.49	0.44
3:I:96:GLU:HA	3:I:100:TRP:CA	2.48	0.44
4:K:232:VAL:CG1	4:K:233:LYS:H	2.25	0.44
5:L:303:ARG:NH2	5:L:316:THR:HG21	2.32	0.44
7:N:50:GLN:OE1	7:N:53:ILE:HD11	2.18	0.44
1:O:169:LEU:O	1:O:169:LEU:HD12	2.17	0.44
1:O:221:THR:O	1:O:221:THR:OG1	2.31	0.44
8:P:105:HIS:HB3	8:P:120:PHE:HD2	1.83	0.44
9:S:14:SER:O	9:S:18:ARG:HB2	2.17	0.44
9:S:24:HIS:CB	16:Q:93:MET:HE3	2.42	0.44
11:W:77:ALA:O	11:W:81:VAL:HG23	2.18	0.44
12:X:42:LEU:HA	12:X:45:PHE:HB2	1.99	0.44
2:H:118:LYS:HG3	2:H:121:ARG:NH1	2.33	0.44
2:H:215:VAL:CG1	4:K:213:HIS:NE2	2.72	0.44
3:I:89:GLU:HG3	3:I:93:LYS:HE3	1.99	0.44
3:I:475:PHE:O	3:I:539:TYR:OH	2.27	0.44
3:I:723:LEU:HD21	3:I:731:LEU:HD23	1.99	0.44
6:M:99:PHE:O	6:M:128:LEU:HD12	2.18	0.44
6:M:170:ARG:HB2	6:M:170:ARG:CZ	2.48	0.44
8:P:227:ASP:CG	8:P:233:PHE:CZ	2.91	0.44
9:S:78:ASN:HB2	9:S:80:GLU:OE1	2.17	0.44
10:T:460:LEU:HD13	10:T:484:GLU:HG2	1.98	0.44
10:T:507:ARG:NH1	10:T:511:LYS:HB2	2.33	0.44
2:H:172:LEU:HB2	4:K:139:LEU:HD11	1.99	0.44
3:I:544:SER:HB2	3:I:561:ILE:HD13	2.00	0.44
3:I:544:SER:HB2	3:I:561:ILE:CD1	2.48	0.44
4:K:216:LEU:HD22	4:K:264:LEU:HB2	1.99	0.44
7:N:190:LYS:HZ1	7:N:194:ARG:HD2	1.81	0.44
1:O:148:LEU:HB3	1:O:174:GLN:HE22	1.81	0.44
9:S:63:LYS:O	9:S:67:MET:HG2	2.17	0.44
9:S:65:LEU:HD11	9:S:82:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:533:VAL:HA	10:T:536:GLU:OE2	2.17	0.44
3:I:195:ASP:OD1	3:I:229:MET:HE2	2.18	0.43
3:I:392:LEU:HD23	3:I:392:LEU:HA	1.71	0.43
3:I:403:TYR:CE1	3:I:411:GLY:HA2	2.53	0.43
5:L:158:TRP:CZ2	5:L:184:PHE:HZ	2.35	0.43
2:H:84:ASP:HA	2:H:87:ASN:OD1	2.18	0.43
2:H:148:TRP:CZ3	3:I:729:GLN:NE2	2.86	0.43
6:M:44:LEU:O	6:M:46:VAL:N	2.51	0.43
16:Q:92:ILE:O	16:Q:95:ILE:HG13	2.18	0.43
16:Q:147:ARG:NE	16:Q:148:ASP:OD1	2.52	0.43
7:N:140:GLN:NE2	16:Q:155:LEU:HD12	2.33	0.43
1:O:229:GLN:CD	1:O:229:GLN:H	2.22	0.43
8:P:83:LYS:HZ3	8:P:105:HIS:HB2	1.83	0.43
9:S:20:LYS:O	16:Q:93:MET:SD	2.77	0.43
12:X:44:VAL:O	12:X:48:GLU:HB3	2.19	0.43
16:Q:153:GLU:O	16:Q:157:LEU:HB3	2.18	0.43
3:I:234:HIS:ND1	3:I:234:HIS:N	2.65	0.43
5:L:244:PRO:HD2	7:N:314:ILE:HD11	2.01	0.43
7:N:108:PHE:CE2	7:N:133:ILE:HG21	2.53	0.43
7:N:167:MET:HE2	14:J:-10:DG:C4'	2.48	0.43
1:O:107:ALA:O	1:O:114:SER:HB2	2.18	0.43
1:O:193:GLN:NE2	1:O:197:LEU:CD2	2.74	0.43
1:O:248:THR:OG1	1:O:249:ASP:N	2.50	0.43
8:P:225:GLN:O	8:P:233:PHE:HD1	2.01	0.43
17:U:359:SER:O	17:U:363:GLN:N	2.36	0.43
3:I:194:ASP:OD1	3:I:197:LEU:HD23	2.19	0.43
3:I:562:LEU:HB3	3:I:602:GLN:HG3	2.01	0.43
3:I:573:ILE:CG2	3:I:609:ARG:HH21	2.23	0.43
4:K:239:TRP:HD1	4:K:242:TYR:CD2	2.36	0.43
4:K:263:ARG:HH12	4:K:266:ALA:HB2	1.83	0.43
5:L:30:ARG:O	5:L:30:ARG:HD3	2.17	0.43
9:S:55:PHE:HE1	12:X:22:HIS:NE2	2.16	0.43
13:G:22:DG:C4	13:G:23:DC:N3	2.87	0.43
17:U:322:GLU:O	17:U:326:GLU:N	2.46	0.43
3:I:565:TYR:CG	3:I:583:PHE:HE1	2.36	0.43
3:I:721:ASP:O	3:I:723:LEU:O	2.36	0.43
5:L:201:GLN:HG2	5:L:206:CYS:O	2.18	0.43
5:L:220:TRP:O	5:L:224:MET:HG3	2.18	0.43
5:L:246:SER:OG	5:L:247:PRO:HD3	2.19	0.43
1:O:145:GLN:OE1	1:O:147:PRO:HD2	2.19	0.43
1:O:268:ARG:O	1:O:272:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:80:ASN:HB3	8:P:108:SER:HB3	1.99	0.43
10:T:472:LYS:N	10:T:472:LYS:HD3	2.33	0.43
10:T:515:LEU:HB3	11:W:42:LEU:HD13	2.00	0.43
10:T:542:GLU:OE1	10:T:542:GLU:N	2.51	0.43
12:X:16:SER:O	12:X:20:HIS:HB2	2.18	0.43
16:Q:83:HIS:NE2	16:Q:132:GLU:OE2	2.51	0.43
16:Q:91:VAL:O	16:Q:95:ILE:HG12	2.18	0.43
3:I:65:ALA:HA	3:I:68:MET:CG	2.48	0.43
4:K:93:GLY:O	4:K:96:GLU:N	2.52	0.43
4:K:160:ASN:O	4:K:164:THR:HG23	2.19	0.43
1:O:296:MET:SD	1:O:296:MET:N	2.91	0.43
9:S:58:CYS:HA	9:S:61:PHE:HD2	1.84	0.43
11:W:72:LYS:O	11:W:76:LEU:HG	2.19	0.43
16:Q:180:LYS:O	16:Q:184:GLN:HG3	2.18	0.43
16:Q:186:LEU:O	16:Q:190:VAL:HG23	2.19	0.43
3:I:146:LYS:HD3	3:I:184:LEU:HD21	2.00	0.43
3:I:499:GLU:O	3:I:503:ASN:ND2	2.45	0.43
4:K:216:LEU:HD13	4:K:264:LEU:CD1	2.48	0.43
4:K:232:VAL:HG13	4:K:233:LYS:N	2.24	0.43
6:M:97:VAL:O	6:M:127:PRO:HD2	2.19	0.43
8:P:197:LEU:HD13	8:P:206:MET:HG2	2.00	0.43
13:G:20:DA:H2"	13:G:21:DG:H8	1.83	0.43
2:H:145:GLN:CA	2:H:148:TRP:CZ3	2.98	0.43
3:I:723:LEU:HD11	3:I:731:LEU:HD23	2.00	0.43
4:K:206:SER:O	4:K:207:VAL:HB	2.17	0.43
5:L:74:LEU:HD12	5:L:320:ILE:CB	2.40	0.43
5:L:218:LEU:HD12	5:L:218:LEU:HA	1.74	0.43
6:M:67:VAL:HG21	6:M:146:LEU:HD21	2.01	0.43
1:O:164:ILE:HG23	1:O:168:TYR:CD1	2.54	0.43
8:P:84:GLN:HG2	8:P:104:ARG:HB3	2.01	0.43
3:I:686:PRO:O	3:I:689:LEU:HB3	2.19	0.43
4:K:63:GLN:O	4:K:67:LEU:HD23	2.19	0.43
5:L:297:ILE:O	5:L:297:ILE:HG13	2.18	0.43
6:M:22:GLY:N	6:M:28:LEU:HD11	2.34	0.43
7:N:43:GLN:HG3	7:N:44:ARG:HG2	2.00	0.43
1:O:284:PHE:HA	1:O:287:PHE:HB2	2.00	0.43
8:P:227:ASP:CB	8:P:233:PHE:CZ	3.00	0.43
8:P:265:LEU:HD13	8:P:278:LEU:HD13	2.01	0.43
9:S:20:LYS:O	9:S:23:VAL:HG13	2.19	0.43
9:S:84:LEU:O	9:S:87:ARG:HB3	2.19	0.43
12:X:15:VAL:HG23	12:X:35:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:143:MET:C	16:Q:143:MET:SD	2.97	0.43
3:I:108:GLU:OE1	3:I:112:LEU:HD22	2.19	0.42
3:I:113:LEU:HD21	3:I:127:THR:HG21	2.00	0.42
3:I:219:VAL:HG22	3:I:249:LEU:HD23	2.01	0.42
3:I:498:LYS:HD3	3:I:567:LYS:HE2	2.01	0.42
4:K:31:MET:O	4:K:35:MET:HG2	2.19	0.42
5:L:197:GLY:O	5:L:201:GLN:HG3	2.19	0.42
5:L:251:ASP:O	7:N:298:SER:N	2.47	0.42
6:M:14:ASN:HB3	6:M:43:GLU:HG2	2.01	0.42
8:P:116:PHE:HB3	8:P:142:MET:SD	2.59	0.42
14:J:-19:DC:H2"	14:J:-18:DG:C8	2.54	0.42
3:I:143:SER:O	3:I:146:LYS:HB3	2.19	0.42
4:K:114:LYS:O	4:K:118:LEU:HD23	2.19	0.42
5:L:238:GLU:O	5:L:308:SER:N	2.52	0.42
6:M:125:GLN:NE2	6:M:170:ARG:HE	2.17	0.42
7:N:194:ARG:HH11	7:N:194:ARG:CB	2.31	0.42
7:N:320:SER:O	7:N:322:LEU:N	2.52	0.42
8:P:265:LEU:HA	8:P:268:LEU:HD23	2.00	0.42
9:S:56:ARG:HA	9:S:56:ARG:NE	2.33	0.42
2:H:155:LEU:HD21	3:I:574:ASN:HB3	2.01	0.42
2:H:162:LEU:HD22	3:I:506:LEU:HB3	2.00	0.42
2:H:163:GLN:HA	2:H:166:GLN:HE21	1.84	0.42
2:H:206:ILE:HD12	2:H:209:THR:HB	2.02	0.42
4:K:49:THR:HG23	6:M:90:ALA:HB3	2.01	0.42
5:L:299:LEU:HD23	5:L:299:LEU:HA	1.72	0.42
7:N:10:LYS:O	7:N:14:LEU:HG	2.19	0.42
7:N:190:LYS:NZ	7:N:192:ASP:HA	2.34	0.42
8:P:105:HIS:CD2	8:P:107:LEU:HB2	2.54	0.42
9:S:88:ARG:NH2	12:X:79:LEU:O	2.43	0.42
11:W:27:LYS:HA	11:W:27:LYS:HD2	1.77	0.42
11:W:76:LEU:HD12	11:W:77:ALA:N	2.34	0.42
16:Q:182:LYS:C	16:Q:182:LYS:HD2	2.40	0.42
3:I:460:SER:OG	3:I:499:GLU:HB3	2.18	0.42
4:K:208:ASN:OD1	4:K:209:LEU:N	2.53	0.42
5:L:75:TYR:HB2	5:L:184:PHE:CD2	2.53	0.42
6:M:17:THR:OG1	6:M:62:ARG:O	2.38	0.42
1:O:110:PHE:CD1	1:O:111:THR:N	2.88	0.42
1:O:136:ASP:OD2	1:O:138:TYR:CE1	2.72	0.42
1:O:229:GLN:HG2	1:O:264:TRP:NE1	2.28	0.42
8:P:84:GLN:HE21	8:P:104:ARG:NE	2.18	0.42
8:P:104:ARG:HA	8:P:121:GLN:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:208:ILE:HD12	8:P:218:LEU:HB3	2.00	0.42
8:P:227:ASP:CG	8:P:233:PHE:HZ	2.23	0.42
16:Q:99:SER:C	16:Q:101:LYS:N	2.72	0.42
16:Q:131:MET:HG2	16:Q:132:GLU:N	2.33	0.42
16:Q:164:LYS:HD3	16:Q:164:LYS:C	2.39	0.42
3:I:204:LEU:HD12	3:I:204:LEU:O	2.20	0.42
3:I:599:ILE:HG21	3:I:599:ILE:HD13	1.69	0.42
7:N:157:GLN:NE2	1:O:212:ASN:HD22	2.18	0.42
1:O:161:LEU:O	1:O:165:ALA:N	2.41	0.42
1:O:293:LYS:HB2	1:O:293:LYS:HE2	1.93	0.42
10:T:496:ASP:OD1	10:T:496:ASP:N	2.44	0.42
13:G:4:DG:H2"	13:G:5:DA:C8	2.54	0.42
2:H:107:ARG:HH11	4:K:81:THR:HG23	1.85	0.42
2:H:198:ILE:HA	2:H:201:ASN:HD21	1.85	0.42
3:I:84:LYS:HB2	3:I:87:THR:HG23	2.02	0.42
3:I:185:TYR:CD2	3:I:213:ASN:HB3	2.55	0.42
3:I:495:GLN:HB2	3:I:560:PHE:CD2	2.54	0.42
4:K:38:CYS:HA	4:K:41:LYS:HD2	2.01	0.42
4:K:209:LEU:O	4:K:213:HIS:HB2	2.19	0.42
1:O:129:ALA:H	8:P:168:ARG:HH12	1.67	0.42
1:O:161:LEU:H	1:O:214:LEU:HD11	1.85	0.42
8:P:275:LEU:O	8:P:279:ILE:HG12	2.19	0.42
13:G:10:DC:H42	14:J:-10:DG:H1	1.67	0.42
7:N:85:VAL:HG22	7:N:162:PHE:HD1	1.84	0.42
1:O:126:ILE:HG13	1:O:185:ASN:ND2	2.34	0.42
1:O:190:ARG:HG2	1:O:245:THR:HA	2.01	0.42
16:Q:134:LEU:CD1	17:U:295:GLU:HA	2.46	0.42
16:Q:141:LEU:HA	16:Q:144:GLU:HB2	2.02	0.42
2:H:113:LYS:HD3	2:H:116:LEU:CD1	2.35	0.42
3:I:85:ASP:N	3:I:85:ASP:OD1	2.52	0.42
3:I:720:LEU:CA	3:I:724:PHE:CE2	3.03	0.42
1:O:194:ALA:HA	1:O:197:LEU:HB2	2.02	0.42
11:W:54:LEU:HA	11:W:82:ILE:CD1	2.50	0.42
12:X:19:LEU:HD12	12:X:19:LEU:HA	1.86	0.42
2:H:138:LYS:N	2:H:141:MET:HE2	2.35	0.42
3:I:609:ARG:O	3:I:613:ASN:ND2	2.41	0.42
5:L:158:TRP:CZ3	5:L:160:GLY:HA3	2.55	0.42
5:L:254:PHE:CD1	5:L:291:PHE:HD2	2.38	0.42
6:M:44:LEU:HD23	6:M:44:LEU:HA	1.88	0.42
6:M:52:LEU:HD23	6:M:84:SER:O	2.19	0.42
6:M:106:ARG:HG2	6:M:109:HIS:ND1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:110:PHE:HE2	8:P:78:ILE:HG12	1.85	0.42
8:P:197:LEU:HA	8:P:206:MET:HA	2.01	0.42
9:S:24:HIS:CG	16:Q:93:MET:HB3	2.55	0.42
2:H:162:LEU:HB2	3:I:429:GLN:OE1	2.19	0.42
4:K:232:VAL:C	4:K:234:ILE:H	2.21	0.42
1:O:123:CYS:HB3	1:O:139:PHE:CZ	2.55	0.42
8:P:213:ARG:NH2	17:U:363:GLN:O	2.53	0.42
9:S:45:GLN:CG	12:X:67:VAL:HG22	2.44	0.42
13:G:21:DG:H2"	13:G:22:DG:C8	2.55	0.42
2:H:99:LYS:HE2	4:K:79:PRO:HA	2.02	0.41
3:I:146:LYS:HD2	3:I:184:LEU:HD11	2.00	0.41
3:I:446:TRP:NE1	3:I:450:CYS:O	2.42	0.41
4:K:216:LEU:HB3	4:K:264:LEU:HD13	2.02	0.41
10:T:542:GLU:HG2	10:T:543:TYR:HD1	1.85	0.41
16:Q:83:HIS:CB	16:Q:131:MET:CE	2.90	0.41
16:Q:181:ASN:HA	16:Q:184:GLN:HG3	2.02	0.41
3:I:632:PHE:O	3:I:636:THR:CB	2.57	0.41
5:L:72:TRP:HB3	5:L:185:LEU:HD22	2.01	0.41
5:L:126:GLY:O	5:L:127:MET:HE2	2.20	0.41
5:L:128:LYS:HB2	5:L:133:ASP:HB2	2.02	0.41
5:L:241:TRP:CE2	5:L:299:LEU:HD13	2.55	0.41
6:M:4:LEU:HD23	6:M:4:LEU:HA	1.88	0.41
6:M:135:VAL:HG11	6:M:138:PHE:HD2	1.84	0.41
7:N:207:LYS:NZ	7:N:330:ARG:HD3	2.34	0.41
7:N:336:ILE:HG22	15:C:303:PHE:HZ	1.85	0.41
1:O:142:LEU:HD23	1:O:150:ILE:HG13	2.01	0.41
1:O:193:GLN:NE2	1:O:197:LEU:HD13	2.24	0.41
8:P:127:ASN:OD1	8:P:128:LYS:N	2.50	0.41
10:T:473:MET:HA	10:T:474:PRO:HD3	1.92	0.41
10:T:511:LYS:HB3	10:T:513:GLU:OE2	2.20	0.41
2:H:52:GLN:HE22	6:M:161:SER:CB	2.32	0.41
2:H:86:GLU:C	2:H:86:GLU:OE1	2.58	0.41
5:L:31:LEU:O	5:L:35:ARG:NE	2.51	0.41
5:L:83:PHE:CE2	5:L:85:TYR:CE1	3.08	0.41
5:L:83:PHE:HE2	5:L:85:TYR:CE1	2.38	0.41
5:L:238:GLU:HB3	5:L:308:SER:HB3	2.01	0.41
6:M:136:GLU:C	6:M:136:GLU:OE2	2.58	0.41
1:O:126:ILE:N	1:O:138:TYR:O	2.53	0.41
1:O:231:PHE:CD1	1:O:257:VAL:HG21	2.55	0.41
8:P:172:PHE:O	8:P:175:GLU:HB2	2.20	0.41
10:T:522:GLN:HG2	11:W:86:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:54:LEU:O	11:W:58:SER:HB3	2.20	0.41
2:H:145:GLN:HA	2:H:148:TRP:HZ3	1.74	0.41
3:I:82:GLN:H	3:I:82:GLN:HG3	1.66	0.41
3:I:137:THR:OG1	3:I:175:ILE:HG13	2.20	0.41
6:M:20:LEU:HD13	6:M:67:VAL:HG22	2.02	0.41
6:M:21:VAL:HB	6:M:68:PHE:HA	2.02	0.41
7:N:273:THR:O	7:N:291:LEU:N	2.52	0.41
1:O:120:ARG:HG3	1:O:120:ARG:O	2.19	0.41
1:O:145:GLN:CD	1:O:147:PRO:HD2	2.40	0.41
8:P:76:ILE:CG2	8:P:111:CYS:HA	2.50	0.41
9:S:95:TYR:CE2	12:X:44:VAL:HG21	2.55	0.41
9:S:106:ILE:H	9:S:106:ILE:HG13	1.69	0.41
12:X:70:LEU:O	12:X:73:VAL:HG22	2.21	0.41
14:J:-11:DG:H2"	14:J:-10:DG:C8	2.56	0.41
3:I:166:ARG:HB2	3:I:200:TYR:CD2	2.56	0.41
3:I:484:THR:O	6:M:145:ARG:HA	2.19	0.41
3:I:498:LYS:O	3:I:502:GLN:OE1	2.38	0.41
3:I:686:PRO:HD2	3:I:687:SER:H	1.85	0.41
3:I:720:LEU:O	3:I:723:LEU:HB3	2.20	0.41
3:I:734:PHE:C	3:I:734:PHE:HD1	2.23	0.41
4:K:132:GLN:HA	4:K:135:ILE:HG22	2.02	0.41
4:K:205:SER:O	4:K:207:VAL:N	2.52	0.41
5:L:42:LEU:HD12	5:L:42:LEU:O	2.20	0.41
6:M:16:ALA:HB1	6:M:150:LEU:HG	2.02	0.41
10:T:471:ALA:HA	11:W:55:ALA:HB1	2.01	0.41
11:W:84:LYS:HA	11:W:87:ARG:HD3	2.01	0.41
16:Q:95:ILE:O	16:Q:99:SER:N	2.35	0.41
18:R:93:VAL:O	18:R:97:SER:N	2.43	0.41
2:H:132:HIS:CD2	2:H:136:LEU:HD21	2.55	0.41
3:I:167:TRP:O	3:I:171:MET:HG2	2.20	0.41
3:I:491:CYS:SG	3:I:557:LEU:HA	2.61	0.41
3:I:584:PRO:HD2	3:I:587:ILE:HD13	2.02	0.41
6:M:53:PRO:CD	6:M:87:HIS:ND1	2.83	0.41
8:P:232:VAL:O	8:P:234:PRO:HD3	2.21	0.41
16:Q:91:VAL:O	16:Q:94:THR:OG1	2.26	0.41
16:Q:105:GLU:O	16:Q:109:HIS:CD2	2.74	0.41
2:H:186:LEU:HD22	2:H:189:MET:CE	2.51	0.41
3:I:222:LEU:HA	3:I:222:LEU:HD23	1.82	0.41
3:I:558:LEU:HD23	3:I:558:LEU:C	2.41	0.41
5:L:134:PRO:HG2	5:L:180:CYS:O	2.21	0.41
7:N:167:MET:HB3	7:N:169:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:77:PRO:HD2	3:I:80:ALA:HB3	2.03	0.41
4:K:217:GLU:HA	4:K:220:ILE:HG22	2.01	0.41
5:L:241:TRP:CZ3	5:L:304:LEU:HG	2.56	0.41
5:L:288:TYR:CD2	5:L:300:SER:HB3	2.56	0.41
5:L:290:HIS:CE1	7:N:291:LEU:HD23	2.55	0.41
6:M:52:LEU:HD23	6:M:84:SER:C	2.41	0.41
7:N:75:GLN:NE2	7:N:124:ARG:HH11	2.15	0.41
7:N:91:GLY:H	7:N:186:HIS:CE1	2.39	0.41
7:N:336:ILE:HD12	15:C:305:ILE:HD11	2.01	0.41
8:P:103:GLN:HB2	8:P:122:ILE:HG13	2.01	0.41
12:X:10:PHE:HD2	12:X:42:LEU:HD11	1.85	0.41
2:H:216:PHE:O	2:H:220:ILE:HD12	2.21	0.41
3:I:418:LEU:HD22	3:I:458:LEU:HD21	2.03	0.41
3:I:546:THR:HG22	3:I:549:ARG:NH2	2.36	0.41
4:K:208:ASN:ND2	4:K:210:ILE:HB	2.35	0.41
4:K:255:HIS:CD2	4:K:261:ARG:HH21	2.38	0.41
5:L:35:ARG:O	5:L:39:SER:OG	2.26	0.41
5:L:158:TRP:CD1	5:L:192:ASN:HB2	2.56	0.41
5:L:221:MET:HB3	5:L:221:MET:HE2	1.83	0.41
5:L:243:VAL:HG12	5:L:302:THR:CG2	2.50	0.41
7:N:261:GLN:NE2	7:N:327:PRO:HB3	2.36	0.41
8:P:104:ARG:HD3	8:P:121:GLN:OE1	2.21	0.41
9:S:40:MET:HE1	12:X:64:ARG:HA	2.03	0.41
11:W:72:LYS:HE3	11:W:76:LEU:HD23	2.02	0.41
5:L:28:GLN:HA	5:L:31:LEU:HD23	2.03	0.41
5:L:230:MET:CE	5:L:311:VAL:HG22	2.50	0.41
1:O:109:HIS:O	1:O:109:HIS:ND1	2.54	0.41
8:P:285:GLU:OE1	17:U:366:GLN:CB	2.69	0.41
10:T:466:LEU:O	10:T:470:TYR:HB2	2.21	0.41
2:H:76:LYS:O	2:H:77:GLN:HG2	2.21	0.40
2:H:124:SER:O	2:H:127:MET:N	2.42	0.40
3:I:235:LEU:HD23	3:I:235:LEU:HA	1.86	0.40
3:I:723:LEU:HG	3:I:724:PHE:N	2.34	0.40
4:K:71:LEU:HD12	4:K:72:SER:N	2.36	0.40
4:K:239:TRP:CE3	4:K:239:TRP:HA	2.56	0.40
4:K:248:ARG:NH1	10:T:544:ARG:HD2	2.36	0.40
5:L:323:LEU:HD13	5:L:323:LEU:HA	1.87	0.40
6:M:48:LEU:O	7:N:240:GLU:HB2	2.21	0.40
7:N:158:THR:OG1	1:O:160:PRO:HG3	2.21	0.40
1:O:113:LEU:CD2	1:O:181:CYS:HB3	2.50	0.40
8:P:84:GLN:HE21	8:P:104:ARG:CZ	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:36:GLU:OE1	11:W:37:LYS:N	2.54	0.40
11:W:51:VAL:HA	11:W:54:LEU:HB2	2.02	0.40
11:W:57:GLU:OE1	11:W:82:ILE:HD11	2.22	0.40
16:Q:134:LEU:CD2	17:U:295:GLU:CB	3.00	0.40
16:Q:155:LEU:HD11	17:U:316:LYS:CA	2.51	0.40
3:I:197:LEU:HB3	3:I:201:VAL:HG23	2.03	0.40
3:I:467:PHE:CD2	3:I:535:LYS:HB3	2.55	0.40
3:I:568:VAL:O	3:I:571:ILE:HG12	2.21	0.40
3:I:615:THR:O	3:I:619:LYS:HG2	2.22	0.40
4:K:28:CYS:O	4:K:32:TRP:CD1	2.73	0.40
4:K:164:THR:O	4:K:167:LEU:HG	2.22	0.40
6:M:65:LEU:HB2	6:M:150:LEU:CD1	2.51	0.40
7:N:258:ASP:HB2	7:N:259:TYR:CD1	2.56	0.40
7:N:264:LEU:HA	7:N:299:SER:O	2.21	0.40
8:P:121:GLN:HB3	8:P:137:ASP:HB2	2.03	0.40
11:W:53:ARG:HB3	11:W:82:ILE:HG21	2.03	0.40
2:H:215:VAL:O	2:H:219:LEU:HB2	2.20	0.40
3:I:64:ASP:O	3:I:67:GLN:HG3	2.21	0.40
3:I:250:ILE:HG22	5:L:101:ALA:CB	2.52	0.40
3:I:601:ASN:OD1	3:I:602:GLN:N	2.53	0.40
3:I:647:MET:CG	3:I:651:LEU:HD23	2.51	0.40
6:M:27:LEU:HD12	6:M:27:LEU:HA	1.95	0.40
6:M:45:LYS:HD3	6:M:45:LYS:HA	1.94	0.40
7:N:84:GLU:CG	7:N:165:SER:HB3	2.46	0.40
7:N:177:GLN:OE1	17:U:320:MET:O	2.39	0.40
7:N:180:THR:HB	7:N:188:ILE:HB	2.04	0.40
3:I:107:GLU:HG2	3:I:141:GLU:HA	2.04	0.40
3:I:447:ASP:OD1	3:I:449:LEU:N	2.55	0.40
4:K:38:CYS:HA	4:K:41:LYS:HB2	2.04	0.40
5:L:55:LEU:HD13	5:L:59:VAL:CG2	2.51	0.40
5:L:140:GLN:HG2	5:L:159:THR:HG23	2.04	0.40
7:N:45:LYS:O	7:N:49:VAL:HG13	2.22	0.40
7:N:170:ARG:H	7:N:170:ARG:HD3	1.86	0.40
8:P:227:ASP:OD1	8:P:231:LYS:N	2.54	0.40
16:Q:167:GLU:O	16:Q:171:LEU:HG	2.22	0.40
2:H:198:ILE:HA	2:H:201:ASN:ND2	2.37	0.40
2:H:216:PHE:CE2	4:K:179:THR:HB	2.57	0.40
3:I:62:GLU:N	3:I:62:GLU:OE2	2.55	0.40
3:I:164:PHE:CZ	3:I:168:LEU:HD21	2.57	0.40
3:I:483:PHE:CE2	6:M:168:LEU:HB3	2.57	0.40
3:I:495:GLN:HB2	3:I:560:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:495:GLN:NE2	3:I:499:GLU:OE1	2.54	0.40
4:K:67:LEU:O	4:K:71:LEU:HG	2.22	0.40
4:K:258:ASP:OD1	4:K:258:ASP:C	2.59	0.40
6:M:31:LEU:HA	6:M:139:ARG:HD3	2.04	0.40
6:M:44:LEU:O	6:M:46:VAL:HG23	2.22	0.40
7:N:169:ARG:HE	7:N:169:ARG:HB2	1.72	0.40
1:O:193:GLN:O	1:O:197:LEU:N	2.47	0.40
8:P:64:GLU:OE2	8:P:64:GLU:N	2.47	0.40
8:P:152:GLU:O	8:P:152:GLU:CD	2.60	0.40
8:P:153:PHE:CE1	8:P:166:PHE:HB2	2.57	0.40
8:P:218:LEU:HD12	8:P:218:LEU:HA	1.82	0.40
8:P:269:LEU:HB3	8:P:273:ALA:HB3	2.04	0.40
10:T:484:GLU:C	10:T:484:GLU:OE2	2.60	0.40
16:Q:245:LEU:O	16:Q:249:SER:N	2.52	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	O	204/300 (68%)	176 (86%)	25 (12%)	3 (2%)	10 44
1	o	10/300 (3%)	10 (100%)	0	0	100 100
2	H	191/253 (76%)	179 (94%)	12 (6%)	0	100 100
3	I	503/756 (66%)	447 (89%)	53 (10%)	3 (1%)	25 61
4	K	224/269 (83%)	202 (90%)	19 (8%)	3 (1%)	12 47
5	L	296/344 (86%)	261 (88%)	32 (11%)	3 (1%)	15 51
6	M	166/180 (92%)	146 (88%)	20 (12%)	0	100 100
7	N	299/345 (87%)	262 (88%)	36 (12%)	1 (0%)	41 74
8	P	220/288 (76%)	195 (89%)	22 (10%)	3 (1%)	11 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	S	95/138 (69%)	94 (99%)	1 (1%)	0	100 100
10	T	97/561 (17%)	93 (96%)	4 (4%)	0	100 100
11	W	73/88 (83%)	72 (99%)	1 (1%)	0	100 100
12	X	72/81 (89%)	71 (99%)	1 (1%)	0	100 100
15	C	3/943 (0%)	1 (33%)	1 (33%)	1 (33%)	0 0
15	c	11/943 (1%)	6 (54%)	4 (36%)	1 (9%)	1 10
16	Q	156/274 (57%)	151 (97%)	4 (3%)	1 (1%)	25 61
17	U	136/418 (32%)	131 (96%)	5 (4%)	0	100 100
18	R	58/177 (33%)	56 (97%)	2 (3%)	0	100 100
All	All	2814/6658 (42%)	2553 (91%)	242 (9%)	19 (1%)	26 59

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L	44	PRO
1	O	156	PRO
15	C	304	ILE
16	Q	100	ILE
4	K	207	VAL
8	P	144	PRO
8	P	192	PRO
3	I	724	PHE
5	L	59	VAL
4	K	233	LYS
5	L	187	ASN
1	O	131	GLU
1	O	132	GLY
15	c	263	SER
3	I	463	PRO
4	K	188	PHE
3	I	135	PRO
7	N	321	PRO
8	P	76	ILE

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	O	170/263 (65%)	159 (94%)	11 (6%)	17 48
1	o	10/263 (4%)	9 (90%)	1 (10%)	7 32
2	H	174/230 (76%)	165 (95%)	9 (5%)	23 54
3	I	440/691 (64%)	422 (96%)	18 (4%)	30 59
4	K	211/260 (81%)	195 (92%)	16 (8%)	13 43
5	L	268/306 (88%)	264 (98%)	4 (2%)	65 81
6	M	147/158 (93%)	142 (97%)	5 (3%)	37 63
7	N	273/317 (86%)	258 (94%)	15 (6%)	21 53
8	P	204/259 (79%)	194 (95%)	10 (5%)	25 55
9	S	86/121 (71%)	80 (93%)	6 (7%)	15 46
10	T	88/461 (19%)	84 (96%)	4 (4%)	27 57
11	W	61/77 (79%)	55 (90%)	6 (10%)	8 33
12	X	65/67 (97%)	62 (95%)	3 (5%)	27 56
15	C	4/875 (0%)	4 (100%)	0	100 100
15	c	12/875 (1%)	11 (92%)	1 (8%)	11 40
16	Q	109/254 (43%)	99 (91%)	10 (9%)	9 36
All	All	2322/5477 (42%)	2203 (95%)	119 (5%)	27 55

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	o	24	LEU
2	H	45	ARG
2	H	96	PHE
2	H	107	ARG
2	H	148	TRP
2	H	180	ASN
2	H	187	ASP
2	H	189	MET
2	H	204	MET
2	H	210	THR
3	I	110	ASP
3	I	133	MET
3	I	150	TRP
3	I	172	PHE

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Mol	Chain	Res	Type
3	I	174	PHE
3	I	195	ASP
3	I	224	ASP
3	I	229	MET
3	I	234	HIS
3	I	381	ASP
3	I	447	ASP
3	I	462	ILE
3	I	514	MET
3	I	647	MET
3	I	688	PHE
3	I	695	PHE
3	I	726	GLN
3	I	734	PHE
4	K	26	ARG
4	K	28	CYS
4	K	62	MET
4	K	71	LEU
4	K	97	PHE
4	K	101	ARG
4	K	115	ASN
4	K	121	ASP
4	K	127	ARG
4	K	180	LEU
4	K	186	ASP
4	K	217	GLU
4	K	221	ASN
4	K	222	ARG
4	K	231	TYR
4	K	248	ARG
5	L	35	ARG
5	L	94	LEU
5	L	293	ARG
5	L	341	PHE
6	M	65	LEU
6	M	93	PHE
6	M	114	ARG
6	M	156	HIS
6	M	166	LEU
7	N	14	LEU
7	N	18	MET
7	N	30	PHE

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Mol	Chain	Res	Type
7	N	60	ARG
7	N	69	LEU
7	N	148	LYS
7	N	170	ARG
7	N	192	ASP
7	N	236	ARG
7	N	247	ARG
7	N	258	ASP
7	N	259	TYR
7	N	292	ARG
7	N	294	LEU
7	N	337	ARG
1	O	110	PHE
1	O	151	HIS
1	O	167	LYS
1	O	170	GLN
1	O	175	HIS
1	O	201	PHE
1	O	204	LEU
1	O	211	ARG
1	O	217	LEU
1	O	258	GLU
1	O	266	GLU
8	P	108	SER
8	P	120	PHE
8	P	142	MET
8	P	143	GLU
8	P	166	PHE
8	P	180	ARG
8	P	193	ASP
8	P	223	ARG
8	P	233	PHE
8	P	283	CYS
9	S	12	ARG
9	S	15	TYR
9	S	37	ASP
9	S	56	ARG
9	S	64	ASP
9	S	101	GLU
10	T	467	PHE
10	T	470	TYR
10	T	476	GLU

Continued on next page...

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Mol	Chain	Res	Type
10	T	477	ARG
11	W	47	CYS
11	W	61	ASN
11	W	63	CYS
11	W	76	LEU
11	W	80	LYS
11	W	83	LEU
12	X	36	GLN
12	X	42	LEU
12	X	81	PHE
15	c	268	GLU
16	Q	83	HIS
16	Q	101	LYS
16	Q	114	LYS
16	Q	115	LYS
16	Q	131	MET
16	Q	147	ARG
16	Q	152	GLU
16	Q	177	GLN
16	Q	182	LYS
16	Q	184	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	52	GLN
2	H	87	ASN
2	H	166	GLN
3	I	123	ASN
3	I	182	ASN
3	I	213	ASN
3	I	397	GLN
3	I	642	HIS
3	I	726	GLN
3	I	729	GLN
4	K	63	GLN
4	K	73	GLN
4	K	132	GLN
4	K	249	ASN
5	L	71	GLN
5	L	187	ASN
5	L	290	HIS

Continued on next page...

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Mol	Chain	Res	Type
6	M	29	GLN
6	M	115	HIS
6	M	156	HIS
7	N	75	GLN
7	N	106	ASN
7	N	157	GLN
7	N	185	HIS
7	N	208	GLN
7	N	239	HIS
1	O	152	HIS
1	O	170	GLN
1	O	185	ASN
1	O	193	GLN
1	O	229	GLN
1	O	281	HIS
8	P	121	GLN
10	T	538	HIS
12	X	36	GLN
16	Q	85	GLN
16	Q	184	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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

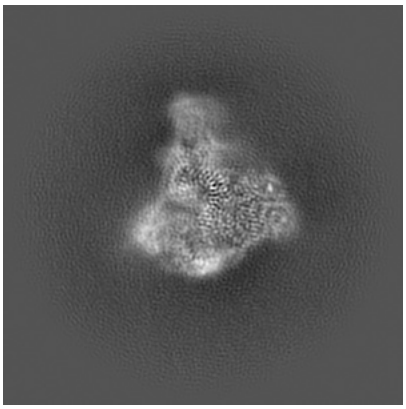
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33196. These allow visual inspection of the internal detail of the map and identification of artifacts.

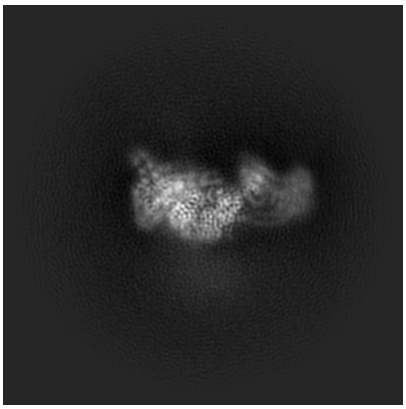
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

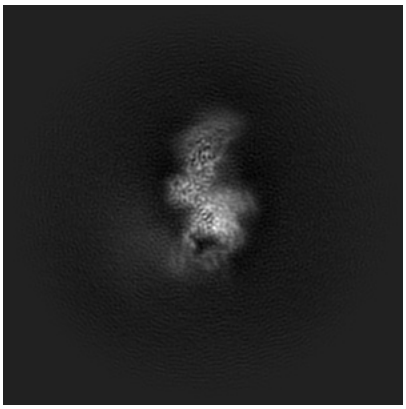
6.1.1 Primary map



X

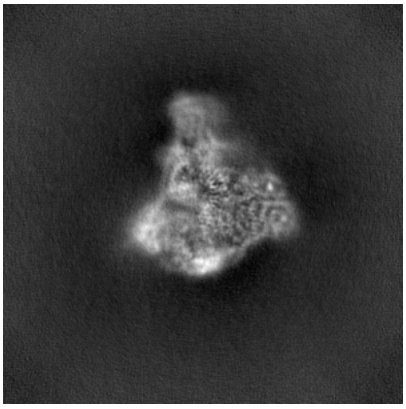


Y

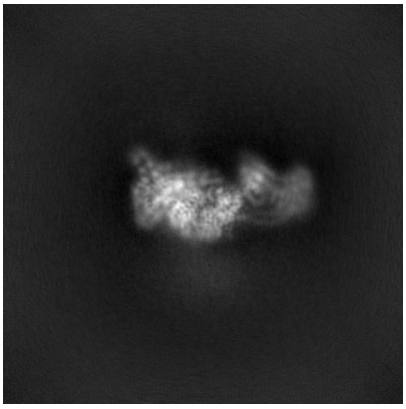


Z

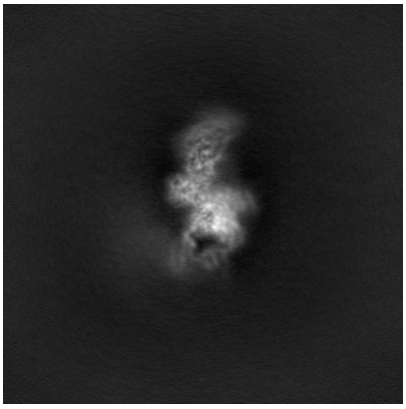
6.1.2 Raw map



X



Y

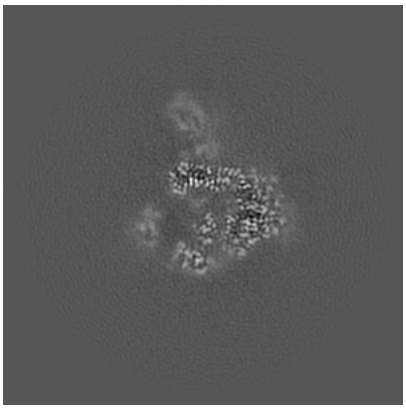


Z

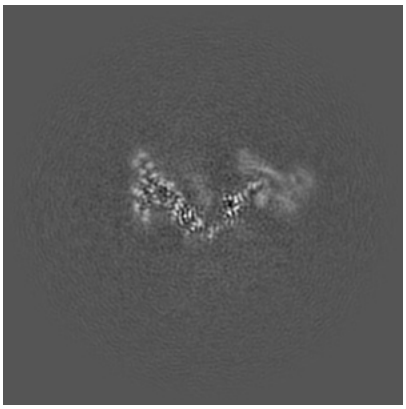
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

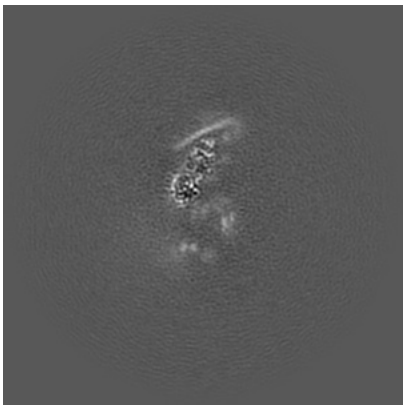
6.2.1 Primary map



X Index: 156

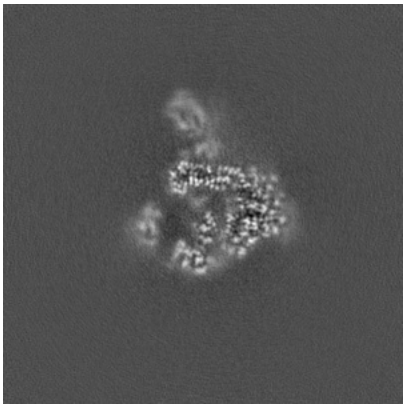


Y Index: 156

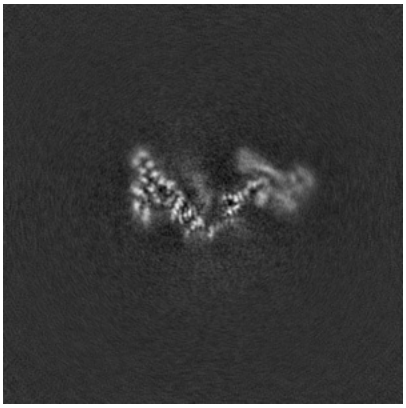


Z Index: 156

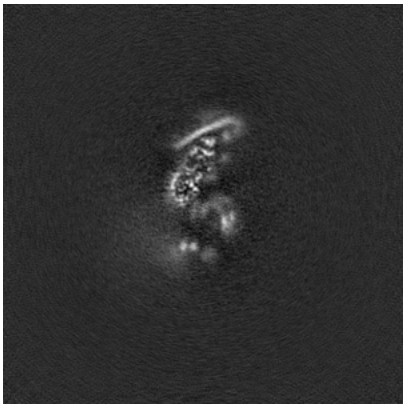
6.2.2 Raw map



X Index: 156



Y Index: 156

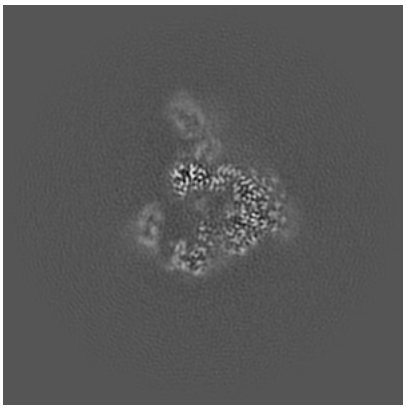


Z Index: 156

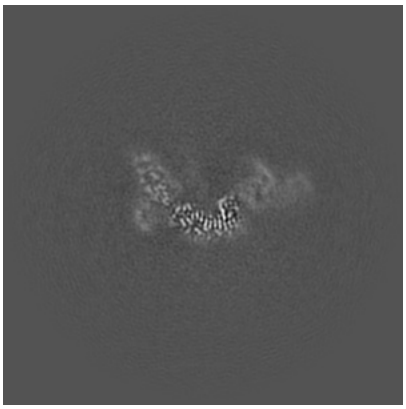
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

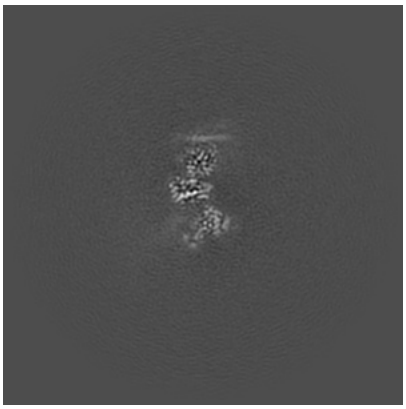
6.3.1 Primary map



X Index: 158

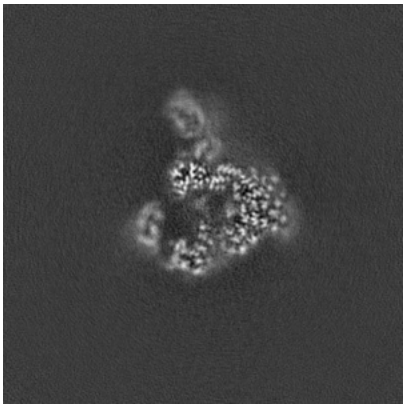


Y Index: 162

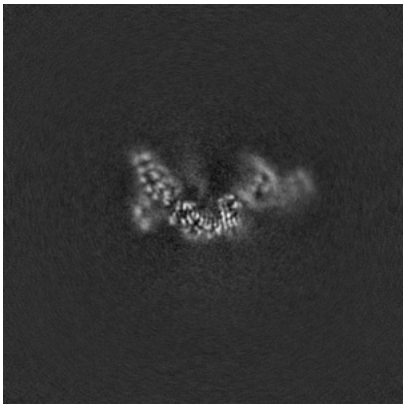


Z Index: 169

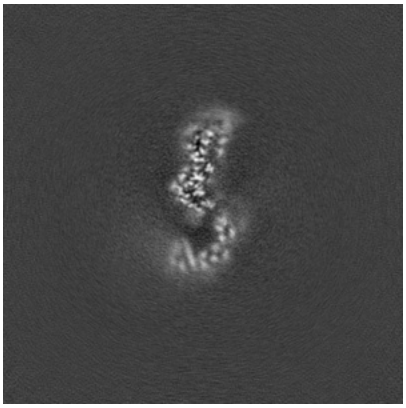
6.3.2 Raw map



X Index: 158



Y Index: 161



Z Index: 139

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 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X

Y

Z

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

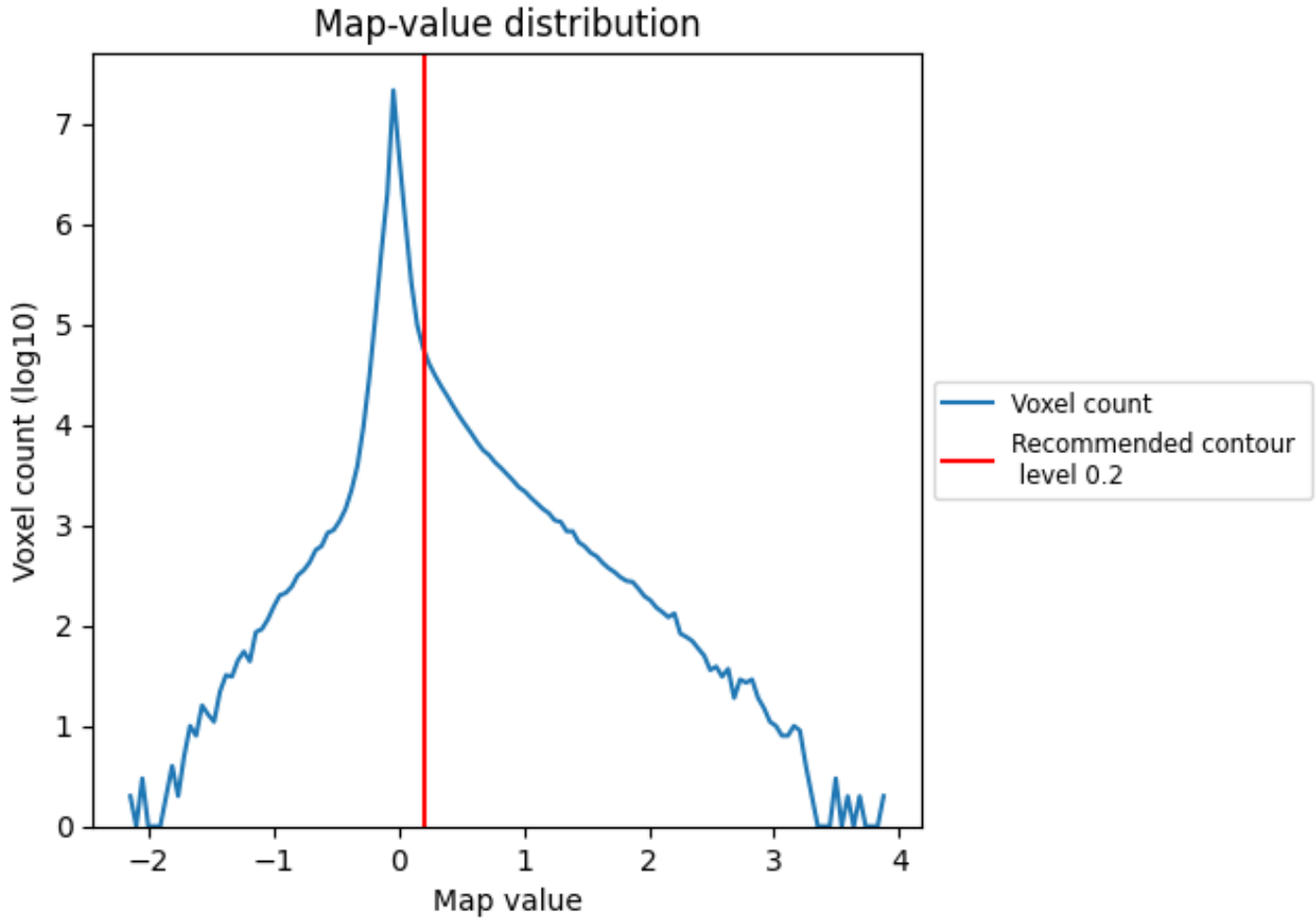
6.5 Mask visualisation (i)

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

7 Map analysis

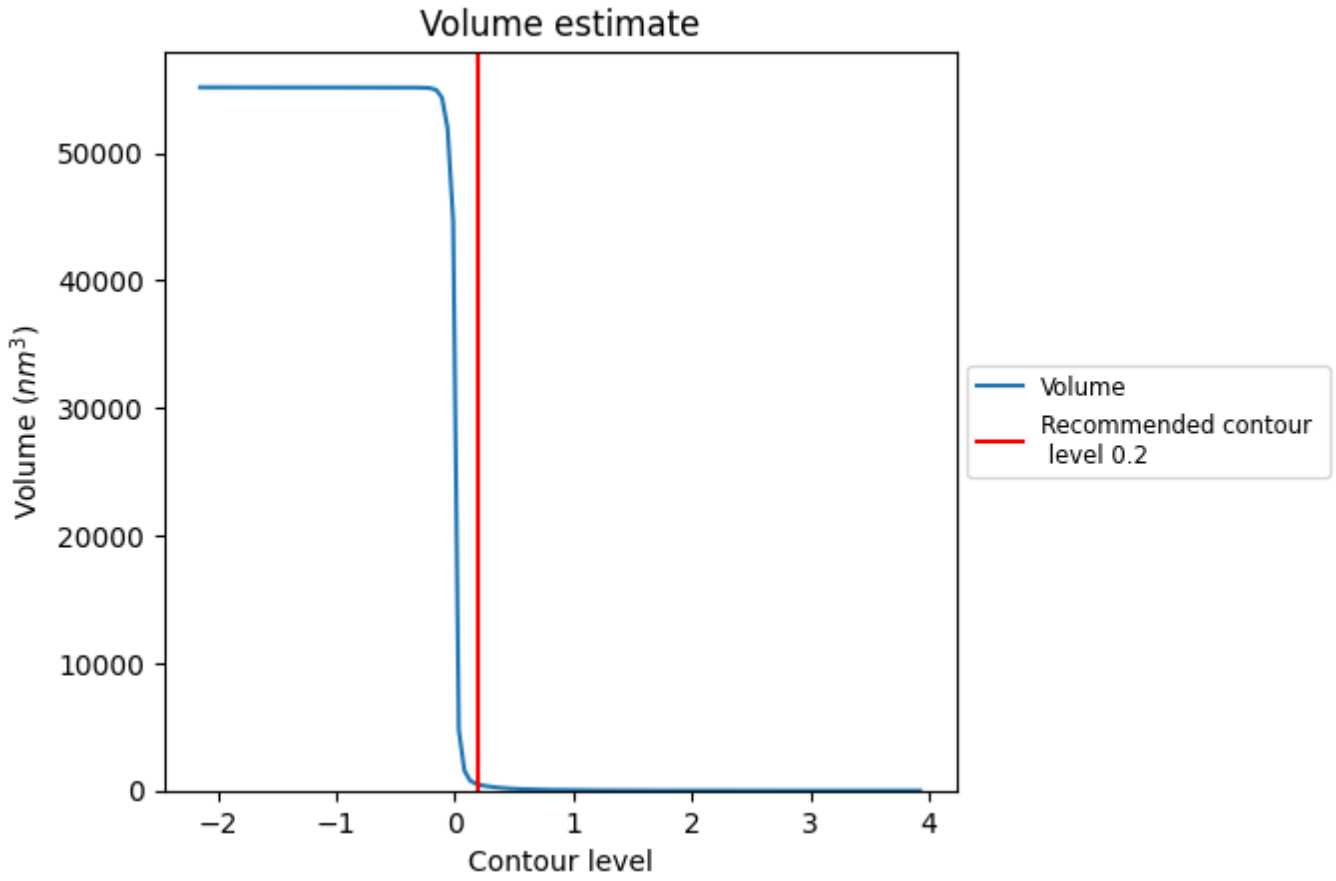
This section contains the results of statistical analysis of the map.

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.

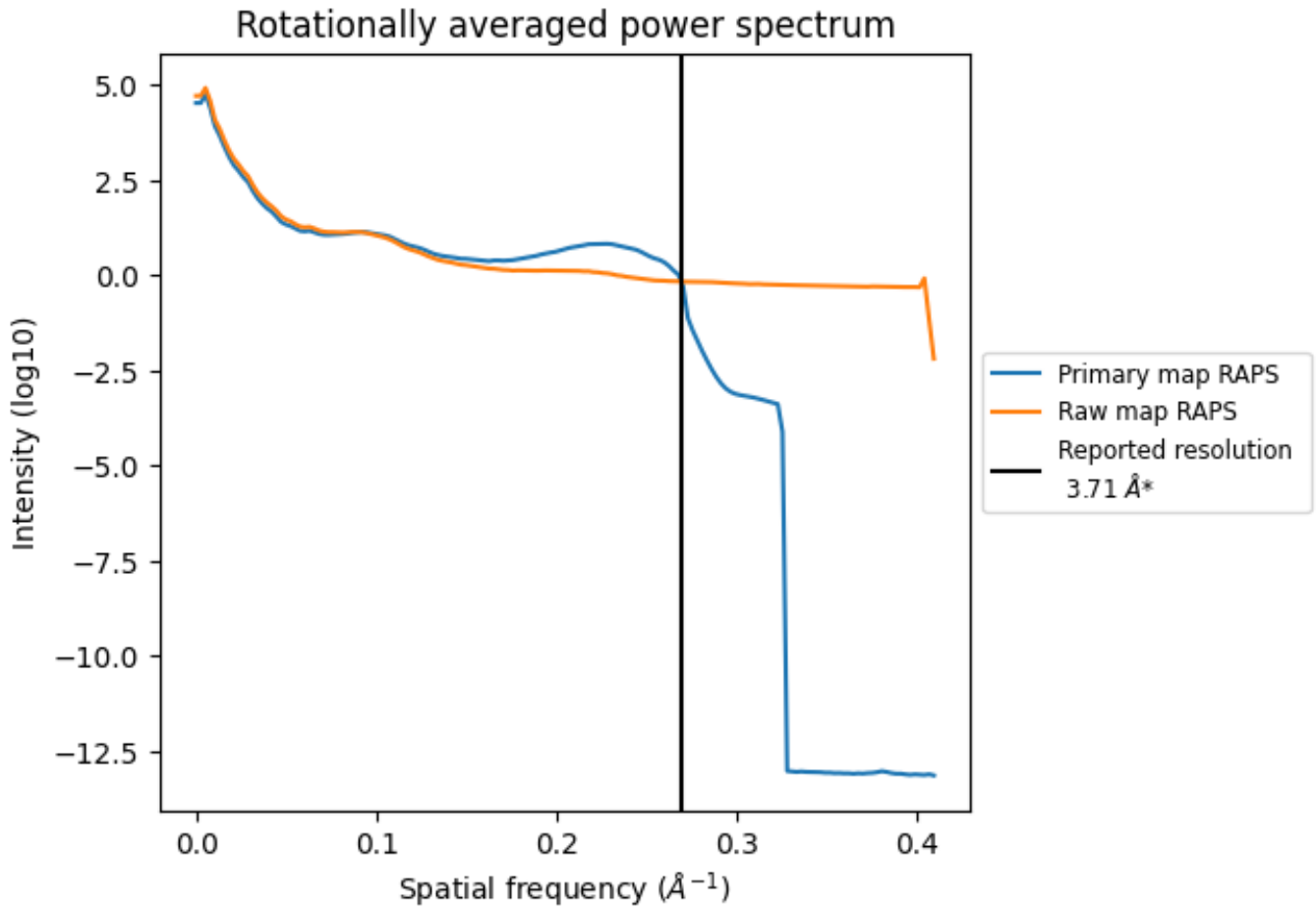
7.2 Volume estimate



The volume at the recommended contour level is 482 nm^3; this corresponds to an approximate mass of 435 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)

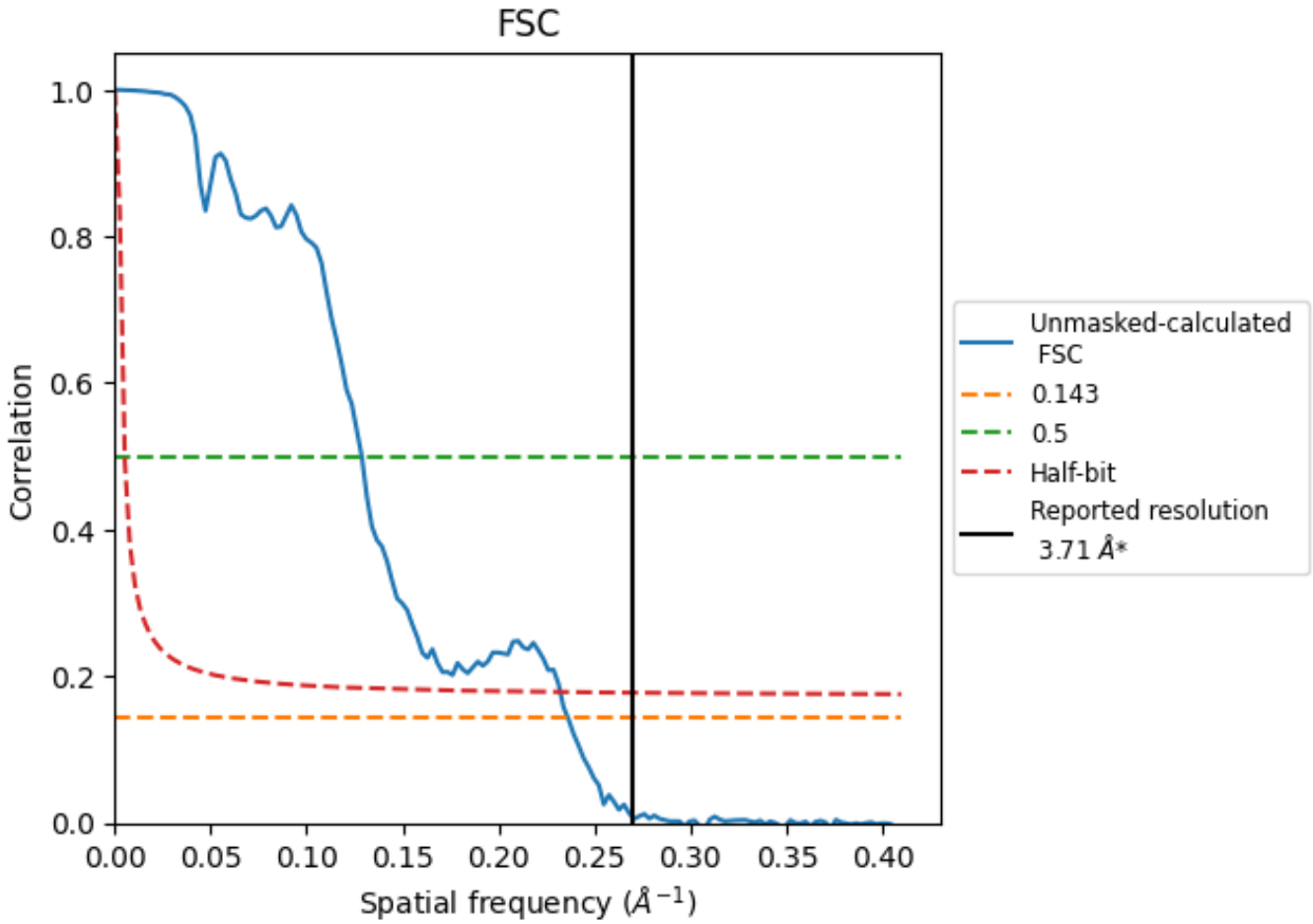


*Reported resolution corresponds to spatial frequency of 0.270 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

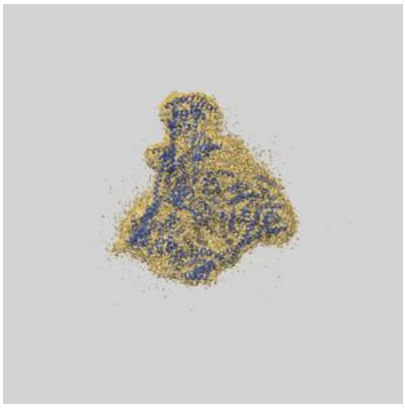
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.71	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	7.77	4.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.71 by more than 10 %

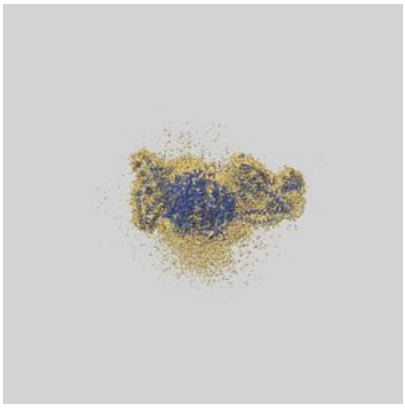
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33196 and PDB model 7XHN. Per-residue inclusion information can be found in section 3 on page 8.

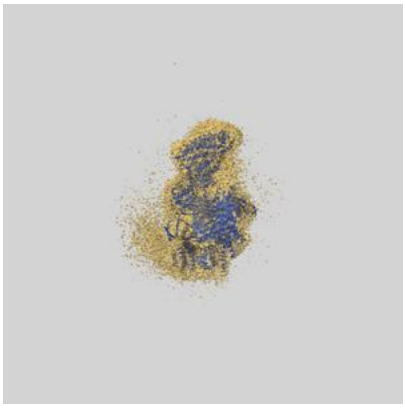
9.1 Map-model overlay



X



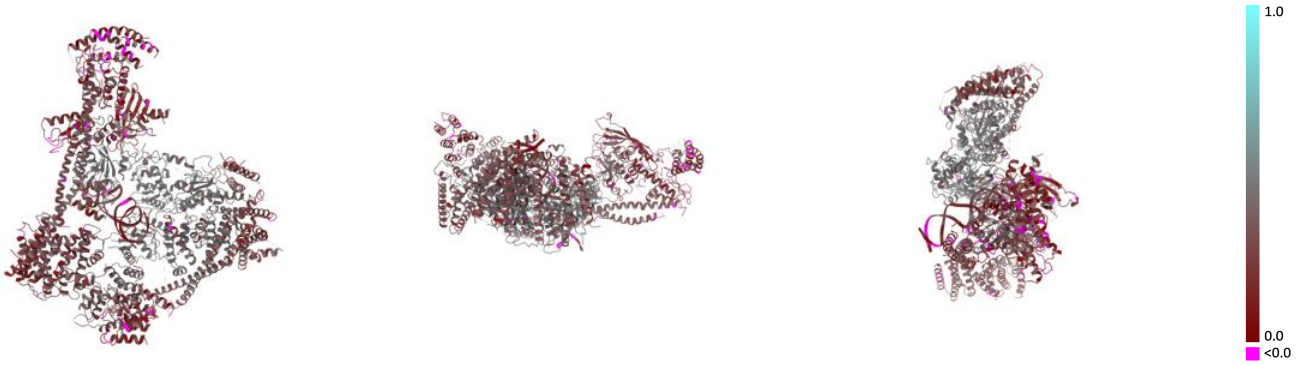
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

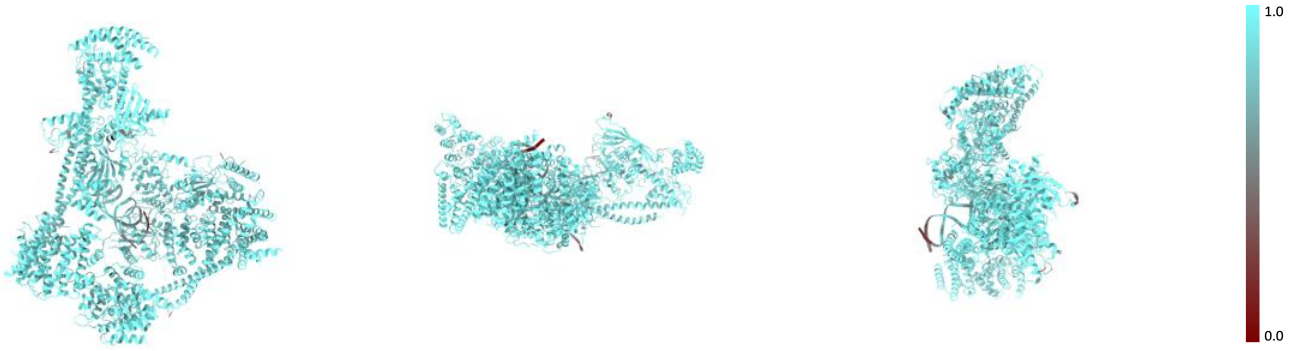
9.2 Q-score mapped to coordinate model (i)



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.

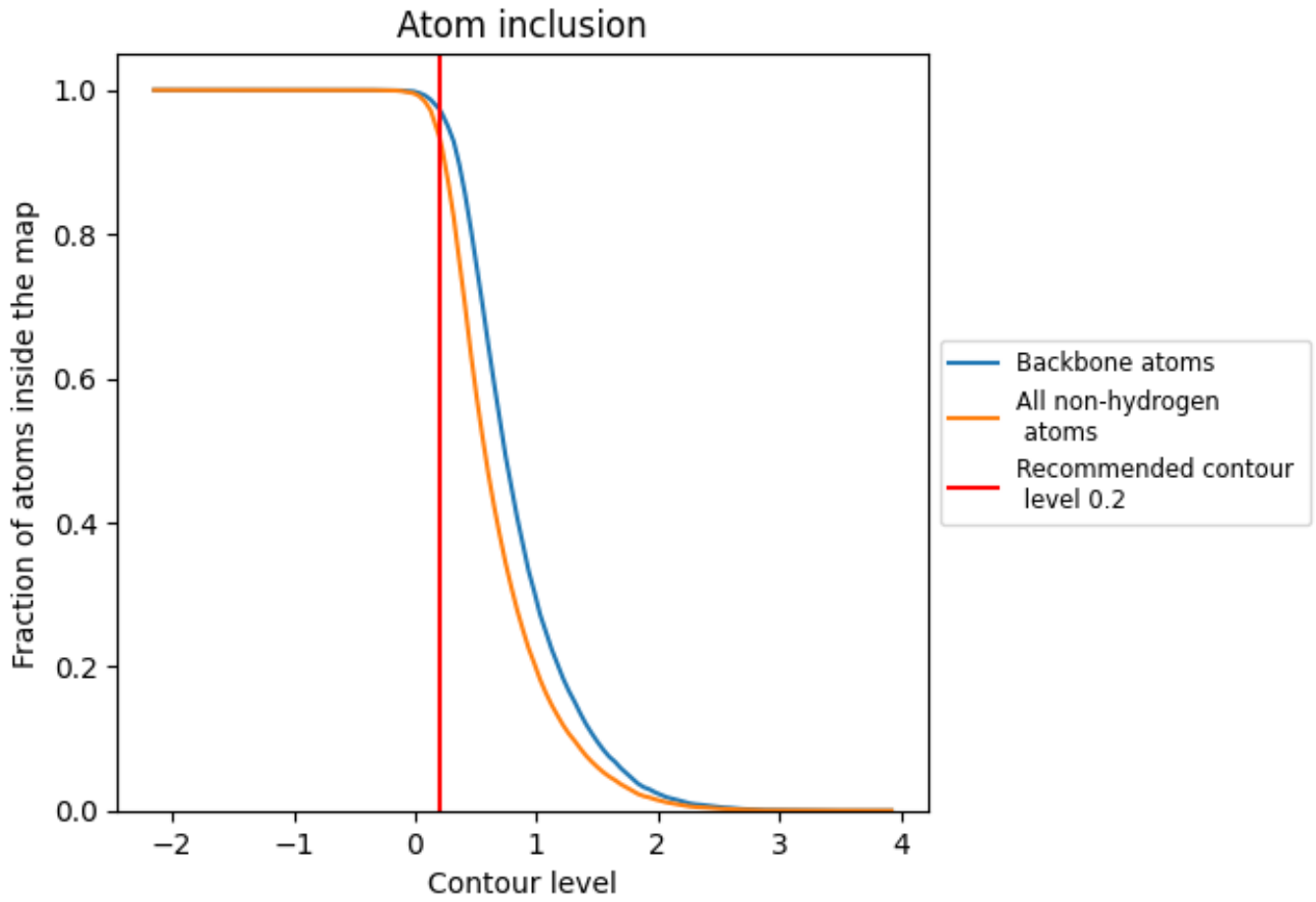
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9351	0.3210
C	0.8750	0.1220
G	0.6745	0.1440
H	0.9279	0.3090
I	0.9459	0.3450
J	0.6445	0.1300
K	0.9251	0.3320
L	0.9589	0.4510
M	0.9459	0.4530
N	0.9611	0.4220
O	0.9271	0.2580
P	0.9600	0.1920
Q	0.9536	0.2150
R	0.9545	0.1730
S	0.9651	0.2430
T	0.9720	0.3410
U	0.9986	0.2840
W	0.9648	0.3230
X	0.9155	0.2020
c	0.7379	0.1720
o	0.8817	0.3490