



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 12:01 AM UTC

PDB ID : 7XHN / pdb_00007xhn
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

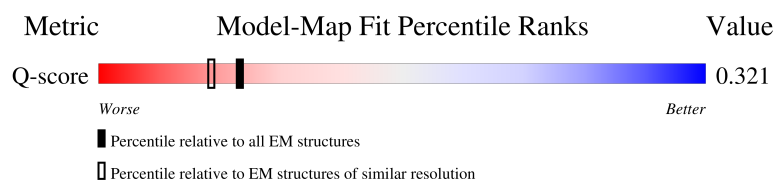
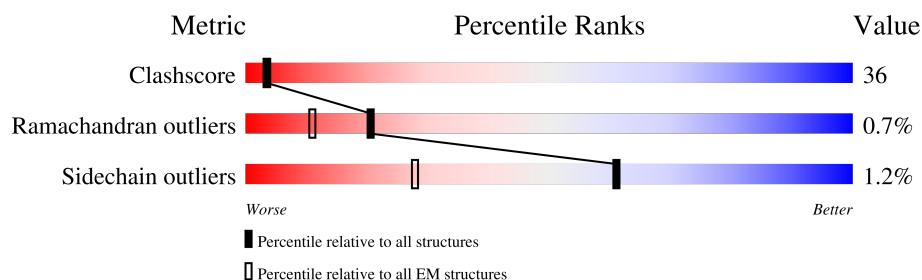
1 Overall quality at a glance

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.



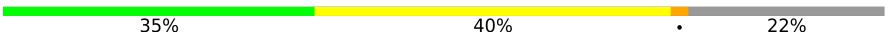
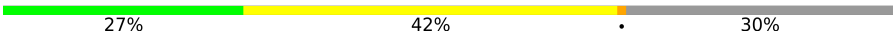
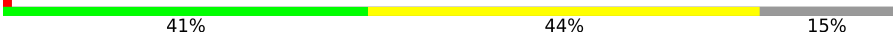
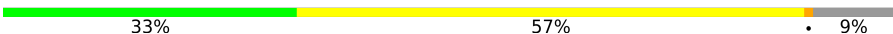
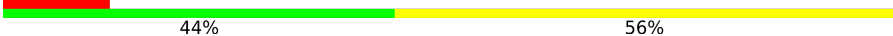
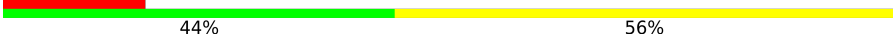
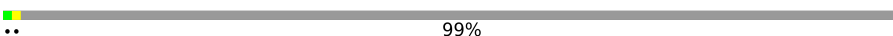
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10534 (3.21 - 4.21)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	O	300	
1	o	300	
2	H	253	
3	I	756	

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Mol	Chain	Length	Quality of chain
4	K	269	
5	L	344	
6	M	180	
7	N	345	
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		0	0
			95	59	18	18			
1	O	206	Total	C	N	O	S	0	0
			1588	1017	269	294	8		

- Molecule 2 is a protein called Centromere protein H.

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

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	0	0
			4111	2700	661	724	26		

- Molecule 4 is a protein called Centromere protein K.

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

- 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		

[illegible]

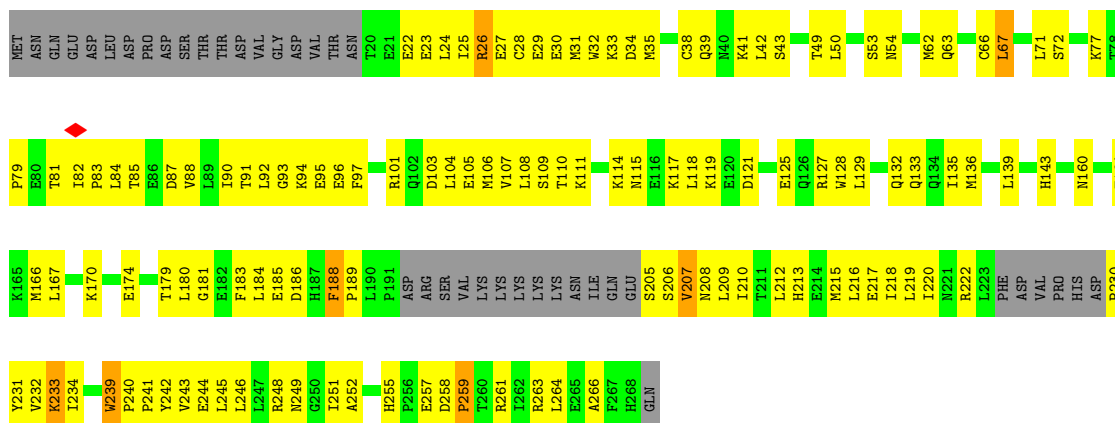
Chain I: 31% 36% 32%

TRP	F583	SER	L449	GLU	ARG	ALA	MET
THR	P584	PRO	C450	LEU	PRO	E62	SER
LYS	I587	LEU	C451	PRO	LEU	E63	PRO
PRO	F588	GLU	R452	SER	C202	M133	GLN
PHE	Y589	THR	S453	GLN	H203	T134	LYS
GLN	S590	THR		MET	L204	P135	ARG
LYS	A591	GLN	Q457	GLY	L205	A136	VAL
GLY	L592	G527	L458	S365	Y206	T137	VAL
ILE	L593	M530	S460	L371	L207	V138	ASN
THR	S594	N531	S461	Y371	L208	I139	VAL
ILE	L595	S532	I462	Y375	T209	S140	GLN
ASP	D596	V533	P463	I376	K210	E141	ALA
PRO	T597	S534	F464	N377	N213	D142	GLN
GLU	S598	K535	C378	C378	S143	V144	ASN
ILE	I599	L536		VAL	V145	G75	ARG
LEU	L600	I537	F467	V379	V219	P77	THR
GLU	N601	H538	K471	E382	R220	K146	SER
LYS	Q602	T539	P472		K221	A147	GLN
THR	L603	V540	L473	Y389	L222	V148	GLY
GLY		G541	L475	Y390	M229	S149	SER
VAL	I606	W542	F476	W391	Y233	W150	SER
ALA	M607	L543	D476	L392	P233	L151	SER
GLU	H608	S544	H477		H234	K86	PHE
THR	R609	T545	L478	T395	L235	T87	GLN
LYS	Y610	T546	A479			L88	THR
ASN	R611	A547	Q480	E399	L249	E89	LEU
LEU	N612	M548	L481	Y403	I250	K90	SER
ASN	L614	R549	F482		S251	H91	ALA
VAL	T615	L550	F483	MET	V252	L92	TRP
VAL		E551	T484	GLU	SER	K93	LYS
VAL		S552		K411	LEU	T94	VAL
HIS	K618	N553	I487	K412	PRO	E95	LYS
H685	K619	L557	K490	N416	ASP	E96	GLN
P686	N620	L558	C491	F417	CTVS		ASP
S687	E621			L418	LEU		PRO
F688	LEU	H559	L494	I421	ASN	A99	SER
L689	VAL	F560	Q495	I422	ARG	W100	ASN
GLM	S690	I561			M171	K101	SER
Y591	LYS	L562		GLY	F172	N102	SER
A692	THR	D563	K498	F427	D173	G103	LYS
V693	LYS	F564	E499	L428	F174	A105	ASN
S694	SER	Y565		Q429	I175	S106	ILE
F695	GLU	E566	Q502	L429	D176	E107	SER
LEU	PHE	K567	N503	G431	L273		LYS
LEU	N631	L568	F504	F432	P283	I181	HIS
GLN	F632	C569	L505	Y433	SER	T109	GLN
GLU		D570	L506	S434	PRO	D110	GLN
SER	T636	I571	W607	C435	GLN	T111	ASN
PRO	Y637	I572	L508	E436	SER	L112	ASN
GLU		I573	S509		PHE	L113	PRO
ARG	N641	T574	M510	Y440	PRO	C186	VAL
THR	H642	Y575		K441	LEU	L117	GLY
VAL	Y643	N576	H513	L442	LYS	F189	ASP
ASN	L644	L577	M514	S443	MET	K120	TYR
VAL	M647	P578	K615	P444	LEU	F121	GLU
SER		L579		L445	GLN	L192	HIS
LEU		V580	PRO	L446	LEU	Q193	ALA
SER		H581	VAL	W446	PRO	D194	ASP
THR	C650	V582	THR	D447	ALA	A124	ASP
LEU	L651	L582	ASN	G448	ASN	T127	GLN
						L193	



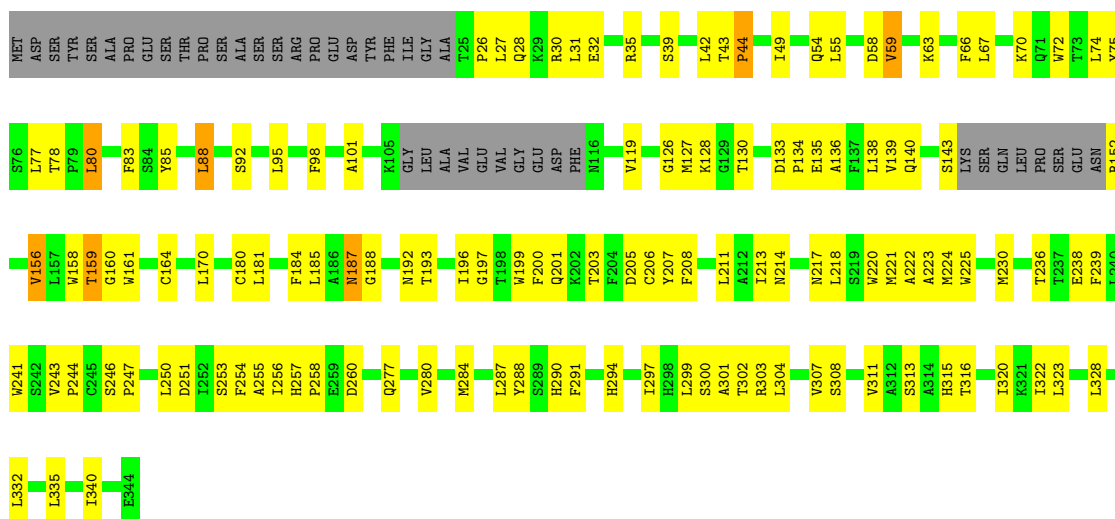
• Molecule 4: Centromere protein K

Chain K: 38% 45% 14%



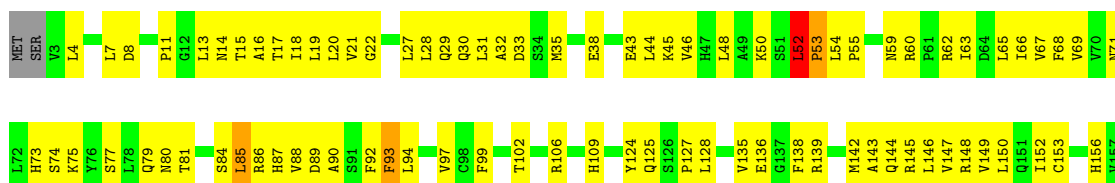
• Molecule 5: Centromere protein L

Chain L: 50% 35% 12%



• Molecule 6: Centromere protein M

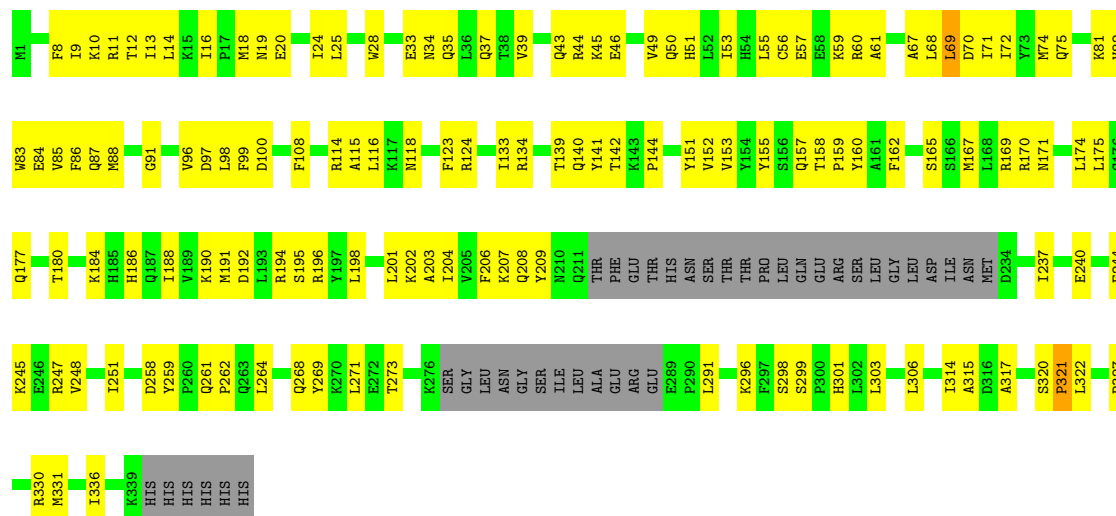
Chain M: 41% 50% 7%





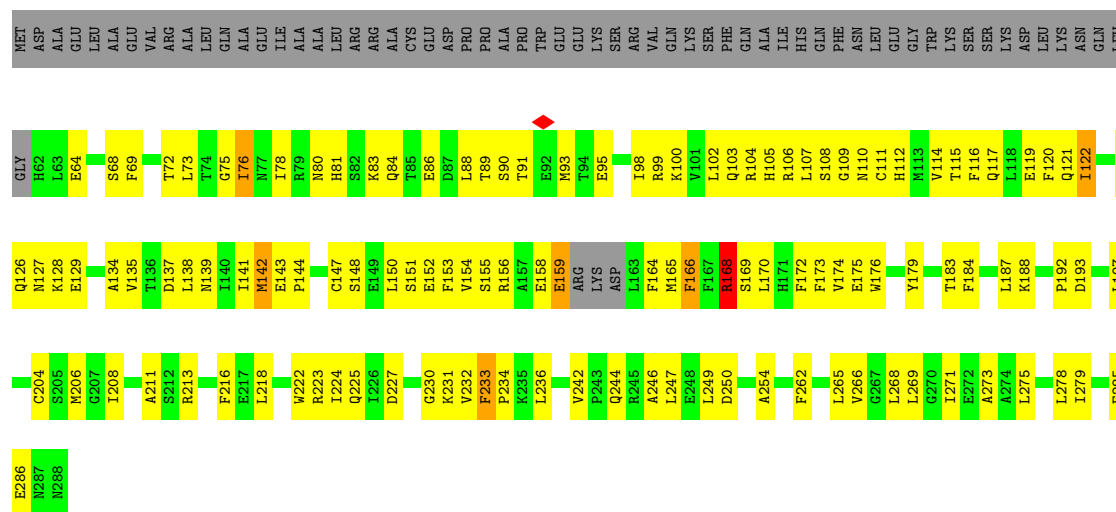
• Molecule 7: Centromere protein N

Chain N: 48% 39% 12%



• Molecule 8: Centromere protein P

Chain P: 35% 40% 22%

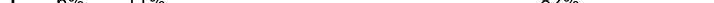


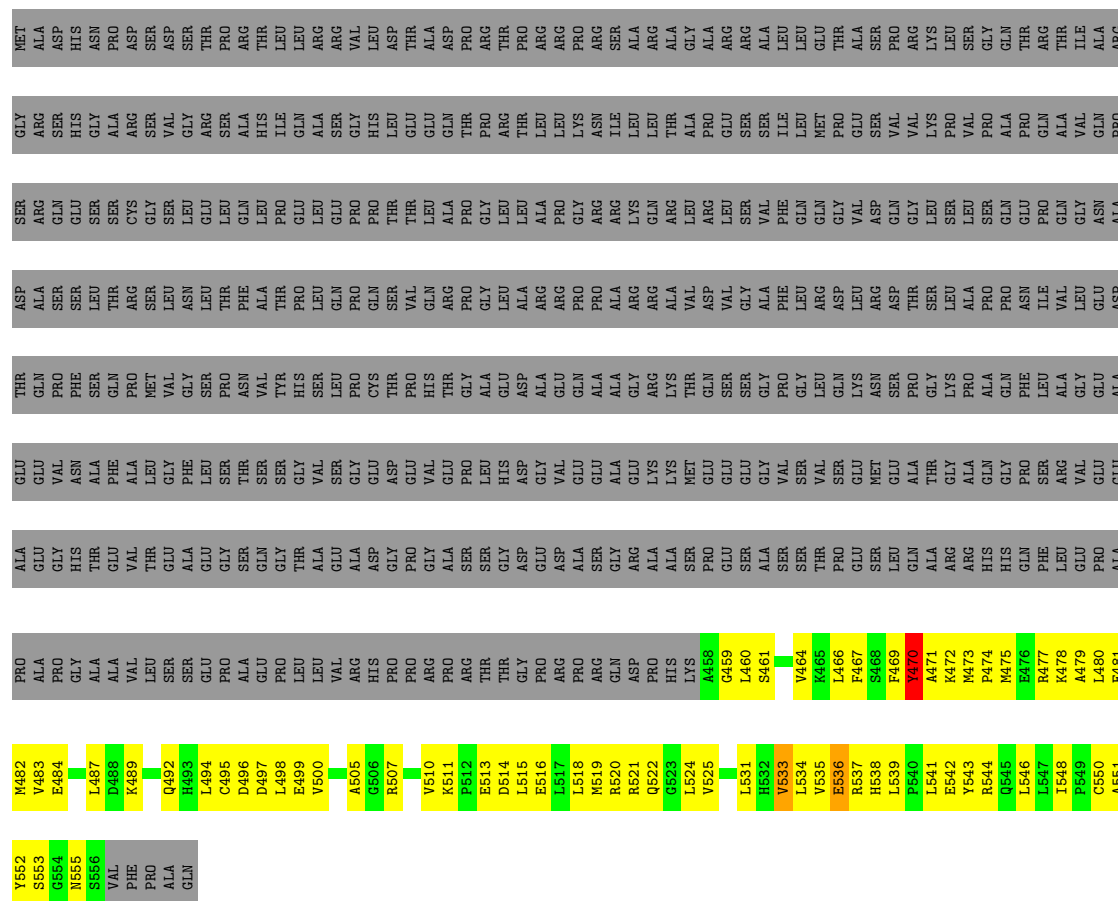
• Molecule 9: Centromere protein S

Chain S: 27% 42% 30%

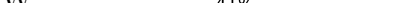


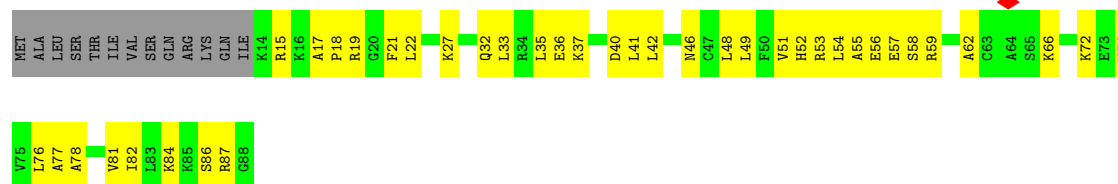
- Molecule 10: Centromere protein T

Chain T:  6% 11% 82%



- Molecule 11: CENP-W

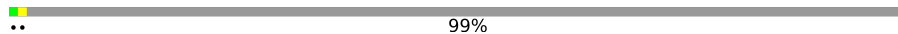
Chain W: 

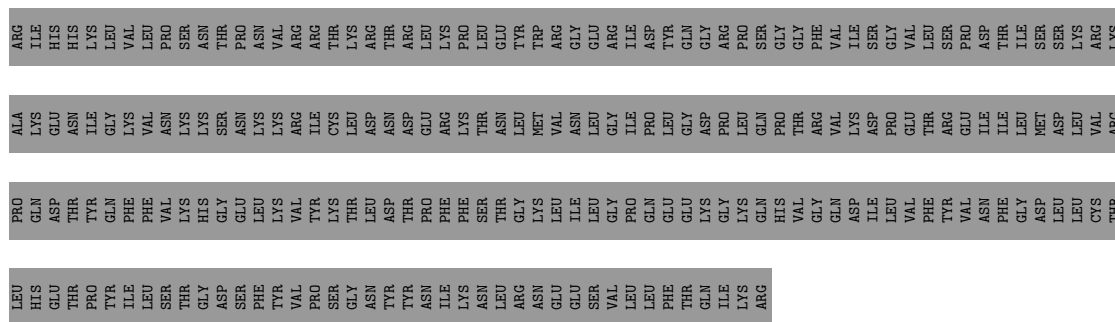


- Molecule 12: Centromere protein X

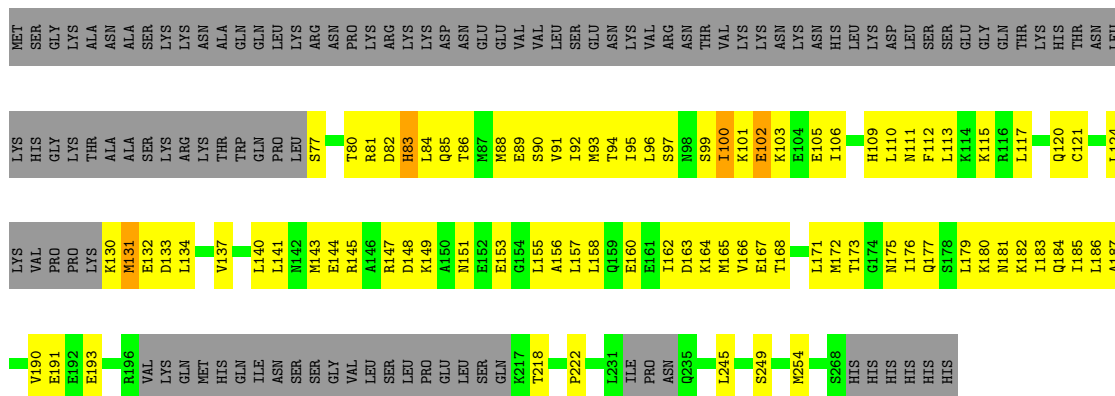
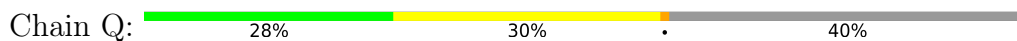
Chain X: 33% 57% 9%

- Molecule 15: Centromere protein C

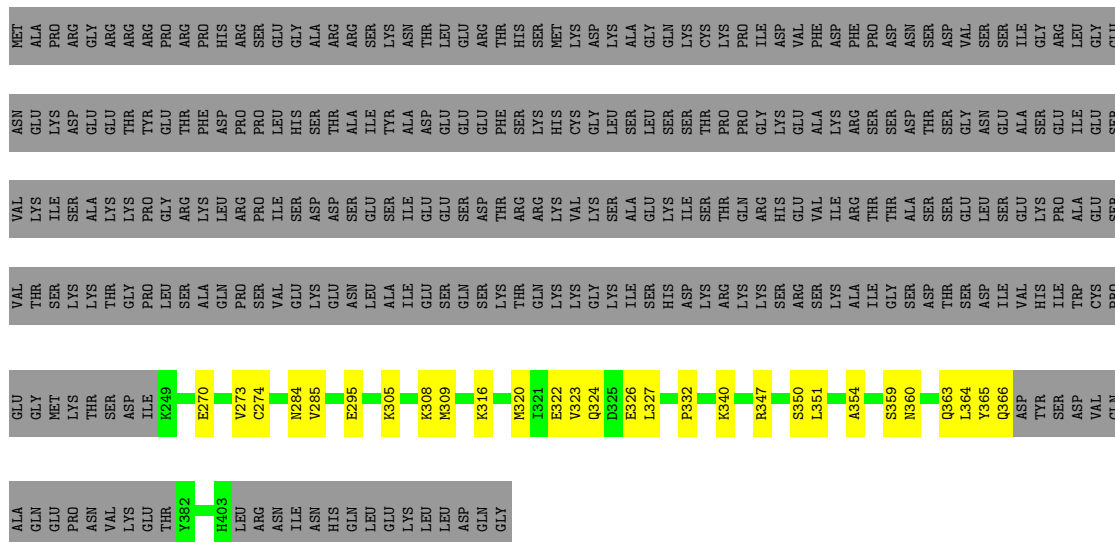
Chain c: ..[illegible]



- Molecule 16: Centromere protein Q

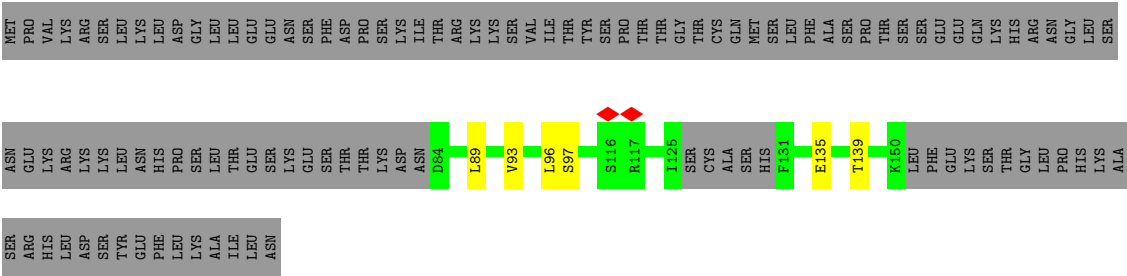


- Molecule 17: Centromere protein U



- Molecule 18: Centromere protein R





4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	380.64, 380.64, 380.64	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.84	7/1624 (0.4%)	1.21	9/2208 (0.4%)
1	o	0.23	0/95	0.50	0/127
2	H	0.36	0/1566	0.69	1/2093 (0.0%)
3	I	0.42	5/4210 (0.1%)	0.63	2/5704 (0.0%)
4	K	0.49	2/1897 (0.1%)	0.66	2/2558 (0.1%)
5	L	0.34	1/2487 (0.0%)	0.53	0/3379
6	M	0.59	2/1320 (0.2%)	0.68	2/1791 (0.1%)
7	N	0.24	0/2547	0.47	0/3440
8	P	0.46	2/1839 (0.1%)	0.66	4/2474 (0.2%)
9	S	0.32	0/799	0.70	2/1070 (0.2%)
10	T	0.46	2/821 (0.2%)	0.61	1/1105 (0.1%)
11	W	0.32	0/590	0.58	0/785
12	X	0.34	0/596	0.68	0/801
13	G	0.18	0/575	0.34	0/885
14	J	0.20	0/573	0.37	0/882
15	C	0.32	0/40	1.00	0/53
15	c	0.17	0/106	0.70	0/141
16	Q	0.39	1/1175 (0.1%)	0.70	1/1580 (0.1%)
17	U	0.26	0/697	0.68	3/972 (0.3%)
18	R	0.18	0/306	0.52	0/424
All	All	0.43	22/23863 (0.1%)	0.67	27/32472 (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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	208	PRO	CB-CG	18.97	2.44	1.49
4	K	259	PRO	CA-CB	14.73	1.62	1.53
1	O	208	PRO	CG-CD	-13.77	1.03	1.50
6	M	52	LEU	CG-CD2	-13.41	1.08	1.52
1	O	208	PRO	N-CA	-8.82	1.36	1.46
3	I	724	PHE	CE1-CZ	-8.55	1.12	1.38
1	O	207	GLY	C-N	8.46	1.44	1.33
1	O	208	PRO	N-CD	7.77	1.58	1.47
3	I	724	PHE	CG-CD2	-7.41	1.23	1.38
5	L	156	VAL	CB-CG1	-6.94	1.29	1.52
10	T	470	TYR	CG-CD2	-6.83	1.25	1.39
6	M	85	LEU	CG-CD2	-6.78	1.30	1.52
4	K	67	LEU	CG-CD2	-6.70	1.30	1.52
3	I	506	LEU	CG-CD2	-6.47	1.31	1.52
3	I	734	PHE	CG-CD2	-6.45	1.25	1.38
8	P	159	GLU	CD-OE2	-6.38	1.13	1.25
1	O	206	THR	C-N	6.35	1.43	1.33
3	I	734	PHE	CE2-CZ	-5.92	1.20	1.38
16	Q	131	MET	SD-CE	-5.63	1.65	1.79
1	O	207	GLY	N-CA	5.46	1.52	1.44
8	P	233	PHE	CE2-CZ	-5.29	1.22	1.38
10	T	470	TYR	CE1-CZ	-5.13	1.25	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	208	PRO	CB-CG-CD	-33.14	0.05	106.10
1	O	208	PRO	CA-N-CD	-21.41	82.02	112.00
6	M	53	PRO	CA-N-CD	-12.84	94.02	112.00
1	O	208	PRO	CA-CB-CG	-12.62	80.52	104.50
1	O	208	PRO	N-CD-CG	-12.45	84.53	103.20
1	O	207	GLY	O-C-N	-11.81	109.96	121.77
6	M	52	LEU	CD1-CG-CD2	-10.02	88.76	110.80
1	O	207	GLY	C-N-CD	9.80	165.16	125.00
8	P	168	ARG	N-CA-C	-9.28	102.53	114.04
3	I	607	MET	CG-SD-CE	-8.97	81.16	100.90
4	K	259	PRO	CA-N-CD	-8.40	100.25	112.00
2	H	220	ILE	N-CA-C	-7.12	105.57	111.91
1	O	207	GLY	CA-C-N	-7.07	112.65	120.14
1	O	207	GLY	C-N-CA	-7.07	112.65	120.14
1	O	208	PRO	N-CA-CB	-6.46	96.89	103.15
16	Q	222	PRO	N-CA-CB	6.45	110.02	103.25
8	P	166	PHE	N-CA-C	-6.44	103.77	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	T	470	TYR	CZ-CE2-CD2	6.26	130.88	119.60
17	U	332	PRO	N-CA-CB	6.23	110.18	103.33
17	U	270	GLU	CA-C-N	-6.17	112.48	122.36
17	U	270	GLU	C-N-CA	-6.17	112.48	122.36
9	S	38	LYS	CA-CB-CG	5.96	126.02	114.10
9	S	93	LEU	CA-CB-CG	5.60	135.91	116.30
4	K	259	PRO	N-CA-CB	-5.46	99.15	102.81
8	P	75	GLY	N-CA-C	-5.38	107.17	115.73
3	I	464	PHE	CA-CB-CG	5.12	118.92	113.80
8	P	159	GLU	OE1-CD-OE2	-5.04	110.81	122.90

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 ⓘ

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	139	0
1	o	95	0	96	10	0
2	H	1560	0	1633	168	0
3	I	4111	0	4032	324	0
4	K	1869	0	1857	161	0
5	L	2422	0	2398	128	0
6	M	1298	0	1349	126	0
7	N	2493	0	2511	146	0
8	P	1808	0	1810	146	0
9	S	790	0	798	79	0
10	T	804	0	814	87	0
11	W	584	0	631	58	0
12	X	590	0	620	77	0
13	G	513	0	279	19	0
14	J	512	0	280	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	40	0	36	3	0
15	c	105	0	106	9	0
16	Q	1175	0	1058	142	0
17	U	699	0	303	45	0
18	R	308	0	127	4	0
All	All	23364	0	22278	1620	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 36.

All (1620) 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:HE1	8:P:168:ARG:CD	1.22	1.55
8:P:165:MET:CE	8:P:168:ARG:HD2	1.10	1.54
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:HE1	8:P:168:ARG:NE	1.54	1.23
8:P:165:MET:CE	8:P:168:ARG:CD	1.93	1.19
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
8:P:165:MET:HE1	8:P:168:ARG:CZ	1.85	1.06
3:I:530:MET:HE3	3:I:530:MET:HA	1.38	1.05
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
1:O:179:SER:HB3	1:O:183:TYR:HE2	1.21	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
2:H:186:LEU:HA	2:H:189:MET:SD	2.03	0.99
8:P:165:MET:HE2	8:P:168:ARG:HD2	1.45	0.98
12:X:15:VAL:HB	12:X:38:MET:HE1	1.44	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:250:ASP:CG	17:U:364:LEU:HA	1.92	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:210:GLN:OE1	1:O:219:SER:OG	1.83	0.94
7:N:18:MET:HE3	7:N:18:MET:H	1.33	0.93
16:Q:83:HIS:CG	16:Q:131:MET:HE2	2.03	0.92
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
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
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
16:Q:83:HIS:HB3	16:Q:131:MET:HE2	1.56	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
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
3:I:607:MET:HE1	3:I:734:PHE:CE2	2.10	0.86
9:S:65:LEU:HD21	9:S:85:LEU:HD22	1.58	0.86
4:K:136:MET:HA	4:K:136:MET:HE2	1.56	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:140:LEU:O	16:Q:143:MET:HE3	1.79	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
8:P:90:SER:O	8:P:93:MET:HE2	1.81	0.80
6:M:52:LEU:HD23	6:M:84:SER:CB	2.11	0.80
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
16:Q:83:HIS:CB	16:Q:131:MET:HE2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:548:MET:HE1	3:I:553:ASN:HA	1.66	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
9:S:24:HIS:ND1	16:Q:93:MET:HE3	1.98	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
2:H:162:LEU:HD23	3:I:510:MET:HE3	1.69	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
5:L:126:GLY:C	5:L:127:MET:HE2	2.11	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
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
16:Q:130:LYS:HZ1	16:Q:132:GLU:HG2	1.51	0.74
4:K:245:LEU:HD12	10:T:551:ALA:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:213:ARG:NH2	17:U:366:GLN:C	2.47	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
16:Q:80:THR:HA	16:Q:131:MET:HE1	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:Q:83:HIS:ND1	16:Q:131:MET:HE2	2.07	0.69
5:L:59:VAL:HG12	5:L:127:MET:HE3	1.72	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:181:ASN:C	16:Q:184:GLN:HE21	2.00	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
2:H:112:LEU:O	2:H:116:LEU:N	2.26	0.67
3:I:510:MET:HB2	3:I:514:MET:HE2	1.77	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
8:P:89:THR:HA	8:P:93:MET:HE1	1.76	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
3:I:573:ILE:HG21	3:I:609:ARG:NH2	2.10	0.67
12:X:48:GLU:CD	12:X:52:ARG:HH12	2.03	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
12:X:60:GLU:CD	12:X:69:GLN:HE21	2.03	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
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
8:P:250:ASP:CG	17:U:364:LEU:CA	2.66	0.66
9:S:95:TYR:O	9:S:99:LYS:HG2	1.95	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:I:195:ASP:OD1	3:I:229:MET:HE3	1.97	0.65
9:S:24:HIS:CG	16:Q:93:MET:HE3	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:510:MET:CB	3:I:514:MET:HE2	2.28	0.63
3:I:530:MET:HA	3:I:530:MET:CE	2.22	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
3:I:530:MET:HE3	3:I:530:MET:CA	2.21	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: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
10:T:467:PHE:HB3	10:T:475:MET:HE1	1.80	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:165:MET:CE	8:P:168:ARG:NE	2.37	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
16:Q:88:MET:HE1	17:U:285:VAL:N	2.14	0.62
16:Q:99:SER:C	16:Q:101:LYS:H	2.06	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
7:N:74:MET:HE1	7:N:81:LYS:HD2	1.82	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
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
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
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
12:X:68:ASP:C	12:X:72:LYS:HE2	2.24	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
7:N:87:GLN:HB2	7:N:191:MET:HE2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:147:CYS:O	8:P:151:SER:N	2.34	0.61
8:P:176:TRP:CZ2	8:P:223:ARG:C	2.79	0.61
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
1:O:294:LEU:O	1:O:296:MET:HE1	2.01	0.60
3:I:93:LYS:HA	3:I:96:GLU:CD	2.26	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
2:H:46:LEU:O	2:H:47:ARG:C	2.43	0.60
2:H:130:MET:HE1	4:K:97:PHE:HB3	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
2:H:42:LEU:O	2:H:46:LEU:HG	2.02	0.60
3:I:644:LEU:HA	3:I:647:MET:HE3	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:MET:HE3	2:H:131:LYS:HE3	1.84	0.59
4:K:29:GLU:HG3	15:c:260:LYS:CB	2.31	0.59
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
1:O:112:GLY:O	1:O:126:ILE:HG13	2.02	0.59
3:I:64:ASP:C	3:I:68:MET:HE3	2.28	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
7:N:167:MET:HE2	14:J:-10:DG:H4'	1.84	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
9:S:40:MET:HE1	12:X:64:ARG:HA	1.83	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
2:H:202:LEU:HG	4:K:166:MET:HE2	1.85	0.59
3:I:685:HIS:O	3:I:689:LEU:N	2.33	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:195:ASP:CG	11:W:15:ARG:HD3	2.28	0.59
3:I:720:LEU:C	3:I:724:PHE:CD2	2.81	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
7:N:44:ARG:HE	7:N:45:LYS:HZ3	1.50	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
3:I:548:MET:HE3	3:I:548:MET:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:64:ASP:O	3:I:68:MET:HE3	2.03	0.58
1:O:110:PHE:O	1:O:111:THR:OG1	2.21	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
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
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
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
3:I:568:VAL:HA	3:I:571:ILE:HD11	1.86	0.57
9:S:40:MET:HE3	9:S:41:GLN:H	1.69	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
2:H:186:LEU:HD22	2:H:189:MET:HE1	1.86	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
16:Q:85:GLN:HA	16:Q:88:MET:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:607:MET:HE1	3:I:734:PHE:HE2	1.70	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
1:O:16:GLY:HA2	4:K:117:LYS:HG3	1.86	0.56
7:N:244:GLU:OE2	7:N:247:ARG:NH1	2.36	0.56
1:O:17:VAL:HG21	3:I:560:PHE:HZ	1.70	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
12:X:53:GLY:O	12:X:56:GLN:NE2	2.33	0.56
1:O:17:VAL:HG23	4:K:110:THR:HG23	1.87	0.56
2:H:156:ASP:HA	2:H:159:LYS:HE3	1.87	0.56
3:I:133:MET:HE3	3:I:133:MET:H	1.69	0.56
7:N:167:MET:HE2	14:J:-10:DG:C4'	2.36	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
10:T:552:TYR:O	10:T:553:SER:OG	2.24	0.56
16:Q:102:GLU:CD	16:Q:105:GLU:HB3	2.31	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
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:13:LEU:HG	15:c:263:SER:HB2	1.86	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
7:N:190:LYS:HZ1	7:N:194:ARG:HD2	1.69	0.56
1:O:258:GLU:CD	1:O:258:GLU:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:K:63:GLN:CD	6:M:166:LEU:HD11	2.30	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:98:ASP:HA	9:S:101:GLU:HG3	1.88	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
4:K:206:SER:OG	4:K:207:VAL:N	2.39	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
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: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
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
1:O:20:HIS:O	1:O:24:LEU:HD12	2.07	0.55
6:M:142:MET:HE1	6:M:145:ARG:NH1	2.22	0.55
7:N:45:LYS:HZ2	14:J:-20:DT:H5''	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:L:127:MET:HE2	5:L:127:MET:N	2.20	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
9:S:24:HIS:HB2	16:Q:93:MET:CE	2.36	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
3:I:490:LYS:HZ1	3:I:550:LEU:HD12	1.72	0.54
5:L:54:GLN:N	5:L:54:GLN:OE1	2.39	0.54
7:N:160:TYR:CE1	7:N:191:MET:HE1	2.42	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
2:H:211:VAL:O	2:H:215:VAL:HG23	2.07	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
6:M:13:LEU:CG	15:c:263:SER:HB2	2.37	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
6:M:94:LEU:C	6:M:166:LEU:HD22	2.32	0.54
16:Q:149:LYS:HD3	16:Q:149:LYS:C	2.32	0.54
3:I:164:PHE:O	3:I:168:LEU:HD22	2.07	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
1:O:18:LEU:HB3	3:I:453:SER:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
12:X:48:GLU:CD	12:X:52:ARG:NH1	2.65	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
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
5:L:126:GLY:O	5:L:127:MET:HE2	2.08	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
8:P:213:ARG:CZ	17:U:366:GLN:C	2.82	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
3:I:548:MET:HE3	3:I:548:MET:CA	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:63:GLN:OE1	6:M:94:LEU:HD22	2.08	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
2:H:202:LEU:CD2	4:K:166:MET:HE2	2.39	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:179:LEU:HG	16:Q:180:LYS:HZ3	1.74	0.53
7:N:140:GLN:HB3	16:Q:151:ASN:CG	2.34	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
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
5:L:43:THR:O	5:L:44:PRO:C	2.52	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
12:X:35:LEU:CD2	12:X:38:MET:HE3	2.39	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
3:I:133:MET:HE2	3:I:137:THR:HG23	1.91	0.52
5:L:223:ALA:HB3	5:L:280:VAL:HG22	1.91	0.52
5:L:284:MET:HE3	5:L:284:MET:HA	1.91	0.52
10:T:520:ARG:HG2	10:T:520:ARG:NH1	2.23	0.52
16:Q:190:VAL:HG11	17:U:347:ARG:HA	1.91	0.52
2:H:112:LEU:C	2:H:116:LEU:HG	2.35	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
5:L:78:THR:HG1	5:L:207:TYR:H	1.56	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
12:X:33:ASP:C	12:X:36:GLN:NE2	2.67	0.52
12:X:60:GLU:CD	12:X:69:GLN:NE2	2.67	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:74:MET:HE2	7:N:151:TYR:CE1	2.44	0.52
7:N:208:GLN:HE22	1:O:154:SER:HA	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:K:32:TRP:CE3	4:K:35:MET:HE3	2.45	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
3:I:734:PHE:CD1	3:I:734:PHE:C	2.88	0.52
4:K:39:GLN:HE22	6:M:8:ASP:HA	1.75	0.52
5:L:28:GLN:CD	5:L:28:GLN:H	2.18	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: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
3:I:580:VAL:O	3:I:580:VAL:HG13	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
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:88:LEU:O	5:L:92:SER:OG	2.27	0.51
5:L:236:THR:HA	5:L:258:PRO:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:O:126:ILE:O	1:O:138:TYR:N	2.29	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
1:O:17:VAL:HG21	3:I:560:PHE:CZ	2.46	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:20:HIS:CE1	1:O:24:LEU:HD11	2.46	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
9:S:40:MET:HE2	12:X:65:VAL:HG23	1.92	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
5:L:205:ASP:OD1	5:L:207:TYR:OH	2.21	0.50
7:N:28:TRP:CD2	7:N:69:LEU:HG	2.46	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:T:470:TYR:HD2	11:W:52:HIS:HA	1.71	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
8:P:156:ARG:HA	8:P:159:GLU:CD	2.30	0.50
8:P:179:TYR:O	8:P:183:THR:OG1	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:70:ASP:OD2	7:N:151:TYR:OH	2.29	0.49
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
3:I:172:PHE:CD1	3:I:172:PHE:C	2.89	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
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
15:c:261:SER:O	15:c:263:SER:OG	2.25	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:43:LEU:HD11	15:c:265:LEU:HD21	1.95	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:644:LEU:HD23	3:I:647:MET:HE1	1.94	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: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:227:ASP:CG	8:P:233:PHE:CZ	2.91	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
6:M:53:PRO:HD2	6:M:87:HIS:HD1	1.77	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
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
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:168:TYR:O	1:O:171:THR:OG1	2.28	0.48
1:O:189:GLY:HA3	8:P:168:ARG:HH22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:O:229:GLN:CD	1:O:229:GLN:H	2.22	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
4:K:62:MET:HE1	6:M:90:ALA:HB1	1.96	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
2:H:168:SER:HG	3:I:378:CYS:HG	1.53	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: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
8:P:165:MET:HE2	8:P:168:ARG:CD	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
16:Q:143:MET:C	16:Q:143:MET:SD	2.97	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
16:Q:164:LYS:HD3	16:Q:164:LYS:C	2.39	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
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
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
4:K:127:ARG:HH21	4:K:128:TRP:HE1	1.63	0.47
5:L:127:MET:HB2	5:L:136:ALA:HB3	1.97	0.47
8:P:227:ASP:CG	8:P:233:PHE:HZ	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:Q:182:LYS:C	16:Q:182:LYS:HD2	2.40	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
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:232:VAL:C	4:K:234:ILE:H	2.21	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
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
6:M:136:GLU:C	6:M:136:GLU:OE2	2.58	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
16:Q:164:LYS:NZ	16:Q:165:MET:HE2	2.29	0.46
1:O:17:VAL:CG2	3:I:560:PHE:HZ	2.28	0.46
2:H:86:GLU:C	2:H:86:GLU:OE1	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:O:145:GLN:CD	1:O:147:PRO:HD2	2.40	0.46
8:P:147:CYS:HA	8:P:150:LEU:HB2	1.96	0.46
8:P:148:SER:O	8:P:151:SER:OG	2.28	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:44:ARG:NE	7:N:45:LYS:HZ3	2.11	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
3:I:558:LEU:HD23	3:I:558:LEU:C	2.41	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
8:P:108:SER:HB2	8:P:117:GLN:HG2	1.97	0.46
14:J:-9:DA:H2"	14:J:-8:DT:C5	2.51	0.46
15:c:263:SER:OG	15:c:264:THR:N	2.48	0.46
2:H:202:LEU:CG	4:K:166:MET:HE2	2.45	0.46
4:K:181:GLY:O	4:K:185:GLU:HG2	2.16	0.46
6:M:52:LEU:HD23	6:M:84:SER:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:O:17:VAL:O	1:O:17:VAL:HG22	2.16	0.45
2:H:225:VAL:HG23	2:H:227:TRP:N	2.31	0.45
3:I:127:THR:C	3:I:131:LYS:HG3	2.42	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:537:ILE:CD1	3:I:568:VAL:HG13	2.41	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
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
3:I:734:PHE:C	3:I:734:PHE:HD1	2.23	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:S:24:HIS:HB2	16:Q:93:MET:HE3	1.98	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
16:Q:99:SER:C	16:Q:101:LYS:N	2.72	0.45
1:o:20:HIS:O	1:o:23:ARG:HG2	2.17	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
4:K:258:ASP:OD1	4:K:258:ASP:C	2.59	0.45
5:L:214:ASN:OD1	5:L:214:ASN:N	2.50	0.45
8:P:152:GLU:CD	8:P:152:GLU:O	2.60	0.45
10:T:484:GLU:C	10:T:484:GLU:OE2	2.60	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
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
4:K:62:MET:HE1	6:M:90:ALA:CB	2.48	0.45
5:L:158:TRP:NE1	5:L:193:THR:OG1	2.44	0.45
5:L:161:TRP:HH2	5:L:328:LEU:HD12	1.82	0.45
1:O:131:GLU:C	1:O:133:ASN:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:262:PHE:HA	15:c:266:PHE:HD2	1.82	0.45
16:Q:158:LEU:HD23	16:Q:158:LEU:HA	1.68	0.45
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:430:GLU:HB3	3:I:507:TRP:CZ2	2.52	0.44
3:I:463:PRO:O	3:I:464:PHE:C	2.61	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
1:O:179:SER:C	1:O:183:TYR:CD2	2.95	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
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:137:ASN:C	2:H:141:MET:HE2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:447:ASP:C	3:I:447:ASP:OD1	2.60	0.44
3:I:607:MET:HB2	3:I:607:MET:HE2	1.69	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:127:MET:HE2	5:L:127:MET:CA	2.47	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
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: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
7:N:97:ASP:OD1	7:N:97:ASP:C	2.60	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:133:MET:HE1	3:I:171:MET:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:T:533:VAL:HA	10:T:536:GLU:OE2	2.17	0.44
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
4:K:215:MET:HE2	4:K:233:LYS:O	2.18	0.43
4:K:219:LEU:C	4:K:230:PRO:HG3	2.43	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
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
3:I:596:ASP:OD2	3:I:598:SER:OG	2.34	0.43
3:I:720:LEU:C	3:I:724:PHE:CE2	2.96	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
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
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:149:SER:HA	3:I:161:LYS:HZ3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:N:82:VAL:HG23	7:N:195:SER:C	2.44	0.43
1:O:172:ASN:C	1:O:172:ASN:OD1	2.61	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
2:H:138:LYS:HZ3	2:H:142:LYS:NZ	2.17	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
7:N:191:MET:HE2	7:N:191:MET:HB2	1.91	0.43
7:N:192:ASP:OD1	7:N:192:ASP:C	2.62	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
15:c:266:PHE:O	15:c:270:VAL:HG22	2.19	0.43
2:H:133:LEU:C	2:H:133:LEU:HD23	2.44	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
15:c:262:PHE:O	15:c:266:PHE:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:N:99:PHE:C	1:O:212:ASN:HD21	2.27	0.43
1:O:248:THR:OG1	1:O:249:ASP:N	2.50	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
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:230:MET:HE1	5:L:311:VAL:HG22	2.00	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
3:I:607:MET:SD	3:I:607:MET:C	3.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:460:SER:OG	3:I:499:GLU:HB3	2.18	0.42
4:K:108:LEU:HD12	4:K:108:LEU:C	2.44	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
6:M:75:LYS:C	6:M:79:GLN:HE21	2.26	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
8:P:208:ILE:HD12	8:P:218:LEU:HB3	2.00	0.42
16:Q:131:MET:HG2	16:Q:132:GLU:N	2.33	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:128:ARG:HB2	3:I:131:LYS:HZ1	1.84	0.42
3:I:145:VAL:C	3:I:148:VAL:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:113:LYS:HD3	2:H:116:LEU:CD1	2.35	0.42
3:I:85:ASP:OD1	3:I:85:ASP:N	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
12:X:56:GLN:HE22	12:X:69:GLN:CD	2.27	0.42
2:H:130:MET:CE	4:K:97:PHE:HB3	2.47	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
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:84:ASP:HA	2:H:87:ASN:CG	2.45	0.42
2:H:127:MET:HE2	2:H:127:MET:HB3	1.95	0.42
2:H:162:LEU:HB2	3:I:429:GLN:OE1	2.19	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
5:L:297:ILE:O	5:L:297:ILE:HG13	2.18	0.41
10:T:542:GLU:HG2	10:T:543:TYR:HD1	1.85	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
11:W:54:LEU:O	11:W:58:SER:HB3	2.20	0.41
16:Q:82:ASP:C	16:Q:85:GLN:HE21	2.28	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
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
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
7:N:50:GLN:O	7:N:50:GLN:CD	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:K:208:ASN:OD1	4:K:208:ASN:C	2.62	0.41
6:M:53:PRO:CD	6:M:87:HIS:ND1	2.83	0.41
6:M:54:LEU:O	6:M:55:PRO:C	2.63	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
3:I:222:LEU:HA	3:I:222:LEU:HD23	1.82	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
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:59:ASN:OD1	6:M:59:ASN:C	2.64	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:243:VAL:HG12	5:L:302:THR:CG2	2.50	0.41
6:M:60:ARG:HE	7:N:240:GLU:CD	2.28	0.41
7:N:118:ASN:C	7:N:144:PRO:HG3	2.46	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
11:W:72:LYS:HE3	11:W:76:LEU:HD23	2.02	0.41
16:Q:164:LYS:HZ2	16:Q:165:MET:HE2	1.86	0.41
2:H:186:LEU:HD22	2:H:189:MET:CE	2.51	0.41
5:L:28:GLN:HA	5:L:31:LEU:HD23	2.03	0.41
1:O:109:HIS:O	1:O:109:HIS:ND1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:80:ASN:OD1	8:P:80:ASN:C	2.64	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:245:LEU:C	4:K:245:LEU:HD23	2.46	0.40
4:K:248:ARG:NH1	10:T:544:ARG:HD2	2.36	0.40
5:L:58:ASP:OD1	5:L:58:ASP:C	2.64	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
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
5:L:127:MET:HE2	5:L:127:MET:HA	2.03	0.40
5:L:230:MET:CE	5:L:311:VAL:HG22	2.50	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:SD	3:I:647:MET:C	3.04	0.40
3:I:647:MET:CG	3:I:651:LEU:HD23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:K:136:MET:HA	4:K:136:MET:CE	2.40	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
11:W:36:GLU:CD	11:W:37:LYS:H	2.30	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
3:I:495:GLN:NE2	3:I:499:GLU:OE1	2.54	0.40
4:K:22:GLU:H	4:K:22:GLU:CD	2.29	0.40
4:K:67:LEU:O	4:K:71:LEU:HG	2.22	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: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
16:Q:245:LEU:O	16:Q:249:SER:N	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	204/300 (68%)	176 (86%)	25 (12%)	3 (2%)	8	36
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%)	21	52
4	K	224/269 (83%)	202 (90%)	19 (8%)	3 (1%)	9	38
5	L	296/344 (86%)	261 (88%)	32 (11%)	3 (1%)	12	43
6	M	166/180 (92%)	146 (88%)	20 (12%)	0	100	100
7	N	299/345 (87%)	262 (88%)	36 (12%)	1 (0%)	36	65
8	P	220/288 (76%)	195 (89%)	22 (10%)	3 (1%)	9	37
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%)	0	8
16	Q	156/274 (57%)	151 (97%)	4 (3%)	1 (1%)	21	52
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%)	20	49

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	167 (98%)	3 (2%)	51	67
1	o	10/263 (4%)	10 (100%)	0	100	100
2	H	174/230 (76%)	172 (99%)	2 (1%)	65	73
3	I	440/691 (64%)	435 (99%)	5 (1%)	65	73
4	K	211/260 (81%)	209 (99%)	2 (1%)	70	75
5	L	268/306 (88%)	265 (99%)	3 (1%)	65	73
6	M	147/158 (93%)	145 (99%)	2 (1%)	59	70
7	N	273/317 (86%)	271 (99%)	2 (1%)	76	77
8	P	204/259 (79%)	200 (98%)	4 (2%)	48	64
9	S	86/121 (71%)	86 (100%)	0	100	100
10	T	88/461 (19%)	85 (97%)	3 (3%)	32	55
11	W	61/77 (79%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	X	65/67 (97%)	64 (98%)	1 (2%)	57	68
15	C	4/875 (0%)	4 (100%)	0	100	100
15	c	12/875 (1%)	12 (100%)	0	100	100
16	Q	109/254 (43%)	107 (98%)	2 (2%)	51	67
All	All	2322/5477 (42%)	2293 (99%)	29 (1%)	61	72

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	96	PHE
2	H	210	THR
3	I	150	TRP
3	I	462	ILE
3	I	494	LEU
3	I	514	MET
3	I	582	LEU
4	K	26	ARG
4	K	239	TRP
5	L	80	LEU
5	L	88	LEU
5	L	159	THR
6	M	52	LEU
6	M	93	PHE
7	N	69	LEU
7	N	331	MET
1	O	185	ASN
1	O	201	PHE
1	O	204	LEU
8	P	122	ILE
8	P	142	MET
8	P	143	GLU
8	P	193	ASP
10	T	470	TYR
10	T	533	VAL
10	T	536	GLU
12	X	38	MET
16	Q	83	HIS
16	Q	102	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	52	GLN
2	H	87	ASN
2	H	166	GLN
2	H	182	GLN
3	I	123	ASN
3	I	182	ASN
3	I	213	ASN
3	I	397	GLN
3	I	477	HIS
3	I	553	ASN
3	I	641	ASN
3	I	642	HIS
3	I	729	GLN
4	K	63	GLN
4	K	73	GLN
4	K	132	GLN
4	K	143	HIS
5	L	187	ASN
5	L	290	HIS
6	M	29	GLN
6	M	73	HIS
6	M	113	HIS
6	M	115	HIS
6	M	156	HIS
7	N	54	HIS
7	N	75	GLN
7	N	106	ASN
7	N	157	GLN
7	N	185	HIS
7	N	208	GLN
1	O	152	HIS
1	O	185	ASN
1	O	193	GLN
1	O	281	HIS
8	P	77	ASN
8	P	84	GLN
8	P	121	GLN
10	T	538	HIS
12	X	56	GLN
16	Q	85	GLN
16	Q	184	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

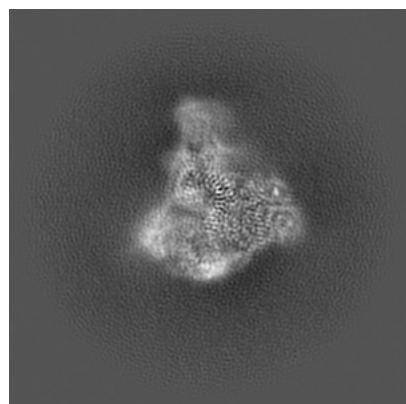
6 Map visualisation [i](#)

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.

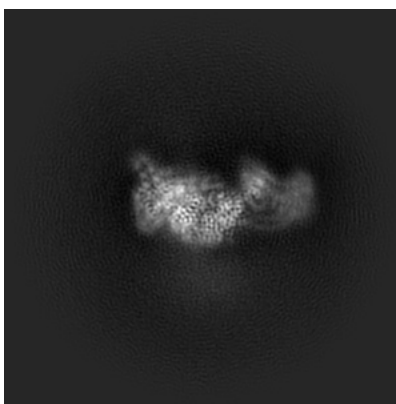
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

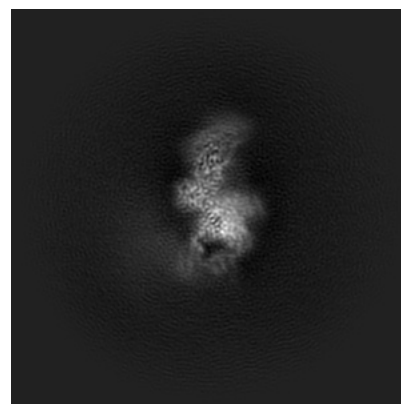
6.1.1 Primary map



X

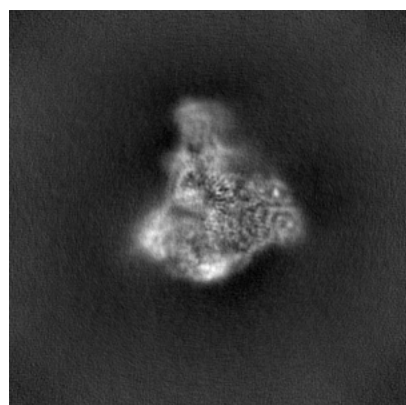


Y

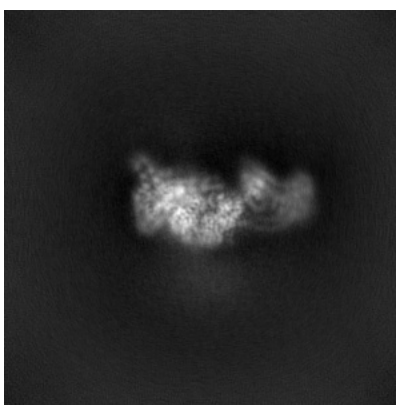


Z

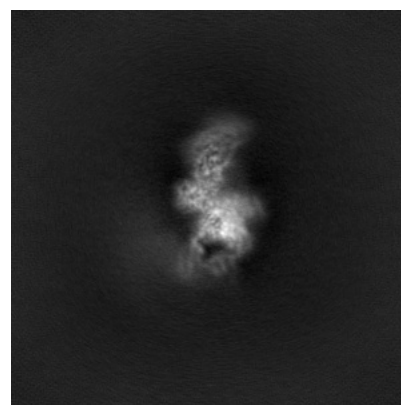
6.1.2 Raw map



X



Y

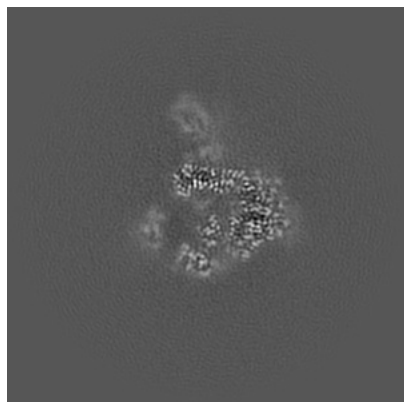


Z

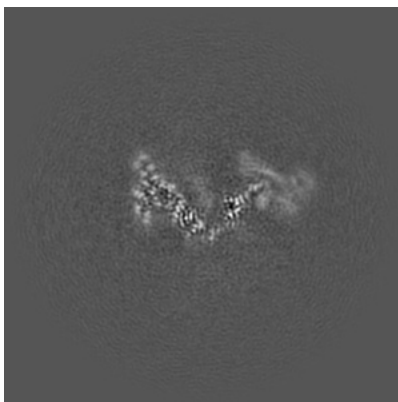
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

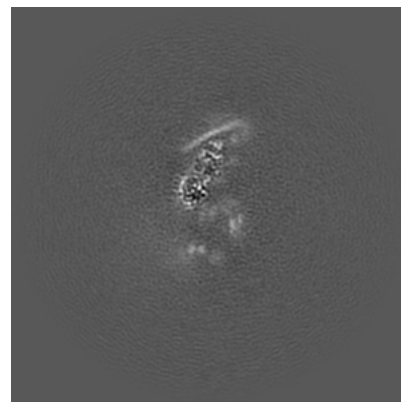
6.2.1 Primary map



X Index: 156

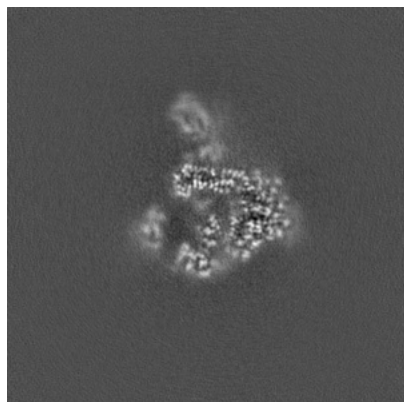


Y Index: 156

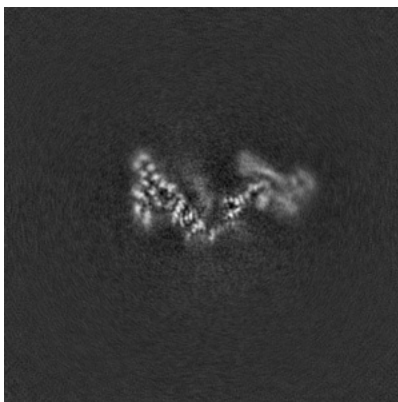


Z Index: 156

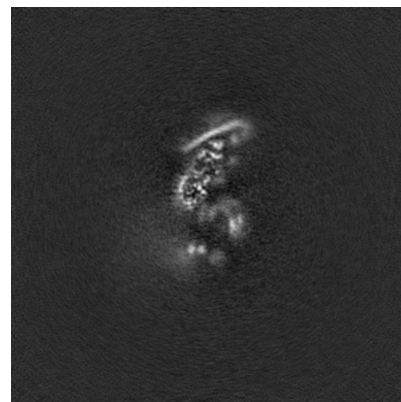
6.2.2 Raw map



X Index: 156



Y Index: 156

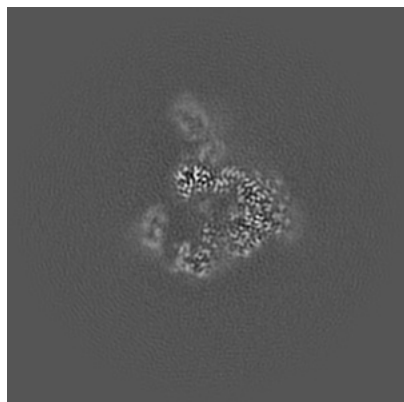


Z Index: 156

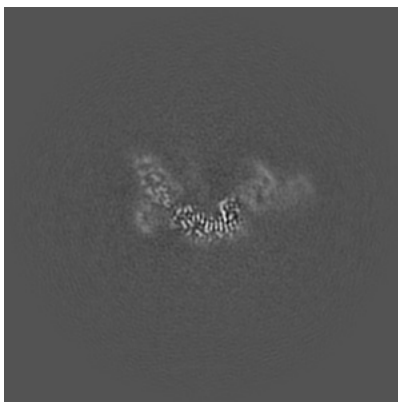
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

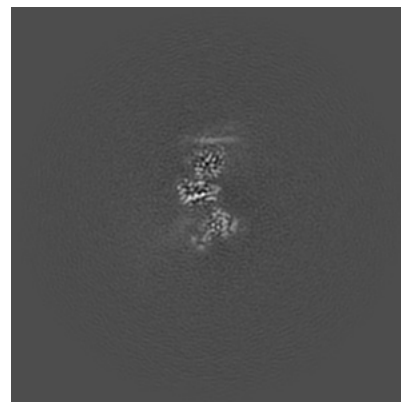
6.3.1 Primary map



X Index: 158

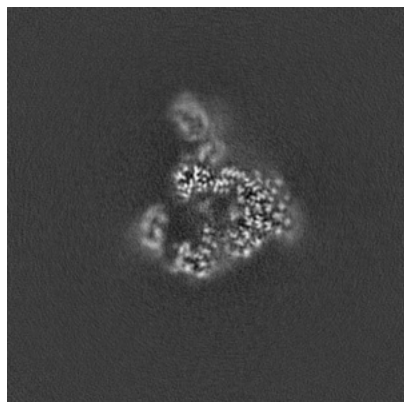


Y Index: 162

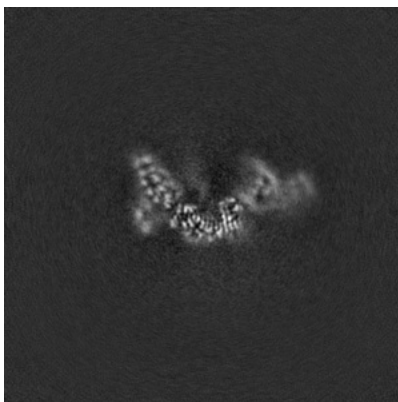


Z Index: 169

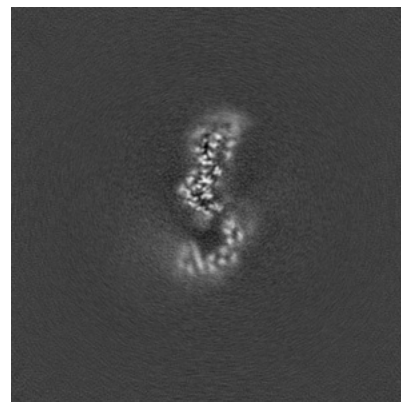
6.3.2 Raw map



X Index: 158



Y Index: 161

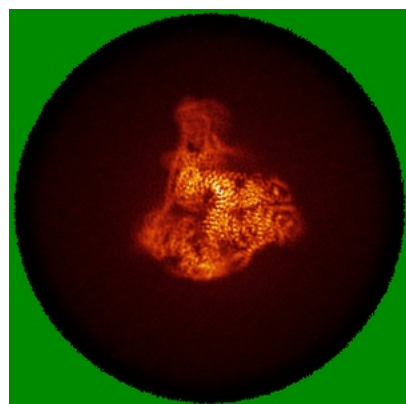


Z Index: 139

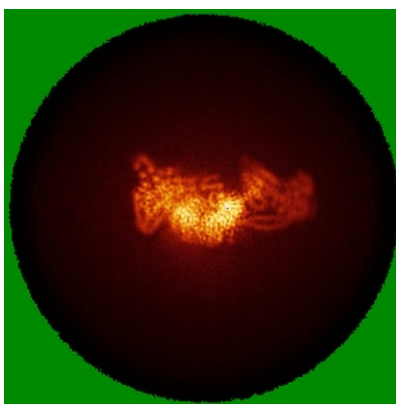
The images above show the largest variance slices of the map in three orthogonal directions.

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

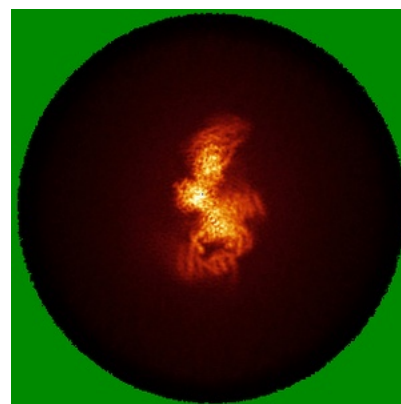
6.4.1 Primary map



X

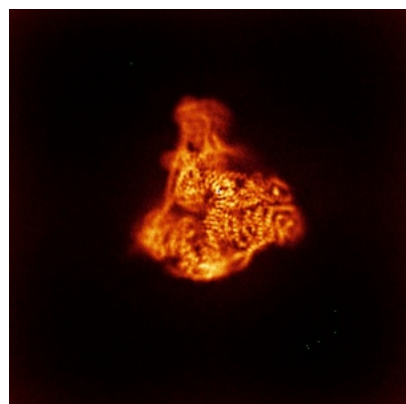


Y

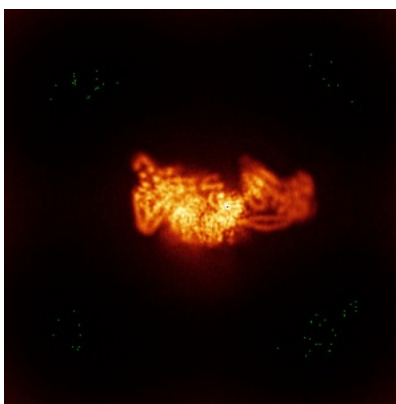


Z

6.4.2 Raw map



X



Y

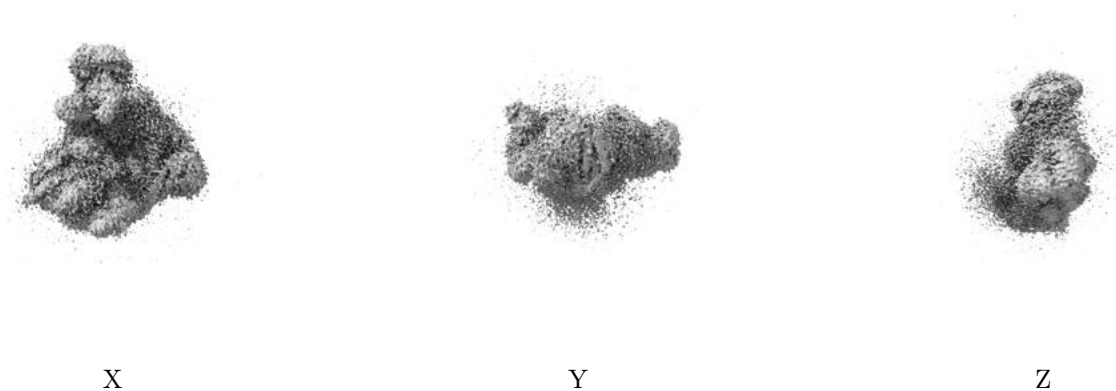


Z

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

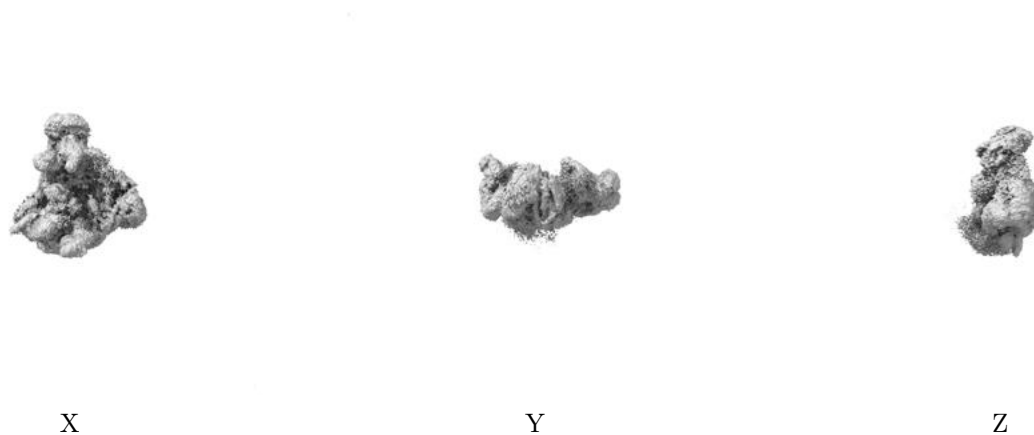
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

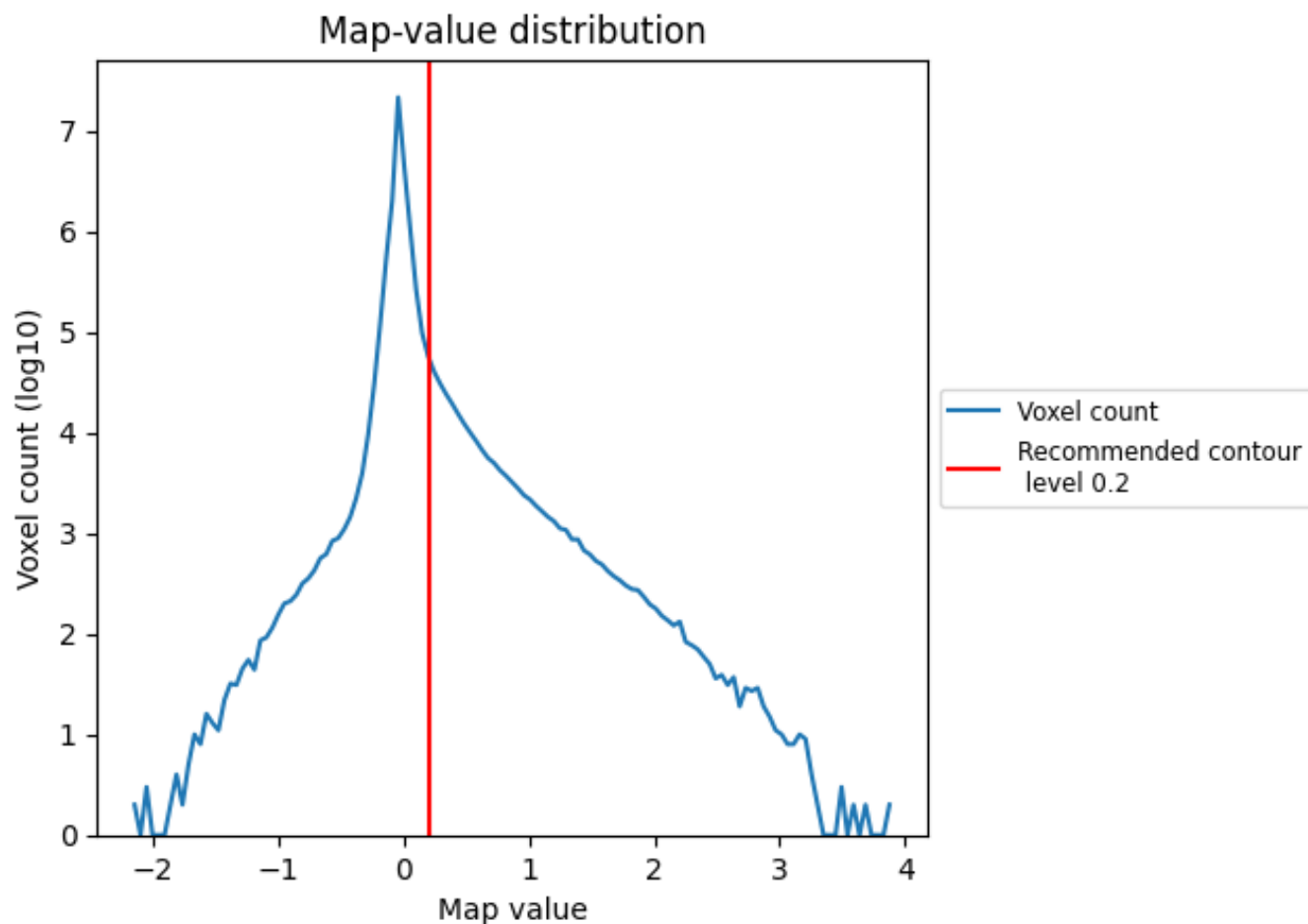
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

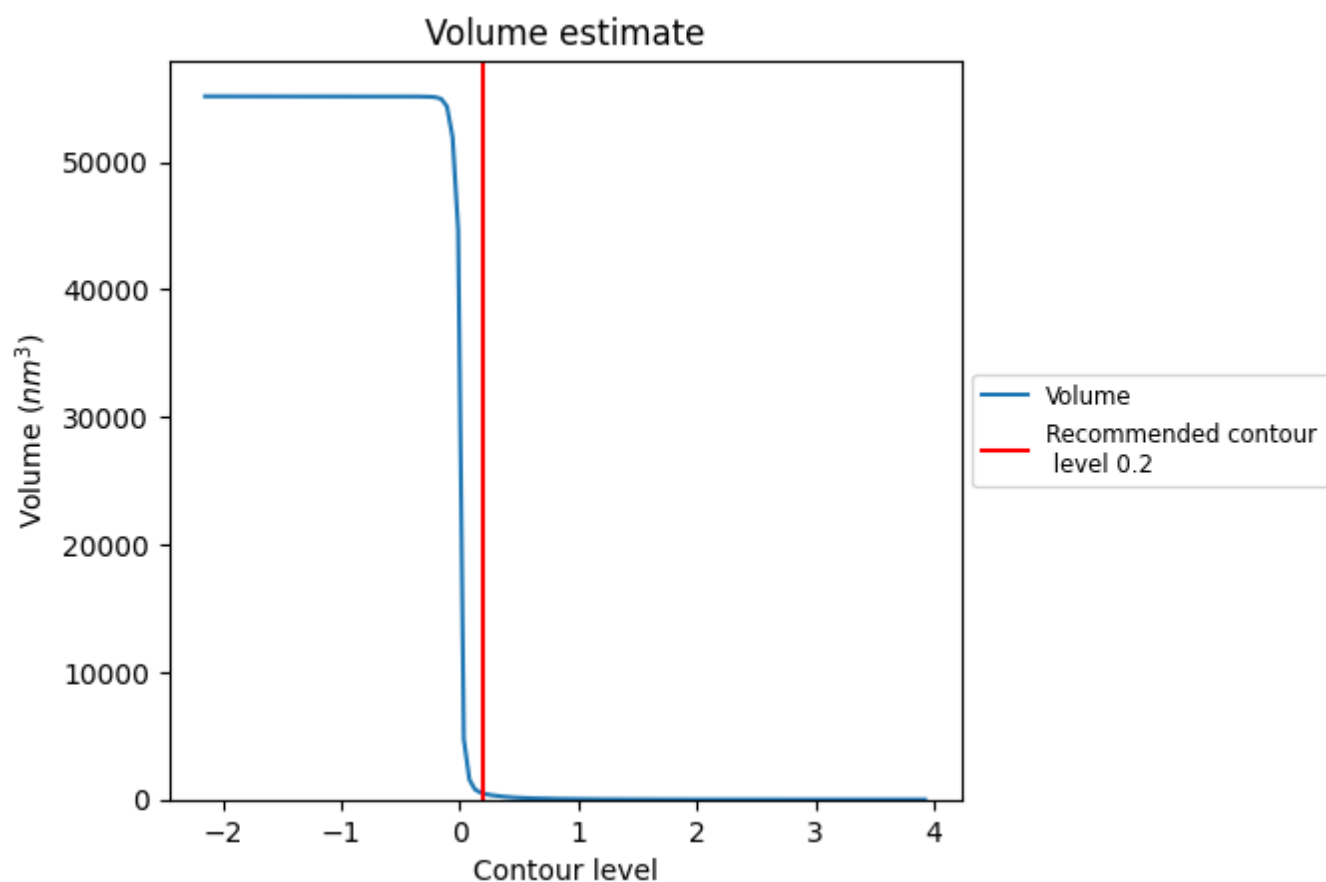
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

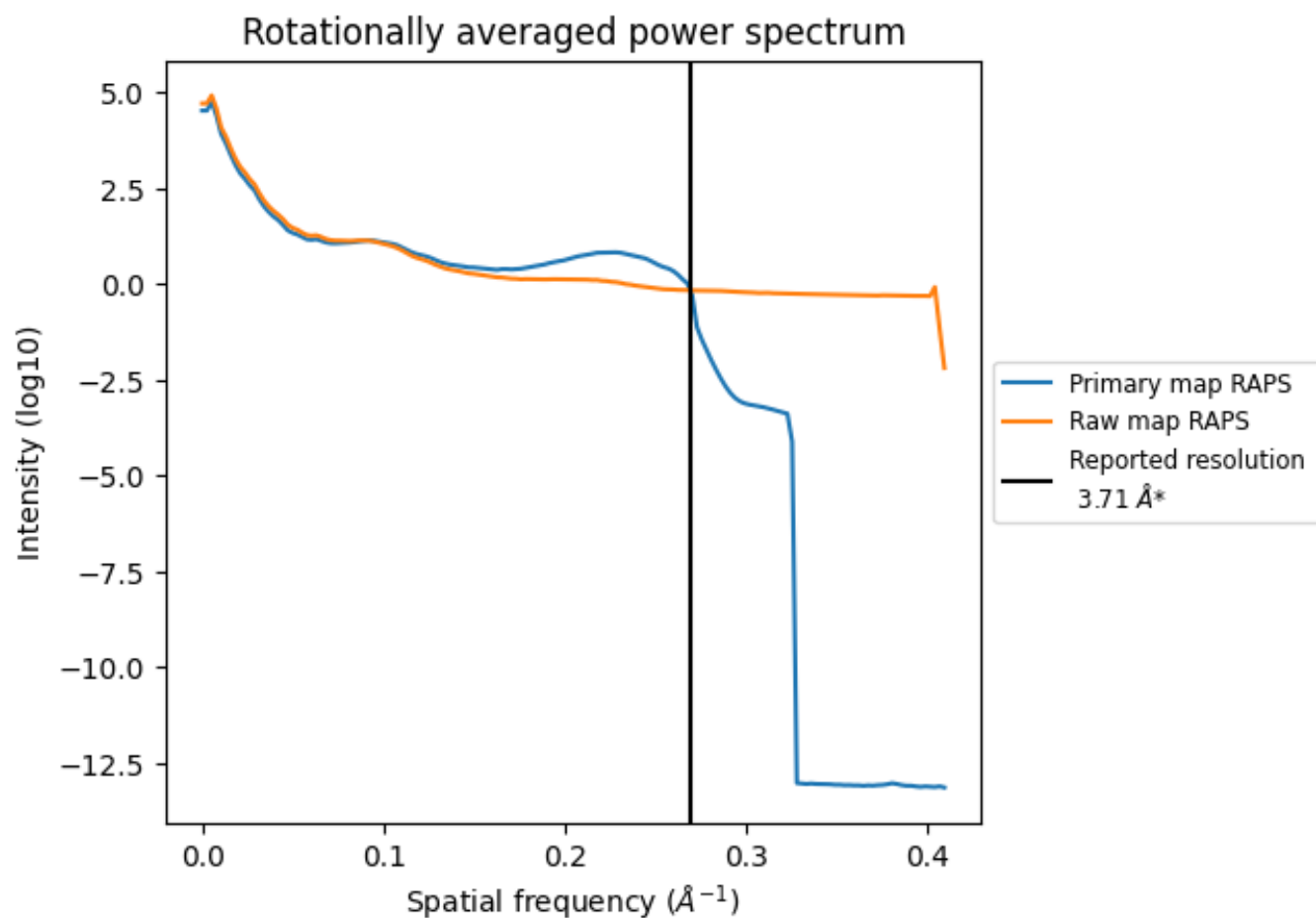
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 482 nm³; 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 ⓘ

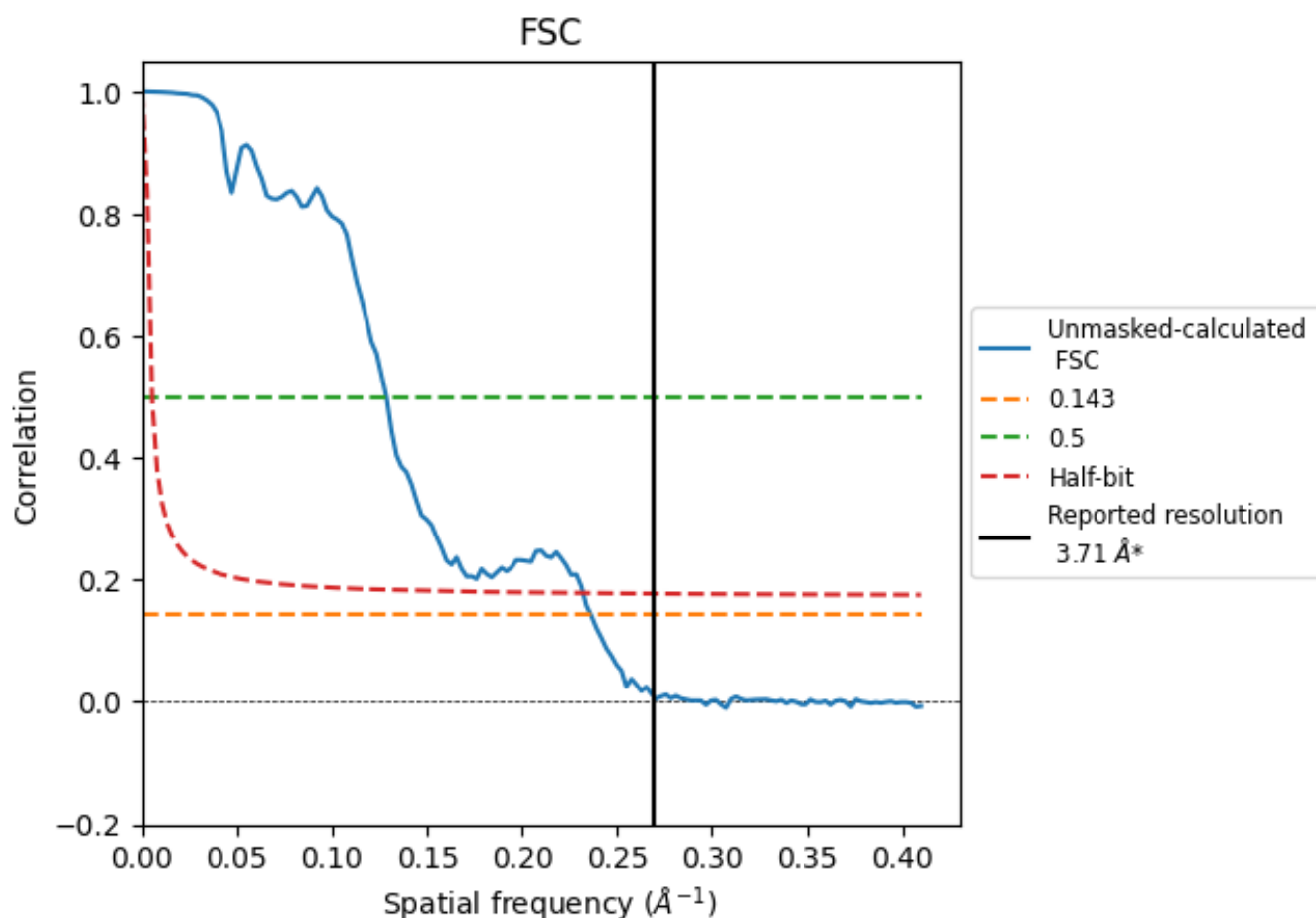


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

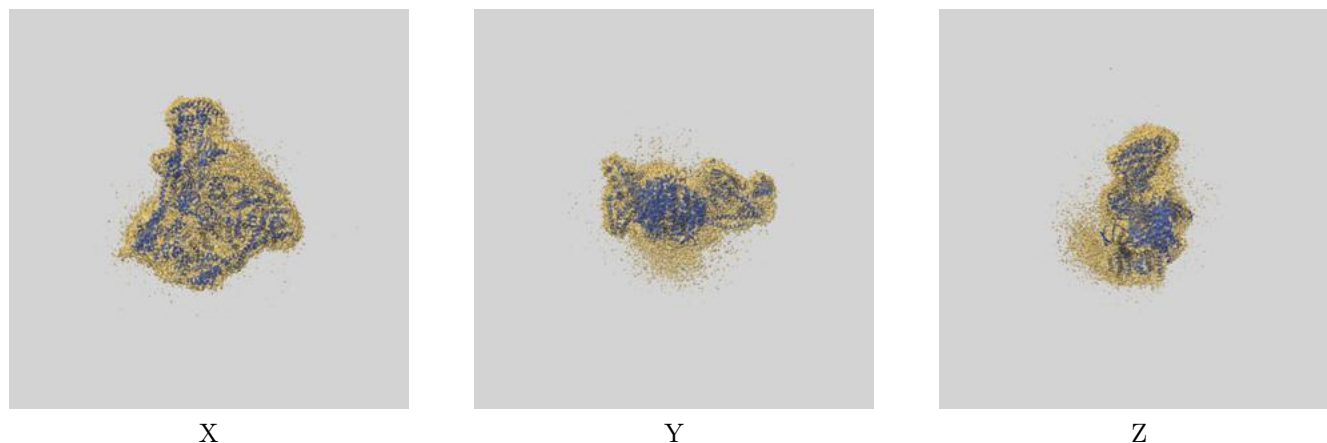
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.71	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	7.77	4.31

*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 [i](#)

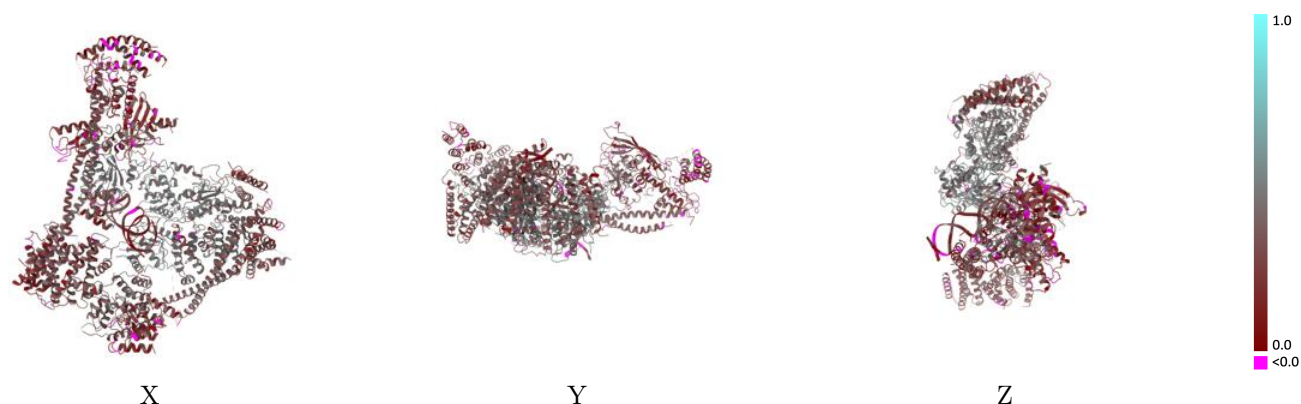
This section contains information regarding the fit between EMDB map EMD-33196 and PDB model 7XHN. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



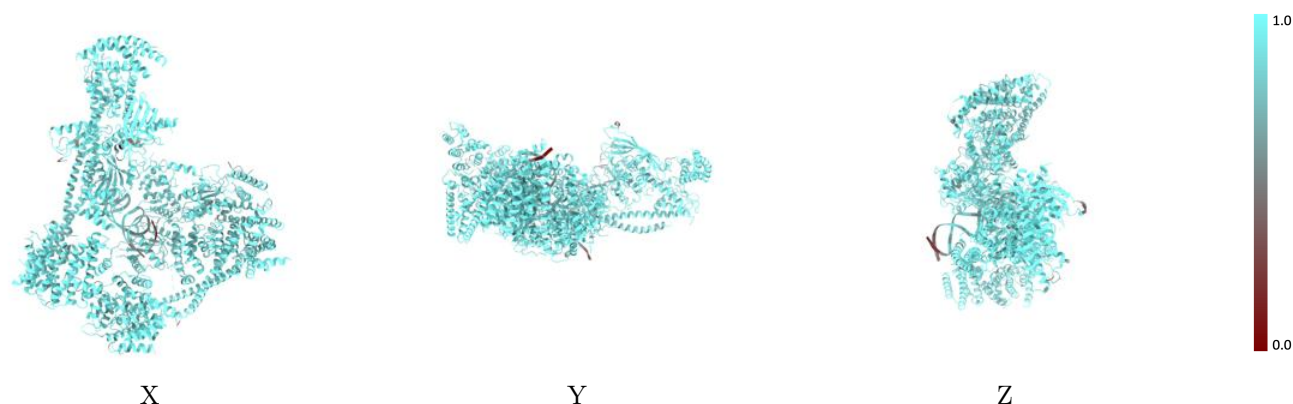
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



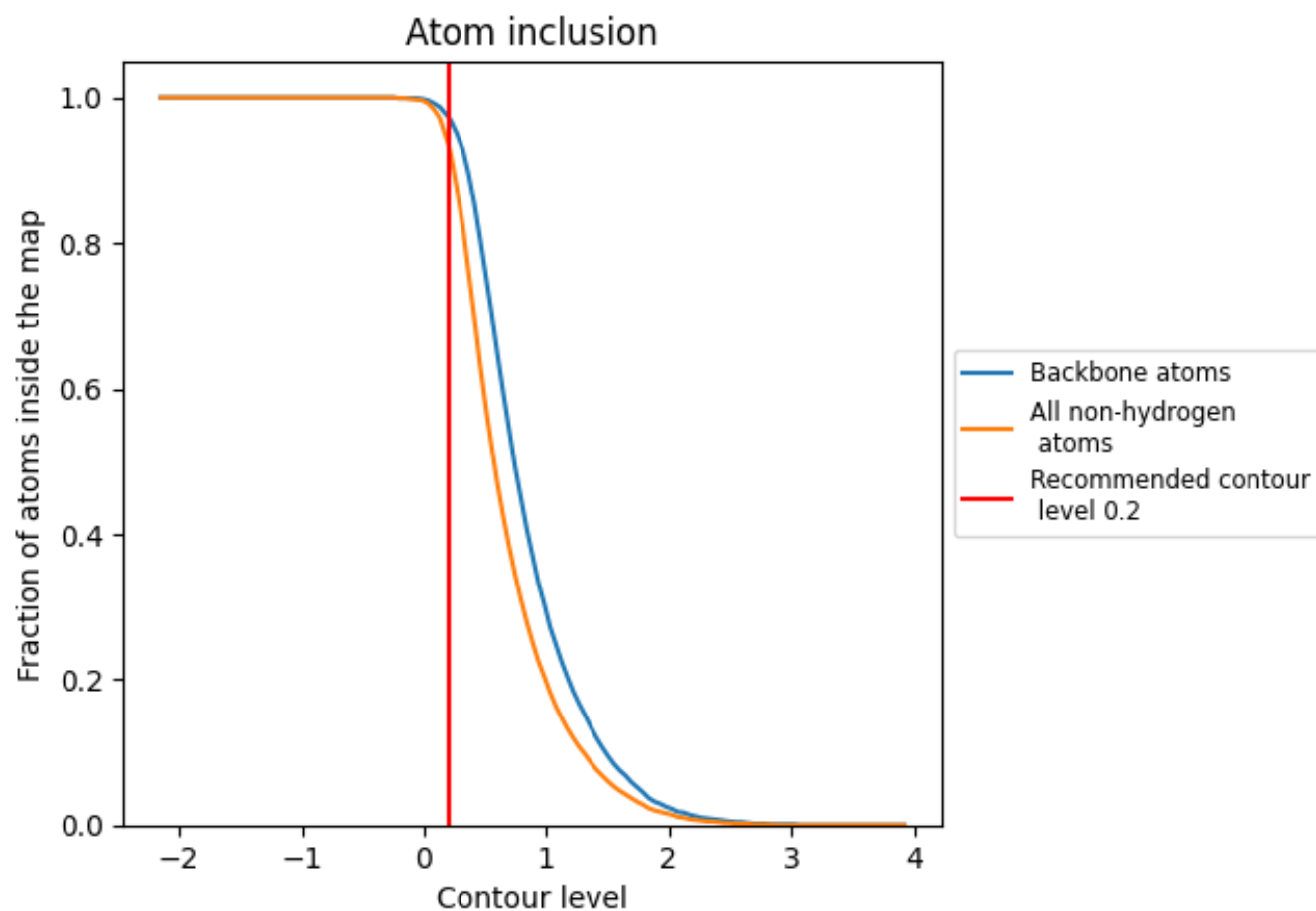
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

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	 0.9350	 0.3210
C	 0.8750	 0.1220
G	 0.6740	 0.1440
H	 0.9280	 0.3090
I	 0.9460	 0.3450
J	 0.6440	 0.1300
K	 0.9250	 0.3320
L	 0.9590	 0.4510
M	 0.9460	 0.4530
N	 0.9610	 0.4220
O	 0.9270	 0.2580
P	 0.9600	 0.1920
Q	 0.9540	 0.2150
R	 0.9550	 0.1730
S	 0.9650	 0.2430
T	 0.9720	 0.3410
U	 0.9990	 0.2840
W	 0.9650	 0.3230
X	 0.9150	 0.2020
c	 0.7380	 0.1720
o	 0.8820	 0.3490

