



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:20 PM UTC

PDB ID : 8OW1 / pdb_00008ow1
EMDB ID : EMD-17227
Title : Cryo-EM structure of the yeast Inner kinetochore bound to a CENP-A nucleosome.
Authors : Dendooven, T.D.; Zhang, Z.; Yang, J.; McLaughlin, S.; Schwabb, J.; Scheres, S.; Yatskevich, S.; Barford, D.
Deposited on : 2023-04-26
Resolution : 3.70 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

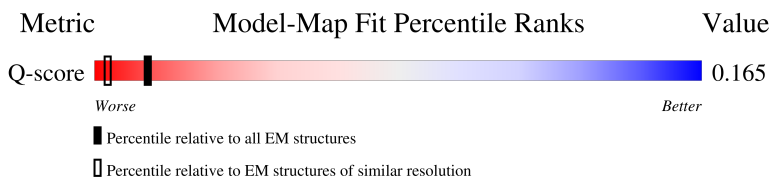
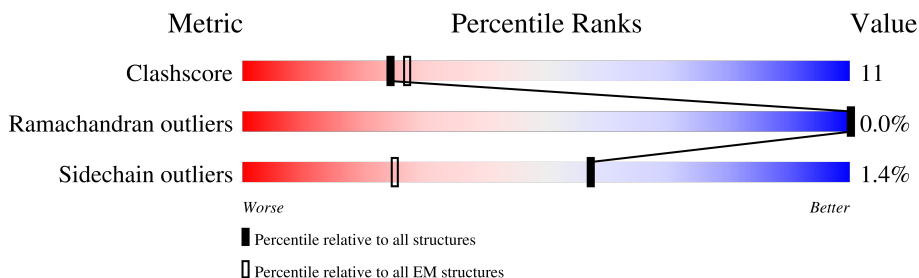
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	A	351	
1	B	351	
2	I	733	
2	II	733	

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Mol	Chain	Length	Quality of chain
3	K	239	
3	KK	239	
4	H	181	
4	HH	181	
5	L	245	
5	LL	245	
6	N	458	
6	NN	458	
7	CT	478	
8	CE	608	
8	ce	608	
9	SK	194	
10	P	369	
10	PP	369	
11	Q	406	
11	QQ	406	
12	O	368	
12	OO	368	
13	T	361	
13	TT	361	
14	U	324	
14	UU	324	
15	W	89	
15	WW	89	
16	Y	238	

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Mol	Chain	Length	Quality of chain
16	YY	238	
17	Z	153	
17	ZZ	153	
18	D	153	
19	E	153	
20	b	103	
20	f	103	
21	d	131	
21	h	131	
22	a	229	
22	e	229	
23	c	132	
23	g	132	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 78671 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-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	110	Total	C	N	O	S	0	0
			898	554	162	179	3		
1	B	116	Total	C	N	O	S	0	0
			957	592	174	188	3		

- Molecule 2 is a protein called Inner kinetochore subunit CTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	659	Total	C	N	O	S	0	0
			5337	3459	890	958	30		
2	II	704	Total	C	N	O	S	0	0
			5705	3692	954	1028	31		

- Molecule 3 is a protein called Inner kinetochore subunit MCM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	219	Total	C	N	O	S	0	0
			1762	1113	304	340	5		
3	KK	227	Total	C	N	O	S	0	0
			1805	1143	307	349	6		

- Molecule 4 is a protein called Inner kinetochore subunit MCM16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	171	Total	C	N	O	S	0	0
			1412	890	247	273	2		
4	HH	176	Total	C	N	O	S	0	0
			1449	912	252	283	2		

- Molecule 5 is a protein called Inner kinetochore subunit IML3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LL	241	Total	C	N	O	S	0	0
			1941	1244	320	366	11		
5	L	241	Total	C	N	O	S	0	0
			1941	1244	320	366	11		

- Molecule 6 is a protein called Inner kinetochore subunit CHL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	NN	385	Total	C	N	O	S	0	0
			3121	2021	530	557	13		
6	N	386	Total	C	N	O	S	0	0
			3129	2027	531	558	13		

- Molecule 7 is a protein called Centromere DNA-binding protein complex CBF3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CT	391	Total	C	N	O	S	0	0
			3298	2154	556	576	12		

- Molecule 8 is a protein called Centromere DNA-binding protein complex CBF3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	ce	524	Total	C	N	O	S	0	0
			4352	2834	700	797	21		
8	CE	557	Total	C	N	O	S	0	0
			4608	2980	758	841	29		

- Molecule 9 is a protein called Suppressor of kinetochore protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SK	151	Total	C	N	O	S	0	0
			1230	769	214	243	4		

- Molecule 10 is a protein called Inner kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	255	Total	C	N	O	S	0	0
			2098	1348	362	374	14		
10	PP	254	Total	C	N	O	S	0	0
			2094	1346	360	374	14		

- Molecule 11 is a protein called Inner kinetochore subunit OKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	261	Total	C	N	O	S	0	0
			2193	1384	388	412	9		
11	QQ	247	Total	C	N	O	S	0	0
			2060	1296	364	391	9		

- Molecule 12 is a protein called Inner kinetochore subunit MCM21.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	OO	240	Total	C	N	O	S	0	0
			1967	1272	323	368	4		
12	O	245	Total	C	N	O	S	0	0
			2015	1302	333	375	5		

- Molecule 13 is a protein called Inner kinetochore subunit CNN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	92	Total	C	N	O	S	0	0
			761	488	125	144	4		
13	TT	92	Total	C	N	O	S	0	0
			761	488	125	144	4		

- Molecule 14 is a protein called Inner kinetochore subunit AME1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	184	Total	C	N	O	S	0	0
			1485	928	255	299	3		
14	UU	179	Total	C	N	O	S	0	0
			1445	904	249	289	3		

- Molecule 15 is a protein called Inner kinetochore subunit WIP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	69	Total	C	N	O	S	0	0
			551	348	96	105	2		
15	WW	69	Total	C	N	O	S	0	0
			550	348	96	104	2		

- Molecule 16 is a protein called Inner kinetochore subunit NKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	223	Total	C	N	O	S	0	0
			1663	1027	281	349	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	YY	223	Total	C	N	O	S	0	0
			1663	1027	281	349	6		

- Molecule 17 is a protein called Inner kinetochore subunit NKP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	151	Total	C	N	O	S	0	0
			1180	740	204	235	1		
17	ZZ	151	Total	C	N	O	S	0	0
			1180	740	204	235	1		

- Molecule 18 is a DNA chain called C0N3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D	153	Total	C	N	O	P	0	0
			3139	1499	574	913	153		

- Molecule 19 is a DNA chain called C0N3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	153	Total	C	N	O	P	0	0
			3134	1499	559	923	153		

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	79	Total	C	N	O		0	0
			625	393	120	112			
20	f	79	Total	C	N	O		0	0
			627	395	120	112			

- Molecule 21 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	95	Total	C	N	O	S	0	0
			735	461	129	144	1		
21	h	97	Total	C	N	O	S	0	0
			745	467	129	148	1		

- Molecule 22 is a protein called Histone H3-like centromeric protein CSE4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	e	97	Total	C	N	O	S	0	0
			781	498	139	140	4		
22	a	97	Total	C	N	O	S	0	0
			781	498	139	140	4		

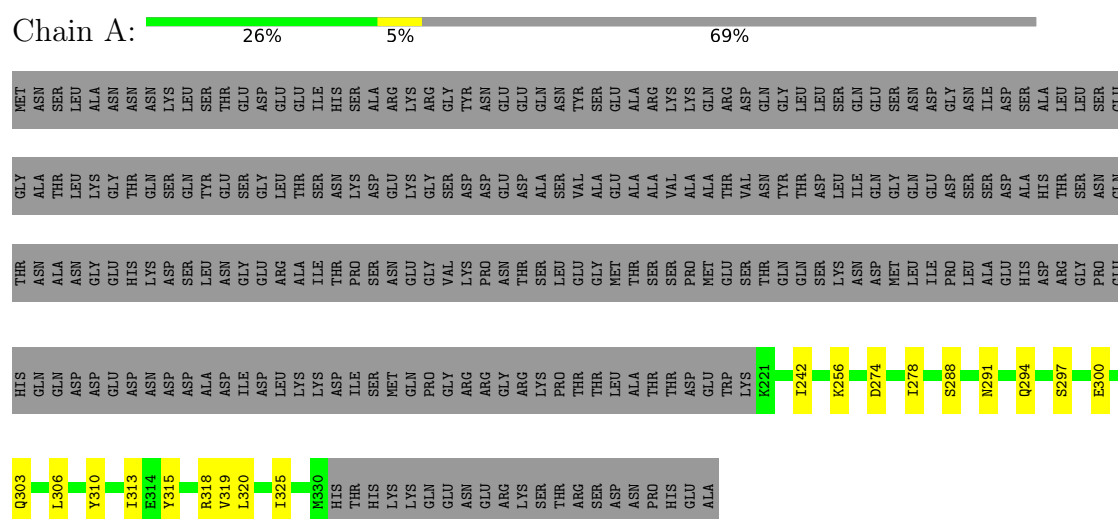
- Molecule 23 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	g	98	Total	C	N	O		0	0
			751	470	147	134			
23	c	97	Total	C	N	O		0	0
			742	464	146	132			

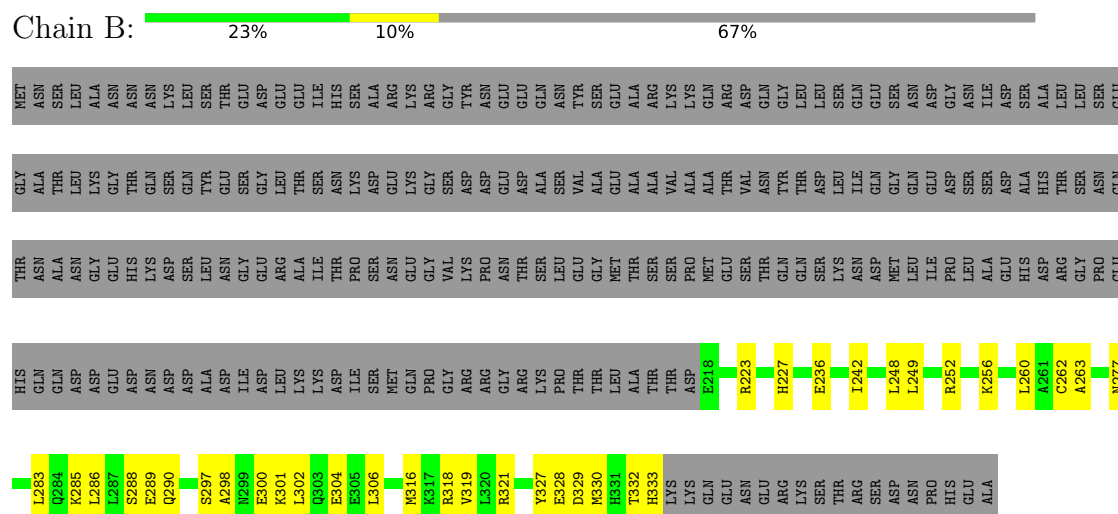
3 Residue-property plots [i](#)

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

• Molecule 1: Centromere-binding protein 1

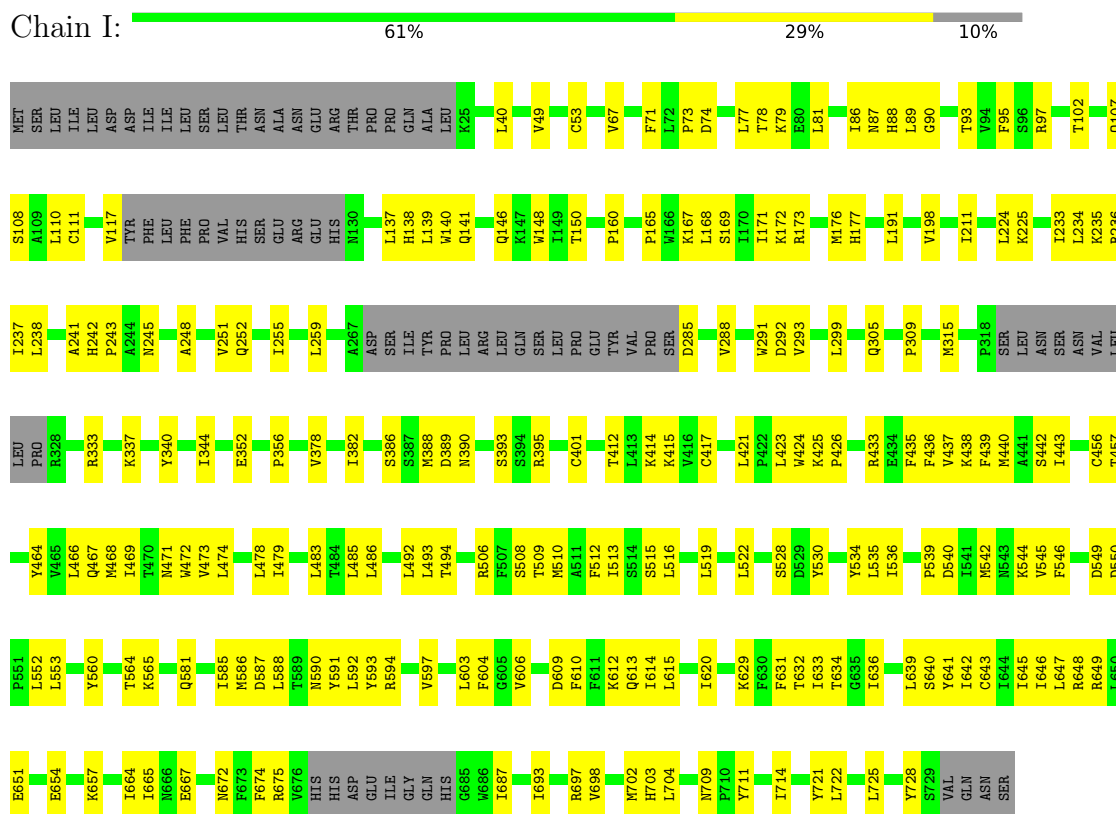


• Molecule 1: Centromere-binding protein 1



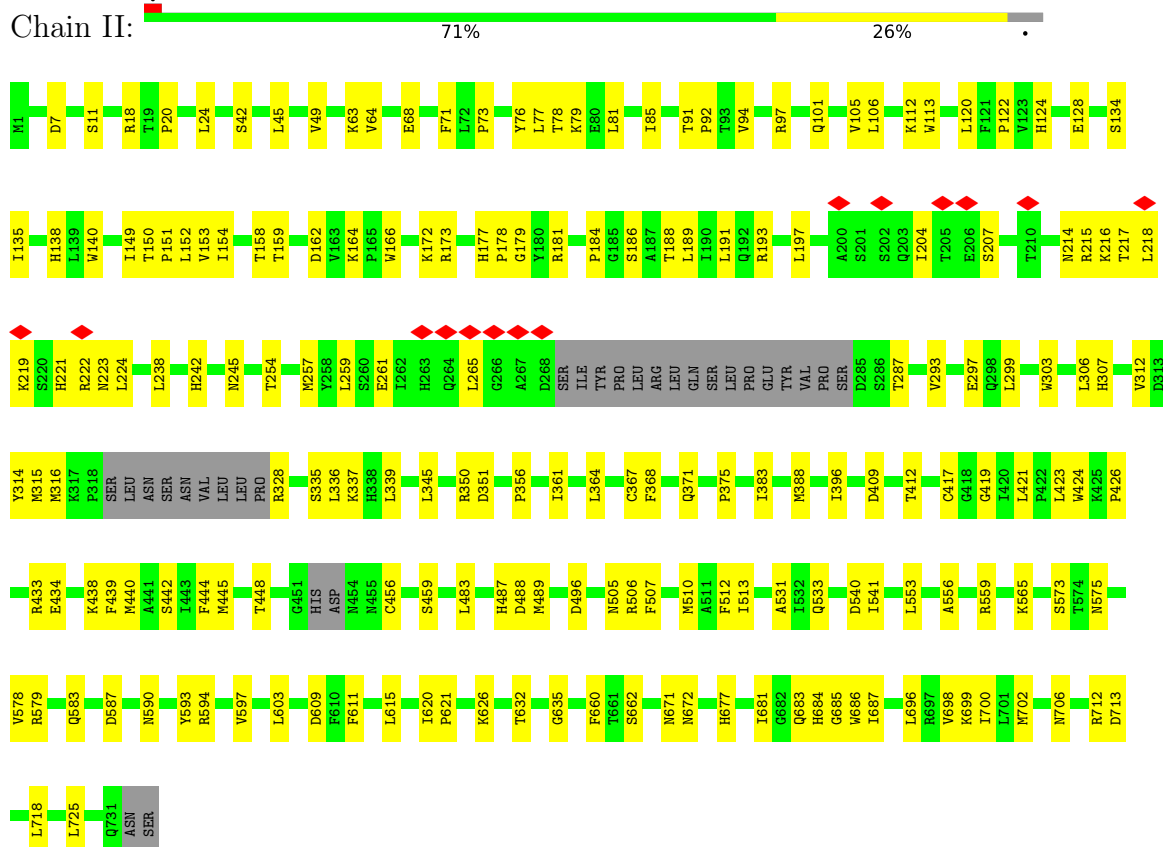
• Molecule 2: Inner kinetochore subunit CTF3

Chain I:

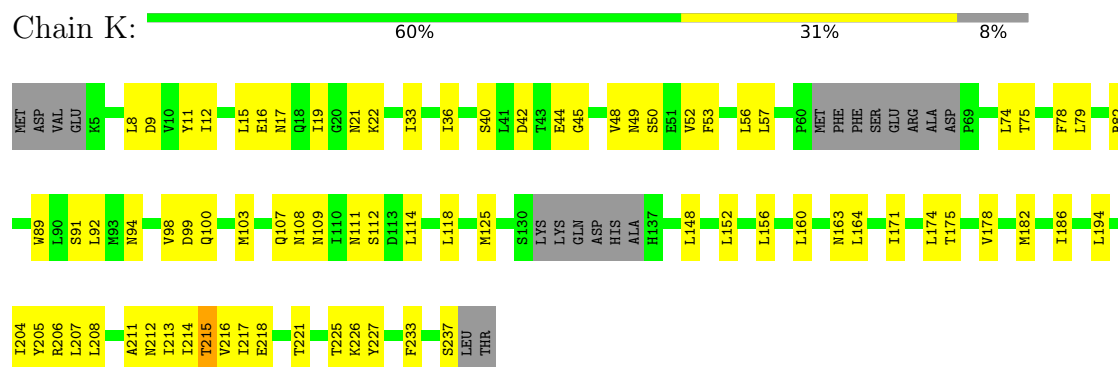


• Molecule 2: Inner kinetochore subunit CTF3

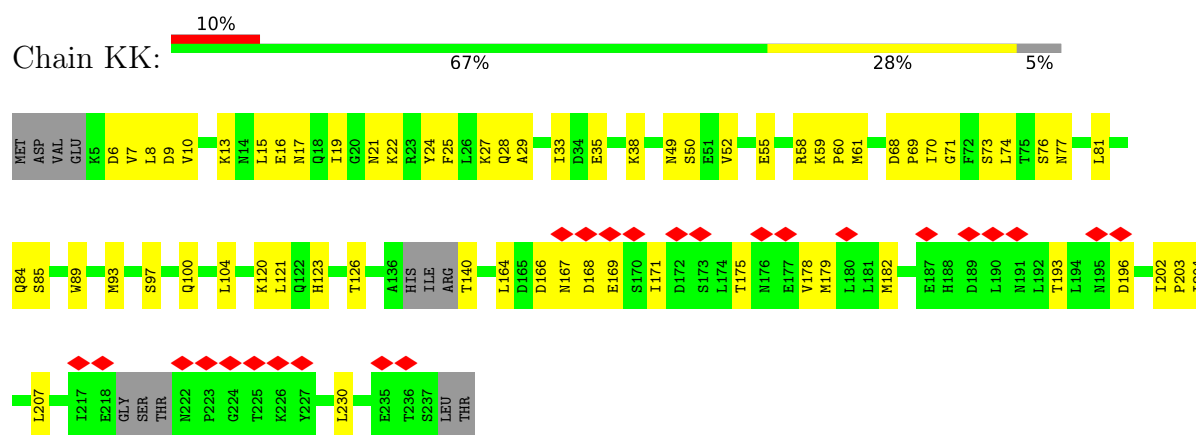
Chain II:



- Molecule 3: Inner kinetochore subunit MCM22



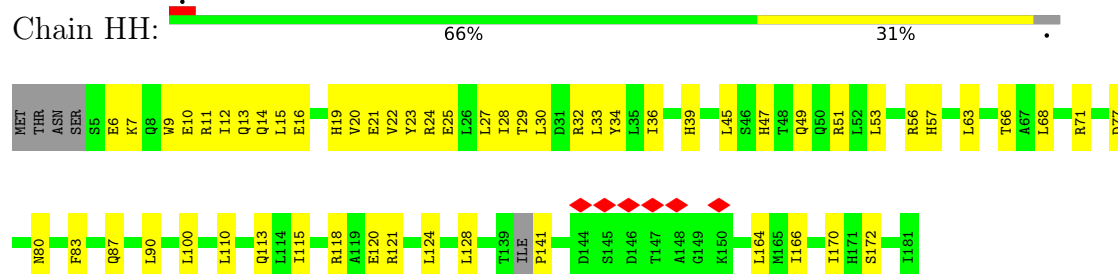
- Molecule 3: Inner kinetochore subunit MCM22



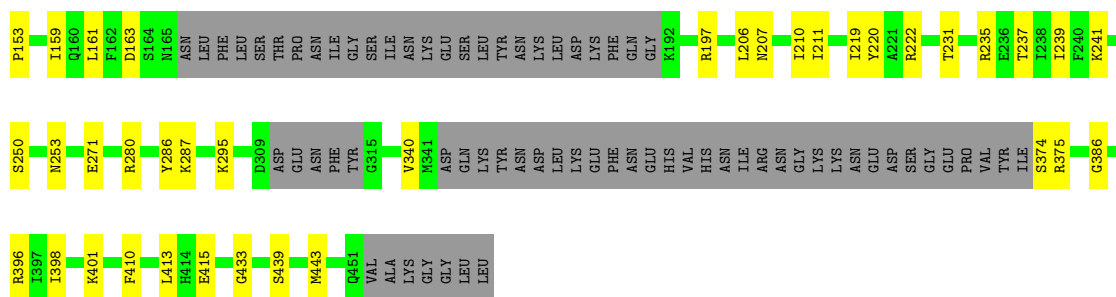
- Molecule 4: Inner kinetochore subunit MCM16



- Molecule 4: Inner kinetochore subunit MCM16

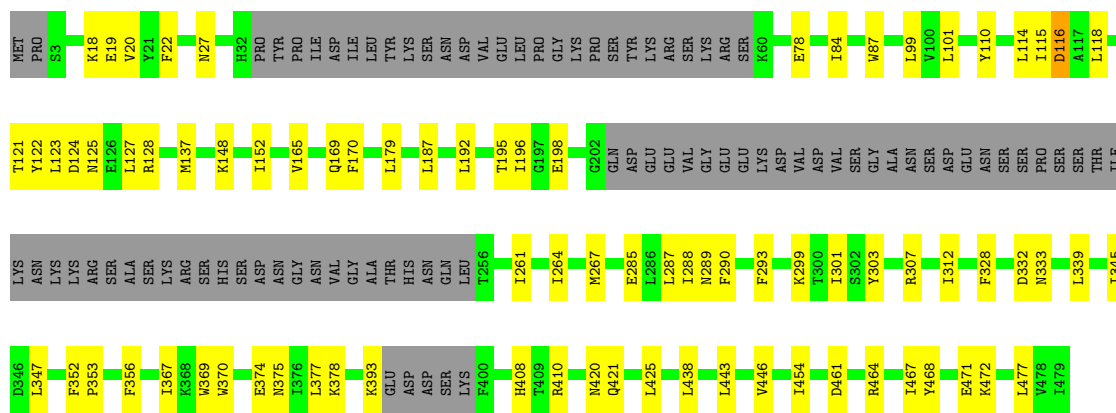


MT	SR	N3	D9	D16	V19	V29	W39	G49	L53	T57	L60	L61	T62	E63	R67	R68	I71	D82	G83	L84	N85	Q88	E91	E102	K110	R113	Y119	V120	V121	I129	E130	N131	I139	Y140	V144	Y145	M146
----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------



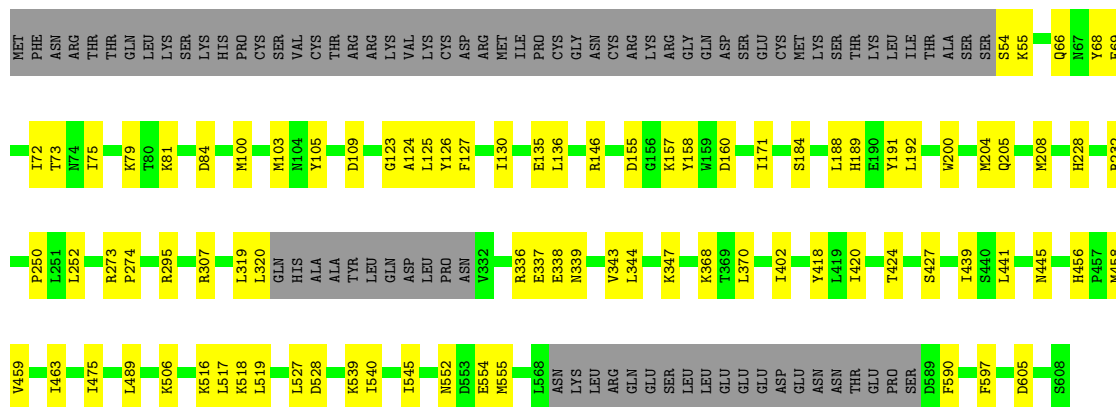
• Molecule 7: Centromere DNA-binding protein complex CBF3 subunit C

Chain CT: 65% 17% 18%



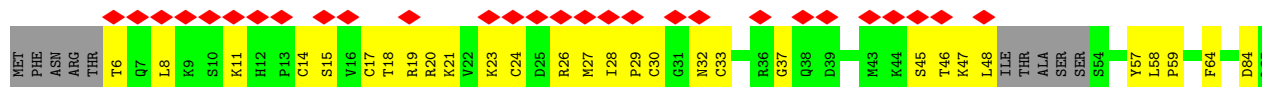
• Molecule 8: Centromere DNA-binding protein complex CBF3 subunit B

Chain ce: 72% 14% 14%

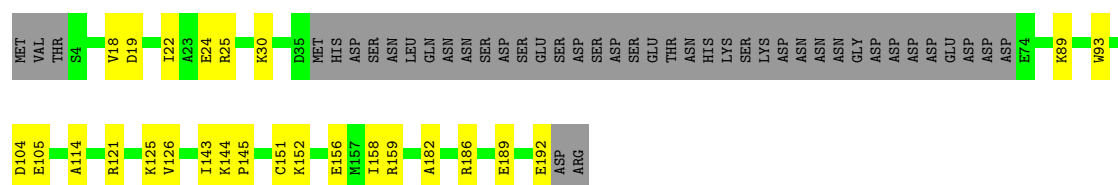


• Molecule 8: Centromere DNA-binding protein complex CBF3 subunit B

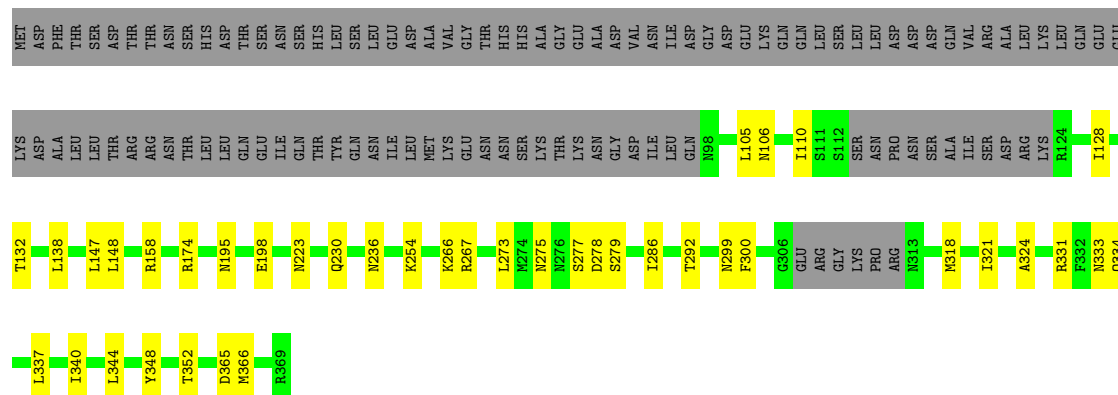
Chain CE: 5% 73% 18% 8%



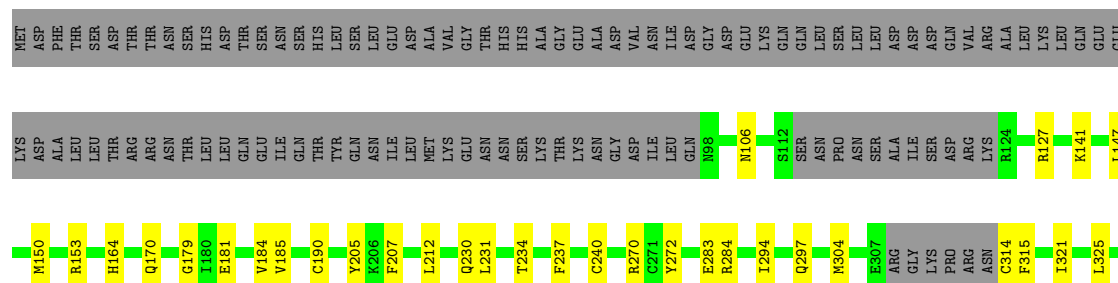
- Molecule 9: Suppressor of kinetochore protein 1



- Molecule 10: Inner kinetochore subunit CTF19



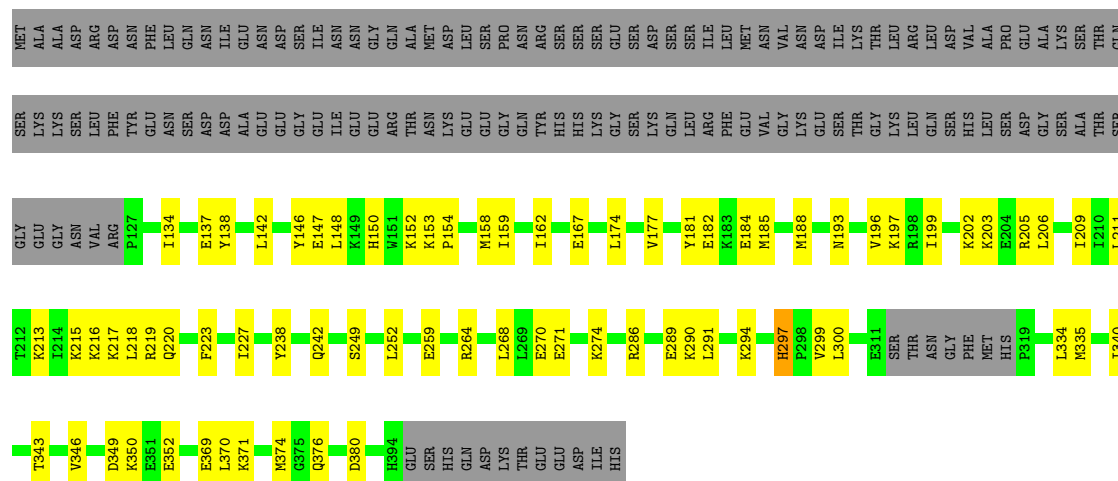
- Molecule 10: Inner kinetochore subunit CTF19





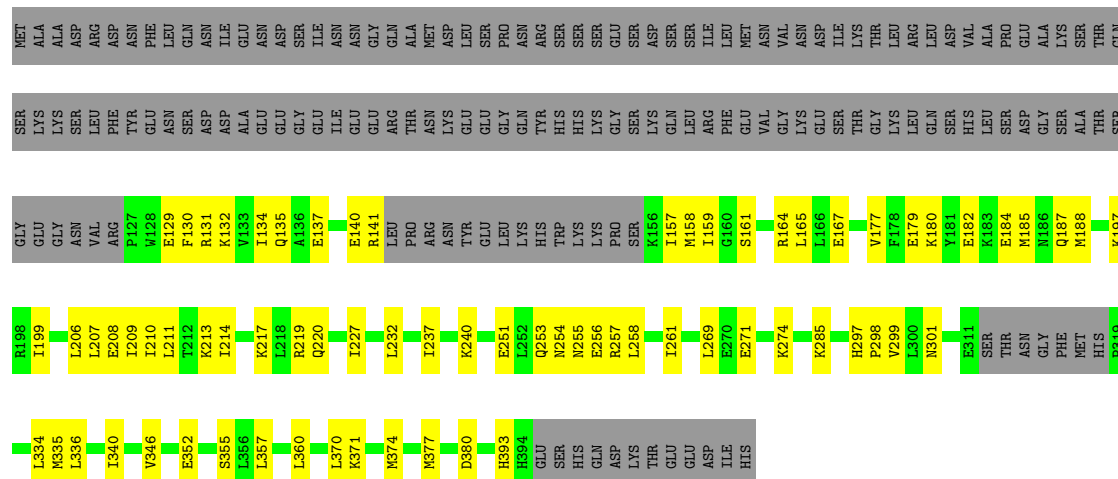
• Molecule 11: Inner kinetochore subunit OKP1

Chain Q: 46% 18% 36%



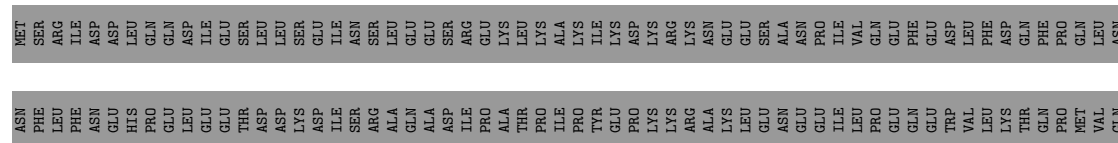
• Molecule 11: Inner kinetochore subunit OKP1

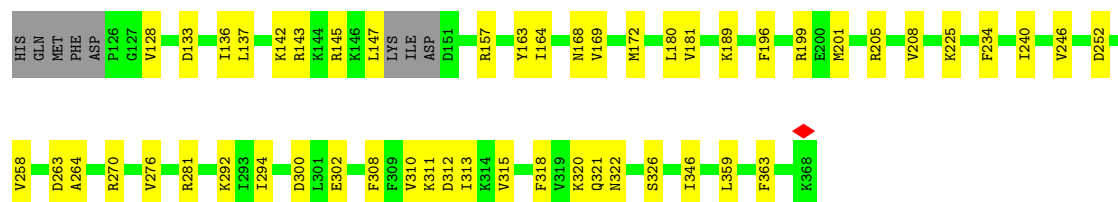
Chain QQ: 43% 18% 39%



• Molecule 12: Inner kinetochore subunit MCM21

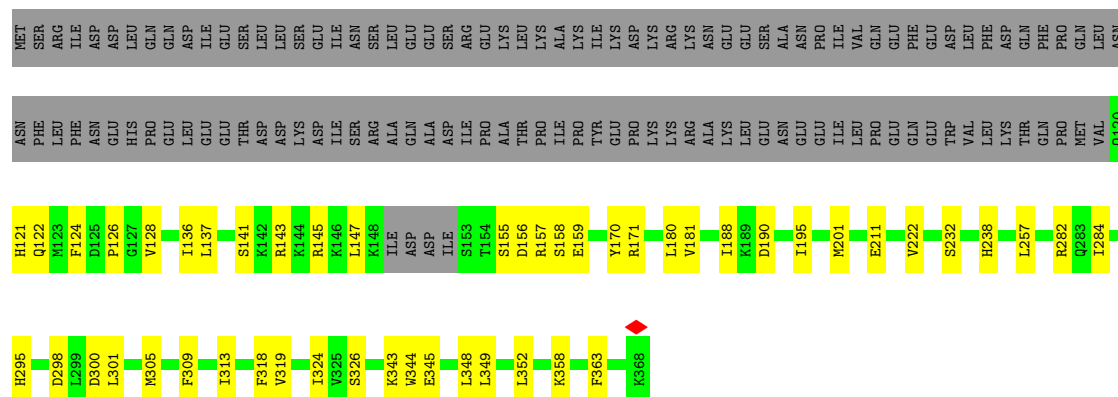
Chain OO: 51% 14% 35%





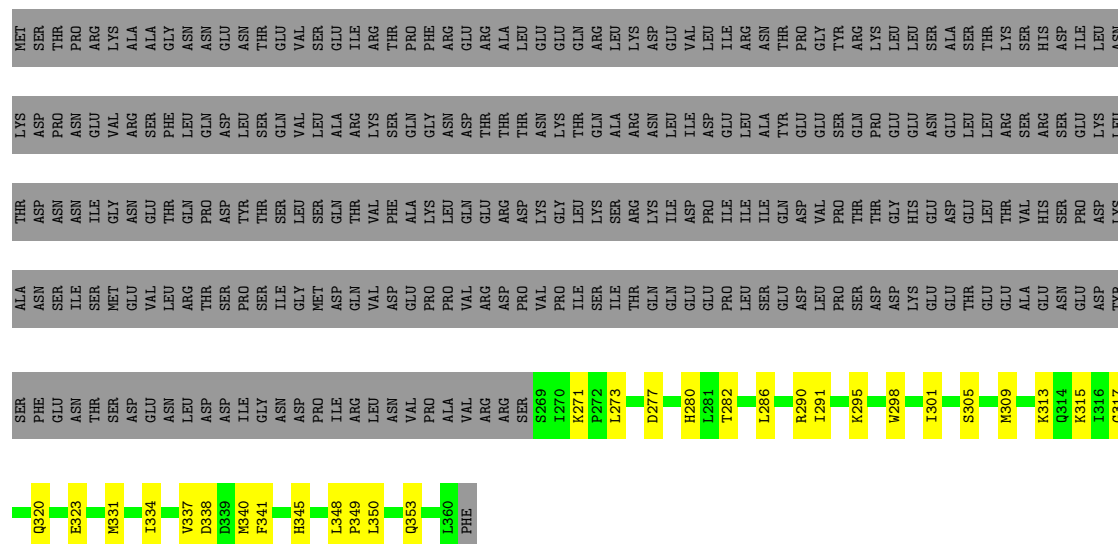
• Molecule 12: Inner kinetochore subunit MCM21

Chain O: 53% 14% 33%



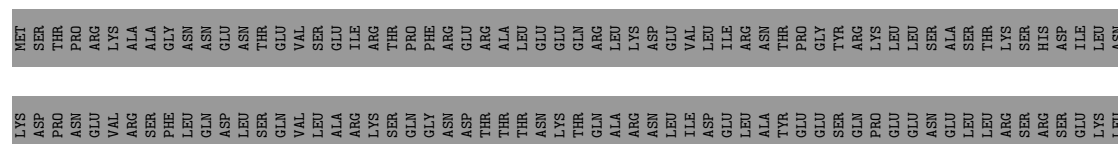
• Molecule 13: Inner kinetochore subunit CNN1

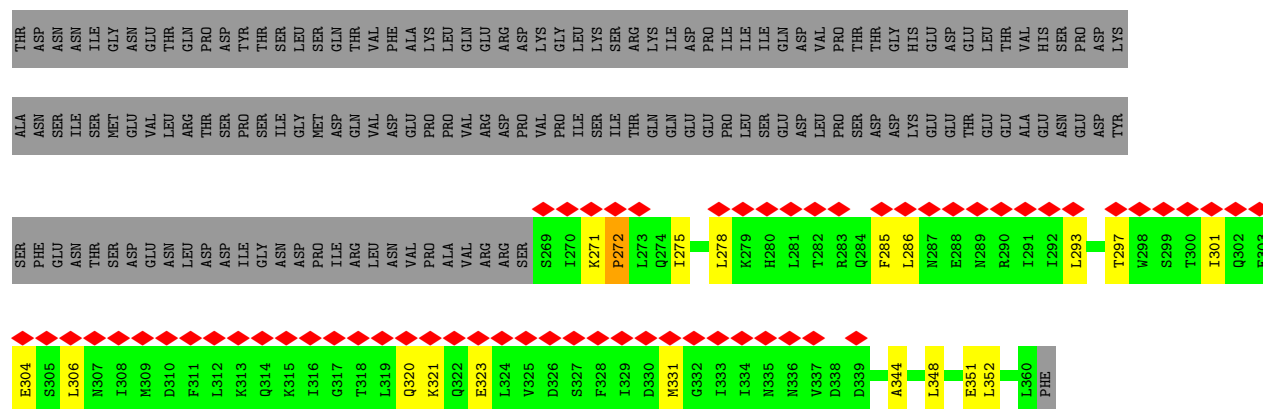
Chain T: 17% 8% 75%



• Molecule 13: Inner kinetochore subunit CNN1

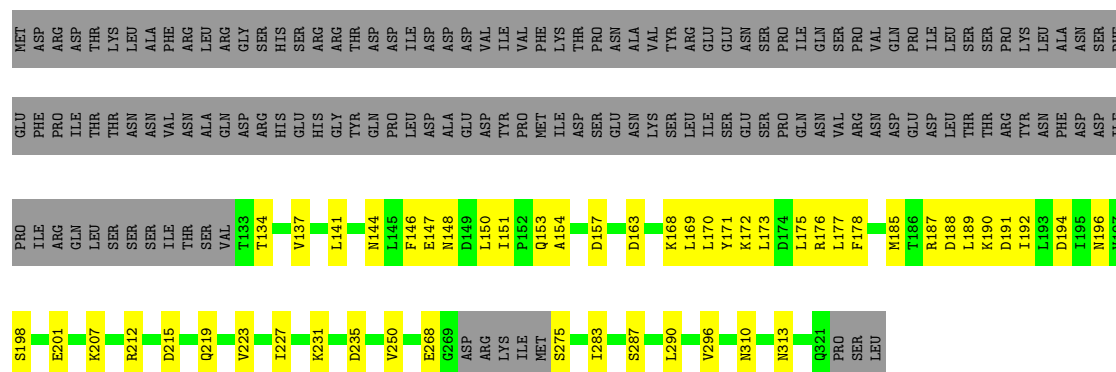
Chain TT: 17% 20% 5% 75%





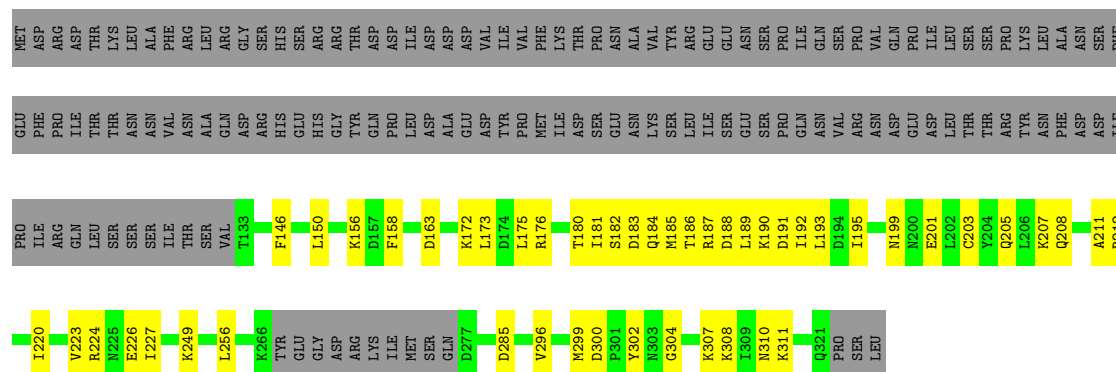
- Molecule 14: Inner kinetochore subunit AME1

Chain U: 41% 16% 43%



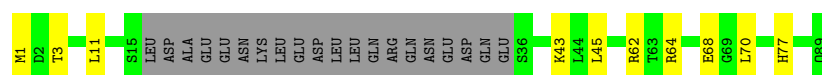
- Molecule 14: Inner kinetochore subunit AME1

Chain UU: 40% 15% 45%

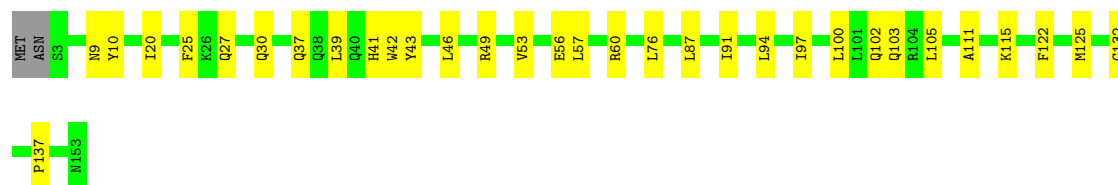


- Molecule 15: Inner kinetochore subunit WIP1

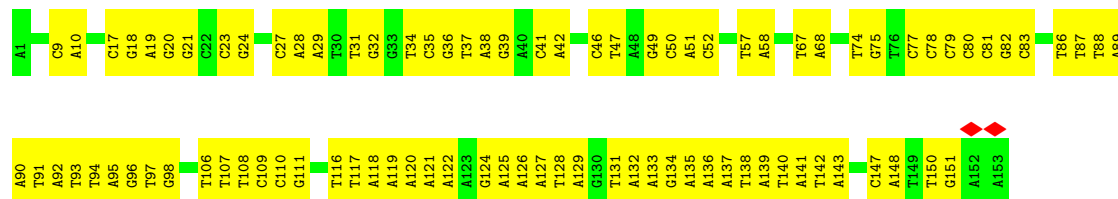
Chain W: 66% 11% 22%



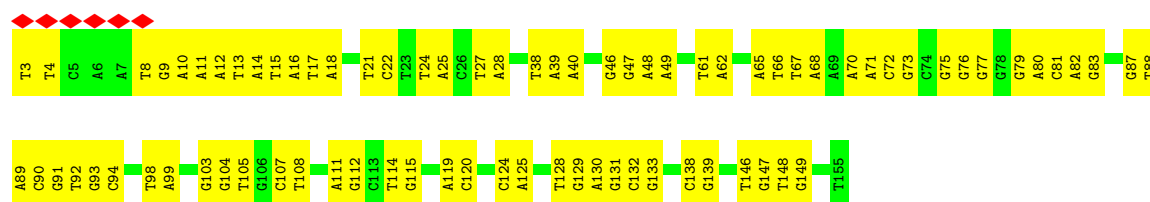
- Molecule 15: Inner kinetochore subunit WIP1



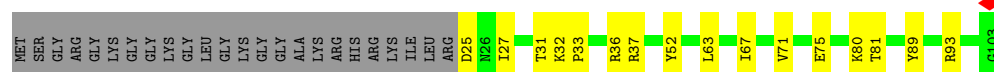
- Molecule 18: C0N3



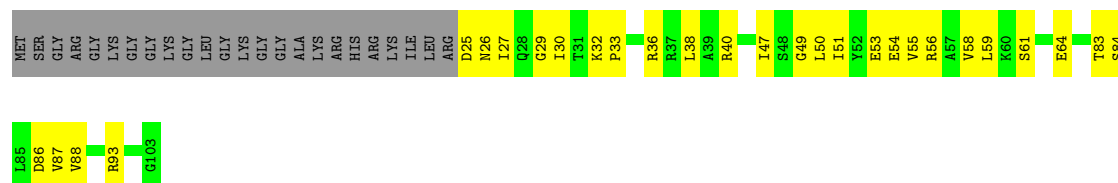
- Molecule 19: C0N3



- Molecule 20: Histone H4



- Molecule 20: Histone H4



- Molecule 21: Histone H2B.1





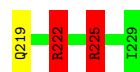
Chain h:



Chain e: 28% 11% 58%



Chain a: 28% 11% .. 58%



Chain g: 64% 10% 26%



LEU

● Molecule 23: Histone H2A.1



THR
LYS
ALA
SER
GLN
GLU
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108672	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00271	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.12	0/905	0.30	0/1210
1	B	0.15	0/968	0.36	0/1296
2	I	0.16	0/5458	0.32	0/7402
2	II	0.10	0/5837	0.28	0/7921
3	K	0.17	0/1784	0.35	0/2404
3	KK	0.14	0/1828	0.35	0/2466
4	H	0.20	0/1429	0.45	0/1923
4	HH	0.18	0/1468	0.36	0/1979
5	L	0.18	0/1981	0.51	3/2684 (0.1%)
5	LL	0.18	0/1981	0.51	3/2684 (0.1%)
6	N	0.11	0/3201	0.27	0/4322
6	NN	0.09	0/3193	0.26	0/4311
7	CT	0.10	0/3369	0.32	0/4544
8	CE	0.09	0/4716	0.27	0/6375
8	ce	0.09	0/4458	0.24	0/6038
9	SK	0.11	0/1251	0.34	0/1692
10	P	0.12	0/2131	0.28	0/2866
10	PP	0.09	0/2127	0.28	0/2860
11	Q	0.19	1/2228 (0.0%)	0.35	0/2983
11	QQ	0.13	0/2087	0.31	0/2791
12	O	0.11	0/2054	0.30	0/2761
12	OO	0.10	0/2004	0.30	0/2695
13	T	0.14	0/772	0.34	0/1040
13	TT	0.44	1/772 (0.1%)	0.67	3/1040 (0.3%)
14	U	0.16	0/1499	0.40	0/2018
14	UU	0.13	0/1458	0.36	0/1963
15	W	0.10	0/557	0.27	0/748
15	WW	0.07	0/556	0.22	0/748
16	Y	0.22	0/1672	0.65	4/2252 (0.2%)
16	YY	0.22	0/1672	0.65	4/2252 (0.2%)
17	Z	0.20	0/1195	0.49	1/1616 (0.1%)
17	ZZ	0.16	0/1195	0.36	1/1616 (0.1%)
18	D	0.18	0/3523	0.37	0/5435
19	E	0.19	0/3513	0.36	0/5420

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	b	0.17	0/632	0.38	0/845
20	f	0.15	0/634	0.39	0/848
21	d	0.14	0/745	0.37	0/1003
21	h	0.11	0/755	0.34	0/1017
22	a	0.26	0/792	0.75	7/1066 (0.7%)
22	e	0.26	0/792	0.76	7/1066 (0.7%)
23	c	0.14	0/751	0.40	0/1015
23	g	0.13	0/760	0.36	0/1027
All	All	0.15	2/80703 (0.0%)	0.37	33/110242 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	4
3	K	0	1
3	KK	0	1
4	H	0	1
7	CT	0	2
11	Q	0	1
16	Y	0	1
16	YY	0	1
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	TT	272	PRO	CG-CD	-11.35	1.12	1.50
11	Q	297	HIS	C-N	5.13	1.41	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	TT	272	PRO	N-CD-CG	-14.38	81.62	103.20
13	TT	272	PRO	CA-N-CD	-9.56	98.62	112.00
16	Y	115	GLU	CA-CB-CG	9.49	133.09	114.10
16	YY	115	GLU	CA-CB-CG	9.49	133.08	114.10
13	TT	272	PRO	CA-CB-CG	-8.57	88.21	104.50
22	e	225	ARG	CG-CD-NE	8.51	130.71	112.00
22	a	225	ARG	CG-CD-NE	8.50	130.71	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	e	222	ARG	CG-CD-NE	8.28	130.21	112.00
22	a	222	ARG	CG-CD-NE	8.28	130.21	112.00
16	YY	115	GLU	CB-CG-CD	7.22	124.88	112.60
16	Y	115	GLU	CB-CG-CD	7.22	124.87	112.60
5	LL	167	ARG	CA-CB-CG	6.99	128.07	114.10
5	L	167	ARG	CA-CB-CG	6.97	128.04	114.10
5	L	115	LYS	CB-CG-CD	6.63	126.55	111.30
5	LL	115	LYS	CB-CG-CD	6.62	126.52	111.30
22	e	225	ARG	CB-CG-CD	6.32	125.83	111.30
22	a	225	ARG	CB-CG-CD	6.31	125.80	111.30
16	Y	223	PRO	N-CA-CB	6.17	110.12	103.33
17	ZZ	137	PRO	N-CA-CB	6.16	110.11	103.33
5	LL	167	ARG	CB-CG-CD	6.01	125.13	111.30
5	L	167	ARG	CB-CG-CD	6.01	125.12	111.30
16	YY	223	PRO	N-CA-CB	5.96	110.11	103.44
17	Z	137	PRO	N-CA-CB	5.94	110.09	103.44
22	e	222	ARG	CD-NE-CZ	5.51	132.11	124.40
16	Y	112	ARG	CA-CB-CG	5.51	125.11	114.10
16	YY	112	ARG	CA-CB-CG	5.50	125.11	114.10
22	e	147	ARG	CG-CD-NE	5.50	124.10	112.00
22	a	147	ARG	CG-CD-NE	5.50	124.09	112.00
22	a	222	ARG	CD-NE-CZ	5.46	132.05	124.40
22	a	225	ARG	CD-NE-CZ	5.22	131.71	124.40
22	e	225	ARG	CD-NE-CZ	5.20	131.68	124.40
22	e	222	ARG	CB-CG-CD	5.05	122.91	111.30
22	a	222	ARG	CB-CG-CD	5.04	122.90	111.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	CT	116	ASP	Peptide
7	CT	125	ASN	Peptide
4	H	70	ILE	Peptide
2	I	425	LYS	Mainchain
2	I	456	CYS	Peptide
2	I	534	TYR	Peptide
2	I	612	LYS	Peptide
3	K	215	THR	Peptide
3	KK	68	ASP	Peptide
11	Q	297	HIS	Mainchain
16	Y	82	MET	Peptide

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Mol	Chain	Res	Type	Group
16	YY	82	MET	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	898	0	912	12	0
1	B	957	0	962	29	0
2	I	5337	0	5460	166	0
2	II	5705	0	5817	141	0
3	K	1762	0	1796	86	0
3	KK	1805	0	1809	49	0
4	H	1412	0	1451	96	0
4	HH	1449	0	1478	65	0
5	L	1941	0	1946	56	0
5	LL	1941	0	1946	58	0
6	N	3129	0	3182	50	0
6	NN	3121	0	3171	42	0
7	CT	3298	0	3368	55	0
8	CE	4608	0	4595	77	0
8	ce	4352	0	4318	54	0
9	SK	1230	0	1198	21	0
10	P	2098	0	2174	33	0
10	PP	2094	0	2172	28	0
11	Q	2193	0	2252	59	0
11	QQ	2060	0	2110	62	0
12	O	2015	0	2035	35	0
12	OO	1967	0	1993	43	0
13	T	761	0	781	27	0
13	TT	761	0	781	16	0
14	U	1485	0	1467	42	0
14	UU	1445	0	1436	42	0
15	W	551	0	559	8	0
15	WW	550	0	559	11	0
16	Y	1663	0	1588	61	0
16	YY	1663	0	1588	47	0
17	Z	1180	0	1108	38	0
17	ZZ	1180	0	1108	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	D	3139	0	1727	89	0
19	E	3134	0	1732	81	0
20	b	625	0	657	13	0
20	f	627	0	664	23	0
21	d	735	0	753	24	0
21	h	745	0	757	19	0
22	a	781	0	803	32	0
22	e	781	0	803	26	0
23	c	742	0	775	15	0
23	g	751	0	789	16	0
All	All	78671	0	76580	1648	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 11.

All (1648) 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)
18:D:82:DG:C2	19:E:75:DG:C2	2.10	1.38
18:D:82:DG:C2	19:E:75:DG:N2	1.96	1.34
18:D:82:DG:N1	19:E:75:DG:N1	1.80	1.27
18:D:80:DC:N4	19:E:76:DG:C6	2.07	1.23
18:D:82:DG:N3	19:E:75:DG:N2	1.89	1.18
18:D:80:DC:N4	19:E:76:DG:O6	1.83	1.12
18:D:82:DG:N2	19:E:75:DG:C2	2.28	1.01
16:Y:24:ASP:HA	17:Z:49:ARG:HH12	1.30	0.96
10:PP:284:ARG:HB3	10:PP:362:LEU:HD22	1.45	0.94
18:D:80:DC:N4	19:E:76:DG:N1	2.11	0.92
4:H:43:VAL:HG13	4:H:44:ILE:HG23	1.54	0.89
22:e:222:ARG:HB3	22:e:222:ARG:HH11	1.38	0.89
17:Z:56:GLU:HB3	17:Z:60:ARG:HH12	1.33	0.89
22:a:222:ARG:HH11	22:a:222:ARG:HB3	1.37	0.86
1:B:252:ARG:HH12	6:N:443:MET:HE2	1.39	0.85
2:II:440:MET:HG3	2:II:489:MET:HE1	1.60	0.84
5:LL:167:ARG:HA	5:LL:170:CYS:HB2	1.60	0.83
2:I:510:MET:HE2	4:H:100:LEU:CD2	2.08	0.83
5:L:167:ARG:HA	5:L:170:CYS:HB2	1.60	0.82
14:U:172:LYS:HB2	14:U:176:ARG:HH12	1.44	0.82
8:ce:171:ILE:HD11	8:ce:208:MET:HE3	1.61	0.82
17:Z:56:GLU:HB3	17:Z:60:ARG:NH1	1.95	0.81
4:H:65:LYS:O	4:H:69:LEU:HB2	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:225:ARG:CB	22:a:225:ARG:HH11	1.95	0.80
13:T:349:PRO:O	13:T:353:GLN:NE2	2.15	0.80
18:D:82:DG:C6	19:E:75:DG:N1	2.36	0.80
2:I:614:ILE:HG21	4:H:64:GLU:HG2	1.63	0.79
5:LL:101:GLN:HA	5:LL:104:LYS:HD2	1.65	0.79
22:e:225:ARG:CB	22:e:225:ARG:HH11	1.95	0.79
22:a:222:ARG:HB3	22:a:222:ARG:NH1	1.98	0.79
5:L:101:GLN:HA	5:L:104:LYS:HD2	1.65	0.79
7:CT:115:ILE:HG13	7:CT:116:ASP:H	1.46	0.78
11:Q:147:GLU:HB2	13:T:315:LYS:HD3	1.65	0.78
22:e:222:ARG:HB3	22:e:222:ARG:NH1	1.98	0.77
2:I:412:THR:HA	2:I:415:LYS:HE2	1.67	0.77
17:Z:26:LYS:HD3	17:Z:29:LEU:HD11	1.67	0.77
3:KK:69:PRO:HD2	3:KK:70:ILE:HD12	1.67	0.77
2:II:590:ASN:HA	2:II:594:ARG:HB2	1.67	0.76
13:T:271:LYS:HG2	13:T:309:MET:HG3	1.66	0.76
16:YY:81:ILE:HG21	17:ZZ:76:LEU:HD13	1.67	0.76
22:a:225:ARG:HH11	22:a:225:ARG:HB3	1.50	0.75
21:d:80:GLU:HG3	21:d:105:ILE:HD11	1.69	0.75
11:QQ:208:GLU:HA	11:QQ:211:LEU:HB2	1.66	0.75
4:H:161:ILE:HG22	4:H:165:MET:HE2	1.69	0.75
2:I:603:LEU:HB3	2:I:606:VAL:HB	1.68	0.75
22:e:225:ARG:HH11	22:e:225:ARG:HB3	1.50	0.74
2:I:506:ARG:HH12	3:K:89:TRP:HE1	1.36	0.74
17:Z:29:LEU:HD13	17:Z:39:LEU:HD13	1.69	0.74
23:c:81:ILE:HG22	23:c:83:ARG:H	1.50	0.74
2:I:388:MET:SD	4:H:121:ARG:NH1	2.59	0.74
3:K:152:LEU:HD13	4:H:165:MET:HG2	1.68	0.74
18:D:80:DC:N4	19:E:76:DG:H1	1.86	0.74
2:I:494:THR:O	4:H:51:ARG:NH2	2.21	0.73
18:D:81:DC:O2	19:E:76:DG:N2	2.21	0.73
4:H:45:LEU:HD11	4:H:49:GLN:HE21	1.53	0.73
14:U:147:GLU:HA	14:U:151:ILE:HD12	1.69	0.73
18:D:81:DC:OP2	20:f:36:ARG:NH2	2.21	0.73
12:OO:346:ILE:HG13	17:ZZ:103:GLN:HE21	1.53	0.73
3:K:56:LEU:HG	4:H:38:LYS:HG2	1.69	0.73
2:I:603:LEU:HD22	4:H:59:LEU:HD22	1.70	0.73
10:P:299:ASN:HD22	14:U:290:LEU:HD21	1.53	0.73
19:E:91:DG:H2'	19:E:92:DT:H71	1.70	0.72
3:K:194:LEU:HD22	3:K:205:TYR:HE2	1.53	0.72
7:CT:148:LYS:HA	7:CT:152:ILE:HD13	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:HH:25:GLU:HA	4:HH:28:ILE:HG22	1.70	0.72
6:N:67:ARG:HB3	19:E:131:DG:H5''	1.70	0.72
10:P:174:ARG:NH2	6:N:286:TYR:OH	2.22	0.72
22:e:154:SER:HB2	22:e:157:PRO:HD2	1.72	0.72
22:a:154:SER:HB2	22:a:157:PRO:HD2	1.72	0.72
13:T:291:ILE:HG23	15:W:62:ARG:HD3	1.70	0.72
10:PP:363:PHE:HB3	10:PP:366:MET:HG2	1.72	0.72
2:I:510:MET:HE2	4:H:100:LEU:HD23	1.72	0.71
6:NN:298:MET:HB2	6:NN:324:LEU:HD13	1.70	0.71
11:Q:346:VAL:HG22	16:Y:148:LYS:HZ3	1.55	0.71
2:II:287:THR:HA	2:II:307:HIS:CD2	2.26	0.71
18:D:82:DG:N1	19:E:75:DG:C6	2.59	0.71
22:e:141:GLU:HA	22:e:144:LYS:HG2	1.73	0.71
3:K:48:VAL:HG13	4:H:39:HIS:HB2	1.71	0.71
16:YY:75:ALA:O	16:YY:79:GLN:NE2	2.24	0.71
10:PP:181:GLU:HB3	10:PP:205:TYR:HB2	1.72	0.70
21:h:47:LYS:O	21:h:51:GLN:NE2	2.24	0.70
16:Y:75:ALA:O	16:Y:79:GLN:NE2	2.24	0.70
22:e:222:ARG:HH11	22:e:222:ARG:CB	2.04	0.70
14:U:172:LYS:HB2	14:U:176:ARG:NH1	2.05	0.70
16:YY:14:ASN:OD1	16:YY:14:ASN:N	2.24	0.70
2:I:586:MET:HG3	2:I:722:LEU:HD21	1.74	0.70
8:CE:587:PRO:HB3	2:II:698:VAL:HG11	1.72	0.70
9:SK:18:VAL:HG23	9:SK:19:ASP:H	1.57	0.69
22:a:222:ARG:HH11	22:a:222:ARG:CB	2.04	0.69
12:OO:310:VAL:HG13	12:OO:311:LYS:HG2	1.72	0.69
12:OO:163:TYR:HB3	10:PP:150:MET:HE2	1.74	0.69
2:II:191:LEU:HD22	2:II:204:ILE:HD11	1.72	0.69
16:Y:14:ASN:OD1	16:Y:14:ASN:N	2.24	0.69
12:O:143:ARG:HH12	12:O:147:LEU:HB2	1.57	0.69
16:YY:70:GLU:O	16:YY:74:ARG:HB2	1.93	0.69
18:D:82:DG:N1	19:E:75:DG:C2	2.40	0.69
2:I:53:CYS:SG	2:I:102:THR:OG1	2.46	0.69
19:E:92:DT:H5''	22:a:134:PRO:HB3	1.74	0.69
16:YY:78:SER:O	16:YY:82:MET:HG2	1.93	0.69
3:K:233:PHE:HB2	4:H:160:THR:HG22	1.75	0.68
16:Y:78:SER:O	16:Y:82:MET:HG2	1.93	0.68
2:I:168:LEU:HD22	2:I:191:LEU:HD23	1.75	0.68
8:ce:370:LEU:HB3	8:ce:418:TYR:HE1	1.58	0.68
16:Y:70:GLU:O	16:Y:74:ARG:HB2	1.93	0.68
11:QQ:137:GLU:HB3	11:QQ:141:ARG:HH22	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:141:GLU:HA	22:a:144:LYS:HG2	1.73	0.68
4:H:16:GLU:HA	4:H:19:HIS:CE1	2.29	0.68
2:I:590:ASN:HA	2:I:594:ARG:HG3	1.74	0.68
2:I:510:MET:HE1	2:I:552:LEU:HD13	1.74	0.68
2:II:510:MET:SD	4:HH:100:LEU:HD21	2.33	0.68
5:LL:153:THR:OG1	6:NN:415:GLU:OE2	2.12	0.68
4:H:19:HIS:HA	4:H:22:VAL:HG12	1.76	0.67
2:II:159:THR:HG23	2:II:162:ASP:H	1.58	0.67
2:II:540:ASP:OD1	4:HH:51:ARG:NH1	2.27	0.67
4:H:35:LEU:HD11	4:H:49:GLN:HE22	1.59	0.67
18:D:96:DG:N2	19:E:61:DT:O2	2.28	0.67
22:a:139:LEU:HD12	22:a:143:ARG:HH12	1.60	0.67
3:K:74:LEU:HD13	4:H:61:ILE:HG23	1.77	0.67
11:Q:370:LEU:HD11	11:Q:374:MET:HE3	1.76	0.67
18:D:50:DC:H4'	22:a:177:ARG:HH12	1.60	0.67
7:CT:303:TYR:O	7:CT:307:ARG:NH1	2.28	0.66
5:L:101:GLN:HA	5:L:104:LYS:HB2	1.77	0.66
5:LL:50:ALA:HA	5:LL:80:LYS:HE2	1.78	0.66
21:d:82:SER:HB2	23:c:41:TYR:HB3	1.77	0.66
5:L:50:ALA:HA	5:L:80:LYS:HE2	1.78	0.66
6:N:235:ARG:NH2	16:Y:95:SER:OG	2.29	0.66
21:h:101:ALA:O	21:h:105:ILE:HG12	1.95	0.66
2:I:550:ASP:OD1	3:K:82:ARG:NH1	2.27	0.66
7:CT:461:ASP:OD2	8:ce:339:ASN:ND2	2.28	0.66
18:D:81:DC:C2	19:E:76:DG:N2	2.63	0.66
22:e:139:LEU:HD12	22:e:143:ARG:HH12	1.60	0.66
2:II:179:GLY:HA2	15:WW:3:THR:H	1.61	0.66
11:QQ:179:GLU:HA	11:QQ:182:GLU:HB2	1.76	0.66
18:D:51:DA:H2''	18:D:52:DC:H5''	1.78	0.66
20:f:25:ASP:OD1	20:f:26:ASN:N	2.28	0.65
2:I:466:LEU:HA	2:I:469:ILE:HD12	1.77	0.65
3:KK:16:GLU:HA	3:KK:19:ILE:HB	1.79	0.65
2:II:367:CYS:HB2	2:II:375:PRO:HB3	1.76	0.65
2:I:610:PHE:HZ	4:H:56:ARG:HG3	1.60	0.65
15:WW:7:ALA:HB2	15:WW:47:ALA:HB2	1.77	0.65
6:NN:382:ILE:HD12	6:NN:437:SER:HB3	1.76	0.65
16:Y:68:ASP:O	16:Y:71:SER:OG	2.09	0.65
2:I:510:MET:CE	4:H:100:LEU:HD23	2.27	0.65
13:T:345:HIS:HA	13:T:353:GLN:HG2	1.78	0.65
20:f:47:ILE:HG23	20:f:51:ILE:HD11	1.78	0.65
8:CE:107:GLN:HB2	8:CE:110:GLN:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:649:ARG:NH2	2:I:709:ASN:OD1	2.30	0.64
5:LL:101:GLN:HA	5:LL:104:LYS:HB2	1.77	0.64
8:CE:372:ALA:HA	8:CE:375:ARG:HH21	1.62	0.64
18:D:86:DT:H2''	18:D:87:DT:H5''	1.77	0.64
2:I:414:LYS:HD3	2:I:457:THR:HG22	1.78	0.64
22:e:181:MET:HG2	20:f:84:SER:HB3	1.80	0.64
5:LL:166:PRO:O	5:LL:169:SER:OG	2.15	0.64
5:L:149:PHE:HZ	5:L:200:VAL:HG13	1.61	0.64
2:I:67:VAL:HG11	2:I:110:LEU:HA	1.79	0.64
2:II:417:CYS:HA	2:II:421:LEU:HD23	1.80	0.64
8:CE:114:LEU:HG	8:CE:174:MET:HE1	1.79	0.64
2:I:389:ASP:O	2:I:393:SER:N	2.31	0.64
5:LL:115:LYS:HA	5:LL:115:LYS:HE2	1.79	0.64
5:LL:149:PHE:HZ	5:LL:200:VAL:HG13	1.62	0.64
11:Q:152:LYS:NZ	11:Q:153:LYS:O	2.30	0.63
5:L:115:LYS:HE2	5:L:115:LYS:HA	1.79	0.63
11:Q:167:GLU:HG3	11:Q:211:LEU:HD11	1.80	0.63
11:Q:371:LYS:NZ	14:U:287:SER:OG	2.30	0.63
16:Y:6:ASN:OD1	16:Y:7:SER:N	2.32	0.63
17:Z:57:LEU:HD23	17:Z:60:ARG:HH21	1.64	0.63
2:I:640:SER:HB3	2:I:664:ILE:HA	1.81	0.63
12:OO:252:ASP:OD1	12:OO:270:ARG:NH1	2.32	0.63
12:O:188:ILE:HG22	12:O:190:ASP:H	1.64	0.63
11:QQ:184:GLU:HG3	11:QQ:187:GLN:HE21	1.63	0.63
11:Q:154:PRO:HG2	11:Q:159:ILE:HD11	1.80	0.63
11:Q:158:MET:HE1	11:Q:227:ILE:HB	1.80	0.63
11:Q:270:GLU:HB3	11:Q:274:LYS:HZ3	1.63	0.63
11:Q:270:GLU:HB3	11:Q:274:LYS:NZ	2.14	0.63
11:Q:193:ASN:HA	11:Q:196:VAL:HG12	1.80	0.62
16:Y:61:LEU:O	16:Y:65:GLU:HG3	1.99	0.62
14:UU:296:VAL:HA	16:YY:177:LEU:HD13	1.79	0.62
18:D:93:DT:H2''	18:D:94:DT:H5''	1.81	0.62
12:OO:281:ARG:NH2	12:OO:302:GLU:O	2.32	0.62
2:II:77:LEU:HD21	2:II:120:LEU:HB3	1.80	0.62
2:I:530:TYR:HB2	2:I:535:LEU:HD12	1.81	0.62
22:e:194:LEU:HD11	20:f:59:LEU:HD13	1.81	0.62
6:N:237:THR:HG21	14:U:231:LYS:HB3	1.81	0.62
16:YY:6:ASN:OD1	16:YY:7:SER:N	2.32	0.62
2:II:215:ARG:NE	18:D:79:DC:OP2	2.28	0.62
11:QQ:297:HIS:ND1	11:QQ:299:VAL:HG22	2.14	0.62
3:KK:22:LYS:NZ	4:HH:22:VAL:HG13	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:82:DG:C2	19:E:75:DG:N1	2.36	0.62
2:I:648:ARG:HA	2:I:651:GLU:HB2	1.82	0.62
5:LL:169:SER:HB2	6:NN:398:ILE:HG23	1.81	0.62
7:CT:123:LEU:O	7:CT:128:ARG:NH2	2.32	0.62
16:Y:74:ARG:O	16:Y:78:SER:HB3	2.00	0.62
16:YY:74:ARG:O	16:YY:78:SER:HB3	2.00	0.62
19:E:40:DA:OP2	23:g:19:ARG:NH2	2.33	0.62
23:g:44:ARG:HB2	21:h:92:THR:HG22	1.80	0.62
4:H:49:GLN:O	4:H:53:LEU:N	2.33	0.62
10:P:236:ASN:ND2	12:O:211:GLU:OE1	2.32	0.62
16:Y:16:LEU:HD12	17:Z:57:LEU:HD22	1.81	0.62
13:TT:293:LEU:HD13	13:TT:301:ILE:HD11	1.81	0.62
8:CE:30:CYS:HB3	8:CE:33:CYS:HB2	1.82	0.61
10:PP:367:TYR:OH	11:QQ:298:PRO:HD2	2.00	0.61
2:I:433:ARG:HG2	2:I:485:LEU:HD12	1.82	0.61
2:I:483:LEU:HD11	2:I:528:SER:HB2	1.82	0.61
6:N:280:ARG:O	12:O:171:ARG:NH2	2.33	0.61
10:PP:272:TYR:HA	11:QQ:393:HIS:HE2	1.65	0.61
2:II:364:LEU:HG	2:II:368:PHE:HE2	1.65	0.61
2:I:73:PRO:HG3	2:I:117:VAL:HG12	1.82	0.61
11:Q:290:LYS:HG2	14:U:250:VAL:HG22	1.83	0.61
10:PP:345:ILE:HD11	11:QQ:336:LEU:HD11	1.80	0.61
3:K:218:GLU:HA	3:K:226:LYS:HA	1.82	0.61
7:CT:393:LYS:HE2	7:CT:410:ARG:HD3	1.82	0.61
12:OO:133:ASP:HB2	3:KK:28:GLN:HE22	1.64	0.61
2:II:215:ARG:NH2	18:D:80:DC:OP1	2.33	0.61
17:Z:118:GLU:O	17:Z:121:GLU:HG3	2.00	0.61
12:OO:240:ILE:HG13	12:OO:246:VAL:HG11	1.83	0.61
2:II:314:TYR:O	2:II:337:LYS:NZ	2.21	0.61
16:Y:150:LEU:HD12	17:Z:94:LEU:HD12	1.81	0.61
14:UU:208:GLN:O	14:UU:212:ARG:N	2.33	0.61
2:II:214:ASN:HB2	2:II:216:LYS:HZ3	1.65	0.61
8:ce:402:ILE:HA	8:ce:458:MET:HE1	1.83	0.60
5:L:115:LYS:HA	5:L:115:LYS:CE	2.31	0.60
5:L:131:HIS:CD2	5:L:229:ARG:HH12	2.19	0.60
13:T:348:LEU:HD21	15:W:3:THR:HB	1.82	0.60
16:YY:8:ILE:O	16:YY:12:ILE:HG23	2.01	0.60
23:c:69:GLY:O	23:c:73:ARG:HD2	2.01	0.60
12:OO:201:MET:HE2	12:OO:225:LYS:HG3	1.84	0.60
2:I:516:LEU:HD23	2:I:519:LEU:HD12	1.82	0.60
18:D:51:DA:H61	19:E:105:DT:H3	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:606:VAL:HA	3:K:57:LEU:HD21	1.84	0.60
3:K:164:LEU:HD22	3:K:204:ILE:HD11	1.84	0.60
5:LL:131:HIS:CD2	5:LL:229:ARG:HH12	2.19	0.60
4:H:72:LEU:HD13	4:H:82:LEU:HD22	1.83	0.60
5:LL:167:ARG:HD2	5:LL:167:ARG:C	2.27	0.60
13:T:286:LEU:HD23	13:T:290:ARG:HA	1.84	0.60
12:O:222:VAL:HG23	12:O:238:HIS:HB3	1.82	0.60
1:B:249:LEU:HD11	1:B:263:ALA:HA	1.83	0.60
5:LL:115:LYS:HA	5:LL:115:LYS:CE	2.31	0.60
11:Q:259:GLU:OE2	14:U:212:ARG:NH1	2.34	0.60
11:QQ:165:LEU:HD22	11:QQ:232:LEU:HD23	1.83	0.60
21:d:58:ILE:HD13	23:c:80:ILE:HD11	1.83	0.60
11:Q:150:HIS:HB3	13:T:317:GLY:H	1.66	0.60
2:I:506:ARG:HH12	3:K:89:TRP:NE1	1.98	0.60
3:K:100:GLN:OE1	4:H:107:GLN:NE2	2.35	0.60
7:CT:408:HIS:HB3	7:CT:471:GLU:HA	1.84	0.60
11:Q:146:TYR:HD2	11:Q:148:LEU:HG	1.66	0.60
2:II:293:VAL:HG11	2:II:299:LEU:HD12	1.84	0.60
7:CT:425:LEU:HD13	8:ce:274:PRO:HG2	1.83	0.60
7:CT:328:PHE:HB2	7:CT:353:PRO:HD3	1.84	0.60
5:L:166:PRO:O	5:L:169:SER:OG	2.15	0.60
16:Y:160:GLY:HA3	17:Z:108:LEU:HD21	1.83	0.60
18:D:74:DT:H2"	18:D:75:DG:H5"	1.83	0.60
6:NN:161:LEU:HD12	6:NN:220:TYR:HB3	1.84	0.59
5:L:167:ARG:HD2	5:L:167:ARG:C	2.26	0.59
10:PP:106:ASN:HD21	4:HH:47:HIS:CG	2.20	0.59
8:CE:24:CYS:SG	8:CE:26:ARG:NH2	2.75	0.59
22:e:217:ASP:OD1	22:a:207:HIS:NE2	2.34	0.59
3:K:118:LEU:HD22	4:H:127:LYS:HZ3	1.67	0.59
5:L:117:GLU:N	5:L:117:GLU:OE1	2.36	0.59
16:Y:8:ILE:O	16:Y:12:ILE:HG23	2.01	0.59
5:LL:191:TYR:HA	5:LL:194:ASN:HB2	1.84	0.59
4:H:99:GLU:HA	4:H:102:GLN:HG3	1.84	0.59
14:UU:172:LYS:HA	14:UU:175:LEU:HB2	1.83	0.59
2:II:409:ASP:HB3	2:II:412:THR:HG22	1.85	0.59
13:T:340:MET:HG3	15:W:45:LEU:HD22	1.84	0.59
12:O:295:HIS:HB2	12:O:309:PHE:HB2	1.84	0.59
16:YY:77:GLN:HA	16:YY:80:GLN:HG3	1.85	0.59
11:QQ:130:PHE:HB2	11:QQ:220:GLN:HE22	1.66	0.59
5:L:191:TYR:HA	5:L:194:ASN:HB2	1.84	0.59
11:Q:182:GLU:HA	11:Q:185:MET:HE3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:134:THR:HA	14:U:137:VAL:HG12	1.85	0.59
2:II:686:TRP:CG	2:II:687:ILE:H	2.20	0.59
3:K:221:THR:OG1	3:K:227:TYR:OH	2.16	0.59
5:LL:36:GLN:HE22	5:LL:38:ILE:HG12	1.68	0.59
8:CE:33:CYS:O	8:CE:37:GLY:N	2.36	0.59
12:OO:136:ILE:HA	12:OO:142:LYS:HB3	1.84	0.59
2:I:550:ASP:HB2	3:K:82:ARG:HH22	1.68	0.58
2:II:91:THR:HG21	13:TT:351:GLU:HB2	1.84	0.58
2:II:388:MET:HE1	4:HH:118:ARG:HG2	1.83	0.58
19:E:27:DT:H2''	19:E:28:DA:C8	2.38	0.58
13:TT:331:MET:HA	15:WW:89:GLN:HG2	1.85	0.58
2:I:540:ASP:HB2	4:H:51:ARG:HG2	1.84	0.58
8:ce:75:ILE:HA	8:ce:79:LYS:HB2	1.85	0.58
14:U:192:ILE:O	14:U:196:ASN:ND2	2.35	0.58
16:Y:77:GLN:HA	16:Y:80:GLN:HG3	1.85	0.58
11:QQ:217:LYS:O	11:QQ:220:GLN:NE2	2.31	0.58
3:K:57:LEU:HG	4:H:56:ARG:HD2	1.83	0.58
8:CE:15:SER:O	8:CE:18:THR:OG1	2.22	0.58
6:N:29:VAL:HG22	6:N:68:ARG:HE	1.67	0.58
8:ce:146:ARG:NH2	8:ce:160:ASP:OD2	2.37	0.58
12:O:136:ILE:HG13	12:O:137:LEU:HD12	1.85	0.58
7:CT:471:GLU:HG2	7:CT:472:LYS:HD3	1.85	0.58
19:E:98:DT:H2''	19:E:99:DA:C8	2.38	0.58
6:N:163:ASP:OD1	6:N:220:TYR:OH	2.19	0.58
2:II:559:ARG:NH1	2:II:713:ASP:OD2	2.36	0.58
21:d:124:LYS:NZ	23:c:22:LYS:O	2.36	0.58
5:LL:117:GLU:N	5:LL:117:GLU:OE1	2.36	0.58
2:II:609:ASP:OD2	3:KK:58:ARG:NH2	2.36	0.58
22:e:152:LEU:HD12	20:f:38:LEU:HD23	1.85	0.58
1:B:236:GLU:OE1	5:L:167:ARG:NH2	2.32	0.58
3:K:16:GLU:HA	3:K:19:ILE:HG22	1.85	0.58
8:CE:21:LYS:HE2	18:D:109:DC:H5	1.68	0.58
21:h:117:GLU:OE1	21:h:120:ARG:NH2	2.37	0.58
7:CT:345:ILE:HB	7:CT:367:ILE:HD13	1.85	0.58
6:NN:282:PRO:O	12:OO:168:ASN:ND2	2.37	0.58
8:ce:66:GLN:HE21	8:ce:420:ILE:HG21	1.69	0.58
2:II:434:GLU:O	2:II:438:LYS:NZ	2.37	0.57
2:I:251:VAL:O	2:I:255:ILE:N	2.34	0.57
5:L:36:GLN:HE22	5:L:38:ILE:HG12	1.68	0.57
14:U:169:LEU:O	14:U:173:LEU:HD23	2.04	0.57
17:Z:65:PHE:O	17:Z:69:ARG:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:E:76:DG:H2''	19:E:77:DG:C8	2.39	0.57
13:TT:320:GLN:HB2	13:TT:323:GLU:HB2	1.86	0.57
8:CE:14:CYS:O	8:CE:18:THR:N	2.37	0.57
13:T:320:GLN:NE2	13:T:323:GLU:OE1	2.37	0.57
14:UU:176:ARG:HH11	11:QQ:177:VAL:HG13	1.68	0.57
19:E:17:DT:H2''	19:E:18:DA:C8	2.40	0.57
10:P:331:ARG:NH2	10:P:334:GLN:OE1	2.38	0.57
13:TT:351:GLU:HG2	13:TT:352:LEU:HD12	1.86	0.57
2:I:87:ASN:HB3	4:H:175:THR:HA	1.86	0.57
14:UU:296:VAL:HG12	16:YY:177:LEU:HB2	1.87	0.57
4:HH:45:LEU:HD12	4:HH:49:GLN:HB2	1.86	0.57
1:B:316:MET:HE2	1:B:316:MET:HA	1.86	0.57
3:K:148:LEU:HD22	4:H:165:MET:HE1	1.87	0.57
4:H:169:GLN:HB3	4:H:177:ILE:HG12	1.86	0.57
7:CT:374:GLU:HA	7:CT:377:LEU:HD12	1.87	0.57
3:KK:171:ILE:O	3:KK:175:THR:OG1	2.20	0.57
22:e:207:HIS:NE2	22:a:217:ASP:OD1	2.38	0.57
8:ce:527:LEU:HD13	8:ce:590:PHE:HZ	1.70	0.57
10:P:273:LEU:HD21	10:P:277:SER:HA	1.86	0.57
2:II:328:ARG:N	2:II:335:SER:O	2.38	0.57
5:L:7:PHE:HB3	5:L:114:ILE:HG13	1.87	0.57
14:U:223:VAL:O	14:U:227:ILE:HG12	2.05	0.57
17:ZZ:105:LEU:HD22	11:QQ:357:LEU:HD13	1.86	0.57
2:II:456:CYS:SG	2:II:505:ASN:ND2	2.78	0.57
6:N:207:ASN:HB2	12:O:301:LEU:HD21	1.86	0.57
1:B:298:ALA:HB1	10:P:366:MET:HG2	1.87	0.56
7:CT:264:ILE:HA	7:CT:267:MET:HE1	1.87	0.56
2:II:433:ARG:NH2	2:II:488:ASP:OD2	2.38	0.56
19:E:21:DT:H2''	19:E:22:DC:C6	2.41	0.56
3:K:107:GLN:HA	4:H:121:ARG:NH2	2.21	0.56
11:Q:199:ILE:HG23	14:U:170:LEU:HB2	1.86	0.56
10:PP:348:TYR:O	10:PP:352:THR:OG1	2.23	0.56
17:ZZ:53:VAL:HA	17:ZZ:56:GLU:HG2	1.87	0.56
11:QQ:158:MET:HE1	11:QQ:227:ILE:HB	1.85	0.56
2:I:592:LEU:HD22	2:I:633:ILE:HB	1.87	0.56
11:Q:376:GLN:NE2	11:Q:380:ASP:OD2	2.38	0.56
10:PP:230:GLN:NE2	10:PP:304:MET:O	2.34	0.56
16:Y:50:ARG:NH1	17:Z:14:SER:O	2.38	0.56
5:LL:7:PHE:HB3	5:LL:114:ILE:HG13	1.87	0.56
14:U:190:LYS:O	14:U:194:ASP:N	2.19	0.56
2:II:303:TRP:HD1	2:II:306:LEU:HD12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:II:388:MET:HA	2:II:388:MET:HE3	1.86	0.56
2:I:613:GLN:HG2	12:O:124:PHE:C	2.31	0.56
5:LL:59:ARG:HG2	5:LL:72:LYS:HG2	1.88	0.56
10:PP:270:ARG:HH12	10:PP:283:GLU:HB2	1.70	0.56
2:II:575:ASN:HB3	2:II:578:VAL:HG22	1.87	0.56
3:KK:22:LYS:HZ1	4:HH:22:VAL:HG13	1.70	0.56
2:I:593:TYR:H	2:I:632:THR:HA	1.71	0.56
8:CE:186:TYR:HA	8:CE:189:HIS:HD2	1.70	0.56
14:U:296:VAL:HG22	16:Y:177:LEU:HD22	1.88	0.56
2:I:90:GLY:O	2:I:107:GLN:NE2	2.39	0.56
3:K:22:LYS:HD2	4:H:26:LEU:HD22	1.88	0.56
10:PP:170:GLN:HB2	10:PP:184:VAL:HG13	1.88	0.56
8:ce:54:SER:OG	8:ce:55:LYS:N	2.39	0.56
5:L:59:ARG:HG2	5:L:72:LYS:HG2	1.88	0.56
3:KK:22:LYS:HA	3:KK:25:PHE:HB2	1.88	0.56
18:D:82:DG:N2	19:E:75:DG:N2	2.45	0.56
19:E:21:DT:H2"	19:E:22:DC:C5	2.41	0.56
2:I:291:TRP:HZ3	2:I:309:PRO:HG2	1.70	0.56
16:Y:174:ILE:HD11	17:Z:122:PHE:CZ	2.41	0.56
8:CE:452:PHE:HA	8:CE:455:ARG:HD3	1.87	0.55
4:HH:12:ILE:O	4:HH:16:GLU:N	2.37	0.55
13:TT:293:LEU:HD22	13:TT:297:THR:HG21	1.88	0.55
2:I:672:ASN:ND2	4:H:74:GLU:OE2	2.39	0.55
5:L:20:ILE:HD12	5:L:33:LEU:HB2	1.89	0.55
12:OO:199:ARG:HE	12:OO:225:LYS:HD3	1.70	0.55
11:QQ:140:GLU:OE2	11:QQ:141:ARG:NH1	2.30	0.55
21:d:46:TYR:O	21:d:50:LYS:HG2	2.07	0.55
21:d:49:LEU:HD22	21:d:58:ILE:HD11	1.88	0.55
2:I:293:VAL:HG21	2:I:299:LEU:HD12	1.88	0.55
14:U:187:ARG:O	14:U:191:ASP:N	2.36	0.55
21:d:106:LEU:HD11	23:c:60:LEU:HD11	1.88	0.55
13:T:338:ASP:HA	13:T:341:PHE:CZ	2.41	0.55
17:ZZ:37:GLN:O	17:ZZ:41:HIS:ND1	2.34	0.55
1:A:320:LEU:HD11	1:A:325:ILE:HB	1.89	0.55
6:NN:279:GLU:OE2	12:OO:205:ARG:NH2	2.35	0.55
6:N:144:VAL:HG12	6:N:159:ILE:HG12	1.87	0.55
14:U:169:LEU:HD12	14:U:172:LYS:HZ3	1.72	0.55
12:O:122:GLN:HE22	12:O:126:PRO:HG3	1.72	0.55
18:D:82:DG:N2	19:E:75:DG:N3	2.55	0.55
20:f:83:THR:HG23	20:f:86:ASP:H	1.72	0.55
3:K:57:LEU:HD23	3:K:57:LEU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:348:TYR:O	10:P:352:THR:OG1	2.25	0.55
2:II:68:GLU:OE2	2:II:112:LYS:NZ	2.38	0.55
19:E:67:DT:H2"	19:E:68:DA:C8	2.41	0.55
20:b:89:TYR:HE1	21:d:87:TYR:CE1	2.25	0.55
1:B:223:ARG:NH1	1:B:227:HIS:HB2	2.22	0.55
11:Q:138:TYR:HE1	14:U:137:VAL:HG11	1.71	0.55
6:N:16:ASP:HB3	6:N:19:VAL:HG22	1.88	0.55
1:B:236:GLU:CD	5:L:167:ARG:HH21	2.15	0.55
3:K:11:TYR:HE2	4:H:12:ILE:HG23	1.71	0.55
9:SK:24:GLU:HA	9:SK:30:LYS:NZ	2.22	0.55
10:PP:164:HIS:ND1	10:PP:190:CYS:O	2.40	0.55
8:CE:254:ASN:OD1	8:CE:303:GLN:NE2	2.38	0.55
12:O:188:ILE:HG12	12:O:195:ILE:HG12	1.89	0.55
13:TT:278:LEU:HD13	13:TT:301:ILE:HG22	1.89	0.54
1:B:290:GLN:OE1	11:Q:294:LYS:NZ	2.28	0.54
5:LL:20:ILE:HD12	5:LL:33:LEU:HB2	1.89	0.54
9:SK:89:LYS:HE3	9:SK:126:VAL:HG11	1.89	0.54
1:B:301:LYS:O	1:B:304:GLU:HG3	2.07	0.54
12:OO:180:LEU:HD22	12:OO:201:MET:SD	2.47	0.54
6:N:239:ILE:HD12	6:N:241:LYS:HE2	1.89	0.54
4:H:47:HIS:HD2	10:P:106:ASN:HB3	1.73	0.54
13:T:340:MET:HE3	15:W:45:LEU:HB3	1.89	0.54
2:II:217:THR:O	2:II:221:HIS:N	2.36	0.54
19:E:146:DT:H2"	19:E:147:DG:C8	2.42	0.54
5:LL:59:ARG:C	5:LL:60:LEU:HD12	2.33	0.54
23:g:65:LEU:HD11	21:h:45:ILE:HG23	1.89	0.54
5:LL:215:LYS:HB3	5:LL:222:VAL:HB	1.89	0.54
7:CT:307:ARG:O	7:CT:333:ASN:ND2	2.41	0.54
10:P:318:MET:HE3	11:Q:335:MET:HE3	1.90	0.54
23:g:36:LEU:HD13	23:g:45:ILE:HD11	1.90	0.54
2:I:86:ILE:HG23	2:I:139:LEU:HD11	1.89	0.54
2:I:565:LYS:HD3	2:I:585:ILE:HD13	1.90	0.54
3:K:194:LEU:HD23	3:K:225:THR:HG23	1.90	0.54
12:O:282:ARG:NH2	12:O:300:ASP:O	2.39	0.54
2:I:587:ASP:O	2:I:591:TYR:N	2.41	0.54
3:K:78:PHE:CD2	4:H:65:LYS:HE2	2.42	0.54
8:ce:319:LEU:HG	8:ce:320:LEU:HG	1.88	0.54
6:N:61:LEU:HD13	6:N:71:ILE:HG22	1.88	0.54
12:O:313:ILE:HD11	12:O:363:PHE:HE1	1.73	0.54
2:II:76:TYR:CE2	2:II:122:PRO:HB3	2.43	0.54
2:I:291:TRP:CZ3	2:I:309:PRO:HG2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:II:632:THR:HG23	2:II:635:GLY:H	1.72	0.54
4:HH:10:GLU:O	4:HH:14:GLN:NE2	2.36	0.54
8:ce:146:ARG:HD2	8:ce:146:ARG:O	2.08	0.54
5:L:147:LEU:HD23	5:L:205:LEU:HD11	1.89	0.54
8:CE:443:VAL:HA	8:CE:446:PHE:HD2	1.72	0.54
6:N:250:SER:O	6:N:253:ASN:N	2.41	0.54
10:PP:147:LEU:O	10:PP:153:ARG:NH2	2.34	0.54
18:D:94:DT:O4	18:D:95:DA:N6	2.41	0.54
2:I:40:LEU:HD12	2:I:71:PHE:HA	1.90	0.53
5:LL:147:LEU:HD23	5:LL:205:LEU:HD11	1.89	0.53
11:Q:268:LEU:HA	11:Q:271:GLU:HG2	1.90	0.53
2:II:140:TRP:NE1	2:II:150:THR:OG1	2.28	0.53
5:L:94:ASN:OD1	5:L:95:ARG:HD2	2.08	0.53
5:L:215:LYS:HB3	5:L:222:VAL:HB	1.89	0.53
11:Q:174:LEU:HD11	11:Q:203:LYS:HD3	1.89	0.53
2:II:388:MET:HG3	4:HH:121:ARG:HD2	1.90	0.53
21:d:46:TYR:CZ	21:d:50:LYS:HD3	2.44	0.53
2:I:148:TRP:HZ3	2:I:225:LYS:HE3	1.74	0.53
16:Y:74:ARG:CG	17:Z:72:LEU:HD21	2.38	0.53
6:NN:9:ASP:HB3	6:NN:43:PHE:HE1	1.74	0.53
5:L:59:ARG:C	5:L:60:LEU:HD12	2.33	0.53
10:P:321:ILE:HD11	11:Q:334:LEU:HD11	1.91	0.53
14:UU:208:GLN:HA	14:UU:211:ALA:HB3	1.90	0.53
2:I:242:HIS:CG	2:I:243:PRO:HD3	2.43	0.53
3:K:9:ASP:OD1	4:H:8:GLN:NE2	2.41	0.53
3:K:45:GLY:H	4:H:42:ALA:HA	1.74	0.53
6:NN:235:ARG:HH22	16:YY:112:ARG:HD2	1.74	0.53
11:Q:215:LYS:HE3	11:Q:219:ARG:HH21	1.73	0.53
4:HH:110:LEU:O	4:HH:113:GLN:HG3	2.09	0.53
11:QQ:177:VAL:HG23	11:QQ:180:LYS:HE3	1.90	0.53
13:T:282:THR:HG21	13:T:298:TRP:HH2	1.73	0.53
2:II:219:LYS:NZ	18:D:80:DC:OP2	2.39	0.53
3:K:36:ILE:HD11	4:H:37:ARG:HD3	1.91	0.53
5:LL:131:HIS:CE1	5:LL:229:ARG:HH22	2.27	0.53
12:OO:320:LYS:HD3	12:OO:321:GLN:N	2.24	0.53
2:II:699:LYS:HD2	2:II:702:MET:HE2	1.90	0.53
3:KK:76:SER:OG	4:HH:16:GLU:OE2	2.25	0.53
13:TT:272:PRO:HA	13:TT:306:LEU:HD21	1.90	0.53
2:II:423:LEU:HD22	4:HH:118:ARG:HG3	1.91	0.53
5:LL:94:ASN:OD1	5:LL:95:ARG:HD2	2.08	0.53
17:ZZ:46:LEU:HD13	17:ZZ:49:ARG:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:41:DC:H2''	18:D:42:DA:C8	2.44	0.53
3:K:152:LEU:HD11	3:K:182:MET:HE3	1.90	0.53
7:CT:443:LEU:HD12	7:CT:467:ILE:HG22	1.91	0.53
5:L:27:LEU:HD21	5:L:60:LEU:HD23	1.91	0.53
6:N:219:ILE:HA	6:N:222:ARG:NH2	2.24	0.53
12:O:305:MET:HE3	12:O:305:MET:HA	1.90	0.53
2:II:94:VAL:HG13	2:II:97:ARG:HH21	1.74	0.53
11:QQ:211:LEU:HA	11:QQ:214:ILE:HG22	1.91	0.53
23:g:19:ARG:HA	23:g:22:LYS:HD3	1.91	0.53
4:H:52:LEU:HA	4:H:55:ILE:HD12	1.91	0.52
7:CT:467:ILE:HG13	7:CT:467:ILE:O	2.09	0.52
8:CE:28:ILE:HD12	8:CE:29:PRO:HA	1.91	0.52
11:Q:205:ARG:NH1	11:Q:206:LEU:HG	2.24	0.52
8:CE:6:THR:HB	8:CE:8:LEU:HD23	1.91	0.52
6:N:39:TRP:NE1	6:N:91:GLU:OE2	2.42	0.52
14:UU:224:ARG:HA	14:UU:227:ILE:HD12	1.91	0.52
17:ZZ:132:GLY:HA3	11:QQ:380:ASP:HB3	1.91	0.52
3:KK:178:VAL:HG22	3:KK:182:MET:HE2	1.90	0.52
11:QQ:258:LEU:HD13	11:QQ:261:ILE:HD12	1.91	0.52
9:SK:24:GLU:HA	9:SK:30:LYS:HZ1	1.74	0.52
17:Z:62:LYS:O	17:Z:66:ILE:HG12	2.09	0.52
3:KK:97:SER:O	3:KK:100:GLN:NE2	2.43	0.52
18:D:67:DT:H2''	18:D:68:DA:N7	2.23	0.52
18:D:134:DG:H2''	18:D:135:DA:C8	2.44	0.52
13:TT:271:LYS:O	15:WW:9:TYR:OH	2.26	0.52
2:I:438:LYS:O	2:I:442:SER:N	2.42	0.52
5:LL:27:LEU:HD21	5:LL:60:LEU:HD23	1.91	0.52
6:NN:341:MET:HE2	6:NN:341:MET:HA	1.90	0.52
5:L:131:HIS:CE1	5:L:229:ARG:HH22	2.27	0.52
3:K:213:ILE:HG13	3:K:214:ILE:HG12	1.91	0.52
13:T:280:HIS:HB2	15:W:1:MET:HG3	1.91	0.52
23:g:17:GLN:O	23:g:22:LYS:NZ	2.42	0.52
11:Q:217:LYS:HG3	11:Q:220:GLN:HE21	1.74	0.52
16:Y:181:ILE:HG23	16:Y:190:ILE:HG21	1.92	0.52
16:YY:11:PHE:HE1	17:ZZ:60:ARG:HB3	1.74	0.52
18:D:140:DT:H2''	18:D:141:DA:C8	2.45	0.52
7:CT:290:PHE:HA	7:CT:293:PHE:HB2	1.92	0.52
16:Y:208:MET:SD	16:Y:212:LEU:HD23	2.49	0.52
16:YY:5:TYR:HA	16:YY:8:ILE:HG22	1.91	0.52
1:B:330:MET:N	1:B:330:MET:HE2	2.25	0.52
2:I:390:ASN:OD1	4:H:118:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:725:LEU:HA	2:I:728:TYR:HD2	1.75	0.52
3:K:42:ASP:HB2	4:H:41:HIS:HD2	1.75	0.52
5:LL:22:LYS:NZ	5:LL:102:TRP:HE1	2.08	0.52
16:Y:98:ARG:HA	16:Y:101:VAL:HG22	1.92	0.52
2:II:154:ILE:HG23	2:II:193:ARG:HG2	1.92	0.52
2:I:437:VAL:HA	2:I:440:MET:HE2	1.90	0.52
2:I:587:ASP:OD1	2:I:588:LEU:N	2.42	0.52
6:NN:162:PHE:HB3	6:NN:194:LEU:HD13	1.92	0.52
16:YY:181:ILE:HG23	16:YY:190:ILE:HG21	1.92	0.52
20:f:27:ILE:HG22	20:f:56:ARG:HD3	1.91	0.52
2:I:352:GLU:OE1	2:I:395:ARG:NH1	2.42	0.51
7:CT:288:ILE:HD12	7:CT:312:ILE:HD13	1.92	0.51
14:U:146:PHE:HE1	14:U:185:MET:HG2	1.76	0.51
16:Y:207:GLU:O	16:Y:210:LEU:HG	2.10	0.51
3:KK:61:MET:HE2	3:KK:61:MET:HA	1.92	0.51
21:h:42:SER:HB3	21:h:63:MET:HE3	1.92	0.51
8:ce:200:TRP:HA	8:ce:204:MET:HB3	1.92	0.51
2:I:426:PRO:HB2	2:I:478:LEU:HD12	1.92	0.51
2:I:486:LEU:HD11	2:I:515:SER:HB3	1.90	0.51
2:I:509:THR:HA	2:I:512:PHE:HD2	1.76	0.51
7:CT:464:ARG:HH12	8:ce:336:ARG:CZ	2.24	0.51
8:CE:116:ASN:OD1	8:CE:137:TYR:OH	2.26	0.51
2:II:345:LEU:HD13	2:II:350:ARG:HH21	1.74	0.51
2:II:510:MET:SD	4:HH:100:LEU:CD2	2.98	0.51
14:UU:299:MET:HE1	16:YY:197:TYR:CE2	2.46	0.51
2:II:361:ILE:HD11	2:II:396:ILE:HG12	1.93	0.51
21:d:117:GLU:OE1	23:c:55:ALA:HB1	2.10	0.51
2:I:603:LEU:HD23	2:I:604:PHE:HD2	1.75	0.51
8:ce:100:MET:HA	8:ce:103:MET:HG3	1.92	0.51
9:SK:182:ALA:O	9:SK:186:ARG:NH2	2.44	0.51
8:CE:442:ILE:HD12	8:CE:492:LEU:HD21	1.92	0.51
17:Z:29:LEU:HD13	17:Z:39:LEU:CD1	2.40	0.51
2:II:214:ASN:HB2	2:II:216:LYS:NZ	2.25	0.51
6:NN:203:ALA:HB3	6:NN:212:PHE:HB2	1.93	0.51
5:L:22:LYS:NZ	5:L:102:TRP:HE1	2.08	0.51
8:CE:158:TYR:HD1	8:CE:232:ARG:HB2	1.75	0.51
12:OO:258:VAL:HG13	12:OO:263:ASP:HB2	1.93	0.51
11:QQ:206:LEU:HD23	11:QQ:209:ILE:HD11	1.93	0.51
2:I:234:LEU:HD23	2:I:238:LEU:HD23	1.92	0.51
3:K:17:ASN:OD1	3:K:21:ASN:ND2	2.43	0.51
7:CT:170:PHE:HB2	7:CT:196:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:II:512:PHE:HD2	2:II:553:LEU:HD11	1.76	0.51
18:D:38:DA:H2"	18:D:39:DG:C8	2.46	0.51
3:K:75:THR:HG22	4:H:86:LEU:HD12	1.92	0.51
5:LL:27:LEU:HG	5:LL:29:LEU:HD23	1.93	0.51
5:LL:207:SER:HB2	5:LL:217:MET:HG2	1.92	0.51
6:NN:207:ASN:ND2	12:OO:300:ASP:OD2	2.43	0.51
5:L:169:SER:HB2	6:N:398:ILE:HG23	1.93	0.51
8:CE:417:MET:HE1	8:CE:421:TYR:CD2	2.46	0.51
12:OO:128:VAL:HG13	4:HH:34:TYR:HD1	1.76	0.51
14:UU:180:THR:HG21	11:QQ:177:VAL:HG11	1.92	0.51
14:UU:300:ASP:HB3	14:UU:304:GLY:H	1.76	0.51
2:II:531:ALA:HB1	2:II:533:GLN:OE1	2.11	0.51
3:KK:24:TYR:HA	3:KK:27:LYS:HG2	1.91	0.51
11:QQ:335:MET:SD	11:QQ:335:MET:N	2.84	0.51
19:E:124:DC:H2"	19:E:125:DA:C8	2.46	0.51
2:I:224:LEU:HB2	2:I:259:LEU:HD13	1.91	0.51
10:P:337:LEU:HA	10:P:340:ILE:HG22	1.92	0.51
16:YY:90:LYS:HD2	16:YY:98:ARG:HD2	1.93	0.51
16:YY:153:LYS:NZ	17:ZZ:102:GLN:OE1	2.41	0.51
3:KK:7:VAL:HG23	3:KK:8:LEU:HD12	1.92	0.51
23:c:72:ALA:HB2	23:c:80:ILE:HG22	1.92	0.51
5:L:27:LEU:HG	5:L:29:LEU:HD23	1.93	0.51
14:UU:184:GLN:O	14:UU:188:ASP:N	2.43	0.51
2:II:506:ARG:HG3	2:II:510:MET:HG2	1.93	0.51
2:II:579:ARG:CZ	2:II:579:ARG:HA	2.41	0.51
3:K:216:VAL:HG13	3:K:217:ILE:H	1.76	0.50
4:H:57:HIS:O	4:H:61:ILE:HG12	2.11	0.50
5:L:207:SER:HB2	5:L:217:MET:HG2	1.92	0.50
10:P:148:LEU:HD11	6:N:295:LYS:HE3	1.93	0.50
11:Q:184:GLU:HB3	11:Q:188:MET:HE1	1.91	0.50
13:T:273:LEU:HB3	13:T:277:ASP:HB2	1.93	0.50
14:UU:192:ILE:HA	14:UU:195:ILE:HG22	1.92	0.50
19:E:47:DG:H2"	19:E:48:DA:C8	2.46	0.50
3:K:11:TYR:CE2	4:H:12:ILE:HG23	2.45	0.50
6:NN:39:TRP:HH2	6:NN:92:ILE:HD11	1.76	0.50
7:CT:169:GLN:HB2	7:CT:198:GLU:HG2	1.92	0.50
16:Y:5:TYR:HA	16:Y:8:ILE:HG22	1.91	0.50
16:Y:90:LYS:HD2	16:Y:98:ARG:HD2	1.93	0.50
2:II:505:ASN:OD1	3:KK:85:SER:OG	2.23	0.50
4:HH:27:LEU:HD12	4:HH:57:HIS:CD2	2.46	0.50
11:QQ:298:PRO:HA	11:QQ:301:ASN:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:23:DC:H2''	18:D:24:DG:C8	2.46	0.50
19:E:148:DT:H2''	19:E:149:DG:H8	1.76	0.50
2:I:423:LEU:O	4:H:118:ARG:NH1	2.44	0.50
6:NN:443:MET:HB3	6:NN:448:GLN:HE22	1.76	0.50
3:KK:123:HIS:O	3:KK:126:THR:OG1	2.29	0.50
18:D:131:DT:H2''	18:D:132:DA:C8	2.46	0.50
1:B:242:ILE:HD13	1:B:256:LYS:HG2	1.94	0.50
2:I:248:ALA:O	2:I:252:GLN:N	2.40	0.50
3:K:40:SER:OG	4:H:36:ILE:O	2.27	0.50
8:ce:475:ILE:HG22	8:ce:518:LYS:HB2	1.94	0.50
16:YY:158:GLN:NE2	11:QQ:340:ILE:HG12	2.26	0.50
16:YY:174:ILE:HD11	17:ZZ:122:PHE:CZ	2.46	0.50
11:QQ:157:ILE:O	11:QQ:161:SER:N	2.41	0.50
20:f:84:SER:HA	20:f:87:VAL:HG12	1.91	0.50
8:ce:68:TYR:HA	8:ce:545:ILE:HD11	1.93	0.50
6:N:60:LEU:HD13	21:d:43:SER:HB2	1.92	0.50
16:YY:98:ARG:HA	16:YY:101:VAL:HG22	1.92	0.50
2:II:172:LYS:HD3	2:II:207:SER:HB3	1.93	0.50
19:E:128:DT:H2''	19:E:129:DG:C8	2.46	0.50
2:I:597:VAL:HB	2:I:631:PHE:CD2	2.47	0.50
11:Q:134:ILE:HG13	14:U:141:LEU:HD13	1.94	0.50
16:Y:49:LYS:HG3	17:Z:19:LEU:HD12	1.94	0.50
17:Z:35:ASP:OD2	17:Z:37:GLN:NE2	2.39	0.50
11:QQ:370:LEU:O	11:QQ:374:MET:HB2	2.11	0.50
21:d:58:ILE:HG21	21:d:63:MET:SD	2.51	0.50
2:I:421:LEU:HD12	2:I:464:TYR:HB3	1.94	0.50
5:LL:20:ILE:HA	5:LL:23:LEU:HD12	1.93	0.50
7:CT:187:LEU:HD22	7:CT:192:LEU:HB2	1.93	0.50
9:SK:105:GLU:OE2	9:SK:144:LYS:NZ	2.41	0.50
15:W:64:ARG:HH21	15:W:77:HIS:HA	1.77	0.50
2:II:134:SER:HB2	4:HH:166:ILE:HD13	1.93	0.50
4:HH:12:ILE:O	4:HH:16:GLU:HG2	2.11	0.50
23:g:80:ILE:HB	21:h:58:ILE:HG22	1.94	0.50
12:OO:180:LEU:HD23	12:OO:181:VAL:N	2.27	0.50
16:YY:207:GLU:O	16:YY:210:LEU:HG	2.11	0.50
2:II:510:MET:CE	4:HH:100:LEU:HG	2.41	0.50
2:I:173:ARG:CZ	3:K:212:ASN:HA	2.41	0.50
3:K:156:LEU:HD13	3:K:178:VAL:HG12	1.94	0.50
10:PP:356:GLU:HA	10:PP:359:ASN:HB2	1.93	0.50
16:Y:189:ASP:C	16:Y:189:ASP:OD1	2.55	0.50
14:UU:307:LYS:HA	14:UU:310:ASN:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:QQ:210:ILE:HA	11:QQ:213:LYS:HB2	1.94	0.50
19:E:38:DT:H2"	19:E:39:DA:C8	2.47	0.50
23:g:56:VAL:HG21	21:h:102:VAL:HG21	1.93	0.50
15:WW:57:ILE:HD13	15:WW:82:THR:HG22	1.93	0.50
7:CT:124:ASP:HB2	7:CT:128:ARG:HH22	1.77	0.49
2:I:160:PRO:HB3	2:I:198:VAL:HA	1.93	0.49
2:I:549:ASP:OD1	2:I:549:ASP:N	2.41	0.49
2:I:654:GLU:HB3	2:I:687:ILE:HG21	1.93	0.49
3:K:99:ASP:O	3:K:103:MET:HG3	2.12	0.49
10:P:286:ILE:O	10:P:292:THR:OG1	2.24	0.49
6:N:121:VAL:HG11	6:N:211:ILE:HD11	1.93	0.49
2:II:7:ASP:O	2:II:11:SER:N	2.44	0.49
6:NN:49:GLY:HA3	6:NN:53:LEU:HD23	1.92	0.49
8:ce:307:ARG:NH2	8:ce:554:GLU:OE1	2.45	0.49
5:L:158:LEU:HD22	6:N:413:LEU:HD22	1.93	0.49
16:Y:114:ILE:O	16:Y:118:LEU:HD23	2.12	0.49
2:II:42:SER:HB2	2:II:77:LEU:H	1.78	0.49
2:II:218:LEU:O	2:II:222:ARG:N	2.42	0.49
2:II:224:LEU:HB3	2:II:259:LEU:HD22	1.94	0.49
2:II:683:GLN:HG2	2:II:684:HIS:N	2.26	0.49
11:QQ:182:GLU:HA	11:QQ:185:MET:HG2	1.94	0.49
3:K:53:PHE:HA	3:K:56:LEU:HB2	1.94	0.49
8:ce:84:ASP:OD1	8:ce:84:ASP:N	2.43	0.49
18:D:82:DG:H2"	18:D:83:DC:H5"	1.94	0.49
2:I:169:SER:HA	2:I:172:LYS:HE3	1.93	0.49
2:I:610:PHE:CZ	4:H:56:ARG:HG3	2.44	0.49
4:H:18:GLU:O	4:H:21:GLU:HG3	2.12	0.49
8:ce:158:TYR:OH	8:ce:228:HIS:O	2.26	0.49
11:Q:152:LYS:HB2	13:T:313:LYS:O	2.13	0.49
10:PP:270:ARG:NH1	10:PP:283:GLU:HB2	2.27	0.49
16:YY:190:ILE:HD11	17:ZZ:125:MET:HE1	1.95	0.49
2:II:77:LEU:HB2	2:II:81:LEU:HD23	1.95	0.49
3:KK:202:ILE:HG22	3:KK:203:PRO:HD3	1.95	0.49
18:D:128:DT:H2"	18:D:129:DA:C8	2.48	0.49
19:E:91:DG:OP2	20:b:36:ARG:NH2	2.32	0.49
2:I:634:THR:HG21	2:I:697:ARG:HG2	1.94	0.49
7:CT:27:ASN:HD21	9:SK:159:ARG:HH12	1.59	0.49
11:Q:146:TYR:CD2	11:Q:148:LEU:HG	2.45	0.49
12:O:156:ASP:HA	12:O:159:GLU:CD	2.38	0.49
2:I:89:LEU:HD21	2:I:111:CYS:HB2	1.94	0.49
2:I:641:TYR:CE2	4:H:91:GLU:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LL:29:LEU:HD12	5:LL:62:ILE:HD13	1.95	0.49
5:L:20:ILE:HA	5:L:23:LEU:HD12	1.93	0.49
8:CE:372:ALA:HA	8:CE:375:ARG:HE	1.78	0.49
11:Q:159:ILE:HG23	11:Q:218:LEU:HG	1.95	0.49
6:N:68:ARG:NH1	19:E:133:DG:OP2	2.35	0.49
14:UU:173:LEU:HD11	14:UU:176:ARG:HH21	1.78	0.49
16:YY:114:ILE:O	16:YY:118:LEU:HD23	2.12	0.49
18:D:91:DT:H2''	18:D:92:DA:C8	2.48	0.49
19:E:103:DG:H2''	19:E:104:DG:H5''	1.94	0.49
3:K:208:LEU:HB3	3:K:214:ILE:HD11	1.93	0.49
5:L:223:THR:HG22	5:L:225:THR:H	1.78	0.49
2:II:18:ARG:HG3	2:II:20:PRO:HD3	1.94	0.49
2:II:328:ARG:HE	2:II:335:SER:HA	1.78	0.49
3:KK:193:THR:HG23	3:KK:196:ASP:H	1.77	0.49
18:D:31:DT:H2''	18:D:32:DG:C8	2.48	0.49
18:D:37:DT:H2''	18:D:38:DA:C8	2.48	0.49
18:D:142:DT:H2''	18:D:143:DA:C8	2.48	0.49
19:E:13:DT:H2''	19:E:14:DA:C8	2.47	0.49
19:E:87:DG:H2''	19:E:88:DT:C6	2.47	0.49
22:e:144:LYS:O	22:e:148:SER:HB2	2.12	0.49
20:f:26:ASN:O	20:f:30:ILE:HD12	2.13	0.49
2:I:643:CYS:O	2:I:647:LEU:N	2.45	0.49
4:H:120:GLU:HA	4:H:123:GLU:CD	2.37	0.49
7:CT:285:GLU:HA	7:CT:289:ASN:HB3	1.95	0.49
8:CE:436:LYS:HA	8:CE:439:ILE:HD12	1.95	0.49
16:YY:142:GLU:HA	16:YY:145:ASN:HD21	1.78	0.49
2:II:621:PRO:HD3	4:HH:71:ARG:HD3	1.94	0.49
4:HH:6:GLU:HA	4:HH:9:TRP:HD1	1.78	0.49
18:D:49:DG:H1'	22:a:177:ARG:HH21	1.77	0.49
21:d:118:GLY:O	21:d:122:VAL:HG23	2.13	0.49
8:ce:528:ASP:OD1	8:ce:528:ASP:N	2.46	0.49
5:L:29:LEU:HD12	5:L:62:ILE:HD13	1.95	0.49
10:P:333:ASN:O	10:P:337:LEU:HD23	2.12	0.49
12:O:319:VAL:HG12	12:O:324:ILE:HA	1.95	0.49
3:KK:81:LEU:HD12	3:KK:84:GLN:HE21	1.77	0.49
18:D:50:DC:O4'	22:a:177:ARG:NH2	2.38	0.49
18:D:124:DG:H2''	18:D:125:DA:C8	2.48	0.49
20:f:32:LYS:HG2	20:f:33:PRO:HD3	1.95	0.49
2:I:648:ARG:HH12	2:I:649:ARG:HG3	1.77	0.48
7:CT:87:TRP:NE1	7:CT:137:MET:HE1	2.28	0.48
5:L:13:GLN:N	5:L:84:PRO:HG2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:PP:141:LYS:HE3	10:PP:147:LEU:HD23	1.94	0.48
16:Y:163:LYS:HE3	16:Y:163:LYS:HA	1.94	0.48
16:YY:163:LYS:HA	16:YY:163:LYS:HE3	1.94	0.48
17:ZZ:94:LEU:HD13	17:ZZ:97:ILE:HD11	1.95	0.48
2:II:215:ARG:HA	2:II:218:LEU:HB2	1.95	0.48
20:f:26:ASN:C	20:f:29:GLY:H	2.21	0.48
13:TT:286:LEU:HD21	15:WW:58:LEU:HD13	1.95	0.48
1:A:274:ASP:O	1:A:278:ILE:HG12	2.13	0.48
1:B:252:ARG:HH12	6:N:443:MET:CE	2.18	0.48
1:B:329:ASP:C	1:B:330:MET:HE2	2.38	0.48
2:I:79:LYS:HB3	4:H:179:TYR:HE2	1.77	0.48
3:K:206:ARG:HH22	13:T:345:HIS:HB2	1.77	0.48
8:ce:424:THR:HG23	8:ce:427:SER:HB2	1.95	0.48
8:ce:516:LYS:HA	8:ce:519:LEU:HD23	1.95	0.48
12:OO:258:VAL:HG11	12:OO:264:ALA:HB2	1.94	0.48
2:II:541:ILE:HA	4:HH:51:ARG:HH22	1.78	0.48
4:HH:10:GLU:HA	4:HH:13:GLN:OE1	2.13	0.48
4:HH:80:ASN:HB3	4:HH:83:PHE:HB3	1.94	0.48
5:LL:13:GLN:N	5:LL:84:PRO:HG2	2.27	0.48
6:NN:89:LEU:HA	6:NN:92:ILE:HD12	1.95	0.48
8:CE:23:LYS:NZ	18:D:110:DC:OP2	2.32	0.48
8:CE:201:GLU:CD	8:CE:201:GLU:H	2.22	0.48
11:Q:264:ARG:HH22	17:Z:83:HIS:CD2	2.32	0.48
13:T:315:LYS:HD2	13:T:331:MET:HE2	1.96	0.48
14:UU:185:MET:O	14:UU:189:LEU:N	2.33	0.48
2:II:699:LYS:HA	2:II:702:MET:HG3	1.95	0.48
22:a:144:LYS:O	22:a:148:SER:HB2	2.12	0.48
22:a:215:LYS:O	22:a:219:GLN:HG2	2.13	0.48
2:I:493:LEU:HD22	2:I:508:SER:HA	1.95	0.48
3:K:42:ASP:HB2	4:H:41:HIS:CD2	2.48	0.48
6:NN:33:TYR:CE1	6:NN:58:LEU:HB3	2.48	0.48
6:N:82:ASP:OD1	6:N:82:ASP:N	2.46	0.48
17:Z:42:TRP:HD1	17:Z:45:LEU:HD12	1.79	0.48
2:II:138:HIS:HB3	4:HH:170:ILE:HG21	1.95	0.48
3:KK:140:THR:HG21	4:HH:141:PRO:HB2	1.95	0.48
11:QQ:352:GLU:O	11:QQ:355:SER:OG	2.28	0.48
22:e:215:LYS:O	22:e:219:GLN:HG2	2.13	0.48
3:K:108:ASN:HA	3:K:111:ASN:HB2	1.95	0.48
11:Q:223:PHE:HZ	14:U:141:LEU:HD22	1.78	0.48
12:OO:164:ILE:HA	10:PP:150:MET:HE1	1.94	0.48
13:T:282:THR:HG21	13:T:298:TRP:CH2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Z:49:ARG:HA	17:Z:52:ARG:HG2	1.96	0.48
2:II:336:LEU:HD23	2:II:339:LEU:HD12	1.96	0.48
2:II:583:GLN:NE2	2:II:587:ASP:OD2	2.46	0.48
19:E:9:DG:H2''	19:E:10:DA:C8	2.48	0.48
2:I:629:LYS:HA	2:I:632:THR:HG22	1.95	0.48
3:K:57:LEU:HG	4:H:56:ARG:HH11	1.78	0.48
3:K:114:LEU:HD22	4:H:125:MET:HE1	1.96	0.48
6:NN:296:LYS:HA	10:PP:127:ARG:HA	1.95	0.48
5:L:172:GLY:HA2	6:N:396:ARG:HE	1.79	0.48
9:SK:93:TRP:HH2	9:SK:145:PRO:HB2	1.78	0.48
10:PP:212:LEU:HD11	10:PP:237:PHE:CZ	2.47	0.48
14:UU:304:GLY:O	14:UU:308:LYS:NZ	2.35	0.48
4:HH:21:GLU:HG2	4:HH:22:VAL:N	2.29	0.48
11:QQ:357:LEU:HD23	11:QQ:360:LEU:HD11	1.95	0.48
18:D:121:DA:H2''	18:D:122:DA:C8	2.49	0.48
19:E:8:DT:H2''	19:E:9:DG:C8	2.49	0.48
19:E:88:DT:H2''	19:E:89:DA:N7	2.28	0.48
20:f:50:LEU:O	20:f:54:GLU:HG3	2.13	0.48
20:f:93:ARG:HH22	21:h:105:ILE:HD13	1.78	0.48
5:LL:223:THR:HG22	5:LL:225:THR:H	1.78	0.48
6:NN:158:ARG:HG3	6:NN:201:TYR:HE1	1.79	0.48
10:P:147:LEU:HD21	12:O:181:VAL:HG12	1.96	0.48
17:Z:5:GLN:HA	17:Z:8:HIS:HD2	1.78	0.48
19:E:46:DG:H2''	19:E:47:DG:C8	2.48	0.48
8:CE:8:LEU:HD11	8:CE:26:ARG:HB3	1.96	0.48
20:b:37:ARG:HE	22:a:152:LEU:HB3	1.78	0.48
2:I:509:THR:HB	2:I:553:LEU:HD22	1.96	0.48
2:I:546:PHE:HB3	2:I:588:LEU:HD13	1.96	0.48
5:LL:59:ARG:HH11	5:LL:59:ARG:CG	2.26	0.48
7:CT:115:ILE:HG13	7:CT:116:ASP:N	2.22	0.48
5:L:59:ARG:CG	5:L:59:ARG:HH11	2.26	0.48
17:Z:90:LEU:O	17:Z:94:LEU:HD23	2.14	0.48
19:E:70:DA:H2''	19:E:71:DA:H8	1.77	0.48
19:E:138:DC:H2''	19:E:139:DG:C8	2.49	0.48
2:I:293:VAL:O	2:I:333:ARG:NH1	2.42	0.48
8:CE:348:ILE:HG21	8:CE:406:GLN:HB3	1.96	0.48
11:Q:199:ILE:HD12	14:U:170:LEU:HB2	1.96	0.48
12:OO:318:PHE:HB3	12:OO:326:SER:HB3	1.96	0.48
16:Y:142:GLU:HA	16:Y:145:ASN:HD21	1.78	0.48
2:II:49:VAL:HG21	2:II:85:ILE:HG12	1.96	0.48
1:A:315:TYR:HA	1:A:318:ARG:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:165:PRO:HG3	3:K:237:SER:HB3	1.95	0.47
5:LL:12:LYS:HG3	5:LL:109:VAL:HG12	1.96	0.47
7:CT:20:VAL:HA	9:SK:151:CYS:SG	2.54	0.47
7:CT:261:ILE:HD11	7:CT:299:LYS:HG2	1.95	0.47
6:N:49:GLY:HA3	6:N:53:LEU:HD23	1.94	0.47
6:N:139:ILE:HG22	6:N:140:TYR:CD1	2.49	0.47
20:b:31:THR:HB	20:b:33:PRO:HD2	1.95	0.47
1:A:297:SER:O	1:A:300:GLU:HG3	2.14	0.47
8:ce:81:LYS:HD3	8:ce:250:PRO:HD2	1.97	0.47
8:CE:474:GLN:HE22	8:CE:486:LEU:HB2	1.80	0.47
12:OO:208:VAL:HG23	12:OO:276:VAL:HG22	1.96	0.47
12:O:232:SER:HB3	12:O:257:LEU:HD12	1.95	0.47
17:ZZ:39:LEU:O	17:ZZ:43:TYR:N	2.39	0.47
11:QQ:159:ILE:HG22	11:QQ:219:ARG:HH21	1.78	0.47
19:E:15:DT:H2''	19:E:16:DA:C8	2.50	0.47
19:E:72:DC:H6	19:E:72:DC:H5'	1.79	0.47
2:I:138:HIS:O	2:I:141:GLN:NE2	2.47	0.47
6:NN:82:ASP:N	6:NN:82:ASP:OD1	2.47	0.47
6:NN:317:GLU:HB3	6:NN:322:ARG:NH2	2.29	0.47
5:L:12:LYS:HG3	5:L:109:VAL:HG12	1.96	0.47
16:Y:115:GLU:OE1	16:Y:115:GLU:C	2.57	0.47
16:YY:39:CYS:SG	16:YY:40:ARG:NH1	2.80	0.47
3:KK:121:LEU:HD12	4:HH:128:LEU:HD22	1.96	0.47
8:CE:58:LEU:HG	8:CE:59:PRO:HD3	1.97	0.47
10:PP:231:LEU:O	10:PP:234:THR:OG1	2.32	0.47
17:Z:58:GLU:HA	17:Z:61:ILE:HG12	1.95	0.47
14:UU:173:LEU:HD22	11:QQ:199:ILE:HD12	1.96	0.47
4:HH:7:LYS:HD3	4:HH:7:LYS:C	2.39	0.47
2:I:702:MET:SD	2:I:703:HIS:N	2.88	0.47
3:K:107:GLN:HA	4:H:121:ARG:HH21	1.78	0.47
3:K:152:LEU:O	3:K:156:LEU:HG	2.14	0.47
3:K:216:VAL:HG13	3:K:217:ILE:N	2.28	0.47
12:OO:172:MET:HE3	12:OO:172:MET:HA	1.95	0.47
14:U:157:ASP:HB3	14:U:171:TYR:CG	2.50	0.47
17:ZZ:27:GLN:HA	17:ZZ:30:GLN:HG2	1.96	0.47
18:D:27:DC:H2''	18:D:28:DA:C8	2.49	0.47
21:d:50:LYS:HE3	21:d:50:LYS:HA	1.96	0.47
1:A:242:ILE:HG21	1:A:256:LYS:HG2	1.96	0.47
2:I:97:ARG:HB2	3:K:163:ASN:HA	1.96	0.47
5:LL:142:TRP:HB2	5:LL:167:ARG:HD3	1.97	0.47
7:CT:122:TYR:CD2	7:CT:179:LEU:HD22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CE:432:ILE:O	8:CE:436:LYS:HG3	2.14	0.47
11:Q:158:MET:HE2	11:Q:162:ILE:HG12	1.96	0.47
14:U:235:ASP:OD1	14:U:235:ASP:N	2.48	0.47
16:YY:201:LEU:O	16:YY:205:LEU:HD23	2.15	0.47
18:D:57:DT:H2''	18:D:58:DA:N7	2.29	0.47
2:I:510:MET:HG3	3:K:89:TRP:CZ2	2.50	0.47
5:LL:190:PRO:O	5:LL:194:ASN:N	2.46	0.47
6:NN:56:GLU:HA	6:NN:59:ASP:HB2	1.95	0.47
7:CT:110:TYR:HB3	7:CT:114:LEU:HD23	1.97	0.47
9:SK:189:GLU:HA	9:SK:192:GLU:HB2	1.97	0.47
8:CE:47:LYS:C	8:CE:48:LEU:HD23	2.40	0.47
8:CE:249:GLU:HG2	8:CE:252:LEU:HD12	1.96	0.47
12:OO:142:LYS:HG2	12:OO:145:ARG:HH12	1.79	0.47
16:Y:175:ASN:HA	16:Y:178:THR:HG22	1.96	0.47
16:Y:201:LEU:O	16:Y:205:LEU:HD23	2.15	0.47
16:YY:175:ASN:HA	16:YY:178:THR:HG22	1.96	0.47
4:HH:23:TYR:O	4:HH:27:LEU:HD23	2.14	0.47
18:D:79:DC:H1'	18:D:80:DC:C6	2.50	0.47
2:I:95:PHE:HZ	3:K:204:ILE:HG13	1.79	0.47
3:K:125:MET:HE2	3:K:125:MET:HA	1.96	0.47
9:SK:121:ARG:C	9:SK:125:LYS:HZ2	2.22	0.47
12:O:348:LEU:HA	12:O:358:LYS:HD2	1.97	0.47
16:YY:148:LYS:HZ3	11:QQ:346:VAL:HG13	1.78	0.47
2:II:184:PRO:O	2:II:188:THR:OG1	2.29	0.47
2:II:303:TRP:HA	2:II:306:LEU:HG	1.95	0.47
18:D:46:DC:H2''	18:D:47:DT:C5	2.49	0.47
18:D:97:DT:H2''	18:D:98:DG:C8	2.50	0.47
18:D:136:DA:H2''	18:D:137:DA:C8	2.49	0.47
1:A:310:TYR:HA	1:A:313:ILE:HG22	1.96	0.47
1:B:328:GLU:OE1	1:B:333:HIS:NE2	2.48	0.47
2:I:615:LEU:HD23	2:I:620:ILE:HG13	1.95	0.47
7:CT:18:LYS:HG3	7:CT:110:TYR:CZ	2.49	0.47
8:CE:109:ASP:N	8:CE:109:ASP:OD1	2.48	0.47
10:P:254:LYS:HG3	10:P:300:PHE:HD2	1.78	0.47
14:U:188:ASP:HA	14:U:191:ASP:HB2	1.97	0.47
4:HH:6:GLU:O	4:HH:9:TRP:HB2	2.15	0.47
2:I:93:THR:HG22	13:T:350:LEU:HD21	1.96	0.47
5:LL:205:LEU:HD21	5:LL:208:VAL:HG23	1.97	0.47
6:NN:7:LEU:HD12	6:NN:11:TYR:CG	2.50	0.47
10:P:275:ASN:HB3	10:P:278:ASP:HB3	1.97	0.47
10:P:344:LEU:O	10:P:348:TYR:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:113:ARG:HG2	6:N:119:TYR:HB2	1.97	0.47
14:UU:180:THR:HA	14:UU:183:ASP:HB2	1.96	0.47
3:KK:55:GLU:HA	3:KK:58:ARG:HB3	1.97	0.47
13:TT:285:PHE:CG	15:WW:55:ARG:HG2	2.50	0.47
2:I:513:ILE:HA	2:I:516:LEU:HB2	1.97	0.46
4:H:24:ARG:NH1	4:H:57:HIS:HB3	2.29	0.46
4:H:62:ASN:OD1	4:H:63:LEU:N	2.48	0.46
7:CT:332:ASP:OD1	7:CT:332:ASP:N	2.46	0.46
7:CT:420:ASN:OD1	7:CT:421:GLN:N	2.48	0.46
10:P:198:GLU:OE1	10:P:198:GLU:N	2.49	0.46
6:N:68:ARG:HA	6:N:71:ILE:HG12	1.97	0.46
13:T:301:ILE:O	13:T:305:SER:HB2	2.14	0.46
2:II:351:ASP:OD1	2:II:351:ASP:N	2.47	0.46
2:II:440:MET:HE2	2:II:440:MET:HA	1.98	0.46
2:II:620:ILE:HD12	2:II:626:LYS:HG3	1.96	0.46
3:KK:74:LEU:HD23	4:HH:20:VAL:HG12	1.97	0.46
23:g:101:ASN:OD1	23:g:102:VAL:N	2.47	0.46
5:LL:163:ILE:HG12	6:NN:402:LEU:HD22	1.96	0.46
6:N:39:TRP:CD1	6:N:88:GLN:HG2	2.50	0.46
6:N:386:GLY:O	6:N:439:SER:HB2	2.14	0.46
14:UU:256:LEU:HG	11:QQ:297:HIS:NE2	2.30	0.46
14:UU:307:LYS:O	14:UU:311:LYS:N	2.48	0.46
2:II:189:LEU:HD22	2:II:265:LEU:HB2	1.97	0.46
2:II:254:THR:HA	2:II:257:MET:HE2	1.97	0.46
4:HH:22:VAL:HA	4:HH:25:GLU:CD	2.40	0.46
11:QQ:161:SER:HA	11:QQ:164:ARG:NE	2.30	0.46
19:E:65:DA:H2"	19:E:66:DT:C5	2.50	0.46
20:f:53:GLU:OE1	20:f:53:GLU:N	2.40	0.46
1:A:315:TYR:O	1:A:319:VAL:HG23	2.16	0.46
2:I:177:HIS:NE2	3:K:215:THR:HG21	2.30	0.46
2:I:467:GLN:O	4:H:111:HIS:NE2	2.49	0.46
2:I:634:THR:HB	2:I:665:ILE:HB	1.97	0.46
11:Q:203:LYS:HB2	14:U:170:LEU:HD11	1.97	0.46
18:D:135:DA:H2"	18:D:136:DA:C8	2.50	0.46
18:D:147:DC:H2"	18:D:148:DA:C8	2.51	0.46
20:b:81:THR:HG23	22:a:177:ARG:HB3	1.96	0.46
1:B:286:LEU:O	1:B:289:GLU:HG3	2.15	0.46
3:K:94:ASN:O	3:K:98:VAL:N	2.33	0.46
4:H:61:ILE:HG22	4:H:65:LYS:NZ	2.30	0.46
5:LL:36:GLN:HE21	5:LL:38:ILE:HG23	1.81	0.46
8:ce:130:ILE:HD11	8:ce:136:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CE:26:ARG:HH12	18:D:108:DT:H5''	1.81	0.46
14:UU:150:LEU:HD21	11:QQ:210:ILE:HG21	1.97	0.46
2:II:383:ILE:HD12	2:II:419:GLY:HA3	1.98	0.46
11:QQ:377:MET:HE3	11:QQ:377:MET:HA	1.97	0.46
18:D:95:DA:N1	19:E:62:DA:N6	2.64	0.46
3:K:194:LEU:HB2	3:K:225:THR:HG23	1.98	0.46
16:Y:192:GLU:OE1	16:Y:192:GLU:N	2.35	0.46
2:II:510:MET:HE2	4:HH:100:LEU:HG	1.97	0.46
1:A:306:LEU:HA	1:B:306:LEU:HD13	1.97	0.46
2:I:140:TRP:CZ3	2:I:171:ILE:HA	2.50	0.46
4:H:110:LEU:O	4:H:114:LEU:HG	2.15	0.46
6:NN:138:LYS:O	11:QQ:257:ARG:NH1	2.43	0.46
11:Q:202:LYS:O	11:Q:205:ARG:HD3	2.15	0.46
11:Q:350:LYS:HE2	14:U:283:ILE:HD13	1.96	0.46
17:Z:53:VAL:O	17:Z:57:LEU:HG	2.16	0.46
2:II:151:PRO:HA	2:II:154:ILE:HD12	1.96	0.46
3:KK:89:TRP:CH2	3:KK:93:MET:HG3	2.51	0.46
3:KK:168:ASP:O	3:KK:169:GLU:HG2	2.16	0.46
2:I:474:LEU:HD13	4:H:112:LYS:HZ2	1.80	0.46
2:I:641:TYR:O	2:I:645:ILE:HG13	2.16	0.46
2:I:667:GLU:HG3	2:I:693:ILE:HG21	1.97	0.46
11:Q:142:LEU:HD13	11:Q:146:TYR:CE2	2.50	0.46
11:Q:369:GLU:OE2	17:Z:127:ARG:NH2	2.48	0.46
16:Y:104:GLU:HB2	16:Y:106:GLN:NE2	2.31	0.46
17:Z:74:ARG:HA	17:Z:74:ARG:NE	2.29	0.46
2:II:312:VAL:HA	2:II:315:MET:HE2	1.97	0.46
2:II:445:MET:HE2	2:II:445:MET:HA	1.97	0.46
2:II:483:LEU:O	2:II:487:HIS:ND1	2.38	0.46
3:KK:230:LEU:HD11	4:HH:164:LEU:HD13	1.97	0.46
18:D:88:DT:H2''	18:D:89:DA:N7	2.31	0.46
22:a:138:ALA:O	22:a:142:ILE:HG13	2.16	0.46
2:I:493:LEU:HB3	2:I:508:SER:OG	2.16	0.46
2:I:594:ARG:HH21	2:I:725:LEU:HD23	1.80	0.46
2:I:610:PHE:HD1	4:H:60:GLN:NE2	2.14	0.46
8:ce:555:MET:HE1	8:CE:269:VAL:HG22	1.96	0.46
5:L:59:ARG:HH11	5:L:59:ARG:HG3	1.81	0.46
5:L:97:GLU:O	5:L:100:LEU:HB3	2.15	0.46
5:L:142:TRP:HB2	5:L:167:ARG:HD3	1.97	0.46
10:PP:358:CYS:O	10:PP:362:LEU:HB2	2.15	0.46
14:UU:163:ASP:OD1	14:UU:163:ASP:N	2.49	0.46
3:KK:6:ASP:HA	3:KK:9:ASP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:QQ:210:ILE:O	11:QQ:214:ILE:N	2.42	0.46
18:D:9:DC:H2''	18:D:10:DA:C8	2.51	0.46
18:D:119:DA:H2''	18:D:120:DA:C8	2.51	0.46
23:g:75:ASN:O	23:g:75:ASN:ND2	2.27	0.46
2:I:95:PHE:C	3:K:163:ASN:HD22	2.24	0.46
2:I:536:ILE:HD11	2:I:539:PRO:HA	1.98	0.46
5:L:36:GLN:HE21	5:L:38:ILE:HG23	1.81	0.46
5:L:205:LEU:HD21	5:L:208:VAL:HG23	1.97	0.46
11:Q:217:LYS:HA	11:Q:220:GLN:HG3	1.97	0.46
13:T:295:LYS:HA	13:T:298:TRP:CD1	2.51	0.46
16:Y:206:GLU:O	16:Y:209:LYS:HB3	2.16	0.46
16:YY:99:ASN:HB3	16:YY:105:PRO:HB3	1.97	0.46
2:II:597:VAL:HG21	2:II:603:LEU:HD22	1.96	0.46
19:E:128:DT:H2''	19:E:129:DG:H8	1.81	0.46
6:NN:33:TYR:HE1	6:NN:58:LEU:HB3	1.81	0.46
8:CE:64:PHE:HE2	8:CE:541:LEU:HD23	1.81	0.46
12:OO:142:LYS:HA	12:OO:145:ARG:NH1	2.31	0.46
16:Y:74:ARG:HG3	17:Z:72:LEU:HD21	1.98	0.46
16:YY:206:GLU:O	16:YY:209:LYS:HB3	2.16	0.46
4:HH:53:LEU:HD11	4:HH:56:ARG:HH21	1.80	0.46
19:E:3:DT:H2''	19:E:4:DT:H5'	1.98	0.46
8:ce:456:HIS:ND1	8:ce:458:MET:HG2	2.31	0.45
9:SK:18:VAL:HG23	9:SK:19:ASP:N	2.27	0.45
11:Q:197:LYS:HE2	11:Q:197:LYS:HA	1.97	0.45
14:U:268:GLU:OE2	14:U:275:SER:OG	2.34	0.45
4:HH:25:GLU:O	4:HH:29:THR:OG1	2.27	0.45
18:D:126:DA:H2''	18:D:127:DA:C8	2.50	0.45
18:D:132:DA:H2''	18:D:133:DA:C8	2.51	0.45
8:ce:273:ARG:HD3	8:ce:337:GLU:HB3	1.98	0.45
16:Y:39:CYS:SG	16:Y:40:ARG:NH1	2.80	0.45
17:Z:93:ALA:O	17:Z:97:ILE:HG12	2.17	0.45
16:YY:190:ILE:HD12	16:YY:194:PHE:HE2	1.81	0.45
2:II:173:ARG:O	2:II:177:HIS:N	2.48	0.45
18:D:150:DT:H2''	18:D:151:DG:C8	2.50	0.45
2:I:536:ILE:HB	2:I:542:MET:HE2	1.97	0.45
7:CT:124:ASP:HB2	7:CT:128:ARG:HH12	1.81	0.45
2:II:63:LYS:HB3	2:II:106:LEU:HD13	1.98	0.45
2:II:216:LYS:HZ2	18:D:80:DC:H5	1.63	0.45
18:D:88:DT:H2''	18:D:89:DA:C8	2.51	0.45
19:E:132:DC:H2''	19:E:133:DG:C8	2.51	0.45
20:b:63:LEU:O	20:b:67:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:g:28:PRO:HD3	21:h:44:TYR:CD2	2.50	0.45
4:H:71:ARG:O	4:H:74:GLU:N	2.49	0.45
5:LL:97:GLU:O	5:LL:100:LEU:HB3	2.15	0.45
8:ce:69:GLU:O	8:ce:73:THR:OG1	2.32	0.45
8:ce:123:GLY:HA2	8:ce:126:TYR:CE2	2.50	0.45
8:ce:157:LYS:HA	8:ce:157:LYS:HD3	1.79	0.45
10:P:174:ARG:HH22	6:N:287:LYS:NZ	2.14	0.45
4:HH:27:LEU:HD12	4:HH:57:HIS:HD2	1.80	0.45
22:e:138:ALA:O	22:e:142:ILE:HG13	2.16	0.45
1:B:318:ARG:NH1	1:B:319:VAL:HG23	2.32	0.45
2:I:639:LEU:HD23	2:I:642:ILE:HD12	1.99	0.45
2:I:665:ILE:HG22	2:I:693:ILE:HD11	1.98	0.45
5:L:77:GLY:HA3	5:L:85:MET:HB3	1.99	0.45
8:CE:516:LYS:NZ	8:CE:601:TYR:OH	2.48	0.45
12:OO:310:VAL:HG11	12:OO:363:PHE:CE2	2.50	0.45
6:N:410:PHE:CE2	6:N:433:GLY:HA2	2.52	0.45
12:O:156:ASP:OD1	12:O:157:ARG:HD2	2.16	0.45
14:UU:249:LYS:HD2	14:UU:249:LYS:HA	1.74	0.45
16:YY:77:GLN:HA	16:YY:80:GLN:CG	2.47	0.45
2:II:593:TYR:HB2	2:II:718:LEU:HD21	1.99	0.45
20:b:71:VAL:O	20:b:75:GLU:HG3	2.17	0.45
1:A:288:SER:OG	1:B:288:SER:OG	2.27	0.45
5:LL:59:ARG:HH11	5:LL:59:ARG:HG3	1.81	0.45
5:LL:158:LEU:HD13	6:NN:409:ILE:HG23	1.97	0.45
7:CT:468:TYR:OH	9:SK:104:ASP:OD2	2.21	0.45
8:CE:376:GLU:HA	8:CE:379:ILE:HG12	1.99	0.45
12:OO:136:ILE:HG13	12:OO:137:LEU:HD12	1.98	0.45
16:Y:99:ASN:HB3	16:Y:105:PRO:HB3	1.97	0.45
18:D:18:DG:H2"	18:D:19:DA:C8	2.52	0.45
4:H:117:SER:O	4:H:120:GLU:HG3	2.17	0.45
5:LL:77:GLY:HA3	5:LL:85:MET:HB3	1.99	0.45
5:LL:173:LEU:HG	6:NN:398:ILE:HD13	1.99	0.45
9:SK:182:ALA:HB1	9:SK:186:ARG:HH22	1.80	0.45
8:CE:588:SER:O	8:CE:590:PHE:N	2.49	0.45
6:N:153:PRO:HB2	6:N:206:LEU:HG	1.99	0.45
12:O:141:SER:OG	12:O:145:ARG:NH1	2.50	0.45
14:UU:201:GLU:O	14:UU:205:GLN:N	2.35	0.45
4:HH:63:LEU:O	4:HH:66:THR:OG1	2.29	0.45
22:e:179:GLN:O	22:e:183:ILE:HG12	2.17	0.45
13:TT:321:LYS:HZ1	15:WW:41:ASN:HB3	1.82	0.45
1:B:283:LEU:HD11	11:Q:291:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:OO:281:ARG:HD2	12:OO:322:ASN:H	1.81	0.45
6:N:161:LEU:HG	6:N:220:TYR:CD1	2.52	0.45
6:N:374:SER:OG	6:N:375:ARG:N	2.49	0.45
13:T:334:ILE:HD13	13:T:340:MET:SD	2.56	0.45
16:Y:77:GLN:HA	16:Y:80:GLN:CG	2.47	0.45
16:YY:155:GLN:HA	16:YY:158:GLN:HG2	1.99	0.45
2:II:439:PHE:O	2:II:442:SER:OG	2.30	0.45
4:HH:32:ARG:HH12	4:HH:45:LEU:HD22	1.82	0.45
20:f:61:SER:O	20:f:64:GLU:HG2	2.16	0.45
2:I:610:PHE:CZ	4:H:59:LEU:HD23	2.52	0.45
2:I:698:VAL:O	2:I:702:MET:HG3	2.17	0.45
8:CE:417:MET:HE1	8:CE:421:TYR:HD2	1.82	0.45
12:OO:294:ILE:HA	12:OO:310:VAL:HG23	1.99	0.45
12:O:143:ARG:O	12:O:143:ARG:NH1	2.43	0.45
16:YY:74:ARG:HA	16:YY:77:GLN:OE1	2.17	0.45
2:II:120:LEU:HD11	2:II:238:LEU:HD11	1.97	0.45
21:d:109:GLU:HA	21:d:112:LYS:NZ	2.32	0.45
20:f:55:VAL:HA	20:f:58:VAL:HG12	1.99	0.45
20:f:93:ARG:NH2	21:h:105:ILE:HD13	2.32	0.45
1:B:297:SER:O	1:B:300:GLU:HG3	2.17	0.45
3:K:79:LEU:HA	3:K:82:ARG:HG2	1.98	0.45
6:NN:287:LYS:HA	6:NN:287:LYS:HD2	1.72	0.45
8:ce:191:TYR:O	8:ce:192:LEU:HD12	2.17	0.45
5:L:190:PRO:O	5:L:194:ASN:N	2.46	0.45
10:P:128:ILE:HA	10:P:132:THR:HG21	1.99	0.45
11:Q:209:ILE:HG22	11:Q:213:LYS:HE2	1.99	0.45
11:Q:352:GLU:OE1	16:Y:152:LEU:HD21	2.17	0.45
12:OO:308:PHE:HD2	12:OO:315:VAL:HB	1.82	0.45
12:O:343:LYS:HZ3	12:O:344:TRP:NE1	2.15	0.45
16:Y:74:ARG:HA	16:Y:77:GLN:OE1	2.17	0.45
14:UU:187:ARG:O	14:UU:191:ASP:HB2	2.17	0.45
2:II:364:LEU:HG	2:II:368:PHE:CE2	2.49	0.45
2:II:424:TRP:CZ2	2:II:426:PRO:HB3	2.52	0.45
19:E:8:DT:H2"	19:E:9:DG:H8	1.82	0.45
21:d:111:ALA:O	21:d:115:VAL:HG22	2.17	0.45
22:e:177:ARG:HD2	22:e:177:ARG:HA	1.64	0.45
2:I:479:ILE:HD11	2:I:528:SER:HB3	1.99	0.44
2:I:603:LEU:H	2:I:606:VAL:H	1.65	0.44
7:CT:454:ILE:HD13	7:CT:477:LEU:HB3	1.99	0.44
8:ce:307:ARG:NH1	8:ce:552:ASN:O	2.50	0.44
8:CE:84:ASP:OD2	8:CE:86:THR:OG1	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:144:ASN:O	14:U:148:ASN:HB2	2.17	0.44
2:II:565:LYS:HA	2:II:565:LYS:HD2	1.76	0.44
3:KK:17:ASN:O	3:KK:21:ASN:ND2	2.50	0.44
19:E:129:DG:H2''	19:E:130:DA:H8	1.81	0.44
23:g:22:LYS:O	21:h:124:LYS:NZ	2.47	0.44
2:I:424:TRP:O	2:I:471:ASN:ND2	2.49	0.44
2:I:646:ILE:HG13	2:I:704:LEU:HD13	1.99	0.44
4:H:65:LYS:O	4:H:69:LEU:CB	2.60	0.44
14:U:150:LEU:O	14:U:153:GLN:HG3	2.17	0.44
14:U:207:LYS:HD3	14:U:207:LYS:HA	1.75	0.44
4:HH:87:GLN:HA	4:HH:90:LEU:HD12	1.99	0.44
18:D:118:DA:H2''	18:D:119:DA:C8	2.52	0.44
19:E:79:DG:H2''	19:E:80:DA:C8	2.53	0.44
19:E:114:DT:H2''	19:E:115:DG:C8	2.52	0.44
21:h:112:LYS:HA	21:h:115:VAL:HG22	1.99	0.44
1:A:278:ILE:HD11	1:B:277:ASN:ND2	2.33	0.44
2:I:243:PRO:HG2	2:I:245:ASN:OD1	2.17	0.44
4:H:134:LYS:HB3	4:H:134:LYS:HE2	1.77	0.44
7:CT:443:LEU:HD22	7:CT:446:VAL:HG11	1.98	0.44
11:Q:238:TYR:O	11:Q:242:GLN:HG2	2.16	0.44
6:N:9:ASP:O	6:N:85:ASN:ND2	2.49	0.44
10:PP:294:ILE:HG22	10:PP:325:LEU:HD11	1.99	0.44
14:UU:182:SER:HA	14:UU:185:MET:HG2	1.99	0.44
17:ZZ:87:LEU:O	17:ZZ:91:ILE:HG12	2.18	0.44
2:II:686:TRP:CG	2:II:687:ILE:N	2.84	0.44
2:I:636:ILE:O	2:I:640:SER:N	2.48	0.44
3:K:156:LEU:HA	3:K:160:LEU:HB3	1.99	0.44
8:ce:188:LEU:HD12	8:ce:189:HIS:N	2.32	0.44
8:CE:301:TYR:CZ	8:CE:353:ARG:HA	2.52	0.44
14:UU:199:ASN:O	14:UU:203:CYS:N	2.31	0.44
17:ZZ:39:LEU:HA	17:ZZ:42:TRP:HB2	2.00	0.44
2:II:513:ILE:HG13	2:II:556:ALA:HB2	2.00	0.44
11:QQ:158:MET:CE	11:QQ:227:ILE:HB	2.47	0.44
18:D:78:DC:H2''	18:D:79:DC:C6	2.53	0.44
19:E:81:DC:H2''	19:E:82:DA:H8	1.82	0.44
3:K:79:LEU:HD12	3:K:82:ARG:HD2	2.00	0.44
5:LL:131:HIS:CE1	5:LL:141:THR:HG1	2.35	0.44
8:CE:586:GLU:HG2	8:CE:591:ARG:HH22	1.83	0.44
10:P:365:ASP:OD1	10:P:366:MET:N	2.50	0.44
16:Y:150:LEU:HD23	16:Y:150:LEU:HA	1.83	0.44
16:Y:155:GLN:HA	16:Y:158:GLN:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:UU:223:VAL:O	14:UU:227:ILE:HG13	2.18	0.44
16:YY:11:PHE:CE1	17:ZZ:60:ARG:HB3	2.52	0.44
19:E:82:DA:H2''	19:E:83:DG:H8	1.81	0.44
13:TT:301:ILE:HA	13:TT:304:GLU:HG2	1.99	0.44
2:I:473:VAL:HB	2:I:522:LEU:HD21	1.99	0.44
2:I:645:ILE:O	2:I:648:ARG:NH1	2.51	0.44
4:H:99:GLU:HA	4:H:102:GLN:CG	2.48	0.44
11:QQ:207:LEU:O	11:QQ:211:LEU:N	2.44	0.44
1:B:249:LEU:HD12	1:B:262:CYS:SG	2.58	0.44
2:I:291:TRP:HZ2	2:I:315:MET:HG2	1.83	0.44
2:I:344:ILE:HG21	2:I:356:PRO:HG2	1.98	0.44
2:I:560:TYR:O	2:I:564:THR:N	2.36	0.44
2:I:648:ARG:NH1	2:I:649:ARG:HG3	2.33	0.44
3:K:89:TRP:HZ2	4:H:100:LEU:HD21	1.81	0.44
4:H:35:LEU:HD11	4:H:49:GLN:NE2	2.28	0.44
7:CT:438:LEU:HD23	7:CT:438:LEU:HA	1.77	0.44
5:L:131:HIS:CE1	5:L:141:THR:HG1	2.35	0.44
8:CE:587:PRO:HG2	2:II:725:LEU:HD13	2.00	0.44
16:Y:190:ILE:HD12	16:Y:194:PHE:HE2	1.82	0.44
17:ZZ:100:LEU:HA	17:ZZ:103:GLN:HE22	1.83	0.44
2:II:76:TYR:C	2:II:77:LEU:HD23	2.43	0.44
18:D:111:DG:H4'	23:g:44:ARG:HB3	2.00	0.44
21:d:94:SER:OG	21:d:97:GLU:OE2	2.30	0.44
22:a:179:GLN:O	22:a:183:ILE:HG12	2.17	0.44
3:K:79:LEU:HD21	4:H:90:LEU:HG	1.99	0.44
5:L:8:LEU:HD21	5:L:111:MET:HB3	2.00	0.44
8:CE:443:VAL:HA	8:CE:446:PHE:CD2	2.51	0.44
10:P:266:LYS:O	10:P:267:ARG:HG2	2.18	0.44
10:PP:321:ILE:HG13	11:QQ:334:LEU:HD11	2.00	0.44
16:Y:38:VAL:HG11	17:Z:42:TRP:CZ3	2.53	0.44
2:II:706:ASN:O	2:II:712:ARG:NH1	2.51	0.44
20:b:32:LYS:HG3	20:b:52:TYR:CE2	2.53	0.44
2:I:544:LYS:HG3	4:H:51:ARG:NH1	2.32	0.44
3:K:33:ILE:HA	3:K:36:ILE:HG22	1.99	0.44
4:H:45:LEU:HD11	4:H:49:GLN:NE2	2.29	0.44
6:NN:39:TRP:HZ3	6:NN:84:LEU:HD12	1.83	0.44
7:CT:27:ASN:ND2	9:SK:159:ARG:HH12	2.16	0.44
5:L:10:ILE:HD11	5:L:87:LEU:HD23	2.00	0.44
8:CE:206:LEU:HD13	8:CE:499:ILE:O	2.17	0.44
11:Q:213:LYS:HG2	11:Q:216:LYS:HZ2	1.83	0.44
12:OO:128:VAL:HG21	4:HH:30:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:189:LEU:HA	14:U:192:ILE:HG12	2.00	0.44
16:Y:24:ASP:HA	17:Z:49:ARG:NH1	2.13	0.44
14:UU:158:PHE:CE1	14:UU:172:LYS:HB3	2.52	0.44
14:UU:190:LYS:HA	14:UU:193:LEU:HB2	2.00	0.44
3:KK:6:ASP:OD1	3:KK:7:VAL:N	2.51	0.44
23:g:19:ARG:HG3	23:g:29:VAL:HG11	1.99	0.44
2:I:108:SER:HG	2:I:148:TRP:HE1	1.65	0.43
8:CE:463:ILE:HA	8:CE:466:VAL:HG12	1.98	0.43
13:T:345:HIS:CA	13:T:353:GLN:HG2	2.45	0.43
15:W:11:LEU:HB3	15:W:43:LYS:HD2	2.00	0.43
12:O:155:SER:O	12:O:158:SER:OG	2.29	0.43
16:Y:163:LYS:O	16:Y:167:ILE:HG12	2.18	0.43
14:UU:156:LYS:HB3	14:UU:156:LYS:HE2	1.79	0.43
14:UU:176:ARG:NH1	11:QQ:177:VAL:HG13	2.32	0.43
2:II:45:LEU:HD11	2:II:73:PRO:HB3	1.99	0.43
4:HH:11:ARG:O	4:HH:14:GLN:HG2	2.18	0.43
19:E:93:DG:H2''	19:E:94:DC:H5''	2.00	0.43
2:I:235:LYS:O	2:I:238:LEU:HG	2.18	0.43
6:NN:39:TRP:CH2	6:NN:88:GLN:HB3	2.53	0.43
8:CE:19:ARG:HG2	8:CE:20:ARG:CZ	2.48	0.43
14:U:310:ASN:HA	14:U:313:ASN:ND2	2.33	0.43
12:O:284:ILE:HG21	12:O:352:LEU:HG	2.00	0.43
2:II:92:PRO:HD3	2:II:101:GLN:HG3	2.00	0.43
2:II:149:ILE:HG22	2:II:153:VAL:HG23	2.00	0.43
2:II:660:PHE:CZ	2:II:662:SER:HB3	2.52	0.43
18:D:34:DT:H2''	18:D:35:DC:C6	2.53	0.43
19:E:88:DT:H2''	19:E:89:DA:C8	2.53	0.43
22:a:177:ARG:HD2	22:a:177:ARG:HA	1.64	0.43
2:I:510:MET:HE2	4:H:100:LEU:HD21	1.94	0.43
5:LL:60:LEU:HB3	5:LL:95:ARG:HG2	2.00	0.43
8:ce:338:GLU:HG2	8:ce:343:VAL:HG21	2.00	0.43
5:L:60:LEU:HB3	5:L:95:ARG:HG2	2.00	0.43
8:CE:103:MET:HG2	8:CE:164:TRP:CZ2	2.52	0.43
12:OO:308:PHE:HZ	12:OO:359:LEU:HD11	1.83	0.43
12:O:318:PHE:HB3	12:O:326:SER:HB3	1.99	0.43
3:KK:24:TYR:HD1	3:KK:27:LYS:HZ3	1.67	0.43
11:QQ:164:ARG:HA	11:QQ:167:GLU:HG2	1.99	0.43
18:D:77:DC:H2''	18:D:78:DC:C5	2.54	0.43
21:h:94:SER:OG	21:h:95:ALA:N	2.50	0.43
2:I:610:PHE:CD1	4:H:60:GLN:NE2	2.87	0.43
3:K:15:LEU:HD13	4:H:19:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CE:414:LEU:O	8:CE:417:MET:HB2	2.18	0.43
10:PP:314:CYS:SG	10:PP:315:PHE:N	2.91	0.43
2:II:181:ARG:HB2	15:WW:2:ASP:HB3	1.99	0.43
2:II:242:HIS:HB3	2:II:245:ASN:HB3	2.01	0.43
4:HH:11:ARG:O	4:HH:15:LEU:HD23	2.19	0.43
1:A:291:ASN:O	1:A:294:GLN:HG3	2.17	0.43
1:B:328:GLU:HG3	1:B:330:MET:HE1	1.99	0.43
2:I:542:MET:O	2:I:545:VAL:HG22	2.17	0.43
2:I:648:ARG:HB2	2:I:657:LYS:HZ1	1.83	0.43
5:LL:214:THR:HG22	5:LL:223:THR:HG23	2.00	0.43
6:NN:393:ILE:HB	6:NN:398:ILE:HD12	2.00	0.43
8:ce:456:HIS:O	8:ce:459:VAL:HG22	2.19	0.43
5:L:164:GLU:OE1	6:N:401:LYS:NZ	2.39	0.43
11:Q:349:ASP:OD2	11:Q:352:GLU:HG3	2.17	0.43
6:N:39:TRP:NE1	6:N:88:GLN:HG2	2.33	0.43
4:HH:19:HIS:O	4:HH:19:HIS:ND1	2.41	0.43
11:QQ:130:PHE:HB3	11:QQ:134:ILE:HD12	1.99	0.43
18:D:35:DC:H2"	18:D:36:DG:C8	2.54	0.43
21:d:53:HIS:CD2	23:c:73:ARG:HH22	2.36	0.43
21:d:55:ASP:OD1	21:d:56:THR:N	2.52	0.43
21:h:85:ALA:HB2	21:h:93:ILE:HG22	2.01	0.43
2:I:146:GLN:O	2:I:150:THR:OG1	2.34	0.43
5:LL:8:LEU:HD21	5:LL:111:MET:HB3	2.00	0.43
7:CT:78:GLU:HA	7:CT:84:ILE:HD11	1.99	0.43
14:U:168:LYS:O	14:U:172:LYS:HG2	2.19	0.43
17:ZZ:20:ILE:HG12	17:ZZ:25:PHE:HD1	1.82	0.43
22:a:184:MET:SD	22:a:184:MET:N	2.92	0.43
2:I:74:ASP:OD1	2:I:74:ASP:N	2.46	0.43
2:I:492:LEU:HD22	10:P:105:LEU:HD22	2.00	0.43
6:NN:198:ARG:HH21	6:NN:218:ASP:HB2	1.84	0.43
16:YY:163:LYS:O	16:YY:167:ILE:HG12	2.17	0.43
2:II:64:VAL:HG21	2:II:105:VAL:HG22	2.00	0.43
2:II:193:ARG:HH22	2:II:261:GLU:HB3	1.84	0.43
3:KK:175:THR:HG22	3:KK:179:MET:HE3	2.00	0.43
19:E:129:DG:H2"	19:E:130:DA:C8	2.53	0.43
2:I:586:MET:O	2:I:590:ASN:N	2.33	0.43
3:K:204:ILE:HD12	3:K:204:ILE:H	1.83	0.43
5:LL:36:GLN:NE2	5:LL:38:ILE:HG12	2.33	0.43
8:ce:125:LEU:O	8:ce:295:ARG:NH2	2.52	0.43
8:CE:456:HIS:CG	8:CE:457:PRO:HD2	2.53	0.43
11:Q:181:TYR:HB3	14:U:173:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:OO:189:LYS:HG3	12:OO:196:PHE:CE1	2.54	0.43
12:O:155:SER:O	12:O:158:SER:N	2.52	0.43
12:O:298:ASP:OD1	12:O:298:ASP:N	2.51	0.43
16:Y:174:ILE:HD12	16:Y:174:ILE:HA	1.81	0.43
14:UU:146:PHE:HA	14:UU:150:LEU:HB2	2.00	0.43
17:ZZ:56:GLU:HG3	17:ZZ:60:ARG:HH12	1.83	0.43
2:II:124:HIS:CE1	2:II:128:GLU:HB2	2.54	0.43
2:II:158:THR:HA	2:II:197:LEU:HD21	2.01	0.43
18:D:20:DG:H2''	18:D:21:DG:C8	2.54	0.43
19:E:72:DC:C2	19:E:73:DG:N7	2.87	0.43
21:d:49:LEU:HD12	21:d:52:THR:OG1	2.18	0.43
22:e:184:MET:SD	22:e:184:MET:N	2.92	0.43
1:B:285:LYS:HB2	1:B:285:LYS:HE3	1.78	0.43
2:I:288:VAL:HB	2:I:292:ASP:HB2	2.01	0.43
4:H:26:LEU:O	4:H:30:LEU:HB2	2.18	0.43
5:LL:81:MET:H	5:LL:81:MET:HG2	1.51	0.43
7:CT:123:LEU:HG	7:CT:128:ARG:NH1	2.34	0.43
8:ce:171:ILE:O	8:ce:205:GLN:NE2	2.51	0.43
5:L:153:THR:OG1	6:N:415:GLU:OE2	2.22	0.43
8:CE:14:CYS:HB3	8:CE:17:CYS:HB2	1.47	0.43
16:Y:139:VAL:HA	16:Y:142:GLU:HG3	2.01	0.43
16:YY:139:VAL:HA	16:YY:142:GLU:HG3	2.01	0.43
11:QQ:251:GLU:HA	11:QQ:254:ASN:HB2	2.00	0.43
22:e:153:ILE:HG13	22:e:191:GLU:OE2	2.19	0.43
22:e:161:LEU:HA	20:f:26:ASN:HD21	1.84	0.43
2:I:78:THR:HG23	2:I:81:LEU:H	1.83	0.43
2:I:176:MET:HG3	2:I:211:ILE:HG22	2.01	0.43
5:LL:242:PHE:HE2	2:II:371:GLN:HG3	1.84	0.43
6:NN:270:TRP:NE1	6:NN:434:GLU:OE2	2.39	0.43
8:ce:252:LEU:HD13	8:CE:227:ALA:HB2	2.00	0.43
9:SK:121:ARG:NH1	9:SK:156:GLU:OE1	2.49	0.43
12:OO:169:VAL:HG11	10:PP:185:VAL:HG21	2.01	0.43
6:N:129:ILE:HD11	6:N:146:MET:HE3	2.01	0.43
2:II:510:MET:HE2	4:HH:100:LEU:CG	2.49	0.43
3:KK:35:GLU:HA	3:KK:38:LYS:NZ	2.34	0.43
4:HH:120:GLU:O	4:HH:124:LEU:HG	2.18	0.43
11:QQ:161:SER:HA	11:QQ:164:ARG:HE	1.84	0.43
11:QQ:285:LYS:HE3	11:QQ:285:LYS:HB3	1.81	0.43
18:D:49:DG:O3'	22:a:177:ARG:NH2	2.52	0.43
18:D:107:DT:H2''	18:D:108:DT:C5	2.54	0.43
19:E:72:DC:H5'	19:E:72:DC:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:37:ARG:HG2	22:a:152:LEU:HD13	2.00	0.43
15:WW:6:LEU:O	15:WW:10:LEU:HG	2.19	0.43
2:I:97:ARG:HA	2:I:97:ARG:HD3	1.87	0.42
2:I:305:GLN:HA	4:H:138:PRO:HA	2.01	0.42
2:I:536:ILE:HG21	2:I:581:GLN:OE1	2.19	0.42
3:K:109:ASN:O	3:K:112:SER:OG	2.34	0.42
5:LL:10:ILE:HD11	5:LL:87:LEU:HD23	2.00	0.42
5:L:214:THR:HG22	5:L:223:THR:HG23	2.00	0.42
8:CE:158:TYR:HB3	8:CE:232:ARG:HD2	2.01	0.42
14:U:150:LEU:HD23	14:U:178:PHE:CD1	2.54	0.42
16:Y:77:GLN:O	16:Y:80:GLN:HG3	2.19	0.42
21:h:115:VAL:O	21:h:119:THR:HG23	2.19	0.42
4:H:168:LEU:HD23	4:H:171:HIS:HD2	1.83	0.42
6:NN:385:VAL:HG22	6:NN:409:ILE:HD13	2.00	0.42
8:ce:540:ILE:HD12	8:ce:597:PHE:CE2	2.54	0.42
12:OO:143:ARG:HH21	12:OO:147:LEU:HD13	1.83	0.42
2:II:20:PRO:HG2	2:II:24:LEU:H	1.84	0.42
2:II:216:LYS:HD2	18:D:79:DC:H2"	2.01	0.42
19:E:11:DA:H2"	19:E:12:DA:C8	2.54	0.42
19:E:24:DT:H2"	19:E:25:DA:C8	2.54	0.42
23:c:38:ARG:HG2	23:c:38:ARG:HH21	1.85	0.42
23:c:97:LYS:HD2	23:c:97:LYS:C	2.45	0.42
22:a:153:ILE:HG13	22:a:191:GLU:OE2	2.19	0.42
3:K:9:ASP:HA	3:K:12:ILE:HD13	2.01	0.42
3:K:164:LEU:HD23	3:K:174:LEU:HD13	2.00	0.42
5:L:36:GLN:NE2	5:L:38:ILE:HG12	2.33	0.42
8:CE:503:LYS:HA	8:CE:503:LYS:HD3	1.79	0.42
11:Q:249:SER:O	11:Q:252:LEU:HG	2.19	0.42
11:Q:286:ARG:HA	11:Q:289:GLU:HG3	2.01	0.42
6:N:163:ASP:OD2	6:N:197:ARG:NE	2.48	0.42
17:Z:39:LEU:HD23	17:Z:39:LEU:HA	1.81	0.42
2:II:297:GLU:OE1	3:KK:120:LYS:NZ	2.35	0.42
18:D:121:DA:H2"	18:D:122:DA:N7	2.34	0.42
23:g:19:ARG:HA	23:g:22:LYS:HB2	2.00	0.42
22:a:154:SER:HB2	22:a:157:PRO:CD	2.47	0.42
3:K:53:PHE:HA	3:K:56:LEU:HD12	1.99	0.42
7:CT:99:LEU:HD21	9:SK:158:ILE:HD12	2.01	0.42
8:CE:45:SER:OG	8:CE:46:THR:N	2.52	0.42
10:P:300:PHE:CE1	10:P:321:ILE:HD12	2.54	0.42
12:OO:164:ILE:HD12	12:OO:164:ILE:H	1.85	0.42
6:N:102:GLU:N	6:N:102:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:KK:164:LEU:HD21	3:KK:204:ILE:HG12	2.01	0.42
3:K:194:LEU:HD22	3:K:205:TYR:CE2	2.43	0.42
8:ce:441:LEU:O	8:ce:445:ASN:ND2	2.53	0.42
8:CE:456:HIS:HD2	8:CE:458:MET:HG3	1.85	0.42
17:ZZ:9:ASN:OD1	17:ZZ:10:TYR:N	2.52	0.42
2:II:135:ILE:HG23	4:HH:170:ILE:HD11	2.01	0.42
11:QQ:129:GLU:HB2	11:QQ:132:LYS:HE2	2.02	0.42
18:D:138:DT:H2''	18:D:139:DA:N7	2.34	0.42
19:E:90:DC:H2''	19:E:91:DG:H8	1.85	0.42
2:I:233:ILE:O	2:I:237:ILE:HG12	2.19	0.42
7:CT:19:GLU:HA	7:CT:22:PHE:HB3	2.02	0.42
7:CT:375:ASN:HA	7:CT:378:LYS:NZ	2.34	0.42
10:P:195:ASN:OD1	10:P:223:ASN:ND2	2.53	0.42
12:OO:157:ARG:NH1	12:OO:157:ARG:HG2	2.35	0.42
6:N:68:ARG:HB3	19:E:132:DC:OP1	2.19	0.42
2:II:78:THR:OG1	2:II:79:LYS:N	2.52	0.42
2:II:315:MET:SD	2:II:356:PRO:HG3	2.60	0.42
2:II:459:SER:HB3	2:II:507:PHE:HB3	2.00	0.42
18:D:20:DG:H2''	18:D:21:DG:H8	1.85	0.42
18:D:138:DT:H2''	18:D:139:DA:C8	2.54	0.42
10:P:138:LEU:HD23	10:P:138:LEU:HA	1.91	0.42
11:Q:152:LYS:HA	13:T:317:GLY:HA2	2.01	0.42
12:O:121:HIS:O	12:O:137:LEU:HD22	2.19	0.42
16:YY:148:LYS:HZ3	11:QQ:346:VAL:HG22	1.85	0.42
17:ZZ:53:VAL:O	17:ZZ:57:LEU:N	2.42	0.42
21:d:50:LYS:HE3	21:d:54:PRO:HA	2.01	0.42
22:e:156:ILE:HB	22:e:157:PRO:HD3	2.02	0.42
2:I:285:ASP:N	2:I:305:GLN:OE1	2.53	0.42
5:L:5:TRP:HB2	5:L:221:ILE:HG23	2.02	0.42
14:U:154:ALA:HB1	14:U:175:LEU:HA	2.02	0.42
14:UU:285:ASP:OD1	14:UU:285:ASP:N	2.53	0.42
2:II:681:ILE:HA	2:II:685:GLY:HA2	2.02	0.42
21:d:82:SER:OG	23:c:41:TYR:O	2.32	0.42
22:e:204:LEU:HD12	22:a:207:HIS:CE1	2.55	0.42
20:f:84:SER:O	20:f:88:VAL:HG22	2.20	0.42
2:I:674:PHE:O	2:II:683:GLN:HB2	2.19	0.42
4:H:30:LEU:HD21	12:O:128:VAL:HG11	2.01	0.42
5:LL:5:TRP:HB2	5:LL:221:ILE:HG23	2.02	0.42
8:ce:463:ILE:HD13	8:ce:463:ILE:HA	1.93	0.42
12:OO:225:LYS:HB3	12:OO:234:PHE:CE1	2.55	0.42
12:OO:312:ASP:OD2	12:OO:312:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:57:THR:HA	6:N:60:LEU:HD12	2.02	0.42
14:U:215:ASP:OD1	14:U:219:GLN:NE2	2.46	0.42
17:Z:70:SER:O	17:Z:74:ARG:HG2	2.20	0.42
14:UU:302:TYR:O	14:UU:307:LYS:HD2	2.20	0.42
16:YY:77:GLN:O	16:YY:80:GLN:HG3	2.19	0.42
2:II:164:LYS:HB3	2:II:166:TRP:CD1	2.54	0.42
2:I:242:HIS:ND1	2:I:243:PRO:HD3	2.35	0.42
2:I:337:LYS:HA	2:I:340:TYR:HB2	2.02	0.42
3:K:44:GLU:OE1	4:H:44:ILE:HG12	2.20	0.42
4:H:150:LYS:O	4:H:154:VAL:HG23	2.20	0.42
8:ce:506:LYS:NZ	8:ce:605:ASP:HB2	2.35	0.42
16:Y:138:LYS:H	16:Y:138:LYS:HG3	1.28	0.42
2:II:681:ILE:HD13	2:II:685:GLY:HA2	2.02	0.42
3:KK:71:GLY:C	4:HH:68:LEU:HD11	2.45	0.42
3:KK:104:LEU:HD22	4:HH:113:GLN:HE22	1.85	0.42
19:E:92:DT:C2	19:E:93:DG:N7	2.88	0.42
13:TT:275:ILE:HD12	13:TT:275:ILE:H	1.84	0.42
2:I:382:ILE:O	2:I:386:SER:OG	2.31	0.41
2:I:469:ILE:HA	2:I:472:TRP:HB2	2.02	0.41
5:LL:81:MET:HB2	5:LL:241:GLN:NE2	2.35	0.41
8:ce:109:ASP:OD1	8:ce:109:ASP:N	2.42	0.41
8:ce:344:LEU:HA	8:ce:347:LYS:HD2	2.02	0.41
16:Y:100:ARG:N	16:Y:100:ARG:HD2	2.35	0.41
14:UU:226:GLU:OE1	11:QQ:269:LEU:HD21	2.20	0.41
2:II:496:ASP:OD2	4:HH:24:ARG:NH2	2.53	0.41
4:HH:12:ILE:HA	4:HH:15:LEU:HB2	2.02	0.41
4:HH:32:ARG:HD2	4:HH:32:ARG:N	2.35	0.41
19:E:48:DA:H2''	19:E:49:DA:C8	2.55	0.41
22:e:225:ARG:HH11	22:e:225:ARG:HB2	1.80	0.41
2:I:436:PHE:CD2	2:I:468:MET:HE1	2.55	0.41
3:K:186:ILE:HD13	3:K:186:ILE:HA	1.92	0.41
7:CT:287:LEU:HD22	7:CT:301:ILE:HG13	2.01	0.41
8:ce:539:LYS:HE3	8:ce:539:LYS:HB3	1.88	0.41
8:CE:264:PHE:CZ	8:CE:293:PHE:HB2	2.55	0.41
6:N:271:GLU:HB3	6:N:340:VAL:HG21	2.01	0.41
16:YY:60:ASP:O	16:YY:63:SER:OG	2.30	0.41
2:II:388:MET:HE1	4:HH:118:ARG:HA	2.02	0.41
2:II:611:PHE:O	2:II:615:LEU:HG	2.20	0.41
3:KK:10:VAL:HA	3:KK:13:LYS:HE2	2.01	0.41
11:QQ:271:GLU:HA	11:QQ:274:LYS:HE2	2.02	0.41
19:E:82:DA:H2''	19:E:83:DG:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLN:HA	1:B:302:LEU:HD21	2.01	0.41
5:L:144:SER:HA	5:L:167:ARG:HB3	2.01	0.41
8:CE:506:LYS:HD2	8:CE:606:ILE:HA	2.01	0.41
10:P:337:LEU:O	10:P:340:ILE:HG22	2.19	0.41
3:KK:29:ALA:O	3:KK:33:ILE:HG12	2.21	0.41
11:QQ:197:LYS:HD2	11:QQ:197:LYS:HA	1.89	0.41
11:QQ:214:ILE:HD12	11:QQ:214:ILE:HA	1.87	0.41
23:c:84:HIS:HA	23:c:87:LEU:HD12	2.01	0.41
1:B:248:LEU:HD23	1:B:248:LEU:HA	1.91	0.41
2:I:137:LEU:HD23	2:I:167:LYS:HD2	2.02	0.41
2:I:510:MET:HE1	2:I:552:LEU:CD1	2.45	0.41
3:K:75:THR:HA	4:H:65:LYS:HE3	2.02	0.41
4:H:15:LEU:O	4:H:19:HIS:ND1	2.53	0.41
7:CT:121:THR:O	7:CT:127:LEU:HD12	2.21	0.41
5:L:81:MET:HB2	5:L:241:GLN:NE2	2.35	0.41
8:CE:475:ILE:HG22	8:CE:518:LYS:HB3	2.01	0.41
8:CE:535:HIS:ND1	8:CE:537:VAL:HG12	2.35	0.41
11:Q:340:ILE:HG23	16:Y:158:GLN:HE21	1.84	0.41
12:O:180:LEU:HD23	12:O:181:VAL:N	2.35	0.41
16:Y:209:LYS:O	16:Y:212:LEU:HG	2.20	0.41
2:II:219:LYS:HE2	20:f:49:GLY:HA3	2.03	0.41
2:II:444:PHE:O	2:II:448:THR:HG23	2.20	0.41
3:KK:175:THR:O	3:KK:179:MET:HG3	2.20	0.41
19:E:111:DA:H2"	19:E:112:DG:H8	1.85	0.41
21:d:53:HIS:HA	21:d:54:PRO:HD3	1.81	0.41
3:K:50:SER:HA	3:K:53:PHE:HB3	2.01	0.41
3:K:89:TRP:HA	3:K:92:LEU:HD12	2.03	0.41
4:H:22:VAL:HA	4:H:25:GLU:OE2	2.21	0.41
7:CT:339:LEU:HD13	7:CT:345:ILE:HD13	2.02	0.41
8:CE:296:LEU:HD23	8:CE:296:LEU:HA	1.88	0.41
11:Q:352:GLU:OE2	16:Y:152:LEU:HD11	2.21	0.41
12:OO:292:LYS:HA	12:OO:292:LYS:HD3	1.79	0.41
12:OO:311:LYS:HG3	12:OO:313:ILE:HG12	2.03	0.41
6:N:84:LEU:HD23	6:N:84:LEU:HA	1.88	0.41
15:W:68:GLU:OE2	15:W:70:LEU:HG	2.20	0.41
16:Y:142:GLU:HA	16:Y:145:ASN:ND2	2.36	0.41
16:YY:43:LYS:O	16:YY:46:VAL:HG22	2.21	0.41
16:YY:100:ARG:N	16:YY:100:ARG:HD2	2.35	0.41
2:II:573:SER:O	2:II:579:ARG:NH2	2.53	0.41
3:KK:77:ASN:C	3:KK:77:ASN:HD22	2.28	0.41
11:QQ:237:ILE:HD12	11:QQ:240:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:82:DG:C6	19:E:75:DG:C6	3.08	0.41
2:I:49:VAL:HG13	2:I:88:HIS:CE1	2.56	0.41
2:I:423:LEU:HD21	3:K:103:MET:HE3	2.02	0.41
3:K:8:LEU:O	3:K:12:ILE:HD12	2.21	0.41
3:K:171:ILE:O	3:K:175:THR:OG1	2.38	0.41
6:NN:33:TYR:OH	6:NN:59:ASP:OD1	2.29	0.41
8:CE:456:HIS:CD2	8:CE:458:MET:HG3	2.55	0.41
8:CE:531:ASP:OD1	8:CE:531:ASP:N	2.53	0.41
8:CE:535:HIS:CG	8:CE:536:PRO:HD2	2.56	0.41
12:O:136:ILE:HG13	12:O:137:LEU:N	2.36	0.41
17:Z:88:GLU:HG2	17:Z:89:THR:N	2.36	0.41
16:YY:142:GLU:HA	16:YY:145:ASN:ND2	2.36	0.41
4:HH:33:LEU:HA	4:HH:36:ILE:HG22	2.01	0.41
4:HH:53:LEU:HD12	4:HH:56:ARG:HE	1.85	0.41
4:HH:115:ILE:HD12	4:HH:115:ILE:HA	1.97	0.41
11:QQ:131:ARG:HG3	11:QQ:135:GLN:HG2	2.02	0.41
18:D:116:DT:C6	18:D:117:DT:H72	2.56	0.41
19:E:107:DC:H2"	19:E:108:DT:C5	2.56	0.41
19:E:119:DA:H2"	19:E:120:DC:C6	2.55	0.41
2:I:77:LEU:HB3	2:I:81:LEU:HD23	2.02	0.41
2:I:545:VAL:HB	2:I:553:LEU:HG	2.03	0.41
5:LL:123:LYS:HA	5:LL:123:LYS:HD3	1.68	0.41
6:NN:96:LEU:HD12	6:NN:96:LEU:HA	1.95	0.41
8:ce:68:TYR:CZ	8:ce:72:ILE:HG13	2.56	0.41
8:ce:130:ILE:HD12	8:ce:135:GLU:HG3	2.01	0.41
8:ce:439:ILE:HD11	8:ce:489:LEU:HD13	2.02	0.41
9:SK:19:ASP:OD2	9:SK:22:ILE:HG12	2.20	0.41
9:SK:25:ARG:HD3	9:SK:25:ARG:HA	1.84	0.41
8:CE:171:ILE:HA	8:CE:174:MET:HE3	2.02	0.41
8:CE:177:GLU:OE1	8:CE:178:LYS:HG3	2.20	0.41
8:CE:445:ASN:O	8:CE:450:SER:OG	2.31	0.41
6:N:110:LYS:HG3	6:N:210:ILE:HD13	2.03	0.41
13:T:286:LEU:HD23	13:T:291:ILE:H	1.86	0.41
14:U:163:ASP:OD1	14:U:163:ASP:N	2.53	0.41
14:UU:186:THR:O	14:UU:190:LYS:HB3	2.21	0.41
2:II:71:PHE:HB3	2:II:113:TRP:NE1	2.36	0.41
2:II:219:LYS:O	2:II:223:ASN:ND2	2.54	0.41
3:KK:167:ASN:C	3:KK:169:GLU:H	2.28	0.41
20:f:51:ILE:O	20:f:55:VAL:HG23	2.20	0.41
23:c:90:ARG:NH1	23:c:96:ASN:OD1	2.43	0.41
2:I:241:ALA:HA	2:I:242:HIS:HA	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:506:ARG:NH1	3:K:89:TRP:HE1	2.12	0.41
2:I:615:LEU:H	2:I:615:LEU:HD12	1.86	0.41
4:H:89:LEU:HA	4:H:92:GLU:HG2	2.02	0.41
5:LL:100:LEU:HG	5:LL:104:LYS:HE3	2.03	0.41
7:CT:165:VAL:O	7:CT:195:THR:OG1	2.37	0.41
8:ce:124:ALA:HA	8:ce:127:PHE:CE2	2.56	0.41
8:ce:155:ASP:OD1	8:ce:232:ARG:NH1	2.54	0.41
9:SK:25:ARG:HG3	9:SK:143:ILE:HG23	2.01	0.41
8:CE:502:SER:OG	8:CE:506:LYS:NZ	2.54	0.41
8:CE:536:PRO:HD3	8:CE:590:PHE:CE1	2.56	0.41
6:N:63:GLU:HG2	21:d:37:ARG:HH11	1.86	0.41
17:ZZ:111:ALA:O	17:ZZ:115:LYS:HG2	2.21	0.41
2:II:671:ASN:OD1	2:II:672:ASN:N	2.53	0.41
3:KK:15:LEU:HB3	4:HH:15:LEU:HD12	2.02	0.41
18:D:106:DT:H2"	18:D:107:DT:C6	2.56	0.41
18:D:109:DC:H2"	18:D:110:DC:C6	2.54	0.41
19:E:76:DG:H2"	19:E:77:DG:N7	2.36	0.41
23:c:87:LEU:O	23:c:91:ASN:HB2	2.21	0.41
22:a:156:ILE:HB	22:a:157:PRO:HD3	2.02	0.41
1:B:329:ASP:O	1:B:332:THR:OG1	2.34	0.41
2:I:609:ASP:HB3	2:I:610:PHE:H	1.60	0.41
2:I:721:TYR:HA	2:I:722:LEU:HA	1.63	0.41
3:K:164:LEU:HD21	3:K:174:LEU:HD22	2.02	0.41
5:LL:144:SER:HA	5:LL:167:ARG:HB3	2.01	0.41
6:NN:416:LEU:HD22	6:NN:421:LEU:HD12	2.01	0.41
7:CT:101:LEU:HD23	7:CT:101:LEU:HA	1.91	0.41
7:CT:347:LEU:HD12	7:CT:369:TRP:HA	2.03	0.41
8:ce:517:LEU:HD13	8:ce:597:PHE:CE1	2.55	0.41
5:L:234:ALA:O	5:L:238:GLN:HG3	2.21	0.41
8:CE:27:MET:SD	8:CE:28:ILE:N	2.94	0.41
8:CE:57:TYR:HB3	8:CE:533:PHE:CD2	2.56	0.41
10:P:230:GLN:OE1	10:P:230:GLN:N	2.50	0.41
10:P:324:ALA:HB1	10:P:331:ARG:HH12	1.86	0.41
11:Q:137:GLU:HB3	14:U:137:VAL:HG23	2.02	0.41
11:Q:177:VAL:HG21	14:U:177:LEU:HA	2.02	0.41
12:O:180:LEU:HD22	12:O:201:MET:SD	2.60	0.41
16:Y:43:LYS:O	16:Y:46:VAL:HG22	2.21	0.41
17:Z:57:LEU:O	17:Z:61:ILE:HG23	2.21	0.41
17:Z:62:LYS:HA	17:Z:62:LYS:HD3	1.89	0.41
14:UU:195:ILE:O	14:UU:199:ASN:HB2	2.21	0.41
2:II:120:LEU:HD11	2:II:238:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:II:177:HIS:HA	2:II:178:PRO:HD3	1.92	0.41
2:II:181:ARG:HD2	2:II:181:ARG:O	2.21	0.41
2:II:677:HIS:O	2:II:681:ILE:HG12	2.21	0.41
3:KK:100:GLN:H	3:KK:100:GLN:HG3	1.75	0.41
11:QQ:132:LYS:HE2	11:QQ:132:LYS:HB2	1.90	0.41
11:QQ:137:GLU:HB3	11:QQ:141:ARG:NH2	2.30	0.41
11:QQ:253:GLN:HA	11:QQ:256:GLU:HB3	2.03	0.41
18:D:17:DC:H2''	18:D:18:DG:C8	2.55	0.41
19:E:88:DT:H2''	19:E:89:DA:C5	2.55	0.41
19:E:111:DA:OP1	20:b:80:LYS:N	2.54	0.41
19:E:148:DT:H2''	19:E:149:DG:C8	2.55	0.41
20:b:25:ASP:CG	20:b:27:ILE:HG22	2.46	0.41
20:b:93:ARG:HG3	20:b:93:ARG:HH11	1.86	0.41
2:I:417:CYS:O	2:I:421:LEU:HG	2.22	0.41
2:I:513:ILE:HD13	2:I:552:LEU:HB3	2.03	0.41
2:I:711:TYR:HB3	2:I:714:ILE:HD13	2.02	0.41
4:H:24:ARG:HH12	4:H:57:HIS:HB3	1.86	0.41
6:NN:71:ILE:O	6:NN:75:ILE:HG12	2.21	0.41
8:CE:169:MET:HE2	8:CE:169:MET:HB3	1.90	0.41
8:CE:440:SER:HA	8:CE:443:VAL:HG22	2.02	0.41
14:UU:212:ARG:HG2	11:QQ:255:ASN:HD21	1.84	0.41
2:II:149:ILE:HG23	2:II:152:LEU:HD23	2.02	0.41
3:KK:73:SER:HA	4:HH:16:GLU:OE2	2.20	0.41
18:D:81:DC:H2''	18:D:82:DG:C8	2.56	0.41
21:h:44:TYR:O	21:h:48:VAL:HG23	2.21	0.41
1:B:321:ARG:HH22	1:B:327:TYR:HB2	1.86	0.40
4:H:13:GLN:HA	4:H:16:GLU:HB2	2.03	0.40
4:H:63:LEU:HA	4:H:66:THR:HG22	2.02	0.40
7:CT:352:PHE:HE2	7:CT:370:TRP:HZ2	1.69	0.40
7:CT:356:PHE:CE2	7:CT:438:LEU:HD21	2.56	0.40
9:SK:114:ALA:O	9:SK:152:LYS:NZ	2.53	0.40
8:CE:460:MET:HA	8:CE:463:ILE:HG12	2.03	0.40
10:P:158:ARG:HG2	12:O:170:TYR:OH	2.21	0.40
10:P:279:SER:HA	10:P:299:ASN:HA	2.04	0.40
12:OO:157:ARG:HG2	12:OO:157:ARG:HH11	1.85	0.40
10:PP:231:LEU:HD12	10:PP:240:CYS:HA	2.03	0.40
11:QQ:184:GLU:O	11:QQ:188:MET:HG2	2.21	0.40
18:D:90:DA:H2'	18:D:91:DT:H71	2.03	0.40
19:E:10:DA:H2''	19:E:11:DA:C8	2.56	0.40
23:g:28:PRO:HD3	21:h:44:TYR:HD2	1.86	0.40
13:TT:344:ALA:O	13:TT:348:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:95:PHE:CZ	3:K:204:ILE:HG13	2.55	0.40
2:I:378:VAL:O	2:I:382:ILE:HG12	2.22	0.40
2:I:439:PHE:O	2:I:443:ILE:HG12	2.22	0.40
3:K:207:LEU:O	3:K:211:ALA:N	2.54	0.40
4:H:47:HIS:NE2	10:P:110:ILE:HG13	2.36	0.40
4:H:159:GLU:O	4:H:162:GLN:HG2	2.20	0.40
6:NN:122:LYS:HA	6:NN:122:LYS:HD2	1.80	0.40
8:CE:11:LYS:HA	8:CE:11:LYS:HD2	1.75	0.40
8:CE:344:LEU:HD13	8:CE:383:LYS:HD3	2.03	0.40
11:Q:343:THR:HB	11:Q:346:VAL:HB	2.02	0.40
10:PP:179:GLY:O	10:PP:207:PHE:HB3	2.22	0.40
16:Y:157:LEU:HD21	17:Z:104:ARG:HG2	2.03	0.40
17:Z:29:LEU:HD12	17:Z:30:GLN:N	2.36	0.40
3:KK:49:ASN:OD1	3:KK:50:SER:N	2.55	0.40
4:HH:49:GLN:H	4:HH:49:GLN:HG2	1.70	0.40
21:h:36:ALA:O	21:h:38:LYS:NZ	2.53	0.40
1:B:256:LYS:O	1:B:260:LEU:HG	2.21	0.40
2:I:233:ILE:O	2:I:236:ARG:HG2	2.22	0.40
2:I:401:CYS:HB3	2:I:435:PHE:CE2	2.56	0.40
4:H:76:PRO:HB3	4:H:83:PHE:CZ	2.56	0.40
4:H:85:LYS:O	4:H:89:LEU:HG	2.21	0.40
5:LL:19:GLY:O	5:LL:22:LYS:HG3	2.21	0.40
6:NN:34:ASP:OD1	6:NN:34:ASP:N	2.52	0.40
7:CT:118:LEU:HD12	7:CT:118:LEU:HA	1.91	0.40
11:Q:299:VAL:HG23	11:Q:300:LEU:HD22	2.02	0.40
6:N:131:ASN:HB2	6:N:231:THR:HG23	2.03	0.40
13:T:337:VAL:HA	13:T:340:MET:HB2	2.02	0.40
16:Y:60:ASP:O	16:Y:63:SER:OG	2.30	0.40
2:II:186:SER:HA	2:II:221:HIS:CE1	2.56	0.40
2:II:510:MET:CE	4:HH:100:LEU:HD21	2.52	0.40
3:KK:52:VAL:HG21	4:HH:39:HIS:NE2	2.36	0.40
3:KK:59:LYS:HD3	3:KK:60:PRO:HD2	2.04	0.40
3:KK:207:LEU:HD11	4:HH:172:SER:HB3	2.03	0.40
22:e:173:ASP:OD1	22:e:174:GLN:N	2.55	0.40
20:f:40:ARG:HA	20:f:40:ARG:HD3	1.72	0.40
3:K:57:LEU:O	4:H:56:ARG:NH1	2.54	0.40
3:K:91:SER:HA	3:K:94:ASN:HB2	2.02	0.40
5:L:100:LEU:HG	5:L:104:LYS:HE3	2.03	0.40
12:OO:359:LEU:HD12	12:OO:359:LEU:HA	1.86	0.40
14:U:198:SER:O	14:U:201:GLU:HG2	2.22	0.40
12:O:345:GLU:O	12:O:349:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:UU:220:ILE:HG22	14:UU:224:ARG:HD2	2.03	0.40
16:YY:138:LYS:H	16:YY:138:LYS:HG3	1.28	0.40
2:II:124:HIS:HE1	2:II:128:GLU:HB2	1.87	0.40
2:II:314:TYR:O	2:II:316:MET:N	2.55	0.40
3:KK:166:ASP:C	3:KK:168:ASP:H	2.28	0.40
18:D:28:DA:H2"	18:D:29:DA:H8	1.87	0.40
20:b:93:ARG:HG3	20:b:93:ARG:NH1	2.36	0.40
22:a:161:LEU:O	22:a:165:VAL:HG23	2.22	0.40
2:I:672:ASN:HA	2:I:675:ARG:HE	1.87	0.40
2:I:711:TYR:CE2	4:H:98:TYR:HE1	2.39	0.40
3:K:49:ASN:OD1	3:K:52:VAL:HG22	2.21	0.40
5:LL:120:THR:O	5:LL:124:LEU:HD23	2.21	0.40
7:CT:110:TYR:HA	8:ce:368:LYS:NZ	2.37	0.40
8:ce:105:TYR:OH	8:ce:184:SER:O	2.38	0.40
8:CE:17:CYS:HB3	8:CE:32:ASN:HD22	1.87	0.40
14:UU:181:ILE:O	14:UU:185:MET:HG2	2.22	0.40
14:UU:207:LYS:HA	14:UU:207:LYS:HD2	1.66	0.40
16:YY:63:SER:O	16:YY:66:ILE:HG22	2.22	0.40
2:II:189:LEU:HD11	2:II:222:ARG:HA	2.04	0.40
2:II:696:LEU:O	2:II:700:ILE:HG12	2.22	0.40
4:HH:77:ASP:OD1	4:HH:77:ASP:N	2.48	0.40
11:QQ:371:LYS:HE2	11:QQ:371:LYS:HB2	1.97	0.40
22:e:207:HIS:CE1	22:a:208:ALA:HB2	2.56	0.40
22:a:156:ILE:CD1	22:a:156:ILE:N	2.85	0.40
22:a:171:THR:OG1	22:a:173:ASP:OD1	2.40	0.40
13:TT:352:LEU:HD23	15:WW:44:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	108/351 (31%)	108 (100%)	0	0	100	100
1	B	114/351 (32%)	113 (99%)	1 (1%)	0	100	100
2	I	649/733 (88%)	624 (96%)	25 (4%)	0	100	100
2	II	696/733 (95%)	676 (97%)	20 (3%)	0	100	100
3	K	213/239 (89%)	207 (97%)	6 (3%)	0	100	100
3	KK	221/239 (92%)	209 (95%)	12 (5%)	0	100	100
4	H	167/181 (92%)	159 (95%)	8 (5%)	0	100	100
4	HH	172/181 (95%)	168 (98%)	4 (2%)	0	100	100
5	L	239/245 (98%)	228 (95%)	11 (5%)	0	100	100
5	LL	239/245 (98%)	228 (95%)	11 (5%)	0	100	100
6	N	378/458 (82%)	365 (97%)	13 (3%)	0	100	100
6	NN	377/458 (82%)	369 (98%)	8 (2%)	0	100	100
7	CT	383/478 (80%)	362 (94%)	21 (6%)	0	100	100
8	CE	549/608 (90%)	532 (97%)	16 (3%)	1 (0%)	43	72
8	ce	518/608 (85%)	506 (98%)	12 (2%)	0	100	100
9	SK	147/194 (76%)	142 (97%)	5 (3%)	0	100	100
10	P	249/369 (68%)	246 (99%)	3 (1%)	0	100	100
10	PP	248/369 (67%)	241 (97%)	7 (3%)	0	100	100
11	Q	257/406 (63%)	253 (98%)	4 (2%)	0	100	100
11	QQ	241/406 (59%)	233 (97%)	8 (3%)	0	100	100
12	O	241/368 (66%)	230 (95%)	11 (5%)	0	100	100
12	OO	236/368 (64%)	228 (97%)	8 (3%)	0	100	100
13	T	90/361 (25%)	87 (97%)	3 (3%)	0	100	100
13	TT	90/361 (25%)	87 (97%)	3 (3%)	0	100	100
14	U	180/324 (56%)	177 (98%)	3 (2%)	0	100	100
14	UU	175/324 (54%)	172 (98%)	3 (2%)	0	100	100
15	W	65/89 (73%)	65 (100%)	0	0	100	100
15	WW	65/89 (73%)	65 (100%)	0	0	100	100
16	Y	217/238 (91%)	208 (96%)	9 (4%)	0	100	100
16	YY	217/238 (91%)	208 (96%)	9 (4%)	0	100	100
17	Z	149/153 (97%)	146 (98%)	3 (2%)	0	100	100
17	ZZ	149/153 (97%)	148 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	b	77/103 (75%)	74 (96%)	3 (4%)	0	100	100
20	f	77/103 (75%)	73 (95%)	4 (5%)	0	100	100
21	d	93/131 (71%)	90 (97%)	3 (3%)	0	100	100
21	h	95/131 (72%)	93 (98%)	2 (2%)	0	100	100
22	a	95/229 (42%)	94 (99%)	1 (1%)	0	100	100
22	e	95/229 (42%)	94 (99%)	1 (1%)	0	100	100
23	c	95/132 (72%)	92 (97%)	3 (3%)	0	100	100
23	g	96/132 (73%)	96 (100%)	0	0	100	100
All	All	8762/12108 (72%)	8496 (97%)	265 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	CE	587	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/305 (32%)	97 (100%)	0	100	100
1	B	103/305 (34%)	103 (100%)	0	100	100
2	I	612/683 (90%)	612 (100%)	0	100	100
2	II	654/683 (96%)	654 (100%)	0	100	100
3	K	202/223 (91%)	202 (100%)	0	100	100
3	KK	202/223 (91%)	202 (100%)	0	100	100
4	H	162/172 (94%)	162 (100%)	0	100	100
4	HH	167/172 (97%)	167 (100%)	0	100	100
5	L	217/221 (98%)	193 (89%)	24 (11%)	6	25
5	LL	217/221 (98%)	193 (89%)	24 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	N	350/416 (84%)	350 (100%)	0	100	100
6	NN	349/416 (84%)	349 (100%)	0	100	100
7	CT	368/449 (82%)	368 (100%)	0	100	100
8	CE	521/569 (92%)	521 (100%)	0	100	100
8	ce	488/569 (86%)	488 (100%)	0	100	100
9	SK	137/179 (76%)	137 (100%)	0	100	100
10	P	240/344 (70%)	240 (100%)	0	100	100
10	PP	240/344 (70%)	239 (100%)	1 (0%)	84	81
11	Q	250/378 (66%)	250 (100%)	0	100	100
11	QQ	234/378 (62%)	234 (100%)	0	100	100
12	O	230/347 (66%)	230 (100%)	0	100	100
12	OO	225/347 (65%)	225 (100%)	0	100	100
13	T	89/339 (26%)	89 (100%)	0	100	100
13	TT	89/339 (26%)	89 (100%)	0	100	100
14	U	168/308 (54%)	168 (100%)	0	100	100
14	UU	164/308 (53%)	164 (100%)	0	100	100
15	W	57/76 (75%)	57 (100%)	0	100	100
15	WW	57/76 (75%)	57 (100%)	0	100	100
16	Y	175/219 (80%)	156 (89%)	19 (11%)	6	26
16	YY	175/219 (80%)	156 (89%)	19 (11%)	6	26
17	Z	121/143 (85%)	120 (99%)	1 (1%)	73	76
17	ZZ	121/143 (85%)	121 (100%)	0	100	100
20	b	65/81 (80%)	65 (100%)	0	100	100
20	f	66/81 (82%)	66 (100%)	0	100	100
21	d	81/109 (74%)	81 (100%)	0	100	100
21	h	81/109 (74%)	81 (100%)	0	100	100
22	a	82/207 (40%)	71 (87%)	11 (13%)	4	20
22	e	82/207 (40%)	71 (87%)	11 (13%)	4	20
23	c	75/99 (76%)	75 (100%)	0	100	100
23	g	77/99 (78%)	76 (99%)	1 (1%)	61	71
All	All	8090/11106 (73%)	7979 (99%)	111 (1%)	57	70

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	LL	6	LYS
5	LL	8	LEU
5	LL	14	LEU
5	LL	20	ILE
5	LL	52	GLU
5	LL	59	ARG
5	LL	62	ILE
5	LL	80	LYS
5	LL	81	MET
5	LL	85	MET
5	LL	99	VAL
5	LL	104	LYS
5	LL	115	LYS
5	LL	123	LYS
5	LL	130	VAL
5	LL	146	LYS
5	LL	155	ASP
5	LL	167	ARG
5	LL	170	CYS
5	LL	215	LYS
5	LL	218	ARG
5	LL	226	ARG
5	LL	238	GLN
5	LL	240	ILE
5	L	6	LYS
5	L	8	LEU
5	L	14	LEU
5	L	20	ILE
5	L	52	GLU
5	L	59	ARG
5	L	62	ILE
5	L	80	LYS
5	L	81	MET
5	L	85	MET
5	L	99	VAL
5	L	104	LYS
5	L	115	LYS
5	L	123	LYS
5	L	130	VAL
5	L	146	LYS
5	L	155	ASP
5	L	167	ARG

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Mol	Chain	Res	Type
5	L	170	CYS
5	L	215	LYS
5	L	218	ARG
5	L	226	ARG
5	L	238	GLN
5	L	240	ILE
10	PP	297	GLN
16	Y	12	ILE
16	Y	14	ASN
16	Y	19	LEU
16	Y	61	LEU
16	Y	65	GLU
16	Y	74	ARG
16	Y	77	GLN
16	Y	112	ARG
16	Y	115	GLU
16	Y	116	ASP
16	Y	138	LYS
16	Y	161	GLU
16	Y	162	SER
16	Y	173	SER
16	Y	176	SER
16	Y	181	ILE
16	Y	189	ASP
16	Y	202	VAL
16	Y	206	GLU
17	Z	38	GLN
16	YY	12	ILE
16	YY	14	ASN
16	YY	19	LEU
16	YY	61	LEU
16	YY	65	GLU
16	YY	74	ARG
16	YY	77	GLN
16	YY	112	ARG
16	YY	115	GLU
16	YY	116	ASP
16	YY	138	LYS
16	YY	161	GLU
16	YY	162	SER
16	YY	173	SER
16	YY	176	SER

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Mol	Chain	Res	Type
16	YY	181	ILE
16	YY	189	ASP
16	YY	202	VAL
16	YY	206	GLU
22	e	147	ARG
22	e	153	ILE
22	e	154	SER
22	e	156	ILE
22	e	184	MET
22	e	190	SER
22	e	191	GLU
22	e	206	LEU
22	e	209	LYS
22	e	222	ARG
22	e	225	ARG
23	g	75	ASN
22	a	147	ARG
22	a	153	ILE
22	a	154	SER
22	a	156	ILE
22	a	184	MET
22	a	190	SER
22	a	191	GLU
22	a	206	LEU
22	a	209	LYS
22	a	222	ARG
22	a	225	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	GLN
2	I	130	ASN
2	I	192	GLN
2	I	214	ASN
2	I	301	GLN
2	I	617	ASN
3	K	234	ASN
4	H	47	HIS
4	H	49	GLN
4	H	60	GLN
4	H	151	GLN

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Mol	Chain	Res	Type
4	H	171	HIS
5	LL	36	GLN
6	NN	73	ASN
6	NN	124	GLN
6	NN	308	ASN
7	CT	319	GLN
8	ce	189	HIS
8	ce	219	GLN
8	ce	399	GLN
8	ce	433	HIS
8	ce	495	ASN
5	L	36	GLN
9	SK	88	GLN
9	SK	139	ASN
8	CE	32	ASN
8	CE	259	GLN
8	CE	445	ASN
10	P	98	ASN
11	Q	242	GLN
11	Q	394	HIS
12	OO	261	HIS
6	N	10	ASN
6	N	160	GLN
6	N	394	ASN
13	T	296	GLN
14	U	144	ASN
14	U	200	ASN
14	U	217	ASN
14	U	257	ASN
14	U	313	ASN
10	PP	98	ASN
10	PP	106	ASN
10	PP	260	ASN
10	PP	333	ASN
12	O	215	GLN
12	O	220	HIS
12	O	283	GLN
12	O	322	ASN
16	Y	79	GLN
17	Z	5	GLN
17	Z	8	HIS
17	Z	9	ASN

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Mol	Chain	Res	Type
17	Z	30	GLN
17	Z	38	GLN
17	Z	47	GLN
17	Z	63	GLN
17	Z	80	GLN
17	Z	102	GLN
14	UU	148	ASN
14	UU	179	GLN
14	UU	205	GLN
14	UU	208	GLN
14	UU	219	GLN
14	UU	241	ASN
16	YY	79	GLN
17	ZZ	113	GLN
2	II	141	GLN
2	II	305	GLN
2	II	307	HIS
2	II	376	GLN
2	II	731	GLN
3	KK	28	GLN
3	KK	77	ASN
3	KK	145	ASN
3	KK	163	ASN
3	KK	191	ASN
4	HH	107	GLN
11	QQ	135	GLN
11	QQ	187	GLN
11	QQ	250	GLN
11	QQ	255	ASN
11	QQ	266	GLN
11	QQ	394	HIS
21	h	88	ASN
23	c	70	ASN
13	TT	284	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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.

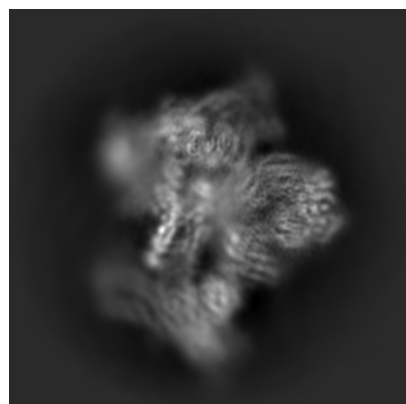
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17227. These allow visual inspection of the internal detail of the map and identification of artifacts.

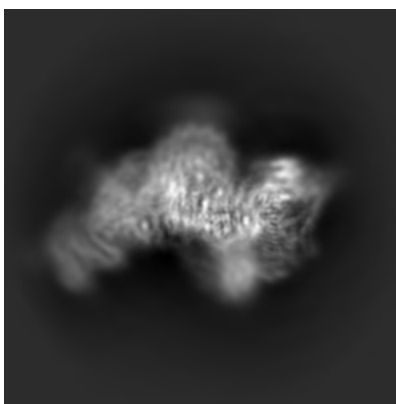
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

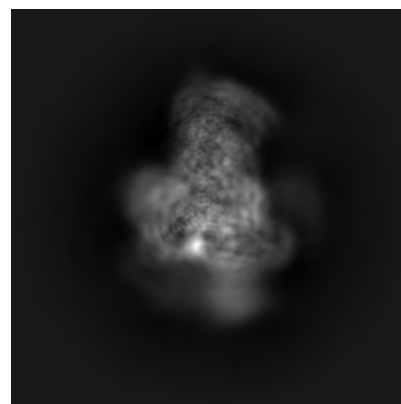
6.1.1 Primary map



X

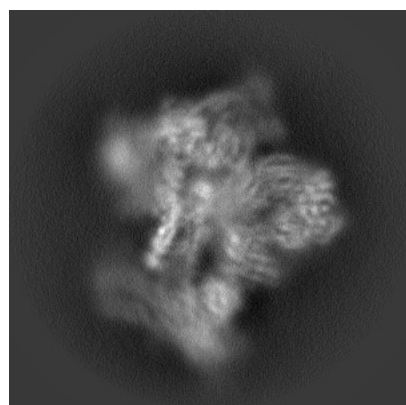


Y

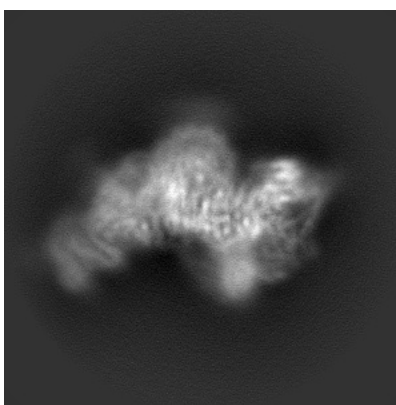


Z

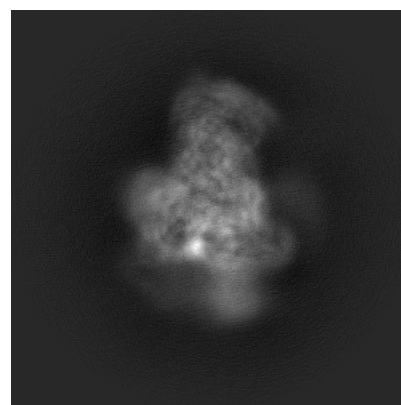
6.1.2 Raw map



X



Y

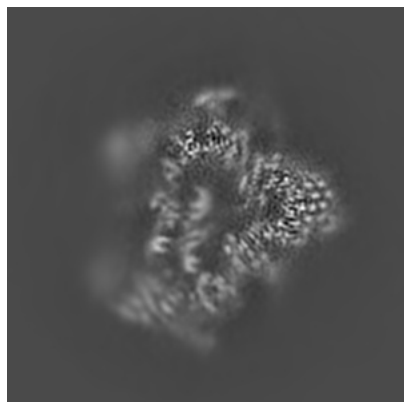


Z

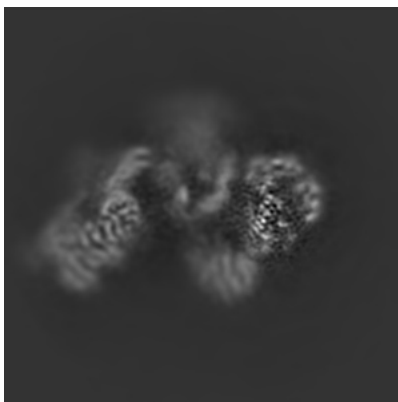
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

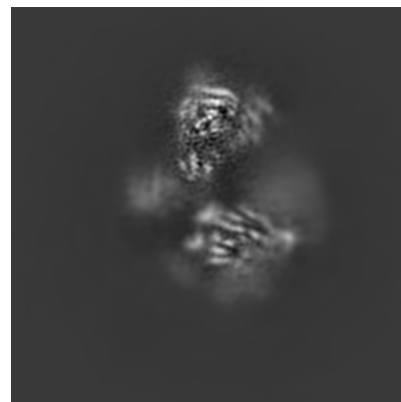
6.2.1 Primary map



X Index: 176

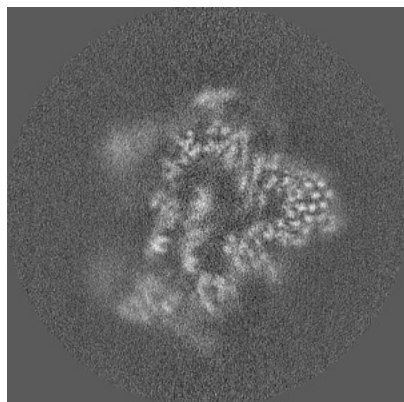


Y Index: 176

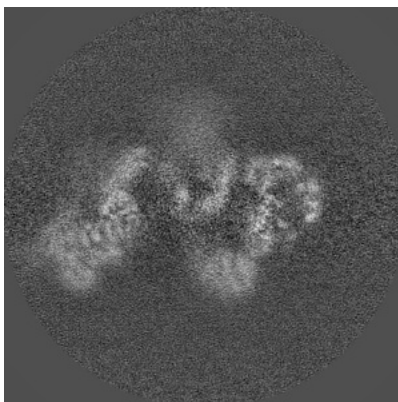


Z Index: 176

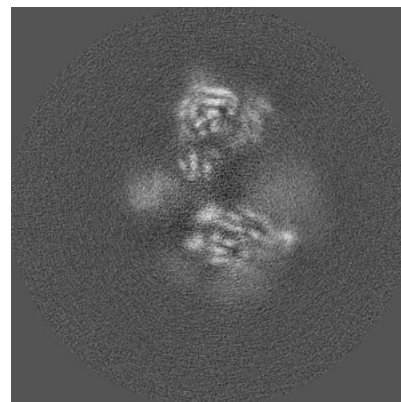
6.2.2 Raw map



X Index: 176



Y Index: 176

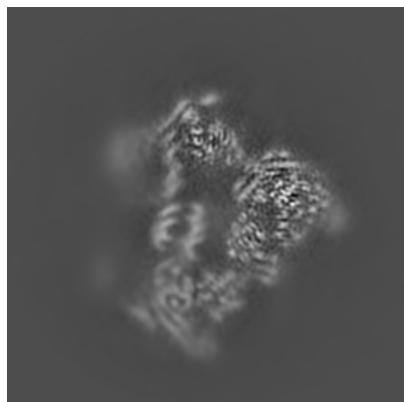


Z Index: 176

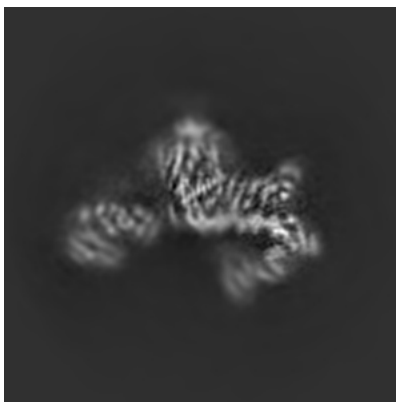
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

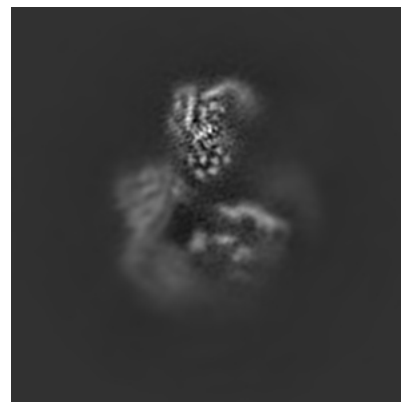
6.3.1 Primary map



X Index: 167

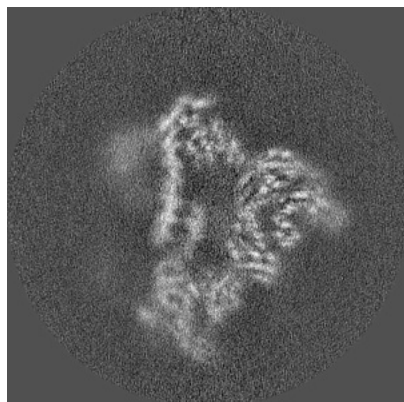


Y Index: 143

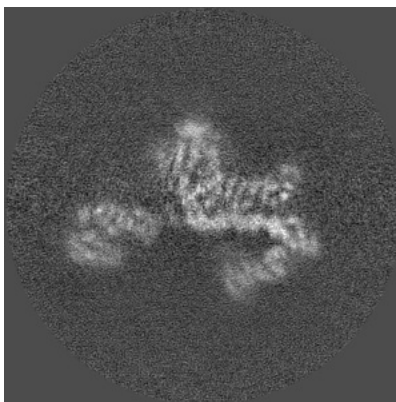


Z Index: 196

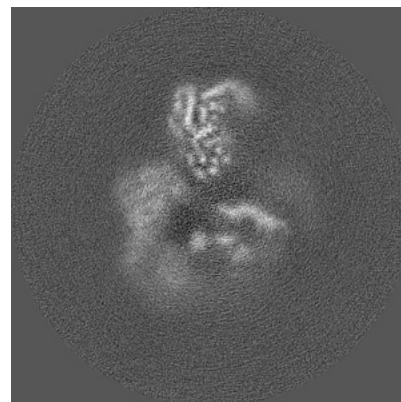
6.3.2 Raw map



X Index: 163



Y Index: 144

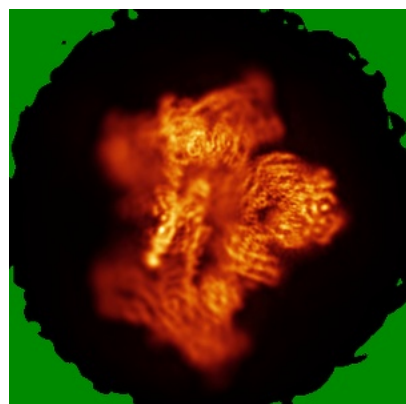


Z Index: 196

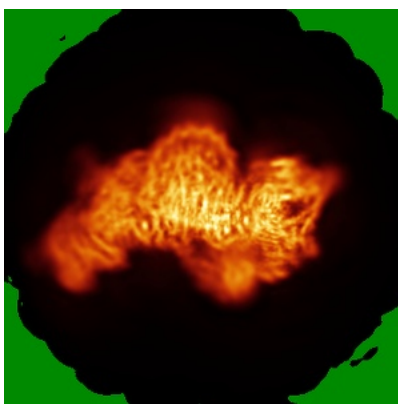
The images above show the largest variance slices of the map in three orthogonal directions.

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

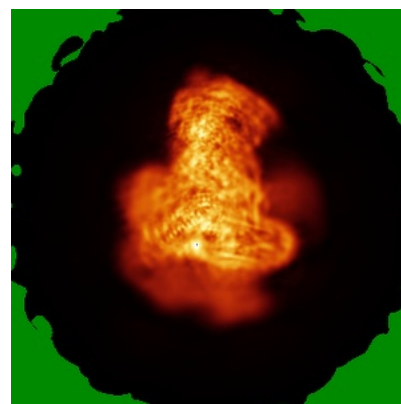
6.4.1 Primary map



X

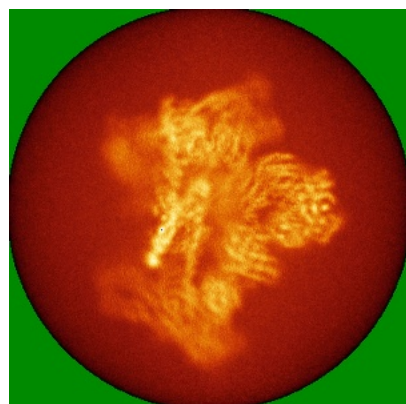


Y

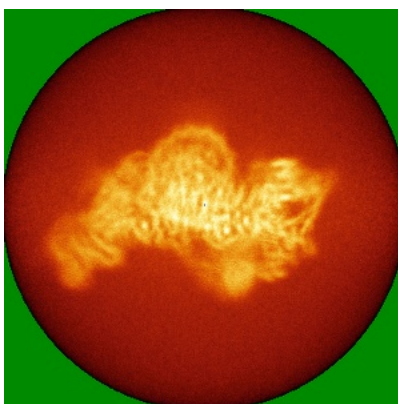


Z

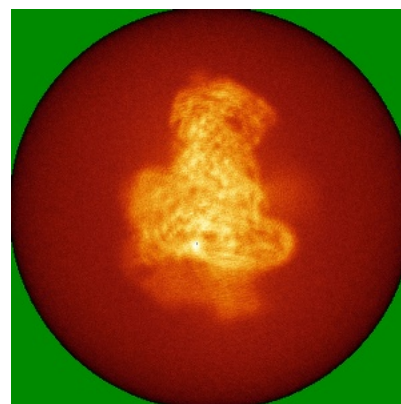
6.4.2 Raw map



X



Y

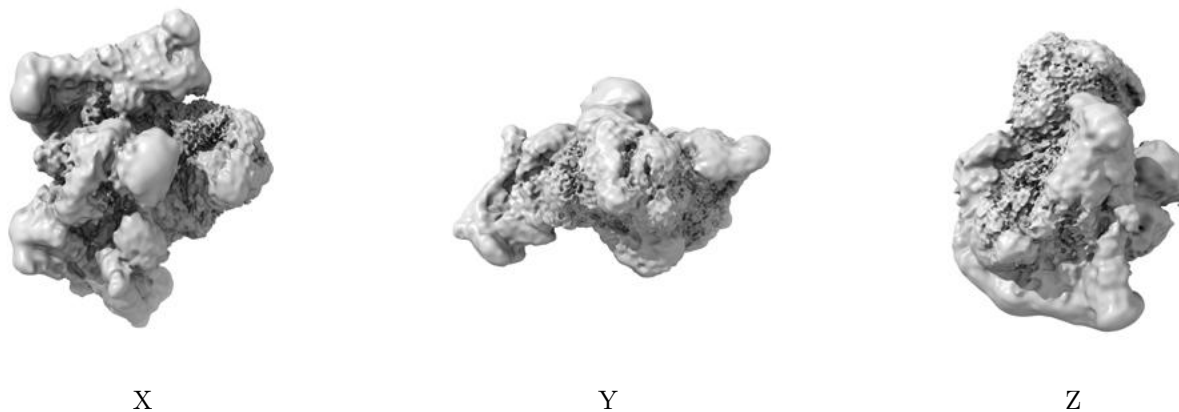


Z

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.

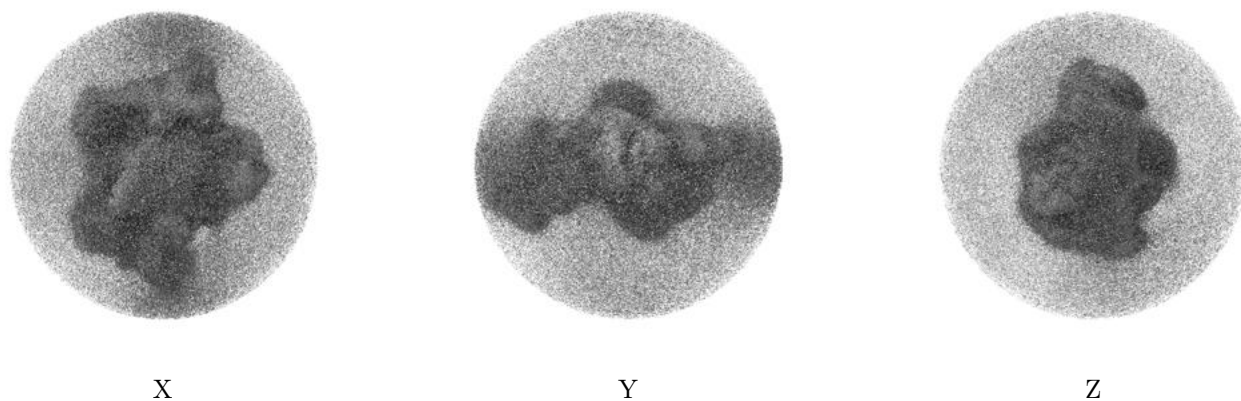
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00271. 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.

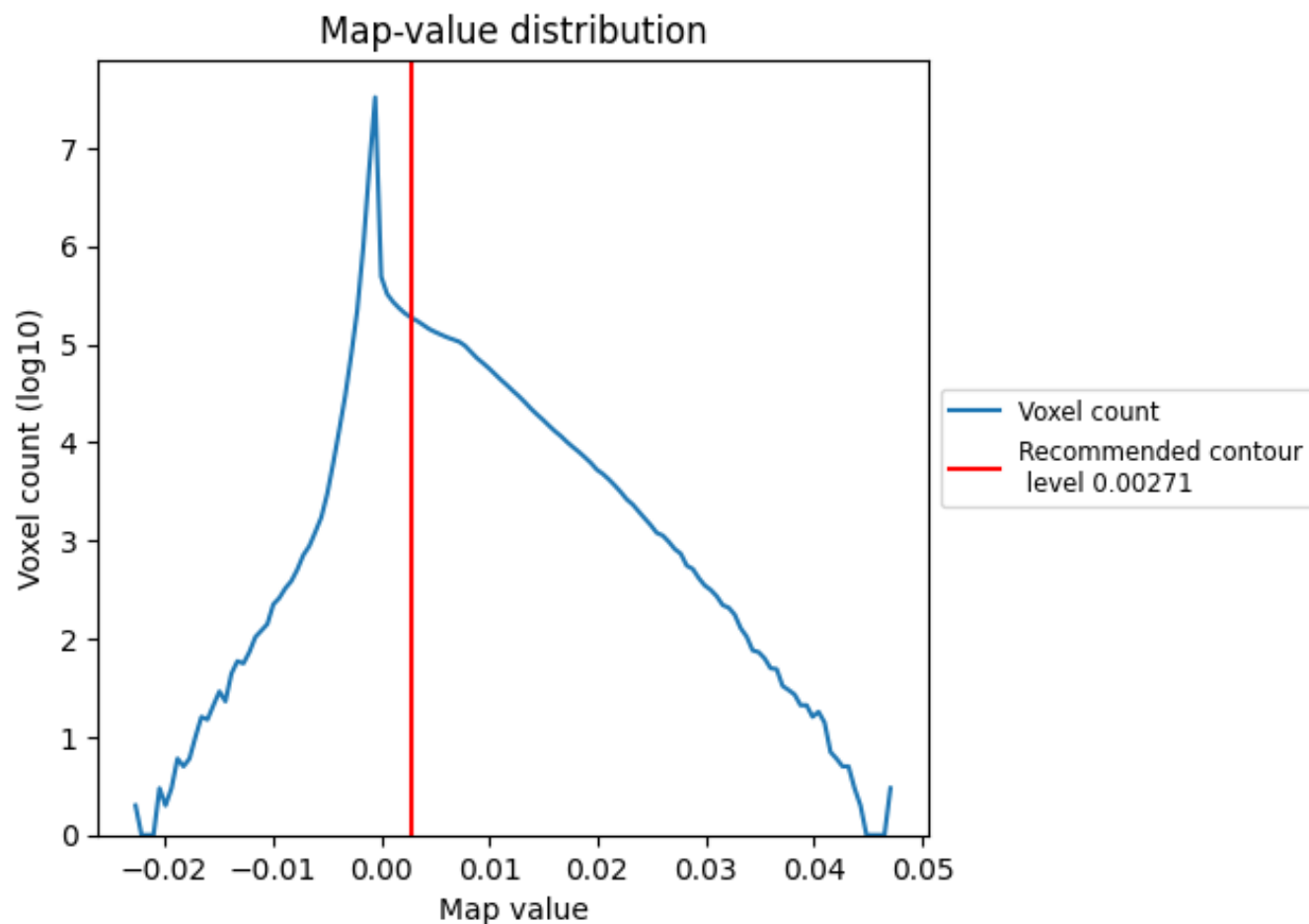
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

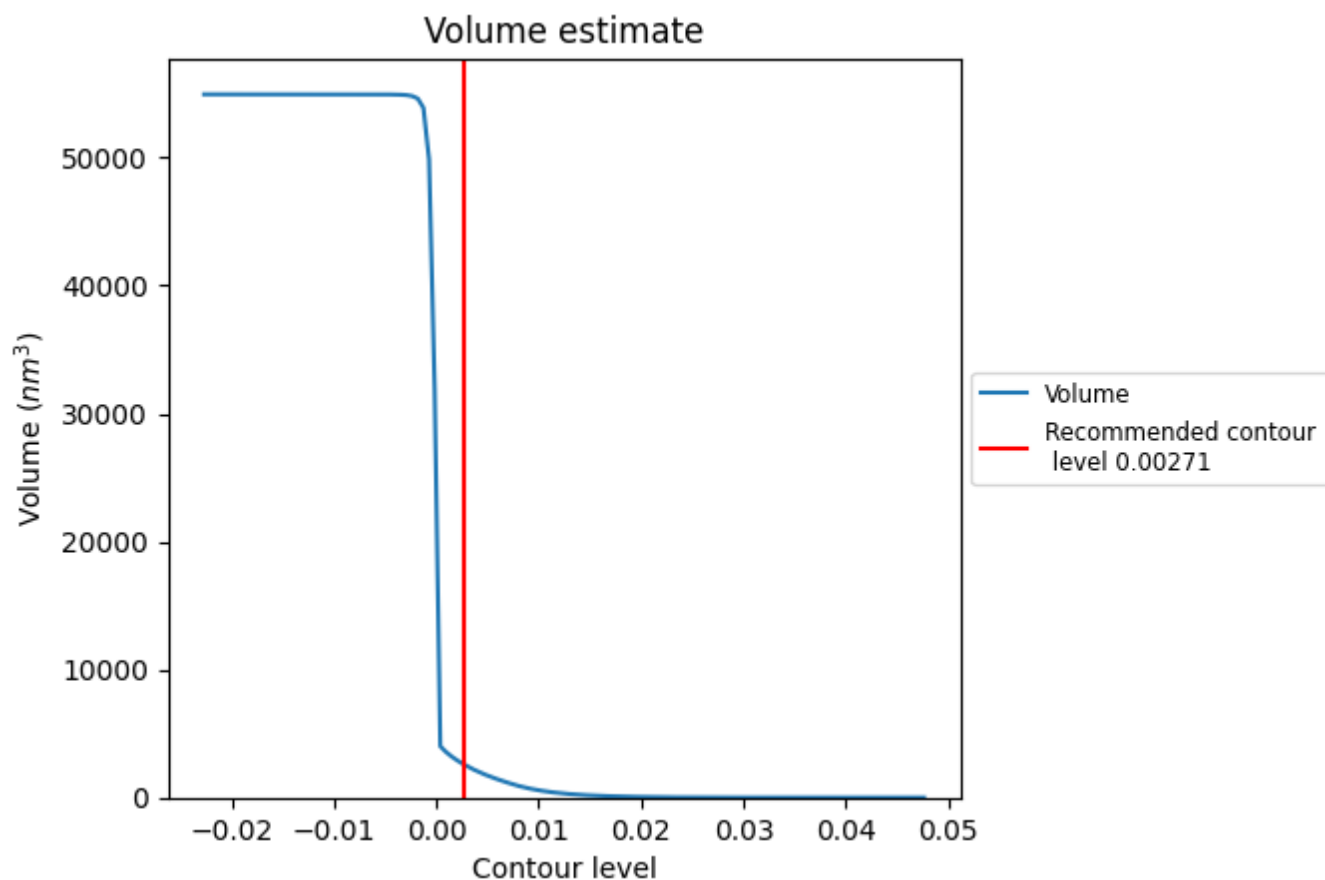
This section contains the results of statistical analysis of the map.

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.

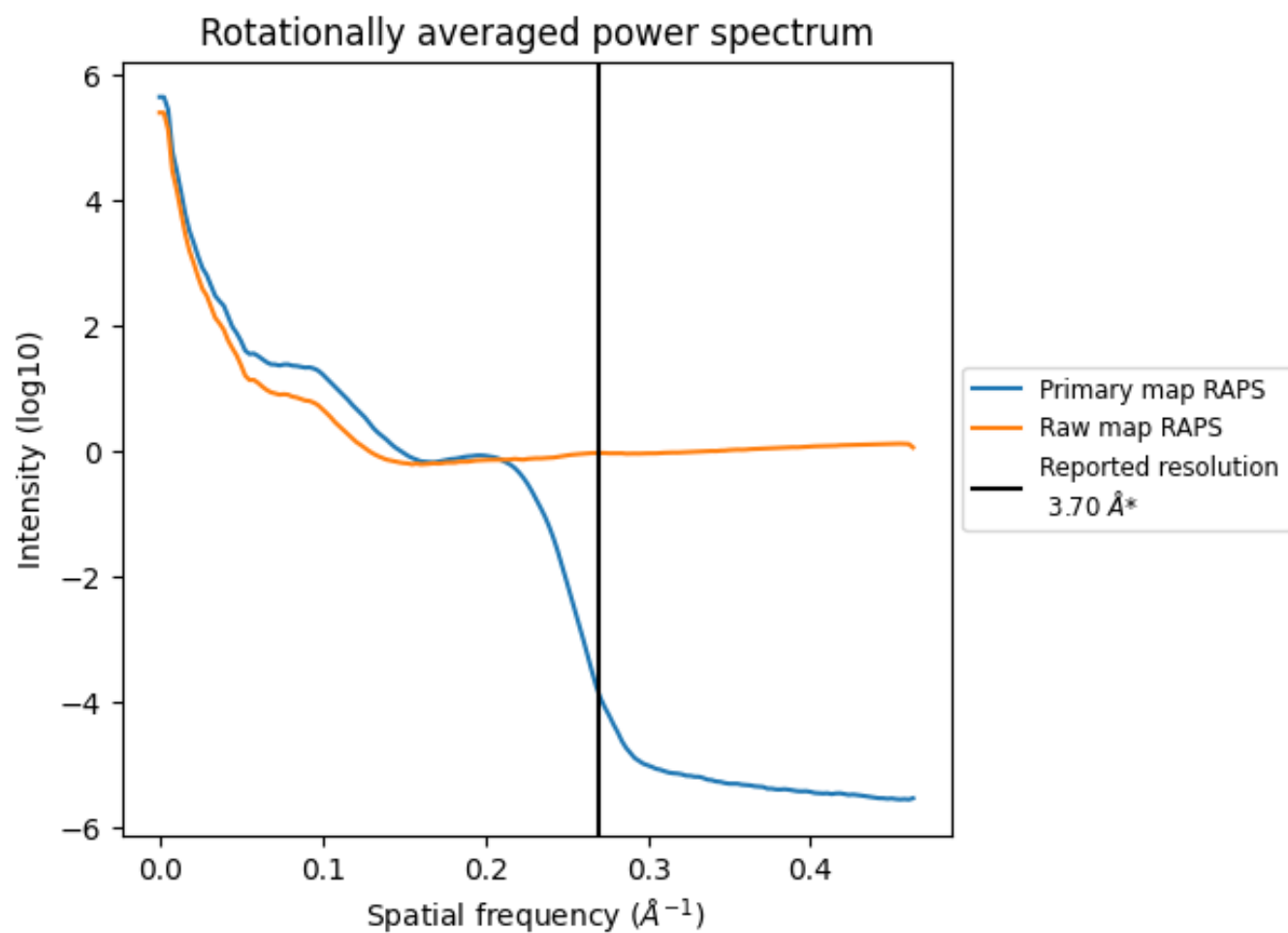
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2581 nm^3 ; this corresponds to an approximate mass of 2331 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 ⓘ

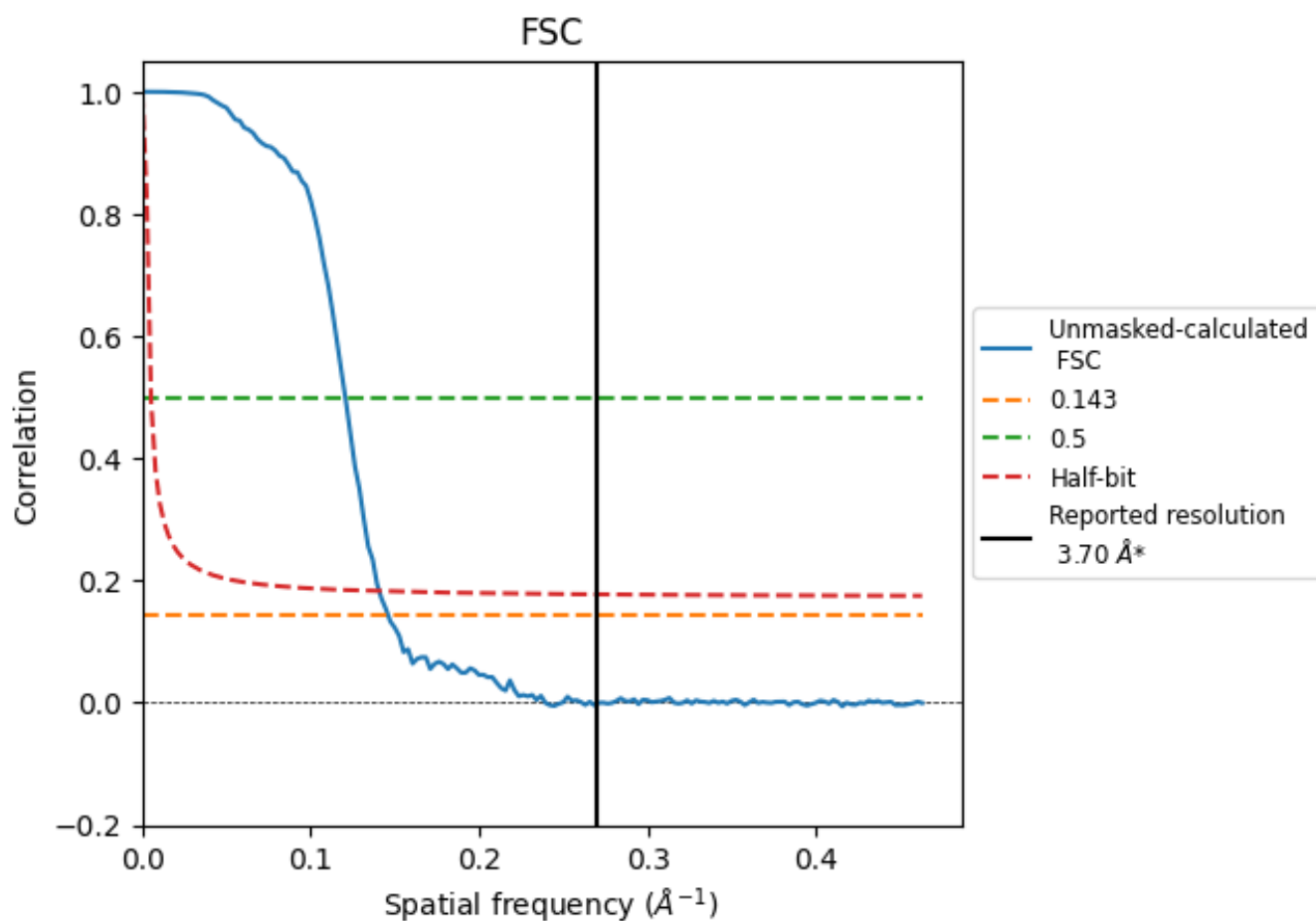


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

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](#)

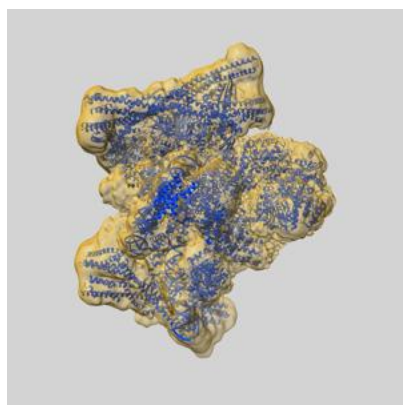
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.85	8.29	7.11

*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 6.85 differs from the reported value 3.7 by more than 10 %

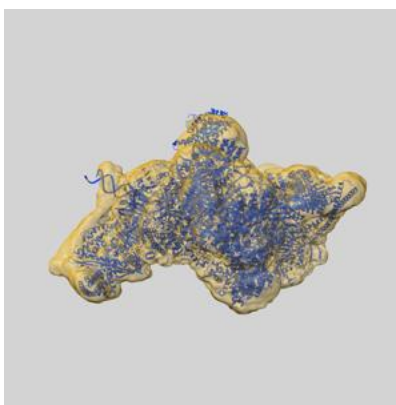
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17227 and PDB model 8OW1. Per-residue inclusion information can be found in section [3](#) on page [10](#).

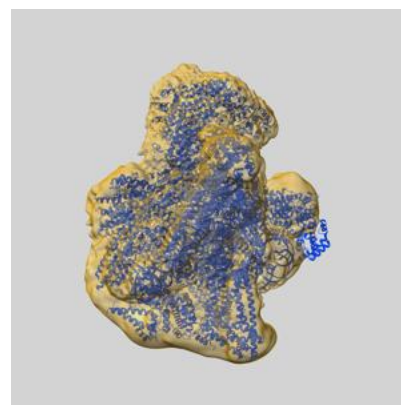
9.1 Map-model overlay [i](#)



X



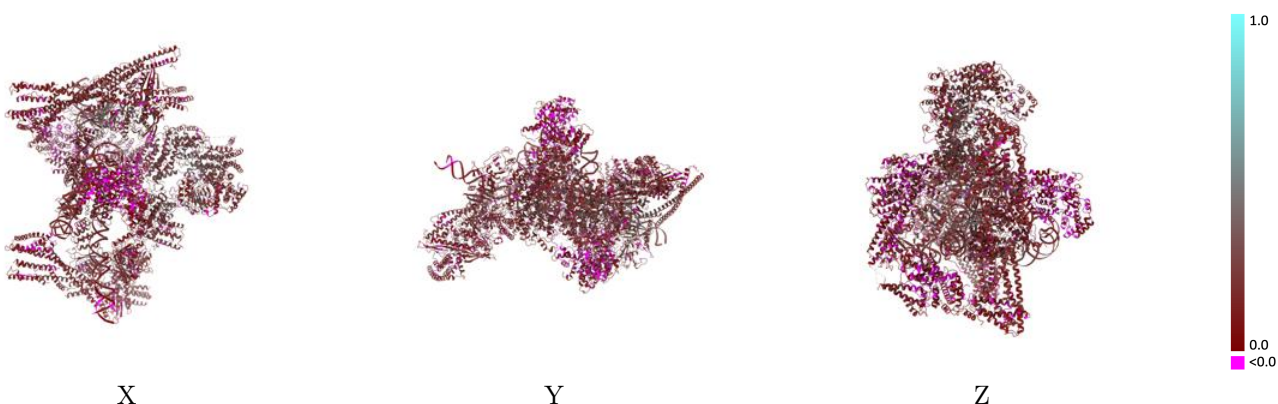
Y



Z

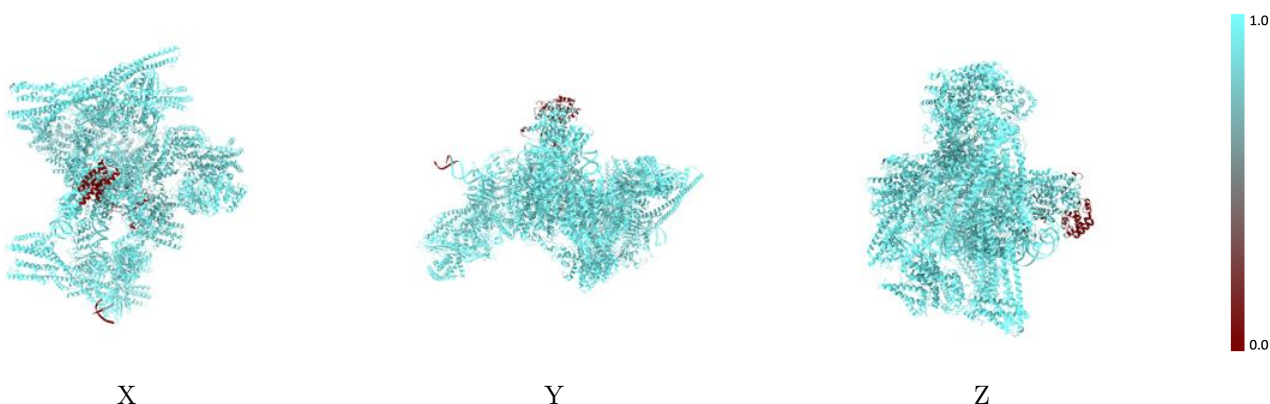
The images above show the 3D surface view of the map at the recommended contour level 0.00271 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



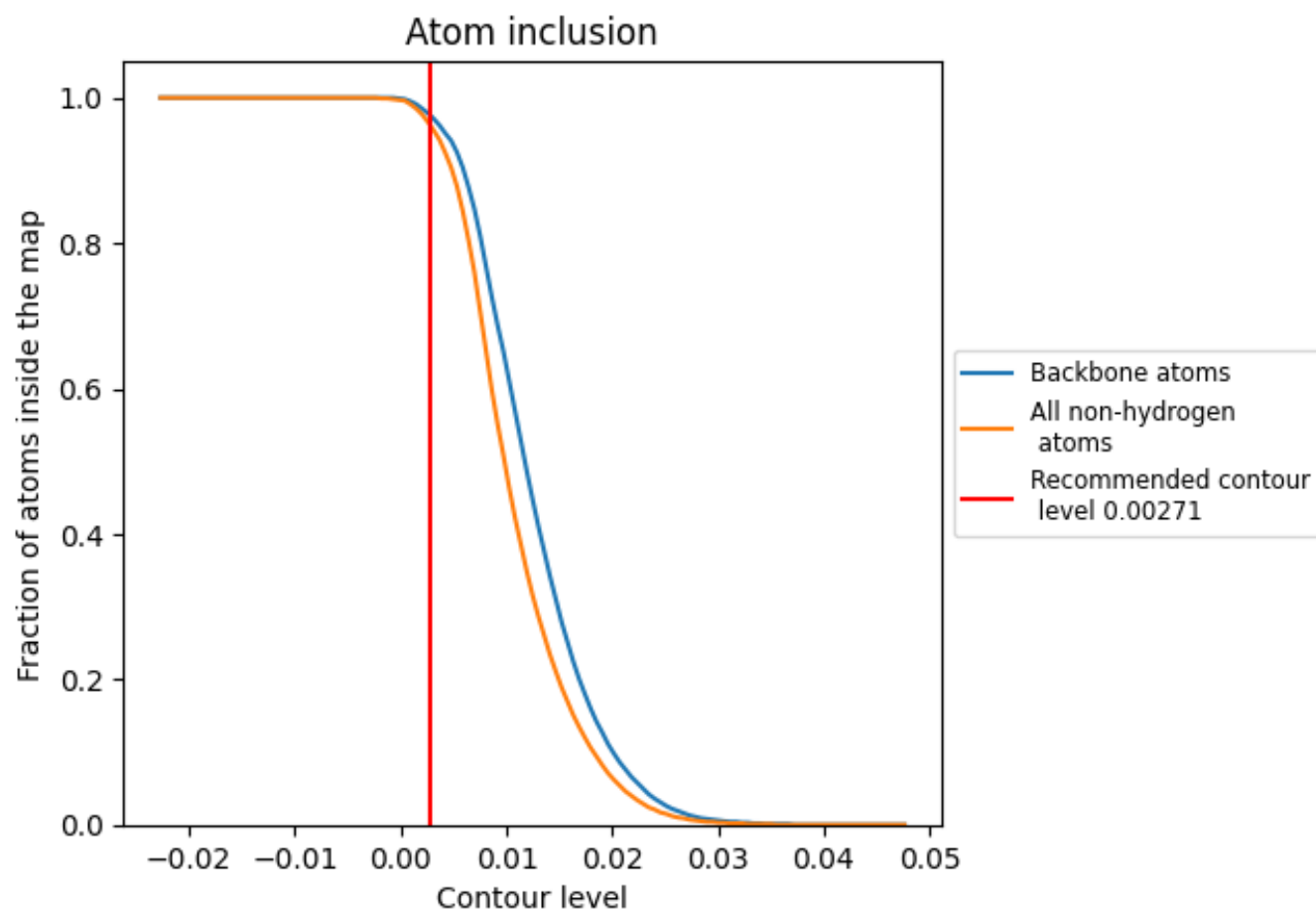
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00271).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.00271) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.1650
A	 0.9900	 0.1660
B	 0.9880	 0.2000
CE	 0.9230	 0.2300
CT	 0.9840	 0.2070
D	 0.9780	 0.1910
E	 0.9630	 0.1940
H	 0.9990	 0.0860
HH	 0.9440	 0.1480
I	 0.9990	 0.0650
II	 0.9650	 0.1480
K	 0.9970	 0.0900
KK	 0.8670	 0.1080
L	 0.9850	 0.1950
LL	 0.9900	 0.1570
N	 0.9600	 0.2510
NN	 0.9910	 0.1860
O	 0.9690	 0.2320
OO	 0.9840	 0.1560
P	 0.9880	 0.1810
PP	 0.9960	 0.1480
Q	 0.9960	 0.1390
QQ	 1.0000	 0.1290
SK	 0.9930	 0.1920
T	 0.9970	 0.0560
TT	 0.3070	 -0.0000
U	 0.9970	 0.1460
UU	 0.9980	 0.1240
W	 1.0000	 0.0940
WW	 0.2070	 0.0250
Y	 0.9950	 0.1540
YY	 0.9950	 0.1510
Z	 0.9830	 0.1560
ZZ	 0.9970	 0.1470
a	 0.9750	 0.1650



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Chain	Atom inclusion	Q-score
b	 0.9670	 0.2090
c	 0.9610	 0.2250
ce	 0.9750	 0.2360
d	 0.9570	 0.2170
e	 0.9650	 0.1700
f	 0.9670	 0.1920
g	 0.9780	 0.1810
h	 0.9600	 0.1950