



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:53 AM UTC

PDB ID : 6LTJ / pdb_00006ltj
EMDB ID : EMD-0974
Title : Structure of nucleosome-bound human BAF complex
Authors : He, S.; Wu, Z.; Tian, Y.; Yu, Z.; Yu, J.; Wang, X.; Li, J.; Liu, B.; Xu, Y.
Deposited on : 2020-01-22
Resolution : 3.70 Å(reported)

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

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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

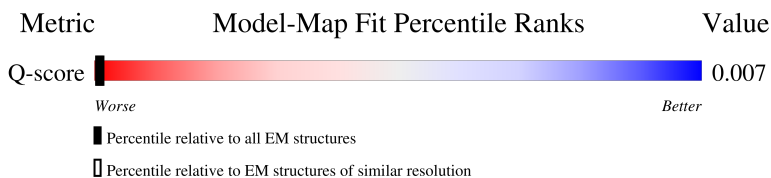
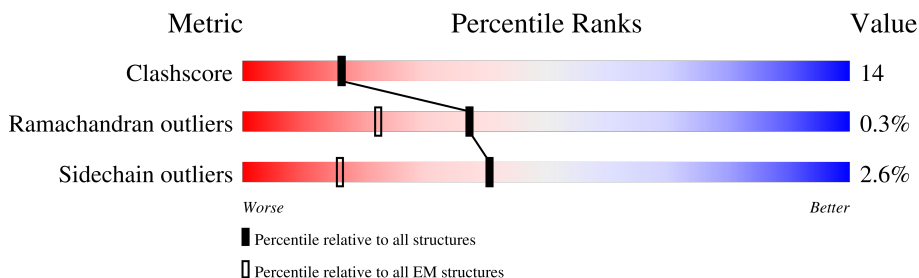
1 Overall quality at a glance

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	136	35% 50% 17% 33%
1	E	136	29% 49% 18% 33%
2	B	103	30% 62% 14% 24%
2	F	103	33% 58% 17% 25%

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Mol	Chain	Length	Quality of chain
3	C	130	
3	G	130	
4	D	126	
4	H	126	
5	I	1647	
6	J	407	
7	K	375	
8	L	1295	
9	M	336	
10	N	1214	
10	O	1214	
11	P	515	
12	Q	411	
13	R	292	
14	X	119	
15	Y	119	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 34283 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 Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	91	Total	C	N	O	S	0	0
			739	466	141	130	2		
1	E	91	Total	C	N	O	S	0	0
			739	466	141	130	2		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	78	Total	C	N	O	S	0	0
			622	393	120	108	1		
2	F	77	Total	C	N	O	S	0	0
			614	389	119	105	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	95	Total	C	N	O	0	0
			726	455	142	129		
3	G	95	Total	C	N	O	0	0
			727	457	142	128		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	88	Total	C	N	O	S	0	0
			682	430	121	129	2		
4	H	90	Total	C	N	O	S	0	0
			700	441	124	133	2		

- Molecule 5 is a protein called Transcription activator BRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	551	Total	C	N	O	S	0	0
			4606	2932	841	809	24		

- Molecule 6 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	334	Total	C	N	O	S	0	0
			2612	1656	441	495	20		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	418	PRO	-	expression tag	UNP O96019

- Molecule 7 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	317	Total	C	N	O	S	0	0
			2482	1575	409	480	18		

- Molecule 8 is a protein called AT-rich interactive domain-containing protein 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	466	Total	C	N	O	S	0	0
			3670	2341	620	688	21		

- Molecule 9 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily B member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	283	Total	C	N	O	S	0	0
			2277	1437	388	440	12		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	163	GLY	-	linker	UNP Q12824
M	164	GLY	-	linker	UNP Q12824
M	165	SER	-	linker	UNP Q12824
M	166	GLY	-	linker	UNP Q12824
M	167	GLY	-	linker	UNP Q12824
M	168	SER	-	linker	UNP Q12824

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Chain	Residue	Modelled	Actual	Comment	Reference
M	169	GLY	-	linker	UNP Q12824
M	170	GLY	-	linker	UNP Q12824
M	171	SER	-	linker	UNP Q12824

- Molecule 10 is a protein called SWI/SNF complex subunit SMARCC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	261	Total	C	N	O	S	0	0
			2120	1346	374	388	12		
10	O	325	Total	C	N	O	S	0	0
			2632	1676	458	485	13		

- Molecule 11 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	239	Total	C	N	O	S	0	0
			2015	1281	362	361	11		

- Molecule 12 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	105	Total	C	N	O	S	0	0
			860	530	161	165	4		

- Molecule 13 is a protein called Zinc finger protein ubi-d4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	70	Total	C	N	O	S	0	0
			580	361	112	102	5		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	101	GLY	-	linker	UNP Q92785
R	102	GLY	-	linker	UNP Q92785
R	103	SER	-	linker	UNP Q92785
R	104	GLY	-	linker	UNP Q92785
R	105	GLY	-	linker	UNP Q92785
R	106	SER	-	linker	UNP Q92785

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Chain	Residue	Modelled	Actual	Comment	Reference
R	107	GLY	-	linker	UNP Q92785
R	108	GLY	-	linker	UNP Q92785
R	109	SER	-	linker	UNP Q92785

- Molecule 14 is a DNA chain called DNA (119-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	119	Total	C	N	O	P	0	0
			2424	1150	440	715	119		

- Molecule 15 is a DNA chain called DNA (119-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Y	119	Total	C	N	O	P	0	0
			2455	1160	463	713	119		

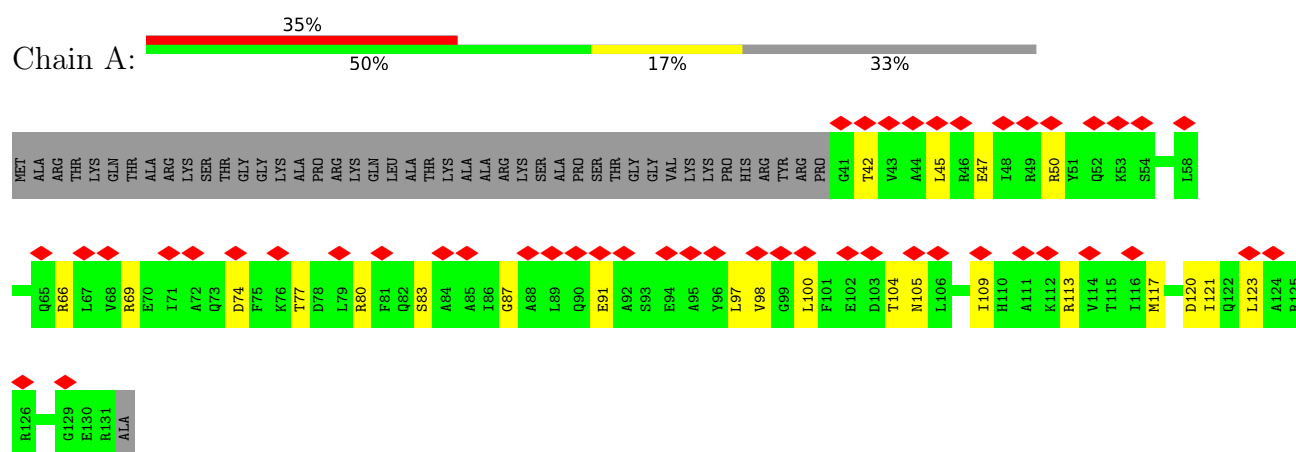
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
16	L	1	Total	Zn	0
			1	1	

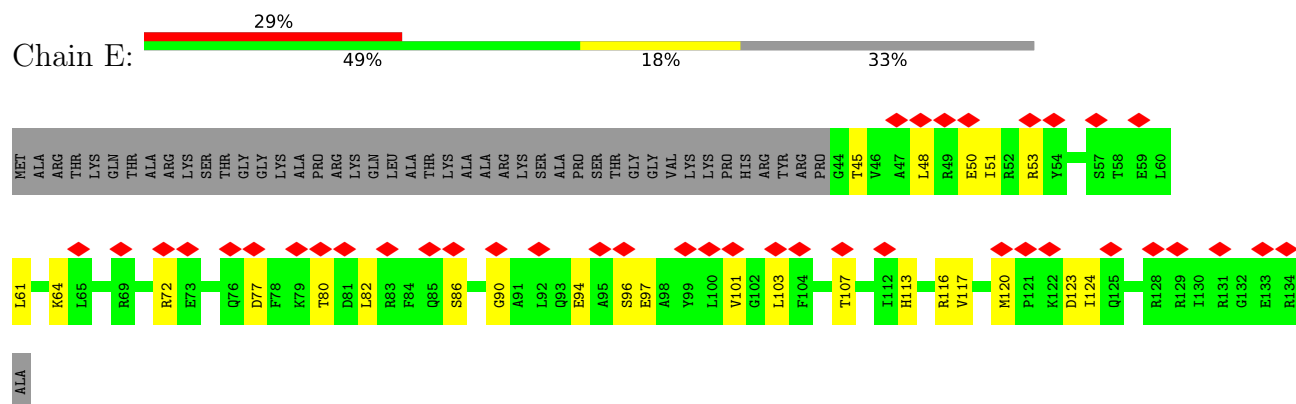
3 Residue-property plots

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

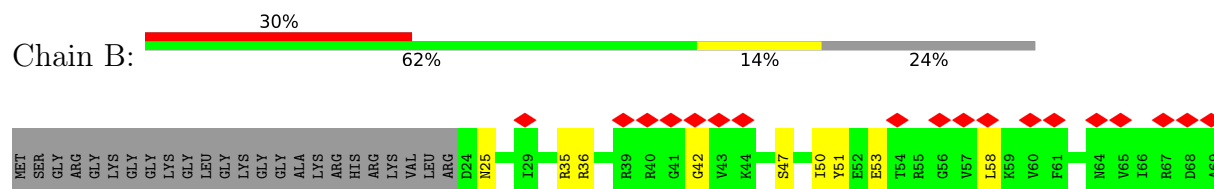
• Molecule 1: Histone H3.3

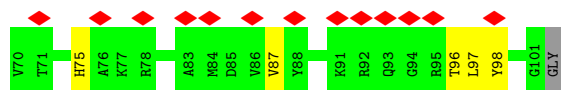


• Molecule 1: Histone H3.3

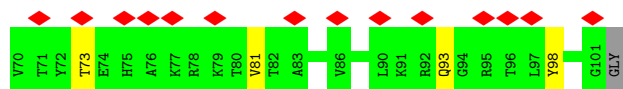


• Molecule 2: Histone H4

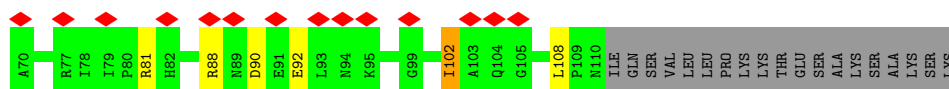
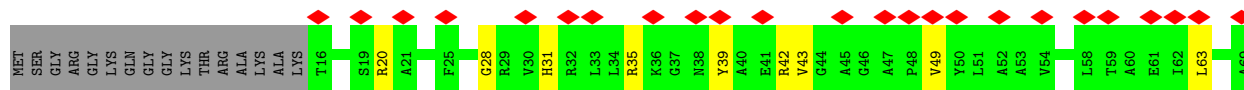




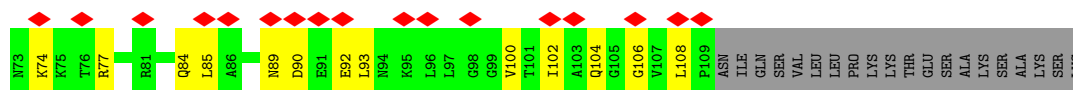
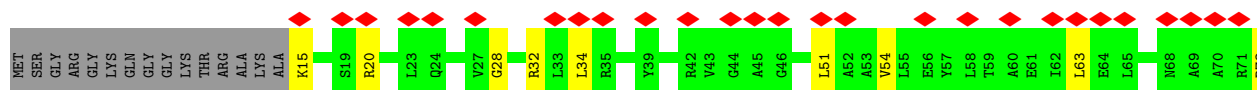
- Molecule 2: Histone H4



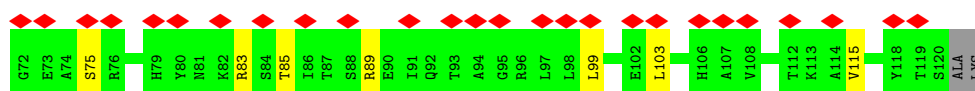
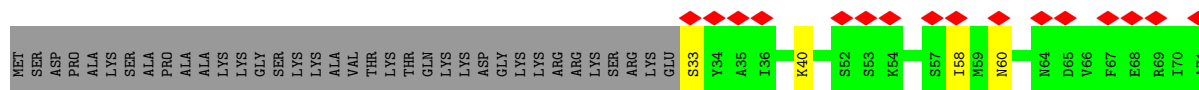
- Molecule 3: Histone H2A type 1



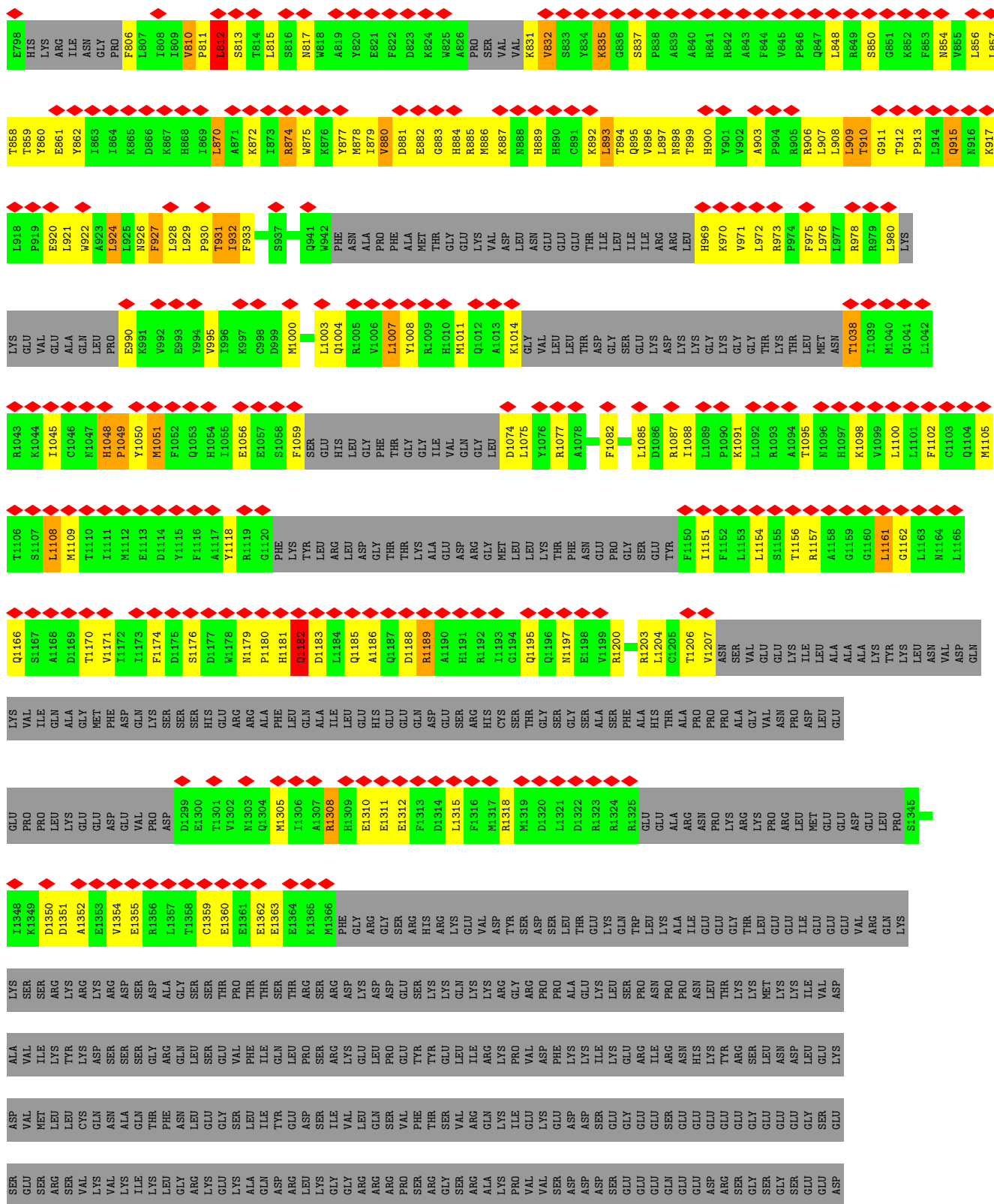
- Molecule 3: Histone H2A type 1

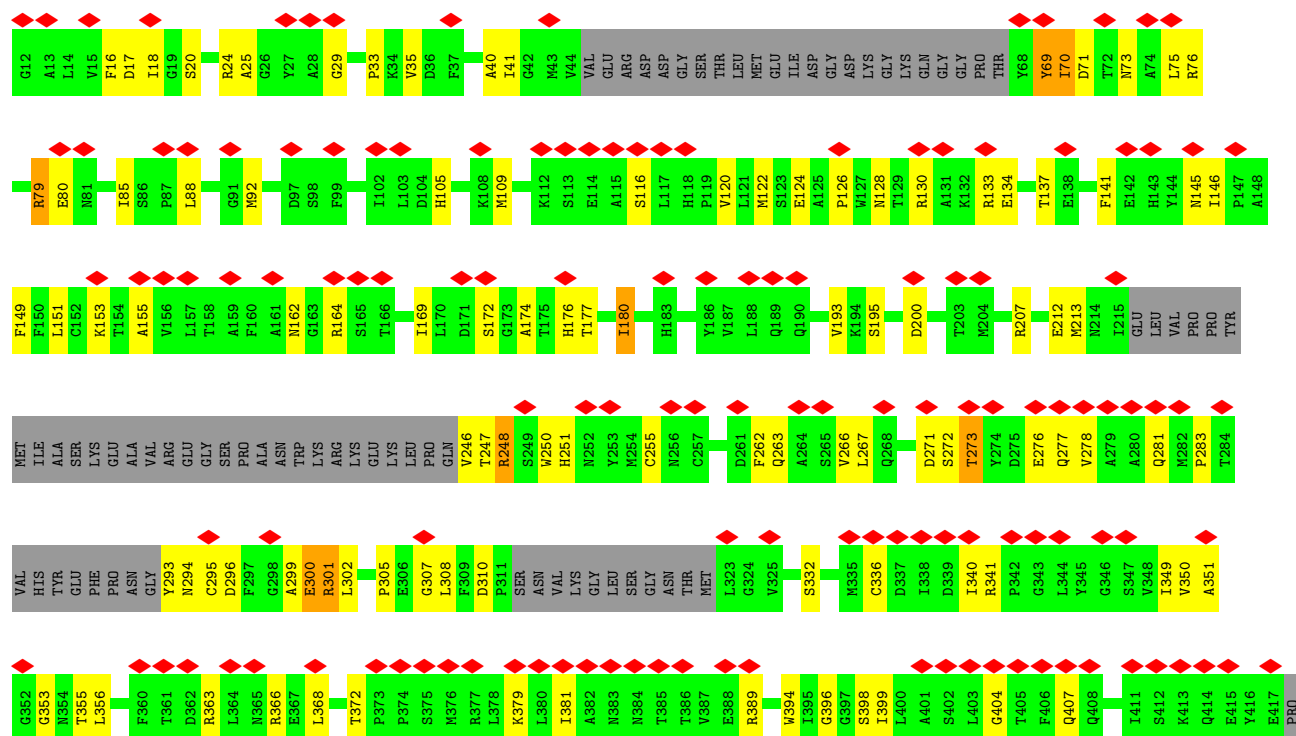


- Molecule 4: Histone H2B

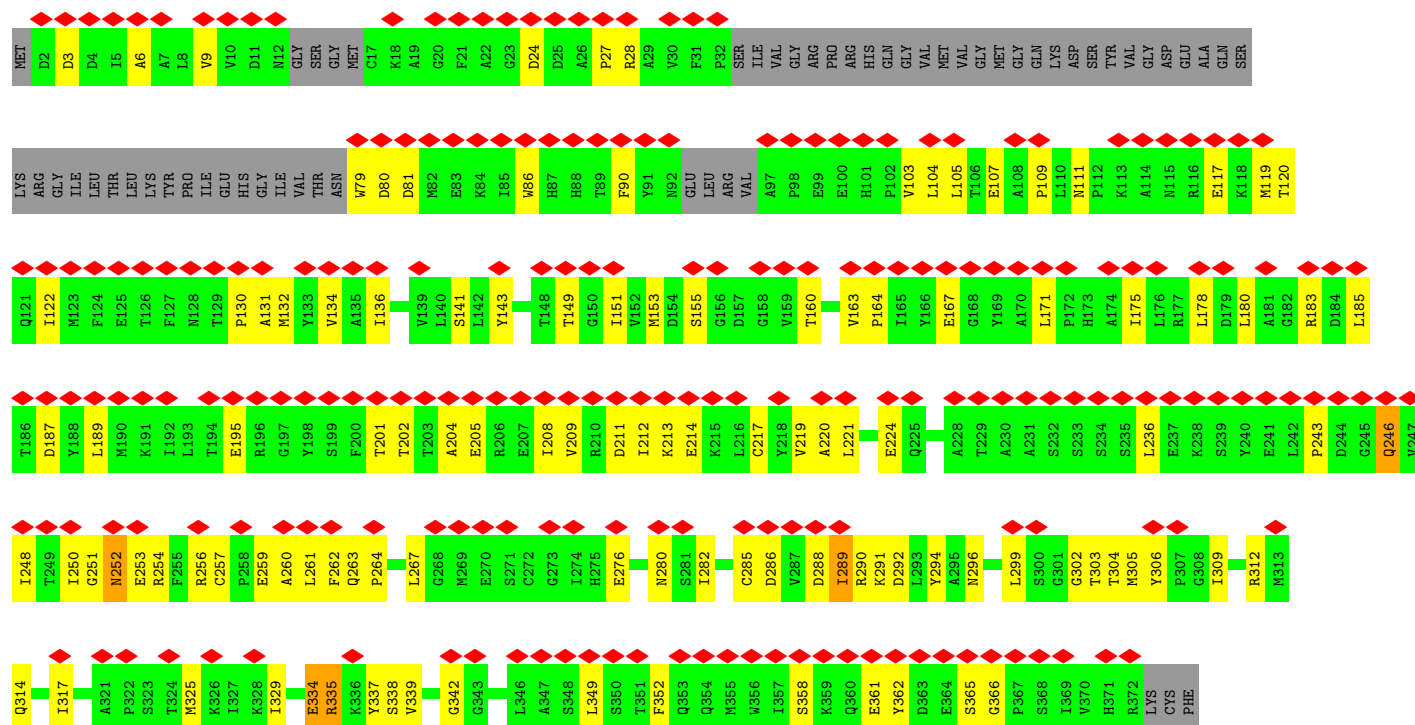


- Molecule 4: Histone H2B





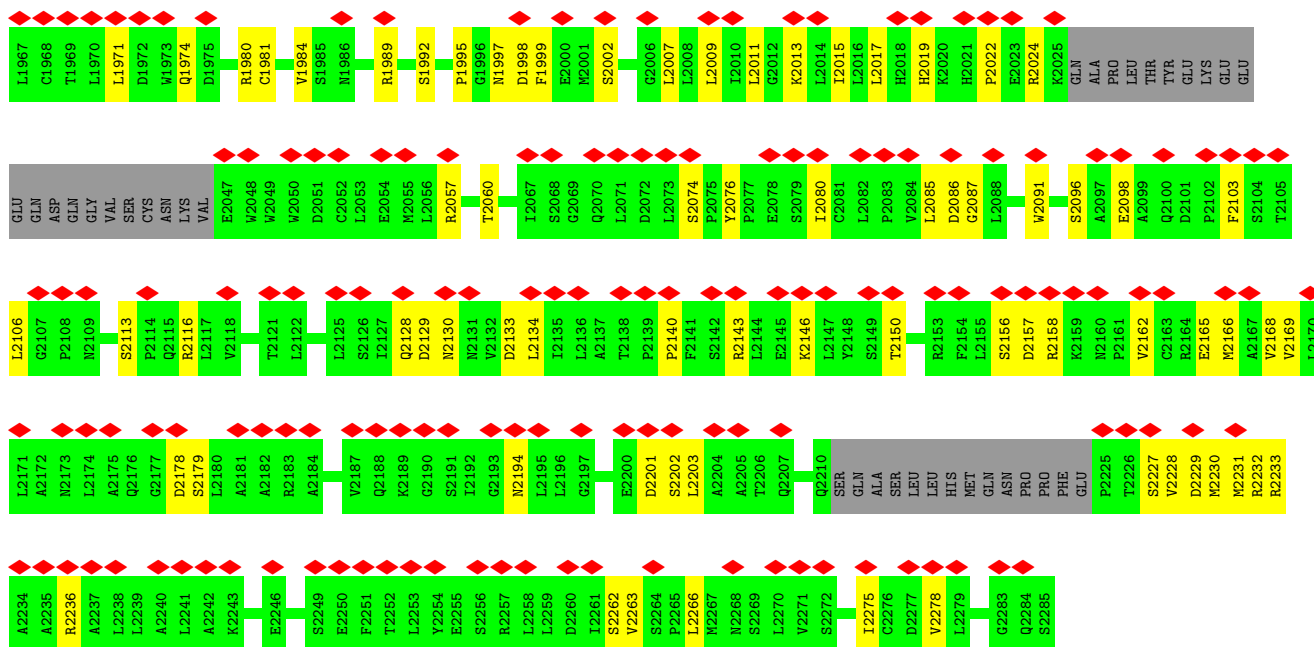
• Molecule 7: Actin, cytoplasmic 1



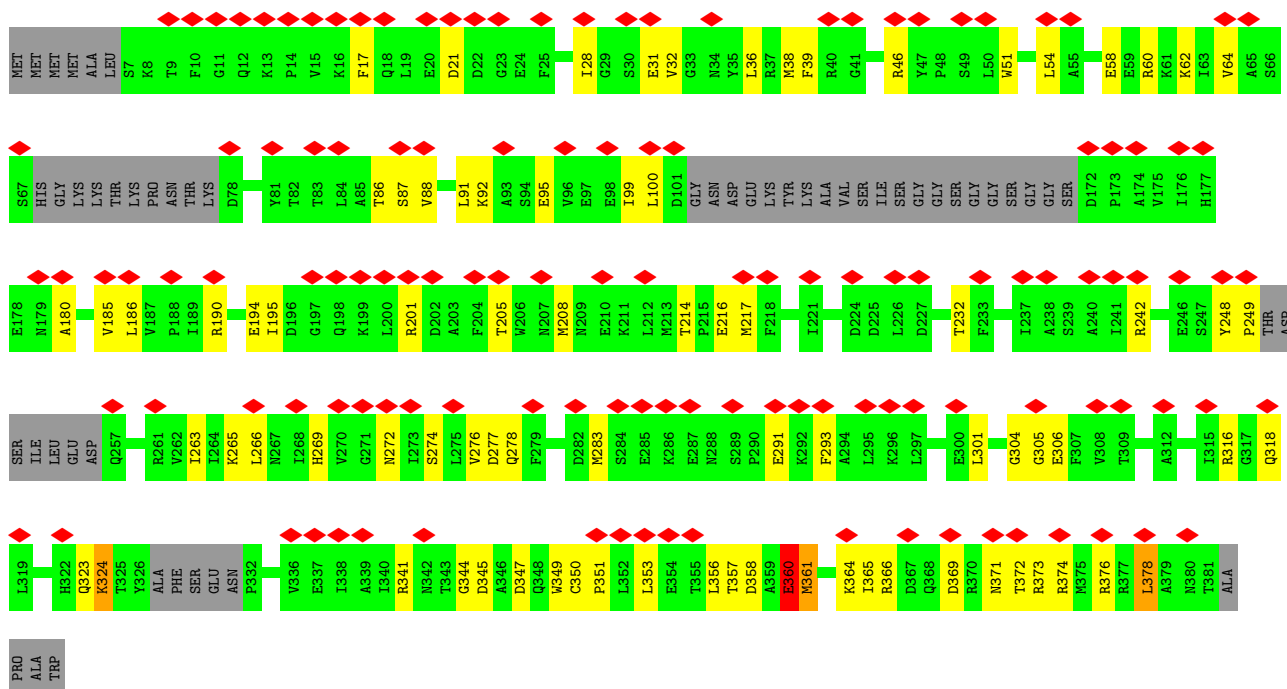
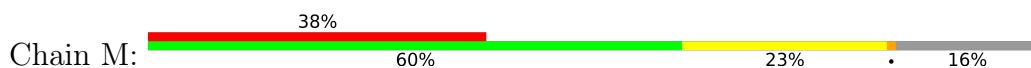
• Molecule 8: AT-rich interactive domain-containing protein 1A







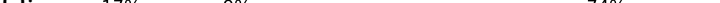
- Molecule 9: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin sub-family B member 1

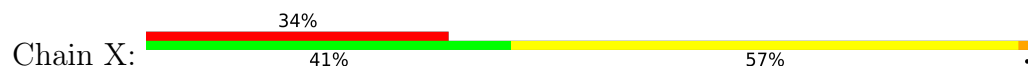


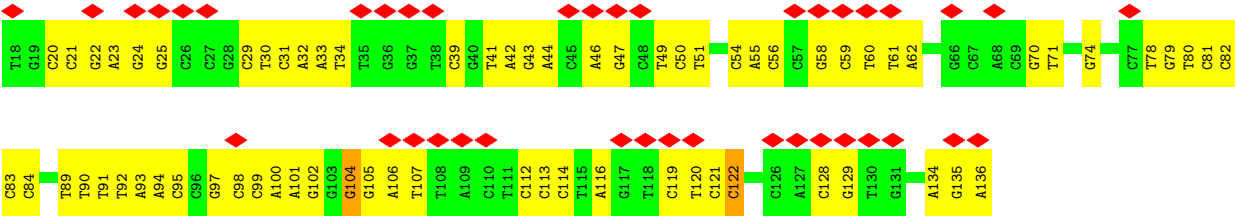
- Molecule 10: SWI/SNF complex subunit SMARCC2



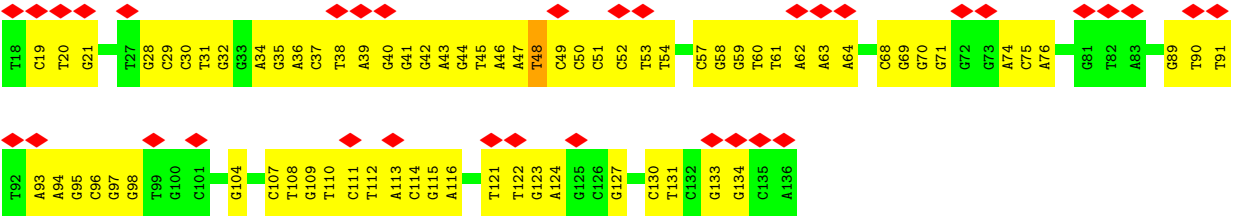


- Chain Q: 





• Molecule 15: DNA (119-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	320658	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.306	Depositor
Minimum map value	-1.288	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.48	Depositor
Map size ($\text{\AA}$)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.71	0/747	0.77	0/1001
1	E	0.71	0/747	0.77	0/1001
2	B	0.77	0/629	0.80	0/843
2	F	0.84	0/621	0.85	0/832
3	C	0.71	0/735	0.66	0/993
3	G	0.71	0/736	0.66	0/993
4	D	0.71	0/693	0.68	0/934
4	H	0.74	0/711	0.69	1/957 (0.1%)
5	I	0.63	0/4682	1.05	21/6281 (0.3%)
6	J	0.48	0/2667	0.85	5/3615 (0.1%)
7	K	0.41	0/2535	0.74	0/3436
8	L	0.26	0/3739	0.41	0/5070
9	M	0.34	0/2317	0.58	4/3129 (0.1%)
10	N	0.27	0/2158	0.44	0/2908
10	O	0.25	0/2692	0.47	1/3646 (0.0%)
11	P	0.24	0/2055	0.45	0/2764
12	Q	0.24	0/871	0.51	0/1168
13	R	0.25	0/595	0.46	0/799
14	X	0.44	0/2715	0.67	7/4184 (0.2%)
15	Y	0.44	0/2757	0.54	2/4257 (0.0%)
All	All	0.48	0/35402	0.69	41/48811 (0.1%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	515	GLN	N-CA-C	-12.52	97.71	111.36
5	I	514	GLU	N-CA-C	-8.84	102.28	113.23
14	X	122	DC	C2'-C3'-O3'	-8.70	98.45	111.50
5	I	913	PRO	N-CA-C	-7.96	99.48	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	X	56	DC	C2'-C3'-O3'	-7.70	99.95	111.50
14	X	60	DT	C2'-C3'-O3'	-7.17	100.75	111.50
6	J	146	ILE	N-CA-C	-6.84	102.66	109.02
14	X	128	DC	C2'-C3'-O3'	-6.82	101.27	111.50
5	I	516	LYS	N-CA-C	-6.51	104.10	111.07
5	I	927	PHE	CB-CA-C	-6.50	102.90	111.42
5	I	476	LEU	N-CA-C	-6.38	104.33	111.28
5	I	861	GLU	N-CA-C	-6.29	105.61	113.28
14	X	129	DG	C4'-C3'-O3'	6.18	119.27	110.00
5	I	1182	GLN	N-CA-C	-6.17	105.47	112.87
4	H	38	VAL	N-CA-C	-6.13	106.83	112.96
14	X	104	DG	C2'-C3'-O3'	-6.09	102.37	111.50
6	J	340	ILE	N-CA-C	-6.04	104.80	113.07
15	Y	48	DT	C2'-C3'-O3'	-5.92	102.62	111.50
5	I	1051	MET	N-CA-C	-5.89	104.26	112.45
5	I	883	GLY	N-CA-C	5.87	119.31	112.50
6	J	273	THR	N-CA-C	5.79	119.25	109.76
6	J	355	THR	CA-C-N	5.79	129.95	120.63
6	J	355	THR	C-N-CA	5.79	129.95	120.63
5	I	810	VAL	N-CA-C	5.76	115.52	109.01
5	I	778	ALA	N-CA-C	5.73	117.32	110.44
5	I	508	HIS	N-CA-C	-5.70	105.15	111.36
15	Y	104	DG	C2'-C3'-O3'	-5.68	102.98	111.50
14	X	55	DA	C2'-C3'-O3'	-5.62	103.08	111.50
5	I	1007	LEU	N-CA-C	-5.61	105.07	111.07
5	I	497	ILE	N-CA-C	-5.57	105.07	110.42
10	O	663	PRO	N-CA-C	-5.56	101.02	112.47
5	I	504	VAL	N-CA-C	-5.35	105.16	110.62
5	I	496	LYS	N-CA-C	-5.27	105.53	111.28
9	M	358	ASP	CB-CA-C	-5.25	102.08	110.79
5	I	500	LEU	N-CA-C	-5.13	105.69	111.28
5	I	1049	PRO	N-CA-C	5.11	123.44	114.75
9	M	360	GLU	N-CA-C	-5.11	105.79	111.36
5	I	475	TYR	N-CA-C	-5.09	105.73	111.28
9	M	304	GLY	CA-C-N	-5.03	112.31	121.32
9	M	304	GLY	C-N-CA	-5.03	112.31	121.32
5	I	502	LYS	CB-CA-C	-5.02	102.46	110.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	739	0	778	17	0
1	E	739	0	778	17	0
2	B	622	0	660	11	0
2	F	614	0	656	14	0
3	C	726	0	761	12	0
3	G	727	0	768	31	0
4	D	682	0	697	10	0
4	H	700	0	716	12	0
5	I	4606	0	4726	211	0
6	J	2612	0	2557	74	0
7	K	2482	0	2432	76	0
8	L	3670	0	3724	91	0
9	M	2277	0	2248	86	0
10	N	2120	0	2116	81	0
10	O	2632	0	2606	93	0
11	P	2015	0	2046	71	0
12	Q	860	0	864	30	0
13	R	580	0	557	20	0
14	X	2424	0	1335	69	0
15	Y	2455	0	1334	85	0
16	L	1	0	0	0	0
All	All	34283	0	32359	944	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 14.

All (944) 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)
3:G:74:LYS:HZ1	9:M:195:ILE:HG21	1.08	1.16
3:G:74:LYS:NZ	9:M:195:ILE:HG21	1.68	1.05
3:G:74:LYS:NZ	9:M:232:THR:HG23	1.74	1.02
6:J:305:PRO:O	6:J:308:LEU:HB2	1.61	1.00
6:J:248:ARG:HA	6:J:248:ARG:CZ	1.92	0.99
3:G:74:LYS:NZ	9:M:232:THR:CG2	2.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:1818:GLN:HA	10:O:428:SER:HB3	1.49	0.93
9:M:249:PRO:HG3	9:M:324:LYS:CE	2.02	0.90
9:M:190:ARG:HD3	9:M:376:ARG:HH22	1.37	0.90
6:J:105:HIS:O	6:J:109:MET:HB2	1.73	0.89
6:J:251:HIS:O	6:J:255:CYS:HB2	1.75	0.84
3:G:74:LYS:HZ1	9:M:232:THR:CG2	1.88	0.84
6:J:213:MET:HE2	6:J:213:MET:HA	1.62	0.82
5:I:1161:LEU:HD11	5:I:1188:ASP:HB2	1.61	0.82
3:G:74:LYS:HZ2	9:M:232:THR:HG23	1.40	0.81
8:L:2263:VAL:HG22	11:P:358:PRO:HD3	1.64	0.80
11:P:352:MET:HE3	11:P:360:ARG:HG2	1.63	0.80
6:J:25:ALA:O	6:J:35:VAL:HB	1.81	0.79
6:J:122:MET:O	6:J:151:LEU:HA	1.83	0.79
5:I:513:ARG:HE	5:I:513:ARG:HA	1.47	0.78
9:M:249:PRO:CG	9:M:324:LYS:NZ	2.46	0.78
5:I:1351:ASP:HB2	5:I:1355:GLU:HG3	1.64	0.78
6:J:248:ARG:HA	6:J:248:ARG:NE	1.98	0.77
8:L:2157:ASP:OD1	8:L:2158:ARG:N	2.17	0.77
10:N:612:ALA:O	10:N:616:TYR:HB2	1.85	0.77
5:I:856:LEU:HD23	5:I:856:LEU:H	1.50	0.76
5:I:1004:GLN:O	5:I:1008:TYR:HB2	1.84	0.76
11:P:300:ARG:HH22	11:P:345:GLN:HB3	1.50	0.76
11:P:296:LYS:HG3	11:P:309:THR:HG22	1.65	0.76
5:I:1180:PRO:HA	5:I:1182:GLN:NE2	2.01	0.76
15:Y:47:DA:H2''	15:Y:48:DT:H2'	1.67	0.76
9:M:249:PRO:HG3	9:M:324:LYS:NZ	2.01	0.76
3:G:74:LYS:NZ	9:M:195:ILE:CG2	2.48	0.76
9:M:51:TRP:HE1	9:M:92:LYS:HG3	1.49	0.76
5:I:487:LYS:HE2	5:I:487:LYS:HA	1.66	0.75
8:L:2140:PRO:HG2	8:L:2143:ARG:HD2	1.67	0.75
9:M:95:GLU:O	9:M:99:ILE:HB	1.87	0.75
15:Y:62:DA:H8	15:Y:62:DA:H5''	1.51	0.74
8:L:2017:LEU:O	8:L:2057:ARG:NH2	2.21	0.73
5:I:785:LYS:HE2	5:I:909:LEU:HB2	1.71	0.73
8:L:2202:SER:HB3	8:L:2231:MET:HE2	1.70	0.73
10:N:683:VAL:HA	12:Q:211:VAL:HG12	1.69	0.73
10:N:909:LEU:HA	10:N:912:ILE:HD12	1.70	0.73
5:I:1180:PRO:C	5:I:1182:GLN:HE21	1.98	0.72
9:M:249:PRO:CG	9:M:324:LYS:HZ3	2.02	0.72
5:I:481:GLN:HA	5:I:484:LYS:HD2	1.71	0.72
9:M:347:ASP:OD1	10:O:488:ARG:NH2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:100:DA:H2'	14:X:101:DA:C8	2.25	0.72
14:X:24:DG:H2''	14:X:25:DG:H5''	1.70	0.71
5:I:1000:MET:HE3	5:I:1004:GLN:HE21	1.55	0.71
15:Y:108:DT:H2''	15:Y:109:DG:H5''	1.71	0.71
7:K:103:VAL:O	7:K:132:MET:HA	1.90	0.71
9:M:361:MET:HE3	9:M:361:MET:HA	1.71	0.71
5:I:1161:LEU:HD11	5:I:1188:ASP:CB	2.20	0.71
5:I:350:SER:OG	5:I:351:ARG:N	2.23	0.71
15:Y:69:DG:H2'	15:Y:70:DG:C8	2.26	0.70
8:L:1823:PHE:O	13:R:60:ARG:NH1	2.24	0.70
15:Y:111:DC:H2''	15:Y:112:DT:H5''	1.73	0.70
9:M:301:LEU:O	13:R:38:ARG:NH1	2.24	0.70
9:M:305:GLY:HA2	10:N:489:ASN:HD22	1.57	0.69
8:L:1736:VAL:HG22	8:L:1850:ASP:HA	1.73	0.69
7:K:185:LEU:HG	7:K:213:LYS:HZ1	1.56	0.68
10:N:464:ALA:HA	13:R:55:ILE:HG22	1.75	0.68
11:P:361:LEU:HG	11:P:365:LEU:HD11	1.74	0.68
3:G:74:LYS:HZ1	9:M:195:ILE:CG2	1.96	0.68
5:I:513:ARG:HA	5:I:513:ARG:NE	2.08	0.67
11:P:349:SER:H	11:P:360:ARG:HH21	1.43	0.67
9:M:249:PRO:HG2	9:M:324:LYS:HZ3	1.56	0.67
8:L:1718:GLU:OE2	8:L:1721:ARG:NH2	2.28	0.67
3:G:74:LYS:HZ2	9:M:232:THR:CG2	2.02	0.67
7:K:205:GLU:HA	7:K:208:ILE:HG12	1.77	0.66
10:N:902:LYS:NZ	11:P:154:GLU:OE2	2.29	0.66
10:N:484:THR:HA	10:N:487:ARG:HG2	1.76	0.66
5:I:1195:GLN:HE22	5:I:1197:ASN:HD22	1.43	0.66
5:I:920:GLU:O	5:I:924:LEU:HB2	1.96	0.65
5:I:1102:PHE:HB3	5:I:1156:THR:HG22	1.79	0.65
7:K:202:THR:HG22	7:K:204:ALA:H	1.61	0.65
12:Q:264:ASP:O	12:Q:268:ASN:ND2	2.29	0.65
15:Y:29:DC:H1'	15:Y:30:DC:C2	2.32	0.65
14:X:113:DC:O2	15:Y:41:DG:N2	2.28	0.65
10:N:687:ARG:NH1	10:O:703:MET:SD	2.70	0.65
10:O:894:THR:HG23	12:Q:241:LEU:HD23	1.79	0.65
6:J:353:GLY:O	6:J:356:LEU:HB3	1.97	0.65
7:K:155:SER:HA	7:K:160:THR:HG22	1.78	0.64
10:O:887:LEU:HD23	12:Q:234:LEU:HB2	1.77	0.64
14:X:106:DA:H2''	14:X:107:DT:H5''	1.79	0.64
15:Y:94:DA:H2''	15:Y:95:DG:C8	2.32	0.64
5:I:978:ARG:HH21	5:I:980:LEU:HD13	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:377:ARG:NH1	10:O:651:ASP:OD2	2.30	0.64
5:I:1360:GLU:HA	5:I:1363:GLU:HB2	1.79	0.64
9:M:249:PRO:HG2	9:M:324:LYS:NZ	2.10	0.64
9:M:190:ARG:CD	9:M:376:ARG:NH2	2.61	0.64
9:M:274:SER:O	9:M:353:LEU:HA	1.97	0.63
1:A:69:ARG:NH1	15:Y:54:DT:OP1	2.29	0.63
9:M:190:ARG:HD3	9:M:376:ARG:NH2	2.11	0.63
3:C:28:GLY:HA3	15:Y:32:DG:H3'	1.81	0.63
14:X:33:DA:H2'	14:X:34:DT:H71	1.81	0.63
10:N:932:GLN:HG2	12:Q:273:LEU:HD21	1.80	0.63
5:I:1351:ASP:HB3	5:I:1354:VAL:HG12	1.81	0.62
8:L:2178:ASP:OD1	8:L:2179:SER:N	2.30	0.62
5:I:922:TRP:NE1	5:I:971:VAL:O	2.30	0.62
6:J:124:GLU:OE2	6:J:128:ASN:ND2	2.31	0.62
5:I:405:LYS:NZ	10:O:614:GLU:OE1	2.30	0.62
8:L:1805:LEU:HD21	10:O:431:ALA:HA	1.80	0.62
7:K:253:GLU:HA	7:K:256:ARG:HB2	1.82	0.62
10:N:424:ILE:HD13	10:N:474:ARG:HD3	1.80	0.62
10:O:662:GLN:HG3	11:P:473:PRO:HG2	1.82	0.62
5:I:512:GLU:O	5:I:515:GLN:HB3	2.00	0.62
15:Y:62:DA:H2'	15:Y:63:DA:C8	2.35	0.62
5:I:483:ALA:HB1	6:J:399:ILE:HG13	1.82	0.62
3:G:74:LYS:HZ1	9:M:232:THR:HG21	1.63	0.61
5:I:468:ARG:HA	5:I:471:LYS:HD2	1.83	0.61
5:I:487:LYS:HE3	6:J:399:ILE:HD13	1.80	0.61
12:Q:188:MET:HA	12:Q:191:THR:HG22	1.81	0.61
10:N:692:ALA:HB2	10:O:696:ALA:HB2	1.82	0.61
1:A:80:ARG:HD2	14:X:104:DG:H5''	1.83	0.61
8:L:2158:ARG:NH1	8:L:2201:ASP:OD2	2.34	0.61
11:P:297:LEU:HD21	11:P:315:ILE:HD13	1.82	0.61
10:N:448:GLU:OE2	10:N:499:ARG:NE	2.29	0.61
15:Y:76:DA:H8	15:Y:76:DA:H5''	1.66	0.61
5:I:1203:ARG:NH1	5:I:1204:LEU:O	2.34	0.61
7:K:86:TRP:O	7:K:90:PHE:HB2	2.01	0.61
9:M:190:ARG:CD	9:M:376:ARG:HH22	2.08	0.61
15:Y:112:DT:H2''	15:Y:113:DA:N7	2.16	0.61
7:K:221:LEU:HD12	7:K:221:LEU:N	2.16	0.61
10:N:901:ILE:HB	11:P:417:ILE:HD11	1.83	0.61
12:Q:180:ASP:OD1	12:Q:181:ASP:N	2.34	0.61
14:X:93:DA:H1'	14:X:94:DA:N7	2.15	0.61
5:I:889:HIS:O	5:I:895:GLN:NE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:223:ARG:HB3	12:Q:224:MET:HE2	1.83	0.60
10:N:913:MET:HE1	10:O:909:LEU:HD23	1.82	0.60
10:O:621:ASN:OD1	10:O:632:GLN:NE2	2.34	0.60
9:M:378:LEU:HD13	9:M:378:LEU:O	2.01	0.60
1:A:113:ARG:NH2	1:A:120:ASP:OD1	2.34	0.60
1:E:116:ARG:NH2	1:E:123:ASP:OD1	2.34	0.60
9:M:249:PRO:HG3	9:M:324:LYS:HE2	1.80	0.60
11:P:300:ARG:NH1	11:P:345:GLN:O	2.23	0.60
7:K:109:PRO:HA	7:K:136:ILE:HD12	1.84	0.59
10:N:877:ALA:HB2	11:P:441:MET:HB2	1.84	0.59
7:K:213:LYS:NZ	7:K:257:CYS:SG	2.74	0.59
7:K:276:GLU:O	7:K:280:ASN:ND2	2.35	0.59
15:Y:52:DC:H2''	15:Y:53:DT:H72	1.83	0.59
3:G:92:GLU:HG2	9:M:366:ARG:HH22	1.68	0.59
5:I:514:GLU:CD	5:I:514:GLU:O	2.46	0.59
8:L:1847:GLY:HA3	8:L:2009:LEU:HD22	1.84	0.59
2:F:50:ILE:O	2:F:53:GLU:HB3	2.02	0.59
5:I:1051:MET:HA	5:I:1051:MET:HE2	1.83	0.59
10:N:489:ASN:ND2	13:R:43:ASP:OD2	2.36	0.59
6:J:69:TYR:CE2	6:J:73:ASN:HB3	2.37	0.58
15:Y:124:DA:H5'	15:Y:124:DA:C8	2.38	0.58
10:N:696:ALA:HB2	10:O:692:ALA:HB2	1.85	0.58
10:O:684:VAL:O	11:P:449:GLN:NE2	2.36	0.58
11:P:297:LEU:HD22	11:P:301:LEU:HD23	1.84	0.58
13:R:58:GLU:H	13:R:61:HIS:HD2	1.51	0.58
15:Y:28:DG:H2''	15:Y:29:DC:H5'	1.84	0.58
15:Y:62:DA:H5''	15:Y:62:DA:C8	2.35	0.58
6:J:141:PHE:O	6:J:145:ASN:ND2	2.36	0.58
8:L:1828:SER:OG	8:L:1835:GLN:NE2	2.36	0.58
5:I:778:ALA:HB2	5:I:910:THR:HG23	1.86	0.58
5:I:896:VAL:HA	5:I:899:THR:HG22	1.86	0.58
8:L:2096:SER:OG	8:L:2098:GLU:OE1	2.21	0.58
11:P:294:GLN:HB2	11:P:311:THR:HG22	1.86	0.58
8:L:2162:VAL:HG22	8:L:2166:MET:HE3	1.85	0.58
5:I:779:ASP:OD1	5:I:779:ASP:N	2.35	0.58
3:G:72:ASP:CG	9:M:194:GLU:O	2.47	0.58
10:N:917:ARG:HH12	10:O:909:LEU:HG	1.68	0.58
15:Y:107:DC:H2'	15:Y:108:DT:C6	2.38	0.58
11:P:294:GLN:HA	11:P:311:THR:HA	1.86	0.58
13:R:17:TYR:O	13:R:21:MET:HG2	2.04	0.58
14:X:23:DA:H5'	14:X:23:DA:H8	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:367:LEU:HD13	10:O:659:LEU:HD12	1.86	0.58
5:I:792:LEU:C	5:I:792:LEU:HD23	2.29	0.57
15:Y:35:DG:H2'	15:Y:36:DA:C8	2.39	0.57
14:X:50:DC:H2''	14:X:51:DT:H71	1.84	0.57
15:Y:127:DG:H5'	15:Y:127:DG:C8	2.40	0.57
9:M:185:VAL:HG13	9:M:208:MET:HB3	1.85	0.57
10:N:618:ASP:OD1	10:N:618:ASP:N	2.36	0.57
10:N:923:GLN:OE1	10:O:924:ARG:NH2	2.37	0.57
10:O:890:LEU:O	10:O:893:GLU:HG3	2.04	0.57
15:Y:45:DT:O4	15:Y:46:DA:N6	2.36	0.57
8:L:1705:ASN:ND2	8:L:1707:SER:OG	2.37	0.57
5:I:451:ARG:NH2	8:L:2165:GLU:OE2	2.36	0.57
6:J:276:GLU:O	6:J:277:GLN:NE2	2.37	0.57
9:M:265:LYS:O	9:M:318:GLN:NE2	2.31	0.57
14:X:113:DC:N4	15:Y:40:DG:O6	2.37	0.57
5:I:774:ASN:HB2	5:I:929:LEU:HB2	1.86	0.57
9:M:357:THR:O	9:M:360:GLU:HG3	2.03	0.57
5:I:1087:ARG:O	5:I:1091:LYS:NZ	2.30	0.57
5:I:1305:MET:HE2	5:I:1318:ARG:HH21	1.70	0.57
9:M:277:ASP:HB3	9:M:351:PRO:HA	1.86	0.57
3:G:90:ASP:OD1	9:M:366:ARG:NH2	2.36	0.56
5:I:513:ARG:HE	5:I:513:ARG:CA	2.17	0.56
7:K:105:LEU:O	7:K:134:VAL:HA	2.05	0.56
2:F:31:LYS:HG3	2:F:35:ARG:HH11	1.69	0.56
6:J:307:GLY:HA2	6:J:310:ASP:HB3	1.86	0.56
3:G:32:ARG:NH1	14:X:33:DA:OP1	2.39	0.56
5:I:406:ALA:HB1	10:O:644:ILE:HG12	1.88	0.56
5:I:513:ARG:O	5:I:516:LYS:HB3	2.05	0.56
5:I:889:HIS:HB3	5:I:924:LEU:HA	1.86	0.56
6:J:262:PHE:O	6:J:266:VAL:HB	2.05	0.56
7:K:3:ASP:HA	7:K:6:ALA:HB3	1.88	0.56
8:L:1686:TRP:CD1	10:O:542:VAL:HG23	2.40	0.56
15:Y:49:DC:H4'	15:Y:50:DC:H5'	1.86	0.56
3:G:74:LYS:HZ3	9:M:195:ILE:HG21	1.69	0.56
6:J:126:PRO:HG3	6:J:153:LYS:HD3	1.87	0.56
6:J:381:ILE:O	6:J:389:ARG:NH2	2.36	0.56
7:K:221:LEU:HA	7:K:312:ARG:HD3	1.87	0.56
10:O:427:PRO:HG3	10:O:512:TYR:CZ	2.41	0.56
14:X:82:DC:H2''	14:X:83:DC:C5	2.41	0.56
7:K:131:ALA:HA	7:K:358:SER:HA	1.88	0.56
15:Y:122:DT:H2''	15:Y:123:DG:N7	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:472:HIS:HA	5:I:475:TYR:CD2	2.41	0.56
7:K:153:MET:HE1	7:K:160:THR:HB	1.88	0.56
10:N:470:ILE:HA	10:N:510:ILE:HD11	1.88	0.56
11:P:331:PRO:O	11:P:334:ARG:NE	2.32	0.56
15:Y:29:DC:H1'	15:Y:30:DC:N3	2.21	0.56
11:P:328:LEU:O	11:P:338:ILE:N	2.39	0.55
15:Y:34:DA:H2''	15:Y:35:DG:H5''	1.88	0.55
5:I:1351:ASP:HB3	5:I:1354:VAL:CG1	2.36	0.55
10:N:602:THR:HG23	10:N:605:GLU:H	1.70	0.55
10:O:908:GLU:OE2	12:Q:252:HIS:NE2	2.33	0.55
5:I:377:ARG:HD2	10:O:648:TYR:HD2	1.72	0.55
5:I:1305:MET:O	5:I:1318:ARG:NH2	2.39	0.55
9:M:305:GLY:HA2	10:N:489:ASN:ND2	2.21	0.55
5:I:786:THR:HG23	5:I:787:ILE:HG13	1.87	0.55
5:I:1315:LEU:HD23	5:I:1315:LEU:O	2.06	0.55
6:J:18:ILE:HG22	6:J:88:LEU:HD11	1.87	0.55
7:K:79:TRP:N	7:K:81:ASP:OD1	2.40	0.55
8:L:1652:VAL:O	12:Q:189:LYS:NZ	2.35	0.55
14:X:50:DC:OP2	14:X:50:DC:H2'	2.06	0.55
5:I:1108:LEU:HD12	5:I:1109:MET:HG2	1.89	0.55
1:E:50:GLU:HA	1:E:53:ARG:HB2	1.89	0.55
2:F:64:ASN:OD1	2:F:64:ASN:N	2.35	0.55
9:M:216:GLU:OE2	9:M:242:ARG:NH1	2.27	0.55
10:O:876:LEU:HA	10:O:879:VAL:HG12	1.89	0.55
10:O:941:TYR:HA	10:O:944:MET:HB2	1.88	0.55
5:I:810:VAL:HA	5:I:882:GLU:HG2	1.89	0.55
5:I:1098:LYS:HD2	5:I:1151:ILE:HD11	1.88	0.55
7:K:236:LEU:HD13	7:K:254:ARG:HH21	1.72	0.55
8:L:2002:SER:O	8:L:2076:TYR:OH	2.23	0.55
8:L:2203:LEU:HD22	8:L:2266:LEU:HD12	1.89	0.55
15:Y:130:DC:H2''	15:Y:131:DT:H72	1.88	0.55
2:B:87:VAL:HG12	2:B:97:LEU:HD23	1.88	0.55
5:I:467:LYS:HG2	5:I:471:LYS:HE3	1.88	0.55
6:J:248:ARG:HH21	6:J:251:HIS:HD2	1.55	0.55
10:O:611:GLU:HG3	10:O:615:MET:HE3	1.88	0.55
5:I:972:LEU:HB3	5:I:976:LEU:HD12	1.89	0.54
7:K:80:ASP:OD1	7:K:80:ASP:N	2.39	0.54
11:P:410:SER:O	11:P:413:SER:OG	2.21	0.54
15:Y:112:DT:H2''	15:Y:113:DA:C8	2.42	0.54
10:O:618:ASP:OD2	11:P:498:LYS:NZ	2.30	0.54
14:X:32:DA:H2''	14:X:33:DA:C8	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:50:DC:H2''	14:X:51:DT:C7	2.37	0.54
1:A:47:GLU:HA	1:A:50:ARG:HB2	1.89	0.54
7:K:183:ARG:NH1	7:K:187:ASP:OD2	2.40	0.54
10:N:909:LEU:HD11	11:P:164:LYS:HB2	1.88	0.54
11:P:300:ARG:NH2	11:P:345:GLN:HB3	2.22	0.54
3:G:74:LYS:CE	9:M:232:THR:HG23	2.37	0.54
5:I:1105:MET:SD	14:X:102:DG:H5'	2.47	0.54
7:K:290:ARG:O	7:K:294:TYR:N	2.39	0.54
1:A:69:ARG:HH22	15:Y:54:DT:P	2.31	0.54
8:L:1706:LEU:H	8:L:1997:ASN:ND2	2.05	0.54
10:N:621:ASN:OD1	10:N:632:GLN:NE2	2.41	0.54
10:O:514:VAL:HB	10:O:519:ARG:HH21	1.73	0.54
13:R:44:SER:C	13:R:46:THR:H	2.16	0.54
6:J:350:VAL:O	6:J:389:ARG:NH1	2.35	0.54
11:P:401:LYS:HG2	11:P:405:ASN:HD21	1.72	0.54
5:I:498:GLN:HA	5:I:498:GLN:OE1	2.07	0.54
8:L:1676:LEU:HD23	8:L:1687:ALA:HB1	1.89	0.53
8:L:1998:ASP:OD1	8:L:1999:PHE:N	2.41	0.53
9:M:51:TRP:NE1	9:M:92:LYS:HG3	2.21	0.53
10:O:661:TYR:CE1	11:P:457:GLN:HG2	2.43	0.53
11:P:425:HIS:O	11:P:429:GLU:HG3	2.09	0.53
14:X:119:DC:O2	15:Y:35:DG:N2	2.41	0.53
3:G:28:GLY:HA3	14:X:33:DA:H3'	1.90	0.53
5:I:903:ALA:O	5:I:906:ARG:NE	2.41	0.53
5:I:1206:THR:OG1	5:I:1207:VAL:N	2.42	0.53
6:J:368:LEU:O	6:J:372:THR:OG1	2.27	0.53
10:O:887:LEU:HD21	12:Q:235:MET:HG3	1.90	0.53
11:P:401:LYS:O	11:P:405:ASN:ND2	2.41	0.53
10:O:439:HIS:CD2	10:O:441:ILE:H	2.27	0.53
14:X:114:DC:H5''	14:X:114:DC:C6	2.43	0.53
5:I:491:ARG:O	5:I:494:THR:OG1	2.25	0.53
5:I:504:VAL:HG21	7:K:143:TYR:CE2	2.43	0.53
5:I:1352:ALA:O	5:I:1355:GLU:HB2	2.09	0.53
7:K:149:THR:HG22	7:K:167:GLU:H	1.74	0.53
8:L:2227:SER:OG	8:L:2228:VAL:N	2.38	0.53
9:M:190:ARG:NH2	9:M:372:THR:HG21	2.23	0.53
3:G:85:LEU:O	3:G:89:ASN:ND2	2.36	0.53
5:I:1091:LYS:HD3	5:I:1318:ARG:HB3	1.90	0.53
6:J:20:SER:HB3	6:J:176:HIS:HE1	1.73	0.53
6:J:271:ASP:OD1	6:J:366:ARG:NH1	2.41	0.53
9:M:361:MET:HA	9:M:361:MET:CE	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:127:DG:H5'	15:Y:127:DG:H8	1.74	0.53
3:G:15:LYS:O	3:G:20:ARG:NH2	2.42	0.53
5:I:1074:ASP:HA	5:I:1077:ARG:HD2	1.90	0.53
6:J:20:SER:HB2	6:J:174:ALA:H	1.74	0.52
11:P:462:ASP:OD1	12:Q:195:ARG:NH1	2.43	0.52
5:I:424:MET:O	5:I:428:THR:OG1	2.23	0.52
5:I:924:LEU:C	5:I:926:ASN:H	2.17	0.52
5:I:990:GLU:N	5:I:1197:ASN:O	2.42	0.52
6:J:271:ASP:O	6:J:363:ARG:NH2	2.42	0.52
5:I:769:TYR:HD1	5:I:907:LEU:HB2	1.74	0.52
5:I:917:LYS:HB3	5:I:920:GLU:HB2	1.89	0.52
10:N:504:LEU:HB3	10:N:510:ILE:HG12	1.90	0.52
2:F:68:ASP:OD2	2:F:93:GLN:NE2	2.43	0.52
8:L:2103:PHE:HB2	8:L:2106:LEU:HD23	1.92	0.52
8:L:1959:PRO:HG3	8:L:2019:HIS:CE1	2.45	0.52
9:M:38:MET:HE3	9:M:46:ARG:HG2	1.90	0.52
9:M:186:LEU:HB3	9:M:205:THR:CG2	2.39	0.52
11:P:321:GLN:NE2	11:P:325:THR:OG1	2.43	0.52
4:H:84:SER:O	4:H:84:SER:OG	2.24	0.52
5:I:361:LEU:HD13	10:N:672:PRO:HG3	1.91	0.52
6:J:75:LEU:HD22	6:J:76:ARG:HG3	1.91	0.52
8:L:1671:ARG:NH2	10:O:539:SER:HB3	2.24	0.52
1:A:104:THR:HG21	1:A:121:ILE:HG12	1.92	0.52
5:I:769:TYR:O	5:I:769:TYR:CG	2.63	0.52
6:J:40:ALA:HA	6:J:85:ILE:O	2.09	0.52
10:N:449:PHE:CG	10:N:462:TYR:HB2	2.45	0.52
10:O:879:VAL:O	10:O:882:ARG:HD3	2.10	0.52
15:Y:20:DT:H2''	15:Y:21:DG:N7	2.25	0.52
5:I:793:ILE:HG12	5:I:806:PHE:HE1	1.75	0.52
6:J:207:ARG:NH1	6:J:255:CYS:SG	2.83	0.52
8:L:1657:ARG:NH1	8:L:1658:ARG:O	2.43	0.52
14:X:93:DA:H1'	14:X:94:DA:C8	2.45	0.52
5:I:894:THR:O	5:I:898:ASN:ND2	2.42	0.51
5:I:1180:PRO:CA	5:I:1182:GLN:NE2	2.72	0.51
2:F:51:TYR:HA	2:F:54:THR:HG22	1.92	0.51
10:N:435:TYR:OH	10:N:471:ASP:OD2	2.24	0.51
10:N:948:GLN:O	10:N:952:GLN:NE2	2.37	0.51
1:E:64:LYS:N	15:Y:95:DG:OP2	2.43	0.51
5:I:504:VAL:HG13	5:I:508:HIS:NE2	2.25	0.51
15:Y:50:DC:OP2	15:Y:50:DC:H2'	2.11	0.51
5:I:481:GLN:O	5:I:484:LYS:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:806:PHE:N	5:I:878:MET:HA	2.26	0.51
5:I:929:LEU:HD22	5:I:931:THR:HG22	1.90	0.51
10:N:483:SER:OG	10:N:498:MET:HG2	2.11	0.51
5:I:1014:LYS:NZ	5:I:1362:GLU:OE2	2.43	0.51
5:I:1315:LEU:HD23	5:I:1315:LEU:C	2.36	0.51
6:J:299:ALA:C	6:J:301:ARG:H	2.17	0.51
10:O:880:GLU:HG2	12:Q:227:LEU:HB3	1.93	0.51
15:Y:51:DC:H4'	15:Y:52:DC:OP1	2.10	0.51
6:J:16:PHE:HB2	6:J:122:MET:HG2	1.93	0.51
7:K:338:SER:O	7:K:342:GLY:N	2.40	0.51
11:P:354:PHE:O	11:P:357:ILE:HG13	2.11	0.51
1:E:107:THR:HG21	1:E:124:ILE:HG12	1.93	0.51
4:H:106:HIS:NE2	9:M:371:ASN:OD1	2.44	0.51
7:K:151:ILE:HD13	7:K:282:ILE:HD11	1.92	0.51
8:L:2165:GLU:HA	8:L:2168:VAL:HG12	1.92	0.51
1:A:66:ARG:HH11	2:B:25:ASN:HD22	1.59	0.51
6:J:271:ASP:HA	6:J:363:ARG:HE	1.75	0.51
14:X:94:DA:H1'	14:X:95:DC:H5'	1.93	0.51
9:M:180:ALA:O	10:N:451:ASN:ND2	2.45	0.50
10:O:708:PRO:HG2	10:O:711:LEU:HD23	1.92	0.50
15:Y:121:DT:H2''	15:Y:122:DT:H5''	1.93	0.50
7:K:302:GLY:HA2	7:K:305:MET:HG2	1.94	0.50
14:X:58:DG:H2'	14:X:59:DC:O4'	2.12	0.50
9:M:32:VAL:HG21	9:M:91:LEU:HD22	1.92	0.50
14:X:112:DC:H4'	14:X:113:DC:OP1	2.10	0.50
1:E:96:SER:HB3	2:F:58:LEU:HD11	1.93	0.50
1:E:97:GLU:HG2	2:F:37:LEU:HD21	1.94	0.50
3:G:54:VAL:HG23	4:H:107:ALA:HB1	1.94	0.50
11:P:361:LEU:HD12	11:P:364:LEU:HB2	1.92	0.50
12:Q:178:ASP:OD1	12:Q:178:ASP:N	2.44	0.50
3:G:102:ILE:HG23	4:H:58:ILE:HD12	1.93	0.50
5:I:1156:THR:OG1	5:I:1157:ARG:N	2.43	0.50
6:J:213:MET:HE2	6:J:213:MET:CA	2.38	0.50
11:P:437:GLN:O	11:P:441:MET:HG2	2.12	0.50
10:O:631:THR:HG22	10:O:632:GLN:H	1.76	0.50
5:I:892:LYS:HD2	5:I:895:GLN:HB2	1.94	0.50
8:L:1971:LEU:HB2	8:L:1974:GLN:HG3	1.93	0.50
9:M:21:ASP:N	9:M:21:ASP:OD1	2.43	0.50
9:M:60:ARG:HH11	9:M:88:VAL:HG12	1.76	0.50
1:E:117:VAL:N	14:X:74:DG:OP1	2.37	0.50
7:K:9:VAL:HG12	7:K:104:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:2113:SER:OG	8:L:2116:ARG:HG3	2.12	0.50
10:N:948:GLN:HE22	10:O:945:ARG:HH11	1.59	0.50
13:R:30:ARG:O	13:R:34:GLU:HG3	2.12	0.50
4:H:109:SER:OG	9:M:374:ARG:NH2	2.45	0.49
5:I:461:LYS:HE3	8:L:2128:GLN:HA	1.93	0.49
7:K:155:SER:HB2	7:K:303:THR:HB	1.94	0.49
8:L:2086:ASP:OD1	8:L:2143:ARG:NH1	2.34	0.49
9:M:369:ASP:OD1	9:M:373:ARG:NH1	2.45	0.49
3:G:84:GLN:HG2	3:G:106:GLY:H	1.77	0.49
6:J:162:ASN:HD22	6:J:349:ILE:HD12	1.77	0.49
8:L:2146:LYS:O	8:L:2150:THR:HG23	2.13	0.49
9:M:269:HIS:CD2	9:M:365:ILE:HG22	2.47	0.49
10:N:939:LEU:O	10:N:943:GLU:HG2	2.12	0.49
5:I:769:TYR:HB2	5:I:907:LEU:HD22	1.95	0.49
6:J:155:ALA:HB2	6:J:180:ILE:HD12	1.93	0.49
10:O:898:LYS:O	10:O:901:ILE:HG22	2.12	0.49
11:P:321:GLN:NE2	11:P:321:GLN:O	2.45	0.49
8:L:1731:LEU:HD21	8:L:2013:LYS:HG3	1.95	0.49
10:O:466:ARG:HB2	10:O:504:LEU:HD11	1.94	0.49
10:O:674:MET:HA	10:O:677:VAL:HG12	1.94	0.49
11:P:137:ILE:HG12	11:P:435:LYS:HD3	1.95	0.49
15:Y:51:DC:H2"	15:Y:52:DC:C6	2.47	0.49
5:I:449:GLU:HG3	5:I:450:ALA:H	1.77	0.49
5:I:1038:THR:O	5:I:1038:THR:OG1	2.29	0.49
7:K:130:PRO:O	7:K:358:SER:OG	2.25	0.49
15:Y:123:DG:H2"	15:Y:124:DA:C8	2.47	0.49
3:G:74:LYS:HZ3	9:M:195:ILE:CG2	2.25	0.49
8:L:1673:MET:O	8:L:1677:LYS:HB2	2.13	0.49
9:M:272:ASN:HB2	9:M:356:LEU:O	2.13	0.49
5:I:893:LEU:HA	5:I:896:VAL:HG12	1.95	0.49
5:I:970:LYS:HE2	5:I:973:ARG:HB3	1.94	0.49
9:M:190:ARG:HD2	9:M:376:ARG:NH2	2.26	0.49
9:M:214:THR:HG23	9:M:217:MET:HE3	1.95	0.49
10:O:598:THR:N	13:R:78:ARG:HA	2.27	0.49
5:I:875:TRP:N	5:I:875:TRP:CD1	2.81	0.49
6:J:75:LEU:O	6:J:75:LEU:HD23	2.13	0.49
6:J:169:ILE:HA	6:J:349:ILE:HB	1.95	0.49
8:L:1648:ALA:O	8:L:1650:GLN:NE2	2.46	0.49
11:P:135:GLN:O	11:P:139:GLU:HG2	2.13	0.49
7:K:189:LEU:HB2	7:K:213:LYS:HZ3	1.78	0.49
10:O:679:PHE:O	10:O:683:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:712:VAL:O	10:O:716:VAL:HG23	2.13	0.49
10:O:882:ARG:HA	10:O:885:LYS:HG2	1.95	0.49
8:L:1714:GLU:O	8:L:1718:GLU:HG2	2.13	0.49
10:N:935:HIS:ND1	12:Q:276:LEU:O	2.31	0.49
10:O:525:PRO:HB3	13:R:48:VAL:HG11	1.94	0.49
8:L:1740:GLY:O	8:L:1744:LEU:N	2.46	0.48
15:Y:68:DC:H2''	15:Y:69:DG:C8	2.48	0.48
15:Y:122:DT:H2''	15:Y:123:DG:C8	2.48	0.48
14:X:23:DA:H2''	14:X:24:DG:O5'	2.12	0.48
2:F:31:LYS:HD3	2:F:51:TYR:CG	2.49	0.48
5:I:441:ARG:NE	12:Q:177:GLU:OE1	2.46	0.48
5:I:929:LEU:O	5:I:931:THR:N	2.47	0.48
5:I:1048:HIS:HB2	5:I:1082:PHE:HE2	1.78	0.48
5:I:769:TYR:O	5:I:769:TYR:CD1	2.67	0.48
8:L:1686:TRP:HD1	10:O:542:VAL:HG23	1.78	0.48
8:L:2275:ILE:HA	8:L:2278:VAL:HG12	1.95	0.48
5:I:810:VAL:HG12	5:I:881:ASP:HB3	1.96	0.48
8:L:1706:LEU:H	8:L:1997:ASN:HD21	1.61	0.48
10:N:611:GLU:O	10:N:615:MET:HG2	2.13	0.48
11:P:343:LEU:O	11:P:347:PHE:N	2.47	0.48
14:X:49:DT:H2''	14:X:50:DC:H5'	1.95	0.48
5:I:1056:GLU:HB2	5:I:1075:LEU:HD21	1.94	0.48
5:I:1161:LEU:CD1	5:I:1188:ASP:CB	2.90	0.48
6:J:79:ARG:NH1	6:J:79:ARG:HA	2.29	0.48
10:N:623:VAL:O	10:N:627:VAL:HG23	2.13	0.48
11:P:488:GLN:O	11:P:491:VAL:HG22	2.14	0.48
5:I:463:GLU:O	5:I:466:ARG:HG3	2.13	0.48
7:K:259:GLU:O	7:K:263:GLN:N	2.47	0.48
8:L:1667:PRO:HG3	8:L:1690:THR:HG21	1.95	0.48
10:N:928:LEU:O	10:N:932:GLN:HG3	2.13	0.48
5:I:485:ASP:O	5:I:488:GLU:HB2	2.14	0.48
7:K:220:ALA:O	7:K:312:ARG:NH1	2.38	0.48
10:N:632:GLN:O	10:N:636:ILE:HG22	2.14	0.48
11:P:498:LYS:O	11:P:502:ARG:HG2	2.14	0.48
14:X:61:DT:H1'	14:X:62:DA:N7	2.28	0.48
15:Y:30:DC:C6	15:Y:30:DC:H5''	2.48	0.48
4:D:83:ARG:HH22	15:Y:43:DA:P	2.36	0.48
3:G:90:ASP:HB3	3:G:93:LEU:HB2	1.95	0.48
5:I:515:GLN:O	5:I:516:LYS:C	2.57	0.48
6:J:169:ILE:HB	6:J:180:ILE:HG13	1.95	0.48
7:K:221:LEU:N	7:K:221:LEU:CD1	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:362:TYR:O	7:K:366:GLY:N	2.42	0.48
15:Y:96:DC:H2''	15:Y:97:DG:C8	2.48	0.48
5:I:929:LEU:C	5:I:931:THR:N	2.72	0.48
7:K:246:GLN:HE22	7:K:248:ILE:HD12	1.79	0.48
10:N:631:THR:O	10:N:635:CYS:N	2.37	0.48
10:O:540:GLY:O	10:O:543:PRO:HD2	2.14	0.48
2:B:50:ILE:O	2:B:53:GLU:HB3	2.14	0.47
5:I:880:VAL:HG13	5:I:897:LEU:HD12	1.96	0.47
5:I:1045:ILE:CD1	5:I:1049:PRO:HA	2.44	0.47
6:J:305:PRO:HB2	6:J:308:LEU:HD12	1.96	0.47
7:K:217:CYS:HA	7:K:254:ARG:HG3	1.96	0.47
8:L:2156:SER:HB3	8:L:2194:ASN:ND2	2.28	0.47
11:P:337:VAL:HB	11:P:354:PHE:CE1	2.49	0.47
2:B:36:ARG:NH2	15:Y:64:DA:OP1	2.46	0.47
2:B:98:TYR:OH	4:H:65:ASP:OD2	2.30	0.47
5:I:781:MET:HG2	5:I:782:GLY:H	1.78	0.47
5:I:929:LEU:H	5:I:932:ILE:HG12	1.79	0.47
5:I:1166:GLN:HG3	5:I:1195:GLN:HG2	1.96	0.47
7:K:361:GLU:O	7:K:365:SER:OG	2.30	0.47
4:H:110:GLU:HG2	9:M:374:ARG:HE	1.78	0.47
14:X:90:DT:C6	14:X:91:DT:H72	2.49	0.47
9:M:293:PHE:HD1	10:O:498:MET:SD	2.36	0.47
10:N:879:VAL:HG12	10:N:883:LYS:HE3	1.96	0.47
10:O:488:ARG:NH1	10:O:489:ASN:OD1	2.47	0.47
14:X:41:DT:H1'	14:X:42:DA:C5	2.50	0.47
14:X:119:DC:H2''	14:X:120:DT:OP2	2.14	0.47
5:I:1008:TYR:HA	5:I:1011:MET:HE3	1.97	0.47
5:I:1051:MET:HE2	5:I:1051:MET:CA	2.44	0.47
7:K:119:MET:HA	7:K:122:ILE:HG22	1.97	0.47
10:N:898:LYS:HG3	11:P:417:ILE:HD12	1.97	0.47
5:I:478:SER:O	5:I:481:GLN:HB2	2.15	0.47
6:J:177:THR:O	6:J:195:SER:OG	2.26	0.47
10:N:602:THR:OG1	10:N:603:GLU:N	2.46	0.47
15:Y:74:DA:H2''	15:Y:75:DC:O5'	2.14	0.47
3:C:42:ARG:HB2	4:D:85:THR:HA	1.94	0.47
3:G:34:LEU:HD11	3:G:51:LEU:HD12	1.95	0.47
5:I:444:ARG:NH2	12:Q:176:ALA:O	2.48	0.47
5:I:777:LEU:O	5:I:785:LYS:NZ	2.42	0.47
7:K:334:GLU:H	7:K:334:GLU:CD	2.22	0.47
8:L:1971:LEU:HD23	11:P:461:ARG:NH2	2.30	0.47
12:Q:224:MET:O	12:Q:228:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:107:DT:H4'	14:X:107:DT:OP1	2.14	0.47
5:I:497:ILE:O	5:I:501:THR:HG23	2.14	0.47
7:K:264:PRO:O	7:K:267:LEU:HB3	2.14	0.47
10:N:673:VAL:HG23	10:O:680:LEU:HD21	1.96	0.47
10:O:480:TYR:CD2	10:O:520:PRO:HD2	2.50	0.47
15:Y:42:DG:H1'	15:Y:43:DA:C8	2.50	0.47
1:E:116:ARG:HB2	14:X:74:DG:OP1	2.14	0.47
2:F:29:ILE:HD13	2:F:58:LEU:HD23	1.96	0.47
5:I:358:PRO:HB3	10:N:676:THR:OG1	2.15	0.47
7:K:253:GLU:O	7:K:257:CYS:N	2.45	0.47
11:P:137:ILE:HD11	11:P:435:LYS:HB2	1.97	0.47
11:P:333:GLU:OE1	11:P:351:ARG:NH2	2.48	0.47
7:K:208:ILE:HD13	7:K:243:PRO:HD3	1.96	0.47
10:O:481:LEU:HA	13:R:28:ASN:ND2	2.29	0.47
10:O:896:MET:HE2	10:O:896:MET:HB2	1.70	0.47
1:A:105:ASN:ND2	2:B:42:GLY:O	2.48	0.46
5:I:490:HIS:O	5:I:494:THR:HG23	2.15	0.46
5:I:1171:VAL:HB	5:I:1200:ARG:O	2.15	0.46
11:P:348:GLU:OE1	11:P:348:GLU:N	2.40	0.46
11:P:356:GLU:N	11:P:356:GLU:OE1	2.48	0.46
15:Y:48:DT:OP2	15:Y:48:DT:H3'	2.14	0.46
5:I:398:THR:HA	5:I:401:THR:HG22	1.98	0.46
6:J:164:ARG:HE	6:J:381:ILE:HD11	1.80	0.46
7:K:252:ASN:OD1	7:K:252:ASN:N	2.47	0.46
8:L:1723:CYS:HB3	8:L:1981:CYS:HB2	1.98	0.46
8:L:1741:GLN:HE21	8:L:1843:HIS:CD2	2.33	0.46
1:E:72:ARG:HH12	14:X:54:DC:P	2.38	0.46
5:I:476:LEU:O	5:I:480:LEU:HG	2.15	0.46
5:I:922:TRP:HZ3	5:I:975:PHE:HB2	1.81	0.46
8:L:1828:SER:C	8:L:1830:LYS:H	2.22	0.46
9:M:28:ILE:HB	9:M:31:GLU:HG3	1.98	0.46
10:O:481:LEU:HD23	10:O:510:ILE:HD11	1.98	0.46
14:X:112:DC:N4	15:Y:41:DG:O6	2.49	0.46
5:I:835:LYS:HD3	5:I:835:LYS:C	2.41	0.46
6:J:172:SER:O	6:J:353:GLY:N	2.48	0.46
8:L:2229:ASP:O	8:L:2233:ARG:HG3	2.15	0.46
10:O:480:TYR:HB2	10:O:514:VAL:HG11	1.96	0.46
3:C:20:ARG:NH1	15:Y:34:DA:OP2	2.46	0.46
5:I:356:GLN:NE2	10:N:675:SER:HB2	2.30	0.46
15:Y:97:DG:H4'	15:Y:98:DG:OP1	2.16	0.46
5:I:810:VAL:N	5:I:858:THR:OG1	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:69:TYR:HD1	6:J:69:TYR:HA	1.66	0.46
3:G:77:ARG:NH1	14:X:24:DG:OP1	2.49	0.46
5:I:478:SER:HA	5:I:481:GLN:CD	2.41	0.46
5:I:837:SER:O	5:I:837:SER:OG	2.21	0.46
5:I:886:MET:HG2	5:I:894:THR:HG22	1.98	0.46
5:I:922:TRP:HH2	5:I:975:PHE:H	1.63	0.46
5:I:1161:LEU:HD22	5:I:1161:LEU:H	1.80	0.46
5:I:1176:SER:HB3	5:I:1203:ARG:HH22	1.81	0.46
14:X:43:DG:H1'	14:X:44:DA:C8	2.49	0.46
15:Y:89:DG:C8	15:Y:89:DG:H5'	2.50	0.46
15:Y:131:DT:H6	15:Y:131:DT:H5''	1.81	0.46
5:I:922:TRP:CZ3	5:I:975:PHE:HB2	2.50	0.46
8:L:1828:SER:O	8:L:1829:ASP:HB2	2.16	0.46
14:X:23:DA:H5'	14:X:23:DA:C8	2.47	0.46
14:X:89:DT:H2''	14:X:90:DT:H5''	1.98	0.46
2:B:96:THR:HB	3:G:100:VAL:HG22	1.97	0.46
7:K:185:LEU:HD22	7:K:261:LEU:HD21	1.98	0.46
8:L:2007:LEU:O	8:L:2011:LEU:HG	2.15	0.46
10:O:705:GLU:O	10:O:705:GLU:HG2	2.16	0.46
12:Q:265:SER:HA	12:Q:268:ASN:HD21	1.81	0.46
14:X:23:DA:H2'	14:X:24:DG:C8	2.51	0.46
15:Y:93:DA:H1'	15:Y:94:DA:C8	2.51	0.46
3:C:102:ILE:HG23	4:D:58:ILE:HD13	1.97	0.46
5:I:487:LYS:HA	5:I:487:LYS:CE	2.40	0.46
6:J:283:PRO:HA	6:J:295:CYS:HB2	1.98	0.46
8:L:1653:LEU:HD11	12:Q:190:HIS:HE1	1.80	0.46
15:Y:40:DG:C4	15:Y:41:DG:C6	3.03	0.46
3:C:43:VAL:N	14:X:116:DA:OP2	2.42	0.45
5:I:1308:ARG:HB2	5:I:1318:ARG:HH22	1.81	0.45
7:K:163:VAL:HG12	7:K:175:ILE:HG23	1.98	0.45
12:Q:254:GLU:O	12:Q:258:LYS:HG2	2.17	0.45
3:C:31:HIS:CD2	3:C:35:ARG:HE	2.35	0.45
5:I:778:ALA:HB2	5:I:976:LEU:HD22	1.98	0.45
5:I:1095:THR:HG21	5:I:1310:GLU:HG3	1.97	0.45
15:Y:36:DA:H2''	15:Y:37:DC:O5'	2.16	0.45
1:A:117:MET:N	1:A:120:ASP:OD2	2.46	0.45
3:C:49:VAL:HG13	4:D:115:VAL:HG22	1.98	0.45
6:J:17:ASP:OD2	6:J:24:ARG:NH1	2.49	0.45
6:J:246:VAL:HG22	6:J:246:VAL:O	2.16	0.45
8:L:1847:GLY:H	8:L:2080:ILE:HD11	1.81	0.45
14:X:98:DC:C4	14:X:99:DC:N4	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:784:GLY:O	5:I:788:GLN:N	2.48	0.45
7:K:246:GLN:CG	7:K:246:GLN:O	2.64	0.45
5:I:917:LYS:HD3	5:I:917:LYS:HA	1.65	0.45
5:I:1100:LEU:HA	5:I:1154:LEU:HD13	1.98	0.45
10:O:424:ILE:HA	10:O:513:GLN:HE22	1.80	0.45
12:Q:229:ARG:O	12:Q:232:GLN:HG3	2.17	0.45
3:G:63:LEU:HD22	4:H:42:LEU:HD13	1.99	0.45
5:I:870:LEU:H	5:I:870:LEU:HG	1.61	0.45
7:K:305:MET:SD	7:K:335:ARG:HG2	2.57	0.45
8:L:1805:LEU:HD23	10:O:426:ILE:HG21	1.98	0.45
9:M:350:CYS:HB2	13:R:27:TYR:CZ	2.52	0.45
10:N:505:GLU:OE2	10:N:511:ASN:ND2	2.43	0.45
11:P:330:ASP:HB3	11:P:333:GLU:O	2.16	0.45
11:P:474:GLU:OE1	11:P:478:ARG:NH1	2.46	0.45
15:Y:133:DG:H2''	15:Y:134:DG:N7	2.32	0.45
8:L:1851:THR:OG1	8:L:1853:GLU:HG3	2.17	0.45
8:L:2011:LEU:O	8:L:2015:ILE:HG13	2.17	0.45
10:N:909:LEU:HD22	10:O:906:PHE:CZ	2.52	0.45
10:O:424:ILE:HA	10:O:513:GLN:NE2	2.32	0.45
11:P:297:LEU:HD23	11:P:297:LEU:HA	1.76	0.45
5:I:889:HIS:HE1	5:I:920:GLU:HA	1.81	0.45
10:O:671:ASN:HB3	10:O:674:MET:HB3	1.98	0.45
1:E:61:LEU:O	2:F:36:ARG:NH2	2.42	0.45
5:I:356:GLN:HE22	5:I:358:PRO:HA	1.81	0.45
5:I:448:ARG:O	5:I:452:ILE:HG12	2.17	0.45
5:I:1085:LEU:HA	5:I:1088:ILE:HB	1.98	0.45
8:L:1854:HIS:HB3	10:N:440:ALA:HB3	1.99	0.45
15:Y:90:DT:H1'	15:Y:91:DT:H5'	1.99	0.45
15:Y:94:DA:H2''	15:Y:95:DG:H5''	1.97	0.45
5:I:1085:LEU:HA	5:I:1088:ILE:HD12	1.99	0.45
5:I:1180:PRO:C	5:I:1182:GLN:NE2	2.69	0.45
5:I:1359:CYS:SG	5:I:1362:GLU:HB3	2.57	0.45
8:L:1980:ARG:O	8:L:1984:VAL:HG23	2.17	0.45
9:M:17:PHE:CE2	9:M:28:ILE:HG13	2.52	0.45
10:N:471:ASP:OD1	10:O:528:THR:OG1	2.21	0.45
10:N:866:LEU:HD11	10:O:681:ALA:HA	1.99	0.45
1:E:51:ILE:HG13	2:F:39:ARG:HD2	2.00	0.44
6:J:116:SER:OG	6:J:145:ASN:O	2.31	0.44
6:J:172:SER:O	6:J:172:SER:OG	2.33	0.44
8:L:2156:SER:HB3	8:L:2194:ASN:HD21	1.81	0.44
10:N:673:VAL:O	10:N:677:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:310:GLN:HB3	11:P:314:VAL:HG21	1.99	0.44
14:X:51:DT:OP2	14:X:51:DT:H2'	2.17	0.44
5:I:1310:GLU:H	5:I:1315:LEU:HD12	1.82	0.44
7:K:209:VAL:HA	7:K:212:ILE:HD12	1.99	0.44
15:Y:76:DA:H5''	15:Y:76:DA:C8	2.47	0.44
5:I:926:ASN:O	5:I:933:PHE:HA	2.17	0.44
9:M:306:GLU:OE1	9:M:306:GLU:N	2.37	0.44
14:X:49:DT:O5'	14:X:49:DT:H6	2.00	0.44
14:X:80:DT:H1'	14:X:81:DC:H5'	2.00	0.44
14:X:120:DT:H2''	14:X:121:DC:C5	2.52	0.44
1:A:97:LEU:HD11	2:B:58:LEU:HD13	1.99	0.44
5:I:778:ALA:HA	5:I:910:THR:O	2.18	0.44
5:I:1077:ARG:NH1	5:I:1118:TYR:OH	2.51	0.44
7:K:224:GLU:H	7:K:224:GLU:CD	2.26	0.44
8:L:2015:ILE:HG21	8:L:2087:GLY:HA3	1.99	0.44
9:M:86:THR:OG1	9:M:87:SER:N	2.50	0.44
10:N:895:GLN:HG2	11:P:150:LEU:HB3	1.99	0.44
10:O:439:HIS:CG	10:O:440:ALA:H	2.35	0.44
14:X:29:DC:H2''	14:X:30:DT:C6	2.52	0.44
15:Y:109:DG:H2'	15:Y:110:DT:H71	1.98	0.44
3:G:63:LEU:HD23	3:G:63:LEU:HA	1.85	0.44
5:I:481:GLN:HA	5:I:484:LYS:CD	2.46	0.44
5:I:897:LEU:HA	5:I:900:HIS:CE1	2.53	0.44
5:I:1176:SER:HB3	5:I:1203:ARG:NH2	2.32	0.44
9:M:283:MET:HE3	9:M:323:GLN:OE1	2.17	0.44
9:M:350:CYS:HB2	13:R:27:TYR:OH	2.17	0.44
10:N:424:ILE:HD11	10:O:531:PHE:HD2	1.83	0.44
10:N:928:LEU:HG	12:Q:266:PHE:HE1	1.82	0.44
10:N:945:ARG:O	10:N:949:GLN:HG2	2.18	0.44
13:R:79:TRP:HZ3	13:R:81:LYS:HE2	1.82	0.44
2:F:31:LYS:HZ3	2:F:51:TYR:HB3	1.82	0.44
4:H:99:LEU:HD12	4:H:103:LEU:HB3	1.99	0.44
7:K:260:ALA:HB1	7:K:267:LEU:HB2	1.99	0.44
8:L:2232:ARG:HE	8:L:2236:ARG:HH22	1.64	0.44
11:P:399:THR:OG1	11:P:400:LEU:N	2.50	0.44
15:Y:115:DG:H2''	15:Y:116:DA:C8	2.53	0.44
6:J:172:SER:N	6:J:351:ALA:O	2.48	0.44
7:K:286:ASP:HB3	7:K:289:ILE:HD13	2.00	0.44
8:L:2232:ARG:HG3	8:L:2236:ARG:NH1	2.33	0.44
9:M:36:LEU:HD21	9:M:100:LEU:HD23	1.98	0.44
11:P:297:LEU:HD13	11:P:301:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:58:GLU:H	13:R:61:HIS:CD2	2.32	0.44
3:C:63:LEU:HD23	3:C:63:LEU:HA	1.83	0.44
4:D:99:LEU:HD12	4:D:103:LEU:HB3	1.99	0.44
6:J:20:SER:HB3	6:J:176:HIS:CE1	2.52	0.44
11:P:359:GLN:HA	11:P:362:HIS:HB2	2.00	0.44
15:Y:46:DA:C5	15:Y:47:DA:C6	3.06	0.44
2:B:35:ARG:NH2	2:B:51:TYR:OH	2.50	0.44
5:I:483:ALA:O	6:J:399:ILE:HD11	2.18	0.44
7:K:251:GLY:N	7:K:253:GLU:OE2	2.49	0.44
10:O:481:LEU:HA	13:R:28:ASN:HD21	1.83	0.44
10:O:900:GLU:C	10:O:904:ARG:HE	2.22	0.44
11:P:299:PRO:O	11:P:303:ARG:HG2	2.18	0.44
4:H:76:ARG:HG2	4:H:80:TYR:CZ	2.53	0.43
7:K:201:THR:OG1	7:K:202:THR:N	2.50	0.43
11:P:432:ASN:O	11:P:436:THR:HG23	2.17	0.43
15:Y:48:DT:C4	15:Y:49:DC:N4	2.86	0.43
15:Y:60:DT:C2	15:Y:61:DT:C2	3.06	0.43
5:I:449:GLU:HG3	5:I:450:ALA:N	2.32	0.43
5:I:929:LEU:C	5:I:931:THR:H	2.26	0.43
8:L:1672:VAL:HG11	8:L:1691:ILE:HD11	2.00	0.43
8:L:1694:LEU:HB3	8:L:1704:PHE:HE2	1.83	0.43
8:L:2024:ARG:HH22	11:P:149:ASP:CG	2.25	0.43
9:M:345:ASP:O	9:M:349:TRP:HD1	2.01	0.43
5:I:776:ILE:HG22	5:I:975:PHE:HB3	2.00	0.43
5:I:892:LYS:O	5:I:895:GLN:C	2.61	0.43
5:I:975:PHE:O	5:I:976:LEU:HD23	2.18	0.43
6:J:92:MET:HE3	6:J:92:MET:HB2	1.90	0.43
7:K:107:GLU:HB2	7:K:111:ASN:HD22	1.82	0.43
7:K:334:GLU:OE1	7:K:334:GLU:N	2.42	0.43
9:M:58:GLU:OE2	9:M:62:LYS:NZ	2.45	0.43
9:M:263:ILE:HD11	9:M:278:GLN:NE2	2.33	0.43
10:N:948:GLN:NE2	10:O:945:ARG:HD3	2.34	0.43
10:O:662:GLN:HE21	11:P:474:GLU:HG2	1.83	0.43
5:I:378:ILE:O	5:I:382:ILE:HG13	2.18	0.43
5:I:806:PHE:CZ	5:I:877:TYR:HB2	2.53	0.43
5:I:835:LYS:HA	5:I:835:LYS:CE	2.48	0.43
5:I:969:HIS:CD2	5:I:970:LYS:H	2.36	0.43
6:J:336:CYS:O	6:J:341:ARG:NH2	2.38	0.43
7:K:282:ILE:HG21	7:K:294:TYR:CZ	2.53	0.43
15:Y:31:DT:H1'	15:Y:32:DG:C5	2.52	0.43
5:I:787:ILE:HA	5:I:790:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:263:GLN:HA	6:J:267:LEU:HD13	2.01	0.43
7:K:117:GLU:O	7:K:120:THR:OG1	2.26	0.43
7:K:317:ILE:HD12	7:K:317:ILE:HA	1.87	0.43
8:L:1645:SER:OG	10:O:669:SER:OG	2.20	0.43
10:N:923:GLN:HB3	10:O:920:LEU:HD21	1.99	0.43
11:P:401:LYS:HG2	11:P:405:ASN:ND2	2.33	0.43
11:P:453:ASN:O	11:P:457:GLN:HG3	2.18	0.43
1:A:123:LEU:HD22	1:E:113:HIS:CG	2.54	0.43
5:I:779:ASP:O	5:I:911:GLY:HA2	2.18	0.43
6:J:248:ARG:C	6:J:250:TRP:N	2.74	0.43
9:M:60:ARG:O	9:M:64:VAL:HG23	2.19	0.43
9:M:341:ARG:NH1	10:O:488:ARG:O	2.51	0.43
12:Q:214:ASP:HA	12:Q:216:ARG:CZ	2.48	0.43
14:X:134:DA:OP2	14:X:134:DA:C8	2.72	0.43
15:Y:46:DA:HI'	15:Y:47:DA:C8	2.53	0.43
4:D:40:LYS:HA	4:D:40:LYS:HD2	1.85	0.43
5:I:417:ARG:HB3	11:P:482:TYR:OH	2.18	0.43
5:I:1045:ILE:HD12	5:I:1045:ILE:HA	1.85	0.43
5:I:1049:PRO:O	5:I:1051:MET:N	2.43	0.43
7:K:27:PRO:HG3	7:K:337:TYR:HB3	2.00	0.43
10:N:428:SER:CB	10:O:538:PRO:HA	2.49	0.43
10:N:640:LEU:HD21	10:N:689:ALA:HB1	2.01	0.43
12:Q:230:GLN:O	12:Q:234:LEU:HG	2.18	0.43
15:Y:49:DC:P	15:Y:49:DC:H3'	2.58	0.43
8:L:1735:GLU:HA	8:L:1849:GLY:O	2.19	0.43
8:L:1989:ARG:O	8:L:1992:SER:OG	2.30	0.43
8:L:2133:ASP:HB3	9:M:39:PHE:CG	2.53	0.43
10:N:946:ALA:O	10:N:950:HIS:HB2	2.19	0.43
6:J:248:ARG:NE	6:J:248:ARG:CA	2.77	0.43
7:K:178:LEU:HG	7:K:180:LEU:HG	2.01	0.43
9:M:201:ARG:NH2	9:M:365:ILE:CD1	2.82	0.43
10:N:488:ARG:HH11	13:R:45:GLN:HG2	1.84	0.43
10:O:540:GLY:HA3	11:P:493:ARG:HH22	1.84	0.43
6:J:70:ILE:HG22	6:J:71:ASP:H	1.84	0.43
15:Y:45:DT:H2''	15:Y:46:DA:H5'	2.01	0.43
5:I:502:LYS:HB2	5:I:502:LYS:HE3	1.81	0.42
6:J:130:ARG:HA	6:J:133:ARG:HG2	2.01	0.42
6:J:137:THR:HG22	6:J:149:PHE:HZ	1.84	0.42
15:Y:52:DC:HI'	15:Y:53:DT:C6	2.54	0.42
7:K:24:ASP:OD2	7:K:28:ARG:NE	2.51	0.42
7:K:141:SER:HB3	7:K:339:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:1673:MET:HE2	8:L:1673:MET:HB3	1.79	0.42
10:O:691:ALA:O	10:O:694:LYS:HG3	2.19	0.42
11:P:133:LEU:HD12	11:P:144:SER:HB2	2.01	0.42
11:P:170:GLU:O	11:P:173:LYS:HG3	2.19	0.42
14:X:135:DG:N2	15:Y:19:DC:O2	2.49	0.42
2:B:47:SER:HA	14:X:84:DC:H5''	2.01	0.42
5:I:350:SER:C	5:I:351:ARG:HD2	2.45	0.42
5:I:885:ARG:C	5:I:887:LYS:H	2.26	0.42
5:I:917:LYS:O	5:I:921:LEU:N	2.49	0.42
8:L:1702:MET:HE1	8:L:1995:PRO:HG2	2.02	0.42
8:L:1955:LEU:HD23	8:L:1955:LEU:HA	1.88	0.42
10:N:674:MET:HA	10:N:677:VAL:HG22	2.01	0.42
10:N:917:ARG:NH1	10:O:909:LEU:HG	2.34	0.42
3:C:39:TYR:O	4:D:75:SER:OG	2.30	0.42
1:E:103:LEU:O	1:E:107:THR:HG23	2.20	0.42
5:I:912:THR:HG23	5:I:912:THR:O	2.18	0.42
5:I:1048:HIS:HB2	5:I:1082:PHE:CE2	2.55	0.42
10:N:948:GLN:HE22	10:O:945:ARG:NH1	2.16	0.42
10:O:708:PRO:C	10:O:710:ALA:H	2.27	0.42
14:X:70:DG:H1'	14:X:71:DT:C5	2.55	0.42
5:I:793:ILE:O	5:I:793:ILE:CG2	2.66	0.42
5:I:887:LYS:HA	5:I:887:LYS:HD2	1.80	0.42
7:K:211:ASP:HA	7:K:214:GLU:HB2	2.00	0.42
7:K:292:ASP:O	7:K:296:ASN:ND2	2.33	0.42
8:L:1956:GLU:HB2	8:L:2022:PRO:HD2	2.02	0.42
14:X:78:DT:H2''	14:X:79:DG:H5''	2.00	0.42
15:Y:41:DG:C5	15:Y:42:DG:C6	3.07	0.42
5:I:1003:LEU:O	5:I:1007:LEU:HG	2.19	0.42
7:K:164:PRO:HB2	7:K:171:LEU:HD23	2.02	0.42
7:K:171:LEU:HD21	7:K:285:CYS:HB2	2.01	0.42
9:M:306:GLU:HA	10:N:488:ARG:O	2.18	0.42
9:M:324:LYS:H	9:M:324:LYS:HG2	1.67	0.42
10:O:685:ASP:N	10:O:685:ASP:OD1	2.50	0.42
14:X:91:DT:C2'	14:X:92:DT:H71	2.49	0.42
5:I:456:LEU:O	5:I:460:GLN:HG3	2.19	0.42
5:I:778:ALA:HB3	5:I:976:LEU:HB3	2.01	0.42
5:I:832:VAL:HG21	5:I:848:LEU:HD11	2.02	0.42
6:J:29:GLY:N	6:J:398:SER:OG	2.52	0.42
6:J:130:ARG:O	6:J:134:GLU:HB2	2.20	0.42
10:N:703:MET:HE3	10:O:687:ARG:HD2	2.01	0.42
12:Q:255:LYS:HD3	12:Q:255:LYS:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:101:DA:H2'	14:X:102:DG:C8	2.54	0.42
1:A:100:LEU:O	1:A:104:THR:HG23	2.20	0.42
5:I:812:LEU:HB3	5:I:813:SER:H	1.57	0.42
6:J:70:ILE:HG22	6:J:71:ASP:N	2.35	0.42
6:J:396:GLY:HA2	6:J:399:ILE:HG22	2.01	0.42
10:O:703:MET:O	10:O:706:GLU:HG2	2.20	0.42
13:R:14:GLU:CD	13:R:14:GLU:H	2.28	0.42
13:R:43:ASP:OD1	13:R:44:SER:N	2.52	0.42
14:X:97:DG:H1'	14:X:98:DC:H5'	2.01	0.42
15:Y:42:DG:C5	15:Y:43:DA:C6	3.07	0.42
1:E:90:GLY:O	1:E:94:GLU:HG2	2.20	0.42
2:F:73:THR:HG21	2:F:81:VAL:HG22	2.01	0.42
5:I:374:LEU:HD23	5:I:374:LEU:HA	1.86	0.42
6:J:379:LYS:HE3	6:J:379:LYS:HB2	1.87	0.42
8:L:1736:VAL:HG23	10:N:443:ARG:HH22	1.85	0.42
9:M:344:GLY:O	9:M:345:ASP:C	2.63	0.42
11:P:457:GLN:O	11:P:461:ARG:HD3	2.20	0.42
14:X:30:DT:H2''	14:X:31:DC:C5	2.55	0.42
14:X:92:DT:H2''	14:X:93:DA:C8	2.55	0.42
1:A:87:GLY:O	1:A:91:GLU:HG2	2.20	0.42
6:J:33:PRO:HB3	6:J:394:TRP:CE2	2.55	0.42
7:K:299:LEU:HB3	7:K:304:THR:HG21	2.02	0.42
8:L:2057:ARG:HA	8:L:2060:THR:HG22	2.02	0.42
10:N:680:LEU:O	10:N:683:VAL:HG22	2.19	0.42
1:A:91:GLU:OE2	3:G:104:GLN:NE2	2.53	0.41
1:E:116:ARG:HB2	14:X:74:DG:P	2.60	0.41
5:I:770:ASN:OD1	5:I:770:ASN:N	2.52	0.41
5:I:1048:HIS:CD2	5:I:1048:HIS:C	2.96	0.41
6:J:404:GLY:HA2	6:J:407:GLN:NE2	2.35	0.41
7:K:246:GLN:O	7:K:246:GLN:CD	2.63	0.41
8:L:2057:ARG:HD3	8:L:2091:TRP:CZ2	2.54	0.41
10:N:624:SER:HB2	10:N:635:CYS:SG	2.59	0.41
10:N:928:LEU:HD23	10:N:928:LEU:HA	1.88	0.41
14:X:79:DG:H2'	14:X:80:DT:H71	2.02	0.41
3:G:72:ASP:HA	9:M:195:ILE:CD1	2.50	0.41
5:I:502:LYS:O	5:I:505:ALA:HB3	2.20	0.41
5:I:1161:LEU:HA	5:I:1189:ARG:HH12	1.85	0.41
9:M:195:ILE:HG21	9:M:232:THR:HG21	2.02	0.41
10:N:903:LEU:O	10:N:906:PHE:HB3	2.20	0.41
10:O:870:ALA:O	10:O:874:LYS:HG2	2.19	0.41
10:O:908:GLU:O	10:O:912:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:258:LYS:O	12:Q:261:GLU:HG3	2.20	0.41
1:A:69:ARG:HH12	15:Y:54:DT:P	2.43	0.41
1:E:120:MET:N	1:E:123:ASP:OD2	2.46	0.41
5:I:507:TYR:O	5:I:511:THR:OG1	2.36	0.41
5:I:874:ARG:HB2	5:I:874:ARG:NH1	2.35	0.41
6:J:174:ALA:O	6:J:200:ASP:N	2.39	0.41
9:M:266:LEU:O	9:M:276:VAL:HA	2.19	0.41
10:N:931:ARG:HG2	12:Q:273:LEU:HG	2.01	0.41
10:O:901:ILE:HG12	10:O:905:HIS:NE2	2.35	0.41
15:Y:57:DC:H1'	15:Y:58:DG:H5'	2.01	0.41
15:Y:107:DC:H2''	15:Y:108:DT:H5'	2.02	0.41
15:Y:114:DC:H2''	15:Y:115:DG:C8	2.55	0.41
5:I:774:ASN:CG	5:I:929:LEU:HD12	2.45	0.41
5:I:1181:HIS:C	5:I:1183:ASP:N	2.74	0.41
8:L:2169:VAL:HG23	8:L:2230:MET:HE1	2.03	0.41
10:O:659:LEU:O	10:O:662:GLN:NE2	2.54	0.41
11:P:136:ARG:HB2	11:P:435:LYS:HD2	2.02	0.41
15:Y:47:DA:C5	15:Y:48:DT:C4	3.09	0.41
15:Y:94:DA:H2''	15:Y:95:DG:H8	1.83	0.41
2:B:75:HIS:O	4:D:89:ARG:NH1	2.53	0.41
3:C:90:ASP:OD1	3:C:92:GLU:N	2.51	0.41
5:I:358:PRO:HG3	10:N:676:THR:HA	2.03	0.41
5:I:859:THR:OG1	5:I:862:TYR:HB2	2.20	0.41
5:I:915:GLN:HA	5:I:915:GLN:HE21	1.85	0.41
5:I:1151:ILE:HD13	5:I:1151:ILE:HA	1.83	0.41
7:K:349:LEU:HB3	7:K:352:PHE:HB2	2.03	0.41
8:L:2074:SER:OG	8:L:2130:ASN:HB3	2.21	0.41
10:O:439:HIS:CG	10:O:440:ALA:N	2.88	0.41
11:P:131:LYS:O	11:P:147:TYR:OH	2.38	0.41
14:X:20:DC:H2''	14:X:21:DC:C5	2.55	0.41
4:D:33:SER:OG	4:D:60:ASN:ND2	2.53	0.41
5:I:908:LEU:HD12	5:I:908:LEU:HA	1.80	0.41
8:L:2085:LEU:HD11	8:L:2134:LEU:HB3	2.02	0.41
10:O:901:ILE:HD11	12:Q:249:GLU:OE1	2.20	0.41
14:X:42:DA:C6	14:X:43:DG:C6	3.09	0.41
15:Y:38:DT:H2''	15:Y:39:DA:C8	2.56	0.41
3:C:88:ARG:HB2	3:C:108:LEU:HD13	2.03	0.41
1:E:82:LEU:HD12	1:E:82:LEU:HA	1.89	0.41
5:I:413:GLN:O	5:I:417:ARG:HG3	2.19	0.41
5:I:461:LYS:HE3	8:L:2129:ASP:H	1.84	0.41
5:I:850:SER:OG	5:I:854:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:193:VAL:HG22	6:J:332:SER:HB3	2.02	0.41
12:Q:229:ARG:CZ	12:Q:229:ARG:HB2	2.50	0.41
14:X:29:DC:H2''	14:X:30:DT:C5	2.54	0.41
14:X:31:DC:H6	14:X:31:DC:H2'	1.69	0.41
4:D:58:ILE:HG23	2:F:98:TYR:HB3	2.02	0.41
6:J:281:GLN:HE21	6:J:296:ASP:HA	1.86	0.41
8:L:2024:ARG:NH2	11:P:149:ASP:OD1	2.54	0.41
9:M:291:GLU:OE2	9:M:316:ARG:NH1	2.54	0.41
10:N:451:ASN:HB3	10:N:453:LYS:HG2	2.03	0.41
10:N:919:ALA:HA	10:N:922:TYR:CD2	2.55	0.41
10:O:487:ARG:HD2	10:O:494:VAL:CG2	2.51	0.41
11:P:357:ILE:N	11:P:358:PRO:HD2	2.36	0.41
15:Y:70:DG:H2''	15:Y:71:DG:C8	2.56	0.41
1:A:109:ILE:HD13	1:A:109:ILE:HA	1.91	0.41
4:H:59:MET:HE3	4:H:59:MET:HB3	1.88	0.41
5:I:498:GLN:O	5:I:501:THR:OG1	2.25	0.41
5:I:832:VAL:HG12	5:I:856:LEU:HA	2.03	0.41
7:K:325:MET:SD	7:K:325:MET:N	2.90	0.41
8:L:1730:ILE:HG23	8:L:1731:LEU:HG	2.02	0.41
8:L:1851:THR:O	10:N:444:ARG:HD2	2.21	0.41
8:L:2232:ARG:NE	8:L:2236:ARG:HH22	2.19	0.41
9:M:269:HIS:CE1	9:M:364:LYS:HB3	2.56	0.41
9:M:324:LYS:HE3	9:M:324:LYS:HB3	1.93	0.41
10:O:488:ARG:HD3	10:O:489:ASN:ND2	2.36	0.41
10:O:521:THR:HG22	10:O:522:PRO:HD2	2.02	0.41
14:X:22:DG:H2''	14:X:23:DA:C8	2.56	0.41
14:X:70:DG:H2''	14:X:71:DT:C7	2.50	0.41
15:Y:43:DA:C5	15:Y:44:DG:C6	3.09	0.41
15:Y:130:DC:H1'	15:Y:131:DT:C6	2.55	0.41
5:I:1189:ARG:HA	5:I:1189:ARG:HD2	1.32	0.41
6:J:134:GLU:O	6:J:137:THR:OG1	2.33	0.41
7:K:314:GLN:HB2	7:K:329:ILE:HG13	2.03	0.41
8:L:1741:GLN:HE21	8:L:1843:HIS:HD2	1.68	0.41
8:L:1850:ASP:OD1	10:N:444:ARG:NH1	2.54	0.41
11:P:141:VAL:HG22	11:P:142:PRO:O	2.21	0.41
11:P:480:GLU:H	11:P:480:GLU:CD	2.28	0.41
5:I:405:LYS:NZ	10:O:611:GLU:OE2	2.53	0.40
5:I:793:ILE:HG12	5:I:806:PHE:CE1	2.55	0.40
5:I:872:LYS:HG2	7:K:291:LYS:NZ	2.36	0.40
5:I:1011:MET:HE3	5:I:1011:MET:HB3	1.90	0.40
5:I:1183:ASP:HA	5:I:1186:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:363:ARG:HA	6:J:366:ARG:HG2	2.03	0.40
8:L:2024:ARG:NH1	11:P:145:GLN:OE1	2.54	0.40
13:R:39:LEU:HD12	13:R:39:LEU:HA	1.88	0.40
15:Y:41:DG:H4'	15:Y:42:DG:OP1	2.22	0.40
4:H:38:VAL:HA	4:H:41:VAL:HG22	2.02	0.40
5:I:381:ARG:HA	5:I:381:ARG:HD2	1.85	0.40
5:I:860:TYR:HD1	5:I:860:TYR:HA	1.82	0.40
5:I:1056:GLU:HA	5:I:1059:PHE:HB2	2.03	0.40
6:J:120:VAL:O	6:J:149:PHE:HA	2.21	0.40
7:K:256:ARG:HB2	7:K:256:ARG:HE	1.65	0.40
14:X:46:DA:C6	14:X:47:DG:C6	3.10	0.40
1:A:97:LEU:HA	1:A:97:LEU:HD23	1.84	0.40
5:I:785:LYS:NZ	5:I:910:THR:O	2.50	0.40
5:I:932:ILE:HD12	5:I:932:ILE:HA	1.91	0.40
5:I:1161:LEU:CD1	5:I:1188:ASP:HB3	2.51	0.40
10:N:469:MET:HG2	10:N:486:CYS:SG	2.61	0.40
10:O:665:PRO:HB3	11:P:459:GLN:HB3	2.04	0.40
14:X:122:DC:N4	15:Y:31:DT:O4	2.53	0.40
5:I:812:LEU:HD21	5:I:862:TYR:CE2	2.56	0.40
5:I:1179:ASN:HD21	5:I:1181:HIS:HB2	1.86	0.40
7:K:213:LYS:HB3	7:K:306:TYR:HE1	1.87	0.40
7:K:219:VAL:HG11	7:K:262:PHE:HE2	1.86	0.40
7:K:219:VAL:HB	7:K:309:ILE:HG22	2.03	0.40
9:M:54:LEU:HA	9:M:54:LEU:HD13	1.90	0.40
9:M:351:PRO:HD3	10:O:487:ARG:NH2	2.36	0.40
14:X:135:DG:H1'	14:X:136:DA:C8	2.55	0.40
3:C:81:ARG:HA	3:C:81:ARG:HD2	1.94	0.40
5:I:1185:GLN:HE21	5:I:1189:ARG:NE	2.20	0.40
8:L:2134:LEU:HD23	8:L:2134:LEU:HA	1.92	0.40
8:L:2262:SER:HB3	8:L:2275:ILE:HG22	2.04	0.40
9:M:248:TYR:CD1	9:M:249:PRO:HD2	2.57	0.40
10:N:425:ILE:H	10:N:513:GLN:NE2	2.19	0.40
10:N:684:VAL:HG21	10:N:871:VAL:HG21	2.02	0.40
14:X:39:DC:H6	14:X:39:DC:H2'	1.74	0.40
14:X:105:DG:H2''	14:X:106:DA:H5''	2.03	0.40
15:Y:58:DG:H2''	15:Y:59:DG:O5'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	89/136 (65%)	87 (98%)	2 (2%)	0	100	100
1	E	89/136 (65%)	87 (98%)	2 (2%)	0	100	100
2	B	76/103 (74%)	73 (96%)	3 (4%)	0	100	100
2	F	75/103 (73%)	74 (99%)	1 (1%)	0	100	100
3	C	93/130 (72%)	88 (95%)	5 (5%)	0	100	100
3	G	93/130 (72%)	90 (97%)	3 (3%)	0	100	100
4	D	86/126 (68%)	82 (95%)	4 (5%)	0	100	100
4	H	88/126 (70%)	84 (96%)	4 (4%)	0	100	100
5	I	527/1647 (32%)	445 (84%)	75 (14%)	7 (1%)	9	38
6	J	324/407 (80%)	288 (89%)	34 (10%)	2 (1%)	21	52
7	K	309/375 (82%)	290 (94%)	18 (6%)	1 (0%)	36	65
8	L	456/1295 (35%)	434 (95%)	22 (5%)	0	100	100
9	M	273/336 (81%)	263 (96%)	10 (4%)	0	100	100
10	N	253/1214 (21%)	247 (98%)	6 (2%)	0	100	100
10	O	317/1214 (26%)	304 (96%)	13 (4%)	0	100	100
11	P	233/515 (45%)	220 (94%)	13 (6%)	0	100	100
12	Q	103/411 (25%)	96 (93%)	7 (7%)	0	100	100
13	R	68/292 (23%)	61 (90%)	7 (10%)	0	100	100
All	All	3552/8696 (41%)	3313 (93%)	229 (6%)	10 (0%)	37	65

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	811	PRO
5	I	874	ARG
5	I	1050	TYR
5	I	1162	GLY

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Mol	Chain	Res	Type
7	K	288	ASP
5	I	930	PRO
5	I	1161	LEU
6	J	212	GLU
6	J	300	GLU
5	I	812	LEU

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	77/110 (70%)	71 (92%)	6 (8%)	11	37
1	E	77/110 (70%)	71 (92%)	6 (8%)	11	37
2	B	64/79 (81%)	64 (100%)	0	100	100
2	F	63/79 (80%)	63 (100%)	0	100	100
3	C	73/100 (73%)	72 (99%)	1 (1%)	59	70
3	G	73/100 (73%)	72 (99%)	1 (1%)	59	70
4	D	74/104 (71%)	74 (100%)	0	100	100
4	H	76/104 (73%)	76 (100%)	0	100	100
5	I	501/1422 (35%)	460 (92%)	41 (8%)	10	36
6	J	287/348 (82%)	271 (94%)	16 (6%)	19	46
7	K	270/318 (85%)	263 (97%)	7 (3%)	40	60
8	L	418/1117 (37%)	417 (100%)	1 (0%)	87	86
9	M	252/294 (86%)	248 (98%)	4 (2%)	55	68
10	N	222/1030 (22%)	222 (100%)	0	100	100
10	O	282/1030 (27%)	281 (100%)	1 (0%)	84	81
11	P	223/442 (50%)	223 (100%)	0	100	100
12	Q	98/361 (27%)	98 (100%)	0	100	100
13	R	59/253 (23%)	59 (100%)	0	100	100
All	All	3189/7401 (43%)	3105 (97%)	84 (3%)	41	60

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	THR
1	A	45	LEU
1	A	74	ASP
1	A	77	THR
1	A	83	SER
1	A	98	VAL
3	C	102	ILE
1	E	45	THR
1	E	48	LEU
1	E	77	ASP
1	E	80	THR
1	E	86	SER
1	E	101	VAL
3	G	108	LEU
5	I	473	GLN
5	I	482	HIS
5	I	490	HIS
5	I	493	VAL
5	I	504	VAL
5	I	510	ASN
5	I	777	LEU
5	I	779	ASP
5	I	793	ILE
5	I	812	LEU
5	I	815	LEU
5	I	817	ASN
5	I	831	LYS
5	I	832	VAL
5	I	835	LYS
5	I	857	LEU
5	I	870	LEU
5	I	879	ILE
5	I	880	VAL
5	I	884	HIS
5	I	893	LEU
5	I	909	LEU
5	I	910	THR
5	I	915	GLN
5	I	924	LEU
5	I	927	PHE
5	I	928	LEU
5	I	931	THR

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Mol	Chain	Res	Type
5	I	932	ILE
5	I	995	VAL
5	I	1038	THR
5	I	1048	HIS
5	I	1108	LEU
5	I	1170	THR
5	I	1174	PHE
5	I	1182	GLN
5	I	1189	ARG
5	I	1308	ARG
5	I	1311	GLU
5	I	1312	GLU
5	I	1350	ASP
6	J	41	ILE
6	J	69	TYR
6	J	70	ILE
6	J	79	ARG
6	J	80	GLU
6	J	180	ILE
6	J	247	THR
6	J	248	ARG
6	J	272	SER
6	J	273	THR
6	J	278	VAL
6	J	293	TYR
6	J	294	ASN
6	J	300	GLU
6	J	301	ARG
6	J	302	LEU
7	K	195	GLU
7	K	246	GLN
7	K	250	ILE
7	K	252	ASN
7	K	289	ILE
7	K	334	GLU
7	K	335	ARG
8	L	1692	ASN
9	M	324	LYS
9	M	360	GLU
9	M	361	MET
9	M	378	LEU
10	O	521	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	90	GLN
2	B	25	ASN
4	D	60	ASN
4	D	106	HIS
1	E	93	GLN
2	F	25	ASN
3	G	24	GLN
4	H	46	HIS
5	I	356	GLN
5	I	472	HIS
5	I	477	ASN
5	I	515	GLN
5	I	817	ASN
5	I	854	ASN
5	I	895	GLN
5	I	941	GLN
5	I	1048	HIS
5	I	1054	HIS
5	I	1096	ASN
5	I	1179	ASN
5	I	1182	GLN
5	I	1191	HIS
5	I	1195	GLN
6	J	105	HIS
6	J	162	ASN
6	J	251	HIS
6	J	268	GLN
6	J	370	GLN
6	J	407	GLN
6	J	408	GLN
7	K	87	HIS
7	K	115	ASN
7	K	246	GLN
7	K	263	GLN
7	K	314	GLN
7	K	353	GLN
8	L	1650	GLN
8	L	1692	ASN
8	L	1705	ASN
8	L	1835	GLN

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Mol	Chain	Res	Type
8	L	1843	HIS
8	L	1858	HIS
8	L	1986	ASN
8	L	1997	ASN
8	L	2268	ASN
9	M	244	GLN
9	M	269	HIS
9	M	322	HIS
10	N	489	ASN
10	N	513	GLN
10	N	621	ASN
10	N	632	GLN
10	N	638	HIS
10	N	925	GLN
10	N	938	GLN
10	N	948	GLN
10	O	439	HIS
10	O	478	GLN
10	O	501	HIS
10	O	513	GLN
10	O	545	GLN
10	O	638	HIS
10	O	662	GLN
11	P	135	GLN
11	P	321	GLN
11	P	326	HIS
11	P	344	GLN
11	P	405	ASN
11	P	432	ASN
11	P	453	ASN
11	P	457	GLN
12	Q	190	HIS
12	Q	238	GLN
12	Q	267	ASN
12	Q	268	ASN
13	R	28	ASN
13	R	61	HIS
13	R	70	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

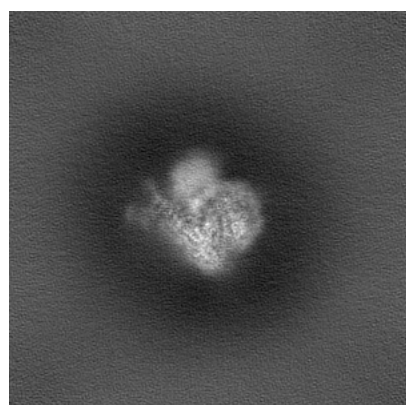
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0974. These allow visual inspection of the internal detail of the map and identification of artifacts.

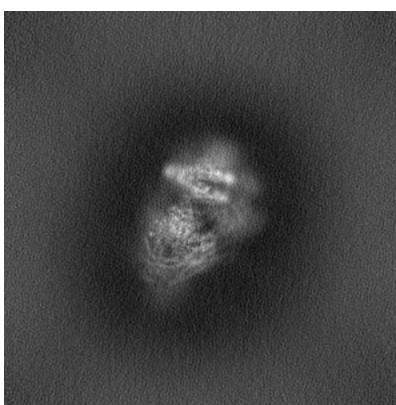
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

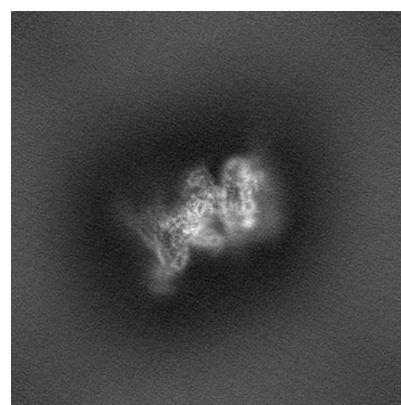
6.1.1 Primary map



X



Y



Z

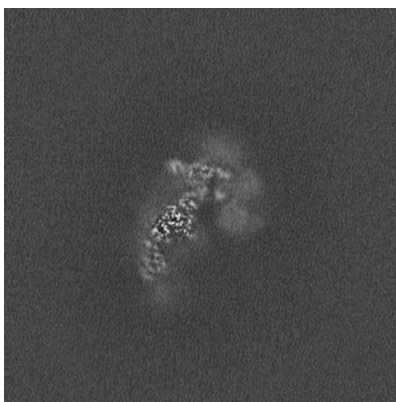
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

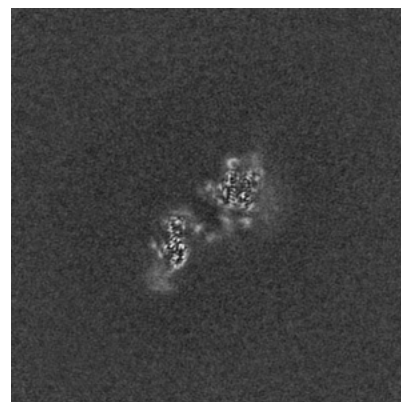
6.2.1 Primary map



X Index: 256



Y Index: 256

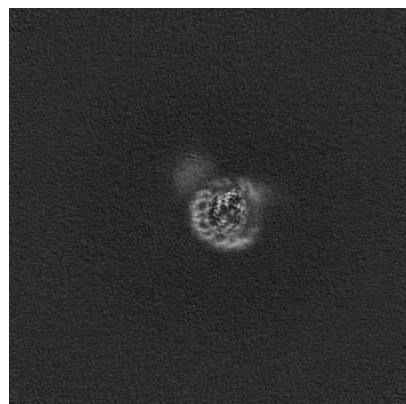


Z Index: 256

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

6.3 Largest variance slices [i](#)

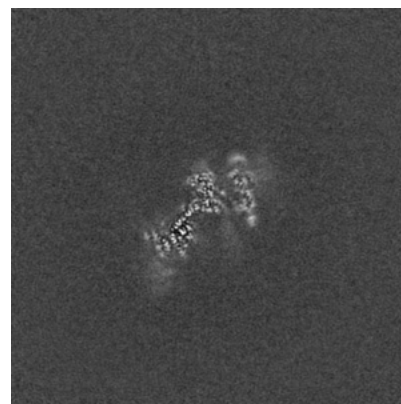
6.3.1 Primary map



X Index: 304



Y Index: 253

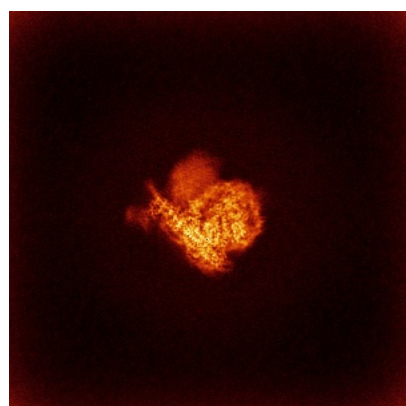


Z Index: 238

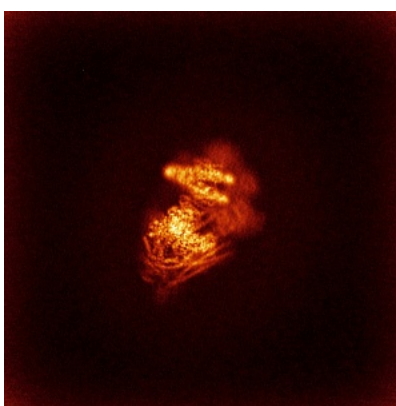
The images above show the largest variance slices of the map in three orthogonal directions.

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

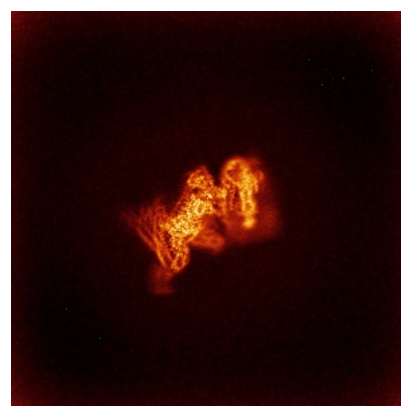
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

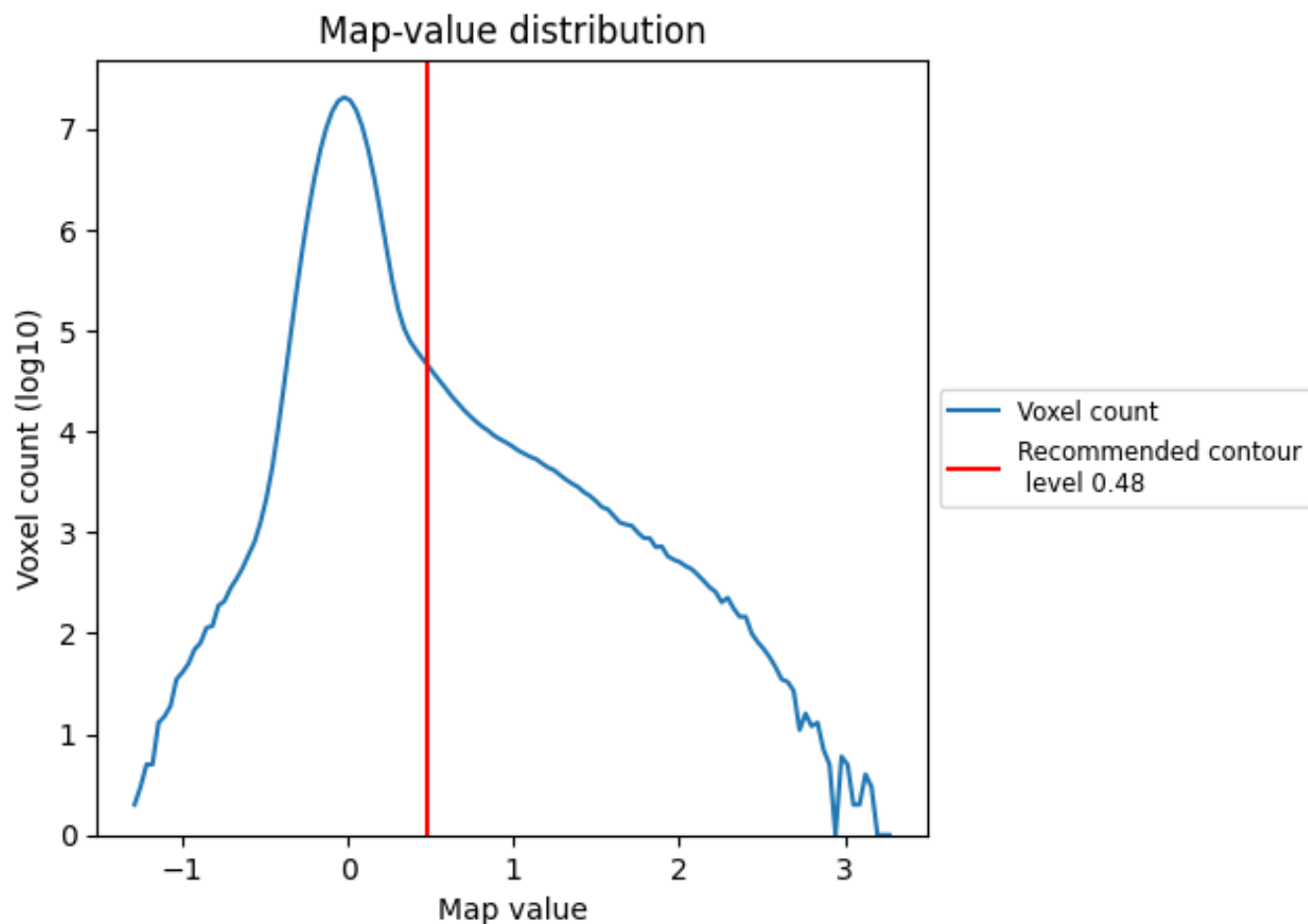
6.6 Mask visualisation

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

7 Map analysis [i](#)

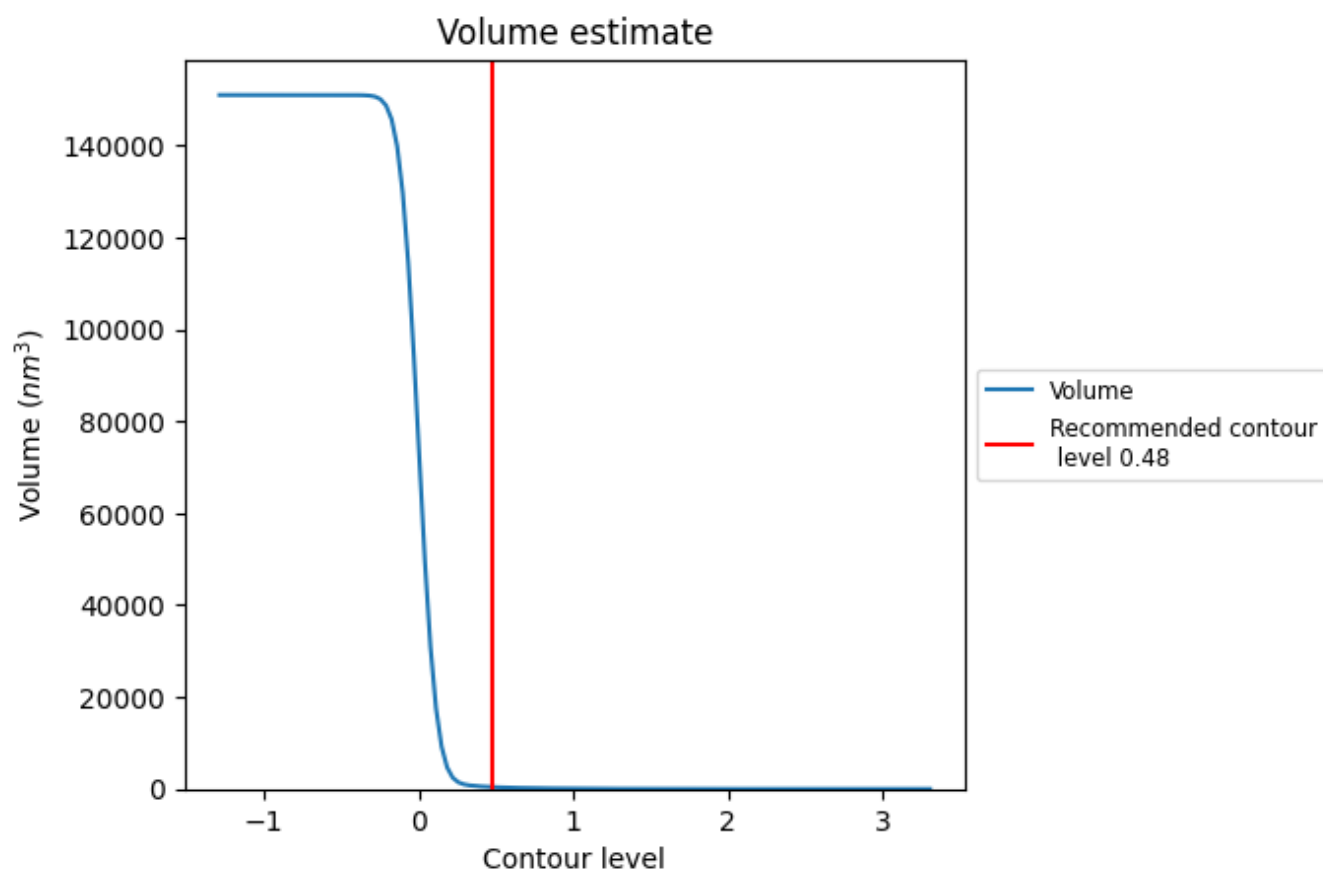
This section contains the results of statistical analysis of the map.

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.

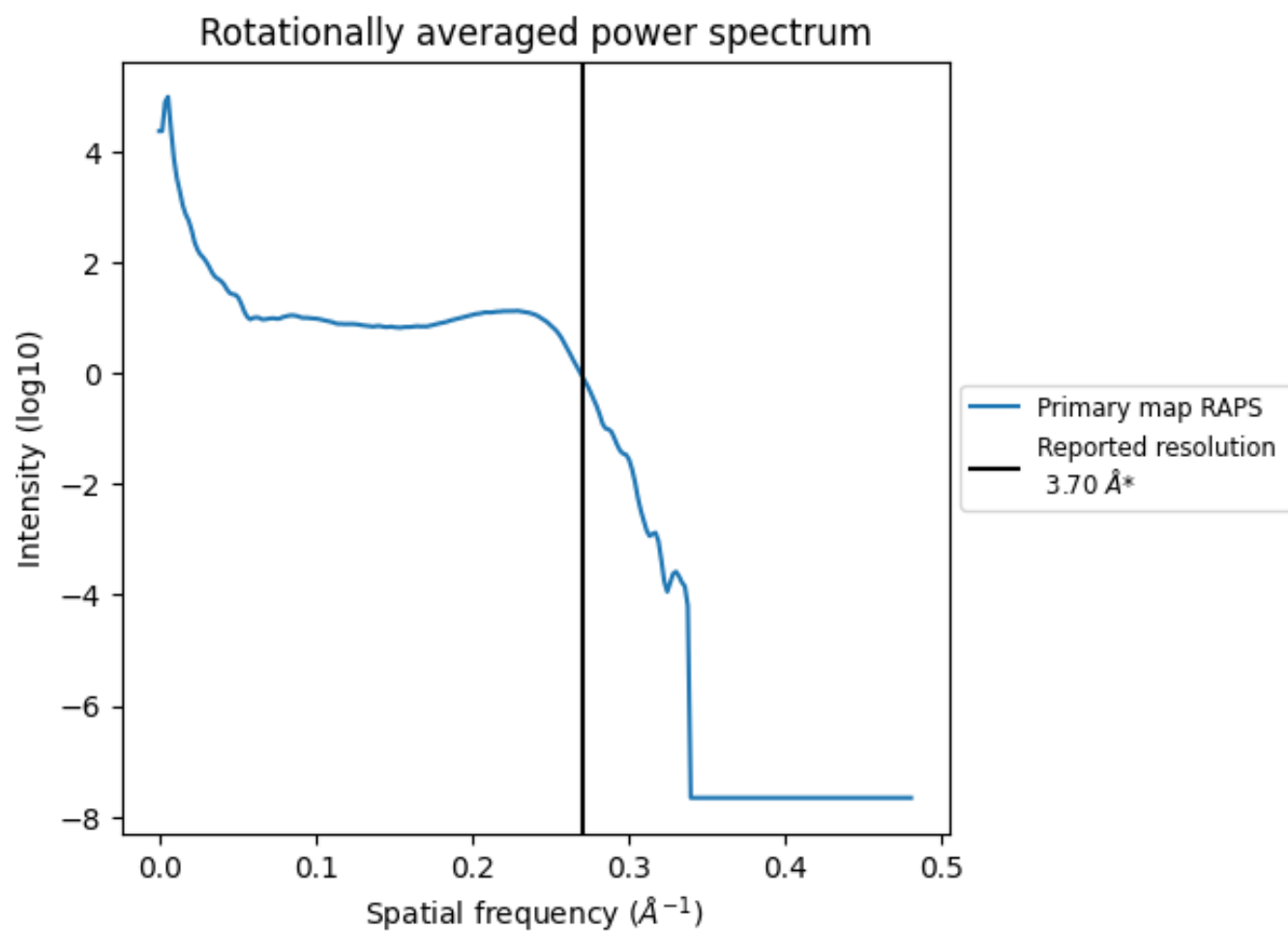
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404 nm^3 ; this corresponds to an approximate mass of 365 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



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

8 Fourier-Shell correlation ⓘ

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

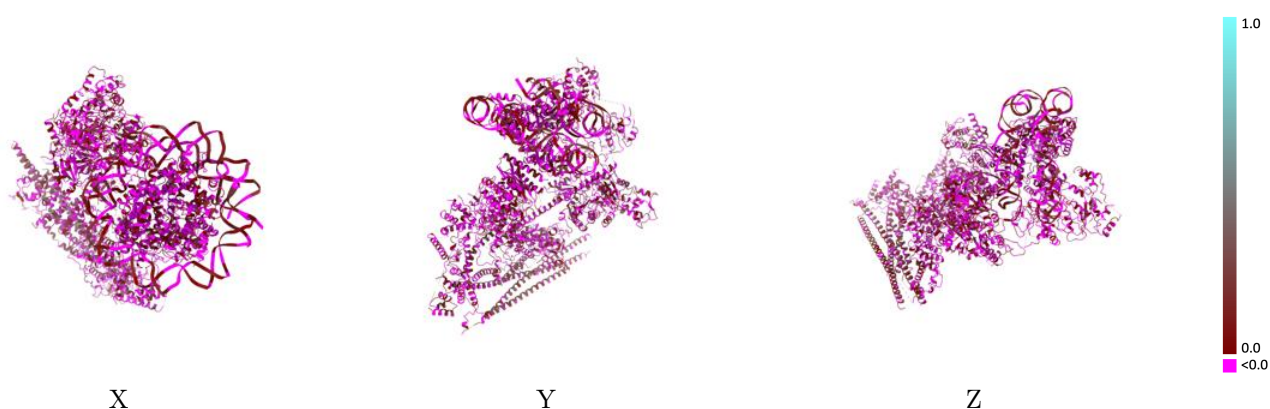
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0974 and PDB model 6LTJ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

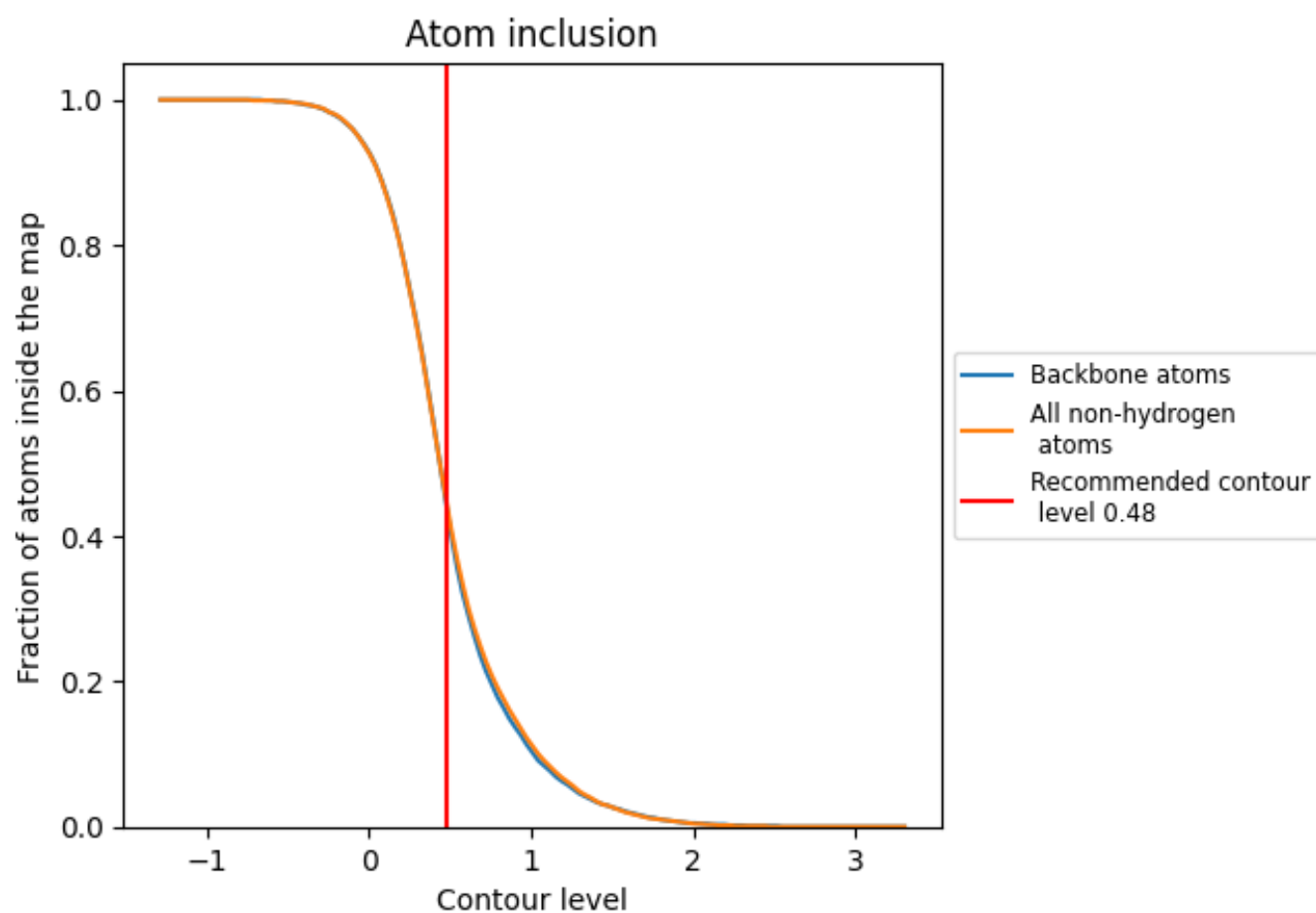


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 44% 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 (0.48) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4430	 0.0070
A	 0.4520	 -0.0070
B	 0.4970	 -0.0090
C	 0.5020	 -0.0140
D	 0.4630	 -0.0280
E	 0.4610	 -0.0760
F	 0.4680	 0.0050
G	 0.4390	 -0.0310
H	 0.3810	 -0.0530
I	 0.2940	 -0.0020
J	 0.5410	 0.0100
K	 0.2800	 0.0300
L	 0.3890	 -0.0050
M	 0.4570	 -0.0130
N	 0.4210	 0.0210
O	 0.5190	 0.0290
P	 0.4480	 0.0110
Q	 0.5510	 0.0880
R	 0.4300	 -0.0440
X	 0.5640	 0.0270
Y	 0.5850	 0.0320

