



Full wwPDB EM Validation Report ⓘ

Jun 8, 2026 – 04:43 PM EDT

PDB ID : 9OKB / pdb_00009okb
EMDB ID : EMD-70558
Title : Structure of the dimeric Bombyx mori CCAN bound to DNA
Authors : Yatskevich, S.; Ciferri, C.
Deposited on : 2025-05-09
Resolution : 4.50 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:

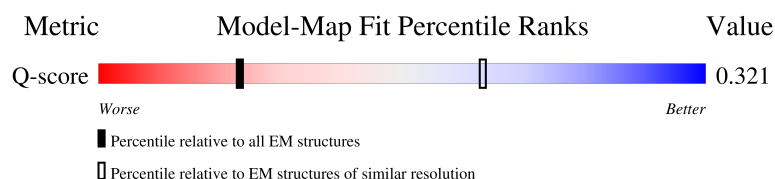
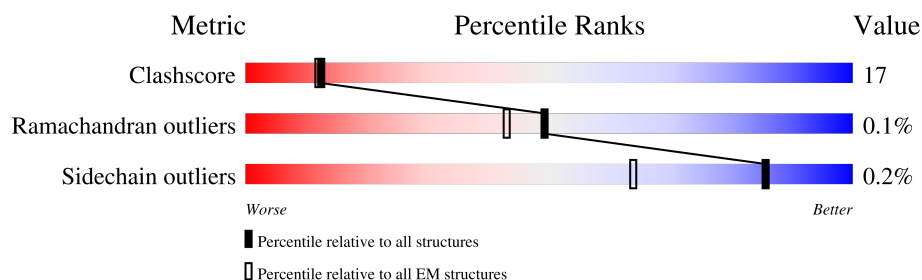
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.50 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	2937 (4.00 - 5.00)

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	95	<div> <div>17%</div> <div>52%</div> <div>21%</div> <div>•</div> <div>26%</div> </div>
1	a	95	<div> <div>51%</div> <div>55%</div> <div>18%</div> <div>•</div> <div>26%</div> </div>
2	B	82	<div> <div>5%</div> <div>54%</div> <div>13%</div> <div>33%</div> </div>
2	b	82	<div> <div>33%</div> <div>50%</div> <div>17%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	72	
3	c	72	
4	D	81	
4	d	81	
5	H	239	
5	h	239	
6	I	661	
6	i	661	
7	J	180	
7	M	180	
8	K	219	
8	k	219	
9	L	302	
9	l	302	
10	N	328	
10	n	328	
11	O	325	
11	o	325	
12	P	638	
12	p	638	
13	T	1016	
13	t	1016	
14	X	58	
15	Y	58	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 84496 atoms, of which 38978 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 CS-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	70	Total	C	H	N	O	S	0	0
			1073	341	527	94	108	3		
1	a	70	Total	C	H	N	O	S	0	0
			1073	341	527	94	108	3		

- Molecule 2 is a protein called CS-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	55	Total	C	H	N	O	0	0
			858	280	419	75	84		
2	b	55	Total	C	H	N	O	0	0
			858	280	419	75	84		

- Molecule 3 is a protein called CS-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	62	Total	C	H	N	O	S	0	0
			1044	323	517	101	100	3		
3	c	62	Total	C	H	N	O	S	0	0
			1044	323	517	101	100	3		

- Molecule 4 is a protein called CS-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	71	Total	C	H	N	O	S	0	0
			1135	346	570	108	110	1		
4	d	71	Total	C	H	N	O	S	0	0
			1135	346	570	108	110	1		

- Molecule 5 is a protein called bmCENP-H.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	H	228	Total	C	H	N	O	S	0	0
			3517	1170	1666	326	345	10		
5	h	228	Total	C	H	N	O	S	0	0
			3517	1170	1666	326	345	10		

- Molecule 6 is a protein called Centromere protein I.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	576	Total	C	H	N	O	S	0	0
			9421	3033	4745	782	842	19		
6	i	576	Total	C	H	N	O	S	0	0
			9421	3033	4745	782	842	19		

- Molecule 7 is a protein called Centromere protein M.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	J	163	Total	C	H	N	O	S	0	0
			2635	818	1349	225	240	3		
7	M	163	Total	C	H	N	O	S	0	0
			2635	818	1349	225	240	3		

- Molecule 8 is a protein called bmCENP-K.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	K	209	Total	C	H	N	O	S	0	0
			3301	1030	1650	273	338	10		
8	k	209	Total	C	H	N	O	S	0	0
			3301	1030	1650	273	338	10		

- Molecule 9 is a protein called Centromere protein L.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	L	239	Total	C	H	N	O	S	0	0
			3880	1237	1974	309	353	7		
9	l	239	Total	C	H	N	O	S	0	0
			3880	1237	1974	309	353	7		

- Molecule 10 is a protein called bmCENP-N.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	N	322	Total	C	H	N	O	S	0	0
			5125	1615	2580	442	476	12		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	n	322	Total	C	H	N	O	S	0	0
			5125	1615	2580	442	476	12		

- Molecule 11 is a protein called Centromere protein O.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	O	254	Total	C	H	N	O	S	0	0
			3716	1300	1666	356	381	13		
11	o	254	Total	C	H	N	O	S	0	0
			3716	1300	1666	356	381	13		

- Molecule 12 is a protein called bmCENP-P.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	P	281	Total	C	H	N	O	S	0	0
			4051	1407	1826	371	435	12		
12	p	281	Total	C	H	N	O	S	0	0
			4051	1407	1826	371	435	12		

- Molecule 13 is a protein called bmCENP-T.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	154	Total	C	N	O	S	0	0
			1304	839	232	228	5		
13	t	154	Total	C	N	O	S	0	0
			1304	839	232	228	5		

- Molecule 14 is a DNA chain called DNA (58-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	58	Total	C	N	O	P	0	0
			1191	568	218	348	57		

- Molecule 15 is a DNA chain called DNA (58-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Y	58	Total	C	N	O	P	0	0
			1184	564	216	346	58		

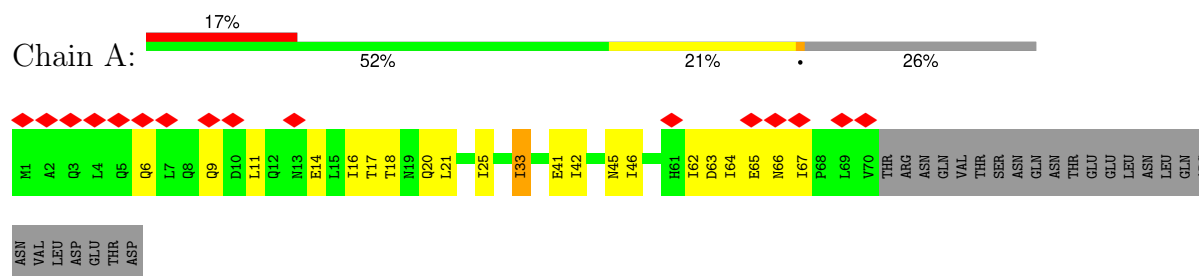
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

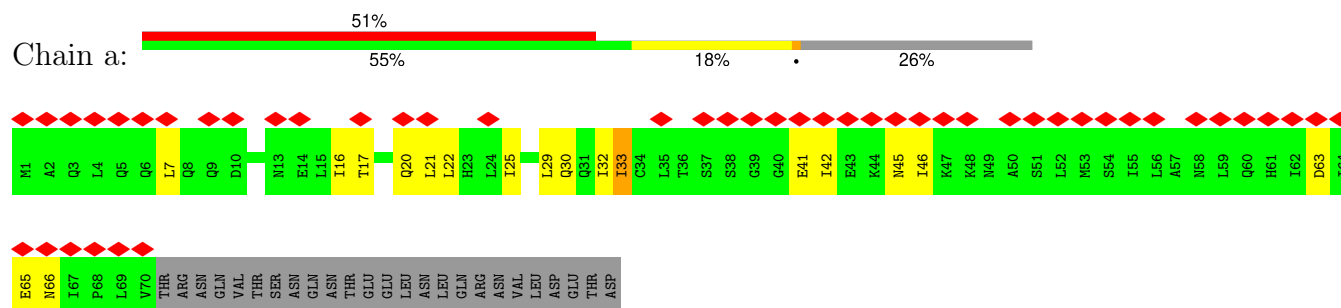
3 Residue-property plots [i](#)

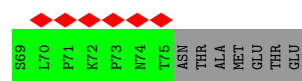
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: CS-1

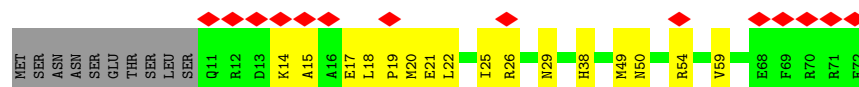


• Molecule 1: CS-1

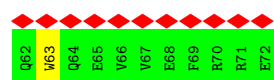
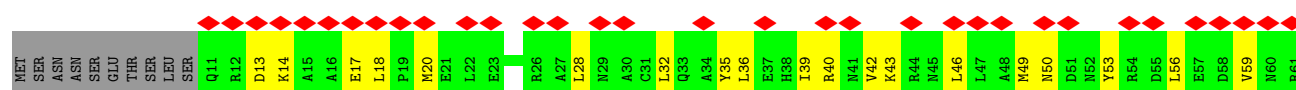




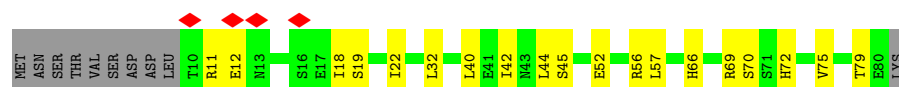
• Molecule 3: CS-3



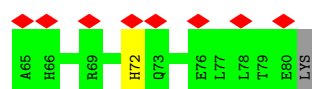
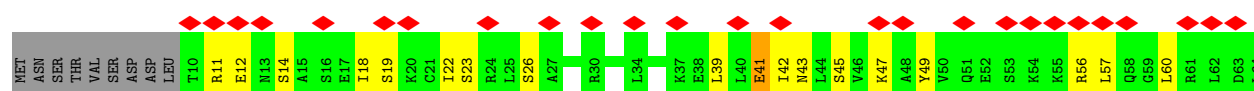
• Molecule 3: CS-3



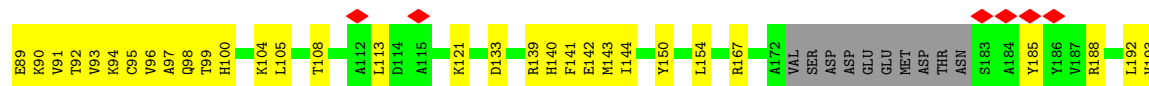
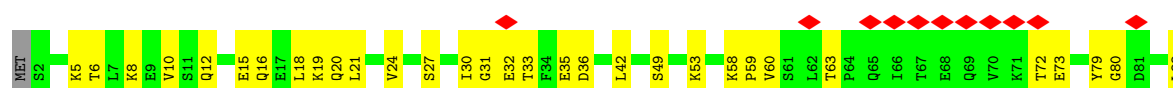
• Molecule 4: CS-4



• Molecule 4: CS-4

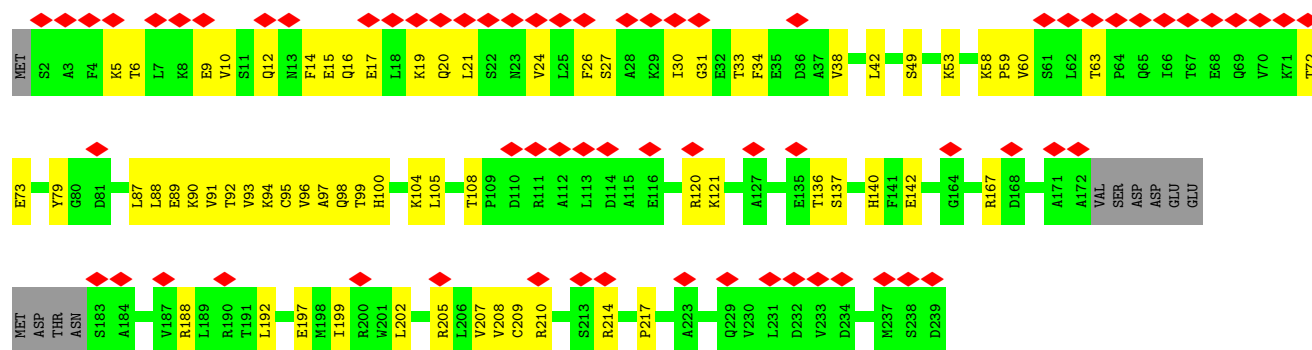


• Molecule 5: bmCENP-H

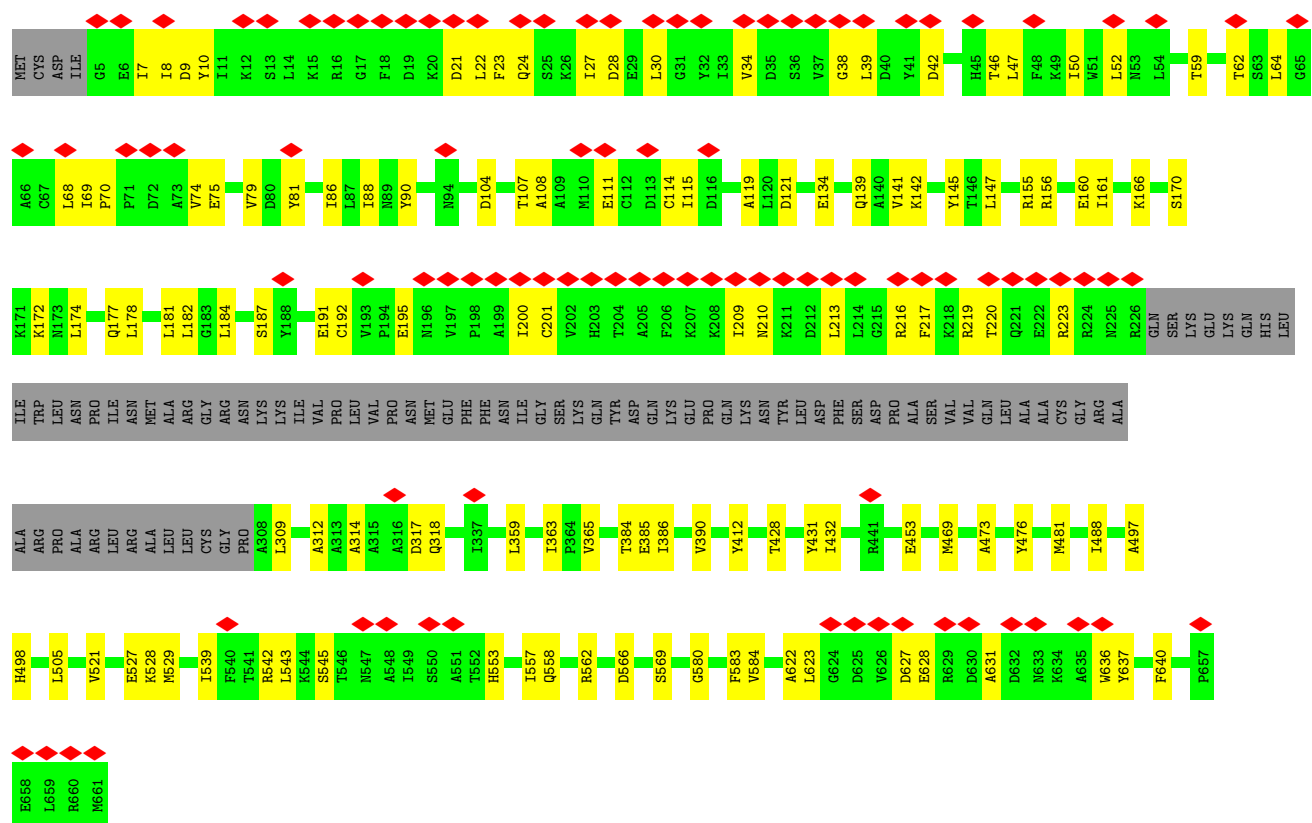




• Molecule 5: bmCENP-H

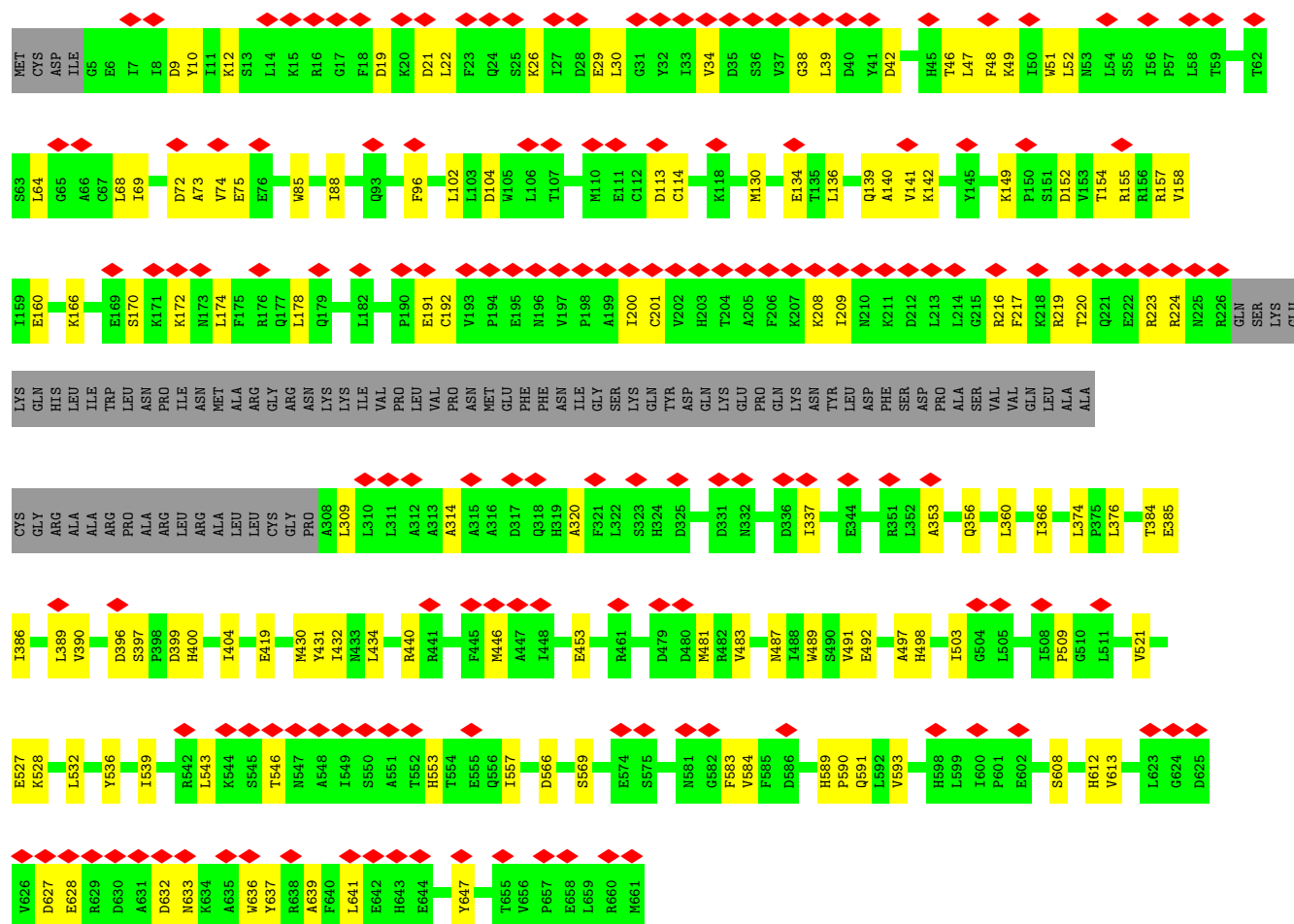


• Molecule 6: Centromere protein I

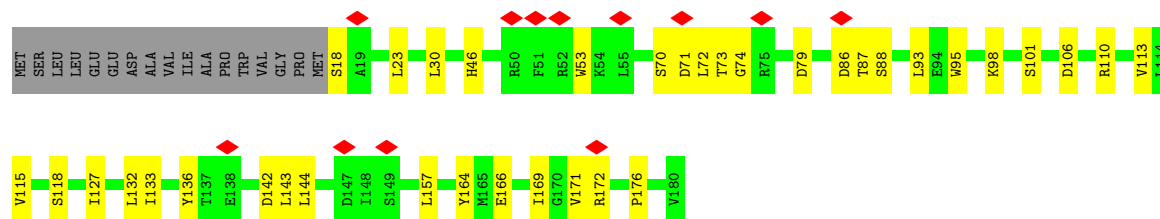


• Molecule 6: Centromere protein I

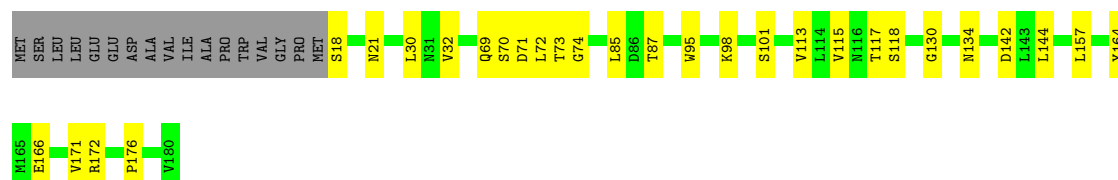
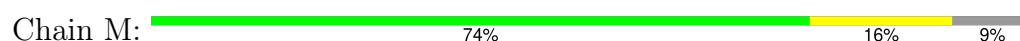




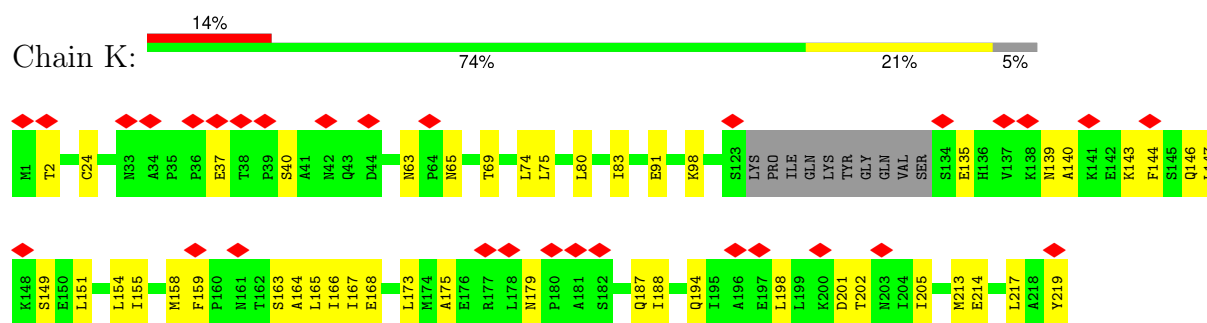
- Molecule 7: Centromere protein M



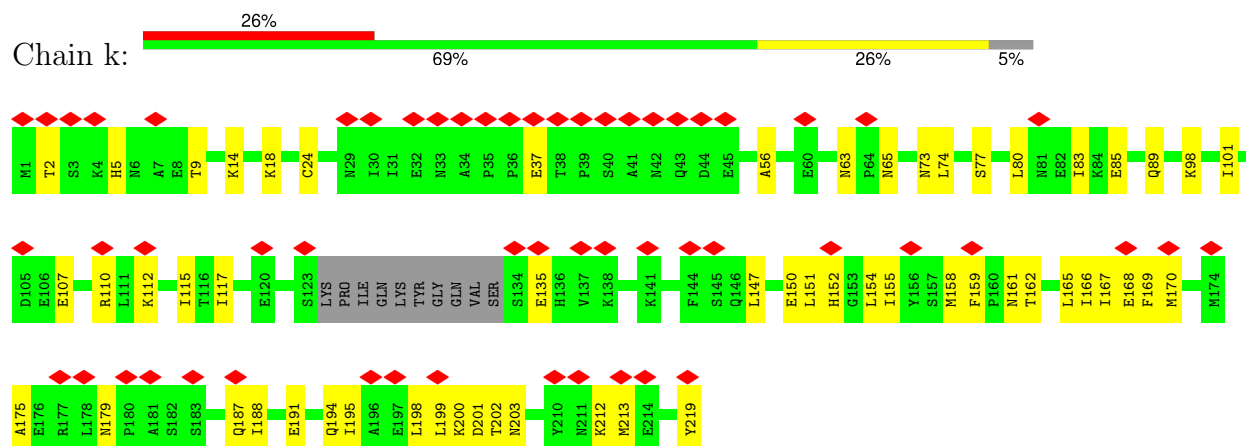
- Molecule 7: Centromere protein M



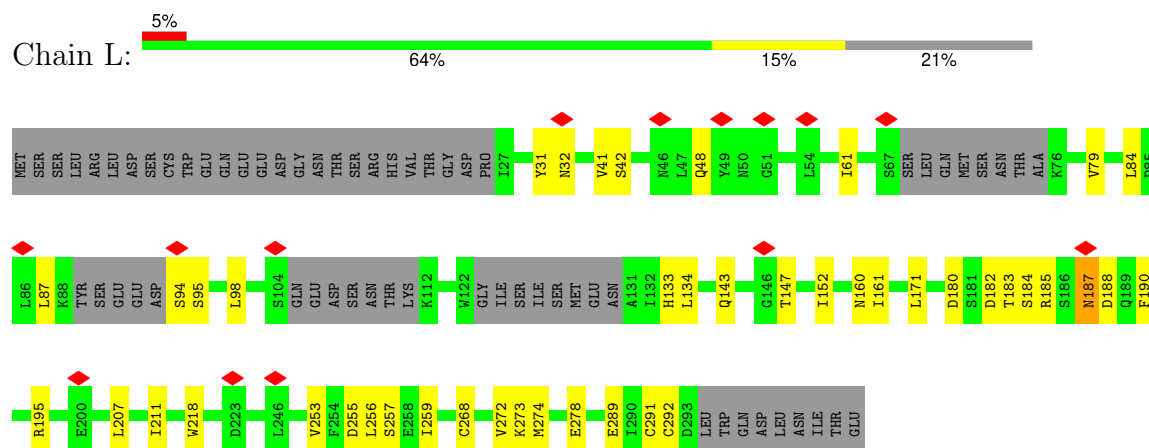
- Molecule 8: bmCENP-K



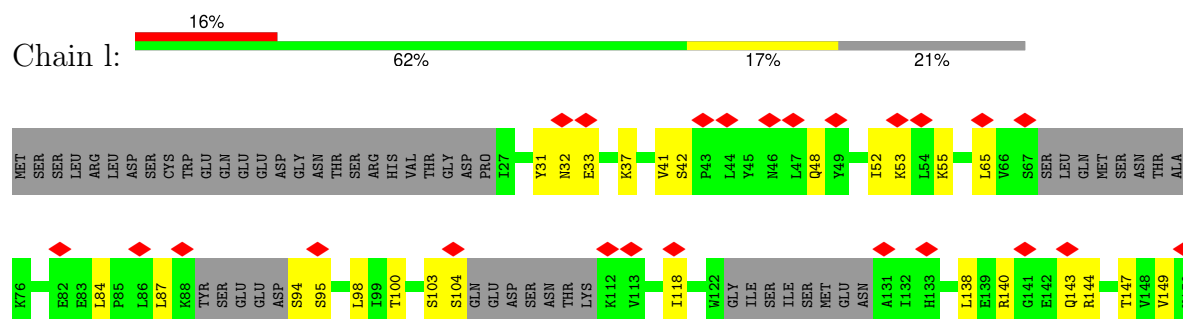
• Molecule 8: bmCENP-K

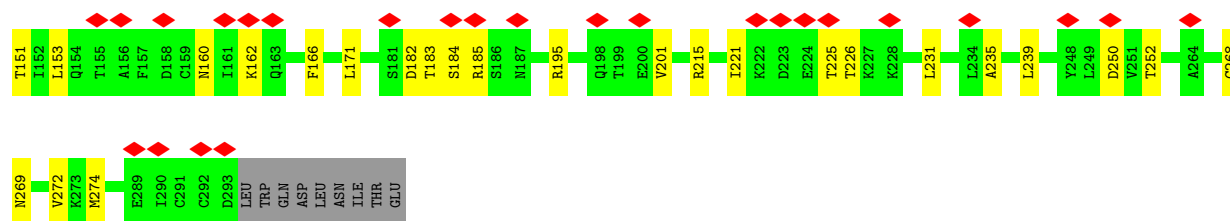


• Molecule 9: Centromere protein L

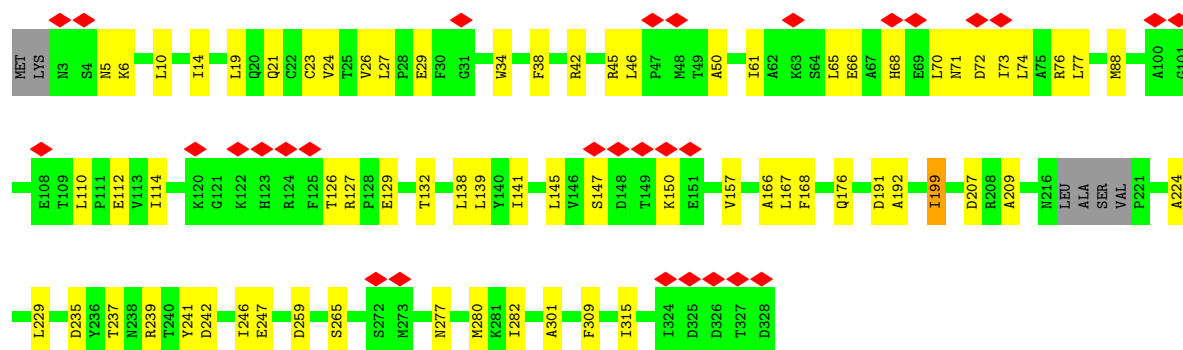
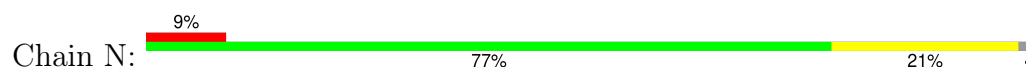


• Molecule 9: Centromere protein L

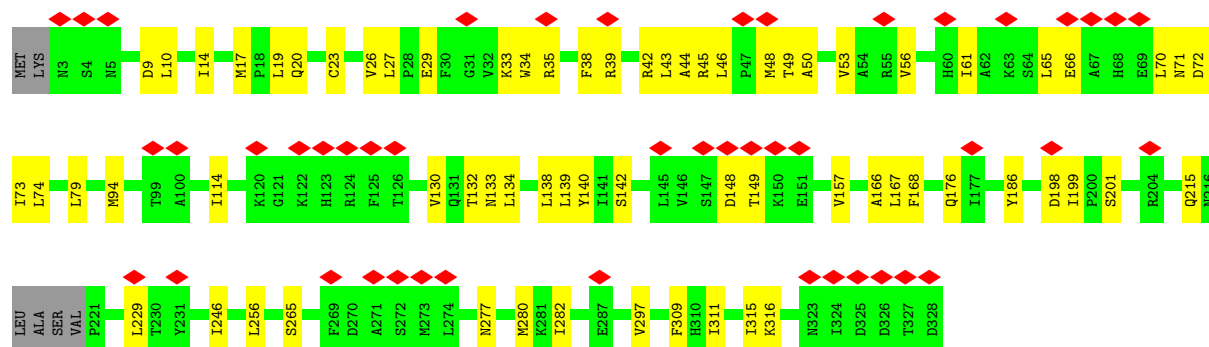
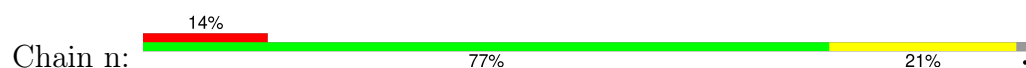




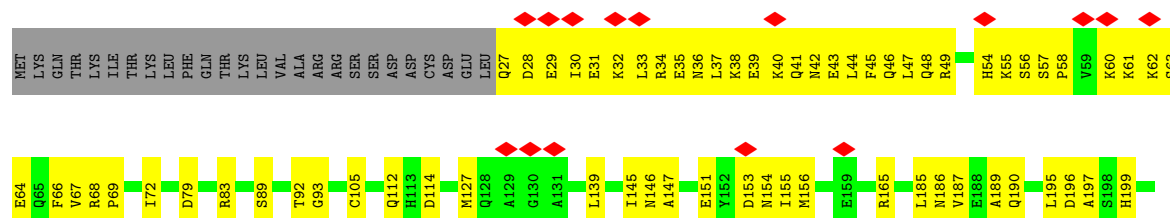
• Molecule 10: bmCENP-N

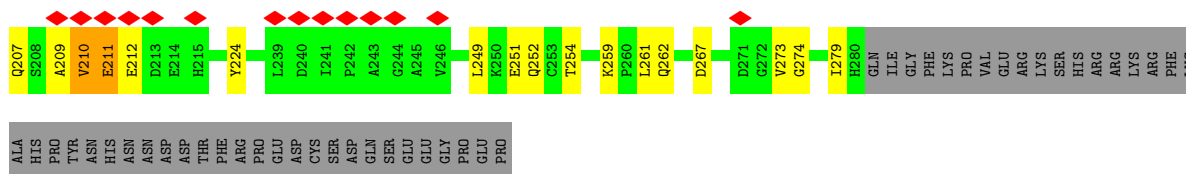


• Molecule 10: bmCENP-N

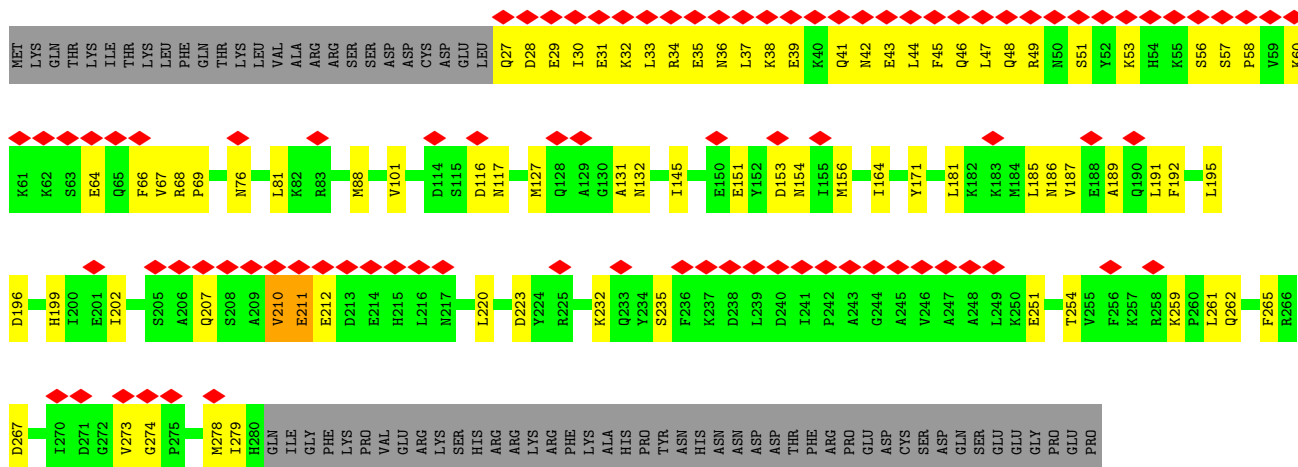


• Molecule 11: Centromere protein O

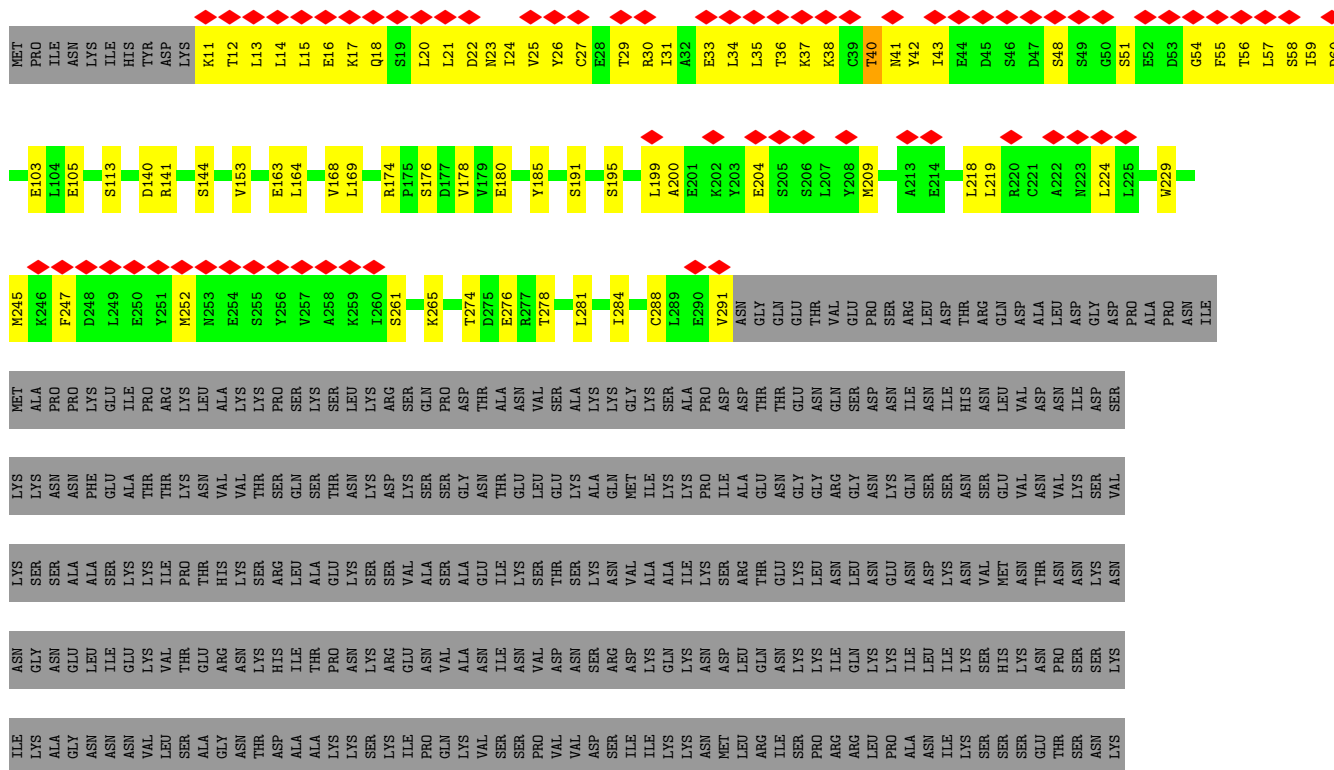
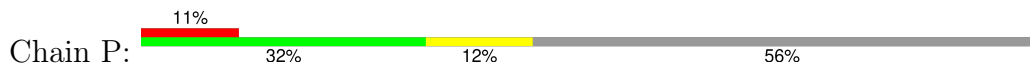




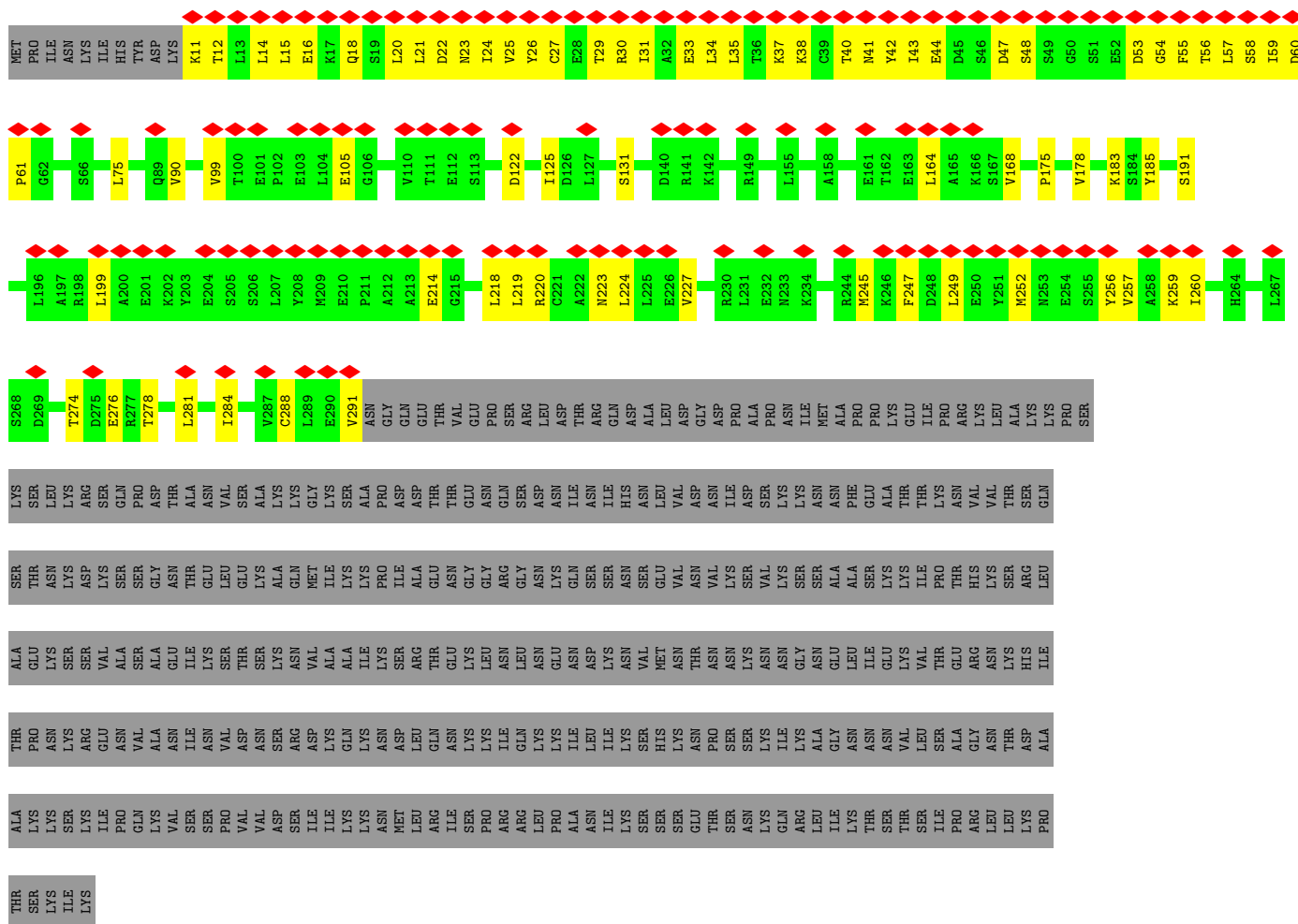
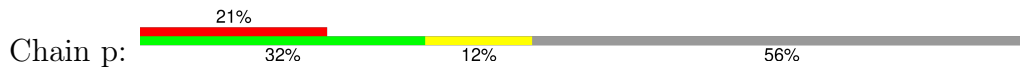
• Molecule 11: Centromere protein O



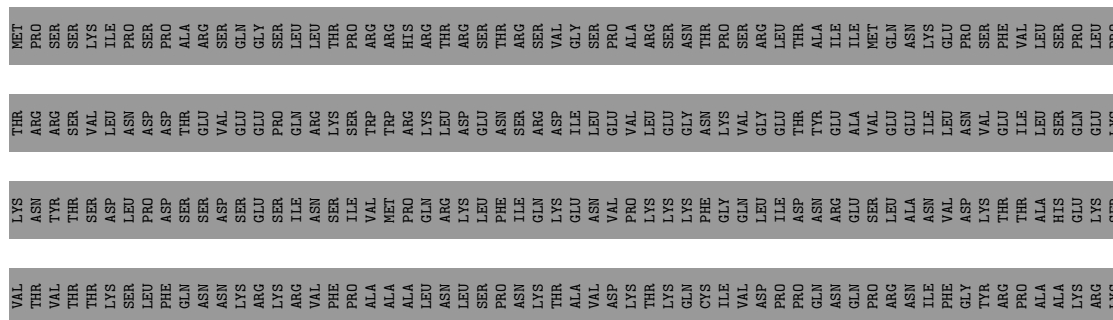
• Molecule 12: bmCENP-P



- Molecule 12: bmCENP-P



- Molecule 13: bmCENP-T



- Molecule 13: bmCENP-T

[illegible]

Chain Y:  5% 34% 95%

T15	A16	A17	C18	C19	G20	C21	C22	A23	A24	G25	G26	G27	G28	A29	T30	T31	A32	C33	T34	C35	C36	C37	T38	A39	G40	T41	C42	T43	C44	C45	A46	G47	G48	C49	A50	C51	G52	T53	G54	T55	C56	A57	G58	A59	T60	A61	T62	A63	T64	A65	C66	A67	T68	C69	G70	A71	T72
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23990	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.00342	Depositor
Map size (Å)	441.525, 441.525, 440.4375	wwPDB
Map dimensions	406, 406, 405	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0875, 1.0875, 1.0875	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	0.10	0/548	0.22	0/740
1	a	0.09	0/548	0.19	0/740
2	B	0.12	0/446	0.27	0/604
2	b	0.11	0/446	0.29	0/604
3	C	0.16	0/533	0.32	0/715
3	c	0.09	0/533	0.21	0/715
4	D	0.15	0/568	0.26	0/761
4	d	0.15	0/568	0.28	0/761
5	H	0.14	0/1872	0.27	0/2508
5	h	0.12	0/1872	0.26	0/2508
6	I	0.11	0/4784	0.24	0/6483
6	i	0.10	0/4784	0.23	0/6483
7	J	0.10	0/1302	0.23	0/1764
7	M	0.13	0/1302	0.25	0/1764
8	K	0.14	0/1670	0.27	0/2253
8	k	0.14	0/1670	0.27	0/2253
9	L	0.12	0/1935	0.29	0/2614
9	l	0.11	0/1935	0.29	1/2614 (0.0%)
10	N	0.13	0/2594	0.30	1/3516 (0.0%)
10	n	0.11	0/2594	0.28	0/3516
11	O	0.13	0/2085	0.26	0/2805
11	o	0.11	0/2085	0.26	0/2805
12	P	0.12	0/2265	0.26	0/3074
12	p	0.10	0/2265	0.27	0/3074
13	T	0.09	0/1334	0.22	0/1790
13	t	0.10	0/1334	0.22	0/1790
14	X	0.19	0/1336	0.38	0/2062
15	Y	0.18	0/1327	0.35	0/2044
All	All	0.12	0/46535	0.27	2/63360 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	221	ILE	CG1-CB-CG2	5.18	126.25	110.70
10	N	199	ILE	CG1-CB-CG2	5.11	126.02	110.70

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	546	527	572	20	0
1	a	546	527	572	21	0
2	B	439	419	453	12	0
2	b	439	419	453	13	0
3	C	527	517	516	19	0
3	c	527	517	516	17	0
4	D	565	570	587	18	0
4	d	565	570	587	19	0
5	H	1851	1666	1938	85	0
5	h	1851	1666	1938	70	0
6	I	4676	4745	4743	86	0
6	i	4676	4745	4743	103	0
7	J	1286	1349	1348	29	0
7	M	1286	1349	1348	19	0
8	K	1651	1650	1658	38	0
8	k	1651	1650	1658	59	0
9	L	1906	1974	1969	33	0
9	l	1906	1974	1969	32	0
10	N	2545	2580	2597	57	0
10	n	2545	2580	2597	59	0
11	O	2050	1666	2072	112	0
11	o	2050	1666	2072	98	0
12	P	2225	1826	2241	104	0
12	p	2225	1826	2241	102	0
13	T	1304	0	1334	167	0
13	t	1304	0	1334	170	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	X	1191	0	656	111	0
15	Y	1184	0	653	99	0
16	T	1	0	0	0	0
All	All	45518	38978	45365	1530	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 17.

All (1530) 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)
14:X:-62:DA:H2'	14:X:-61:DT:H71	1.32	1.07
11:O:30:ILE:HG22	12:P:17:LYS:HE2	1.40	1.03
14:X:-61:DT:H2'	14:X:-60:DA:C8	2.00	0.96
11:o:47:LEU:HD12	12:p:31:ILE:HD12	1.48	0.95
15:Y:37:DC:H2''	15:Y:38:DT:C7	1.99	0.92
13:T:932:LEU:HD21	13:T:964:LEU:HD22	1.52	0.90
13:T:996:LYS:HE2	13:T:996:LYS:HA	1.54	0.90
6:I:622:ALA:HB1	13:T:815:ILE:HG21	1.55	0.89
15:Y:36:DC:H2''	15:Y:37:DC:C5	2.09	0.88
12:p:220:ARG:NH2	12:p:223:ASN:OD1	2.08	0.86
12:P:37:LYS:NZ	12:P:38:LYS:O	2.08	0.86
14:X:-51:DG:C8	14:X:-50:DT:H72	2.08	0.86
15:Y:30:DT:H2'	15:Y:31:DT:H71	1.56	0.86
13:T:910:TYR:O	13:T:914:GLU:HG2	1.75	0.86
14:X:-39:DT:H2''	14:X:-38:DA:C8	2.10	0.85
5:h:27:SER:HB2	11:o:56:SER:HA	1.59	0.85
13:T:916:LYS:HD2	13:T:966:ILE:HG23	1.59	0.84
12:p:122:ASP:OD1	12:p:131:SER:OG	1.94	0.84
13:t:978:HIS:HB2	13:t:986:ARG:HH21	1.43	0.84
13:T:895:LYS:NZ	14:X:-34:DA:OP1	2.09	0.83
13:T:904:TRP:HB3	13:T:982:PRO:HD3	1.58	0.83
13:T:947:GLU:HG2	13:T:948:VAL:HG23	1.61	0.83
15:Y:47:DG:H5''	13:t:900:LYS:HE2	1.57	0.83
5:H:167:ARG:NH1	6:I:314:ALA:O	2.14	0.81
13:T:958:LYS:HE3	13:T:1008:ILE:HD13	1.63	0.81
11:o:259:LYS:NZ	11:o:267:ASP:OD2	2.12	0.81
6:i:155:ARG:NH1	6:i:192:CYS:SG	2.53	0.81
11:O:27:GLN:O	11:O:30:ILE:HG12	1.80	0.81
13:t:817:LYS:HE2	13:t:817:LYS:HA	1.62	0.80
13:t:943:VAL:HG22	13:t:988:LYS:HD2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:962:ALA:HB2	13:T:1008:ILE:HG21	1.63	0.80
5:H:79:TYR:OH	7:M:176:PRO:O	1.98	0.80
15:Y:55:DT:H2''	15:Y:56:DC:C5	2.17	0.79
6:i:566:ASP:O	6:i:569:SER:OG	1.98	0.79
8:K:187:GLN:NE2	8:K:188:ILE:O	2.16	0.79
7:M:166:GLU:OE2	7:M:172:ARG:NE	2.15	0.79
11:O:35:GLU:O	11:O:38:LYS:HG3	1.81	0.79
14:X:-31:DA:H2''	14:X:-30:DA:C8	2.18	0.79
2:b:60:GLU:OE1	4:d:42:ILE:HD13	1.83	0.79
15:Y:37:DC:H2''	15:Y:38:DT:H71	1.63	0.78
7:J:18:SER:OG	8:k:24:CYS:SG	2.39	0.78
14:X:-69:DG:H2''	14:X:-68:DA:C8	2.18	0.78
10:n:42:ARG:NH2	13:t:890:LYS:O	2.16	0.78
11:O:31:GLU:O	11:O:35:GLU:HG2	1.83	0.78
1:A:18:THR:OG1	3:C:29:ASN:OD1	2.00	0.78
1:a:42:ILE:O	1:a:46:ILE:HG12	1.83	0.78
9:l:33:GLU:OE2	9:l:140:ARG:NH2	2.17	0.78
14:X:-37:DG:H2'	14:X:-37:DG:OP2	1.83	0.77
11:o:30:ILE:HB	11:o:34:ARG:HH21	1.50	0.77
10:N:14:ILE:HD13	10:N:26:VAL:HG11	1.66	0.77
6:I:155:ARG:NH1	6:I:192:CYS:SG	2.58	0.76
4:D:12:GLU:N	4:D:12:GLU:OE1	2.18	0.76
5:h:167:ARG:NH1	6:i:314:ALA:O	2.19	0.76
13:T:941:LYS:O	13:T:944:LYS:HG2	1.84	0.76
8:k:212:LYS:NZ	13:t:975:GLN:HG3	2.00	0.76
13:t:947:GLU:N	13:t:947:GLU:OE1	2.19	0.76
10:N:42:ARG:NH2	13:T:890:LYS:O	2.20	0.75
13:t:947:GLU:HG2	13:t:948:VAL:HG23	1.69	0.75
11:o:36:ASN:O	11:o:39:GLU:HG3	1.85	0.75
13:t:905:THR:HG23	13:t:910:TYR:HE2	1.52	0.74
8:k:169:PHE:CD2	8:k:195:ILE:HD12	2.22	0.74
5:H:16:GLN:HA	5:H:19:LYS:HZ3	1.51	0.74
13:T:915:ASP:OD1	13:T:916:LYS:N	2.21	0.74
13:T:817:LYS:HE2	13:T:817:LYS:HA	1.70	0.74
7:M:87:THR:OG1	7:M:118:SER:OG	2.06	0.74
11:O:43:GLU:O	11:O:47:LEU:HG	1.87	0.74
12:P:31:ILE:O	12:P:35:LEU:HG	1.87	0.74
13:t:916:LYS:HD3	13:t:966:ILE:HA	1.69	0.74
13:t:917:LEU:HD11	13:t:966:ILE:HD11	1.68	0.74
5:H:212:GLU:N	5:H:212:GLU:OE1	2.21	0.73
12:p:214:GLU:OE1	12:p:214:GLU:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:207:VAL:HG13	5:H:208:VAL:HG13	1.70	0.73
8:k:194:GLN:OE1	13:t:992:ASP:HA	1.87	0.73
7:J:70:SER:O	7:J:74:GLY:N	2.22	0.73
13:t:955:ASP:OD1	13:t:958:LYS:NZ	2.17	0.73
10:N:21:GLN:N	10:N:21:GLN:OE1	2.22	0.73
11:o:185:LEU:HD12	11:o:185:LEU:O	1.88	0.73
5:H:12:GLN:O	5:H:16:GLN:HG2	1.89	0.73
12:P:276:GLU:N	12:P:276:GLU:OE1	2.22	0.73
14:X:-59:DT:H2''	14:X:-58:DC:C5	2.24	0.73
14:X:-24:DT:C6	14:X:-23:DT:H72	2.23	0.73
6:i:166:LYS:CE	13:t:908:ARG:HD3	2.19	0.73
10:n:29:GLU:N	10:n:29:GLU:OE1	2.22	0.73
13:T:818:SER:O	13:T:821:GLU:HG3	1.89	0.72
5:H:139:ARG:NH1	6:I:527:GLU:OE1	2.22	0.72
14:X:-20:DC:H2''	14:X:-19:DG:C8	2.23	0.72
8:k:2:THR:HG21	12:p:41:ASN:HB2	1.69	0.72
13:t:1007:GLU:HB2	13:t:1010:SER:OG	1.88	0.72
6:I:34:VAL:HG22	6:I:39:LEU:HD23	1.71	0.72
14:X:-60:DA:H2'	14:X:-59:DT:H71	1.71	0.72
15:Y:45:DC:H2''	15:Y:46:DA:C8	2.25	0.72
11:O:42:ASN:O	11:O:46:GLN:HG2	1.90	0.72
11:O:207:GLN:HG2	11:O:279:ILE:HD12	1.72	0.72
12:P:15:LEU:HD12	12:P:16:GLU:N	2.05	0.72
12:P:26:TYR:O	12:P:30:ARG:HG2	1.90	0.72
2:b:30:SER:OG	11:o:76:ASN:OD1	2.07	0.72
11:o:37:LEU:HD11	12:p:23:ASN:OD1	1.89	0.72
5:H:142:GLU:OE1	6:I:528:LYS:NZ	2.16	0.72
11:o:37:LEU:HD22	12:p:20:LEU:HD13	1.71	0.72
13:t:895:LYS:HG2	13:t:896:ARG:H	1.55	0.72
6:i:34:VAL:HG22	6:i:39:LEU:HD23	1.71	0.71
1:A:41:GLU:OE1	1:A:41:GLU:N	2.22	0.71
5:H:16:GLN:O	5:H:20:GLN:HG2	1.91	0.71
10:N:29:GLU:N	10:N:29:GLU:OE1	2.23	0.71
10:N:147:SER:OG	10:N:150:LYS:O	2.03	0.71
5:H:35:GLU:OE1	5:H:35:GLU:N	2.23	0.71
11:O:31:GLU:O	11:O:34:ARG:HG2	1.90	0.71
15:Y:21:DC:H2'	15:Y:22:DC:C6	2.25	0.71
1:a:30:GLN:O	1:a:33:ILE:HG22	1.90	0.71
7:J:176:PRO:O	5:h:79:TYR:OH	2.09	0.70
5:h:205:ARG:NH2	6:i:160:GLU:OE2	2.24	0.70
11:O:273:VAL:HG13	11:O:274:GLY:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:59:ILE:HG22	12:P:60:ASP:H	1.56	0.70
1:a:29:LEU:HD13	2:b:41:ASP:OD1	1.90	0.70
6:I:75:GLU:N	6:I:75:GLU:OE1	2.25	0.70
11:O:64:GLU:N	11:O:64:GLU:OE1	2.24	0.70
11:O:262:GLN:N	11:O:262:GLN:OE1	2.23	0.70
15:Y:30:DT:C2'	15:Y:31:DT:H71	2.19	0.70
13:t:936:ILE:HD11	13:t:961:MET:HE1	1.74	0.70
6:I:139:GLN:N	6:I:139:GLN:OE1	2.24	0.70
12:P:163:GLU:OE1	12:P:185:TYR:OH	2.09	0.70
15:Y:39:DA:H1'	15:Y:40:DG:H5'	1.73	0.70
6:i:360:LEU:O	6:i:440:ARG:NH1	2.24	0.70
8:k:212:LYS:CE	13:t:975:GLN:HG3	2.21	0.70
11:O:29:GLU:O	11:O:32:LYS:HG2	1.91	0.70
11:O:151:GLU:N	11:O:151:GLU:OE1	2.23	0.70
13:T:959:HIS:O	13:T:963:ARG:HG3	1.91	0.70
11:o:31:GLU:O	11:o:34:ARG:HG2	1.90	0.70
8:K:2:THR:CG2	12:P:41:ASN:HB2	2.22	0.70
4:d:23:SER:O	4:d:26:SER:OG	2.09	0.70
6:i:75:GLU:N	6:i:75:GLU:OE1	2.25	0.70
6:i:166:LYS:HE2	13:t:908:ARG:HD3	1.73	0.70
11:O:37:LEU:HA	12:P:24:ILE:HD11	1.74	0.70
11:O:185:LEU:HD12	11:O:185:LEU:O	1.92	0.69
13:T:937:TYR:CE2	13:T:941:LYS:HE2	2.27	0.69
13:T:993:ILE:HD12	13:T:993:ILE:H	1.57	0.69
11:O:29:GLU:HA	11:O:32:LYS:HE2	1.73	0.69
11:O:36:ASN:O	11:O:39:GLU:HG3	1.92	0.69
11:O:60:LYS:NZ	12:P:51:SER:OG	2.17	0.69
2:b:68:HIS:CE1	11:o:41:GLN:HB3	2.28	0.69
6:I:640:PHE:HB3	13:T:816:LYS:HE3	1.74	0.69
8:k:63:ASN:ND2	8:k:65:ASN:OD1	2.25	0.69
12:P:38:LYS:NZ	12:P:40:THR:HA	2.05	0.69
12:P:30:ARG:O	12:P:33:GLU:HG2	1.91	0.69
8:k:169:PHE:HZ	8:k:199:LEU:HD11	1.56	0.69
13:t:905:THR:HG23	13:t:910:TYR:CE2	2.26	0.69
14:X:-28:DC:H2''	14:X:-27:DC:C6	2.27	0.69
5:h:60:VAL:O	5:h:63:THR:OG1	2.05	0.69
13:t:984:GLU:OE1	13:t:984:GLU:N	2.24	0.69
8:k:85:GLU:OE2	8:k:89:GLN:NE2	2.24	0.69
6:i:170:SER:OG	13:t:903:SER:HA	1.92	0.69
12:p:105:GLU:N	12:p:105:GLU:OE1	2.26	0.69
13:t:820:MET:O	13:t:824:MET:HG2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:t:897:TYR:CE2	13:t:899:PRO:HG3	2.28	0.69
5:H:5:LYS:O	5:H:8:LYS:HG2	1.93	0.68
5:H:197:GLU:OE1	8:K:219:TYR:OH	2.10	0.68
12:P:105:GLU:N	12:P:105:GLU:OE1	2.26	0.68
14:X:-50:DT:H2''	14:X:-49:DG:OP2	1.93	0.68
14:X:-30:DA:C8	14:X:-29:DT:H72	2.27	0.68
8:k:169:PHE:CZ	8:k:199:LEU:HD11	2.28	0.68
11:o:151:GLU:N	11:o:151:GLU:OE1	2.26	0.68
13:t:908:ARG:O	13:t:911:LYS:HG2	1.93	0.68
8:K:2:THR:HG21	12:P:41:ASN:HB2	1.74	0.68
11:o:47:LEU:HD12	12:p:31:ILE:CD1	2.23	0.68
9:L:182:ASP:OD1	9:L:183:THR:N	2.25	0.68
15:Y:42:DC:H2''	15:Y:43:DT:O5'	1.93	0.68
5:H:31:GLY:HA3	12:P:42:TYR:CD1	2.29	0.68
12:P:18:GLN:O	12:P:21:LEU:HG	1.93	0.68
13:T:954:VAL:O	13:T:958:LYS:HG3	1.94	0.68
15:Y:45:DC:H2''	15:Y:46:DA:N7	2.09	0.68
5:h:5:LYS:O	5:h:9:GLU:HG2	1.93	0.68
6:I:23:PHE:CE2	6:I:27:ILE:HD11	2.29	0.68
11:o:57:SER:HA	12:p:44:GLU:OE2	1.94	0.68
12:p:15:LEU:HD12	12:p:16:GLU:N	2.09	0.68
4:d:12:GLU:N	4:d:12:GLU:OE1	2.26	0.67
12:p:57:LEU:HD23	12:p:58:SER:N	2.09	0.67
9:L:41:VAL:HG22	9:L:161:ILE:HD12	1.76	0.67
1:a:22:LEU:O	1:a:25:ILE:HG22	1.94	0.67
12:p:16:GLU:O	12:p:20:LEU:HD23	1.94	0.67
13:t:952:ASP:O	13:t:956:VAL:HG23	1.94	0.67
5:H:60:VAL:O	5:H:63:THR:OG1	2.05	0.67
14:X:-63:DT:H2''	14:X:-62:DA:C8	2.28	0.67
13:t:916:LYS:CD	13:t:966:ILE:HA	2.25	0.67
1:A:20:GLN:NE2	11:O:67:VAL:O	2.26	0.67
13:T:985:ILE:O	13:T:989:VAL:HG12	1.95	0.67
15:Y:30:DT:H2''	15:Y:31:DT:O5'	1.94	0.67
6:i:52:LEU:HD12	6:i:85:TRP:CE3	2.30	0.67
14:X:-31:DA:H2''	14:X:-30:DA:H8	1.57	0.67
8:k:5:HIS:O	8:k:9:THR:HG23	1.95	0.67
13:t:936:ILE:HD11	13:t:961:MET:CE	2.23	0.67
14:X:-18:DG:H2'	14:X:-18:DG:OP2	1.95	0.67
5:h:16:GLN:O	5:h:20:GLN:HG2	1.95	0.67
5:h:34:PHE:H	12:p:41:ASN:HD21	1.42	0.67
11:O:47:LEU:CD1	12:P:31:ILE:HG23	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:k:152:HIS:O	8:k:155:ILE:HG22	1.95	0.67
11:o:29:GLU:HA	11:o:32:LYS:HE2	1.76	0.67
12:P:30:ARG:O	12:P:34:LEU:HD23	1.94	0.66
13:T:970:HIS:NE2	13:T:1008:ILE:HA	2.11	0.66
11:o:273:VAL:HG13	11:o:274:GLY:H	1.58	0.66
12:p:21:LEU:HD12	12:p:22:ASP:N	2.11	0.66
8:K:135:GLU:OE1	8:K:135:GLU:N	2.27	0.66
11:o:262:GLN:N	11:o:262:GLN:OE1	2.28	0.66
11:O:30:ILE:HG21	12:P:13:LEU:CD1	2.26	0.66
11:O:105:CYS:SG	11:O:156:MET:HE1	2.35	0.66
9:l:182:ASP:OD1	9:l:183:THR:N	2.29	0.66
2:B:68:HIS:CE1	11:O:41:GLN:HB3	2.30	0.66
13:T:917:LEU:HD21	13:T:966:ILE:HD11	1.77	0.66
5:h:207:VAL:HG13	5:h:208:VAL:HG13	1.76	0.66
11:o:64:GLU:N	11:o:64:GLU:OE1	2.25	0.66
12:P:153:VAL:HG21	12:P:178:VAL:HG21	1.78	0.66
14:X:-34:DA:H2''	14:X:-33:DG:H8	1.61	0.66
5:H:141:PHE:CZ	13:T:830:VAL:HG23	2.30	0.66
15:Y:67:DA:H2'	15:Y:68:DT:H71	1.77	0.66
11:O:47:LEU:HD11	12:P:31:ILE:HG23	1.77	0.66
14:X:-25:DC:H2''	14:X:-24:DT:C6	2.31	0.66
1:a:41:GLU:OE1	1:a:41:GLU:N	2.29	0.66
10:n:215:GLN:N	10:n:215:GLN:OE1	2.27	0.66
13:t:897:TYR:O	13:t:910:TYR:OH	2.13	0.66
10:N:38:PHE:CZ	13:T:889:MET:HA	2.30	0.65
11:O:55:LYS:HD3	11:O:56:SER:H	1.59	0.65
13:t:970:HIS:CD2	13:t:1008:ILE:HG13	2.31	0.65
8:K:194:GLN:HE21	13:T:992:ASP:HA	1.60	0.65
11:O:29:GLU:HG2	12:P:17:LYS:HZ1	1.60	0.65
13:T:899:PRO:HB2	13:T:902:ALA:HB2	1.78	0.65
9:l:250:ASP:OD2	9:l:252:THR:OG1	2.15	0.65
6:I:79:VAL:HG11	6:I:115:ILE:HD11	1.78	0.65
11:O:259:LYS:NZ	11:O:267:ASP:OD2	2.27	0.65
9:l:195:ARG:NH2	9:l:268:CYS:SG	2.69	0.65
13:t:918:GLU:OE1	13:t:922:ASP:HA	1.96	0.65
1:a:20:GLN:NE2	11:o:67:VAL:O	2.30	0.65
5:H:16:GLN:HA	5:H:19:LYS:NZ	2.11	0.65
15:Y:26:DG:H2''	15:Y:27:DG:C8	2.32	0.65
15:Y:47:DG:H4'	13:t:900:LYS:HD3	1.79	0.65
12:p:27:CYS:O	12:p:31:ILE:HG12	1.97	0.65
5:H:27:SER:HB2	11:O:56:SER:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:249:LEU:HD12	11:O:252:GLN:NE2	2.12	0.65
15:Y:36:DC:H2''	15:Y:37:DC:C6	2.31	0.65
13:t:914:GLU:OE2	13:t:926:ARG:HA	1.97	0.65
10:n:176:GLN:N	10:n:176:GLN:OE1	2.30	0.65
12:P:224:LEU:HD21	12:P:252:MET:CG	2.27	0.65
14:X:-34:DA:H2''	14:X:-33:DG:C8	2.31	0.65
15:Y:67:DA:C8	15:Y:67:DA:H5'	2.32	0.65
10:n:138:LEU:HD11	10:n:199:ILE:HG21	1.79	0.65
13:T:929:ALA:O	13:T:933:VAL:HG23	1.97	0.64
13:T:947:GLU:N	13:T:947:GLU:OE1	2.27	0.64
11:O:29:GLU:HB2	11:O:32:LYS:HE2	1.79	0.64
15:Y:15:DT:H2''	15:Y:16:DA:C8	2.31	0.64
5:h:19:LYS:HA	5:h:19:LYS:HE3	1.79	0.64
12:P:113:SER:OG	12:P:140:ASP:OD2	2.14	0.64
14:X:-36:DG:H2''	14:X:-35:DG:N7	2.13	0.64
6:I:488:ILE:HD12	6:I:529:MET:HE1	1.79	0.64
10:n:9:ASP:OD1	10:n:10:LEU:N	2.31	0.64
14:X:-62:DA:H2'	14:X:-61:DT:C7	2.20	0.64
13:T:909:LEU:HD23	13:T:913:LEU:HG	1.80	0.64
6:I:566:ASP:OD2	6:I:584:VAL:N	2.30	0.64
13:T:904:TRP:O	13:T:906:THR:HG23	1.96	0.64
5:H:198:MET:CE	8:K:217:LEU:HD21	2.28	0.64
10:N:280:MET:HE3	10:N:282:ILE:HD11	1.78	0.64
13:T:984:GLU:OE1	13:T:984:GLU:N	2.24	0.64
5:h:12:GLN:O	5:h:15:GLU:HG2	1.97	0.64
12:p:276:GLU:N	12:p:276:GLU:OE1	2.30	0.64
13:t:957:LEU:O	13:t:961:MET:HG2	1.98	0.64
8:K:214:GLU:N	8:K:214:GLU:OE1	2.31	0.64
11:O:112:GLN:OE1	12:P:176:SER:OG	2.05	0.64
5:h:142:GLU:OE1	6:i:528:LYS:NZ	2.19	0.64
10:N:42:ARG:CZ	13:T:891:TYR:HB2	2.28	0.63
5:h:120:ARG:NH1	8:k:77:SER:OG	2.30	0.63
12:p:14:LEU:HD12	12:p:15:LEU:N	2.13	0.63
13:t:820:MET:HE3	13:t:824:MET:CE	2.29	0.63
11:O:37:LEU:HA	12:P:24:ILE:CD1	2.29	0.63
3:c:17:GLU:O	3:c:20:MET:N	2.30	0.63
12:p:281:LEU:O	12:p:284:ILE:HG22	1.98	0.63
13:t:1003:GLY:O	13:t:1006:SER:OG	2.15	0.63
1:A:20:GLN:NE2	11:O:66:PHE:HB2	2.14	0.63
6:I:134:GLU:N	6:I:134:GLU:OE1	2.31	0.63
7:J:132:LEU:HD21	7:J:143:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:249:LEU:HD12	11:O:252:GLN:HE21	1.63	0.63
6:i:48:PHE:O	6:i:52:LEU:HD23	1.98	0.63
5:H:140:HIS:HB3	13:T:830:VAL:HG11	1.78	0.63
12:P:164:LEU:HD23	12:P:169:LEU:HD22	1.81	0.63
9:L:143:GLN:OE1	9:L:143:GLN:N	2.32	0.63
12:P:14:LEU:HD12	12:P:15:LEU:N	2.12	0.63
13:t:993:ILE:HD12	13:t:993:ILE:H	1.64	0.63
11:o:27:GLN:N	11:o:29:GLU:OE1	2.32	0.63
11:o:42:ASN:O	11:o:46:GLN:HG2	1.99	0.63
13:t:970:HIS:HD2	13:t:1008:ILE:HG13	1.62	0.63
5:H:133:ASP:OD1	13:T:822:LYS:HE3	1.99	0.63
12:P:281:LEU:O	12:P:284:ILE:HG22	1.98	0.63
15:Y:54:DG:H2'	15:Y:55:DT:H72	1.81	0.63
11:o:29:GLU:O	11:o:33:LEU:HD23	1.98	0.63
11:o:185:LEU:HD13	11:o:189:ALA:HB3	1.80	0.63
8:k:155:ILE:HD11	8:k:166:ILE:HG22	1.81	0.63
1:A:33:ILE:HG13	2:B:45:ILE:HG12	1.80	0.62
12:P:40:THR:HG23	12:P:42:TYR:CE2	2.34	0.62
15:Y:49:DC:H2''	15:Y:50:DA:C8	2.34	0.62
15:Y:61:DA:C8	15:Y:62:DT:H72	2.34	0.62
15:Y:64:DT:H2''	15:Y:65:DA:C8	2.34	0.62
10:n:17:MET:HE1	10:n:26:VAL:HG13	1.79	0.62
2:b:43:LEU:HD12	12:p:99:VAL:HG13	1.81	0.62
12:p:58:SER:O	12:p:59:ILE:HD13	1.99	0.62
15:Y:29:DA:C8	15:Y:30:DT:H72	2.34	0.62
13:t:963:ARG:HG3	13:t:964:LEU:CD2	2.29	0.62
11:O:45:PHE:CE2	11:O:49:ARG:HD2	2.35	0.62
12:p:30:ARG:O	12:p:34:LEU:HD23	2.00	0.62
11:o:27:GLN:N	11:o:27:GLN:OE1	2.32	0.62
13:T:1007:GLU:OE1	13:T:1009:LEU:N	2.29	0.62
15:Y:49:DC:H2''	15:Y:50:DA:H8	1.64	0.62
13:t:910:TYR:O	13:t:914:GLU:HG2	2.00	0.62
7:M:70:SER:O	7:M:74:GLY:N	2.32	0.62
12:P:15:LEU:O	12:P:18:GLN:HG3	2.00	0.62
13:T:896:ARG:HB2	13:T:898:GLN:OE1	1.99	0.62
14:X:-17:DT:H3	15:Y:17:DA:H61	1.48	0.62
15:Y:35:DC:H2''	15:Y:36:DC:C6	2.34	0.62
6:i:636:TRP:O	13:t:816:LYS:NZ	2.25	0.62
13:t:986:ARG:O	13:t:990:VAL:HG12	2.00	0.62
6:I:566:ASP:OD2	6:I:583:PHE:N	2.33	0.62
12:P:58:SER:O	12:P:59:ILE:HD13	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:566:ASP:OD2	6:i:583:PHE:N	2.29	0.62
13:t:909:LEU:O	13:t:913:LEU:HG	1.99	0.62
14:X:-25:DC:C2'	14:X:-24:DT:H71	2.30	0.62
13:T:943:VAL:HG12	13:T:988:LYS:HD2	1.80	0.61
14:X:-17:DT:H4'	14:X:-16:DT:OP1	1.99	0.61
13:T:916:LYS:HD3	13:T:966:ILE:HA	1.82	0.61
13:t:1008:ILE:HD12	13:t:1008:ILE:H	1.65	0.61
6:I:385:GLU:N	6:I:385:GLU:OE1	2.33	0.61
10:N:19:LEU:HD13	10:N:50:ALA:HA	1.81	0.61
5:h:188:ARG:O	5:h:192:LEU:HD23	1.99	0.61
10:n:79:LEU:HD13	10:n:142:SER:OG	2.00	0.61
10:N:66:GLU:OE1	10:N:66:GLU:N	2.33	0.61
15:Y:16:DA:H1'	15:Y:17:DA:C8	2.36	0.61
4:D:52:GLU:OE2	4:D:56:ARG:NE	2.33	0.61
11:O:146:ASN:OD1	11:O:147:ALA:N	2.34	0.61
14:X:-25:DC:H2''	14:X:-24:DT:H71	1.81	0.61
5:h:136:THR:HG22	13:t:826:ILE:HD13	1.81	0.61
6:i:149:LYS:N	6:i:152:ASP:OD2	2.30	0.61
6:i:385:GLU:N	6:i:385:GLU:OE1	2.34	0.61
12:p:31:ILE:O	12:p:35:LEU:HG	2.00	0.61
13:t:928:ARG:HH11	13:t:931:LYS:HD3	1.66	0.61
5:H:15:GLU:O	5:H:19:LYS:HG3	2.00	0.61
11:O:30:ILE:HG13	11:O:34:ARG:HH21	1.65	0.61
11:O:185:LEU:HD13	11:O:189:ALA:HB3	1.82	0.61
6:I:412:TYR:CG	6:I:469:MET:HE3	2.35	0.61
11:O:54:HIS:NE2	12:P:42:TYR:HB3	2.16	0.61
14:X:-33:DG:H2'	14:X:-32:DT:H71	1.82	0.61
15:Y:37:DC:H2''	15:Y:38:DT:H73	1.83	0.61
11:o:44:LEU:HB2	12:p:31:ILE:HD11	1.83	0.61
6:i:134:GLU:OE1	6:i:134:GLU:N	2.34	0.61
6:i:419:GLU:N	6:i:419:GLU:OE1	2.31	0.61
15:Y:35:DC:H2''	15:Y:36:DC:C5	2.36	0.60
11:O:127:MET:SD	11:O:156:MET:HE3	2.41	0.60
11:O:153:ASP:OD1	11:O:154:ASN:N	2.33	0.60
12:P:54:GLY:O	12:P:56:THR:HG22	2.01	0.60
14:X:-19:DG:H2''	14:X:-18:DG:C8	2.35	0.60
12:p:191:SER:OG	12:p:274:THR:HG22	2.01	0.60
7:M:71:ASP:OD1	7:M:72:LEU:N	2.33	0.60
12:p:22:ASP:O	12:p:25:VAL:HG12	2.02	0.60
4:D:75:VAL:O	4:D:79:THR:OG1	2.15	0.60
11:O:139:LEU:HD11	11:O:145:ILE:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:191:SER:OG	12:P:274:THR:HG22	2.02	0.60
12:P:247:PHE:CE2	12:P:284:ILE:HD13	2.35	0.60
12:p:15:LEU:O	12:p:18:GLN:HG3	2.00	0.60
13:t:907:LYS:HA	13:t:910:TYR:HD2	1.65	0.60
13:t:983:ARG:O	13:t:986:ARG:HG2	2.02	0.60
13:T:822:LYS:O	13:T:826:ILE:HG12	2.02	0.60
6:I:453:GLU:OE1	6:I:453:GLU:N	2.35	0.60
10:N:176:GLN:N	10:N:176:GLN:OE1	2.35	0.60
12:P:12:THR:HA	12:P:15:LEU:HD21	1.82	0.60
1:A:45:ASN:ND2	3:C:50:ASN:OD1	2.34	0.60
14:X:-24:DT:H2'	14:X:-23:DT:H72	1.83	0.60
15:Y:27:DG:H2''	15:Y:28:DG:C8	2.37	0.60
13:T:908:ARG:HH11	13:T:980:PHE:HZ	1.48	0.60
14:X:-32:DT:H2''	14:X:-31:DA:OP2	2.02	0.60
9:L:182:ASP:OD1	9:L:184:SER:N	2.33	0.59
11:O:190:GLN:OE1	11:O:190:GLN:N	2.35	0.59
12:P:18:GLN:HA	12:P:21:LEU:CD2	2.32	0.59
13:T:969:THR:HA	13:T:1007:GLU:HA	1.83	0.59
1:a:25:ILE:HD11	3:c:35:TYR:CE2	2.37	0.59
13:t:974:TYR:CE1	13:t:991:PRO:HD3	2.37	0.59
11:O:114:ASP:OD1	12:P:174:ARG:NH2	2.35	0.59
11:O:224:TYR:OH	11:O:261:LEU:HD21	2.02	0.59
14:X:-60:DA:C2'	14:X:-59:DT:H71	2.31	0.59
8:K:151:LEU:O	8:K:155:ILE:HG13	2.00	0.59
13:T:896:ARG:O	13:T:898:GLN:NE2	2.35	0.59
14:X:-58:DC:H2''	14:X:-57:DT:OP2	2.02	0.59
8:K:63:ASN:ND2	8:K:65:ASN:OD1	2.35	0.59
14:X:-46:DT:H2''	14:X:-45:DG:C8	2.38	0.59
12:p:57:LEU:HD22	12:p:59:ILE:HD11	1.84	0.59
3:C:38:HIS:CG	5:H:18:LEU:HD11	2.37	0.59
15:Y:19:DC:H2''	15:Y:20:DG:C8	2.37	0.59
13:t:951:ASN:O	13:t:954:VAL:HG12	2.03	0.59
4:d:47:LYS:HZ3	5:h:30:ILE:HA	1.67	0.59
9:l:182:ASP:O	9:l:215:ARG:NH2	2.35	0.59
12:P:12:THR:HA	12:P:15:LEU:CD2	2.32	0.59
13:T:896:ARG:HD3	13:T:926:ARG:CZ	2.32	0.59
12:p:38:LYS:NZ	12:p:40:THR:HA	2.18	0.59
7:M:85:LEU:O	7:M:117:THR:OG1	2.20	0.59
11:O:29:GLU:O	11:O:33:LEU:HD23	2.03	0.59
11:O:62:LYS:HE3	11:O:63:SER:O	2.03	0.59
14:X:-68:DA:H2''	14:X:-67:DT:C6	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:141:PHE:CE1	13:T:830:VAL:HG23	2.38	0.58
2:b:41:ASP:O	2:b:45:ILE:HG13	2.03	0.58
5:h:42:LEU:HD21	8:k:74:LEU:HD11	1.86	0.58
6:i:521:VAL:HG22	6:i:521:VAL:O	2.02	0.58
3:c:49:MET:HE3	4:d:43:ASN:HB2	1.84	0.58
6:i:52:LEU:HD11	6:i:102:LEU:HD12	1.85	0.58
5:H:193:VAL:HG21	5:H:232:ASP:C	2.28	0.58
8:K:24:CYS:HG	7:M:18:SER:HG	0.60	0.58
15:Y:67:DA:C2'	15:Y:68:DT:H71	2.34	0.58
15:Y:69:DC:H2''	15:Y:70:DG:OP2	2.03	0.58
11:O:207:GLN:CG	11:O:279:ILE:HD12	2.33	0.58
14:X:-33:DG:C2'	14:X:-32:DT:H71	2.32	0.58
13:T:888:ASP:OD1	13:T:890:LYS:NZ	2.24	0.58
13:T:904:TRP:HB2	13:T:980:PHE:O	2.03	0.58
14:X:-59:DT:H2'	14:X:-59:DT:OP2	2.03	0.58
11:o:37:LEU:HA	12:p:24:ILE:HD11	1.85	0.58
13:t:825:ARG:O	13:t:829:GLU:HG3	2.03	0.58
14:X:-38:DA:H2''	14:X:-37:DG:C8	2.39	0.58
11:O:29:GLU:CA	11:O:32:LYS:HE2	2.34	0.58
12:p:41:ASN:OD1	12:p:42:TYR:N	2.37	0.58
3:C:18:LEU:HB3	3:C:19:PRO:HD3	1.86	0.57
15:Y:67:DA:H2''	15:Y:68:DT:OP2	2.03	0.57
11:o:29:GLU:HA	11:o:32:LYS:HG2	1.86	0.57
13:t:929:ALA:O	13:t:933:VAL:HG23	2.04	0.57
13:T:917:LEU:HD13	13:T:928:ARG:CG	2.34	0.57
14:X:-55:DA:OP1	13:t:892:LYS:NZ	2.37	0.57
15:Y:34:DT:H2''	15:Y:35:DC:C6	2.39	0.57
15:Y:43:DT:H2''	15:Y:44:DC:OP2	2.05	0.57
6:I:166:LYS:O	13:T:906:THR:HG21	2.04	0.57
6:I:170:SER:OG	13:T:903:SER:HA	2.03	0.57
9:L:289:GLU:OE1	9:L:289:GLU:N	2.37	0.57
11:O:40:LYS:O	11:O:43:GLU:HG2	2.04	0.57
12:P:21:LEU:HD12	12:P:22:ASP:N	2.19	0.57
15:Y:53:DT:H2''	15:Y:54:DG:H8	1.69	0.57
11:o:68:ARG:HE	11:o:69:PRO:HD2	1.69	0.57
12:p:12:THR:HA	12:p:15:LEU:HD21	1.86	0.57
13:t:906:THR:O	13:t:907:LYS:HB2	2.05	0.57
6:I:521:VAL:HG22	6:I:521:VAL:O	2.05	0.57
13:T:827:GLU:OE2	13:T:831:ARG:NH2	2.37	0.57
14:X:-57:DT:H2''	14:X:-56:DG:C8	2.39	0.57
15:Y:29:DA:H2''	15:Y:30:DT:OP2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:104:ASP:OD1	6:i:209:ILE:HD12	2.04	0.57
13:t:831:ARG:O	13:t:834:LEU:HG	2.04	0.57
13:t:963:ARG:HG3	13:t:964:LEU:HD23	1.86	0.57
10:N:246:ILE:HD12	10:N:309:PHE:CZ	2.38	0.57
11:O:37:LEU:CA	12:P:24:ILE:HD11	2.35	0.57
13:T:916:LYS:CD	13:T:966:ILE:HA	2.34	0.57
14:X:-22:DG:H2''	14:X:-21:DG:H8	1.70	0.57
15:Y:53:DT:H2''	15:Y:54:DG:C8	2.40	0.57
11:o:31:GLU:O	11:o:35:GLU:HG2	2.03	0.57
13:t:899:PRO:HB2	13:t:902:ALA:HB2	1.87	0.57
11:O:30:ILE:HG21	12:P:13:LEU:HD11	1.87	0.57
10:n:45:ARG:CD	13:t:894:PRO:HD2	2.35	0.57
13:t:993:ILE:HD12	13:t:993:ILE:N	2.20	0.57
11:O:31:GLU:HA	11:O:34:ARG:HE	1.68	0.57
11:O:165:ARG:NH2	12:P:180:GLU:OE1	2.38	0.57
5:H:104:LYS:O	5:H:108:THR:OG1	2.23	0.57
11:O:36:ASN:O	11:O:40:LYS:HG2	2.05	0.57
13:T:957:LEU:HD22	13:T:973:PHE:CZ	2.40	0.57
5:h:15:GLU:O	5:h:19:LYS:HG2	2.04	0.57
13:t:960:GLU:O	13:t:963:ARG:HG2	2.05	0.57
13:t:990:VAL:O	13:t:995:ASN:ND2	2.38	0.57
11:O:211:GLU:OE1	11:O:212:GLU:N	2.37	0.56
12:P:11:LYS:O	12:P:14:LEU:HG	2.05	0.56
15:Y:42:DC:H2'	15:Y:43:DT:H71	1.86	0.56
6:i:566:ASP:OD2	6:i:584:VAL:N	2.37	0.56
13:t:937:TYR:O	13:t:940:THR:HG22	2.04	0.56
1:A:65:GLU:N	1:A:65:GLU:OE1	2.38	0.56
13:T:817:LYS:HE2	13:T:817:LYS:CA	2.33	0.56
10:n:19:LEU:HD13	10:n:50:ALA:HA	1.86	0.56
11:o:44:LEU:HA	12:p:31:ILE:HD11	1.88	0.56
7:J:79:ASP:OD2	7:J:169:ILE:HD11	2.05	0.56
15:Y:42:DC:H2'	15:Y:43:DT:C6	2.40	0.56
8:k:175:ALA:O	8:k:179:ASN:ND2	2.38	0.56
9:l:182:ASP:OD1	9:l:184:SER:N	2.38	0.56
12:p:199:LEU:HD11	12:p:281:LEU:HD13	1.87	0.56
5:H:188:ARG:O	5:H:192:LEU:HD23	2.05	0.56
13:T:928:ARG:HH22	13:T:931:LYS:HE2	1.68	0.56
15:Y:48:DG:H2''	15:Y:49:DC:C6	2.41	0.56
8:k:187:GLN:NE2	8:k:188:ILE:O	2.39	0.56
13:T:932:LEU:O	13:T:936:ILE:HG13	2.05	0.56
15:Y:27:DG:H2''	15:Y:28:DG:N7	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:o:27:GLN:O	11:o:30:ILE:HG12	2.06	0.56
11:o:44:LEU:O	11:o:48:GLN:HG2	2.05	0.56
13:t:916:LYS:HD2	13:t:966:ILE:HD13	1.86	0.56
4:d:18:ILE:O	4:d:22:ILE:HG12	2.05	0.56
13:t:928:ARG:HH11	13:t:931:LYS:CD	2.19	0.56
7:M:73:THR:HA	12:P:59:ILE:HD12	1.86	0.56
11:O:36:ASN:HD21	11:O:40:LYS:HE3	1.71	0.56
6:i:453:GLU:N	6:i:453:GLU:OE1	2.38	0.56
10:N:71:ASN:OD1	10:N:72:ASP:N	2.39	0.56
15:Y:47:DG:C5'	13:t:900:LYS:HE2	2.32	0.56
13:T:906:THR:O	13:T:907:LYS:HB3	2.05	0.56
9:l:48:GLN:N	9:l:48:GLN:OE1	2.39	0.56
10:n:61:ILE:O	10:n:65:LEU:HD22	2.05	0.56
13:t:888:ASP:O	13:t:889:MET:HG2	2.05	0.56
1:A:20:GLN:CD	11:O:66:PHE:HB2	2.31	0.56
5:H:31:GLY:HA3	12:P:42:TYR:CE1	2.41	0.56
8:K:188:ILE:HG22	8:K:213:MET:O	2.06	0.56
15:Y:38:DT:H2''	15:Y:39:DA:N7	2.21	0.56
6:i:34:VAL:HG12	6:i:219:ARG:HH22	1.71	0.56
11:o:186:ASN:OD1	11:o:187:VAL:N	2.39	0.56
12:p:12:THR:HA	12:p:15:LEU:CD2	2.36	0.56
13:t:827:GLU:O	13:t:831:ARG:HG2	2.06	0.56
5:h:136:THR:CG2	13:t:826:ILE:HD13	2.36	0.55
10:n:246:ILE:HD12	10:n:309:PHE:CZ	2.40	0.55
6:I:317:ASP:OD1	6:I:318:GLN:N	2.39	0.55
7:J:73:THR:HA	12:p:59:ILE:HD12	1.89	0.55
11:O:28:ASP:HA	11:O:31:GLU:OE1	2.05	0.55
11:O:29:GLU:CB	11:O:32:LYS:HE2	2.36	0.55
13:T:993:ILE:HD12	13:T:993:ILE:N	2.20	0.55
14:X:-19:DG:H22	15:Y:19:DC:H42	1.52	0.55
13:t:940:THR:HA	13:t:943:VAL:HG12	1.87	0.55
6:I:562:ARG:NH2	6:I:580:GLY:O	2.39	0.55
11:o:67:VAL:HG22	11:o:68:ARG:H	1.71	0.55
13:t:978:HIS:HB2	13:t:986:ARG:NH2	2.19	0.55
13:T:1001:ARG:HH12	10:n:33:LYS:NZ	2.03	0.55
11:o:48:GLN:O	11:o:51:SER:OG	2.21	0.55
11:O:195:LEU:O	11:O:196:ASP:OD1	2.24	0.55
12:P:22:ASP:O	12:P:25:VAL:HG12	2.06	0.55
5:h:9:GLU:O	5:h:12:GLN:HG3	2.07	0.55
13:t:978:HIS:HA	13:t:986:ARG:HE	1.70	0.55
10:N:229:LEU:HD11	12:P:59:ILE:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:56:DC:H2''	15:Y:57:DA:N7	2.21	0.55
8:k:166:ILE:HA	8:k:169:PHE:CE2	2.42	0.55
5:H:31:GLY:HA3	12:P:42:TYR:HD1	1.71	0.55
10:n:134:LEU:HD11	11:o:192:PHE:CE1	2.41	0.55
3:C:15:ALA:O	3:C:19:PRO:HD2	2.05	0.55
11:O:68:ARG:HG3	11:O:69:PRO:HD2	1.89	0.55
13:T:939:PHE:CG	13:T:957:LEU:HD12	2.41	0.55
13:T:961:MET:HE3	13:T:966:ILE:CG2	2.37	0.55
14:X:-39:DT:H2''	14:X:-38:DA:N7	2.22	0.55
6:I:220:THR:HG22	6:I:223:ARG:HH21	1.72	0.55
14:X:-24:DT:H2'	14:X:-23:DT:C7	2.37	0.55
11:o:31:GLU:HA	11:o:34:ARG:CD	2.37	0.55
11:o:196:ASP:OD1	11:o:196:ASP:O	2.25	0.55
12:p:30:ARG:O	12:p:33:GLU:HG2	2.06	0.55
12:p:59:ILE:HG22	12:p:60:ASP:N	2.22	0.55
10:N:132:THR:HG23	10:N:139:LEU:HD11	1.89	0.54
6:i:528:LYS:O	6:i:532:LEU:HD23	2.08	0.54
11:o:44:LEU:CA	12:p:31:ILE:HD11	2.37	0.54
12:p:33:GLU:HG3	12:p:34:LEU:HD22	1.90	0.54
12:p:274:THR:O	12:p:278:THR:HG23	2.07	0.54
11:O:196:ASP:OD1	11:O:196:ASP:O	2.25	0.54
13:t:913:LEU:O	13:t:917:LEU:HD13	2.07	0.54
13:t:1008:ILE:HD12	13:t:1008:ILE:N	2.22	0.54
10:N:45:ARG:CD	13:T:894:PRO:HG2	2.37	0.54
13:T:928:ARG:NH2	13:T:931:LYS:HB3	2.22	0.54
13:T:957:LEU:HD22	13:T:973:PHE:HZ	1.73	0.54
13:T:993:ILE:C	13:T:996:LYS:HE3	2.32	0.54
14:X:-56:DG:H2''	14:X:-55:DA:N7	2.22	0.54
5:h:49:SER:OG	5:h:53:LYS:NZ	2.40	0.54
6:i:10:TYR:OH	6:i:19:ASP:OD1	2.25	0.54
6:i:481:MET:N	8:k:89:GLN:OE1	2.37	0.54
10:n:166:ALA:C	10:n:167:LEU:HD12	2.31	0.54
11:o:195:LEU:O	11:o:196:ASP:OD1	2.25	0.54
12:p:11:LYS:O	12:p:14:LEU:HG	2.06	0.54
9:L:41:VAL:HG22	9:L:161:ILE:CD1	2.38	0.54
13:T:909:LEU:HD23	13:T:909:LEU:O	2.07	0.54
10:N:26:VAL:HG12	10:N:77:LEU:HD13	1.88	0.54
5:H:21:LEU:HA	5:H:24:VAL:HG12	1.90	0.54
6:I:104:ASP:O	6:I:107:THR:OG1	2.18	0.54
12:P:103:GLU:OE1	12:P:103:GLU:N	2.32	0.54
14:X:-69:DG:H2''	14:X:-68:DA:N7	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:-51:DG:H2''	14:X:-50:DT:OP2	2.08	0.54
14:X:-27:DC:H1'	14:X:-26:DC:C5	2.43	0.54
5:h:217:PRO:HD3	6:i:88:ILE:HD11	1.90	0.54
6:i:96:PHE:HD1	6:i:136:LEU:HD11	1.73	0.54
6:i:521:VAL:HG23	6:i:613:VAL:HG12	1.89	0.54
11:o:153:ASP:OD1	11:o:154:ASN:N	2.41	0.54
3:C:38:HIS:CB	5:H:18:LEU:HD11	2.37	0.54
6:I:488:ILE:HD12	6:I:529:MET:CE	2.38	0.54
10:N:166:ALA:C	10:N:167:LEU:HD12	2.32	0.54
13:T:937:TYR:CZ	13:T:941:LYS:HE2	2.42	0.54
14:X:-52:DC:OP2	6:i:172:LYS:NZ	2.41	0.54
15:Y:68:DT:H2''	15:Y:69:DC:C5	2.43	0.54
1:a:17:THR:O	1:a:21:LEU:HD23	2.07	0.54
13:t:943:VAL:CG2	13:t:949:ALA:HB2	2.38	0.54
9:l:42:SER:OG	9:l:160:ASN:N	2.37	0.54
11:O:37:LEU:O	11:O:41:GLN:HG3	2.07	0.54
14:X:-52:DC:H2''	14:X:-51:DG:OP2	2.07	0.54
4:d:56:ARG:O	4:d:60:LEU:HD23	2.06	0.54
12:p:249:LEU:HD21	12:p:260:ILE:HG21	1.90	0.54
4:D:32:LEU:O	4:D:32:LEU:HD23	2.08	0.54
14:X:-61:DT:H2''	14:X:-60:DA:H5'	1.90	0.54
15:Y:21:DC:H2''	15:Y:22:DC:C5'	2.38	0.54
3:c:63:TRP:CE2	4:d:57:LEU:HD21	2.42	0.54
7:J:132:LEU:HD23	7:J:136:TYR:CD2	2.43	0.53
10:N:112:GLU:N	10:N:112:GLU:OE1	2.39	0.53
15:Y:47:DG:H4'	13:t:900:LYS:CD	2.38	0.53
6:i:353:ALA:HB2	6:i:389:LEU:HD22	1.91	0.53
6:i:399:ASP:OD1	6:i:400:HIS:N	2.41	0.53
5:H:234:ASP:OD1	5:H:235:THR:N	2.40	0.53
14:X:-37:DG:H2''	14:X:-36:DG:C8	2.43	0.53
9:l:84:LEU:HD22	9:l:87:LEU:HD11	1.89	0.53
9:l:143:GLN:O	9:l:147:THR:HG23	2.09	0.53
13:t:958:LYS:HG2	13:t:973:PHE:CD2	2.43	0.53
13:T:993:ILE:O	13:T:996:LYS:HE3	2.08	0.53
13:T:999:ILE:HG23	13:T:1000:PRO:HD2	1.91	0.53
15:Y:64:DT:H2''	15:Y:65:DA:H8	1.72	0.53
1:a:25:ILE:HD11	3:c:35:TYR:HE2	1.72	0.53
10:n:42:ARG:CZ	13:t:891:TYR:HB2	2.38	0.53
2:B:60:GLU:OE1	4:D:42:ILE:HG12	2.08	0.53
4:D:44:LEU:HD21	11:O:49:ARG:O	2.09	0.53
13:T:986:ARG:HA	13:T:989:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:t:1000:PRO:HG2	13:t:1004:VAL:HA	1.91	0.53
12:P:224:LEU:HD23	12:P:224:LEU:C	2.33	0.53
2:b:68:HIS:ND1	11:o:41:GLN:HB3	2.22	0.53
10:n:66:GLU:N	10:n:66:GLU:OE1	2.41	0.53
11:o:251:GLU:O	11:o:254:THR:HG22	2.08	0.53
12:p:18:GLN:HA	12:p:21:LEU:CD2	2.39	0.53
12:p:38:LYS:HZ3	12:p:40:THR:HA	1.71	0.53
12:p:54:GLY:O	12:p:56:THR:HG22	2.08	0.53
3:C:50:ASN:O	3:C:54:ARG:HG3	2.08	0.53
14:X:-22:DG:H2''	14:X:-21:DG:C8	2.44	0.53
6:i:21:ASP:OD1	6:i:22:LEU:N	2.42	0.53
11:o:29:GLU:O	11:o:32:LYS:HG2	2.09	0.53
13:t:966:ILE:HG22	13:t:967:VAL:HG13	1.91	0.53
13:t:973:PHE:CZ	13:t:977:PHE:HE2	2.27	0.53
7:J:166:GLU:OE2	7:J:172:ARG:NH1	2.38	0.53
12:P:57:LEU:HG	12:P:59:ILE:HD11	1.91	0.53
13:T:939:PHE:O	13:T:943:VAL:HG23	2.09	0.53
13:T:957:LEU:O	13:T:957:LEU:HD23	2.08	0.53
12:P:27:CYS:O	12:P:31:ILE:HG13	2.08	0.53
8:k:14:LYS:HE2	12:p:47:ASP:HB2	1.91	0.53
12:p:26:TYR:OH	12:p:30:ARG:NH1	2.42	0.53
13:t:967:VAL:HG12	13:t:972:ASP:OD2	2.09	0.53
14:X:-30:DA:H8	14:X:-30:DA:OP2	1.92	0.53
13:t:961:MET:CB	13:t:967:VAL:HG22	2.38	0.53
11:O:62:LYS:HD2	11:O:63:SER:N	2.24	0.52
6:i:26:LYS:NZ	6:i:29:GLU:OE2	2.42	0.52
13:T:827:GLU:O	13:T:830:VAL:HG12	2.09	0.52
14:X:-20:DC:H2''	14:X:-19:DG:N7	2.23	0.52
10:n:39:ARG:O	10:n:43:LEU:HD13	2.09	0.52
11:o:32:LYS:HG3	11:o:33:LEU:HD22	1.91	0.52
12:p:12:THR:O	12:p:15:LEU:HG	2.09	0.52
12:p:224:LEU:HD21	12:p:252:MET:HB2	1.90	0.52
13:t:958:LYS:C	13:t:1008:ILE:HG21	2.33	0.52
13:t:961:MET:HB3	13:t:967:VAL:HG22	1.91	0.52
7:J:87:THR:HG1	7:J:118:SER:HG	1.48	0.52
9:L:143:GLN:O	9:L:147:THR:HG23	2.09	0.52
11:O:45:PHE:CZ	11:O:49:ARG:HD2	2.45	0.52
14:X:-52:DC:OP2	14:X:-52:DC:H2'	2.09	0.52
13:t:999:ILE:HG13	13:t:1000:PRO:HD2	1.91	0.52
7:J:71:ASP:OD1	7:J:72:LEU:N	2.42	0.52
10:N:73:ILE:HG22	10:N:76:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:983:ARG:HG3	13:T:986:ARG:CZ	2.39	0.52
15:Y:41:DT:H2''	15:Y:42:DC:C6	2.45	0.52
2:b:39:ASN:O	2:b:43:LEU:HD23	2.10	0.52
6:i:356:GLN:NE2	6:i:366:ILE:HG21	2.24	0.52
4:D:69:ARG:O	4:D:70:SER:OG	2.11	0.52
7:J:127:ILE:HD11	7:J:132:LEU:HD12	1.89	0.52
8:K:164:ALA:O	8:K:167:ILE:HG22	2.09	0.52
13:T:896:ARG:HA	13:T:930:GLU:OE2	2.09	0.52
13:T:936:ILE:O	13:T:940:THR:HG23	2.10	0.52
13:T:966:ILE:N	13:T:966:ILE:HD12	2.24	0.52
15:Y:28:DG:H2''	15:Y:29:DA:C8	2.44	0.52
6:i:74:VAL:N	6:i:114:CYS:O	2.42	0.52
6:i:166:LYS:HE3	13:t:908:ARG:HD3	1.90	0.52
13:t:899:PRO:HB2	13:t:902:ALA:CB	2.39	0.52
13:t:932:LEU:O	13:t:935:THR:HG22	2.09	0.52
6:I:386:ILE:O	6:I:390:VAL:HG23	2.10	0.52
9:L:84:LEU:HD22	9:L:87:LEU:HD22	1.92	0.52
7:M:30:LEU:HD21	7:M:95:TRP:CD1	2.44	0.52
12:P:12:THR:O	12:P:15:LEU:HG	2.09	0.52
14:X:-71:DT:H2''	14:X:-70:DC:C6	2.45	0.52
3:c:20:MET:SD	5:h:5:LYS:HD3	2.48	0.52
12:p:18:GLN:O	12:p:21:LEU:HG	2.08	0.52
6:I:566:ASP:O	6:I:569:SER:OG	2.10	0.52
10:N:224:ALA:N	10:N:241:TYR:OH	2.39	0.52
13:T:917:LEU:HD13	13:T:928:ARG:HG3	1.92	0.52
10:N:5:ASN:OD1	10:N:6:LYS:N	2.43	0.52
11:O:154:ASN:OD1	11:O:155:ILE:N	2.43	0.52
14:X:-38:DA:OP2	14:X:-38:DA:H3'	2.10	0.52
12:p:18:GLN:HA	12:p:21:LEU:HG	1.91	0.52
13:t:896:ARG:HD3	13:t:926:ARG:NH1	2.24	0.52
13:t:917:LEU:CD1	13:t:966:ILE:HD11	2.38	0.52
6:I:481:MET:HA	6:I:481:MET:HE2	1.91	0.52
13:T:983:ARG:HG3	13:T:986:ARG:NH2	2.25	0.52
13:T:1008:ILE:HG23	13:T:1009:LEU:HG	1.92	0.52
15:Y:22:DC:H2''	15:Y:23:DA:C8	2.45	0.52
9:l:147:THR:O	9:l:151:THR:HG23	2.09	0.52
13:t:955:ASP:HA	13:t:958:LYS:NZ	2.25	0.52
12:P:224:LEU:HD21	12:P:252:MET:SD	2.50	0.52
14:X:-63:DT:H2''	14:X:-62:DA:H8	1.74	0.52
15:Y:25:DG:H2''	15:Y:26:DG:N7	2.25	0.52
15:Y:38:DT:H2''	15:Y:39:DA:OP2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:h:21:LEU:HA	5:h:24:VAL:HG12	1.91	0.52
10:n:46:LEU:HD11	13:t:923:TYR:HB2	1.92	0.52
10:n:70:LEU:O	10:n:73:ILE:HG22	2.09	0.52
11:o:37:LEU:CD2	12:p:20:LEU:HD13	2.40	0.52
11:O:37:LEU:HD11	12:P:23:ASN:HB3	1.92	0.51
5:h:6:THR:O	5:h:10:VAL:HG23	2.09	0.51
13:T:990:VAL:O	13:T:995:ASN:ND2	2.43	0.51
15:Y:46:DA:H2''	15:Y:47:DG:N7	2.25	0.51
9:l:65:LEU:O	9:l:144:ARG:NH2	2.43	0.51
12:p:33:GLU:O	12:p:37:LYS:N	2.41	0.51
7:M:98:LYS:O	7:M:101:SER:OG	2.26	0.51
13:T:910:TYR:HE1	13:T:933:VAL:HG21	1.75	0.51
14:X:-26:DC:H2''	14:X:-25:DC:C6	2.45	0.51
13:t:960:GLU:HA	13:t:963:ARG:HG2	1.91	0.51
4:D:45:SER:HB2	11:O:49:ARG:HE	1.75	0.51
5:H:32:GLU:O	12:P:43:ILE:HG22	2.09	0.51
9:L:195:ARG:NH2	9:L:268:CYS:SG	2.81	0.51
12:P:16:GLU:O	12:P:20:LEU:HD13	2.11	0.51
6:i:139:GLN:OE1	6:i:139:GLN:N	2.41	0.51
9:l:225:THR:HG22	9:l:225:THR:O	2.10	0.51
13:t:953:ALA:O	13:t:957:LEU:HD23	2.10	0.51
14:X:-36:DG:H2''	14:X:-35:DG:C8	2.45	0.51
13:t:943:VAL:HG22	13:t:988:LYS:CD	2.38	0.51
12:P:169:LEU:CD1	12:P:178:VAL:HG23	2.40	0.51
15:Y:58:DG:H2''	15:Y:59:DA:C8	2.46	0.51
5:h:210:ARG:NH2	8:k:198:LEU:HD13	2.25	0.51
6:i:498:HIS:HA	6:i:503:ILE:HG22	1.93	0.51
11:o:273:VAL:HG13	11:o:274:GLY:N	2.26	0.51
8:K:69:THR:HG23	8:K:75:LEU:HD21	1.93	0.51
5:h:202:LEU:HD22	8:k:151:LEU:HD21	1.92	0.51
13:t:921:TYR:O	13:t:924:LYS:HB2	2.10	0.51
13:t:954:VAL:O	13:t:958:LYS:HG3	2.11	0.51
6:I:7:ILE:CD1	6:I:30:LEU:HD12	2.40	0.51
7:M:69:GLN:O	7:M:73:THR:HG22	2.11	0.51
13:T:926:ARG:O	13:T:930:GLU:HG2	2.11	0.51
15:Y:23:DA:H2''	15:Y:24:DA:OP2	2.08	0.51
1:a:63:ASP:OD2	1:a:66:ASN:ND2	2.43	0.51
5:h:26:PHE:CD1	11:o:53:LYS:HE3	2.46	0.51
12:p:224:LEU:C	12:p:224:LEU:HD23	2.35	0.51
12:p:245:MET:SD	12:p:245:MET:N	2.83	0.51
6:I:623:LEU:HD21	6:I:631:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:66:DC:H2''	15:Y:67:DA:OP2	2.10	0.51
6:i:385:GLU:O	6:i:389:LEU:HD23	2.11	0.51
3:C:20:MET:HE1	5:H:5:LYS:HE2	1.93	0.51
6:I:432:ILE:HD12	6:I:497:ALA:HB2	1.93	0.51
9:L:190:PHE:HB2	9:L:211:ILE:HD13	1.93	0.51
11:O:210:VAL:HG12	11:O:211:GLU:H	1.76	0.51
15:Y:22:DC:H2''	15:Y:23:DA:H8	1.75	0.51
5:h:20:GLN:O	5:h:24:VAL:HG12	2.11	0.51
11:o:116:ASP:OD1	11:o:117:ASN:N	2.44	0.51
11:O:251:GLU:O	11:O:254:THR:HG22	2.11	0.50
8:k:166:ILE:HA	8:k:169:PHE:CD2	2.46	0.50
3:C:38:HIS:HB2	5:H:18:LEU:HD11	1.93	0.50
5:H:49:SER:OG	5:H:53:LYS:NZ	2.44	0.50
6:I:174:LEU:O	6:I:178:LEU:HD23	2.11	0.50
10:N:207:ASP:OD1	10:N:209:ALA:N	2.44	0.50
13:T:895:LYS:HG2	13:T:896:ARG:N	2.26	0.50
15:Y:21:DC:H2''	15:Y:22:DC:H5'	1.93	0.50
6:i:216:ARG:O	6:i:220:THR:HG23	2.11	0.50
9:l:149:VAL:O	9:l:153:LEU:HD23	2.10	0.50
6:I:7:ILE:HD13	6:I:30:LEU:HD12	1.94	0.50
6:I:363:ILE:HG22	6:I:365:VAL:HG12	1.93	0.50
12:P:200:ALA:O	12:P:204:GLU:N	2.40	0.50
12:P:229:TRP:HZ3	12:P:281:LEU:HD11	1.76	0.50
14:X:-33:DG:H2'	14:X:-33:DG:OP2	2.12	0.50
15:Y:54:DG:C2'	15:Y:55:DT:H72	2.41	0.50
6:i:48:PHE:CE1	6:i:52:LEU:HD21	2.47	0.50
6:I:64:LEU:C	6:I:64:LEU:HD23	2.37	0.50
10:N:46:LEU:HD11	13:T:923:TYR:HB2	1.93	0.50
12:P:38:LYS:HZ2	12:P:40:THR:HA	1.77	0.50
14:X:-17:DT:H2''	14:X:-16:DT:O5'	2.12	0.50
6:i:627:ASP:OD1	6:i:628:GLU:N	2.44	0.50
8:k:2:THR:CG2	12:p:41:ASN:HB2	2.41	0.50
12:p:40:THR:HG21	12:p:42:TYR:CE2	2.46	0.50
12:p:59:ILE:HG22	12:p:60:ASP:H	1.76	0.50
6:I:637:TYR:HA	6:I:640:PHE:CD2	2.47	0.50
8:k:200:LYS:NZ	13:t:975:GLN:OE1	2.39	0.50
6:I:213:LEU:HD11	6:I:217:PHE:HE2	1.76	0.50
8:K:194:GLN:NE2	13:T:992:ASP:HA	2.27	0.50
11:O:60:LYS:HD3	12:P:48:SER:C	2.37	0.50
14:X:-64:DA:C8	14:X:-63:DT:H72	2.47	0.50
14:X:-51:DG:N9	14:X:-50:DT:H72	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:i:47:LEU:HD23	6:i:68:LEU:HD13	1.93	0.50
8:k:188:ILE:HG22	8:k:213:MET:O	2.12	0.50
1:A:63:ASP:OD2	1:A:66:ASN:ND2	2.43	0.50
9:L:42:SER:OG	9:L:160:ASN:N	2.41	0.50
14:X:-27:DC:H2''	14:X:-26:DC:C5	2.47	0.50
8:k:18:LYS:O	8:k:18:LYS:NZ	2.43	0.50
8:k:107:GLU:OE1	8:k:110:ARG:NH2	2.43	0.50
9:l:98:LEU:HD21	9:l:100:THR:OG1	2.12	0.50
13:t:967:VAL:HG11	13:t:973:PHE:HA	1.92	0.50
12:P:59:ILE:HG22	12:P:60:ASP:N	2.25	0.50
13:T:907:LYS:HA	13:T:910:TYR:CD2	2.46	0.50
13:T:952:ASP:OD1	13:T:953:ALA:N	2.44	0.50
14:X:-35:DG:H2''	14:X:-34:DA:H8	1.77	0.50
12:p:26:TYR:O	12:p:30:ARG:HG2	2.12	0.50
6:I:38:GLY:C	6:I:39:LEU:HD22	2.37	0.49
9:L:187:ASN:O	9:L:187:ASN:ND2	2.38	0.49
14:X:-24:DT:H2''	14:X:-23:DT:C6	2.47	0.49
5:h:17:GLU:O	5:h:21:LEU:HG	2.12	0.49
6:i:22:LEU:HD23	6:i:22:LEU:O	2.12	0.49
6:i:51:TRP:HE3	6:i:52:LEU:HD22	1.77	0.49
13:t:826:ILE:O	13:t:830:VAL:HG23	2.12	0.49
13:t:970:HIS:HE2	13:t:1008:ILE:HA	1.76	0.49
10:N:19:LEU:HD23	10:N:19:LEU:C	2.38	0.49
11:O:27:GLN:N	11:O:29:GLU:OE1	2.45	0.49
8:K:201:ASP:OD1	13:T:986:ARG:NH2	2.18	0.49
10:N:70:LEU:O	10:N:73:ILE:HG12	2.12	0.49
4:d:19:SER:HB2	5:h:10:VAL:HG21	1.94	0.49
2:B:68:HIS:ND1	11:O:41:GLN:HB3	2.27	0.49
5:H:30:ILE:HD12	5:H:31:GLY:H	1.76	0.49
5:H:198:MET:HE2	8:K:217:LEU:HD21	1.93	0.49
6:I:431:TYR:OH	6:I:498:HIS:NE2	2.40	0.49
13:T:961:MET:CG	13:T:967:VAL:HG22	2.42	0.49
6:i:160:GLU:OE1	8:k:203:ASN:ND2	2.46	0.49
12:p:249:LEU:HB3	12:p:257:VAL:HG22	1.93	0.49
13:t:958:LYS:HG2	13:t:973:PHE:CE2	2.48	0.49
5:H:150:TYR:CZ	5:H:154:LEU:HD11	2.48	0.49
6:I:8:ILE:HD11	6:I:50:ILE:HD12	1.95	0.49
11:O:38:LYS:HD2	11:O:39:GLU:N	2.27	0.49
12:P:12:THR:HA	12:P:15:LEU:HG	1.95	0.49
14:X:-38:DA:H2''	14:X:-37:DG:OP2	2.12	0.49
6:i:30:LEU:O	6:i:34:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:t:909:LEU:HB3	13:t:980:PHE:CD2	2.48	0.49
1:A:21:LEU:O	1:A:25:ILE:HG13	2.12	0.49
6:i:64:LEU:HD23	6:i:64:LEU:C	2.38	0.49
2:b:31:VAL:O	2:b:35:LEU:HD23	2.11	0.49
5:h:197:GLU:OE1	8:k:219:TYR:OH	2.18	0.49
11:O:60:LYS:HE2	12:P:48:SER:HA	1.94	0.49
12:P:41:ASN:OD1	12:P:42:TYR:N	2.45	0.49
13:T:918:GLU:N	13:T:919:PRO:HD2	2.28	0.49
13:T:960:GLU:O	13:T:964:LEU:HD13	2.12	0.49
15:Y:19:DC:H2''	15:Y:20:DG:H8	1.77	0.49
9:L:273:LYS:NZ	15:Y:22:DC:H5''	2.28	0.49
13:T:902:ALA:HA	13:T:904:TRP:CZ3	2.48	0.49
6:i:431:TYR:HH	6:i:498:HIS:CE1	2.28	0.49
11:o:60:LYS:HD3	12:p:48:SER:C	2.38	0.49
11:o:185:LEU:HD11	11:o:191:LEU:CD1	2.42	0.49
13:t:909:LEU:HB3	13:t:980:PHE:HD2	1.78	0.49
13:T:976:PHE:HA	13:T:979:ASP:OD1	2.13	0.49
2:b:67:LEU:HD23	11:o:45:PHE:HE1	1.77	0.49
8:k:2:THR:CG2	12:p:43:ILE:HD13	2.42	0.49
11:o:44:LEU:HA	12:p:31:ILE:CD1	2.43	0.49
11:o:44:LEU:CB	12:p:31:ILE:HD11	2.41	0.49
14:X:-49:DG:H2''	14:X:-48:DC:C6	2.48	0.48
15:Y:21:DC:H2''	15:Y:22:DC:O4'	2.13	0.48
5:h:12:GLN:HA	5:h:15:GLU:HG2	1.94	0.48
10:n:19:LEU:C	10:n:19:LEU:HD23	2.37	0.48
12:p:218:LEU:C	12:p:219:LEU:HD12	2.38	0.48
13:t:907:LYS:HA	13:t:910:TYR:CD2	2.46	0.48
13:T:1007:GLU:OE2	13:T:1010:SER:N	2.47	0.48
12:p:18:GLN:HA	12:p:21:LEU:HD21	1.95	0.48
8:K:37:GLU:OE1	8:K:37:GLU:N	2.45	0.48
8:K:159:PHE:O	8:K:163:SER:N	2.46	0.48
12:P:245:MET:SD	12:P:245:MET:N	2.86	0.48
6:i:130:MET:HG3	6:i:136:LEU:HD12	1.96	0.48
10:n:229:LEU:HD11	12:p:57:LEU:H	1.78	0.48
13:t:890:LYS:HG3	13:t:891:TYR:N	2.28	0.48
1:A:14:GLU:O	1:A:17:THR:OG1	2.26	0.48
5:H:20:GLN:O	5:H:24:VAL:HG12	2.13	0.48
6:I:195:GLU:OE1	6:I:195:GLU:N	2.38	0.48
10:N:127:ARG:NH2	10:N:129:GLU:OE2	2.45	0.48
15:Y:28:DG:H2''	15:Y:29:DA:H8	1.78	0.48
15:Y:65:DA:H8	15:Y:65:DA:OP2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:20:GLN:OE1	11:o:66:PHE:HA	2.14	0.48
6:i:38:GLY:C	6:i:39:LEU:HD22	2.38	0.48
6:i:374:LEU:CD1	6:i:404:ILE:HG23	2.43	0.48
5:H:5:LYS:HA	5:H:8:LYS:HE2	1.95	0.48
5:H:210:ARG:NH2	13:T:993:ILE:HG21	2.29	0.48
7:J:142:ASP:OD2	7:J:164:TYR:OH	2.12	0.48
7:M:142:ASP:OD2	7:M:164:TYR:OH	2.12	0.48
5:h:104:LYS:O	5:h:108:THR:OG1	2.31	0.48
6:I:627:ASP:OD1	6:I:628:GLU:N	2.44	0.48
12:P:12:THR:HA	12:P:15:LEU:CG	2.44	0.48
12:P:55:PHE:CE2	12:P:57:LEU:HB2	2.48	0.48
3:c:13:ASP:OD1	3:c:14:LYS:N	2.46	0.48
6:I:309:LEU:O	6:I:309:LEU:HD23	2.14	0.48
13:T:812:LEU:O	13:T:815:ILE:HB	2.13	0.48
13:T:902:ALA:HA	13:T:904:TRP:CH2	2.48	0.48
14:X:-28:DC:H2'	14:X:-28:DC:O5'	2.14	0.48
10:n:132:THR:HG23	10:n:139:LEU:HD11	1.96	0.48
3:C:15:ALA:O	3:C:18:LEU:N	2.47	0.48
8:K:198:LEU:CD1	13:T:993:ILE:HD13	2.43	0.48
11:O:29:GLU:HG2	12:P:17:LYS:NZ	2.29	0.48
14:X:-29:DT:H2''	14:X:-28:DC:C6	2.49	0.48
5:h:72:THR:OG1	5:h:73:GLU:N	2.45	0.48
6:i:637:TYR:O	6:i:641:LEU:HD23	2.13	0.48
13:t:905:THR:HG22	13:t:905:THR:O	2.13	0.48
13:t:999:ILE:CG1	13:t:1000:PRO:HD2	2.44	0.48
7:J:30:LEU:HD11	7:J:95:TRP:CG	2.49	0.48
9:L:48:GLN:N	9:L:48:GLN:OE1	2.47	0.48
10:N:242:ASP:O	10:N:246:ILE:HG12	2.14	0.48
5:h:214:ARG:O	6:i:88:ILE:HD13	2.14	0.48
6:i:154:THR:HG22	6:i:157:ARG:HD2	1.96	0.48
6:i:639:ALA:HB3	13:t:816:LYS:HE2	1.95	0.48
8:k:169:PHE:CD1	8:k:169:PHE:C	2.90	0.48
10:n:53:VAL:HA	10:n:56:VAL:HG12	1.96	0.48
13:t:943:VAL:HG23	13:t:949:ALA:CA	2.44	0.48
9:L:291:CYS:SG	9:L:292:CYS:N	2.83	0.48
14:X:-24:DT:H2''	14:X:-23:DT:H6	1.79	0.48
2:b:53:ILE:HD11	4:d:39:LEU:HB2	1.96	0.48
11:o:210:VAL:HG12	11:o:211:GLU:H	1.78	0.48
11:o:211:GLU:OE1	11:o:212:GLU:N	2.47	0.48
13:t:812:LEU:O	13:t:815:ILE:HG12	2.14	0.48
6:I:121:ASP:HA	6:I:147:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:412:TYR:CD2	6:I:469:MET:HE3	2.48	0.47
14:X:-33:DG:H2''	14:X:-32:DT:OP2	2.12	0.47
15:Y:18:DC:H2''	15:Y:19:DC:C6	2.49	0.47
1:a:7:LEU:HD13	3:c:18:LEU:HD22	1.96	0.47
2:b:33:GLU:O	2:b:37:LEU:HD23	2.13	0.47
8:k:169:PHE:CD1	8:k:170:MET:N	2.82	0.47
13:t:917:LEU:HD21	13:t:932:LEU:HD11	1.97	0.47
5:H:21:LEU:HA	5:H:24:VAL:CG1	2.44	0.47
5:H:212:GLU:O	5:H:215:ASN:ND2	2.47	0.47
7:J:132:LEU:HD23	7:J:136:TYR:HD2	1.79	0.47
10:N:27:LEU:HD13	10:N:34:TRP:HA	1.95	0.47
10:N:282:ILE:HD12	10:N:282:ILE:H	1.80	0.47
14:X:-65:DT:H2''	14:X:-64:DA:H8	1.78	0.47
15:Y:35:DC:H6	15:Y:35:DC:OP2	1.97	0.47
4:d:41:GLU:N	4:d:41:GLU:OE1	2.47	0.47
13:t:895:LYS:HD2	13:t:898:GLN:NE2	2.29	0.47
1:A:11:LEU:HD12	3:C:22:LEU:HD22	1.95	0.47
5:H:6:THR:O	5:H:10:VAL:HG23	2.13	0.47
8:K:198:LEU:HD13	13:T:993:ILE:HD13	1.96	0.47
6:i:608:SER:O	6:i:612:HIS:N	2.45	0.47
8:k:212:LYS:HZ3	13:t:975:GLN:HG3	1.77	0.47
5:H:105:LEU:HD21	5:H:121:LYS:HB2	1.96	0.47
10:N:138:LEU:HD11	10:N:199:ILE:HG21	1.95	0.47
13:T:953:ALA:O	13:T:956:VAL:HG12	2.15	0.47
13:T:1001:ARG:HH12	10:n:33:LYS:HZ1	1.62	0.47
6:i:432:ILE:HD12	6:i:497:ALA:HB2	1.96	0.47
10:n:199:ILE:H	10:n:199:ILE:HD12	1.78	0.47
11:o:58:PRO:HD3	12:p:44:GLU:OE2	2.15	0.47
11:O:29:GLU:HG2	12:P:17:LYS:CE	2.45	0.47
11:O:30:ILE:CG2	12:P:13:LEU:HD11	2.44	0.47
11:O:199:HIS:O	11:O:199:HIS:ND1	2.46	0.47
13:T:827:GLU:HA	13:T:830:VAL:HG12	1.97	0.47
13:T:921:TYR:O	13:T:924:LYS:HB2	2.14	0.47
13:T:1000:PRO:HG2	13:T:1004:VAL:HA	1.96	0.47
5:h:38:VAL:O	5:h:42:LEU:HD23	2.15	0.47
8:k:150:GLU:O	8:k:154:LEU:HD23	2.15	0.47
11:O:30:ILE:CG2	12:P:17:LYS:HE2	2.28	0.47
11:O:60:LYS:HD3	12:P:48:SER:O	2.15	0.47
12:P:195:SER:O	12:P:199:LEU:HD13	2.15	0.47
12:P:219:LEU:HD12	12:P:219:LEU:N	2.29	0.47
13:T:984:GLU:O	13:T:987:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:986:ARG:HG3	13:T:987:VAL:N	2.29	0.47
15:Y:39:DA:H2''	15:Y:40:DG:C8	2.49	0.47
15:Y:40:DG:H1'	15:Y:41:DT:H5'	1.97	0.47
1:a:16:ILE:HG23	11:o:69:PRO:HB3	1.97	0.47
12:p:164:LEU:HD21	12:p:185:TYR:CD1	2.49	0.47
8:K:175:ALA:O	8:K:179:ASN:ND2	2.47	0.47
11:O:39:GLU:OE2	11:O:40:LYS:HE3	2.14	0.47
12:P:229:TRP:CZ3	12:P:281:LEU:HD11	2.50	0.47
12:P:274:THR:O	12:P:278:THR:HG23	2.15	0.47
3:c:40:ARG:O	3:c:43:LYS:HG2	2.15	0.47
6:i:220:THR:HG22	6:i:223:ARG:HH21	1.80	0.47
6:I:86:ILE:O	6:I:90:TYR:N	2.47	0.47
11:O:196:ASP:O	11:O:196:ASP:CG	2.58	0.47
12:p:30:ARG:HA	12:p:33:GLU:HG2	1.97	0.47
12:P:218:LEU:C	12:P:219:LEU:HD12	2.40	0.47
13:T:958:LYS:HG2	13:T:973:PHE:CE2	2.50	0.47
14:X:-56:DG:H2''	14:X:-55:DA:C8	2.50	0.47
9:l:272:VAL:HG22	9:l:274:MET:SD	2.55	0.47
11:o:47:LEU:CD1	12:p:31:ILE:HG23	2.44	0.47
11:o:202:ILE:O	11:o:202:ILE:HG23	2.14	0.47
11:o:220:LEU:HD12	11:o:235:SER:O	2.14	0.47
1:A:33:ILE:HG13	2:B:45:ILE:CG1	2.43	0.46
3:C:15:ALA:O	3:C:19:PRO:CD	2.63	0.46
10:N:45:ARG:HD2	13:T:894:PRO:HG2	1.97	0.46
11:O:92:THR:O	11:O:165:ARG:NH1	2.47	0.46
6:i:51:TRP:CE3	6:i:52:LEU:HD22	2.50	0.46
11:o:202:ILE:HD13	11:o:265:PHE:CE1	2.49	0.46
13:t:932:LEU:HA	13:t:935:THR:HG22	1.97	0.46
13:t:990:VAL:CG2	13:t:991:PRO:HD2	2.45	0.46
5:H:93:VAL:O	5:H:94:LYS:C	2.58	0.46
6:I:216:ARG:O	6:I:220:THR:HG23	2.15	0.46
8:K:144:PHE:HA	8:K:147:LEU:CD2	2.46	0.46
10:N:21:GLN:O	10:N:24:VAL:HG22	2.15	0.46
15:Y:24:DA:H2''	15:Y:25:DG:C8	2.50	0.46
6:i:30:LEU:C	6:i:30:LEU:HD23	2.41	0.46
10:n:246:ILE:HG13	10:n:297:VAL:HG11	1.97	0.46
11:o:37:LEU:HA	12:p:24:ILE:CD1	2.45	0.46
5:H:33:THR:HA	12:P:41:ASN:OD1	2.15	0.46
7:J:46:HIS:NE2	7:J:53:TRP:O	2.43	0.46
11:O:186:ASN:OD1	11:O:187:VAL:N	2.47	0.46
12:P:38:LYS:HZ1	12:P:40:THR:HA	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:831:ARG:O	13:T:835:LYS:HG2	2.14	0.46
15:Y:40:DG:H2'	15:Y:41:DT:H71	1.97	0.46
9:l:274:MET:SD	9:l:274:MET:N	2.89	0.46
10:n:157:VAL:HG22	10:n:168:PHE:CD2	2.51	0.46
11:o:207:GLN:HB2	11:o:279:ILE:HB	1.97	0.46
13:t:890:LYS:HG3	13:t:891:TYR:H	1.80	0.46
13:t:969:THR:C	13:t:1008:ILE:HD11	2.40	0.46
9:L:187:ASN:HD22	9:L:187:ASN:C	2.22	0.46
10:N:45:ARG:HD3	13:T:894:PRO:HG2	1.97	0.46
11:O:40:LYS:HA	11:O:43:GLU:HG2	1.96	0.46
13:T:983:ARG:HA	13:T:986:ARG:NH1	2.30	0.46
13:T:1003:GLY:O	13:T:1006:SER:OG	2.26	0.46
15:Y:58:DG:H2''	15:Y:59:DA:N7	2.30	0.46
6:i:217:PHE:O	6:i:220:THR:OG1	2.28	0.46
6:i:590:PRO:O	6:i:593:VAL:HG12	2.16	0.46
10:n:71:ASN:OD1	10:n:72:ASP:N	2.48	0.46
11:o:28:ASP:HA	11:o:31:GLU:OE1	2.15	0.46
11:o:199:HIS:O	11:o:199:HIS:ND1	2.48	0.46
5:H:140:HIS:NE2	13:T:823:ASN:OD1	2.49	0.46
14:X:-65:DT:H2''	14:X:-64:DA:C8	2.50	0.46
6:i:174:LEU:O	6:i:178:LEU:HD23	2.15	0.46
10:n:256:LEU:C	10:n:256:LEU:HD23	2.40	0.46
12:p:57:LEU:HD22	12:p:59:ILE:CD1	2.46	0.46
13:t:962:ALA:CB	13:t:1009:LEU:HG	2.46	0.46
6:I:52:LEU:HD12	6:I:81:TYR:CE2	2.51	0.46
9:L:256:LEU:HD21	9:L:259:ILE:HD11	1.97	0.46
12:P:224:LEU:HD21	12:P:252:MET:HG3	1.97	0.46
14:X:-21:DG:H2''	14:X:-20:DC:OP2	2.15	0.46
15:Y:25:DG:H2''	15:Y:26:DG:C8	2.51	0.46
15:Y:30:DT:H2'	15:Y:31:DT:C7	2.37	0.46
5:h:21:LEU:HA	5:h:24:VAL:CG1	2.45	0.46
6:i:396:ASP:OD1	6:i:397:SER:N	2.48	0.46
8:k:161:ASN:OD1	8:k:162:THR:N	2.49	0.46
9:l:166:PHE:HB3	9:l:171:LEU:HD22	1.97	0.46
10:n:246:ILE:HG23	10:n:309:PHE:CE1	2.51	0.46
12:p:125:ILE:HD12	12:p:183:LYS:HA	1.97	0.46
12:p:219:LEU:HD12	12:p:219:LEU:N	2.31	0.46
13:T:937:TYR:O	13:T:940:THR:OG1	2.29	0.46
13:T:943:VAL:CG1	13:T:988:LYS:HD2	2.44	0.46
6:i:69:ILE:HD13	6:i:216:ARG:HB3	1.96	0.46
6:i:320:ALA:HA	6:i:446:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:k:169:PHE:CZ	8:k:199:LEU:CD1	2.98	0.46
9:l:94:SER:OG	9:l:95:SER:N	2.49	0.46
3:c:49:MET:HE1	4:d:39:LEU:HD11	1.96	0.46
11:o:37:LEU:CA	12:p:24:ILE:HD11	2.45	0.46
13:t:895:LYS:HG2	13:t:896:ARG:N	2.28	0.46
13:t:906:THR:H	13:t:909:LEU:HD22	1.80	0.46
5:H:206:LEU:HD21	8:K:158:MET:HG2	1.98	0.46
7:M:130:GLY:O	7:M:134:ASN:ND2	2.41	0.46
12:P:33:GLU:O	12:P:37:LYS:HB3	2.16	0.46
13:T:920:LYS:HG3	13:T:921:TYR:CD1	2.51	0.46
15:Y:17:DA:H2''	15:Y:18:DC:C6	2.51	0.46
15:Y:37:DC:OP2	15:Y:37:DC:H2'	2.16	0.46
3:c:42:VAL:O	3:c:46:LEU:HD23	2.16	0.46
5:h:105:LEU:HD21	5:h:121:LYS:HB2	1.98	0.46
6:i:9:ASP:OD1	6:i:10:TYR:N	2.49	0.46
6:i:10:TYR:CZ	6:i:22:LEU:HD22	2.51	0.46
5:H:15:GLU:OE1	5:H:16:GLN:NE2	2.49	0.46
7:J:86:ASP:OD2	7:J:88:SER:OG	2.33	0.46
13:T:909:LEU:HB2	13:T:980:PHE:CD1	2.51	0.46
13:T:993:ILE:HA	13:T:996:LYS:HZ1	1.81	0.46
1:a:45:ASN:ND2	3:c:50:ASN:OD1	2.48	0.46
10:n:265:SER:OG	10:n:277:ASN:ND2	2.49	0.46
3:C:14:LYS:O	3:C:17:GLU:HG3	2.17	0.45
4:D:66:HIS:O	8:K:98:LYS:NZ	2.40	0.45
5:H:42:LEU:HD11	8:K:74:LEU:HD11	1.98	0.45
13:T:984:GLU:HA	13:T:987:VAL:HG12	1.98	0.45
13:T:993:ILE:O	13:T:993:ILE:HG22	2.15	0.45
14:X:-55:DA:H5'	10:n:48:MET:CE	2.45	0.45
5:h:140:HIS:NE2	13:t:826:ILE:HG23	2.32	0.45
11:o:67:VAL:HG22	11:o:68:ARG:N	2.31	0.45
12:p:288:CYS:O	12:p:291:VAL:HG22	2.16	0.45
13:t:918:GLU:N	13:t:919:PRO:HD2	2.31	0.45
13:t:932:LEU:O	13:t:936:ILE:HG12	2.16	0.45
5:H:141:PHE:O	5:H:144:ILE:HG22	2.16	0.45
7:J:93:LEU:HD21	7:J:127:ILE:CD1	2.47	0.45
10:N:235:ASP:OD1	10:N:237:THR:OG1	2.20	0.45
11:O:55:LYS:HD3	11:O:56:SER:N	2.30	0.45
13:T:1000:PRO:HG2	13:T:1004:VAL:CA	2.47	0.45
7:J:166:GLU:HG3	7:J:171:VAL:HG22	1.97	0.45
9:L:185:ARG:N	9:L:188:ASP:OD2	2.50	0.45
13:T:982:PRO:HB2	13:T:984:GLU:CD	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:-60:DA:H2''	14:X:-59:DT:OP2	2.17	0.45
6:i:309:LEU:CD1	8:k:117:ILE:HG21	2.46	0.45
13:t:977:PHE:O	13:t:981:MET:HB2	2.16	0.45
5:H:8:LYS:O	5:H:12:GLN:HG2	2.15	0.45
14:X:-53:DA:H2''	14:X:-52:DC:OP2	2.15	0.45
5:h:31:GLY:HA3	12:p:42:TYR:CE1	2.52	0.45
5:h:199:ILE:HG21	8:k:147:LEU:HG	1.97	0.45
12:p:12:THR:O	12:p:16:GLU:HG2	2.17	0.45
6:I:9:ASP:OD1	6:I:10:TYR:N	2.49	0.45
11:O:31:GLU:HA	11:O:34:ARG:NE	2.31	0.45
12:P:288:CYS:O	12:P:291:VAL:HG22	2.16	0.45
6:i:536:TYR:HA	6:i:539:ILE:HG22	1.98	0.45
9:l:84:LEU:HD22	9:l:87:LEU:CD1	2.46	0.45
11:o:210:VAL:HG12	11:o:211:GLU:N	2.31	0.45
13:t:812:LEU:HG	13:t:815:ILE:HD13	1.98	0.45
6:I:636:TRP:CD1	13:T:812:LEU:HB2	2.52	0.45
9:L:94:SER:OG	9:L:95:SER:N	2.50	0.45
9:L:278:GLU:OE1	9:L:278:GLU:N	2.34	0.45
11:O:30:ILE:CG1	11:O:34:ARG:HH21	2.30	0.45
13:T:928:ARG:NH2	13:T:931:LYS:HE2	2.31	0.45
13:T:961:MET:HG3	13:T:967:VAL:HG22	1.98	0.45
1:a:22:LEU:HA	1:a:25:ILE:HG22	1.97	0.45
5:h:33:THR:HA	12:p:41:ASN:OD1	2.17	0.45
9:l:98:LEU:C	9:l:98:LEU:HD23	2.41	0.45
10:n:133:ASN:O	10:n:139:LEU:HD12	2.17	0.45
11:o:185:LEU:HD11	11:o:191:LEU:HD13	1.98	0.45
13:t:812:LEU:O	13:t:812:LEU:HG	2.17	0.45
11:O:30:ILE:HG21	12:P:13:LEU:HD12	1.96	0.45
14:X:-54:DC:H2''	14:X:-53:DA:C8	2.51	0.45
4:D:18:ILE:O	4:D:22:ILE:HG12	2.16	0.45
5:H:185:TYR:HA	5:H:188:ARG:HG2	1.99	0.45
9:L:253:VAL:HG21	10:N:301:ALA:HB2	1.99	0.45
11:O:54:HIS:CD2	12:P:42:TYR:HB3	2.52	0.45
11:O:273:VAL:HG13	11:O:274:GLY:N	2.27	0.45
13:T:932:LEU:HA	13:T:935:THR:HG22	1.98	0.45
13:T:996:LYS:HA	13:T:996:LYS:CE	2.38	0.45
1:a:30:GLN:HA	1:a:33:ILE:HG22	1.98	0.45
5:h:42:LEU:HD21	8:k:74:LEU:CD1	2.46	0.45
12:p:18:GLN:HA	12:p:21:LEU:CG	2.47	0.45
12:p:55:PHE:CE2	12:p:57:LEU:HB2	2.52	0.45
13:t:982:PRO:HB2	13:t:984:GLU:CD	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:274:MET:SD	9:L:274:MET:N	2.90	0.45
7:M:32:VAL:HG21	10:N:239:ARG:HG2	1.99	0.45
5:h:210:ARG:HH21	8:k:198:LEU:HD13	1.82	0.45
6:i:386:ILE:O	6:i:390:VAL:HG23	2.17	0.45
11:o:88:MET:HE1	12:p:90:VAL:CG2	2.47	0.45
13:t:917:LEU:HD23	13:t:928:ARG:HB3	1.99	0.45
2:B:41:ASP:O	2:B:45:ILE:HG13	2.16	0.45
5:H:98:GLN:O	5:H:99:THR:C	2.59	0.45
8:K:2:THR:HG22	12:P:41:ASN:HB2	1.97	0.45
14:X:-47:DC:H2''	14:X:-46:DT:C5	2.52	0.45
3:C:19:PRO:HA	3:C:22:LEU:HB2	1.99	0.44
3:C:22:LEU:O	3:C:26:ARG:HG3	2.16	0.44
5:H:33:THR:HG23	5:H:36:ASP:H	1.82	0.44
6:I:156:ARG:NH2	6:I:160:GLU:OE2	2.49	0.44
12:P:58:SER:C	12:P:59:ILE:HD13	2.42	0.44
8:k:112:LYS:HA	8:k:115:ILE:HG22	1.99	0.44
9:l:31:TYR:O	9:l:32:ASN:OD1	2.35	0.44
10:n:20:GLN:OE1	13:t:889:MET:HE1	2.17	0.44
10:n:79:LEU:HD11	10:n:140:TYR:HB3	1.98	0.44
13:t:926:ARG:HD3	13:t:926:ARG:O	2.17	0.44
13:t:971:PHE:O	13:t:975:GLN:HG2	2.17	0.44
7:M:166:GLU:HG3	7:M:171:VAL:HG22	1.99	0.44
13:T:950:PRO:O	13:T:954:VAL:HG12	2.17	0.44
5:h:98:GLN:O	5:h:99:THR:C	2.60	0.44
6:i:102:LEU:C	6:i:102:LEU:HD23	2.42	0.44
11:o:32:LYS:HG3	11:o:33:LEU:CD2	2.48	0.44
11:o:81:LEU:HD23	12:p:75:LEU:HB3	1.99	0.44
12:p:25:VAL:O	12:p:29:THR:HG23	2.16	0.44
13:t:943:VAL:HG21	13:t:949:ALA:HB2	1.99	0.44
6:I:172:LYS:HE2	14:X:-36:DG:H5'	1.98	0.44
9:L:133:HIS:C	9:L:134:LEU:HD22	2.43	0.44
5:h:93:VAL:O	5:h:94:LYS:C	2.60	0.44
1:A:62:ILE:HG13	1:A:62:ILE:O	2.16	0.44
4:D:19:SER:HB2	5:H:10:VAL:HG21	1.99	0.44
13:T:989:VAL:HG13	13:T:990:VAL:N	2.33	0.44
5:h:137:SER:N	13:t:826:ILE:HD11	2.32	0.44
5:h:209:CYS:SG	5:h:210:ARG:N	2.90	0.44
6:i:72:ASP:OD1	6:i:73:ALA:N	2.50	0.44
11:o:30:ILE:HB	11:o:34:ARG:NH2	2.27	0.44
11:o:181:LEU:HD22	11:o:261:LEU:HG	1.99	0.44
13:t:896:ARG:HA	13:t:930:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:t:963:ARG:HG3	13:t:964:LEU:HD22	1.98	0.44
5:H:228:ARG:O	5:H:228:ARG:NH1	2.50	0.44
6:I:178:LEU:O	6:I:182:LEU:HD23	2.17	0.44
11:O:44:LEU:O	11:O:48:GLN:HG3	2.18	0.44
15:Y:37:DC:OP2	15:Y:37:DC:H6	2.00	0.44
5:h:89:GLU:O	5:h:90:LYS:C	2.60	0.44
10:n:65:LEU:HD23	10:n:65:LEU:H	1.82	0.44
11:o:29:GLU:CA	11:o:32:LYS:HE2	2.44	0.44
11:o:34:ARG:CZ	11:o:34:ARG:HB3	2.48	0.44
11:o:101:VAL:HG13	11:o:101:VAL:O	2.18	0.44
1:A:6:GLN:O	1:A:9:GLN:NE2	2.50	0.44
5:H:92:THR:O	5:H:93:VAL:C	2.61	0.44
5:H:141:PHE:CE2	13:T:830:VAL:HG23	2.52	0.44
6:I:428:THR:O	6:I:432:ILE:HG12	2.18	0.44
9:L:31:TYR:O	9:L:32:ASN:OD1	2.36	0.44
11:O:32:LYS:HG3	11:O:33:LEU:HD22	1.98	0.44
11:O:34:ARG:HB3	12:P:20:LEU:HD21	1.98	0.44
11:O:210:VAL:HG12	11:O:211:GLU:N	2.33	0.44
13:T:986:ARG:HA	13:T:989:VAL:CG1	2.48	0.44
14:X:-48:DC:H2''	14:X:-47:DC:C6	2.53	0.44
15:Y:60:DT:H2''	15:Y:61:DA:OP2	2.18	0.44
10:n:20:GLN:HE21	11:o:187:VAL:HG21	1.83	0.44
10:n:114:ILE:HG23	10:n:130:VAL:HG21	1.99	0.44
10:n:311:ILE:O	10:n:316:LYS:N	2.44	0.44
11:o:171:TYR:CE2	11:o:196:ASP:HA	2.53	0.44
5:H:105:LEU:HD23	5:H:105:LEU:C	2.43	0.44
9:L:195:ARG:NE	9:L:257:SER:OG	2.50	0.44
7:M:113:VAL:CG2	7:M:144:LEU:HD13	2.48	0.44
11:O:57:SER:OG	11:O:58:PRO:HD2	2.18	0.44
11:O:67:VAL:CG2	11:O:72:ILE:HD11	2.48	0.44
11:O:196:ASP:O	11:O:197:ALA:C	2.60	0.44
14:X:-33:DG:H2''	14:X:-32:DT:O5'	2.18	0.44
15:Y:54:DG:H8	15:Y:54:DG:OP2	2.01	0.44
11:o:29:GLU:CB	11:o:32:LYS:HE2	2.48	0.44
6:I:640:PHE:CD1	6:I:640:PHE:C	2.95	0.44
14:X:-66:DG:H2'	14:X:-65:DT:H72	2.00	0.44
14:X:-41:DA:C5	14:X:-40:DC:N4	2.85	0.44
2:b:63:LEU:HD22	4:d:49:TYR:CG	2.53	0.44
6:i:553:HIS:O	6:i:557:ILE:HG12	2.18	0.44
8:K:165:LEU:O	8:K:166:ILE:C	2.61	0.44
10:N:73:ILE:HG22	10:N:76:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:948:VAL:HA	13:T:988:LYS:HG3	1.99	0.44
5:h:88:LEU:O	5:h:89:GLU:C	2.61	0.44
6:i:491:VAL:HG21	6:i:509:PRO:HG3	2.00	0.44
9:l:52:ILE:O	9:l:55:LYS:HG3	2.18	0.44
12:p:227:VAL:HG22	12:p:247:PHE:HD1	1.82	0.44
13:t:834:LEU:C	13:t:834:LEU:HD12	2.42	0.44
13:t:926:ARG:NH1	13:t:930:GLU:OE2	2.37	0.44
6:I:42:ASP:O	6:I:46:THR:HG23	2.18	0.43
10:N:88:MET:HE1	10:N:259:ASP:OD2	2.18	0.43
12:P:168:VAL:HG22	12:P:168:VAL:O	2.18	0.43
1:a:65:GLU:OE1	1:a:65:GLU:N	2.48	0.43
4:d:72:HIS:CD2	6:i:384:THR:HG23	2.53	0.43
5:h:209:CYS:SG	8:k:158:MET:HE2	2.57	0.43
6:i:130:MET:HE3	6:i:140:ALA:HB2	1.99	0.43
6:i:589:HIS:CD2	6:i:591:GLN:HB3	2.52	0.43
9:l:118:ILE:HG22	9:l:138:LEU:HB2	1.99	0.43
10:n:38:PHE:CE1	13:t:889:MET:HA	2.53	0.43
10:n:280:MET:SD	10:n:282:ILE:HD11	2.58	0.43
10:N:10:LEU:HD23	10:N:10:LEU:C	2.43	0.43
1:a:30:GLN:C	1:a:33:ILE:HG22	2.42	0.43
6:i:46:THR:O	6:i:49:LYS:HG2	2.18	0.43
11:o:47:LEU:CD1	12:p:31:ILE:HD12	2.33	0.43
13:t:817:LYS:HE2	13:t:817:LYS:CA	2.41	0.43
12:P:261:SER:O	12:P:265:LYS:HG2	2.18	0.43
13:T:818:SER:C	13:T:821:GLU:HG3	2.43	0.43
14:X:-66:DG:C8	14:X:-65:DT:H72	2.53	0.43
5:h:99:THR:O	5:h:100:HIS:C	2.62	0.43
13:t:937:TYR:HA	13:t:940:THR:HG22	2.01	0.43
2:B:67:LEU:C	2:B:67:LEU:HD23	2.44	0.43
5:H:58:LYS:HB3	5:H:59:PRO:HD3	1.99	0.43
6:I:542:ARG:O	6:I:545:SER:OG	2.28	0.43
10:N:157:VAL:HG22	10:N:168:PHE:CD2	2.54	0.43
11:O:209:ALA:C	11:O:210:VAL:HG23	2.43	0.43
14:X:-42:DG:C6	14:X:-41:DA:N6	2.86	0.43
6:i:483:VAL:O	6:i:487:ASN:ND2	2.50	0.43
9:l:235:ALA:O	9:l:239:LEU:HD23	2.18	0.43
13:t:909:LEU:HD23	13:t:910:TYR:H	1.82	0.43
13:t:928:ARG:O	13:t:932:LEU:HG	2.18	0.43
5:H:91:VAL:O	5:H:92:THR:C	2.60	0.43
5:H:108:THR:HG21	5:H:113:LEU:HD21	2.01	0.43
6:I:141:VAL:HG21	6:I:177:GLN:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:200:ILE:HG22	6:I:201:CYS:N	2.33	0.43
8:k:80:LEU:O	8:k:83:ILE:HG22	2.19	0.43
11:o:131:ALA:O	11:o:132:ASN:OD1	2.37	0.43
11:o:223:ASP:O	11:o:232:LYS:N	2.49	0.43
2:B:38:ILE:O	2:B:42:ILE:HG12	2.18	0.43
5:H:89:GLU:O	5:H:90:LYS:C	2.62	0.43
5:H:99:THR:O	5:H:100:HIS:C	2.61	0.43
5:H:214:ARG:O	6:I:88:ILE:HD13	2.19	0.43
6:I:47:LEU:HD23	6:I:68:LEU:HD13	2.00	0.43
6:I:209:ILE:HG22	6:I:210:ASN:N	2.34	0.43
7:J:98:LYS:O	7:J:101:SER:OG	2.32	0.43
8:K:173:LEU:HD21	8:K:205:ILE:HG22	1.99	0.43
14:X:-43:DA:H2''	14:X:-42:DG:H8	1.83	0.43
3:c:28:LEU:O	3:c:32:LEU:HD23	2.18	0.43
10:n:48:MET:H	13:t:893:PRO:HG3	1.82	0.43
11:o:60:LYS:HE2	12:p:48:SER:HA	2.01	0.43
13:t:905:THR:CG2	13:t:910:TYR:HE2	2.28	0.43
5:H:94:LYS:O	5:H:95:CYS:C	2.60	0.43
13:T:951:ASN:HA	13:T:954:VAL:HG12	2.01	0.43
5:h:14:PHE:HA	5:h:17:GLU:HG2	1.99	0.43
6:i:543:LEU:HA	6:i:546:THR:HG22	2.00	0.43
10:n:10:LEU:C	10:n:10:LEU:HD23	2.43	0.43
12:p:281:LEU:HA	12:p:284:ILE:HG22	1.99	0.43
6:I:539:ILE:O	6:I:543:LEU:HD23	2.18	0.43
10:N:19:LEU:HD12	10:N:50:ALA:O	2.19	0.43
13:T:896:ARG:HD2	13:T:930:GLU:OE2	2.19	0.43
13:T:899:PRO:CB	13:T:902:ALA:HB2	2.48	0.43
13:T:906:THR:C	13:T:908:ARG:H	2.26	0.43
14:X:-60:DA:H2''	14:X:-59:DT:C6	2.53	0.43
14:X:-55:DA:H2''	14:X:-54:DC:C6	2.54	0.43
15:Y:67:DA:H2'	15:Y:68:DT:C7	2.48	0.43
4:d:11:ARG:O	4:d:14:SER:OG	2.31	0.43
6:i:320:ALA:CA	6:i:446:MET:HE1	2.49	0.43
10:n:26:VAL:HG23	10:n:27:LEU:N	2.33	0.43
13:t:940:THR:O	13:t:943:VAL:HG12	2.19	0.43
6:I:34:VAL:HG12	6:I:219:ARG:HH22	1.84	0.43
10:N:265:SER:OG	10:N:277:ASN:ND2	2.52	0.43
13:T:890:LYS:HG3	13:T:891:TYR:H	1.84	0.43
5:h:31:GLY:HA3	12:p:42:TYR:CZ	2.53	0.43
3:C:21:GLU:O	3:C:25:ILE:HG12	2.19	0.43
9:L:180:ASP:OD2	9:L:218:TRP:NE1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:21:ASN:O	7:M:21:ASN:CG	2.61	0.43
10:N:34:TRP:CH2	13:T:889:MET:HE2	2.53	0.43
13:T:992:ASP:OD1	13:T:995:ASN:ND2	2.51	0.43
14:X:-62:DA:H8	14:X:-62:DA:OP2	2.01	0.43
10:n:27:LEU:HD13	10:n:34:TRP:HA	1.99	0.43
13:t:898:GLN:OE1	13:t:898:GLN:N	2.52	0.43
13:t:984:GLU:HG2	13:t:985:ILE:N	2.34	0.43
6:I:24:GLN:NE2	6:I:28:ASP:OD2	2.52	0.42
7:J:133:ILE:HD11	6:i:376:LEU:CD2	2.49	0.42
9:L:61:ILE:HD13	9:L:152:ILE:HG21	2.01	0.42
10:N:110:LEU:HD21	10:N:141:ILE:HD13	2.01	0.42
12:P:22:ASP:HA	12:P:25:VAL:HG12	2.00	0.42
13:T:907:LYS:O	13:T:907:LYS:HD3	2.19	0.42
14:X:-30:DA:N6	15:Y:29:DA:N6	2.67	0.42
5:h:94:LYS:O	5:h:95:CYS:C	2.61	0.42
6:i:208:LYS:C	6:i:209:ILE:HD13	2.44	0.42
10:n:20:GLN:HG3	11:o:187:VAL:HG11	2.00	0.42
10:n:73:ILE:HG23	10:n:74:LEU:N	2.34	0.42
13:t:993:ILE:HG22	13:t:993:ILE:O	2.18	0.42
3:C:18:LEU:O	3:C:22:LEU:HD23	2.19	0.42
10:N:14:ILE:CD1	10:N:26:VAL:HG11	2.45	0.42
11:O:29:GLU:OE1	11:O:29:GLU:N	2.48	0.42
13:T:831:ARG:O	13:T:835:LYS:HE3	2.19	0.42
13:T:942:GLU:OE1	13:T:942:GLU:HA	2.19	0.42
2:B:49:LEU:O	2:B:53:ILE:HG13	2.19	0.42
5:H:207:VAL:O	5:H:207:VAL:HG22	2.20	0.42
7:J:133:ILE:HD13	7:J:136:TYR:CE2	2.54	0.42
10:N:23:CYS:HA	10:N:27:LEU:HD12	2.01	0.42
11:O:40:LYS:HD3	11:O:43:GLU:OE2	2.18	0.42
13:T:995:ASN:OD1	13:T:997:ILE:HG13	2.19	0.42
15:Y:22:DC:H2''	15:Y:23:DA:OP2	2.18	0.42
15:Y:25:DG:H1'	15:Y:26:DG:C8	2.54	0.42
4:d:47:LYS:NZ	5:h:30:ILE:HA	2.32	0.42
5:h:60:VAL:HG23	8:k:56:ALA:HB1	2.00	0.42
5:h:207:VAL:O	5:h:207:VAL:HG22	2.18	0.42
8:k:73:ASN:HD22	8:k:73:ASN:N	2.17	0.42
9:l:52:ILE:HG23	9:l:53:LYS:N	2.34	0.42
9:l:226:THR:HG21	9:l:231:LEU:HD21	2.01	0.42
10:n:198:ASP:OD2	10:n:201:SER:OG	2.34	0.42
11:o:195:LEU:O	11:o:196:ASP:CG	2.63	0.42
6:I:145:TYR:CD2	6:I:184:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:25:VAL:O	12:P:29:THR:HG23	2.19	0.42
13:T:968:LYS:HD2	13:T:968:LYS:N	2.34	0.42
1:a:29:LEU:HA	1:a:32:ILE:HG22	2.01	0.42
4:d:22:ILE:CG2	5:h:10:VAL:HG12	2.49	0.42
13:t:904:TRP:CE2	13:t:981:MET:HE1	2.55	0.42
5:H:202:LEU:C	5:H:202:LEU:HD23	2.44	0.42
5:H:205:ARG:NH2	8:K:202:THR:O	2.53	0.42
8:K:139:ASN:O	8:K:143:LYS:HG2	2.20	0.42
14:X:-71:DT:H2''	14:X:-70:DC:C5	2.54	0.42
6:i:200:ILE:HG22	6:i:201:CYS:N	2.34	0.42
6:i:489:TRP:O	6:i:492:GLU:HG2	2.19	0.42
8:k:155:ILE:HD13	8:k:167:ILE:HB	2.02	0.42
9:l:103:SER:O	9:l:104:SER:OG	2.36	0.42
12:p:12:THR:HA	12:p:15:LEU:HG	2.00	0.42
3:C:59:VAL:HG13	4:D:57:LEU:HD11	2.01	0.42
5:H:140:HIS:CD2	13:T:827:GLU:HA	2.55	0.42
6:I:363:ILE:CG2	6:I:365:VAL:HG12	2.49	0.42
8:K:146:GLN:O	8:K:149:SER:OG	2.32	0.42
11:O:224:TYR:OH	11:O:261:LEU:HD11	2.19	0.42
12:P:57:LEU:CD2	12:P:59:ILE:HD11	2.50	0.42
5:h:92:THR:O	5:h:93:VAL:C	2.61	0.42
9:l:41:VAL:HG12	9:l:42:SER:O	2.19	0.42
10:n:14:ILE:CD1	10:n:26:VAL:HG11	2.50	0.42
13:t:983:ARG:O	13:t:987:VAL:HG12	2.20	0.42
4:D:11:ARG:HA	4:D:11:ARG:NE	2.35	0.42
6:I:69:ILE:HD13	6:I:216:ARG:HB3	2.02	0.42
6:I:505:LEU:HD13	6:I:539:ILE:HG21	2.02	0.42
12:P:36:THR:O	12:P:37:LYS:C	2.63	0.42
13:T:904:TRP:CH2	13:T:937:TYR:HD1	2.38	0.42
3:c:56:LEU:HA	3:c:59:VAL:HG22	2.02	0.42
5:h:91:VAL:O	5:h:92:THR:C	2.62	0.42
8:k:198:LEU:O	8:k:201:ASP:HB3	2.20	0.42
6:I:141:VAL:HG13	6:I:142:LYS:N	2.35	0.42
14:X:-43:DA:H2''	14:X:-42:DG:C8	2.54	0.42
5:h:58:LYS:HB3	5:h:59:PRO:HD3	2.00	0.42
5:h:140:HIS:CD2	13:t:826:ILE:HG23	2.54	0.42
5:h:209:CYS:HB2	8:k:202:THR:HG22	2.00	0.42
13:t:897:TYR:CZ	13:t:899:PRO:HG3	2.55	0.42
1:A:64:ILE:HG22	2:B:62:GLN:OE1	2.20	0.42
2:B:46:GLU:OE1	4:D:32:LEU:HA	2.20	0.42
5:H:196:MET:HE2	8:K:140:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:932:LEU:HD21	13:T:964:LEU:CD2	2.36	0.42
14:X:-61:DT:H2''	14:X:-60:DA:C5'	2.49	0.42
15:Y:48:DG:OP1	13:t:900:LYS:HA	2.19	0.42
8:k:191:GLU:OE1	8:k:191:GLU:N	2.44	0.42
12:p:33:GLU:HG3	12:p:34:LEU:CD2	2.49	0.42
13:t:992:ASP:OD1	13:t:995:ASN:ND2	2.53	0.42
13:t:1014:VAL:HG12	13:t:1014:VAL:O	2.20	0.42
1:A:42:ILE:O	1:A:46:ILE:HG13	2.19	0.42
4:D:22:ILE:CG2	5:H:10:VAL:HG12	2.50	0.42
5:H:79:TYR:O	5:H:80:GLY:C	2.63	0.42
5:H:88:LEU:O	5:H:89:GLU:C	2.61	0.42
10:N:191:ASP:OD1	10:N:192:ALA:N	2.53	0.42
11:O:79:ASP:O	11:O:83:ARG:HG2	2.20	0.42
12:P:141:ARG:O	12:P:144:SER:OG	2.36	0.42
13:T:832:ASN:HA	13:T:835:LYS:HG2	2.00	0.42
14:X:-36:DG:H4'	14:X:-35:DG:OP1	2.20	0.42
6:i:166:LYS:O	13:t:906:THR:HG21	2.19	0.42
10:n:42:ARG:NH2	13:t:891:TYR:HB2	2.35	0.42
10:n:315:ILE:HD12	10:n:315:ILE:H	1.85	0.42
12:p:53:ASP:CG	12:p:54:GLY:H	2.28	0.42
6:I:21:ASP:OD1	6:I:22:LEU:N	2.49	0.41
6:I:217:PHE:O	6:I:220:THR:OG1	2.29	0.41
7:M:144:LEU:HD12	7:M:144:LEU:N	2.35	0.41
10:N:38:PHE:CE1	13:T:889:MET:HA	2.54	0.41
12:P:200:ALA:HB2	12:P:209:MET:HE2	2.02	0.41
12:P:281:LEU:HA	12:P:284:ILE:HG22	2.01	0.41
13:T:824:MET:HE3	13:T:824:MET:HB3	1.92	0.41
13:T:993:ILE:H	13:T:993:ILE:CD1	2.30	0.41
6:i:632:ASP:OD1	6:i:633:ASN:N	2.53	0.41
10:n:148:ASP:OD1	10:n:149:THR:N	2.53	0.41
13:T:818:SER:HA	13:T:821:GLU:CG	2.50	0.41
13:T:932:LEU:HD11	13:T:964:LEU:CD2	2.50	0.41
13:T:964:LEU:C	13:T:966:ILE:HD12	2.45	0.41
13:T:967:VAL:HG21	13:T:973:PHE:HD1	1.85	0.41
13:T:984:GLU:HG2	13:T:985:ILE:N	2.36	0.41
14:X:-25:DC:H2'	14:X:-24:DT:H71	1.99	0.41
5:h:95:CYS:O	5:h:96:VAL:C	2.63	0.41
12:p:175:PRO:HA	12:p:178:VAL:HG22	2.02	0.41
13:t:890:LYS:C	13:t:892:LYS:H	2.28	0.41
13:t:926:ARG:HD3	13:t:926:ARG:C	2.45	0.41
3:C:49:MET:CE	4:D:40:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:30:LEU:O	6:I:34:VAL:HG23	2.20	0.41
7:J:143:LEU:C	7:J:144:LEU:HD12	2.46	0.41
8:K:165:LEU:O	8:K:168:GLU:HG3	2.20	0.41
9:L:272:VAL:HG22	9:L:274:MET:SD	2.61	0.41
10:N:6:LYS:HE2	10:N:74:LEU:HD13	2.02	0.41
15:Y:50:DA:H2''	15:Y:51:DC:H6	1.85	0.41
9:l:37:LYS:NZ	9:l:269:ASN:O	2.47	0.41
10:n:23:CYS:HA	10:n:27:LEU:HD12	2.01	0.41
12:p:168:VAL:HG22	12:p:168:VAL:O	2.20	0.41
13:t:825:ARG:NE	13:t:829:GLU:OE2	2.52	0.41
13:t:990:VAL:HG22	13:t:991:PRO:HD2	2.02	0.41
6:I:108:ALA:O	6:I:111:GLU:HG3	2.21	0.41
6:I:312:ALA:HA	6:I:359:LEU:HD21	2.02	0.41
7:J:115:VAL:HG11	7:J:157:LEU:HD21	2.03	0.41
8:K:80:LEU:O	8:K:83:ILE:HG22	2.19	0.41
9:L:61:ILE:HG22	9:L:79:VAL:HG21	2.03	0.41
14:X:-32:DT:C2	14:X:-31:DA:C5	3.08	0.41
15:Y:31:DT:H2''	15:Y:32:DA:C8	2.55	0.41
1:a:20:GLN:HE22	11:o:67:VAL:HG12	1.84	0.41
3:c:36:LEU:O	3:c:39:ILE:HG22	2.21	0.41
6:i:337:ILE:O	9:l:162:LYS:NZ	2.45	0.41
8:k:188:ILE:O	8:k:188:ILE:HG23	2.20	0.41
4:D:69:ARG:C	4:D:70:SER:HG	2.14	0.41
6:I:59:THR:O	6:I:62:THR:HG22	2.21	0.41
6:I:70:PRO:HG3	6:I:74:VAL:HG22	2.01	0.41
6:I:79:VAL:HG21	6:I:119:ALA:HB1	2.02	0.41
9:L:171:LEU:O	9:L:259:ILE:HD12	2.20	0.41
13:T:915:ASP:OD1	13:T:915:ASP:C	2.63	0.41
13:T:982:PRO:HB2	13:T:984:GLU:OE2	2.21	0.41
15:Y:32:DA:H1'	15:Y:33:DC:H5'	2.03	0.41
3:c:49:MET:HE2	3:c:53:TYR:HE2	1.85	0.41
5:h:96:VAL:O	5:h:97:ALA:C	2.63	0.41
6:i:64:LEU:HD23	6:i:64:LEU:O	2.20	0.41
6:i:430:MET:O	6:i:434:LEU:HD23	2.21	0.41
8:k:165:LEU:HA	8:k:168:GLU:HG3	2.02	0.41
8:k:212:LYS:HE2	13:t:975:GLN:HG3	1.99	0.41
13:t:961:MET:HB2	13:t:967:VAL:HG22	2.03	0.41
1:A:67:ILE:HG21	2:B:62:GLN:HE21	1.85	0.41
6:I:473:ALA:HA	6:I:476:TYR:CE2	2.56	0.41
7:J:93:LEU:HD21	7:J:127:ILE:HD13	2.03	0.41
7:J:113:VAL:CG2	7:J:144:LEU:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:89:SER:O	11:O:93:GLY:N	2.48	0.41
13:T:1014:VAL:HG12	13:T:1014:VAL:O	2.21	0.41
14:X:-47:DC:H2''	14:X:-46:DT:C7	2.51	0.41
14:X:-23:DT:C2	14:X:-22:DG:C8	3.08	0.41
6:i:51:TRP:CD1	6:i:64:LEU:HD22	2.55	0.41
12:p:12:THR:HA	12:p:15:LEU:CG	2.51	0.41
12:p:38:LYS:HD2	12:p:38:LYS:C	2.45	0.41
5:H:72:THR:OG1	5:H:73:GLU:N	2.54	0.41
14:X:-26:DC:H6	14:X:-26:DC:H2'	1.70	0.41
4:d:45:SER:HB2	11:o:49:ARG:HE	1.85	0.41
6:i:9:ASP:HA	6:i:12:LYS:HG2	2.02	0.41
6:i:141:VAL:HG13	6:i:142:LYS:N	2.36	0.41
6:i:527:GLU:OE2	6:i:647:TYR:N	2.49	0.41
13:t:952:ASP:N	13:t:952:ASP:OD1	2.54	0.41
6:I:74:VAL:N	6:I:114:CYS:O	2.53	0.41
10:N:110:LEU:O	10:N:114:ILE:HG22	2.21	0.41
10:N:315:ILE:HD12	10:N:315:ILE:H	1.86	0.41
11:O:38:LYS:HD2	11:O:38:LYS:C	2.46	0.41
12:P:21:LEU:HD12	12:P:21:LEU:C	2.46	0.41
12:P:169:LEU:HD13	12:P:178:VAL:HG23	2.01	0.41
15:Y:22:DC:C2	15:Y:23:DA:N7	2.89	0.41
15:Y:48:DG:H2''	15:Y:49:DC:H6	1.84	0.41
15:Y:62:DT:H2''	15:Y:63:DA:C8	2.56	0.41
8:k:2:THR:HG23	12:p:43:ILE:HD13	2.01	0.41
8:k:98:LYS:O	8:k:101:ILE:HG22	2.21	0.41
11:o:43:GLU:O	11:o:47:LEU:HG	2.21	0.41
11:o:145:ILE:HD12	11:o:164:ILE:HD12	2.02	0.41
13:t:915:ASP:OD1	13:t:916:LYS:N	2.54	0.41
4:D:72:HIS:CE1	6:I:384:THR:HG23	2.56	0.41
6:I:191:GLU:OE1	6:I:191:GLU:N	2.41	0.41
6:I:553:HIS:O	6:I:557:ILE:HG12	2.21	0.41
7:J:110:ARG:HG3	7:J:110:ARG:O	2.20	0.41
9:L:98:LEU:HD23	9:L:98:LEU:C	2.46	0.41
9:L:255:ASP:OD1	9:L:255:ASP:N	2.47	0.41
7:M:115:VAL:HG11	7:M:157:LEU:HD21	2.02	0.41
10:N:26:VAL:HG23	10:N:27:LEU:N	2.36	0.41
10:N:42:ARG:NH2	13:T:891:TYR:HB2	2.35	0.41
10:N:126:THR:HG21	10:N:145:LEU:HB3	2.02	0.41
11:O:67:VAL:HG21	11:O:72:ILE:HD11	2.02	0.41
13:T:818:SER:HA	13:T:821:GLU:HG3	2.02	0.41
13:T:932:LEU:HD11	13:T:964:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:-72:DA:C2'	14:X:-71:DT:H71	2.50	0.41
14:X:-40:DC:H2''	14:X:-39:DT:OP2	2.21	0.41
14:X:-38:DA:C2'	14:X:-37:DG:C8	3.04	0.41
4:d:22:ILE:HB	5:h:10:VAL:HG11	2.03	0.41
6:i:155:ARG:O	6:i:158:VAL:HG22	2.21	0.41
11:o:37:LEU:HD13	12:p:24:ILE:HG12	2.03	0.41
12:p:60:ASP:N	12:p:61:PRO:HD3	2.35	0.41
12:p:256:TYR:HA	12:p:259:LYS:HG2	2.03	0.41
13:t:917:LEU:HD23	13:t:928:ARG:CG	2.51	0.41
5:H:140:HIS:CB	13:T:830:VAL:HG11	2.47	0.41
5:H:203:ILE:HD11	8:K:154:LEU:HD22	2.03	0.41
7:J:106:ASP:OD1	7:J:106:ASP:N	2.54	0.41
15:Y:56:DC:H1'	15:Y:57:DA:C5	2.56	0.41
8:k:37:GLU:OE1	8:k:37:GLU:N	2.41	0.41
13:t:909:LEU:HD23	13:t:909:LEU:N	2.36	0.41
5:H:209:CYS:HB2	8:K:202:THR:HG22	2.02	0.40
6:I:184:LEU:O	6:I:187:SER:OG	2.31	0.40
7:J:23:LEU:HD13	7:J:169:ILE:CD1	2.50	0.40
7:J:144:LEU:HD12	7:J:144:LEU:N	2.36	0.40
8:K:91:GLU:OE1	8:K:91:GLU:HA	2.21	0.40
9:L:207:LEU:HD12	9:L:207:LEU:N	2.36	0.40
11:O:68:ARG:CG	11:O:69:PRO:HD2	2.50	0.40
14:X:-51:DG:C4	14:X:-50:DT:C5	3.09	0.40
10:n:73:ILE:HG23	10:n:74:LEU:HD12	2.02	0.40
10:n:94:MET:HB3	10:n:186:TYR:CG	2.57	0.40
11:o:38:LYS:HE3	11:o:38:LYS:HB3	1.94	0.40
1:A:16:ILE:HG12	11:O:69:PRO:HB3	2.03	0.40
5:H:95:CYS:O	5:H:96:VAL:C	2.63	0.40
5:H:232:ASP:O	5:H:235:THR:HG22	2.20	0.40
14:X:-61:DT:H2'	14:X:-60:DA:H8	1.73	0.40
6:i:191:GLU:OE1	6:i:191:GLU:N	2.42	0.40
9:l:185:ARG:NE	9:l:185:ARG:HA	2.36	0.40
10:n:44:ALA:HB3	10:n:46:LEU:CD2	2.52	0.40
5:H:140:HIS:O	5:H:143:MET:HG2	2.22	0.40
6:I:161:ILE:HG21	6:I:181:LEU:HD22	2.04	0.40
10:N:68:HIS:C	10:N:68:HIS:HD1	2.28	0.40
11:O:61:LYS:N	11:O:61:LYS:HD3	2.36	0.40
13:T:926:ARG:O	13:T:926:ARG:HD3	2.20	0.40
14:X:-62:DA:C2'	14:X:-61:DT:C6	3.04	0.40
14:X:-50:DT:H2''	14:X:-49:DG:H8	1.86	0.40
15:Y:34:DT:H2''	15:Y:35:DC:OP2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:59:DA:C2'	15:Y:60:DT:H71	2.51	0.40
8:k:135:GLU:OE1	8:k:135:GLU:N	2.41	0.40
10:n:35:ARG:NE	10:n:35:ARG:HA	2.36	0.40
11:o:31:GLU:HA	11:o:34:ARG:NE	2.36	0.40
11:o:278:MET:SD	11:o:278:MET:C	3.05	0.40
10:N:61:ILE:HB	10:N:65:LEU:HD13	2.04	0.40
12:P:18:GLN:HA	12:P:21:LEU:HG	2.03	0.40
13:T:999:ILE:CG2	13:T:1000:PRO:HD2	2.50	0.40
15:Y:67:DA:H1'	15:Y:68:DT:O5'	2.21	0.40
1:a:46:ILE:HD12	3:c:53:TYR:CZ	2.57	0.40
5:h:210:ARG:CZ	8:k:159:PHE:CD1	3.04	0.40
8:k:162:THR:O	8:k:166:ILE:HG13	2.21	0.40
11:o:127:MET:SD	11:o:156:MET:HE3	2.61	0.40
13:t:957:LEU:HB3	13:t:973:PHE:HZ	1.87	0.40
1:A:11:LEU:HD23	1:A:11:LEU:C	2.46	0.40
5:H:5:LYS:HA	5:H:8:LYS:HG2	2.04	0.40
5:H:96:VAL:O	5:H:97:ALA:C	2.62	0.40
15:Y:67:DA:H5'	15:Y:67:DA:H8	1.83	0.40
5:h:87:LEU:O	5:h:88:LEU:C	2.64	0.40
6:i:42:ASP:O	6:i:46:THR:HG23	2.22	0.40
6:i:113:ASP:OD2	6:i:224:ARG:NH2	2.54	0.40
10:n:48:MET:O	10:n:49:THR:C	2.64	0.40
11:o:131:ALA:O	11:o:132:ASN:C	2.63	0.40
13:t:916:LYS:CD	13:t:966:ILE:HD13	2.49	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	68/95 (72%)	67 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	68/95 (72%)	68 (100%)	0	0	100	100
2	B	53/82 (65%)	53 (100%)	0	0	100	100
2	b	53/82 (65%)	53 (100%)	0	0	100	100
3	C	60/72 (83%)	59 (98%)	1 (2%)	0	100	100
3	c	60/72 (83%)	60 (100%)	0	0	100	100
4	D	69/81 (85%)	68 (99%)	1 (1%)	0	100	100
4	d	69/81 (85%)	68 (99%)	1 (1%)	0	100	100
5	H	224/239 (94%)	210 (94%)	14 (6%)	0	100	100
5	h	224/239 (94%)	211 (94%)	13 (6%)	0	100	100
6	I	572/661 (86%)	560 (98%)	12 (2%)	0	100	100
6	i	572/661 (86%)	560 (98%)	12 (2%)	0	100	100
7	J	161/180 (89%)	156 (97%)	5 (3%)	0	100	100
7	M	161/180 (89%)	155 (96%)	6 (4%)	0	100	100
8	K	205/219 (94%)	201 (98%)	4 (2%)	0	100	100
8	k	205/219 (94%)	202 (98%)	3 (2%)	0	100	100
9	L	229/302 (76%)	217 (95%)	12 (5%)	0	100	100
9	l	229/302 (76%)	216 (94%)	12 (5%)	1 (0%)	30	67
10	N	318/328 (97%)	307 (96%)	11 (4%)	0	100	100
10	n	318/328 (97%)	306 (96%)	12 (4%)	0	100	100
11	O	252/325 (78%)	236 (94%)	14 (6%)	2 (1%)	16	53
11	o	252/325 (78%)	236 (94%)	14 (6%)	2 (1%)	16	53
12	P	279/638 (44%)	266 (95%)	13 (5%)	0	100	100
12	p	279/638 (44%)	259 (93%)	20 (7%)	0	100	100
13	T	150/1016 (15%)	140 (93%)	10 (7%)	0	100	100
13	t	150/1016 (15%)	138 (92%)	12 (8%)	0	100	100
All	All	5280/8476 (62%)	5072 (96%)	203 (4%)	5 (0%)	49	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	O	210	VAL
11	o	210	VAL
11	O	211	GLU

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Mol	Chain	Res	Type
11	o	211	GLU
9	l	201	VAL

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	64/89 (72%)	63 (98%)	1 (2%)	55	69
1	a	64/89 (72%)	63 (98%)	1 (2%)	55	69
2	B	52/76 (68%)	52 (100%)	0	100	100
2	b	52/76 (68%)	52 (100%)	0	100	100
3	C	56/66 (85%)	56 (100%)	0	100	100
3	c	56/66 (85%)	56 (100%)	0	100	100
4	D	65/75 (87%)	65 (100%)	0	100	100
4	d	65/75 (87%)	64 (98%)	1 (2%)	57	70
5	H	206/217 (95%)	206 (100%)	0	100	100
5	h	206/217 (95%)	206 (100%)	0	100	100
6	I	511/584 (88%)	510 (100%)	1 (0%)	87	85
6	i	511/584 (88%)	511 (100%)	0	100	100
7	J	147/161 (91%)	147 (100%)	0	100	100
7	M	147/161 (91%)	147 (100%)	0	100	100
8	K	189/198 (96%)	188 (100%)	1 (0%)	81	81
8	k	189/198 (96%)	189 (100%)	0	100	100
9	L	218/277 (79%)	217 (100%)	1 (0%)	81	81
9	l	218/277 (79%)	218 (100%)	0	100	100
10	N	285/290 (98%)	284 (100%)	1 (0%)	84	82
10	n	285/290 (98%)	285 (100%)	0	100	100
11	O	228/295 (77%)	228 (100%)	0	100	100
11	o	228/295 (77%)	228 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	P	255/579 (44%)	254 (100%)	1 (0%)	84	82
12	p	255/579 (44%)	255 (100%)	0	100	100
13	T	144/942 (15%)	143 (99%)	1 (1%)	76	79
13	t	144/942 (15%)	144 (100%)	0	100	100
All	All	4840/7698 (63%)	4831 (100%)	9 (0%)	85	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ILE
6	I	558	GLN
8	K	40	SER
9	L	187	ASN
10	N	247	GLU
12	P	40	THR
13	T	889	MET
1	a	33	ILE
4	d	41	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
2	B	48	ASN
3	C	62	GLN
4	D	72	HIS
5	H	20	GLN
6	I	553	HIS
6	I	561	HIS
6	I	612	HIS
9	L	189	GLN
11	O	104	HIS
12	P	96	ASN
12	P	160	HIS
1	a	20	GLN
1	a	45	ASN
2	b	55	HIS
2	b	74	ASN
4	d	72	HIS
5	h	123	ASN

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Mol	Chain	Res	Type
5	h	152	HIS
5	h	153	ASN
6	i	328	HIS
6	i	361	GLN
6	i	553	HIS
6	i	561	HIS
6	i	612	HIS
8	k	114	GLN
9	l	189	GLN
9	l	260	ASN
11	o	27	GLN
11	o	117	ASN
13	t	819	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

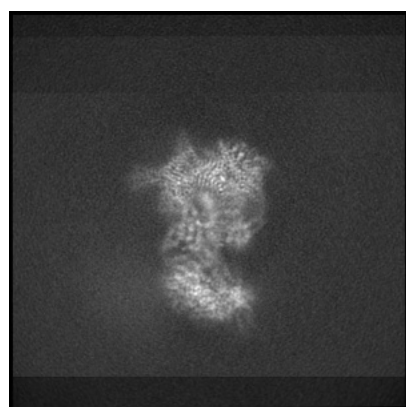
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70558. These allow visual inspection of the internal detail of the map and identification of artifacts.

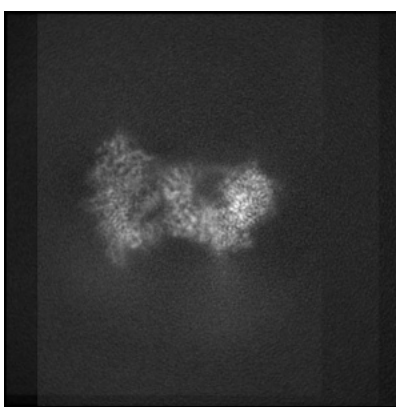
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

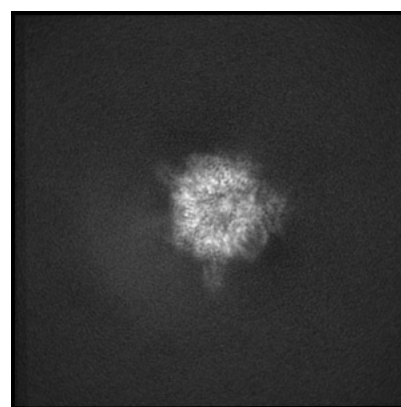
6.1.1 Primary map



X



Y

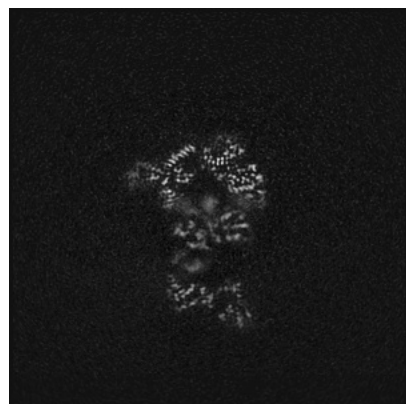


Z

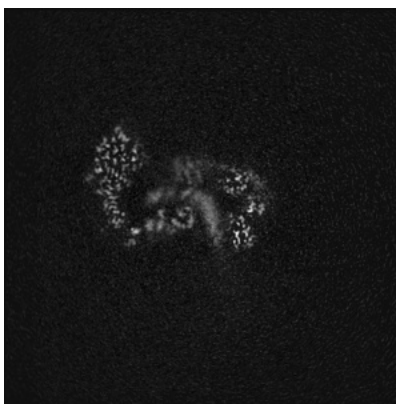
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

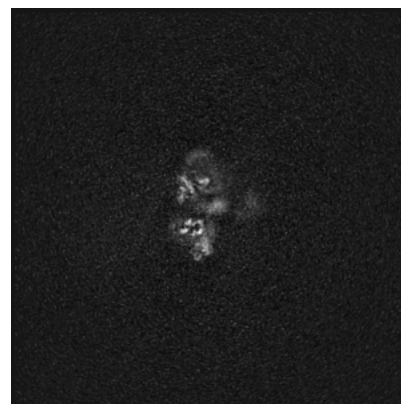
6.2.1 Primary map



X Index: 203



Y Index: 203

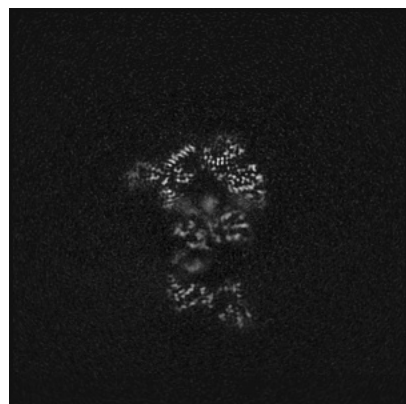


Z Index: 202

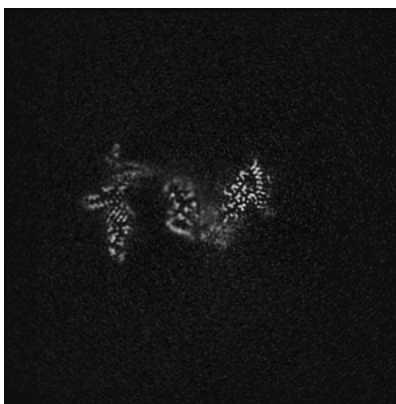
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

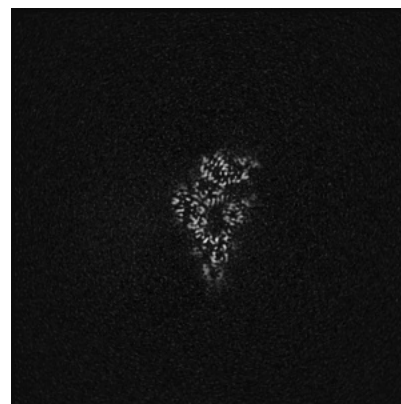
6.3.1 Primary map



X Index: 203



Y Index: 233

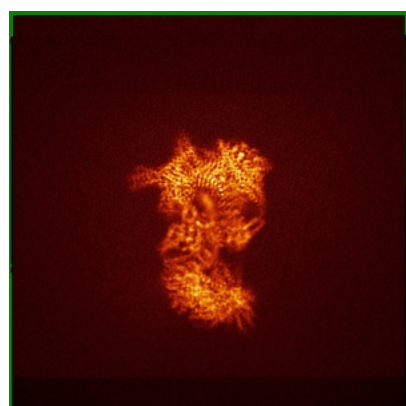


Z Index: 240

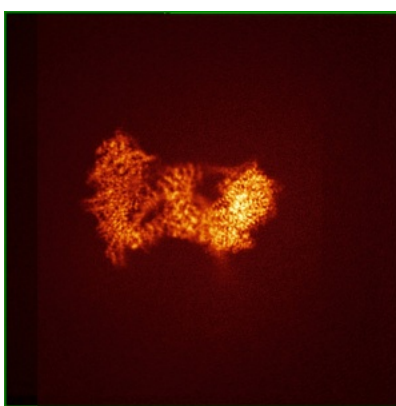
The images above show the largest variance slices of the map in three orthogonal directions.

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

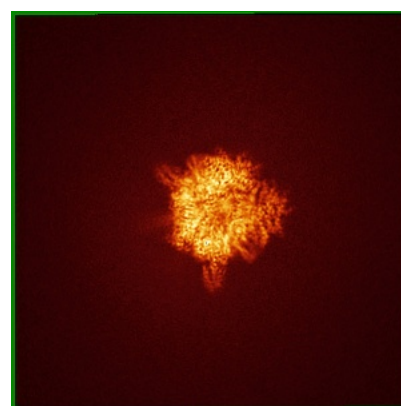
6.4.1 Primary map



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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00342. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

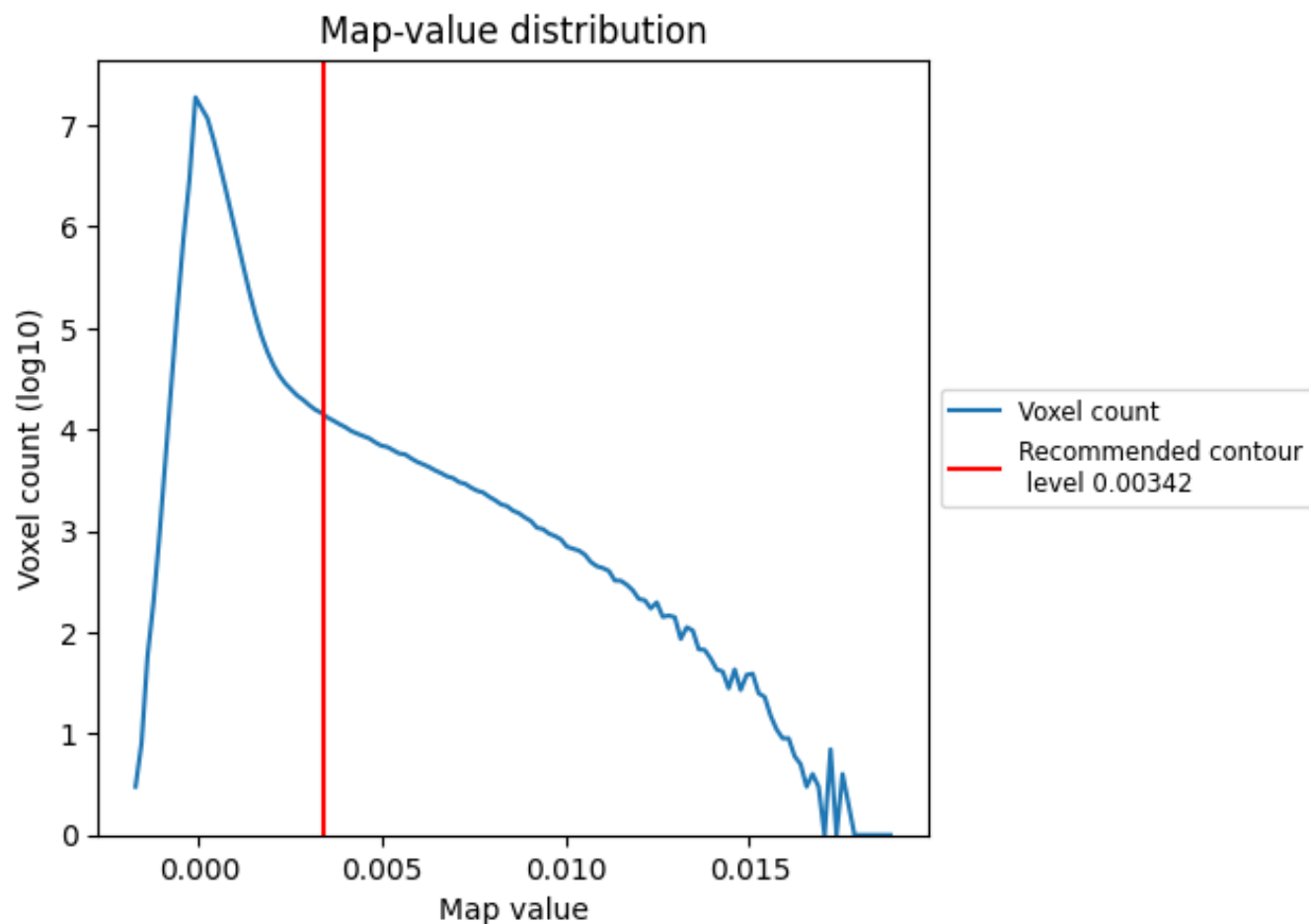
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

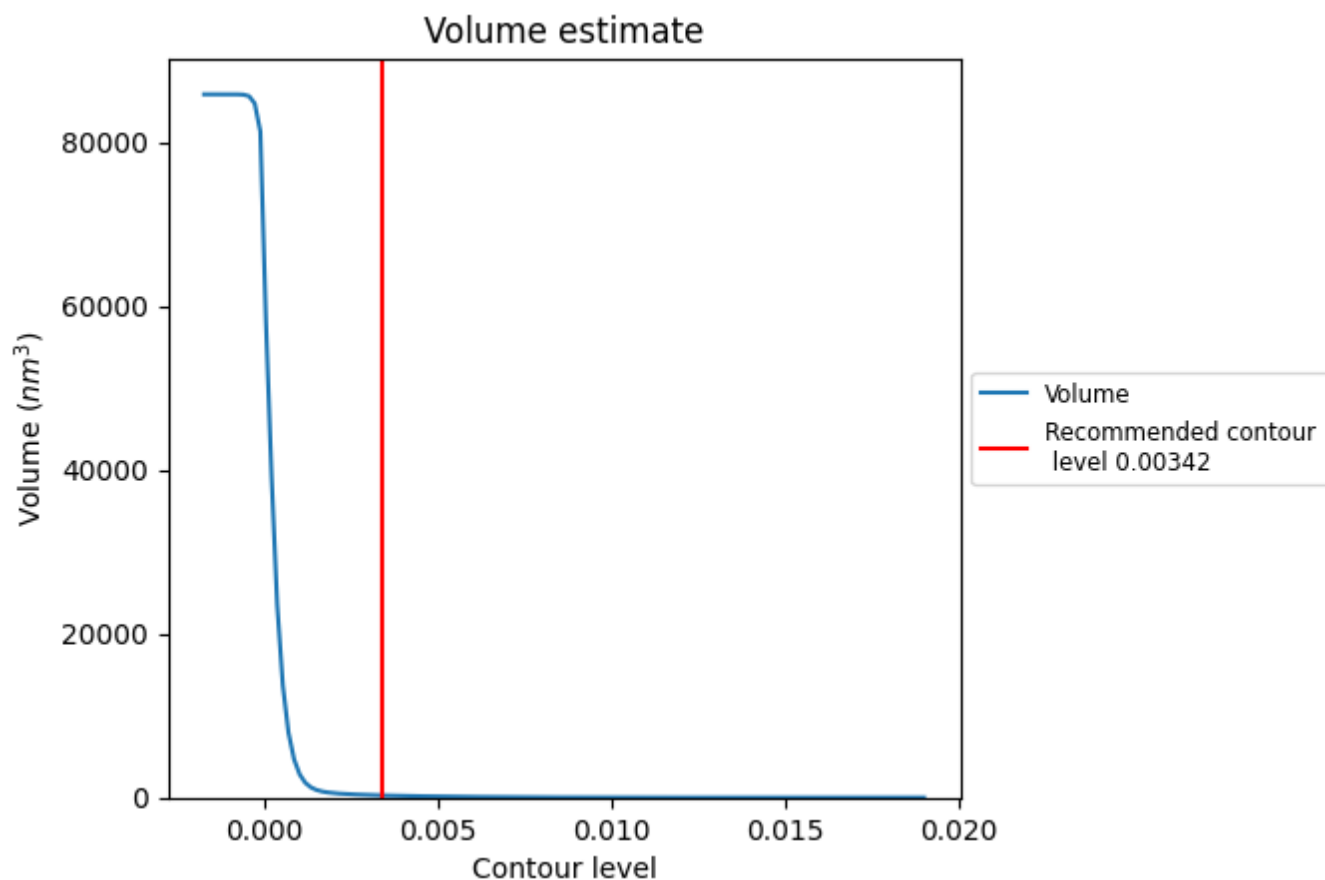
This section contains the results of statistical analysis of the map.

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 260 nm³; this corresponds to an approximate mass of 235 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

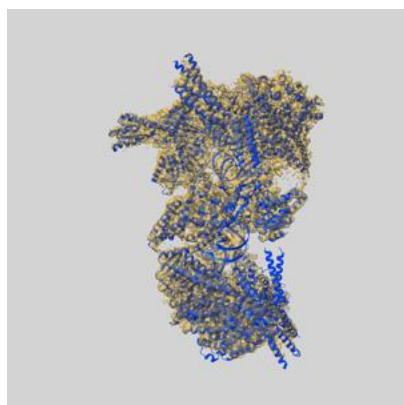
8 Fourier-Shell correlation ⓘ

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

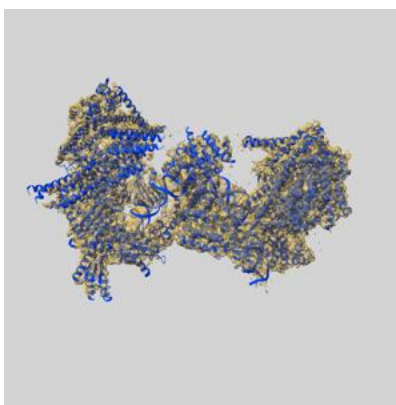
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70558 and PDB model 9OKB. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

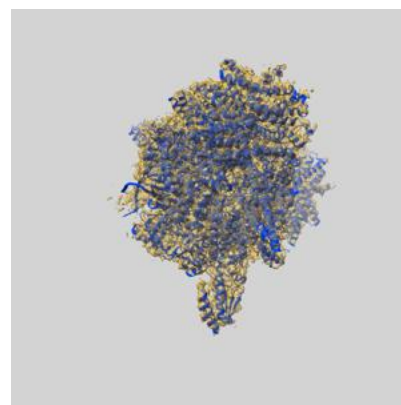
9.1 Map-model overlay [i](#)



X



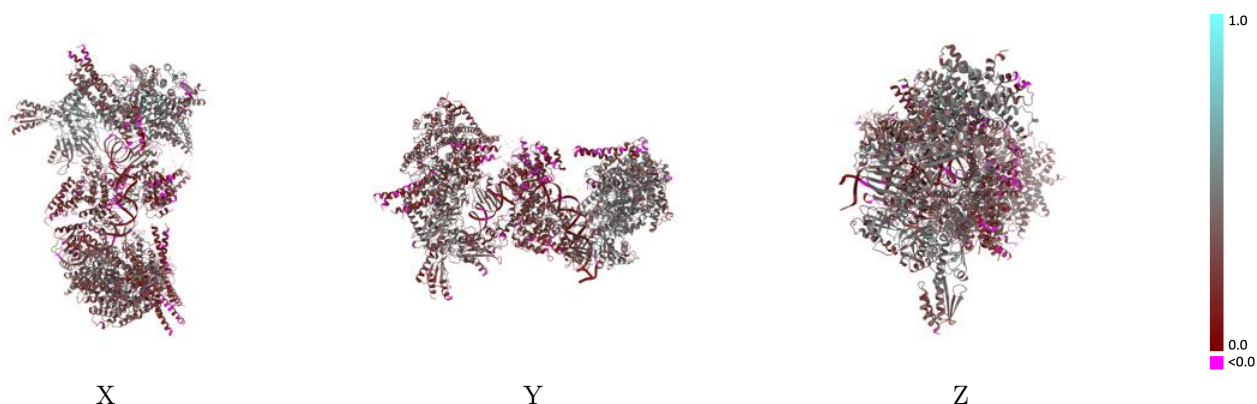
Y



Z

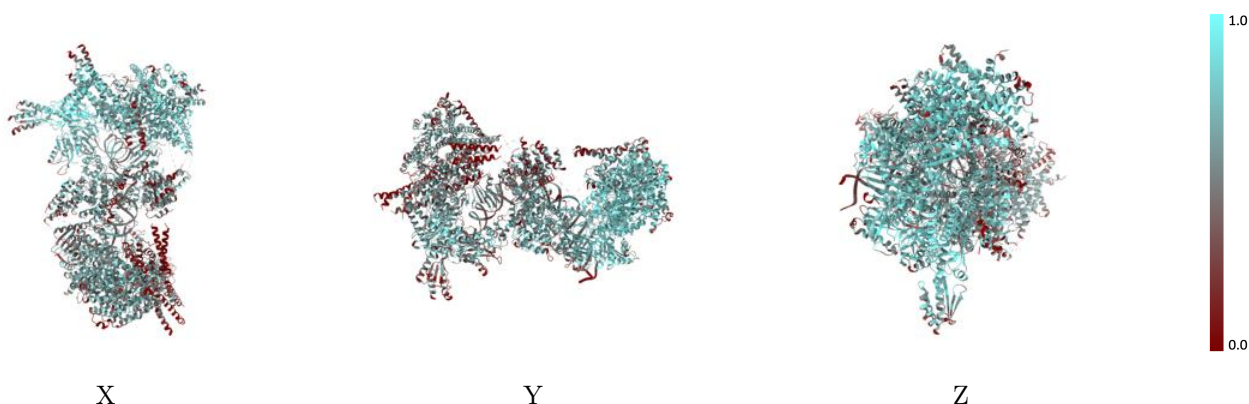
The images above show the 3D surface view of the map at the recommended contour level 0.00342 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



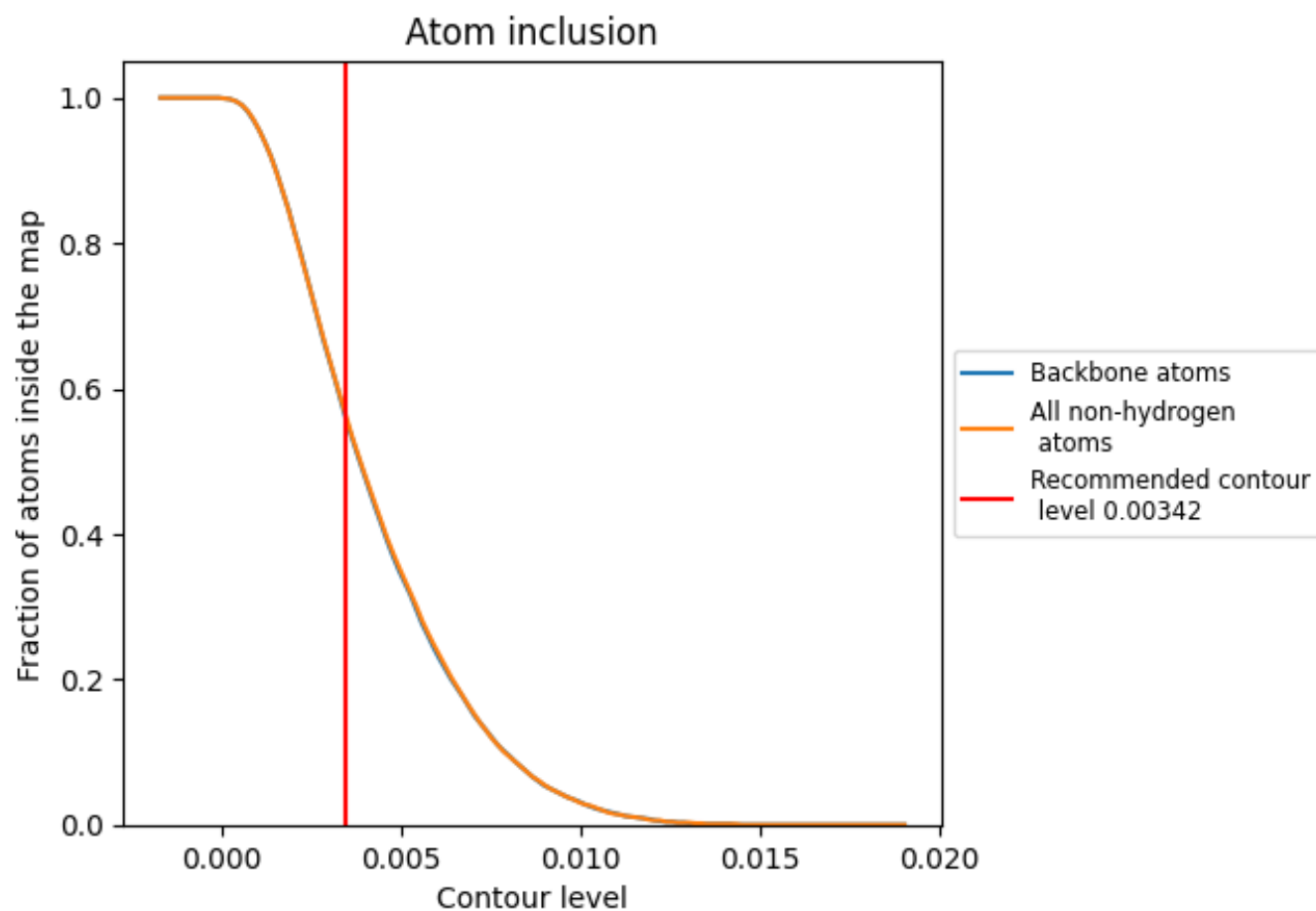
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00342).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 57% 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 (0.00342) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5670	 0.3210
A	 0.6010	 0.3400
B	 0.6760	 0.3920
C	 0.6100	 0.3110
D	 0.7250	 0.3980
H	 0.6750	 0.3610
I	 0.6410	 0.3430
J	 0.6090	 0.4130
K	 0.6580	 0.3240
L	 0.7390	 0.3700
M	 0.8090	 0.4740
N	 0.7370	 0.3760
O	 0.7190	 0.3920
P	 0.6260	 0.3550
T	 0.6030	 0.3130
X	 0.4740	 0.1210
Y	 0.4620	 0.1160
a	 0.2490	 0.2700
b	 0.3880	 0.3150
c	 0.2540	 0.1940
d	 0.4060	 0.3060
h	 0.4980	 0.2790
i	 0.5160	 0.2780
k	 0.5220	 0.2640
l	 0.5540	 0.3170
n	 0.6210	 0.3300
o	 0.4810	 0.3260
p	 0.4120	 0.2900
t	 0.5220	 0.3030

