



Full wwPDB EM Validation Report ⓘ

May 14, 2026 – 01:48 pm BST

PDB ID : 9TAY / pdb_00009tay
EMDB ID : EMD-55759
Title : Structure of the human inner kinetochore CCAN bound to a di-CENP-A nucleosome
Authors : Yu, C.; Barford, D.
Deposited on : 2025-11-18
Resolution : 15.50 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

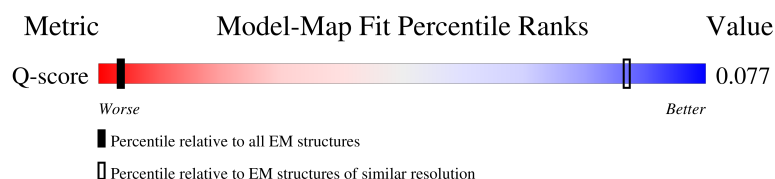
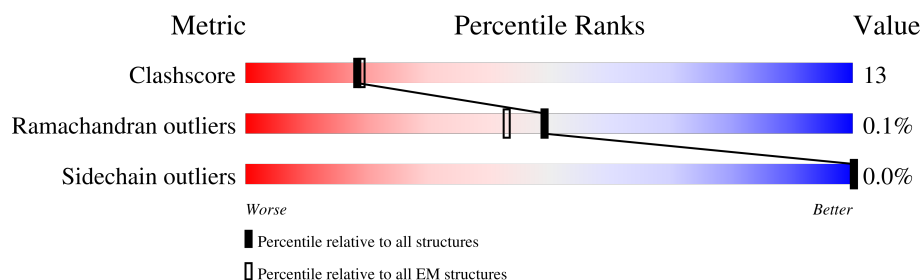
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 15.50 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	53 (15.00 - 16.00)

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	H	247	
2	I	762	
3	K	269	
4	L	348	

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Mol	Chain	Length	Quality of chain
5	M	180	
6	N	347	
7	O	300	
8	Q	215	
9	U	211	
10	P	288	
11	R	177	
12	T	777	
13	W	88	
14	S	138	
15	X	81	
16	A	140	
16	E	140	
16	c	140	
16	g	140	
17	B	103	
17	F	103	
17	d	103	
17	h	103	
18	C	153	
18	G	153	
18	e	153	
18	i	153	
19	D	126	
19	J	126	

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Mol	Chain	Length	Quality of chain
19	f	126	
19	j	126	
20	V	324	
21	Y	324	
22	Z	266	
22	a	266	
22	m	266	
22	n	266	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 57462 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Centromere protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	204	Total	C	N	O	S	0	0
			1652	1036	286	319	11		

- Molecule 2 is a protein called Centromere protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	622	Total	C	N	O	S	0	0
			5014	3283	810	890	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	757	GLU	-	expression tag	UNP Q92674
I	758	ASN	-	expression tag	UNP Q92674
I	759	LEU	-	expression tag	UNP Q92674
I	760	TYR	-	expression tag	UNP Q92674
I	761	PHE	-	expression tag	UNP Q92674
I	762	GLN	-	expression tag	UNP Q92674

- Molecule 3 is a protein called Centromere protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	233	Total	C	N	O	S	0	0
			1922	1220	318	374	10		

- Molecule 4 is a protein called Centromere protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	312	Total	C	N	O	S	0	0
			2502	1628	409	451	14		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-3	GLY	-	expression tag	UNP Q8N0S6
L	-2	PRO	-	expression tag	UNP Q8N0S6
L	-1	LEU	-	expression tag	UNP Q8N0S6
L	0	GLY	-	expression tag	UNP Q8N0S6

- Molecule 5 is a protein called Centromere protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	172	Total	C	N	O	S	0	0
			1325	839	236	243	7		

- Molecule 6 is a protein called Centromere protein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	318	Total	C	N	O	S	0	0
			2617	1681	454	472	10		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	288	LYS	GLU	conflict	UNP Q96H22
N	340	SER	-	expression tag	UNP Q96H22
N	341	ASP	-	expression tag	UNP Q96H22
N	342	LEU	-	expression tag	UNP Q96H22
N	343	GLU	-	expression tag	UNP Q96H22
N	344	VAL	-	expression tag	UNP Q96H22
N	345	LEU	-	expression tag	UNP Q96H22
N	346	PHE	-	expression tag	UNP Q96H22
N	347	GLN	-	expression tag	UNP Q96H22

- Molecule 7 is a protein called Centromere protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	210	Total	C	N	O	S	0	0
			1642	1060	277	298	7		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	1	MET	-	initiating methionine	UNP Q9BU64
O	2	GLU	-	expression tag	UNP Q9BU64
O	3	GLN	-	expression tag	UNP Q9BU64

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Chain	Residue	Modelled	Actual	Comment	Reference
O	4	ALA	-	expression tag	UNP Q9BU64
O	5	ASN	-	expression tag	UNP Q9BU64
O	6	PRO	-	expression tag	UNP Q9BU64
O	7	LEU	-	expression tag	UNP Q9BU64
O	8	ARG	-	expression tag	UNP Q9BU64
O	9	PRO	-	expression tag	UNP Q9BU64
O	10	ASP	-	expression tag	UNP Q9BU64
O	11	GLY	-	expression tag	UNP Q9BU64
O	12	GLU	-	expression tag	UNP Q9BU64
O	13	SER	-	expression tag	UNP Q9BU64
O	14	LYS	-	expression tag	UNP Q9BU64
O	15	GLY	-	expression tag	UNP Q9BU64
O	16	GLY	-	expression tag	UNP Q9BU64
O	17	VAL	-	expression tag	UNP Q9BU64
O	18	LEU	-	expression tag	UNP Q9BU64
O	19	ALA	-	expression tag	UNP Q9BU64
O	20	HIS	-	expression tag	UNP Q9BU64
O	21	LEU	-	expression tag	UNP Q9BU64
O	22	GLU	-	expression tag	UNP Q9BU64
O	23	ARG	-	expression tag	UNP Q9BU64
O	24	LEU	-	expression tag	UNP Q9BU64
O	25	GLU	-	expression tag	UNP Q9BU64
O	26	THR	-	expression tag	UNP Q9BU64
O	27	GLN	-	expression tag	UNP Q9BU64
O	28	VAL	-	expression tag	UNP Q9BU64
O	29	SER	-	expression tag	UNP Q9BU64
O	30	ARG	-	expression tag	UNP Q9BU64
O	31	SER	-	expression tag	UNP Q9BU64
O	32	ARG	-	expression tag	UNP Q9BU64
O	33	LYS	-	expression tag	UNP Q9BU64
O	34	GLN	-	expression tag	UNP Q9BU64
O	35	SER	-	expression tag	UNP Q9BU64
O	36	GLU	-	expression tag	UNP Q9BU64
O	37	GLU	-	expression tag	UNP Q9BU64
O	38	LEU	-	expression tag	UNP Q9BU64
O	39	GLN	-	expression tag	UNP Q9BU64
O	40	SER	-	expression tag	UNP Q9BU64
O	41	VAL	-	expression tag	UNP Q9BU64
O	42	GLN	-	expression tag	UNP Q9BU64
O	43	ALA	-	expression tag	UNP Q9BU64
O	44	GLN	-	expression tag	UNP Q9BU64
O	45	GLU	-	expression tag	UNP Q9BU64

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Chain	Residue	Modelled	Actual	Comment	Reference
O	46	GLY	-	expression tag	UNP Q9BU64
O	47	ALA	-	expression tag	UNP Q9BU64
O	48	LEU	-	expression tag	UNP Q9BU64
O	49	GLY	-	expression tag	UNP Q9BU64
O	50	THR	-	expression tag	UNP Q9BU64
O	51	LYS	-	expression tag	UNP Q9BU64
O	52	ILE	-	expression tag	UNP Q9BU64
O	53	HIS	-	expression tag	UNP Q9BU64
O	54	LYS	-	expression tag	UNP Q9BU64
O	55	LEU	-	expression tag	UNP Q9BU64
O	56	ARG	-	expression tag	UNP Q9BU64
O	57	ARG	-	expression tag	UNP Q9BU64
O	58	LEU	-	expression tag	UNP Q9BU64
O	59	ARG	-	expression tag	UNP Q9BU64
O	60	ASP	-	expression tag	UNP Q9BU64
O	61	GLU	-	expression tag	UNP Q9BU64
O	62	LEU	-	expression tag	UNP Q9BU64
O	63	ARG	-	expression tag	UNP Q9BU64
O	64	ALA	-	expression tag	UNP Q9BU64
O	65	VAL	-	expression tag	UNP Q9BU64
O	66	VAL	-	expression tag	UNP Q9BU64
O	67	ARG	-	expression tag	UNP Q9BU64
O	68	HIS	-	expression tag	UNP Q9BU64
O	69	ARG	-	expression tag	UNP Q9BU64
O	70	ARG	-	expression tag	UNP Q9BU64
O	71	ALA	-	expression tag	UNP Q9BU64
O	72	SER	-	expression tag	UNP Q9BU64
O	73	VAL	-	expression tag	UNP Q9BU64
O	74	LYS	-	expression tag	UNP Q9BU64
O	75	ALA	-	expression tag	UNP Q9BU64
O	76	CYS	-	expression tag	UNP Q9BU64
O	77	ILE	-	expression tag	UNP Q9BU64
O	78	ALA	-	expression tag	UNP Q9BU64
O	79	ASN	-	expression tag	UNP Q9BU64
O	80	VAL	-	expression tag	UNP Q9BU64
O	81	GLU	-	expression tag	UNP Q9BU64
O	82	PRO	-	expression tag	UNP Q9BU64
O	83	ASN	-	expression tag	UNP Q9BU64
O	84	GLN	-	expression tag	UNP Q9BU64
O	85	THR	-	expression tag	UNP Q9BU64
O	86	VAL	-	expression tag	UNP Q9BU64
O	87	GLU	-	expression tag	UNP Q9BU64

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Chain	Residue	Modelled	Actual	Comment	Reference
O	88	ILE	-	expression tag	UNP Q9BU64

- Molecule 8 is a protein called Centromere protein Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	191	Total	C	N	O	S	0	0
			1526	953	258	304	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	54	MET	-	initiating methionine	UNP Q7L2Z9

- Molecule 9 is a protein called Centromere protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U	166	Total	C	N	O	S	0	0
			1365	861	242	257	5		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	419	GLU	-	expression tag	UNP Q71F23
U	420	ASN	-	expression tag	UNP Q71F23
U	421	LEU	-	expression tag	UNP Q71F23
U	422	TYR	-	expression tag	UNP Q71F23
U	423	PHE	-	expression tag	UNP Q71F23
U	424	GLN	-	expression tag	UNP Q71F23
U	425	SER	-	expression tag	UNP Q71F23
U	426	TRP	-	expression tag	UNP Q71F23
U	427	SER	-	expression tag	UNP Q71F23
U	428	HIS	-	expression tag	UNP Q71F23
U	429	PRO	-	expression tag	UNP Q71F23
U	430	GLN	-	expression tag	UNP Q71F23
U	431	PHE	-	expression tag	UNP Q71F23
U	432	GLU	-	expression tag	UNP Q71F23
U	433	LYS	-	expression tag	UNP Q71F23
U	434	GLY	-	expression tag	UNP Q71F23
U	435	GLY	-	expression tag	UNP Q71F23
U	436	GLY	-	expression tag	UNP Q71F23
U	437	SER	-	expression tag	UNP Q71F23
U	438	GLY	-	expression tag	UNP Q71F23

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Chain	Residue	Modelled	Actual	Comment	Reference
U	439	GLY	-	expression tag	UNP Q71F23
U	440	GLY	-	expression tag	UNP Q71F23
U	441	SER	-	expression tag	UNP Q71F23
U	442	GLY	-	expression tag	UNP Q71F23
U	443	GLY	-	expression tag	UNP Q71F23
U	444	GLY	-	expression tag	UNP Q71F23
U	445	SER	-	expression tag	UNP Q71F23
U	446	TRP	-	expression tag	UNP Q71F23
U	447	SER	-	expression tag	UNP Q71F23
U	448	HIS	-	expression tag	UNP Q71F23
U	449	PRO	-	expression tag	UNP Q71F23
U	450	GLN	-	expression tag	UNP Q71F23
U	451	PHE	-	expression tag	UNP Q71F23
U	452	GLU	-	expression tag	UNP Q71F23
U	453	LYS	-	expression tag	UNP Q71F23

- Molecule 10 is a protein called Centromere protein P.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	224	Total	C	N	O	S	0	0
			1788	1141	310	329	8		

- Molecule 11 is a protein called Centromere protein R.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	80	Total	C	N	O	S	0	0
			649	412	105	125	7		

- Molecule 12 is a protein called Methylated-DNA--protein-cysteine methyltransferase, Centromere protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	112	Total	C	N	O	S	0	0
			915	586	163	159	7		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-215	MET	-	initiating methionine	UNP P16455
T	-214	SER	-	expression tag	UNP P16455
T	-213	TYR	-	expression tag	UNP P16455
T	-212	TYR	-	expression tag	UNP P16455

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-211	HIS	-	expression tag	UNP P16455
T	-210	HIS	-	expression tag	UNP P16455
T	-209	HIS	-	expression tag	UNP P16455
T	-208	HIS	-	expression tag	UNP P16455
T	-207	HIS	-	expression tag	UNP P16455
T	-206	HIS	-	expression tag	UNP P16455
T	-205	ASP	-	expression tag	UNP P16455
T	-204	TYR	-	expression tag	UNP P16455
T	-203	ASP	-	expression tag	UNP P16455
T	-202	ILE	-	expression tag	UNP P16455
T	-201	PRO	-	expression tag	UNP P16455
T	-200	THR	-	expression tag	UNP P16455
T	-199	THR	-	expression tag	UNP P16455
T	-198	GLU	-	expression tag	UNP P16455
T	-197	ASN	-	expression tag	UNP P16455
T	-196	LEU	-	expression tag	UNP P16455
T	-195	TYR	-	expression tag	UNP P16455
T	-194	PHE	-	expression tag	UNP P16455
T	-193	GLN	-	expression tag	UNP P16455
T	-192	GLY	-	expression tag	UNP P16455
T	-162	ARG	GLU	conflict	UNP P16455
T	-160	ILE	LYS	conflict	UNP P16455
T	-159	PHE	LEU	conflict	UNP P16455
T	-130	ALA	CYS	conflict	UNP P16455
T	-77	SER	GLN	conflict	UNP P16455
T	-76	HIS	GLN	conflict	UNP P16455
T	-67	ALA	LYS	conflict	UNP P16455
T	-65	THR	ALA	conflict	UNP P16455
T	-64	ALA	ARG	conflict	UNP P16455
T	-61	LYS	GLY	conflict	UNP P16455
T	-60	THR	GLY	conflict	UNP P16455
T	-58	LEU	MET	conflict	UNP P16455
T	-57	SER	ARG	conflict	UNP P16455
T	-42	GLN	CYS	conflict	UNP P16455
T	-41	GLY	SER	conflict	UNP P16455
T	-40	ASP	SER	conflict	UNP P16455
T	-39	LEU	GLY	conflict	UNP P16455
T	-38	ASP	ALA	conflict	UNP P16455
T	-35	GLY	ASN	conflict	UNP P16455
T	-33	GLU	SER	conflict	UNP P16455
T	-9	SER	-	linker	UNP P16455
T	-8	ASP	-	linker	UNP P16455

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-7	LEU	-	linker	UNP P16455
T	-6	GLU	-	linker	UNP P16455
T	-5	VAL	-	linker	UNP P16455
T	-4	LEU	-	linker	UNP P16455
T	-3	PHE	-	linker	UNP P16455
T	-2	GLN	-	linker	UNP P16455
T	-1	GLY	-	linker	UNP P16455
T	0	PRO	-	linker	UNP P16455

- Molecule 13 is a protein called Centromere protein W.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	88	Total	C	N	O	S	0	0
			704	445	143	112	4		

- Molecule 14 is a protein called Centromere protein S.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	120	Total	C	N	O	S	0	0
			982	607	174	195	6		

- Molecule 15 is a protein called Centromere protein X.

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

- Molecule 16 is a protein called Histone H3-like centromeric protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A	99	Total	C	N	O	S	0	0
			816	526	156	133	1		
16	E	99	Total	C	N	O	S	0	0
			816	526	156	133	1		
16	c	99	Total	C	N	O	S	0	0
			816	526	156	133	1		
16	g	98	Total	C	N	O	S	0	0
			811	523	155	132	1		

- Molecule 17 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
17	F	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
17	d	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
17	h	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

- Molecule 18 is a protein called Histone H2A type 1-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	C	107	Total	C	N	O	0	0
			822	517	163	142		
18	G	108	Total	C	N	O	0	0
			831	523	165	143		
18	e	107	Total	C	N	O	0	0
			822	517	163	142		
18	i	108	Total	C	N	O	0	0
			831	523	165	143		

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-23	MET	-	initiating methionine	UNP Q93077
C	-22	GLY	-	expression tag	UNP Q93077
C	-21	SER	-	expression tag	UNP Q93077
C	-20	SER	-	expression tag	UNP Q93077
C	-19	HIS	-	expression tag	UNP Q93077
C	-18	HIS	-	expression tag	UNP Q93077
C	-17	HIS	-	expression tag	UNP Q93077
C	-16	HIS	-	expression tag	UNP Q93077
C	-15	HIS	-	expression tag	UNP Q93077
C	-14	HIS	-	expression tag	UNP Q93077
C	-13	SER	-	expression tag	UNP Q93077
C	-12	PRO	-	expression tag	UNP Q93077
C	-11	GLY	-	expression tag	UNP Q93077
C	-10	LEU	-	expression tag	UNP Q93077
C	-9	GLU	-	expression tag	UNP Q93077
C	-8	VAL	-	expression tag	UNP Q93077
C	-7	LEU	-	expression tag	UNP Q93077
C	-6	PHE	-	expression tag	UNP Q93077
C	-5	GLN	-	expression tag	UNP Q93077

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP Q93077
C	-3	PRO	-	expression tag	UNP Q93077
C	-2	ARG	-	expression tag	UNP Q93077
C	-1	GLY	-	expression tag	UNP Q93077
G	-23	MET	-	initiating methionine	UNP Q93077
G	-22	GLY	-	expression tag	UNP Q93077
G	-21	SER	-	expression tag	UNP Q93077
G	-20	SER	-	expression tag	UNP Q93077
G	-19	HIS	-	expression tag	UNP Q93077
G	-18	HIS	-	expression tag	UNP Q93077
G	-17	HIS	-	expression tag	UNP Q93077
G	-16	HIS	-	expression tag	UNP Q93077
G	-15	HIS	-	expression tag	UNP Q93077
G	-14	HIS	-	expression tag	UNP Q93077
G	-13	SER	-	expression tag	UNP Q93077
G	-12	PRO	-	expression tag	UNP Q93077
G	-11	GLY	-	expression tag	UNP Q93077
G	-10	LEU	-	expression tag	UNP Q93077
G	-9	GLU	-	expression tag	UNP Q93077
G	-8	VAL	-	expression tag	UNP Q93077
G	-7	LEU	-	expression tag	UNP Q93077
G	-6	PHE	-	expression tag	UNP Q93077
G	-5	GLN	-	expression tag	UNP Q93077
G	-4	GLY	-	expression tag	UNP Q93077
G	-3	PRO	-	expression tag	UNP Q93077
G	-2	ARG	-	expression tag	UNP Q93077
G	-1	GLY	-	expression tag	UNP Q93077
e	-23	MET	-	initiating methionine	UNP Q93077
e	-22	GLY	-	expression tag	UNP Q93077
e	-21	SER	-	expression tag	UNP Q93077
e	-20	SER	-	expression tag	UNP Q93077
e	-19	HIS	-	expression tag	UNP Q93077
e	-18	HIS	-	expression tag	UNP Q93077
e	-17	HIS	-	expression tag	UNP Q93077
e	-16	HIS	-	expression tag	UNP Q93077
e	-15	HIS	-	expression tag	UNP Q93077
e	-14	HIS	-	expression tag	UNP Q93077
e	-13	SER	-	expression tag	UNP Q93077
e	-12	PRO	-	expression tag	UNP Q93077
e	-11	GLY	-	expression tag	UNP Q93077
e	-10	LEU	-	expression tag	UNP Q93077
e	-9	GLU	-	expression tag	UNP Q93077

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Chain	Residue	Modelled	Actual	Comment	Reference
e	-8	VAL	-	expression tag	UNP Q93077
e	-7	LEU	-	expression tag	UNP Q93077
e	-6	PHE	-	expression tag	UNP Q93077
e	-5	GLN	-	expression tag	UNP Q93077
e	-4	GLY	-	expression tag	UNP Q93077
e	-3	PRO	-	expression tag	UNP Q93077
e	-2	ARG	-	expression tag	UNP Q93077
e	-1	GLY	-	expression tag	UNP Q93077
i	-23	MET	-	initiating methionine	UNP Q93077
i	-22	GLY	-	expression tag	UNP Q93077
i	-21	SER	-	expression tag	UNP Q93077
i	-20	SER	-	expression tag	UNP Q93077
i	-19	HIS	-	expression tag	UNP Q93077
i	-18	HIS	-	expression tag	UNP Q93077
i	-17	HIS	-	expression tag	UNP Q93077
i	-16	HIS	-	expression tag	UNP Q93077
i	-15	HIS	-	expression tag	UNP Q93077
i	-14	HIS	-	expression tag	UNP Q93077
i	-13	SER	-	expression tag	UNP Q93077
i	-12	PRO	-	expression tag	UNP Q93077
i	-11	GLY	-	expression tag	UNP Q93077
i	-10	LEU	-	expression tag	UNP Q93077
i	-9	GLU	-	expression tag	UNP Q93077
i	-8	VAL	-	expression tag	UNP Q93077
i	-7	LEU	-	expression tag	UNP Q93077
i	-6	PHE	-	expression tag	UNP Q93077
i	-5	GLN	-	expression tag	UNP Q93077
i	-4	GLY	-	expression tag	UNP Q93077
i	-3	PRO	-	expression tag	UNP Q93077
i	-2	ARG	-	expression tag	UNP Q93077
i	-1	GLY	-	expression tag	UNP Q93077

- Molecule 19 is a protein called Histone H2B type 1-C/E/F/G/I.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	D	95	Total	C	N	O	S	0	0
			745	467	136	140	2		
19	J	94	Total	C	N	O	S	0	0
			736	461	134	139	2		
19	f	95	Total	C	N	O	S	0	0
			745	467	136	140	2		
19	j	94	Total	C	N	O	S	0	0
			736	461	134	139	2		

- Molecule 20 is a DNA chain called DNA (318-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	318	Total	C	N	O	P	0	0
			6501	3097	1178	1908	318		

- Molecule 21 is a DNA chain called DNA (318-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	318	Total	C	N	O	P	0	0
			6537	3109	1202	1908	318		

- Molecule 22 is a protein called scFv.

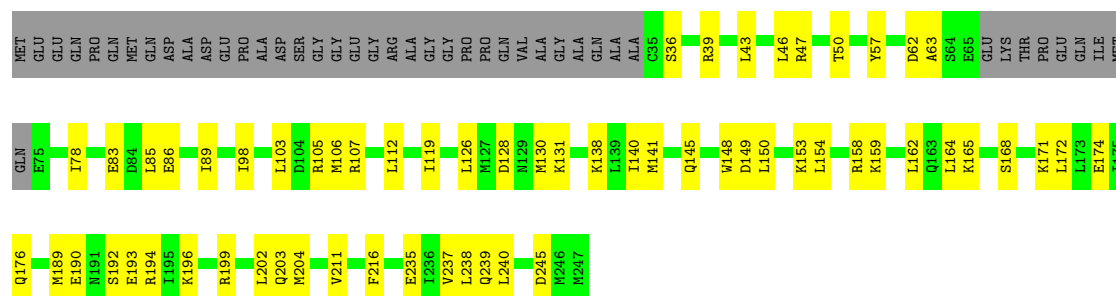
Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	229	Total	C	N	O	S	0	0
			1789	1126	292	362	9		
22	a	229	Total	C	N	O	S	0	0
			1787	1125	292	361	9		
22	m	229	Total	C	N	O	S	0	0
			1789	1126	292	362	9		
22	n	229	Total	C	N	O	S	0	0
			1787	1125	292	361	9		

3 Residue-property plots

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

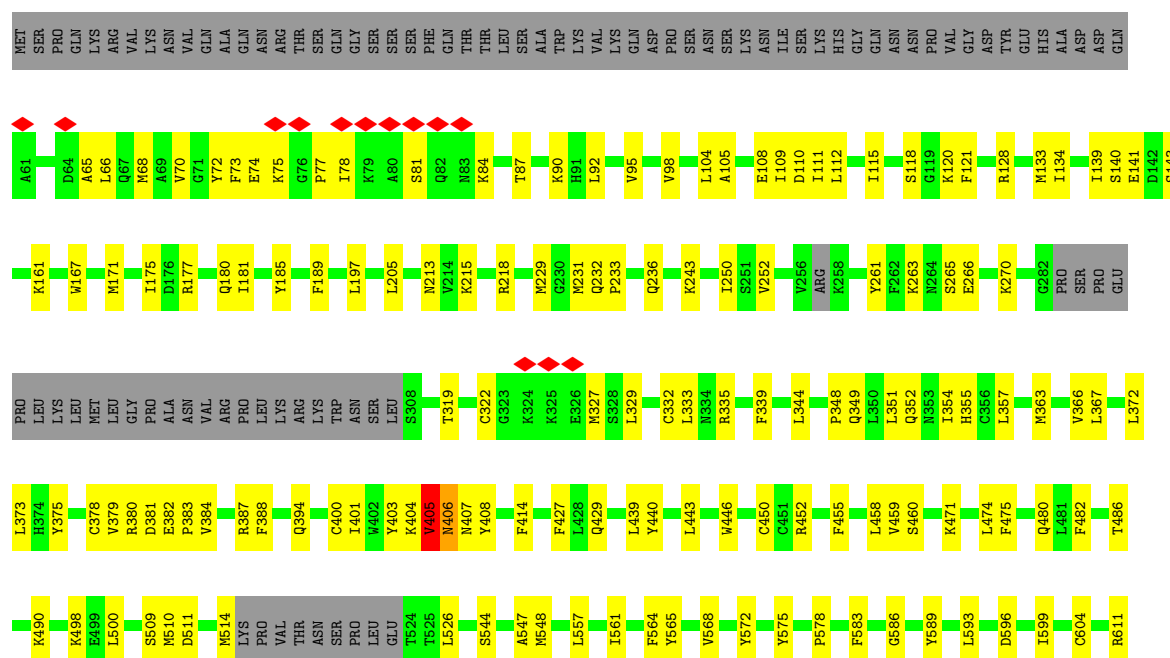
• Molecule 1: Centromere protein H

Chain H: 



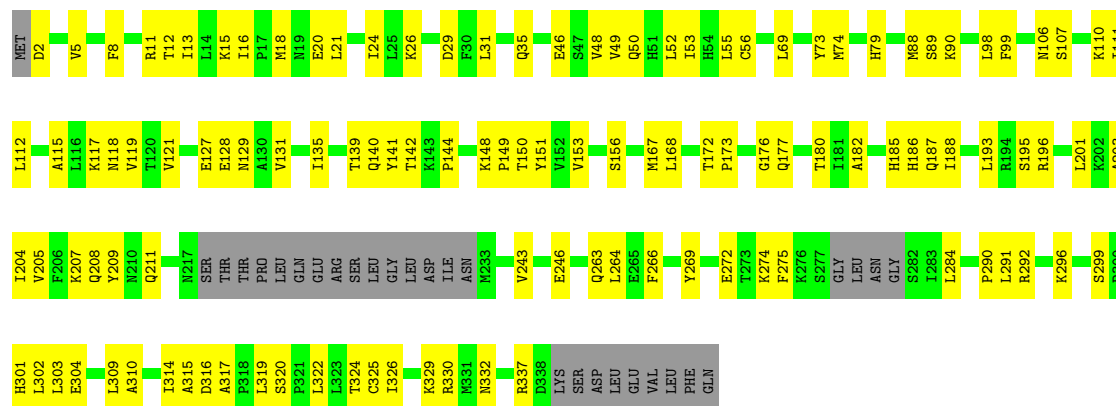
• Molecule 2: Centromere protein I

Chain I: 



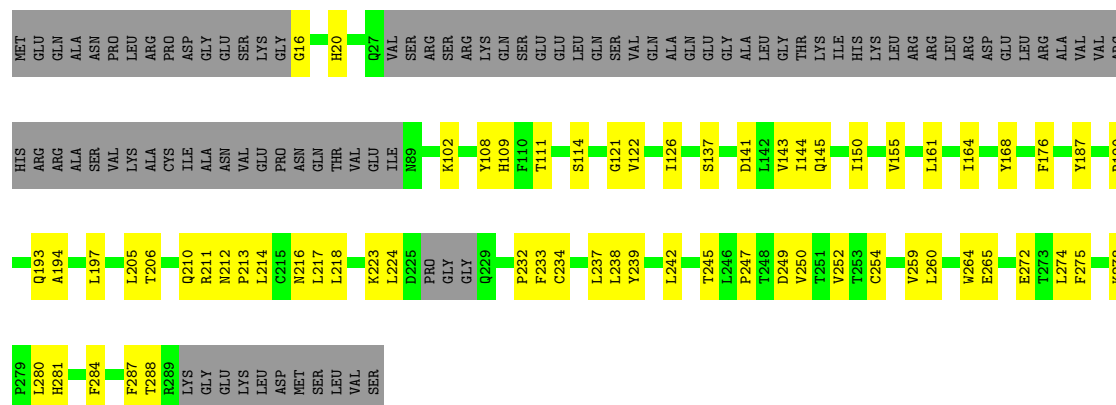
- Molecule 6: Centromere protein N

Chain N:  58% 34% 8%



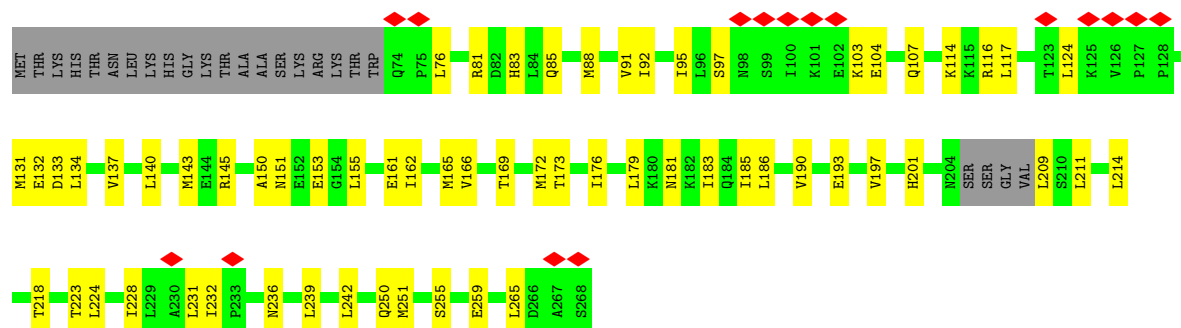
- Molecule 7: Centromere protein O

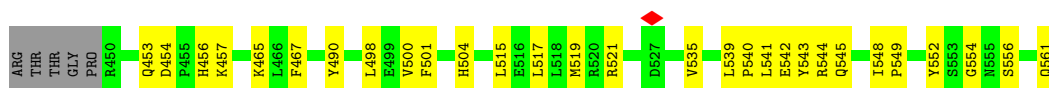
Chain O: 49% 21% 30%



- Molecule 8: Centromere protein Q

Chain Q: 

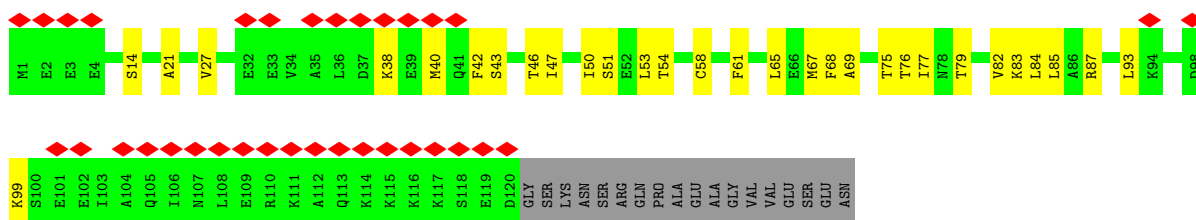


[illegible]

- Molecule 13: Centromere protein W



- Molecule 14: Centromere protein S



- Molecule 15: Centromere protein X



- Molecule 17: Histone H4

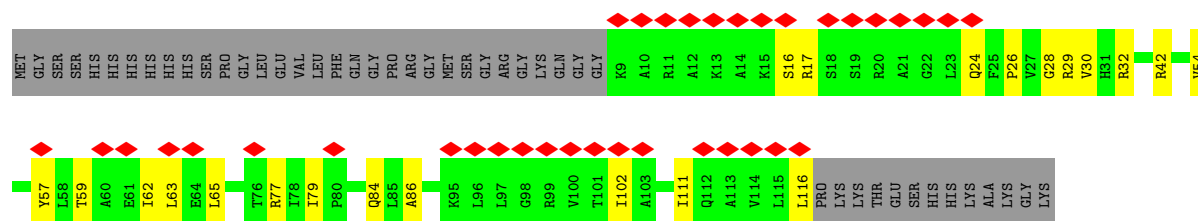
- Molecule 17: Histone H4

- Molecule 17: Histone H4

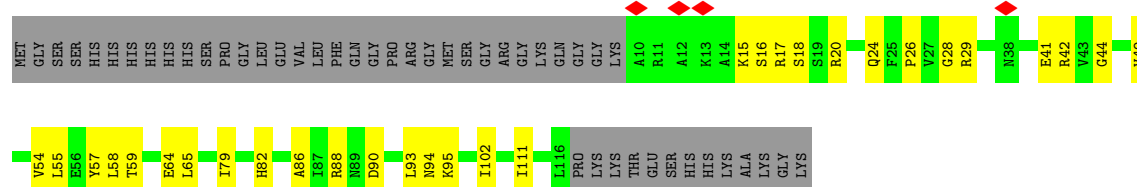
- Molecule 18: Histone H2A type 1-C

- Molecule 18: Histone H2A type 1-C

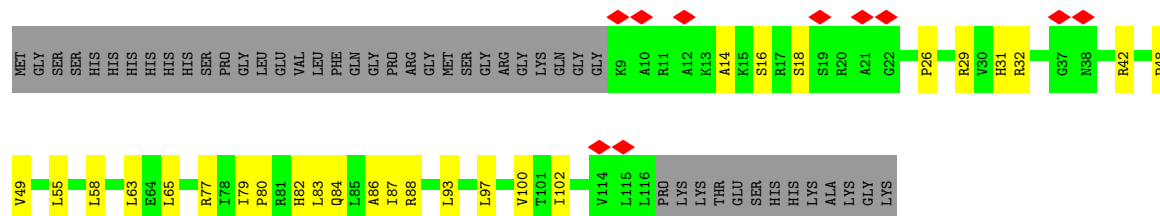




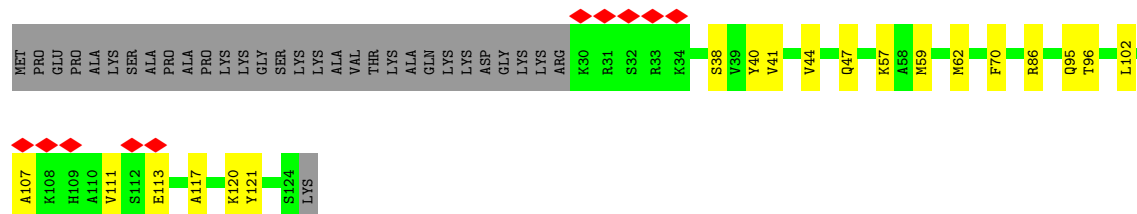
• Molecule 18: Histone H2A type 1-C



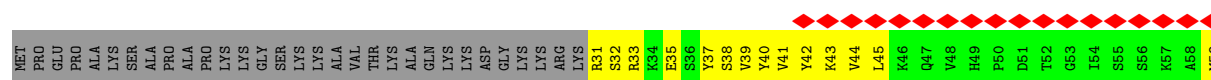
• Molecule 18: Histone H2A type 1-C

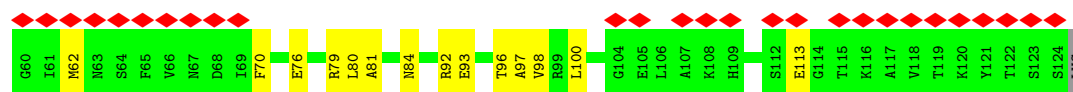


• Molecule 19: Histone H2B type 1-C/E/F/G/I

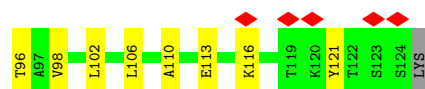
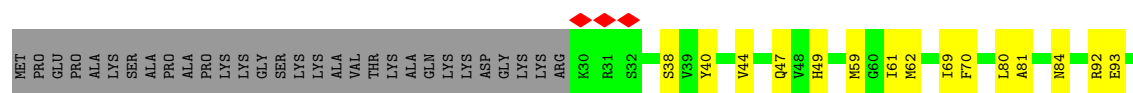


• Molecule 19: Histone H2B type 1-C/E/F/G/I

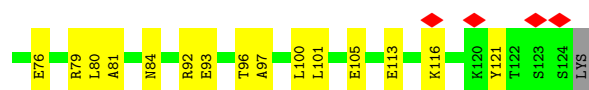
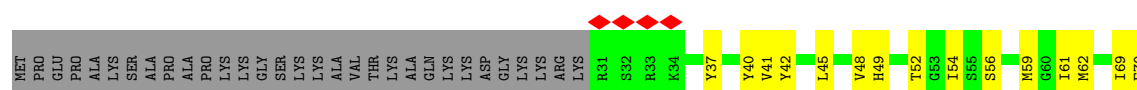




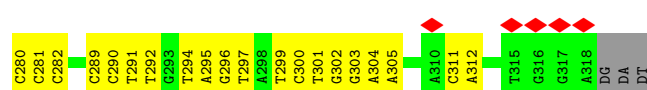
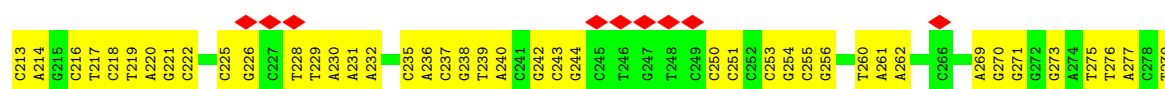
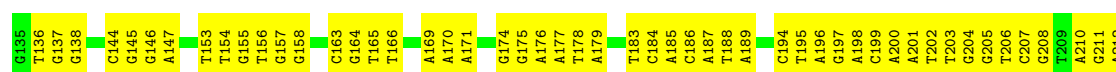
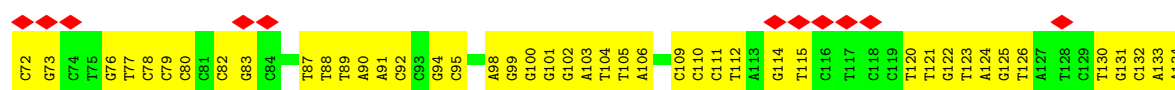
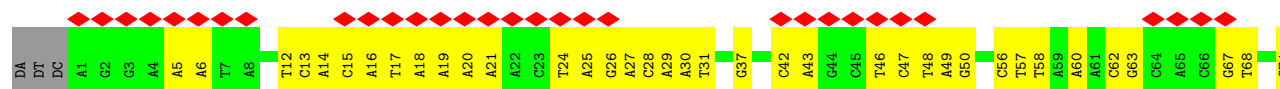
- Molecule 19: Histone H2B type 1-C/E/F/G/I



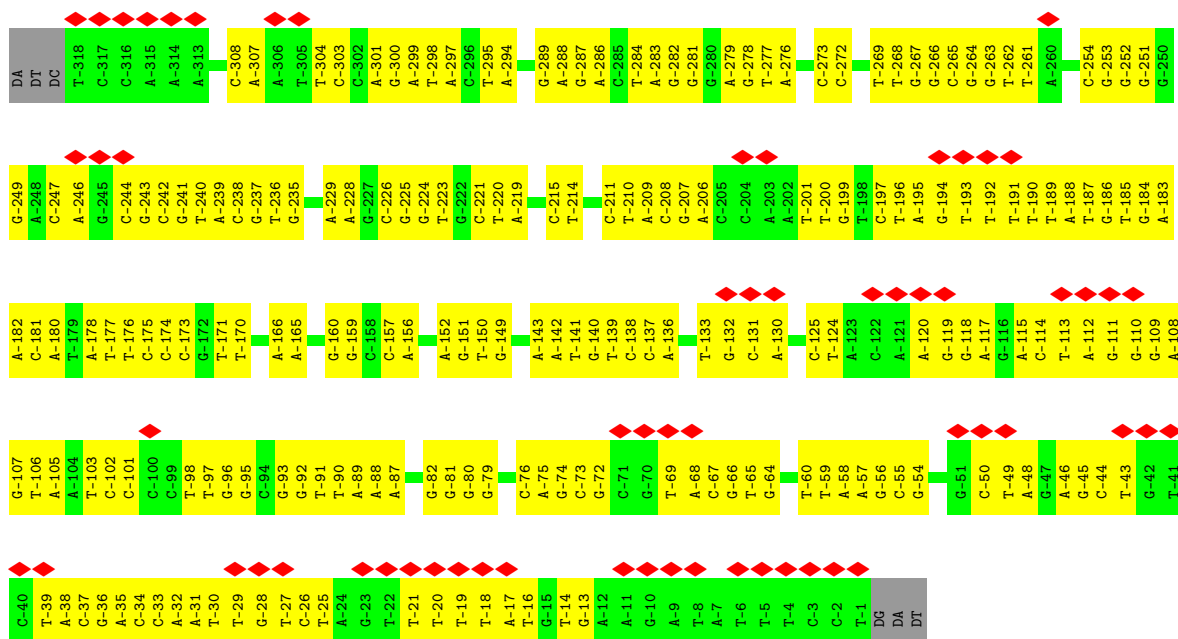
- Molecule 19: Histone H2B type 1-C/E/F/G/I



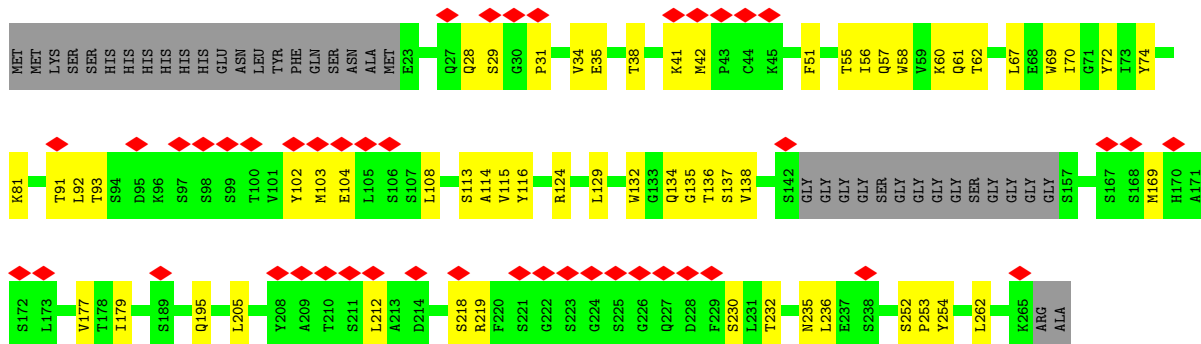
- Molecule 20: DNA (318-MER)



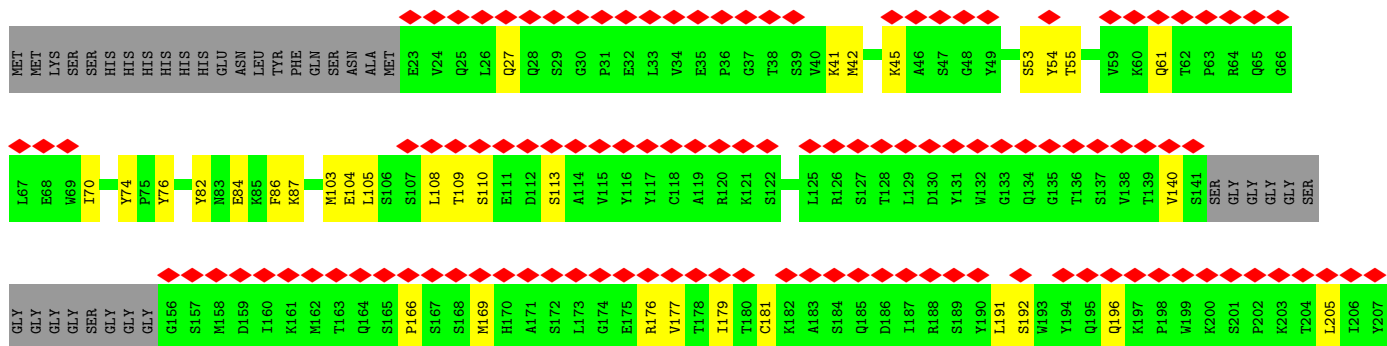
- Molecule 21: DNA (318-MER)



• Molecule 22: scFv

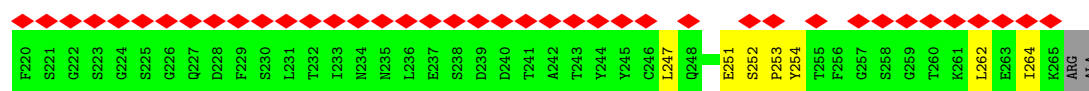
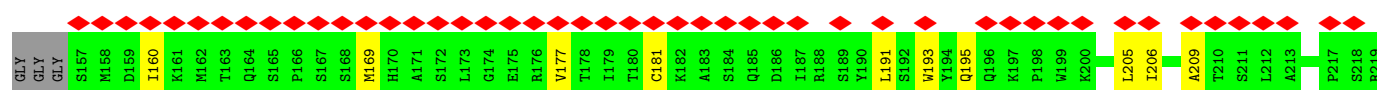
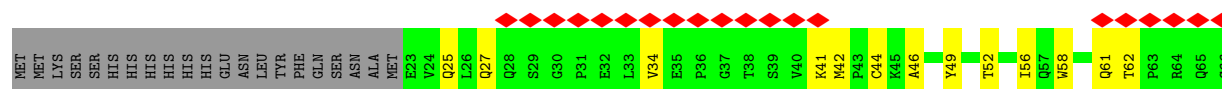


• Molecule 22: scFv

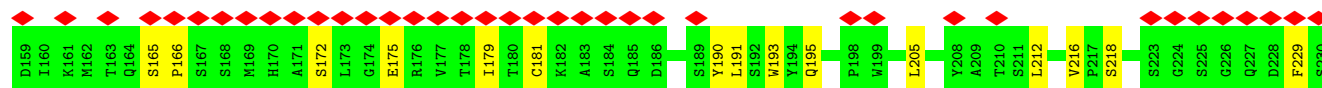
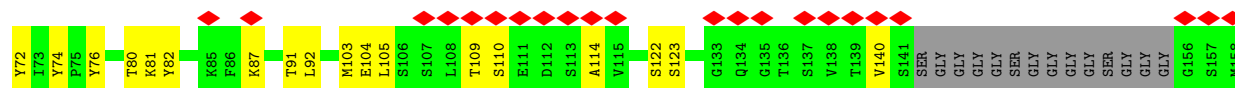
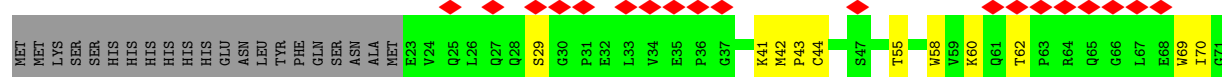




• Molecule 22: scFv



• Molecule 22: scFv



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15057	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.006	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0015	Depositor
Map size (Å)	371.19998, 371.19998, 371.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.928, 0.928, 0.928	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	H	0.16	0/1660	0.37	0/2218
2	I	0.17	0/5137	0.37	0/6955
3	K	0.19	0/1953	0.41	0/2634
4	L	0.15	0/2569	0.36	0/3485
5	M	0.12	0/1347	0.32	0/1827
6	N	0.16	0/2674	0.41	0/3610
7	O	0.15	0/1678	0.37	0/2280
8	Q	0.16	0/1538	0.42	0/2062
9	U	0.19	0/1383	0.45	0/1856
10	P	0.15	0/1820	0.38	0/2451
11	R	0.13	0/653	0.38	0/865
12	T	0.13	0/937	0.34	0/1263
13	W	0.12	0/711	0.32	0/944
14	S	0.12	0/991	0.33	0/1322
15	X	0.12	0/596	0.29	0/801
16	A	0.17	0/831	0.37	0/1116
16	E	0.17	0/831	0.37	0/1116
16	c	0.15	0/831	0.40	1/1116 (0.1%)
16	g	0.13	0/825	0.39	1/1106 (0.1%)
17	B	0.16	0/645	0.40	0/862
17	F	0.15	0/645	0.37	0/862
17	d	0.12	0/645	0.32	0/862
17	h	0.13	0/645	0.33	0/862
18	C	0.14	0/831	0.32	0/1120
18	G	0.11	0/840	0.29	0/1131
18	e	0.13	0/831	0.30	0/1120
18	i	0.11	0/840	0.28	0/1131
19	D	0.11	0/756	0.30	0/1015
19	J	0.13	0/747	0.35	0/1004
19	f	0.14	0/756	0.34	0/1015
19	j	0.13	0/747	0.37	0/1004
20	V	0.22	0/7289	0.45	0/11243
21	Y	0.20	0/7337	0.41	0/11327
22	Z	0.14	0/1831	0.38	0/2480

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	a	0.18	0/1829	0.39	0/2477
22	m	0.13	0/1831	0.39	0/2480
22	n	0.16	0/1829	0.41	0/2477
All	All	0.17	0/59839	0.39	2/83499 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	g	119	VAL	N-CA-C	-6.27	107.13	113.47
16	c	119	VAL	N-CA-C	-6.25	107.15	113.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1652	0	1728	64	0
2	I	5014	0	5036	132	0
3	K	1922	0	1924	78	0
4	L	2502	0	2492	78	0
5	M	1325	0	1370	33	0
6	N	2617	0	2638	82	0
7	O	1642	0	1616	54	0
8	Q	1526	0	1586	72	0
9	U	1365	0	1396	65	0
10	P	1788	0	1791	57	0
11	R	649	0	673	34	0
12	T	915	0	924	24	0
13	W	704	0	789	18	0
14	S	982	0	987	31	0
15	X	590	0	623	19	0
16	A	816	0	857	33	0
16	E	816	0	857	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	c	816	0	857	27	0
16	g	811	0	851	25	0
17	B	638	0	676	27	0
17	F	638	0	676	40	0
17	d	638	0	676	14	0
17	h	638	0	676	19	0
18	C	822	0	880	22	0
18	G	831	0	893	27	0
18	e	822	0	880	29	0
18	i	831	0	893	23	0
19	D	745	0	769	17	0
19	J	736	0	756	30	0
19	f	745	0	769	22	0
19	j	736	0	756	26	0
20	V	6501	0	3581	162	0
21	Y	6537	0	3581	193	0
22	Z	1789	0	1727	38	0
22	a	1787	0	1725	31	0
22	m	1789	0	1727	30	0
22	n	1787	0	1725	32	0
All	All	57462	0	52361	1433	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 13.

All (1433) 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)
22:n:92:LEU:HD23	22:n:103:MET:HE1	1.34	1.03
22:Z:113:SER:HA	22:Z:138:VAL:O	1.70	0.92
8:Q:183:ILE:HG22	9:U:341:TYR:HB2	1.57	0.86
22:n:29:SER:HB3	22:n:43:PRO:HD2	1.58	0.84
16:c:105:LEU:HA	16:c:133:ARG:HH22	1.44	0.82
1:H:105:ARG:HG3	2:I:593:LEU:HB3	1.62	0.81
14:S:53:LEU:HD11	15:X:71:LEU:HD11	1.62	0.81
22:m:169:MET:HE3	22:m:262:LEU:HD13	1.61	0.81
19:J:80:LEU:HD13	19:J:96:THR:HG23	1.64	0.79
19:f:38:SER:HA	19:f:59:MET:HE2	1.63	0.79
4:L:165:VAL:HG21	4:L:332:LEU:HB3	1.65	0.79
19:D:38:SER:HA	19:D:59:MET:HE2	1.64	0.79
7:O:168:TYR:HB3	7:O:176:PHE:HB2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:ILE:HG21	3:K:60:LEU:HB3	1.65	0.78
3:K:219:LEU:HB3	3:K:264:LEU:HB2	1.65	0.78
16:E:133:ARG:HB3	16:E:137:GLU:HB3	1.64	0.78
21:Y:-187:DT:H4'	21:Y:-186:DG:H5'	1.66	0.78
22:a:41:LYS:HG2	22:a:104:GLU:HG2	1.66	0.77
21:Y:-282:DG:H21	18:i:42:ARG:HH22	1.31	0.77
19:J:41:VAL:HB	19:J:59:MET:HE1	1.66	0.77
7:O:259:VAL:HG21	7:O:265:GLU:HG2	1.67	0.76
1:H:50:THR:HB	3:K:31:MET:HE3	1.66	0.76
21:Y:-288:DA:H5''	18:i:16:SER:HA	1.65	0.76
19:j:80:LEU:HD13	19:j:96:THR:HG23	1.67	0.76
21:Y:-190:DT:H4'	21:Y:-189:DT:H5'	1.67	0.75
17:B:34:ILE:HG21	17:B:51:TYR:HA	1.69	0.74
16:A:130:ARG:HH21	16:A:140:GLY:H	1.35	0.74
14:S:82:VAL:HG11	15:X:30:LEU:HD22	1.69	0.74
8:Q:166:VAL:HG12	9:U:323:VAL:HG21	1.69	0.73
4:L:218:LEU:HD23	4:L:304:LEU:HG	1.69	0.73
18:C:45:ALA:HB1	19:D:121:TYR:HE2	1.52	0.73
6:N:118:ASN:HB3	6:N:144:PRO:HD3	1.71	0.73
6:N:325:CYS:HB3	6:N:329:LYS:HG3	1.71	0.73
20:V:136:DT:H2''	20:V:137:DG:H3'	1.71	0.72
10:P:209:ARG:HD3	10:P:214:PRO:HA	1.72	0.72
22:n:91:THR:HB	22:n:104:GLU:HB2	1.72	0.72
7:O:206:THR:HG21	7:O:223:LYS:HE2	1.70	0.71
1:H:62:ASP:HB3	3:K:69:ALA:HB1	1.70	0.71
2:I:141:GLU:H	2:I:177:ARG:HH21	1.37	0.71
6:N:303:LEU:HD21	6:N:326:ILE:HB	1.71	0.71
7:O:259:VAL:HG23	7:O:264:TRP:HB2	1.72	0.71
21:Y:-235:DG:H5'	16:c:43:ARG:HG2	1.74	0.70
18:G:16:SER:HA	20:V:31:DT:H5''	1.73	0.70
22:m:113:SER:HA	22:m:138:VAL:O	1.91	0.70
6:N:150:THR:HG21	6:N:168:LEU:HD12	1.73	0.70
2:I:649:GLY:HA2	2:I:653:THR:HB	1.74	0.69
17:d:65:VAL:HA	17:d:93:GLN:HE22	1.56	0.69
10:P:178:GLU:HB3	10:P:182:ARG:HH21	1.58	0.69
17:B:34:ILE:HA	17:B:37:LEU:HD12	1.74	0.69
16:E:69:ARG:HA	16:E:72:ARG:HD2	1.74	0.69
2:I:344:LEU:HA	2:I:349:GLN:HG2	1.72	0.69
16:E:102:LEU:HD11	17:F:58:LEU:HB2	1.73	0.69
22:a:27:GLN:HE21	22:a:45:LYS:HB3	1.57	0.69
1:H:98:ILE:HD11	2:I:586:GLY:HA2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:189:MET:HE3	3:K:155:GLU:HA	1.72	0.69
8:Q:214:LEU:HD23	8:Q:218:THR:HG21	1.73	0.69
4:L:280:VAL:HG12	4:L:284:MET:HE2	1.73	0.69
18:C:53:ALA:HB1	19:D:113:GLU:HG3	1.75	0.68
10:P:263:ARG:HA	10:P:266:VAL:HG12	1.76	0.68
2:I:471:LYS:HA	2:I:475:PHE:HD2	1.58	0.68
9:U:408:ASN:HD21	11:R:139:THR:HG22	1.59	0.68
4:L:164:CYS:HB2	4:L:182:PRO:HD2	1.75	0.68
10:P:218:LEU:HD11	10:P:278:LEU:HD21	1.76	0.68
21:Y:-171:DT:H2''	21:Y:-170:DT:C5	2.28	0.68
14:S:46:THR:HG23	15:X:63:LEU:HD22	1.75	0.68
1:H:112:LEU:HD21	2:I:689:LEU:HD22	1.75	0.68
20:V:188:DT:H2''	20:V:189:DA:C8	2.28	0.67
16:A:102:LEU:HD11	17:B:58:LEU:HB2	1.76	0.67
16:A:85:ASN:HB3	21:Y:-98:DT:H4'	1.75	0.67
6:N:107:SER:HB2	6:N:182:ALA:HA	1.76	0.67
20:V:269:DA:H2''	20:V:270:DG:C8	2.30	0.67
11:R:89:LEU:HA	11:R:92:LYS:HG2	1.75	0.67
16:g:74:ILE:HA	16:g:77:LYS:HE2	1.76	0.66
10:P:245:ARG:O	10:P:249:LEU:HB2	1.96	0.66
16:A:50:GLU:HA	16:A:53:LYS:HG2	1.75	0.66
8:Q:190:VAL:HG12	9:U:348:LYS:HB2	1.77	0.66
4:L:33:SER:HA	4:L:36:LYS:HG2	1.77	0.66
22:Z:31:PRO:HB3	22:Z:137:SER:HB3	1.77	0.66
6:N:18:MET:HE1	6:N:48:VAL:HG21	1.77	0.66
18:G:42:ARG:HH22	20:V:37:DG:H21	1.44	0.66
20:V:300:DC:H2''	20:V:301:DT:C5	2.31	0.66
8:Q:97:SER:HA	14:S:21:ALA:HB1	1.77	0.66
2:I:401:ILE:HG23	2:I:408:TYR:HA	1.77	0.65
18:C:55:LEU:HD11	19:D:70:PHE:HD2	1.59	0.65
8:Q:134:LEU:HD12	9:U:292:MET:HE2	1.76	0.65
18:G:59:THR:HA	19:J:62:MET:HE2	1.78	0.65
20:V:109:DC:H2''	20:V:110:DC:C5	2.32	0.65
1:H:162:LEU:HD22	2:I:510:MET:SD	2.36	0.65
12:T:544:ARG:HG3	12:T:548:ILE:HD12	1.78	0.65
17:h:84:MET:HE2	17:h:88:TYR:HE2	1.61	0.65
2:I:104:LEU:HD12	2:I:108:GLU:HG3	1.79	0.65
4:L:55:LEU:HD13	4:L:59:VAL:HG11	1.79	0.65
16:A:63:ARG:HD3	20:V:91:DA:H4'	1.77	0.65
7:O:121:GLY:HA2	7:O:144:ILE:HG12	1.79	0.65
8:Q:250:GLN:HG2	11:R:96:LEU:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:219:DT:H2''	20:V:220:DA:C8	2.32	0.65
11:R:146:VAL:HG13	11:R:151:LEU:HB2	1.80	0.64
14:S:27:VAL:HG21	14:S:51:SER:HA	1.79	0.64
20:V:296:DG:H2''	20:V:297:DT:H5''	1.78	0.64
22:Z:169:MET:HE3	22:Z:262:LEU:HD13	1.79	0.64
22:n:74:TYR:CE2	22:n:76:TYR:HB3	2.32	0.64
1:H:130:MET:SD	2:I:690:SER:HA	2.37	0.64
8:Q:124:LEU:HD13	9:U:257:GLU:HG2	1.78	0.64
20:V:218:DC:H2''	20:V:219:DT:H71	1.77	0.64
2:I:443:LEU:HD22	2:I:474:LEU:HD12	1.80	0.64
10:P:188:LYS:HA	10:P:195:VAL:HG11	1.78	0.64
16:E:54:LEU:HD11	17:F:36:ARG:HG2	1.79	0.64
16:c:130:ARG:HH21	16:c:139:LEU:HA	1.62	0.64
19:j:80:LEU:HD11	19:j:100:LEU:HD12	1.80	0.64
2:I:229:MET:HE2	2:I:232:GLN:HE21	1.63	0.64
21:Y:-19:DT:H2''	21:Y:-18:DT:C5	2.33	0.63
11:R:146:VAL:HA	11:R:151:LEU:HD13	1.79	0.63
16:A:69:ARG:HA	16:A:72:ARG:HD2	1.81	0.63
2:I:72:TYR:HA	2:I:75:LYS:HD2	1.80	0.63
19:J:81:ALA:HB2	19:J:93:GLU:HG2	1.80	0.63
4:L:301:ALA:HB3	6:N:314:ILE:HG23	1.81	0.63
12:T:517:LEU:HD11	14:S:67:MET:SD	2.39	0.63
17:F:65:VAL:HA	17:F:93:GLN:HE22	1.63	0.63
18:e:57:TYR:HB2	19:f:113:GLU:HG3	1.81	0.63
6:N:31:LEU:HD21	6:N:56:CYS:HA	1.80	0.63
6:N:269:TYR:HE2	6:N:322:LEU:HB3	1.63	0.63
19:f:80:LEU:HD13	19:f:96:THR:HB	1.81	0.63
11:R:98:GLU:O	11:R:102:GLU:HG2	2.00	0.62
16:E:120:THR:HA	17:F:45:ARG:HB2	1.81	0.62
21:Y:-240:DT:H2''	21:Y:-239:DA:C8	2.33	0.62
16:c:140:GLY:HA2	17:d:60:VAL:HG12	1.80	0.62
8:Q:104:GLU:HA	8:Q:107:GLN:HE21	1.63	0.62
16:A:99:GLU:HG2	17:B:37:LEU:HD21	1.82	0.62
4:L:246:SER:HB2	4:L:247:PRO:HD3	1.81	0.62
6:N:205:VAL:HA	6:N:330:ARG:HD2	1.81	0.62
8:Q:201:HIS:CE1	10:P:277:SER:HB3	2.34	0.62
20:V:198:DA:H2''	20:V:199:DC:C5	2.35	0.62
1:H:193:GLU:HG2	1:H:194:ARG:HG3	1.82	0.62
21:Y:-238:DC:H2''	21:Y:-237:DG:C8	2.34	0.62
2:I:333:LEU:HD11	3:K:158:ILE:HG23	1.81	0.62
3:K:233:LYS:HE3	3:K:261:ARG:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:162:LEU:HB3	2:I:510:MET:HE1	1.82	0.62
6:N:135:ILE:O	6:N:149:PRO:HA	2.00	0.62
11:R:120:GLU:HB3	11:R:126:SER:HA	1.82	0.61
18:G:24:GLN:HE21	19:J:44:VAL:HG22	1.65	0.61
6:N:74:MET:HG3	6:N:151:TYR:CZ	2.35	0.61
8:Q:124:LEU:HD21	9:U:254:VAL:HB	1.82	0.61
6:N:79:HIS:HB3	6:N:196:ARG:HH11	1.65	0.61
10:P:255:ILE:O	10:P:258:ALA:HB2	2.00	0.61
12:T:453:GLN:HB2	21:Y:-143:DA:H5''	1.83	0.61
14:S:54:THR:HG21	15:X:39:VAL:HG22	1.80	0.61
14:S:99:LYS:HD3	15:X:33:GLU:HG3	1.82	0.61
22:a:74:TYR:CE2	22:a:76:TYR:HB3	2.35	0.61
2:I:78:ILE:H	2:I:84:LYS:HD3	1.65	0.61
18:G:54:VAL:HG21	19:J:98:VAL:HG21	1.81	0.61
16:A:62:ILE:HD11	17:B:37:LEU:HD11	1.83	0.61
16:c:42:ARG:HH12	16:c:44:ARG:HH11	1.49	0.61
5:M:19:LEU:HD22	5:M:54:LEU:HD11	1.83	0.61
9:U:382:TYR:HB3	9:U:386:SER:HB2	1.83	0.61
3:K:215:MET:HE1	3:K:242:TYR:HB3	1.82	0.60
6:N:275:PHE:HD2	6:N:284:LEU:HB2	1.66	0.60
2:I:548:MET:HE3	2:I:548:MET:HA	1.83	0.60
2:I:642:HIS:HB3	2:I:659:LYS:HE2	1.82	0.60
14:S:42:PHE:HA	15:X:58:VAL:HB	1.83	0.60
22:n:41:LYS:HG2	22:n:104:GLU:HG2	1.83	0.60
5:M:5:ARG:HB3	5:M:8:ASP:HB2	1.83	0.60
6:N:117:LYS:HB3	6:N:140:GLN:HA	1.82	0.60
20:V:123:DT:H2''	20:V:124:DA:N7	2.16	0.60
20:V:155:DG:H1'	20:V:156:DT:H5'	1.83	0.60
19:j:49:HIS:HB3	19:j:52:THR:HB	1.83	0.60
18:e:26:PRO:HB2	18:e:29:ARG:HB3	1.83	0.60
12:T:498:LEU:HD11	12:T:515:LEU:HD21	1.84	0.60
4:L:31:LEU:HB2	4:L:173:THR:HB	1.84	0.60
20:V:90:DA:H1'	20:V:91:DA:C8	2.37	0.60
19:j:54:ILE:HG23	19:j:59:MET:HE2	1.84	0.60
3:K:248:ARG:HH21	12:T:544:ARG:HG2	1.67	0.60
16:E:67:PHE:HE1	17:F:58:LEU:HD11	1.67	0.60
9:U:372:GLN:HE22	10:P:215:GLY:H	1.48	0.59
4:L:213:ILE:HB	4:L:316:THR:HA	1.84	0.59
8:Q:134:LEU:HG	9:U:292:MET:HG3	1.84	0.59
22:n:60:LYS:HB2	22:n:70:ILE:HD11	1.83	0.59
1:H:46:LEU:HD11	3:K:32:TRP:HE1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:77:LEU:HD21	4:L:80:LEU:HD21	1.85	0.59
16:A:68:SER:HA	16:A:91:LEU:HD22	1.83	0.59
6:N:139:THR:HG23	6:N:141:TYR:H	1.66	0.59
20:V:132:DC:H2''	20:V:133:DA:C8	2.37	0.59
20:V:275:DT:H2'	20:V:276:DT:H71	1.85	0.59
13:W:53:ARG:HB3	13:W:82:ILE:HD12	1.83	0.59
2:I:92:LEU:HD21	2:I:128:ARG:HG3	1.85	0.59
8:Q:145:ARG:NH2	9:U:302:LEU:HG	2.18	0.59
8:Q:169:THR:HA	8:Q:172:MET:HG2	1.83	0.59
20:V:197:DG:H2''	20:V:198:DA:C8	2.38	0.59
12:T:549:PRO:HG3	12:T:561:GLN:HG3	1.85	0.59
12:T:552:TYR:O	12:T:556:SER:HB3	2.03	0.59
14:S:38:LYS:HG3	15:X:47:VAL:HG21	1.84	0.59
18:C:111:ILE:HD11	16:E:52:ARG:HG3	1.83	0.59
21:Y:-225:DG:H2'	21:Y:-224:DG:H8	1.68	0.59
22:m:41:LYS:HA	22:m:103:MET:O	2.03	0.59
22:m:42:MET:SD	22:m:103:MET:HB2	2.43	0.59
2:I:354:ILE:HG12	3:K:139:LEU:HD21	1.84	0.58
4:L:233:TYR:HB3	4:L:258:PRO:HG2	1.85	0.58
20:V:217:DT:H2''	20:V:218:DC:C6	2.38	0.58
16:g:133:ARG:HB3	16:g:137:GLU:HB3	1.85	0.58
10:P:266:VAL:HG23	10:P:271:ILE:HA	1.85	0.58
18:G:30:VAL:HG13	19:J:70:PHE:HE2	1.68	0.58
22:a:55:THR:HG22	22:a:74:TYR:HD1	1.68	0.58
1:H:36:SER:HA	1:H:39:ARG:HH21	1.68	0.58
4:L:75:TYR:HB2	4:L:184:PHE:HB3	1.86	0.58
19:D:41:VAL:HB	19:D:59:MET:HE1	1.85	0.58
21:Y:-193:DT:H2'	21:Y:-192:DT:H71	1.85	0.58
3:K:20:THR:HG21	3:K:84:LEU:HG	1.86	0.58
4:L:165:VAL:H	4:L:336:THR:HG21	1.69	0.58
2:I:327:MET:HE3	2:I:332:CYS:HA	1.84	0.58
8:Q:88:MET:HA	8:Q:91:VAL:HG12	1.84	0.58
9:U:411:LEU:HD22	11:R:146:VAL:HG21	1.84	0.58
16:A:140:GLY:HA2	17:B:60:VAL:HG12	1.84	0.58
17:B:65:VAL:HA	17:B:93:GLN:HE22	1.68	0.58
20:V:176:DA:H2''	20:V:177:DA:C8	2.38	0.58
18:i:83:LEU:HD22	19:j:62:MET:HE3	1.86	0.58
4:L:127:MET:HE1	4:L:164:CYS:H	1.69	0.57
8:Q:107:GLN:NE2	14:S:14:SER:HB2	2.18	0.57
10:P:126:GLN:HG2	10:P:131:LEU:HD22	1.86	0.57
1:H:106:MET:HG2	2:I:668:LEU:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:223:LYS:HG2	7:O:232:PRO:HA	1.85	0.57
18:G:65:LEU:HB3	18:G:86:ALA:HB1	1.86	0.57
20:V:79:DC:H2''	20:V:80:DC:C5	2.39	0.57
22:Z:195:GLN:HB3	22:Z:205:LEU:HD11	1.85	0.57
16:c:102:LEU:HD11	17:d:58:LEU:HB2	1.84	0.57
2:I:263:LYS:HE2	2:I:265:SER:HB3	1.85	0.57
4:L:221:MET:HE2	4:L:314:ALA:HB3	1.87	0.57
6:N:315:ALA:HB1	6:N:319:LEU:HD21	1.85	0.57
10:P:244:GLN:HA	10:P:247:LEU:HD12	1.86	0.57
22:a:191:LEU:HB3	22:a:209:ALA:HB2	1.87	0.57
16:c:128:LEU:HD11	16:g:111:LEU:HB3	1.87	0.57
18:e:54:VAL:HG13	19:f:110:ALA:HB1	1.86	0.57
1:H:103:LEU:O	1:H:107:ARG:HG3	2.05	0.57
21:Y:-30:DT:H2''	21:Y:-29:DT:C5	2.40	0.57
7:O:197:LEU:HD11	7:O:284:PHE:CE2	2.39	0.57
17:h:84:MET:HE2	17:h:88:TYR:CE2	2.40	0.57
1:H:172:LEU:O	1:H:176:GLN:HG2	2.05	0.57
5:M:99:PHE:CE2	5:M:126:SER:HB2	2.40	0.57
9:U:375:GLU:HB2	10:P:245:ARG:HH12	1.69	0.57
22:m:61:GLN:HB2	22:m:67:LEU:HD23	1.86	0.57
22:Z:42:MET:HB2	22:Z:103:MET:HB2	1.87	0.57
22:a:84:GLU:HA	22:a:87:LYS:HG2	1.87	0.57
22:a:212:LEU:HD11	22:a:218:SER:HA	1.87	0.57
2:I:681:ASN:O	2:I:685:HIS:HB2	2.05	0.56
22:Z:91:THR:HB	22:Z:104:GLU:HB2	1.86	0.56
22:a:82:TYR:HB2	22:a:87:LYS:HD2	1.87	0.56
22:m:195:GLN:HB3	22:m:205:LEU:HD11	1.86	0.56
2:I:511:ASP:HA	2:I:514:MET:HE3	1.87	0.56
4:L:59:VAL:HG22	4:L:126:GLY:HA3	1.86	0.56
16:c:111:LEU:HB3	16:g:128:LEU:HD11	1.87	0.56
7:O:284:PHE:HD1	7:O:287:PHE:CE1	2.23	0.56
10:P:255:ILE:O	10:P:258:ALA:CB	2.54	0.56
21:Y:-224:DG:H2'	21:Y:-223:DT:H71	1.87	0.56
17:d:84:MET:HE2	17:d:88:TYR:HE2	1.70	0.56
2:I:648:VAL:HG12	2:I:734:PHE:HZ	1.68	0.56
2:I:77:PRO:HD3	2:I:121:PHE:CE1	2.41	0.56
4:L:56:GLN:HB2	4:L:59:VAL:HG23	1.86	0.56
8:Q:132:GLU:O	9:U:292:MET:HE1	2.06	0.56
11:R:94:GLU:HG3	11:R:140:LYS:HE3	1.88	0.56
15:X:58:VAL:HG13	15:X:62:GLN:HE21	1.70	0.56
16:A:64:LYS:HE3	16:A:92:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:30:THR:HB	17:B:32:PRO:HD2	1.88	0.56
3:K:50:LEU:HD13	3:K:55:ALA:HA	1.88	0.56
7:O:237:LEU:HD23	7:O:247:PRO:HG3	1.87	0.56
8:Q:183:ILE:HD12	9:U:340:LYS:HD2	1.88	0.56
17:B:34:ILE:HD11	17:B:55:ARG:HG3	1.88	0.56
20:V:47:DC:H2''	20:V:48:DT:H72	1.88	0.56
21:Y:-237:DG:H2'	21:Y:-236:DT:H71	1.88	0.56
20:V:290:DC:H2''	20:V:291:DT:C5	2.41	0.56
22:Z:72:TYR:HE2	22:Z:81:LYS:HD2	1.71	0.56
18:e:26:PRO:HB3	19:f:40:TYR:CZ	2.41	0.56
2:I:366:VAL:HG13	2:I:372:LEU:HB3	1.86	0.56
13:W:68:ARG:HG3	13:W:69:VAL:HG23	1.87	0.56
20:V:177:DA:H2''	20:V:178:DT:C6	2.41	0.56
2:I:565:TYR:HA	2:I:568:VAL:HB	1.88	0.56
10:P:140:ILE:HG13	10:P:154:VAL:HG13	1.88	0.56
20:V:27:DA:H2''	20:V:28:DC:C5	2.41	0.56
20:V:201:DA:H3'	18:e:28:GLY:HA3	1.88	0.55
6:N:121:VAL:HG12	6:N:135:ILE:HG12	1.89	0.55
10:P:226:ILE:HG12	10:P:232:VAL:HG22	1.88	0.55
20:V:120:DT:H2''	20:V:121:DT:C5	2.41	0.55
16:A:133:ARG:HB3	16:A:137:GLU:HB3	1.88	0.55
21:Y:-82:DG:H2''	21:Y:-81:DG:C8	2.41	0.55
20:V:253:DC:H2''	20:V:254:DG:C8	2.42	0.55
21:Y:-229:DA:H2''	21:Y:-228:DA:H8	1.71	0.55
22:a:42:MET:SD	22:a:103:MET:HB3	2.47	0.55
16:E:110:TYR:OH	17:F:44:LYS:HB3	2.07	0.55
2:I:639:GLU:O	2:I:642:HIS:HB2	2.06	0.55
4:L:96:ASN:HB2	4:L:119:VAL:HB	1.88	0.55
6:N:12:THR:O	6:N:16:ILE:HG13	2.06	0.55
6:N:35:GLN:HB3	6:N:55:LEU:HD23	1.89	0.55
7:O:187:TYR:HD1	7:O:190:ARG:HH12	1.52	0.55
15:X:58:VAL:HG13	15:X:62:GLN:NE2	2.22	0.55
2:I:596:ASP:HB3	2:I:599:ILE:HB	1.89	0.55
6:N:115:ALA:HA	9:U:320:MET:HE2	1.89	0.55
6:N:310:ALA:HB1	6:N:317:ALA:HA	1.88	0.55
20:V:26:DG:H2''	20:V:27:DA:C8	2.42	0.55
21:Y:-229:DA:H2''	21:Y:-228:DA:C8	2.41	0.55
22:Z:115:VAL:HA	22:Z:136:THR:O	2.07	0.55
3:K:235:SER:H	3:K:238:PHE:HD2	1.53	0.54
20:V:89:DT:H1'	20:V:90:DA:C4	2.42	0.54
18:e:102:ILE:HG23	19:f:61:ILE:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:642:HIS:HB3	2:I:659:LYS:HG2	1.89	0.54
14:S:65:LEU:HB3	14:S:77:ILE:HD13	1.88	0.54
21:Y:-269:DT:H4'	16:g:85:ASN:HB3	1.89	0.54
16:c:133:ARG:HG2	16:c:137:GLU:HB3	1.89	0.54
22:a:70:ILE:HG21	22:a:103:MET:HE3	1.90	0.54
1:H:47:ARG:HA	3:K:31:MET:HE1	1.88	0.54
3:K:110:THR:HG22	7:O:20:HIS:CD2	2.43	0.54
22:a:113:SER:HB2	22:a:140:VAL:HG12	1.89	0.54
18:e:59:THR:HG23	19:f:62:MET:HE2	1.89	0.54
8:Q:83:HIS:HB2	8:Q:134:LEU:HD13	1.88	0.54
10:P:153:PHE:CZ	10:P:169:SER:HB2	2.43	0.54
16:E:130:ARG:HE	16:E:139:LEU:HA	1.71	0.54
18:G:62:ILE:HB	19:J:62:MET:HE1	1.90	0.54
18:e:24:GLN:O	19:f:40:TYR:HD1	1.90	0.54
9:U:368:TYR:HE1	10:P:245:ARG:HB3	1.73	0.54
18:e:54:VAL:HG21	19:f:98:VAL:HG21	1.90	0.54
18:e:55:LEU:HD11	19:f:70:PHE:HD2	1.72	0.54
2:I:363:MET:HG3	2:I:388:PHE:HD2	1.73	0.54
20:V:204:DG:H2''	20:V:205:DG:H5''	1.90	0.54
22:n:55:THR:HG22	22:n:74:TYR:HD1	1.72	0.54
4:L:236:THR:HA	4:L:258:PRO:HG3	1.89	0.54
7:O:143:VAL:HG12	7:O:145:GLN:HG3	1.89	0.54
21:Y:-249:DG:H5''	17:h:45:ARG:HD2	1.90	0.54
21:Y:-181:DC:H2''	21:Y:-180:DA:C8	2.42	0.54
21:Y:-21:DT:H2''	21:Y:-20:DT:C5	2.43	0.54
2:I:381:ASP:HB3	2:I:384:VAL:HG12	1.90	0.54
10:P:72:THR:HG21	11:R:175:ILE:HG12	1.89	0.54
20:V:237:DC:H2''	20:V:238:DG:C8	2.43	0.54
22:n:69:TRP:HZ2	22:n:72:TYR:HD2	1.55	0.54
16:E:121:LEU:HD22	17:F:43:VAL:HG21	1.90	0.54
20:V:156:DT:H2''	20:V:157:DG:N7	2.22	0.54
20:V:291:DT:H1'	20:V:292:DT:C4	2.43	0.54
17:h:75:HIS:CG	19:j:96:THR:HG21	2.43	0.54
6:N:12:THR:HG21	6:N:69:LEU:HG	1.89	0.53
7:O:193:GLN:HA	7:O:281:HIS:HD2	1.73	0.53
14:S:46:THR:HG21	15:X:58:VAL:HG11	1.90	0.53
20:V:136:DT:H2''	20:V:137:DG:H5'	1.91	0.53
21:Y:-138:DC:H1'	21:Y:-137:DC:H5'	1.90	0.53
6:N:99:PHE:N	7:O:212:ASN:HD22	2.06	0.53
8:Q:155:LEU:HB2	9:U:313:ILE:HG22	1.90	0.53
15:X:12:LEU:HD11	15:X:31:MET:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Z:212:LEU:HD11	22:Z:218:SER:HA	1.90	0.53
22:a:105:LEU:HB3	22:a:108:LEU:HD21	1.90	0.53
22:m:58:TRP:CZ3	22:m:118:CYS:HB3	2.43	0.53
2:I:73:PHE:HE2	2:I:95:VAL:HG21	1.73	0.53
2:I:400:CYS:SG	2:I:403:TYR:HB3	2.48	0.53
3:K:117:LYS:HD2	7:O:16:GLY:HA2	1.90	0.53
6:N:90:LYS:HB2	6:N:185:HIS:ND1	2.23	0.53
10:P:103:GLN:O	10:P:121:GLN:HA	2.07	0.53
12:T:515:LEU:HB3	12:T:519:MET:HE1	1.89	0.53
16:E:103:VAL:HG21	17:F:40:ARG:HD2	1.91	0.53
19:J:80:LEU:HD11	19:J:100:LEU:HD12	1.90	0.53
20:V:125:DG:H4'	20:V:126:DT:OP1	2.08	0.53
18:i:63:LEU:HD13	19:j:45:LEU:HB2	1.89	0.53
6:N:204:ILE:HG22	6:N:330:ARG:HG2	1.90	0.53
19:J:38:SER:HA	19:J:59:MET:HE2	1.89	0.53
18:i:49:VAL:HG21	19:j:121:TYR:CG	2.43	0.53
17:d:84:MET:HE2	17:d:88:TYR:CE2	2.42	0.53
2:I:400:CYS:HB3	2:I:403:TYR:O	2.09	0.53
3:K:210:ILE:HG12	3:K:237:SER:HB3	1.89	0.53
21:Y:-36:DG:H2''	21:Y:-35:DA:H8	1.72	0.53
21:Y:-120:DA:H2''	21:Y:-119:DG:C8	2.43	0.53
21:Y:-36:DG:H2''	21:Y:-35:DA:C8	2.43	0.53
22:Z:116:TYR:O	22:Z:135:GLY:HA2	2.08	0.53
11:R:135:GLU:O	11:R:139:THR:HG23	2.09	0.53
14:S:40:MET:HE1	15:X:58:VAL:HG23	1.91	0.53
21:Y:-139:DT:H2''	21:Y:-138:DC:OP2	2.09	0.53
1:H:202:LEU:HD22	3:K:166:MET:HE3	1.91	0.53
6:N:98:LEU:HB3	7:O:217:LEU:HD12	1.91	0.53
17:F:84:MET:HE2	17:F:88:TYR:CE2	2.43	0.53
20:V:56:DC:H2'	20:V:57:DT:H71	1.91	0.53
20:V:262:DA:H4'	16:g:63:ARG:HD3	1.90	0.53
2:I:621:GLU:OE2	2:I:632:PHE:HB2	2.09	0.53
16:g:120:THR:HA	17:h:45:ARG:HB2	1.92	0.53
2:I:189:PHE:HA	2:I:205:LEU:HD11	1.90	0.52
20:V:17:DT:H2''	20:V:18:DA:N7	2.25	0.52
20:V:231:DA:H2''	20:V:232:DA:C8	2.44	0.52
2:I:243:LYS:HD2	2:I:252:VAL:HB	1.90	0.52
2:I:367:LEU:HD13	2:I:388:PHE:HZ	1.73	0.52
8:Q:107:GLN:CD	14:S:14:SER:HB2	2.34	0.52
16:E:47:TRP:CD2	17:F:44:LYS:HG3	2.43	0.52
20:V:261:DA:H1'	20:V:262:DA:N7	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:n:205:LEU:HA	22:n:216:VAL:HG21	1.91	0.52
6:N:21:LEU:HD21	6:N:52:LEU:HD11	1.91	0.52
2:I:139:ILE:HB	2:I:175:ILE:HG13	1.91	0.52
2:I:446:TRP:HH2	2:I:452:ARG:HA	1.74	0.52
2:I:604:CYS:HB3	2:I:734:PHE:HB3	1.91	0.52
3:K:91:THR:HA	3:K:94:LYS:HD3	1.91	0.52
20:V:228:DT:H2''	20:V:229:DT:C6	2.45	0.52
4:L:127:MET:HE2	4:L:163:CYS:HB2	1.92	0.52
17:d:71:THR:HG22	19:f:96:THR:HG23	1.91	0.52
12:T:541:LEU:O	12:T:545:GLN:HG3	2.10	0.52
2:I:480:GLN:HA	5:M:169:LEU:HD22	1.89	0.52
6:N:148:LYS:HB3	6:N:167:MET:HG2	1.92	0.52
9:U:367:ASP:HB3	10:P:249:LEU:HD21	1.91	0.52
16:E:105:LEU:HD11	16:E:130:ARG:HG3	1.92	0.52
18:G:111:ILE:HD12	18:G:116:LEU:HD11	1.91	0.52
22:Z:41:LYS:HG3	22:Z:104:GLU:HG2	1.90	0.52
22:a:110:SER:HA	22:a:140:VAL:HG11	1.91	0.52
4:L:246:SER:CB	4:L:247:PRO:HD3	2.40	0.52
21:Y:-210:DT:H2''	21:Y:-209:DA:N7	2.25	0.52
2:I:111:ILE:O	2:I:115:ILE:HG12	2.10	0.52
2:I:572:TYR:HD1	2:I:578:PRO:HA	1.75	0.52
16:A:126:VAL:HG21	17:B:50:ILE:HD11	1.92	0.52
17:F:76:ALA:HA	19:J:84:ASN:OD1	2.10	0.52
21:Y:-304:DT:H4'	21:Y:-303:DC:OP1	2.09	0.52
19:f:102:LEU:HD13	19:f:106:LEU:HG	1.92	0.52
3:K:131:GLU:O	3:K:135:ILE:HG13	2.09	0.51
5:M:19:LEU:HD21	5:M:54:LEU:HD21	1.92	0.51
13:W:18:PRO:HB2	13:W:21:PHE:HB3	1.91	0.51
21:Y:-221:DC:H2''	21:Y:-220:DT:C5	2.46	0.51
1:H:171:LYS:HG2	3:K:139:LEU:HB3	1.93	0.51
2:I:646:SER:HA	2:I:658:GLY:HA3	1.92	0.51
21:Y:-287:DG:H5''	18:i:14:ALA:HA	1.92	0.51
17:h:30:THR:HB	17:h:32:PRO:HD2	1.92	0.51
22:m:25:GLN:HG3	22:m:27:GLN:HE22	1.76	0.51
2:I:652:TRP:CZ3	2:I:735:ILE:HG12	2.46	0.51
3:K:254:ARG:HA	3:K:262:ILE:HG22	1.93	0.51
11:R:90:LEU:HD22	11:R:140:LYS:NZ	2.26	0.51
20:V:213:DC:H2''	20:V:214:DA:C8	2.45	0.51
2:I:611:ARG:HH12	2:I:738:SER:HB3	1.75	0.51
5:M:138:PHE:HA	5:M:141:THR:HG22	1.93	0.51
21:Y:-188:DA:H4'	21:Y:-187:DT:OP1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:-66:DG:H2'	21:Y:-65:DT:H71	1.91	0.51
1:H:199:ARG:O	1:H:203:GLN:HG2	2.10	0.51
2:I:118:SER:HB2	2:I:120:LYS:NZ	2.26	0.51
4:L:66:PHE:O	4:L:70:LYS:HE2	2.11	0.51
4:L:303:ARG:HD2	5:M:109:HIS:HA	1.92	0.51
20:V:77:DT:H2''	20:V:78:DC:C6	2.45	0.51
22:Z:69:TRP:CG	22:Z:254:TYR:HB2	2.46	0.51
1:H:189:MET:SD	2:I:329:LEU:HD21	2.50	0.51
2:I:618:LYS:HB2	2:I:637:TYR:HE2	1.76	0.51
17:F:34:ILE:HG21	17:F:51:TYR:HA	1.92	0.51
20:V:15:DC:H4'	20:V:16:DA:OP1	2.11	0.51
20:V:130:DT:H2''	20:V:131:DG:C8	2.46	0.51
20:V:211:DG:H1'	20:V:212:DA:C8	2.45	0.51
21:Y:-183:DA:H2''	21:Y:-182:DA:C8	2.46	0.51
1:H:150:LEU:HB3	3:K:118:LEU:HB3	1.93	0.51
9:U:256:PRO:O	9:U:259:GLU:HB3	2.11	0.51
4:L:311:VAL:HG23	4:L:324:CYS:HB3	1.92	0.51
19:D:57:LYS:HZ1	17:F:99:GLY:HA3	1.75	0.51
20:V:228:DT:H3	21:Y:-228:DA:H61	1.59	0.51
21:Y:-225:DG:H2'	21:Y:-224:DG:C8	2.45	0.51
2:I:109:ILE:HG12	2:I:133:MET:HE1	1.92	0.51
3:K:112:GLU:O	3:K:116:GLU:HG2	2.11	0.51
16:E:45:GLN:HB2	16:E:47:TRP:CD1	2.46	0.51
20:V:137:DG:H2''	20:V:138:DG:H5''	1.91	0.51
20:V:174:DG:H2''	20:V:175:DG:C8	2.46	0.51
21:Y:-110:DG:H2''	21:Y:-109:DG:N7	2.26	0.51
21:Y:-90:DT:H1'	21:Y:-89:DA:C4	2.46	0.51
22:Z:60:LYS:HB2	22:Z:70:ILE:HD11	1.92	0.51
18:i:79:ILE:HG12	18:i:82:HIS:CE1	2.45	0.51
6:N:127:GLU:O	6:N:128:GLU:HG3	2.11	0.51
8:Q:239:LEU:HB3	9:U:387:LEU:HD13	1.91	0.51
12:T:535:VAL:HB	12:T:548:ILE:HD11	1.93	0.51
20:V:20:DA:H2''	20:V:21:DA:C8	2.46	0.51
21:Y:-200:DT:H2''	21:Y:-199:DG:C8	2.45	0.51
22:Z:92:LEU:HD23	22:Z:103:MET:SD	2.51	0.51
1:H:202:LEU:HD13	3:K:166:MET:HE3	1.92	0.50
4:L:88:LEU:HB3	4:L:121:PHE:HB3	1.93	0.50
7:O:218:LEU:HD13	7:O:239:TYR:HE1	1.76	0.50
8:Q:76:LEU:HB3	8:Q:81:ARG:HH12	1.76	0.50
8:Q:83:HIS:CB	8:Q:134:LEU:HD13	2.41	0.50
18:C:21:ALA:C	19:D:120:LYS:HD2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:243:DC:H2''	20:V:244:DG:C8	2.46	0.50
22:n:42:MET:SD	22:n:103:MET:HB2	2.51	0.50
1:H:141:MET:O	1:H:145:GLN:HG3	2.10	0.50
9:U:309:MET:O	9:U:313:ILE:HG23	2.11	0.50
20:V:250:DC:H2''	20:V:251:DC:C5	2.46	0.50
21:Y:-187:DT:H2''	21:Y:-186:DG:C8	2.46	0.50
21:Y:-142:DA:H2'	21:Y:-141:DT:H71	1.93	0.50
22:n:92:LEU:CD2	22:n:103:MET:HE1	2.24	0.50
8:Q:179:LEU:O	8:Q:183:ILE:HG23	2.11	0.50
19:J:76:GLU:HB3	19:J:97:ALA:HB1	1.93	0.50
21:Y:-208:DC:H2''	21:Y:-207:DG:C8	2.46	0.50
19:f:113:GLU:O	19:f:116:LYS:HG3	2.11	0.50
1:H:211:VAL:HG23	3:K:268:HIS:HB3	1.93	0.50
2:I:728:LEU:HD23	2:I:731:LEU:HD23	1.93	0.50
4:L:95:LEU:HD13	4:L:199:TRP:CG	2.46	0.50
4:L:218:LEU:HD22	4:L:316:THR:HG23	1.94	0.50
6:N:117:LYS:HB2	6:N:140:GLN:HG3	1.94	0.50
12:T:521:ARG:HD2	14:S:68:PHE:CZ	2.46	0.50
21:Y:-252:DG:H21	16:g:43:ARG:HH22	1.59	0.50
21:Y:-133:DT:H2''	21:Y:-132:DG:C8	2.47	0.50
22:a:181:CYS:SG	22:a:191:LEU:HD11	2.51	0.50
19:f:44:VAL:O	19:f:47:GLN:HG2	2.12	0.50
18:i:55:LEU:HD11	19:j:70:PHE:HD2	1.76	0.50
3:K:243:VAL:HG13	3:K:262:ILE:HD13	1.92	0.50
4:L:88:LEU:HD22	4:L:121:PHE:HD2	1.77	0.50
6:N:15:LYS:HB3	6:N:73:TYR:CZ	2.47	0.50
17:B:62:LEU:HB3	17:B:66:ILE:HD12	1.93	0.50
20:V:89:DT:H1'	20:V:90:DA:C5	2.47	0.50
22:a:191:LEU:HD13	22:a:229:PHE:CG	2.46	0.50
22:a:192:SER:O	22:a:246:CYS:HA	2.10	0.50
1:H:171:LYS:HD2	3:K:143:HIS:CB	2.42	0.50
3:K:28:CYS:HA	3:K:31:MET:HE2	1.94	0.50
6:N:243:VAL:O	6:N:246:GLU:HG2	2.11	0.50
20:V:270:DG:H2''	20:V:271:DG:N7	2.27	0.50
21:Y:-264:DG:H2''	21:Y:-263:DG:C8	2.47	0.50
2:I:509:SER:HB3	2:I:575:TYR:HB3	1.93	0.50
9:U:371:VAL:HB	10:P:245:ARG:HE	1.77	0.50
16:E:112:LEU:HD13	16:E:128:LEU:HD23	1.93	0.50
16:E:140:GLY:HA3	17:F:64:ASN:ND2	2.26	0.50
20:V:153:DT:H2''	20:V:154:DT:H71	1.94	0.50
21:Y:-76:DC:H2''	21:Y:-75:DA:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:-26:DC:H2''	21:Y:-25:DT:H71	1.94	0.50
22:Z:61:GLN:HB2	22:Z:67:LEU:HD23	1.93	0.50
1:H:119:ILE:HD12	1:H:126:LEU:HD13	1.93	0.50
2:I:112:LEU:HD11	2:I:133:MET:SD	2.51	0.50
7:O:238:LEU:HB2	7:O:249:ASP:HB2	1.94	0.50
4:L:239:PHE:HD2	4:L:307:VAL:HG22	1.76	0.50
6:N:272:GLU:HB2	6:N:337:ARG:HG3	1.94	0.50
18:C:62:ILE:HB	19:D:62:MET:HE1	1.92	0.50
21:Y:-283:DA:H2''	21:Y:-282:DG:C8	2.46	0.50
21:Y:-174:DC:H2''	21:Y:-173:DC:C6	2.47	0.50
21:Y:-114:DC:H2'	21:Y:-113:DT:H71	1.94	0.50
6:N:26:LYS:O	6:N:29:ASP:HB3	2.13	0.49
8:Q:134:LEU:CD1	9:U:292:MET:HE2	2.41	0.49
16:A:105:LEU:HD11	16:A:126:VAL:HG13	1.93	0.49
16:g:94:LEU:HD21	17:h:66:ILE:HD11	1.94	0.49
2:I:348:PRO:HA	2:I:351:LEU:HB2	1.94	0.49
6:N:49:VAL:O	6:N:53:ILE:HG12	2.12	0.49
6:N:269:TYR:CE2	6:N:322:LEU:HB3	2.47	0.49
7:O:197:LEU:HD13	7:O:280:LEU:HG	1.94	0.49
18:G:77:ARG:NE	21:Y:-16:DT:H5''	2.27	0.49
20:V:210:DA:H1'	20:V:211:DG:O4'	2.13	0.49
21:Y:-201:DT:H2''	21:Y:-200:DT:C5	2.47	0.49
21:Y:-186:DG:H2''	21:Y:-185:DT:H71	1.93	0.49
21:Y:-157:DC:H2''	21:Y:-156:DA:N7	2.27	0.49
22:Z:58:TRP:NE1	22:Z:103:MET:HE3	2.27	0.49
5:M:30:GLN:HB3	5:M:139:ARG:CZ	2.42	0.49
8:Q:150:ALA:O	8:Q:153:GLU:HG2	2.12	0.49
8:Q:223:THR:HG21	10:P:260:LEU:HD22	1.94	0.49
9:U:404:LEU:HD22	11:R:139:THR:HG21	1.94	0.49
21:Y:-14:DT:C2	21:Y:-13:DG:N7	2.81	0.49
18:e:65:LEU:HB3	18:e:86:ALA:HB1	1.95	0.49
22:m:72:TYR:HE2	22:m:81:LYS:HD2	1.77	0.49
1:H:171:LYS:HD2	3:K:143:HIS:HB2	1.95	0.49
7:O:211:ARG:HA	7:O:217:LEU:O	2.12	0.49
7:O:250:VAL:HG21	7:O:275:PHE:CB	2.43	0.49
21:Y:-201:DT:H2''	21:Y:-200:DT:C6	2.47	0.49
7:O:214:LEU:HD21	7:O:242:LEU:HD11	1.94	0.49
20:V:207:DC:H2''	20:V:208:DG:C8	2.48	0.49
19:j:61:ILE:HG22	19:j:62:MET:HE2	1.93	0.49
22:m:34:VAL:HG21	22:m:108:LEU:HD13	1.94	0.49
1:H:168:SER:HB3	2:I:378:CYS:SG	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:162:ILE:HD11	9:U:316:LYS:O	2.13	0.49
10:P:69:PHE:HD1	11:R:175:ILE:HG23	1.77	0.49
16:c:108:ASP:HB2	16:c:133:ARG:HH21	1.78	0.49
3:K:70:GLU:HG2	3:K:74:TRP:CD1	2.48	0.49
7:O:155:VAL:HG11	7:O:161:LEU:HD22	1.94	0.49
21:Y:-253:DG:H2''	21:Y:-252:DG:C8	2.48	0.49
5:M:75:LYS:HA	5:M:112:ILE:HD11	1.94	0.49
7:O:108:TYR:HB2	10:P:78:ILE:HG21	1.94	0.49
16:E:104:HIS:C	16:E:133:ARG:HH22	2.20	0.49
18:i:29:ARG:HG3	18:i:32:ARG:NH2	2.28	0.49
1:H:199:ARG:O	1:H:202:LEU:HB2	2.13	0.49
6:N:275:PHE:HB2	6:N:291:LEU:HB2	1.95	0.49
4:L:334:TYR:O	4:L:337:GLU:HG2	2.13	0.49
20:V:18:DA:H2''	20:V:19:DA:N7	2.28	0.49
20:V:178:DT:H3	21:Y:-178:DA:H61	1.60	0.49
2:I:105:ALA:O	2:I:109:ILE:HG13	2.13	0.48
3:K:255:HIS:HB3	3:K:258:ASP:O	2.13	0.48
10:P:121:GLN:HG2	10:P:137:ASP:HB3	1.94	0.48
18:i:65:LEU:HB3	18:i:86:ALA:HB1	1.94	0.48
4:L:257:HIS:CG	6:N:292:ARG:HH21	2.31	0.48
6:N:131:VAL:O	6:N:153:VAL:HA	2.13	0.48
6:N:204:ILE:HD11	6:N:264:LEU:HD11	1.94	0.48
16:E:51:ILE:HG13	17:F:39:ARG:HD2	1.95	0.48
17:F:78:ARG:HD2	21:Y:-46:DA:H3'	1.95	0.48
19:J:92:ARG:O	19:J:96:THR:HG22	2.14	0.48
21:Y:-299:DA:H4'	18:i:77:ARG:CZ	2.43	0.48
21:Y:-59:DT:H2''	21:Y:-58:DA:C8	2.49	0.48
22:n:166:PRO:HG2	22:n:179:ILE:HG23	1.95	0.48
6:N:264:LEU:HD13	6:N:303:LEU:HD12	1.95	0.48
8:Q:166:VAL:HG11	9:U:319:ARG:HH21	1.77	0.48
18:G:28:GLY:HA3	20:V:30:DA:H3'	1.95	0.48
19:J:37:TYR:HA	19:J:40:TYR:HD2	1.78	0.48
19:J:39:VAL:HG12	19:J:43:LYS:HE3	1.95	0.48
20:V:46:DT:H2''	20:V:47:DC:C6	2.47	0.48
18:i:87:ILE:HG23	18:i:93:LEU:HB3	1.95	0.48
22:m:92:LEU:HD23	22:m:103:MET:HG2	1.95	0.48
22:n:41:LYS:HA	22:n:103:MET:O	2.12	0.48
5:M:102:THR:HG23	5:M:133:LEU:H	1.78	0.48
17:F:30:THR:HB	17:F:32:PRO:HD2	1.95	0.48
17:F:34:ILE:HB	17:F:51:TYR:HD1	1.78	0.48
19:f:81:ALA:HB2	19:f:93:GLU:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:83:GLU:O	1:H:86:GLU:HG2	2.14	0.48
17:B:31:LYS:HB3	17:B:35:ARG:NH2	2.28	0.48
17:F:35:ARG:HA	17:F:46:ILE:HD13	1.95	0.48
20:V:88:DT:H2''	20:V:89:DT:C5	2.49	0.48
21:Y:-55:DC:H2''	21:Y:-54:DG:H8	1.77	0.48
6:N:112:LEU:HB3	6:N:119:VAL:HG11	1.96	0.48
8:Q:131:MET:HE3	8:Q:132:GLU:N	2.28	0.48
10:P:129:GLU:OE2	10:P:130:ARG:HD2	2.14	0.48
17:F:75:HIS:CG	19:J:96:THR:HG21	2.49	0.48
20:V:184:DC:H42	21:Y:-184:DG:H1	1.61	0.48
22:Z:69:TRP:CD2	22:Z:254:TYR:HB2	2.49	0.48
17:h:35:ARG:HA	17:h:46:ILE:HD13	1.96	0.48
22:m:193:TRP:HZ3	22:m:209:ALA:HA	1.79	0.48
22:n:212:LEU:HD11	22:n:218:SER:HA	1.95	0.48
2:I:482:PHE:HZ	2:I:547:ALA:HB2	1.78	0.48
3:K:102:GLN:O	3:K:105:GLU:HG2	2.13	0.48
7:O:237:LEU:HD22	7:O:280:LEU:HD13	1.94	0.48
7:O:274:LEU:HD22	7:O:278:LYS:HD2	1.95	0.48
9:U:408:ASN:ND2	11:R:142:LEU:HD21	2.28	0.48
20:V:221:DG:H2''	20:V:222:DC:OP2	2.13	0.48
21:Y:-277:DT:H2''	21:Y:-276:DA:C8	2.49	0.48
21:Y:-112:DA:H2''	21:Y:-111:DG:C8	2.49	0.48
22:n:80:THR:HB	22:n:92:LEU:HD12	1.96	0.48
16:g:119:VAL:HG21	17:h:44:LYS:HD3	1.95	0.48
4:L:250:LEU:HD23	6:N:309:LEU:HD11	1.96	0.48
11:R:146:VAL:HG22	11:R:151:LEU:HD22	1.95	0.48
14:S:75:THR:HG23	14:S:76:THR:HG23	1.95	0.48
19:D:44:VAL:O	19:D:47:GLN:HG2	2.14	0.48
20:V:57:DT:H2''	20:V:58:DT:C6	2.49	0.48
20:V:133:DA:H2''	20:V:134:DA:OP2	2.14	0.48
21:Y:-175:DC:H2''	21:Y:-174:DC:C6	2.49	0.48
2:I:110:ASP:HB2	2:I:143:SER:OG	2.14	0.48
5:M:23:THR:HG21	5:M:77:SER:HA	1.96	0.48
8:Q:83:HIS:HB3	8:Q:134:LEU:HD22	1.96	0.48
8:Q:250:GLN:HB3	11:R:100:ILE:HD11	1.95	0.48
9:U:408:ASN:ND2	11:R:139:THR:HG22	2.28	0.48
16:A:65:LEU:HB3	16:A:66:PRO:HD3	1.95	0.48
17:F:34:ILE:HA	17:F:37:LEU:HD12	1.95	0.48
18:G:77:ARG:HE	21:Y:-16:DT:H5''	1.79	0.48
21:Y:-207:DG:H2''	21:Y:-206:DA:C8	2.49	0.48
12:T:500:VAL:HG21	14:S:87:ARG:CZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:D:102:LEU:HB2	19:D:107:ALA:HB2	1.95	0.47
20:V:98:DA:H2''	20:V:99:DG:C8	2.48	0.47
21:Y:-252:DG:H2''	21:Y:-251:DG:C8	2.49	0.47
21:Y:-174:DC:H2''	21:Y:-173:DC:C5	2.49	0.47
2:I:333:LEU:HD22	3:K:161:GLU:HB2	1.95	0.47
4:L:49:ILE:HD11	4:L:269:HIS:CE1	2.49	0.47
15:X:35:LEU:O	15:X:39:VAL:HG23	2.14	0.47
16:A:73:GLU:O	16:A:76:VAL:HG12	2.14	0.47
16:E:74:ILE:HA	16:E:77:LYS:HE2	1.96	0.47
20:V:24:DT:H2''	20:V:25:DA:C8	2.49	0.47
2:I:596:ASP:OD2	3:K:104:LEU:HD21	2.14	0.47
4:L:79:PRO:HB2	4:L:178:PHE:HB3	1.95	0.47
6:N:129:ASN:CG	7:O:213:PRO:HG3	2.39	0.47
8:Q:251:MET:HE1	11:R:100:ILE:HG23	1.97	0.47
18:G:77:ARG:HD2	21:Y:-16:DT:H5''	1.95	0.47
21:Y:-50:DC:H2''	21:Y:-49:DT:C6	2.49	0.47
17:h:76:ALA:HA	19:j:84:ASN:OD1	2.13	0.47
4:L:265:TRP:HH2	4:L:275:VAL:HG13	1.79	0.47
5:M:73:HIS:HE1	5:M:106:ARG:NE	2.12	0.47
7:O:260:LEU:HD23	7:O:260:LEU:H	1.79	0.47
11:R:136:MET:HE3	11:R:140:LYS:NZ	2.29	0.47
19:J:38:SER:HA	19:J:59:MET:CE	2.44	0.47
20:V:238:DG:H2''	20:V:239:DT:C6	2.49	0.47
21:Y:-284:DT:H2''	21:Y:-283:DA:C8	2.49	0.47
21:Y:-228:DA:H4'	16:c:63:ARG:HD3	1.96	0.47
1:H:89:ILE:HG12	3:K:71:LEU:HA	1.96	0.47
1:H:189:MET:HE3	3:K:155:GLU:CA	2.43	0.47
1:H:238:LEU:HD11	2:I:180:GLN:HB3	1.96	0.47
2:I:78:ILE:N	2:I:84:LYS:HZ3	2.12	0.47
2:I:617:ALA:O	2:I:621:GLU:HG3	2.14	0.47
6:N:266:PHE:CZ	6:N:296:LYS:HD2	2.50	0.47
19:D:57:LYS:NZ	17:F:99:GLY:HA3	2.30	0.47
21:Y:-282:DG:H2''	21:Y:-281:DG:C8	2.50	0.47
16:c:126:VAL:HG21	17:d:50:ILE:HD11	1.96	0.47
16:g:69:ARG:HA	16:g:72:ARG:HD2	1.97	0.47
18:C:65:LEU:HD11	22:Z:124:ARG:HH21	1.80	0.47
21:Y:-55:DC:C2	21:Y:-54:DG:N7	2.82	0.47
17:h:77:LYS:HG3	19:j:92:ARG:NH2	2.30	0.47
1:H:43:LEU:HD11	3:K:25:ILE:HG12	1.97	0.47
2:I:498:LYS:HD3	2:I:564:PHE:HA	1.97	0.47
5:M:102:THR:HA	5:M:131:CYS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:214:LEU:HG	10:P:234:PRO:HG2	1.97	0.47
8:Q:228:ILE:HG21	9:U:388:PRO:HB3	1.97	0.47
13:W:26:PHE:CE2	13:W:35:LEU:HB2	2.50	0.47
19:J:33:ARG:HE	21:Y:-25:DT:H4'	1.80	0.47
21:Y:-273:DC:H2''	21:Y:-272:DC:C5	2.49	0.47
21:Y:-226:DC:H2''	21:Y:-225:DG:H8	1.78	0.47
21:Y:-110:DG:H2''	21:Y:-109:DG:C8	2.50	0.47
16:g:75:CYS:HB2	16:g:86:TRP:HZ2	1.79	0.47
18:i:58:LEU:HD12	19:j:69:ILE:HG21	1.96	0.47
6:N:193:LEU:HD12	6:N:332:ASN:HB2	1.97	0.47
13:W:34:ARG:HD3	20:V:136:DT:OP2	2.15	0.47
15:X:31:MET:HE2	15:X:31:MET:HA	1.95	0.47
21:Y:-80:DG:H2''	21:Y:-79:DG:C8	2.49	0.47
16:c:136:GLU:HG2	16:c:137:GLU:N	2.29	0.47
12:T:501:PHE:HZ	12:T:521:ARG:HD3	1.80	0.47
16:A:62:ILE:HD13	17:B:29:ILE:HD12	1.97	0.47
21:Y:-262:DT:H2''	21:Y:-261:DT:C6	2.50	0.47
18:i:63:LEU:HD11	19:j:41:VAL:HG13	1.96	0.47
7:O:214:LEU:HD23	7:O:216:ASN:ND2	2.30	0.47
16:A:66:PRO:HB3	17:B:28:GLY:HA3	1.97	0.47
20:V:290:DC:H2''	20:V:291:DT:C7	2.45	0.47
16:c:119:VAL:HG11	17:d:44:LYS:HD3	1.97	0.47
8:Q:145:ARG:HA	8:Q:145:ARG:NE	2.31	0.46
9:U:259:GLU:HA	9:U:282:TYR:OH	2.16	0.46
9:U:262:HIS:HB2	9:U:282:TYR:CZ	2.49	0.46
10:P:56:LEU:O	10:P:60:LEU:HD23	2.15	0.46
18:G:57:TYR:HB2	19:J:113:GLU:HG3	1.96	0.46
20:V:49:DA:H1'	20:V:50:DG:C8	2.50	0.46
20:V:82:DC:H2''	20:V:83:DG:H8	1.81	0.46
20:V:199:DC:H2''	20:V:200:DA:N7	2.30	0.46
18:e:111:ILE:HD11	16:g:52:ARG:HG3	1.96	0.46
1:H:57:TYR:HB3	3:K:38:CYS:SG	2.55	0.46
16:A:62:ILE:HB	16:A:95:GLN:HE21	1.79	0.46
17:F:39:ARG:HD3	17:F:43:VAL:O	2.15	0.46
20:V:145:DG:H2''	20:V:146:DG:C8	2.50	0.46
20:V:276:DT:H2''	20:V:277:DA:C8	2.50	0.46
21:Y:-211:DC:H2''	21:Y:-210:DT:C5	2.50	0.46
16:c:94:LEU:HD21	17:d:66:ILE:HD11	1.97	0.46
4:L:240:LEU:O	4:L:304:LEU:HD12	2.16	0.46
5:M:67:VAL:HG22	5:M:98:CYS:HB3	1.97	0.46
8:Q:151:ASN:C	9:U:309:MET:HE1	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:103:VAL:HG11	17:F:40:ARG:HG2	1.98	0.46
20:V:194:DC:H2'	20:V:195:DT:H71	1.96	0.46
20:V:202:DT:H5''	18:e:16:SER:HA	1.97	0.46
20:V:304:DA:H2''	20:V:305:DA:H8	1.80	0.46
21:Y:-226:DC:H2''	21:Y:-225:DG:C8	2.50	0.46
21:Y:-195:DA:H2''	21:Y:-194:DG:H8	1.79	0.46
22:n:172:SER:HB3	22:n:175:GLU:OE1	2.15	0.46
2:I:446:TRP:CH2	2:I:452:ARG:HA	2.49	0.46
3:K:61:ILE:HG22	3:K:65:LYS:HE3	1.97	0.46
5:M:19:LEU:HD23	5:M:66:ILE:HD13	1.98	0.46
5:M:28:LEU:HB3	5:M:48:LEU:HD22	1.97	0.46
7:O:194:ALA:HB1	7:O:211:ARG:HH11	1.81	0.46
21:Y:-279:DA:H2''	21:Y:-278:DG:C8	2.50	0.46
22:Z:252:SER:OG	22:Z:253:PRO:HD3	2.15	0.46
22:m:52:THR:HA	22:m:75:PRO:HB2	1.97	0.46
2:I:572:TYR:CD1	2:I:578:PRO:HA	2.50	0.46
6:N:172:THR:HB	6:N:173:PRO:HD3	1.97	0.46
6:N:186:HIS:CE1	9:U:332:PRO:HG3	2.51	0.46
6:N:301:HIS:ND1	6:N:304:GLU:HB2	2.31	0.46
8:Q:224:LEU:HD22	10:P:221:VAL:HG11	1.98	0.46
18:G:59:THR:HG23	19:J:62:MET:HE2	1.98	0.46
19:J:76:GLU:HA	19:J:79:ARG:HE	1.80	0.46
20:V:273:DG:H3'	17:h:78:ARG:HD2	1.96	0.46
4:L:95:LEU:HD23	4:L:121:PHE:HE1	1.81	0.46
9:U:362:LYS:HB2	10:P:281:SER:HB2	1.98	0.46
10:P:89:THR:HG23	10:P:99:ARG:HA	1.98	0.46
10:P:105:HIS:O	10:P:119:GLU:HA	2.16	0.46
10:P:120:PHE:HB3	10:P:138:LEU:HD12	1.98	0.46
11:R:139:THR:HB	11:R:143:MET:HE2	1.96	0.46
13:W:44:HIS:O	13:W:48:LEU:HG	2.16	0.46
20:V:146:DG:H2''	20:V:147:DA:C8	2.51	0.46
22:a:70:ILE:HG23	22:a:86:PHE:HD2	1.80	0.46
17:h:75:HIS:CE1	19:j:93:GLU:HG3	2.50	0.46
17:h:92:ARG:NH2	19:j:101:LEU:HA	2.31	0.46
2:I:373:LEU:HB3	2:I:427:PHE:CD2	2.51	0.46
2:I:645:THR:O	2:I:648:VAL:HG22	2.16	0.46
7:O:250:VAL:HG21	7:O:275:PHE:HB2	1.97	0.46
8:Q:88:MET:HE1	8:Q:114:LYS:HB2	1.97	0.46
9:U:326:GLU:O	9:U:330:LEU:HD23	2.15	0.46
12:T:465:LYS:HE3	13:W:13:ILE:HD13	1.96	0.46
12:T:540:PRO:HD2	12:T:543:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:225:DC:H2''	20:V:226:DG:C8	2.51	0.46
22:Z:102:TYR:C	22:Z:103:MET:HE2	2.41	0.46
17:d:68:ASP:OD2	17:d:92:ARG:HD3	2.15	0.46
18:e:17:ARG:HG2	18:e:20:ARG:HH11	1.80	0.46
1:H:216:PHE:HD2	1:H:240:LEU:HD21	1.81	0.46
3:K:27:GLU:O	3:K:31:MET:HG2	2.16	0.46
7:O:252:VAL:HG12	7:O:272:GLU:HG2	1.98	0.46
8:Q:134:LEU:HA	9:U:292:MET:SD	2.56	0.46
9:U:310:ILE:HA	9:U:313:ILE:HG12	1.98	0.46
15:X:30:LEU:HA	15:X:33:GLU:CD	2.41	0.46
20:V:299:DT:H2''	20:V:300:DC:C5	2.51	0.46
20:V:300:DC:H2''	20:V:301:DT:C6	2.50	0.46
20:V:311:DC:H2''	20:V:312:DA:C8	2.50	0.46
19:j:76:GLU:HB3	19:j:97:ALA:HB1	1.97	0.46
22:m:262:LEU:HD21	22:m:264:ILE:HD11	1.98	0.46
2:I:87:THR:HA	2:I:90:LYS:HE3	1.97	0.46
2:I:637:TYR:O	2:I:640:PHE:HB3	2.16	0.46
10:P:141:ILE:O	10:P:142:MET:HE2	2.16	0.46
11:R:120:GLU:HA	11:R:123:ILE:HG22	1.96	0.46
11:R:132:LEU:O	11:R:136:MET:HB2	2.16	0.46
18:G:42:ARG:HD3	21:Y:-36:DG:H4'	1.97	0.46
20:V:218:DC:H2''	20:V:219:DT:C7	2.44	0.46
7:O:218:LEU:HD13	7:O:239:TYR:CE1	2.51	0.46
7:O:234:CYS:O	7:O:252:VAL:HA	2.16	0.46
8:Q:176:ILE:HG12	9:U:334:LEU:HB2	1.98	0.46
16:E:63:ARG:HD2	20:V:60:DA:H4'	1.98	0.46
18:G:30:VAL:HG13	19:J:70:PHE:CE2	2.50	0.46
20:V:292:DT:H6	20:V:292:DT:H2''	1.63	0.46
21:Y:-185:DT:H2''	21:Y:-184:DG:C8	2.51	0.46
22:a:166:PRO:HG2	22:a:179:ILE:HG23	1.98	0.46
1:H:154:LEU:HD22	1:H:158:ARG:CZ	2.45	0.45
1:H:235:GLU:O	1:H:239:GLN:HG2	2.16	0.45
2:I:66:LEU:HD22	2:I:98:VAL:HG11	1.98	0.45
2:I:161:LYS:HB3	2:I:197:LEU:HD21	1.98	0.45
4:L:256:ILE:HG13	6:N:292:ARG:O	2.15	0.45
9:U:392:PHE:O	9:U:395:ARG:HB3	2.16	0.45
16:A:62:ILE:HG12	17:B:33:ALA:HB1	1.97	0.45
20:V:242:DG:H3'	16:c:118:ARG:HD3	1.99	0.45
20:V:294:DT:H2''	20:V:295:DA:N7	2.31	0.45
21:Y:-88:DA:H2''	21:Y:-87:DA:H8	1.80	0.45
22:Z:62:THR:HG22	22:Z:114:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:164:LEU:HD11	3:K:133:GLN:HG3	1.97	0.45
3:K:62:MET:HG3	5:M:94:LEU:HD11	1.98	0.45
3:K:223:LEU:HA	3:K:230:PRO:HB3	1.98	0.45
9:U:412:GLU:HG3	9:U:415:LEU:HD12	1.98	0.45
14:S:58:CYS:SG	15:X:11:LEU:HD13	2.56	0.45
17:F:31:LYS:CG	17:F:32:PRO:HD3	2.47	0.45
21:Y:-139:DT:H6	21:Y:-139:DT:H2'	1.59	0.45
21:Y:-97:DT:C2	21:Y:-96:DG:C8	3.04	0.45
21:Y:-49:DT:H2''	21:Y:-48:DA:N7	2.32	0.45
21:Y:-34:DC:C2	21:Y:-33:DC:C5	3.05	0.45
1:H:237:VAL:HA	1:H:240:LEU:HD12	1.99	0.45
2:I:455:PHE:O	2:I:459:VAL:HG23	2.16	0.45
3:K:24:LEU:HD21	3:K:82:ILE:HG12	1.99	0.45
4:L:243:VAL:HG22	4:L:302:THR:HG21	1.97	0.45
7:O:141:ASP:O	7:O:150:ILE:HA	2.17	0.45
8:Q:161:GLU:O	8:Q:165:MET:HG2	2.16	0.45
11:R:141:GLU:HG2	11:R:142:LEU:N	2.32	0.45
16:E:50:GLU:HA	16:E:53:LYS:HG2	1.96	0.45
16:E:63:ARG:HD3	21:Y:-57:DA:H4'	1.98	0.45
16:E:110:TYR:CE2	16:E:114:LEU:HD11	2.51	0.45
16:g:110:TYR:HB2	17:h:43:VAL:HG22	1.98	0.45
18:i:29:ARG:HG3	18:i:32:ARG:HH21	1.80	0.45
4:L:233:TYR:CG	4:L:258:PRO:HB2	2.51	0.45
4:L:236:THR:HG22	4:L:258:PRO:HD3	1.96	0.45
8:Q:186:LEU:O	8:Q:190:VAL:HG13	2.15	0.45
9:U:329:ARG:O	9:U:332:PRO:HD2	2.17	0.45
14:S:87:ARG:HA	14:S:93:LEU:HD22	1.98	0.45
18:G:24:GLN:NE2	19:J:44:VAL:HG22	2.29	0.45
20:V:91:DA:H1'	20:V:92:DC:H5'	1.97	0.45
20:V:155:DG:H2''	20:V:156:DT:OP2	2.17	0.45
21:Y:-268:DT:C2	21:Y:-267:DG:C8	3.04	0.45
19:j:76:GLU:HA	19:j:79:ARG:HE	1.81	0.45
2:I:589:TYR:CZ	2:I:660:GLY:HA3	2.51	0.45
2:I:618:LYS:HB2	2:I:637:TYR:CE2	2.51	0.45
3:K:51:THR:HG23	3:K:53:SER:H	1.81	0.45
3:K:62:MET:HE2	3:K:62:MET:HA	1.99	0.45
3:K:106:MET:O	3:K:110:THR:HG23	2.16	0.45
4:L:222:ALA:HB1	4:L:239:PHE:HE2	1.82	0.45
6:N:106:ASN:O	6:N:110:LYS:HG2	2.16	0.45
6:N:176:GLY:HA2	6:N:188:ILE:HD13	1.99	0.45
6:N:274:LYS:HA	6:N:290:PRO:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:412:GLU:HA	9:U:415:LEU:HB2	1.98	0.45
20:V:5:DA:H2''	20:V:6:DA:C8	2.52	0.45
20:V:144:DC:H2''	20:V:145:DG:C8	2.51	0.45
20:V:289:DC:H2''	20:V:290:DC:C5	2.51	0.45
21:Y:-177:DT:H2''	21:Y:-176:DT:C6	2.51	0.45
21:Y:-103:DT:H2''	21:Y:-102:DC:C5	2.52	0.45
21:Y:-102:DC:H2''	21:Y:-101:DC:C6	2.52	0.45
22:a:236:LEU:HD21	22:a:262:LEU:HD21	1.98	0.45
22:n:92:LEU:HD23	22:n:103:MET:CE	2.25	0.45
1:H:164:LEU:HD13	3:K:132:GLN:HB3	1.98	0.45
2:I:547:ALA:HB1	2:I:557:LEU:HD21	1.98	0.45
4:L:32:GLU:O	4:L:35:ARG:HG3	2.17	0.45
8:Q:239:LEU:HA	8:Q:242:LEU:HG	1.98	0.45
9:U:278:ILE:HA	9:U:281:PHE:CE1	2.51	0.45
14:S:43:SER:O	14:S:47:ILE:HD12	2.17	0.45
18:C:16:SER:HA	21:Y:-117:DA:H5''	1.97	0.45
18:C:28:GLY:HA3	21:Y:-118:DG:H3'	1.97	0.45
20:V:12:DT:C2	20:V:13:DC:C5	3.05	0.45
20:V:239:DT:H2''	20:V:240:DA:N7	2.32	0.45
21:Y:-225:DG:H2''	21:Y:-224:DG:O5'	2.15	0.45
21:Y:-215:DC:H2'	21:Y:-214:DT:H71	1.99	0.45
16:c:108:ASP:HB2	16:c:133:ARG:NH2	2.32	0.45
8:Q:131:MET:HE2	9:U:292:MET:HE3	1.99	0.45
10:P:240:THR:HB	10:P:242:VAL:HG23	1.99	0.45
21:Y:-29:DT:H2''	21:Y:-28:DG:C8	2.52	0.45
22:Z:58:TRP:CE2	22:Z:103:MET:HE3	2.52	0.45
22:Z:179:ILE:O	22:Z:230:SER:HA	2.17	0.45
2:I:348:PRO:O	2:I:352:GLN:OE1	2.35	0.45
2:I:668:LEU:HD12	2:I:673:VAL:HG21	1.98	0.45
5:M:53:PRO:HD3	5:M:87:HIS:CD2	2.52	0.45
10:P:206:MET:HE2	10:P:206:MET:HA	1.99	0.45
11:R:85:GLU:HA	11:R:88:MET:HG3	1.98	0.45
12:T:454:ASP:HB3	12:T:457:LYS:HB2	1.99	0.45
12:T:539:LEU:HD22	12:T:543:TYR:HD2	1.82	0.45
16:E:67:PHE:HZ	17:F:62:LEU:HD21	1.82	0.45
20:V:111:DC:H2''	20:V:112:DT:C5	2.50	0.45
21:Y:-187:DT:OP2	21:Y:-187:DT:H3'	2.16	0.45
2:I:339:PHE:HE2	2:I:344:LEU:HB2	1.82	0.45
2:I:357:LEU:HD12	2:I:375:TYR:CD1	2.52	0.45
2:I:405:VAL:O	2:I:406:ASN:C	2.59	0.45
4:L:70:LYS:O	4:L:321:LYS:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:137:VAL:HG11	9:U:292:MET:SD	2.56	0.45
12:T:504:HIS:ND1	14:S:84:LEU:HD11	2.32	0.45
16:g:65:LEU:HB3	16:g:66:PRO:HD3	1.99	0.45
22:n:165:SER:OG	22:n:166:PRO:HD3	2.17	0.45
2:I:70:VAL:O	2:I:74:GLU:OE1	2.34	0.45
8:Q:179:LEU:HD21	9:U:338:GLN:HB2	1.99	0.45
14:S:27:VAL:HG12	14:S:47:ILE:HG23	1.98	0.45
18:C:45:ALA:HB2	20:V:112:DT:OP2	2.16	0.45
21:Y:-166:DA:H2''	21:Y:-165:DA:C8	2.52	0.45
16:c:119:VAL:HG12	16:c:119:VAL:O	2.17	0.45
19:j:45:LEU:HA	19:j:48:VAL:HG22	1.99	0.45
2:I:565:TYR:CE1	2:I:583:PHE:HB3	2.53	0.44
4:L:158:TRP:CZ3	4:L:196:ILE:HG13	2.52	0.44
4:L:290:HIS:CE1	6:N:291:LEU:HD23	2.52	0.44
5:M:106:ARG:HB3	5:M:109:HIS:ND1	2.31	0.44
6:N:107:SER:O	6:N:111:ILE:HG12	2.17	0.44
6:N:302:LEU:O	6:N:303:LEU:HB2	2.18	0.44
9:U:284:ASN:O	9:U:288:GLN:HG2	2.17	0.44
16:A:74:ILE:HD11	17:B:59:LYS:HG3	1.99	0.44
20:V:123:DT:H2''	20:V:124:DA:C8	2.52	0.44
20:V:280:DC:H2''	20:V:281:DC:C5	2.52	0.44
21:Y:-242:DC:H2''	21:Y:-241:DG:C8	2.52	0.44
21:Y:-150:DT:H2''	21:Y:-149:DG:C8	2.52	0.44
21:Y:-20:DT:H2''	21:Y:-19:DT:C5	2.52	0.44
22:Z:34:VAL:HG21	22:Z:108:LEU:HD13	1.98	0.44
2:I:348:PRO:HA	2:I:351:LEU:HD12	1.98	0.44
6:N:127:GLU:HG3	6:N:128:GLU:H	1.82	0.44
7:O:190:ARG:HG3	7:O:245:THR:HA	1.98	0.44
7:O:210:GLN:O	7:O:218:LEU:HA	2.17	0.44
16:E:136:GLU:HG2	16:E:137:GLU:N	2.32	0.44
20:V:169:DA:H2''	20:V:170:DA:C8	2.52	0.44
20:V:302:DG:H2''	20:V:303:DG:C8	2.53	0.44
21:Y:-189:DT:H4'	21:Y:-188:DA:OP2	2.16	0.44
21:Y:-143:DA:H2''	21:Y:-142:DA:H8	1.81	0.44
21:Y:-106:DT:C2	21:Y:-105:DA:N7	2.85	0.44
22:Z:93:THR:OG1	22:Z:102:TYR:HB2	2.16	0.44
18:i:87:ILE:HD13	18:i:97:LEU:HD12	1.98	0.44
22:m:252:SER:OG	22:m:253:PRO:HD3	2.16	0.44
2:I:382:GLU:HB3	2:I:383:PRO:HD3	1.99	0.44
2:I:486:THR:O	2:I:490:LYS:HG3	2.17	0.44
7:O:164:ILE:HG22	7:O:176:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:65:LEU:HD12	14:S:77:ILE:HG21	2.00	0.44
18:G:29:ARG:HG3	18:G:32:ARG:NH2	2.32	0.44
20:V:154:DT:H2"	20:V:155:DG:N7	2.31	0.44
20:V:219:DT:H2"	20:V:220:DA:N7	2.32	0.44
21:Y:-200:DT:H2"	21:Y:-199:DG:N7	2.32	0.44
16:c:61:LEU:HD13	17:d:36:ARG:HB3	1.98	0.44
22:n:44:CYS:HB2	22:n:58:TRP:CZ2	2.52	0.44
4:L:74:LEU:HB3	4:L:211:LEU:HD23	1.99	0.44
4:L:76:SER:HB2	4:L:343:ILE:HG23	1.99	0.44
4:L:301:ALA:HA	5:M:74:SER:OG	2.16	0.44
7:O:102:LYS:HE3	10:P:63:LEU:HD13	2.00	0.44
7:O:187:TYR:HA	7:O:190:ARG:CZ	2.47	0.44
10:P:106:ARG:HG3	10:P:117:GLN:NE2	2.32	0.44
18:C:79:ILE:HG12	18:C:82:HIS:ND1	2.32	0.44
21:Y:-221:DC:H2"	21:Y:-220:DT:C6	2.53	0.44
21:Y:-193:DT:H4'	21:Y:-192:DT:OP1	2.18	0.44
21:Y:-131:DC:H2"	21:Y:-130:DA:C8	2.53	0.44
1:H:85:LEU:HB3	3:K:67:LEU:HB3	1.99	0.44
1:H:171:LYS:O	1:H:174:GLU:HG2	2.17	0.44
4:L:92:SER:HB2	4:L:119:VAL:O	2.17	0.44
4:L:127:MET:CE	4:L:164:CYS:H	2.30	0.44
4:L:340:ILE:HA	4:L:343:ILE:HG12	1.99	0.44
16:E:119:VAL:HG12	20:V:71:DG:OP1	2.18	0.44
20:V:42:DC:H2"	20:V:43:DA:C8	2.52	0.44
20:V:163:DC:H2"	20:V:164:DG:C8	2.52	0.44
1:H:145:GLN:HA	1:H:148:TRP:CE3	2.53	0.44
1:H:172:LEU:HD11	2:I:355:HIS:HA	1.99	0.44
2:I:366:VAL:HG22	2:I:372:LEU:HD13	2.00	0.44
2:I:647:MET:SD	2:I:734:PHE:CZ	3.11	0.44
7:O:197:LEU:HD21	7:O:205:LEU:HD11	2.00	0.44
8:Q:83:HIS:HE1	8:Q:133:ASP:HB2	1.83	0.44
14:S:65:LEU:HD11	14:S:82:VAL:HG22	2.00	0.44
16:A:102:LEU:HD22	17:B:54:THR:HG23	1.98	0.44
16:E:136:GLU:HG2	16:E:137:GLU:H	1.83	0.44
22:a:61:GLN:HE22	22:a:196:GLN:HE22	1.65	0.44
17:d:35:ARG:O	17:d:39:ARG:HG2	2.18	0.44
18:i:80:PRO:HA	18:i:83:LEU:HD12	1.98	0.44
17:F:44:LYS:HG2	17:F:45:ARG:HG3	2.00	0.44
18:G:24:GLN:O	19:J:40:TYR:HD1	2.01	0.44
21:Y:-236:DT:H2"	21:Y:-235:DG:C8	2.53	0.44
2:I:141:GLU:HG3	2:I:181:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:126:ILE:O	7:O:137:SER:HA	2.18	0.44
8:Q:231:LEU:HG	8:Q:232:ILE:HG23	2.00	0.44
17:B:84:MET:HE2	17:B:88:TYR:CE2	2.52	0.44
18:G:63:LEU:HD13	19:J:45:LEU:HB2	1.99	0.44
21:Y:-269:DT:H2'	21:Y:-268:DT:H71	1.98	0.44
22:a:169:MET:SD	22:a:177:VAL:HG13	2.58	0.44
22:a:205:LEU:HA	22:a:216:VAL:HG21	2.00	0.44
18:e:26:PRO:HB3	19:f:40:TYR:OH	2.18	0.44
2:I:73:PHE:O	2:I:121:PHE:HZ	2.01	0.44
5:M:140:ALA:O	5:M:144:GLN:HG2	2.18	0.44
8:Q:162:ILE:O	8:Q:166:VAL:HG13	2.18	0.44
20:V:82:DC:H2''	20:V:83:DG:C8	2.52	0.44
20:V:242:DG:H1'	20:V:243:DC:H5'	1.99	0.44
21:Y:-151:DG:H2'	21:Y:-150:DT:H71	2.00	0.44
21:Y:-108:DA:H2''	21:Y:-107:DG:C8	2.53	0.44
19:j:92:ARG:O	19:j:96:THR:HG22	2.18	0.44
22:n:241:THR:HB	22:n:264:ILE:HG12	1.99	0.44
2:I:440:TYR:HD2	4:L:35:ARG:HH12	1.65	0.43
3:K:160:ASN:HA	3:K:163:LYS:HZ3	1.83	0.43
4:L:214:ASN:HD21	4:L:216:PHE:HB3	1.83	0.43
4:L:306:ARG:HB2	4:L:315:HIS:CD2	2.52	0.43
6:N:320:SER:O	6:N:324:THR:HG23	2.17	0.43
8:Q:140:LEU:HA	8:Q:143:MET:HG3	1.99	0.43
8:Q:201:HIS:NE2	10:P:269:LEU:HD11	2.33	0.43
15:X:41:GLU:O	15:X:45:ARG:HG2	2.17	0.43
20:V:90:DA:H1'	20:V:91:DA:N7	2.32	0.43
22:a:27:GLN:HE21	22:a:45:LYS:CB	2.29	0.43
16:c:79:THR:O	16:c:79:THR:HG22	2.19	0.43
16:g:47:TRP:CD2	17:h:44:LYS:HG3	2.52	0.43
1:H:138:LYS:HE2	1:H:138:LYS:HB3	1.65	0.43
1:H:172:LEU:HD13	3:K:139:LEU:HD11	2.00	0.43
3:K:88:VAL:O	3:K:92:LEU:HG	2.18	0.43
6:N:13:ILE:HA	6:N:16:ILE:HD12	2.00	0.43
6:N:204:ILE:HA	6:N:209:TYR:CD2	2.52	0.43
10:P:209:ARG:HE	10:P:217:GLU:CD	2.26	0.43
13:W:26:PHE:CD2	13:W:35:LEU:HB2	2.53	0.43
14:S:69:ALA:HB2	14:S:77:ILE:HG12	1.99	0.43
21:Y:-115:DA:H2''	21:Y:-114:DC:H5''	2.00	0.43
16:g:45:GLN:HB2	16:g:47:TRP:CD1	2.53	0.43
3:K:47:THR:HB	5:M:89:ASP:HB3	2.01	0.43
5:M:5:ARG:HD2	5:M:8:ASP:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:88:MET:HE2	6:N:185:HIS:HB2	2.01	0.43
9:U:262:HIS:HB2	9:U:282:TYR:CE2	2.54	0.43
10:P:142:MET:CG	10:P:154:VAL:HG21	2.49	0.43
17:B:54:THR:O	17:B:58:LEU:HB3	2.17	0.43
18:G:17:ARG:NH2	18:G:28:GLY:HA2	2.33	0.43
20:V:235:DC:H2''	20:V:236:DA:C8	2.53	0.43
21:Y:-98:DT:H1'	21:Y:-97:DT:H5'	2.01	0.43
18:e:15:LYS:HB2	18:e:15:LYS:HE2	1.80	0.43
22:n:191:LEU:HD13	22:n:229:PHE:CG	2.53	0.43
2:I:319:THR:O	2:I:322:CYS:HB2	2.18	0.43
2:I:544:SER:HB3	2:I:561:ILE:HD13	2.00	0.43
3:K:82:ILE:O	3:K:84:LEU:HD12	2.19	0.43
3:K:184:LEU:HD11	3:K:216:LEU:HD12	2.00	0.43
13:W:32:GLN:HG2	13:W:33:LEU:HD23	2.00	0.43
18:C:37:GLY:HA3	18:C:39:TYR:CE2	2.54	0.43
20:V:62:DC:H2''	20:V:63:DG:H8	1.83	0.43
20:V:88:DT:H2''	20:V:89:DT:C7	2.48	0.43
20:V:104:DT:H2'	20:V:105:DT:H71	1.99	0.43
21:Y:-308:DC:H2''	21:Y:-307:DA:H8	1.84	0.43
22:m:44:CYS:HB2	22:m:58:TRP:CZ2	2.53	0.43
22:m:160:ILE:HD11	22:m:251:GLU:HG3	2.00	0.43
2:I:233:PRO:O	2:I:261:TYR:HB3	2.18	0.43
2:I:446:TRP:HE1	2:I:450:CYS:HB3	1.83	0.43
6:N:203:ALA:HA	6:N:208:GLN:HG2	2.00	0.43
8:Q:209:LEU:HD23	8:Q:209:LEU:HA	1.87	0.43
12:T:490:TYR:HE1	13:W:86:SER:HB2	1.84	0.43
18:C:50:TYR:OH	19:D:111:VAL:HA	2.18	0.43
16:E:102:LEU:HD22	17:F:54:THR:HG23	1.99	0.43
20:V:243:DC:H2''	20:V:244:DG:H8	1.83	0.43
20:V:279:DT:H2''	20:V:280:DC:C6	2.54	0.43
21:Y:-16:DT:H6	21:Y:-16:DT:H2'	1.67	0.43
22:Z:57:GLN:HG3	22:Z:129:LEU:CD2	2.49	0.43
22:Z:169:MET:HE1	22:Z:179:ILE:HD11	1.99	0.43
18:e:18:SER:OG	18:e:26:PRO:HA	2.17	0.43
22:m:181:CYS:SG	22:m:191:LEU:HD11	2.58	0.43
2:I:266:GLU:HG2	2:I:270:LYS:NZ	2.33	0.43
2:I:439:LEU:HG	2:I:455:PHE:CE1	2.54	0.43
5:M:138:PHE:O	5:M:142:MET:HG3	2.18	0.43
6:N:129:ASN:CB	7:O:213:PRO:HG3	2.48	0.43
6:N:129:ASN:HB3	6:N:156:SER:OG	2.18	0.43
8:Q:228:ILE:HA	8:Q:231:LEU:CD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:405:ARG:NH1	11:R:131:PHE:HZ	2.16	0.43
11:R:134:ARG:HB3	11:R:138:LYS:NZ	2.33	0.43
16:A:86:TRP:HB3	16:A:91:LEU:HG	2.01	0.43
17:B:75:HIS:HB2	19:D:96:THR:HG21	2.01	0.43
20:V:178:DT:H2''	20:V:179:DA:N7	2.33	0.43
21:Y:-308:DC:C2	21:Y:-307:DA:N7	2.86	0.43
21:Y:-282:DG:H2''	21:Y:-281:DG:N7	2.33	0.43
18:e:88:ARG:HA	18:e:88:ARG:HD3	1.79	0.43
1:H:165:LYS:HB2	3:K:132:GLN:NE2	2.34	0.43
4:L:127:MET:SD	4:L:127:MET:C	3.02	0.43
4:L:161:TRP:CE3	4:L:185:LEU:HD13	2.54	0.43
7:O:224:LEU:H	7:O:224:LEU:HD23	1.82	0.43
8:Q:92:ILE:HA	8:Q:95:ILE:HG12	2.01	0.43
9:U:351:LEU:HB2	10:P:268:LEU:HD11	2.00	0.43
14:S:79:THR:O	14:S:83:LYS:HG3	2.19	0.43
16:E:119:VAL:CG2	17:F:44:LYS:HD3	2.49	0.43
19:J:31:ARG:HE	19:J:32:SER:H	1.66	0.43
22:n:110:SER:HA	22:n:140:VAL:HG11	2.00	0.43
2:I:691:TYR:CD2	2:I:726:GLN:HG3	2.54	0.43
6:N:177:GLN:HA	6:N:180:THR:HG22	2.00	0.43
10:P:118:LEU:CB	10:P:140:ILE:HG22	2.48	0.43
17:F:26:ILE:HD12	17:F:29:ILE:HG13	2.01	0.43
21:Y:-247:DC:H2''	21:Y:-246:DA:H8	1.83	0.43
21:Y:-73:DC:H2''	21:Y:-72:DG:C8	2.54	0.43
16:c:133:ARG:HD3	16:c:137:GLU:HG2	2.01	0.43
16:c:135:LEU:HD11	18:e:94:ASN:ND2	2.34	0.43
18:i:31:HIS:CD2	18:i:48:PRO:HG3	2.54	0.43
18:i:84:GLN:NE2	18:i:102:ILE:HB	2.34	0.43
2:I:185:TYR:CE2	2:I:213:ASN:HB3	2.54	0.43
2:I:229:MET:HE3	13:W:14:LYS:HE2	2.00	0.43
2:I:387:ARG:HG3	4:L:178:PHE:CZ	2.54	0.43
2:I:405:VAL:O	2:I:407:ASN:N	2.52	0.43
2:I:427:PHE:C	2:I:429:GLN:H	2.27	0.43
16:A:63:ARG:HD2	21:Y:-88:DA:O3'	2.18	0.43
16:A:98:ALA:HB1	17:B:58:LEU:CD1	2.49	0.43
21:Y:-96:DG:C4	21:Y:-95:DG:N7	2.87	0.43
21:Y:-65:DT:C2	21:Y:-64:DG:N7	2.86	0.43
21:Y:-45:DG:C4	21:Y:-44:DC:C5	3.07	0.43
22:a:109:THR:HG22	22:a:110:SER:N	2.34	0.43
2:I:243:LYS:HG3	2:I:250:ILE:O	2.19	0.43
4:L:161:TRP:NE1	4:L:163:CYS:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:20:GLU:O	6:N:24:ILE:HG12	2.19	0.43
8:Q:117:LEU:HD21	9:U:265:HIS:NE2	2.34	0.43
8:Q:173:THR:HA	8:Q:176:ILE:HD12	2.01	0.43
10:P:111:CYS:O	10:P:114:VAL:HG12	2.19	0.43
16:A:112:LEU:HD13	16:A:128:LEU:HB3	2.01	0.43
21:Y:-93:DG:C6	21:Y:-92:DG:C6	3.06	0.43
18:e:79:ILE:HG12	18:e:82:HIS:CE1	2.53	0.43
2:I:140:SER:HB3	2:I:143:SER:OG	2.18	0.42
2:I:167:TRP:CD1	2:I:171:MET:HE3	2.54	0.42
4:L:72:TRP:O	4:L:319:LYS:HA	2.19	0.42
4:L:99:ILE:HG12	4:L:195:ILE:HG21	2.01	0.42
4:L:100:VAL:HG21	4:L:115:PHE:CG	2.54	0.42
4:L:165:VAL:N	4:L:336:THR:HG21	2.32	0.42
6:N:195:SER:HB3	6:N:201:LEU:HG	2.01	0.42
18:G:26:PRO:HD3	19:J:40:TYR:CD1	2.53	0.42
19:J:33:ARG:HD2	19:J:33:ARG:HA	1.89	0.42
19:J:35:GLU:OE2	20:V:29:DA:H5''	2.20	0.42
20:V:165:DT:H2''	20:V:166:DT:C5	2.53	0.42
21:Y:-298:DT:H3'	19:j:42:TYR:OH	2.19	0.42
21:Y:-287:DG:C6	21:Y:-286:DA:C6	3.07	0.42
21:Y:-141:DT:H2''	21:Y:-140:DG:C8	2.54	0.42
21:Y:-69:DT:H2''	21:Y:-68:DA:C8	2.54	0.42
16:c:73:GLU:O	16:c:76:VAL:HG12	2.19	0.42
18:e:41:GLU:HG3	18:e:42:ARG:HG3	2.01	0.42
2:I:526:LEU:HD12	2:I:526:LEU:HA	1.79	0.42
6:N:21:LEU:HD21	6:N:52:LEU:CD1	2.49	0.42
8:Q:103:LYS:O	8:Q:107:GLN:HG2	2.19	0.42
20:V:100:DG:H2''	20:V:101:DG:C8	2.54	0.42
21:Y:-295:DT:H2''	21:Y:-294:DA:N7	2.34	0.42
18:e:26:PRO:HD3	19:f:40:TYR:CD1	2.54	0.42
18:e:64:GLU:HA	19:f:49:HIS:CE1	2.54	0.42
18:i:18:SER:OG	18:i:26:PRO:HA	2.19	0.42
2:I:81:SER:O	2:I:84:LYS:HG2	2.20	0.42
8:Q:85:GLN:HA	8:Q:88:MET:HG3	2.00	0.42
8:Q:145:ARG:NH1	9:U:298:MET:HE1	2.35	0.42
16:A:67:PHE:HE1	17:B:58:LEU:HD11	1.84	0.42
16:E:66:PRO:HB3	17:F:28:GLY:HA3	2.01	0.42
22:Z:177:VAL:CG2	22:Z:236:LEU:HD11	2.49	0.42
22:a:176:ARG:HD3	22:a:234:ASN:HA	2.02	0.42
16:c:47:TRP:HE3	16:c:51:ILE:HD12	1.84	0.42
16:g:86:TRP:HB3	16:g:91:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:159:LYS:HE3	1:H:159:LYS:HB2	1.85	0.42
2:I:65:ALA:HA	2:I:68:MET:HG3	2.01	0.42
5:M:27:LEU:HD13	5:M:133:LEU:HB2	2.01	0.42
7:O:284:PHE:O	7:O:288:THR:HG23	2.19	0.42
8:Q:116:ARG:HH22	9:U:265:HIS:CD2	2.38	0.42
8:Q:181:ASN:O	8:Q:185:ILE:HG12	2.19	0.42
11:R:86:PHE:O	11:R:89:LEU:HG	2.19	0.42
12:T:542:GLU:HG2	12:T:543:TYR:N	2.34	0.42
20:V:60:DA:H61	21:Y:-60:DT:H3	1.67	0.42
20:V:122:DG:H1'	20:V:123:DT:H5'	2.01	0.42
20:V:184:DC:H2''	20:V:185:DA:C8	2.54	0.42
21:Y:-210:DT:H2''	21:Y:-209:DA:C8	2.54	0.42
21:Y:-50:DC:H2''	21:Y:-49:DT:C5	2.54	0.42
21:Y:-32:DA:C6	21:Y:-31:DA:C6	3.08	0.42
22:Z:177:VAL:O	22:Z:232:THR:HA	2.20	0.42
16:c:69:ARG:HA	16:c:72:ARG:HD2	2.01	0.42
4:L:292:HIS:O	4:L:296:LYS:HD3	2.18	0.42
5:M:93:PHE:CE1	5:M:124:TYR:HB3	2.55	0.42
9:U:271:SER:O	9:U:275:LYS:HG3	2.19	0.42
9:U:294:LYS:O	9:U:298:MET:HG3	2.19	0.42
11:R:90:LEU:HD13	11:R:140:LYS:HD2	2.02	0.42
15:X:4:ARG:HB2	15:X:7:LEU:HB2	2.02	0.42
16:A:73:GLU:HB2	17:B:25:ASN:HD22	1.84	0.42
21:Y:-196:DT:H2''	21:Y:-195:DA:C8	2.54	0.42
22:m:52:THR:HG22	22:m:75:PRO:HB2	2.02	0.42
1:H:192:SER:HA	1:H:196:LYS:HE2	2.02	0.42
2:I:133:MET:HE3	2:I:134:ILE:N	2.35	0.42
5:M:31:LEU:O	5:M:35:MET:HG2	2.20	0.42
8:Q:255:SER:O	8:Q:259:GLU:HG3	2.19	0.42
12:T:456:HIS:HA	13:W:21:PHE:CE1	2.55	0.42
16:A:130:ARG:NH1	17:B:57:VAL:HG22	2.34	0.42
20:V:13:DC:C2	20:V:14:DA:N7	2.87	0.42
20:V:62:DC:H2''	20:V:63:DG:C8	2.55	0.42
20:V:170:DA:H2''	20:V:171:DA:C8	2.55	0.42
20:V:195:DT:H2''	20:V:196:DA:C8	2.53	0.42
21:Y:-273:DC:H2''	21:Y:-272:DC:C6	2.55	0.42
21:Y:-160:DG:H2''	21:Y:-159:DG:H8	1.84	0.42
21:Y:-59:DT:OP2	21:Y:-59:DT:H2'	2.19	0.42
21:Y:-55:DC:H2''	21:Y:-54:DG:C8	2.54	0.42
18:e:58:LEU:HD12	19:f:69:ILE:HG21	2.00	0.42
18:e:90:ASP:HB3	18:e:93:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:m:58:TRP:CE3	22:m:118:CYS:HB3	2.55	0.42
22:n:190:TYR:HD2	22:n:250:GLY:HA2	1.85	0.42
3:K:189:PRO:HD2	12:T:554:GLY:HA2	2.02	0.42
4:L:250:LEU:HD13	6:N:299:SER:HB2	2.02	0.42
10:P:77:ASN:HB3	10:P:110:ASN:OD1	2.19	0.42
10:P:106:ARG:NH2	10:P:119:GLU:HG3	2.35	0.42
11:R:86:PHE:O	11:R:90:LEU:HG	2.20	0.42
18:C:26:PRO:HD3	19:D:40:TYR:CG	2.54	0.42
16:E:69:ARG:HH22	21:Y:-57:DA:P	2.43	0.42
21:Y:-254:DC:H2''	21:Y:-253:DG:C8	2.54	0.42
21:Y:-137:DC:H2''	21:Y:-136:DA:C8	2.54	0.42
21:Y:-75:DA:H2''	21:Y:-74:DG:H8	1.85	0.42
22:m:62:THR:HG22	22:m:114:ALA:HB2	2.02	0.42
22:m:109:THR:HG22	22:m:110:SER:H	1.85	0.42
22:m:169:MET:HE1	22:m:177:VAL:HG11	2.01	0.42
4:L:26:PRO:HG2	4:L:29:LYS:HD3	2.02	0.42
5:M:30:GLN:HB3	5:M:139:ARG:NE	2.35	0.42
16:A:63:ARG:HB2	16:A:66:PRO:HG2	2.02	0.42
18:C:18:SER:OG	18:C:26:PRO:HA	2.20	0.42
16:E:119:VAL:HG22	17:F:44:LYS:HD3	2.01	0.42
17:F:33:ALA:HA	17:F:36:ARG:NH1	2.35	0.42
20:V:67:DG:H2''	20:V:68:DT:C6	2.55	0.42
20:V:94:DG:H2''	20:V:95:DC:O5'	2.20	0.42
20:V:205:DG:H2'	20:V:206:DT:H71	2.02	0.42
20:V:231:DA:H2''	20:V:232:DA:H8	1.85	0.42
21:Y:-289:DG:H2''	21:Y:-288:DA:H8	1.85	0.42
21:Y:-265:DC:C2	21:Y:-264:DG:N7	2.88	0.42
21:Y:-207:DG:O5'	18:e:44:GLY:HA2	2.20	0.42
22:Z:28:GLN:H	22:Z:134:GLN:NE2	2.18	0.42
22:a:70:ILE:HG23	22:a:86:PHE:CD2	2.55	0.42
22:n:74:TYR:HE1	22:n:123:SER:HB3	1.83	0.42
22:n:195:GLN:HB2	22:n:205:LEU:HD11	2.02	0.42
2:I:379:VAL:HG13	2:I:380:ARG:N	2.35	0.42
3:K:135:ILE:O	3:K:139:LEU:HD23	2.20	0.42
6:N:8:PHE:HA	6:N:11:ARG:NH2	2.34	0.42
8:Q:172:MET:O	8:Q:176:ILE:HG13	2.18	0.42
13:W:44:HIS:NE2	13:W:48:LEU:HD11	2.35	0.42
16:E:70:LEU:HA	16:E:73:GLU:HG2	2.02	0.42
19:J:42:TYR:OH	20:V:21:DA:H3'	2.20	0.42
21:Y:-209:DA:H2''	21:Y:-208:DC:C6	2.55	0.42
18:e:49:VAL:HG21	19:f:121:TYR:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:n:62:THR:HG22	22:n:114:ALA:HB2	2.02	0.42
4:L:100:VAL:HG21	4:L:115:PHE:CD1	2.54	0.42
4:L:290:HIS:NE2	4:L:294:HIS:HE1	2.17	0.42
6:N:129:ASN:HB3	7:O:213:PRO:HG3	2.01	0.42
7:O:216:ASN:HA	7:O:239:TYR:HB2	2.02	0.42
9:U:408:ASN:HD22	11:R:142:LEU:HD11	1.85	0.42
17:B:50:ILE:O	17:B:53:GLU:HB3	2.20	0.42
18:C:49:VAL:HG12	19:D:117:ALA:HB1	2.01	0.42
20:V:72:DC:H2''	20:V:73:DG:C8	2.55	0.42
20:V:87:DT:H3	21:Y:-87:DA:H61	1.66	0.42
21:Y:-267:DG:C2	21:Y:-266:DG:C5	3.08	0.42
21:Y:-236:DT:C2	21:Y:-235:DG:N7	2.87	0.42
21:Y:-220:DT:H2''	21:Y:-219:DA:N7	2.34	0.42
21:Y:-191:DT:H2''	21:Y:-190:DT:N1	2.34	0.42
21:Y:-111:DG:H2''	21:Y:-110:DG:C8	2.55	0.42
21:Y:-76:DC:H2''	21:Y:-75:DA:C8	2.54	0.42
22:Z:219:ARG:HD2	22:Z:235:ASN:O	2.20	0.42
18:i:79:ILE:HG12	18:i:82:HIS:ND1	2.35	0.42
19:j:81:ALA:HB2	19:j:93:GLU:HG2	2.01	0.42
22:n:109:THR:HG22	22:n:110:SER:N	2.35	0.42
4:L:182:PRO:HG2	4:L:336:THR:HG23	2.02	0.41
7:O:284:PHE:CD1	7:O:287:PHE:CE1	3.07	0.41
8:Q:209:LEU:HB3	8:Q:211:LEU:HD23	2.02	0.41
22:Z:29:SER:O	22:Z:136:THR:HG22	2.20	0.41
1:H:63:ALA:HB2	3:K:66:CYS:HA	2.01	0.41
2:I:664:ASP:HB2	2:I:667:ILE:HG13	2.00	0.41
3:K:160:ASN:HA	3:K:163:LYS:NZ	2.36	0.41
7:O:109:HIS:HA	7:O:114:SER:OG	2.20	0.41
7:O:233:PHE:HD1	7:O:254:CYS:HA	1.84	0.41
9:U:357:PHE:CZ	10:P:258:ALA:HA	2.56	0.41
14:S:67:MET:HE1	14:S:68:PHE:CZ	2.54	0.41
18:C:50:TYR:OH	19:D:95:GLN:HG3	2.21	0.41
20:V:229:DT:H2''	20:V:230:DA:N7	2.35	0.41
21:Y:-279:DA:H2''	21:Y:-278:DG:H8	1.85	0.41
21:Y:-197:DC:H2''	21:Y:-196:DT:H71	2.02	0.41
21:Y:-37:DC:H2''	21:Y:-36:DG:C8	2.55	0.41
22:Z:35:GLU:O	22:Z:38:THR:HG22	2.20	0.41
22:m:193:TRP:HE3	22:m:206:ILE:HB	1.86	0.41
6:N:207:LYS:HA	6:N:209:TYR:CE2	2.56	0.41
7:O:108:TYR:O	7:O:111:THR:HG22	2.20	0.41
8:Q:265:LEU:HD11	9:U:407:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:55:ASP:O	10:P:59:GLN:OE1	2.38	0.41
10:P:78:ILE:HG12	10:P:79:ARG:O	2.20	0.41
13:W:25:VAL:O	13:W:29:LYS:HG3	2.20	0.41
14:S:61:PHE:HD1	14:S:85:LEU:HD11	1.84	0.41
16:E:107:GLU:HG3	17:F:41:GLY:HA2	2.02	0.41
20:V:103:DA:H2'	20:V:104:DT:H71	2.02	0.41
20:V:105:DT:H2''	20:V:106:DA:H8	1.84	0.41
21:Y:-244:DC:H2''	21:Y:-243:DG:C8	2.55	0.41
21:Y:-44:DC:H2'	21:Y:-43:DT:H71	2.02	0.41
22:n:181:CYS:HB2	22:n:193:TRP:CH2	2.56	0.41
1:H:149:ASP:OD1	1:H:153:LYS:HE3	2.19	0.41
2:I:400:CYS:HA	2:I:414:PHE:CE2	2.55	0.41
2:I:565:TYR:CZ	2:I:583:PHE:HB3	2.54	0.41
2:I:691:TYR:HD2	2:I:726:GLN:HG3	1.86	0.41
16:A:124:LYS:HE2	16:E:115:HIS:CE1	2.55	0.41
18:G:84:GLN:HE22	18:G:102:ILE:HB	1.85	0.41
21:Y:-304:DT:H6	21:Y:-304:DT:H2'	1.74	0.41
21:Y:-288:DA:H2''	21:Y:-287:DG:H8	1.85	0.41
21:Y:-269:DT:O5'	16:g:87:GLN:HA	2.20	0.41
22:a:219:ARG:HD2	22:a:235:ASN:O	2.20	0.41
16:c:112:LEU:HB3	16:g:115:HIS:NE2	2.35	0.41
17:d:76:ALA:HA	19:f:84:ASN:OD1	2.20	0.41
16:g:53:LYS:HA	16:g:53:LYS:HD3	1.76	0.41
16:g:54:LEU:HD11	17:h:36:ARG:HG2	2.02	0.41
19:j:37:TYR:HA	19:j:40:TYR:HD2	1.85	0.41
1:H:189:MET:O	1:H:190:GLU:HG3	2.20	0.41
3:K:212:LEU:HD11	3:K:246:LEU:HD21	2.02	0.41
6:N:46:GLU:O	6:N:50:GLN:HG2	2.21	0.41
16:E:98:ALA:HB1	17:F:58:LEU:CD1	2.50	0.41
20:V:98:DA:H2''	20:V:99:DG:H8	1.85	0.41
20:V:101:DG:H2''	20:V:102:DG:N7	2.36	0.41
20:V:165:DT:H3	21:Y:-165:DA:H61	1.68	0.41
21:Y:-59:DT:H4'	21:Y:-58:DA:H5'	2.01	0.41
21:Y:-18:DT:H2''	21:Y:-17:DA:N7	2.36	0.41
22:Z:51:PHE:HE1	22:Z:56:ILE:HD11	1.84	0.41
22:a:41:LYS:HA	22:a:103:MET:O	2.20	0.41
22:a:247:LEU:HD11	22:a:254:TYR:HB3	2.02	0.41
16:g:119:VAL:CG2	17:h:44:LYS:HD3	2.50	0.41
2:I:231:MET:HB3	2:I:236:GLN:NE2	2.36	0.41
2:I:643:TYR:O	2:I:644:LEU:C	2.63	0.41
3:K:184:LEU:HD23	3:K:184:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:2:ASP:HB3	6:N:5:VAL:HG22	2.02	0.41
6:N:208:GLN:HA	6:N:211:GLN:OE1	2.19	0.41
6:N:263:GLN:HA	6:N:301:HIS:CE1	2.55	0.41
9:U:333:GLN:O	9:U:337:LEU:HG	2.20	0.41
11:R:120:GLU:O	11:R:123:ILE:HG22	2.20	0.41
18:C:17:ARG:HA	18:C:20:ARG:HB3	2.02	0.41
20:V:76:DG:H2'	20:V:77:DT:H71	2.02	0.41
20:V:88:DT:H2''	20:V:89:DT:H71	2.02	0.41
20:V:157:DG:C6	20:V:158:DG:C6	3.09	0.41
21:Y:-176:DT:H2''	21:Y:-175:DC:C6	2.55	0.41
22:a:53:SER:HB2	22:a:54:TYR:CD1	2.56	0.41
22:m:44:CYS:HB2	22:m:58:TRP:CH2	2.55	0.41
3:K:247:LEU:HD23	3:K:252:ALA:O	2.20	0.41
4:L:27:LEU:HD23	4:L:30:ARG:NH1	2.36	0.41
4:L:214:ASN:ND2	4:L:216:PHE:HB3	2.35	0.41
4:L:296:LYS:HB3	6:N:316:ASP:HB2	2.01	0.41
5:M:18:ILE:HG13	5:M:65:LEU:O	2.20	0.41
5:M:21:VAL:HA	5:M:49:ALA:O	2.21	0.41
8:Q:193:GLU:O	8:Q:197:VAL:HG23	2.21	0.41
10:P:79:ARG:HD3	10:P:79:ARG:HA	1.88	0.41
10:P:118:LEU:HB3	10:P:140:ILE:HG22	2.03	0.41
14:S:50:ILE:O	14:S:54:THR:HG23	2.20	0.41
20:V:18:DA:H2''	20:V:19:DA:C8	2.56	0.41
20:V:110:DC:H2''	20:V:111:DC:C5	2.56	0.41
20:V:183:DT:H2''	20:V:184:DC:C5	2.55	0.41
21:Y:-35:DA:C4	21:Y:-34:DC:C5	3.08	0.41
22:Z:129:LEU:HD12	22:Z:132:TRP:CZ2	2.56	0.41
22:m:116:TYR:O	22:m:135:GLY:HA2	2.21	0.41
22:m:247:LEU:HD11	22:m:254:TYR:HB3	2.02	0.41
1:H:130:MET:HA	1:H:130:MET:HE2	2.02	0.41
1:H:140:ILE:HG13	3:K:108:LEU:HD12	2.01	0.41
1:H:165:LYS:HB2	3:K:132:GLN:HE22	1.86	0.41
3:K:84:LEU:HB3	3:K:88:VAL:HG21	2.02	0.41
4:L:161:TRP:O	4:L:184:PHE:HA	2.21	0.41
6:N:53:ILE:HA	6:N:56:CYS:SG	2.61	0.41
8:Q:251:MET:CE	11:R:100:ILE:HD12	2.51	0.41
13:W:1:MET:HE1	21:Y:-152:DA:H2''	2.02	0.41
13:W:62:ALA:HA	13:W:74:HIS:ND1	2.35	0.41
16:E:93:ALA:HB2	17:F:100:PHE:CG	2.55	0.41
20:V:165:DT:H3	21:Y:-165:DA:N6	2.18	0.41
20:V:281:DC:H2''	20:V:282:DC:C5	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:-268:DT:P	16:g:86:TRP:H	2.43	0.41
21:Y:-139:DT:H1'	21:Y:-138:DC:O4'	2.20	0.41
16:c:65:LEU:O	16:c:69:ARG:HG2	2.20	0.41
18:e:95:LYS:HB2	18:e:95:LYS:HE3	1.88	0.41
22:m:56:ILE:HD12	22:m:101:VAL:HG21	2.03	0.41
1:H:171:LYS:HG3	3:K:139:LEU:HD12	2.03	0.41
2:I:439:LEU:HD11	2:I:458:LEU:HB3	2.02	0.41
2:I:611:ARG:HH11	2:I:644:LEU:HD11	1.86	0.41
3:K:124:ARG:HG3	3:K:127:ARG:NH2	2.36	0.41
3:K:177:LEU:HD12	3:K:180:LEU:HD23	2.02	0.41
3:K:247:LEU:HA	3:K:252:ALA:O	2.21	0.41
5:M:23:THR:HG22	5:M:50:LYS:HZ2	1.86	0.41
5:M:75:LYS:O	5:M:79:GLN:HG3	2.21	0.41
6:N:89:SER:OG	6:N:187:GLN:HB2	2.21	0.41
8:Q:155:LEU:HD13	9:U:313:ILE:HG22	2.02	0.41
9:U:319:ARG:O	9:U:322:GLU:HG2	2.21	0.41
9:U:412:GLU:HA	9:U:415:LEU:HD12	2.02	0.41
10:P:179:TYR:O	10:P:182:ARG:HG2	2.20	0.41
13:W:14:LYS:HD3	13:W:14:LYS:HA	1.90	0.41
16:A:106:PHE:CD2	17:B:38:ALA:HA	2.56	0.41
18:C:95:LYS:HB2	18:C:95:LYS:HE3	1.86	0.41
16:E:62:ILE:HD13	17:F:29:ILE:HD12	2.03	0.41
16:E:66:PRO:HG3	21:Y:-57:DA:OP1	2.21	0.41
20:V:114:DG:H2'	20:V:115:DT:H71	2.02	0.41
20:V:260:DT:H2''	20:V:261:DA:N7	2.36	0.41
21:Y:-301:DA:H2''	21:Y:-300:DG:C8	2.56	0.41
21:Y:-141:DT:H2''	21:Y:-140:DG:H8	1.84	0.41
22:Z:42:MET:O	22:Z:102:TYR:HA	2.21	0.41
22:Z:72:TYR:CE2	22:Z:81:LYS:HB3	2.56	0.41
17:d:77:LYS:HG3	19:f:92:ARG:NH2	2.36	0.41
18:i:88:ARG:HD3	18:i:88:ARG:HA	1.82	0.41
19:j:113:GLU:O	19:j:116:LYS:HG2	2.20	0.41
6:N:16:ILE:HG21	6:N:21:LEU:HA	2.03	0.41
6:N:139:THR:HG22	6:N:142:THR:OG1	2.21	0.41
7:O:234:CYS:C	7:O:252:VAL:HG23	2.46	0.41
10:P:153:PHE:HZ	10:P:166:PHE:HA	1.86	0.41
12:T:467:PHE:HE1	13:W:54:LEU:HG	1.85	0.41
15:X:4:ARG:NH2	15:X:7:LEU:HD13	2.36	0.41
16:A:102:LEU:HB2	17:B:37:LEU:HD22	2.02	0.41
17:F:31:LYS:HG2	17:F:32:PRO:HD3	2.03	0.41
20:V:279:DT:H2''	20:V:280:DC:C5	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:-30:DT:H2''	21:Y:-29:DT:C6	2.56	0.41
21:Y:-28:DG:H4'	21:Y:-27:DT:H5'	2.02	0.41
19:j:105:GLU:HG3	22:n:122:SER:HB2	2.02	0.41
1:H:245:ASP:O	3:K:165:LYS:HE3	2.21	0.40
4:L:55:LEU:HD23	4:L:55:LEU:HA	1.88	0.40
4:L:95:LEU:HD11	4:L:196:ILE:HD13	2.03	0.40
7:O:122:VAL:HG21	10:P:69:PHE:HZ	1.85	0.40
12:T:504:HIS:CG	14:S:84:LEU:HD11	2.56	0.40
16:E:65:LEU:HB3	16:E:66:PRO:HD3	2.03	0.40
16:E:75:CYS:HA	17:F:66:ILE:HG21	2.03	0.40
20:V:186:DC:H2''	20:V:187:DA:N7	2.35	0.40
20:V:216:DC:H2'	20:V:217:DT:H71	2.03	0.40
21:Y:-298:DT:H2''	21:Y:-297:DA:H8	1.86	0.40
21:Y:-68:DA:H2''	21:Y:-67:DC:C6	2.56	0.40
19:j:56:SER:O	19:j:59:MET:HB2	2.21	0.40
22:m:72:TYR:CE2	22:m:81:LYS:HD2	2.56	0.40
2:I:394:GLN:HB3	4:L:207:TYR:CE1	2.55	0.40
3:K:215:MET:HG2	3:K:238:PHE:CD1	2.57	0.40
3:K:226:VAL:HG12	3:K:229:ASP:H	1.87	0.40
18:C:103:ALA:HB2	17:F:97:LEU:HD11	2.03	0.40
19:D:86:ARG:HD2	21:Y:-108:DA:P	2.61	0.40
20:V:120:DT:H2''	20:V:121:DT:H72	2.03	0.40
20:V:255:DC:H2''	20:V:256:DG:C8	2.56	0.40
21:Y:-125:DC:H2'	21:Y:-124:DT:C4	2.56	0.40
21:Y:-56:DG:C4	21:Y:-55:DC:C5	3.09	0.40
22:a:109:THR:HG22	22:a:110:SER:H	1.86	0.40
16:g:112:LEU:HD13	16:g:128:LEU:HD23	2.02	0.40
17:h:38:ALA:HB3	17:h:46:ILE:HD11	2.04	0.40
18:i:97:LEU:HB3	18:i:100:VAL:HB	2.01	0.40
7:O:237:LEU:CD2	7:O:280:LEU:HD13	2.51	0.40
8:Q:145:ARG:HH22	9:U:302:LEU:HG	1.86	0.40
10:P:150:LEU:O	10:P:154:VAL:HG23	2.22	0.40
18:C:29:ARG:HA	21:Y:-118:DG:OP1	2.21	0.40
20:V:42:DC:H2''	20:V:43:DA:H8	1.86	0.40
21:Y:-91:DT:H1'	21:Y:-90:DT:C2	2.57	0.40
22:n:72:TYR:HE2	22:n:81:LYS:HD2	1.87	0.40
1:H:47:ARG:HG2	3:K:31:MET:HE1	2.02	0.40
1:H:105:ARG:HD3	1:H:105:ARG:HA	1.88	0.40
1:H:107:ARG:HG2	2:I:671:THR:HG21	2.02	0.40
1:H:128:ASP:OD1	1:H:131:LYS:HE3	2.21	0.40
1:H:204:MET:HE3	1:H:204:MET:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:333:LEU:HB2	2:I:335:ARG:HG2	2.04	0.40
2:I:460:SER:HA	2:I:500:LEU:HB2	2.03	0.40
3:K:104:LEU:HA	3:K:107:VAL:HG12	2.03	0.40
4:L:107:LEU:H	4:L:107:LEU:HD23	1.87	0.40
8:Q:236:ASN:HA	8:Q:239:LEU:HG	2.03	0.40
9:U:278:ILE:HD13	9:U:281:PHE:CZ	2.56	0.40
18:G:77:ARG:H	18:G:77:ARG:HD3	1.86	0.40
20:V:203:DT:P	18:e:20:ARG:HH22	2.45	0.40
22:n:82:TYR:HB2	22:n:87:LYS:HD2	2.04	0.40
2:I:215:LYS:HD2	2:I:218:ARG:NH1	2.37	0.40
2:I:354:ILE:HG21	3:K:139:LEU:HD22	2.02	0.40
2:I:611:ARG:HH21	2:I:737:SER:HB2	1.87	0.40
5:M:92:PHE:O	5:M:96:LYS:HB2	2.21	0.40
10:P:88:LEU:O	10:P:100:LYS:HB2	2.21	0.40
11:R:94:GLU:CG	11:R:140:LYS:HE3	2.51	0.40
18:C:15:LYS:HE2	18:C:15:LYS:HB2	1.77	0.40
16:E:130:ARG:O	16:E:138:GLY:HA3	2.22	0.40
18:G:77:ARG:HH22	18:G:79:ILE:HD13	1.86	0.40
18:G:77:ARG:CD	21:Y:-16:DT:H5''	2.50	0.40
20:V:19:DA:H2''	20:V:20:DA:C8	2.56	0.40
20:V:110:DC:H2''	20:V:111:DC:C6	2.55	0.40
20:V:261:DA:H1'	20:V:262:DA:C5	2.55	0.40
21:Y:-39:DT:H2''	21:Y:-38:DA:N7	2.36	0.40
22:Z:55:THR:HG22	22:Z:74:TYR:CD1	2.56	0.40
22:m:46:ALA:HB1	22:m:49:TYR:CE1	2.56	0.40
22:n:42:MET:HE1	22:n:105:LEU:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	200/247 (81%)	195 (98%)	5 (2%)	0	100	100
2	I	610/762 (80%)	583 (96%)	24 (4%)	3 (0%)	24	63
3	K	227/269 (84%)	223 (98%)	4 (2%)	0	100	100
4	L	308/348 (88%)	305 (99%)	2 (1%)	1 (0%)	36	72
5	M	170/180 (94%)	168 (99%)	2 (1%)	0	100	100
6	N	312/347 (90%)	296 (95%)	16 (5%)	0	100	100
7	O	204/300 (68%)	197 (97%)	7 (3%)	0	100	100
8	Q	187/215 (87%)	184 (98%)	3 (2%)	0	100	100
9	U	164/211 (78%)	164 (100%)	0	0	100	100
10	P	220/288 (76%)	212 (96%)	8 (4%)	0	100	100
11	R	76/177 (43%)	72 (95%)	4 (5%)	0	100	100
12	T	110/777 (14%)	108 (98%)	2 (2%)	0	100	100
13	W	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	S	118/138 (86%)	117 (99%)	1 (1%)	0	100	100
15	X	72/81 (89%)	72 (100%)	0	0	100	100
16	A	97/140 (69%)	96 (99%)	1 (1%)	0	100	100
16	E	97/140 (69%)	96 (99%)	1 (1%)	0	100	100
16	c	97/140 (69%)	95 (98%)	2 (2%)	0	100	100
16	g	94/140 (67%)	93 (99%)	1 (1%)	0	100	100
17	B	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
17	F	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
17	d	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
17	h	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
18	C	105/153 (69%)	102 (97%)	3 (3%)	0	100	100
18	G	106/153 (69%)	104 (98%)	2 (2%)	0	100	100
18	e	105/153 (69%)	103 (98%)	2 (2%)	0	100	100
18	i	106/153 (69%)	104 (98%)	2 (2%)	0	100	100
19	D	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
19	J	92/126 (73%)	88 (96%)	4 (4%)	0	100	100
19	f	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
19	j	92/126 (73%)	88 (96%)	4 (4%)	0	100	100
22	Z	225/266 (85%)	210 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	a	225/266 (85%)	213 (95%)	12 (5%)	0	100	100
22	m	225/266 (85%)	211 (94%)	14 (6%)	0	100	100
22	n	225/266 (85%)	211 (94%)	14 (6%)	0	100	100
All	All	5453/7580 (72%)	5279 (97%)	170 (3%)	4 (0%)	49	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	406	ASN
4	L	246	SER
2	I	405	VAL
2	I	404	LYS

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	H	188/224 (84%)	188 (100%)	0	100	100
2	I	560/697 (80%)	559 (100%)	1 (0%)	87	87
3	K	221/260 (85%)	221 (100%)	0	100	100
4	L	277/308 (90%)	277 (100%)	0	100	100
5	M	151/158 (96%)	151 (100%)	0	100	100
6	N	288/319 (90%)	288 (100%)	0	100	100
7	O	177/263 (67%)	177 (100%)	0	100	100
8	Q	179/200 (90%)	179 (100%)	0	100	100
9	U	152/190 (80%)	152 (100%)	0	100	100
10	P	197/259 (76%)	197 (100%)	0	100	100
11	R	75/166 (45%)	75 (100%)	0	100	100
12	T	100/635 (16%)	100 (100%)	0	100	100
13	W	77/77 (100%)	77 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	S	107/121 (88%)	107 (100%)	0	100	100
15	X	65/67 (97%)	65 (100%)	0	100	100
16	A	83/118 (70%)	83 (100%)	0	100	100
16	E	83/118 (70%)	83 (100%)	0	100	100
16	c	83/118 (70%)	83 (100%)	0	100	100
16	g	83/118 (70%)	83 (100%)	0	100	100
17	B	65/79 (82%)	65 (100%)	0	100	100
17	F	65/79 (82%)	65 (100%)	0	100	100
17	d	65/79 (82%)	65 (100%)	0	100	100
17	h	65/79 (82%)	65 (100%)	0	100	100
18	C	82/118 (70%)	82 (100%)	0	100	100
18	G	83/118 (70%)	83 (100%)	0	100	100
18	e	82/118 (70%)	82 (100%)	0	100	100
18	i	83/118 (70%)	83 (100%)	0	100	100
19	D	82/106 (77%)	82 (100%)	0	100	100
19	J	81/106 (76%)	81 (100%)	0	100	100
19	f	82/106 (77%)	82 (100%)	0	100	100
19	j	81/106 (76%)	81 (100%)	0	100	100
22	Z	202/225 (90%)	202 (100%)	0	100	100
22	a	201/225 (89%)	201 (100%)	0	100	100
22	m	202/225 (90%)	202 (100%)	0	100	100
22	n	201/225 (89%)	201 (100%)	0	100	100
All	All	4868/6528 (75%)	4867 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	405	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	49	GLN

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Mol	Chain	Res	Type
1	H	137	ASN
1	H	166	GLN
2	I	232	GLN
2	I	236	GLN
2	I	314	ASN
2	I	353	ASN
2	I	362	GLN
2	I	502	GLN
3	K	63	GLN
3	K	134	GLN
3	K	249	ASN
4	L	269	HIS
5	M	73	HIS
6	N	241	ASN
7	O	153	HIS
7	O	281	HIS
8	Q	107	GLN
8	Q	177	GLN
9	U	372	GLN
9	U	408	ASN
10	P	225	GLN
11	R	130	HIS
12	T	453	GLN
12	T	532	HIS
12	T	545	GLN
12	T	561	GLN
13	W	74	HIS
14	S	17	GLN
16	A	59	HIS
17	B	27	GLN
18	C	112	GLN
19	D	82	HIS
19	J	47	GLN
22	Z	195	GLN
22	a	27	GLN
22	a	61	GLN
22	a	195	GLN
22	a	196	GLN
16	c	87	GLN
18	e	112	GLN
18	i	73	ASN
18	i	112	GLN

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Mol	Chain	Res	Type
22	m	27	GLN
22	m	235	ASN
22	n	195	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

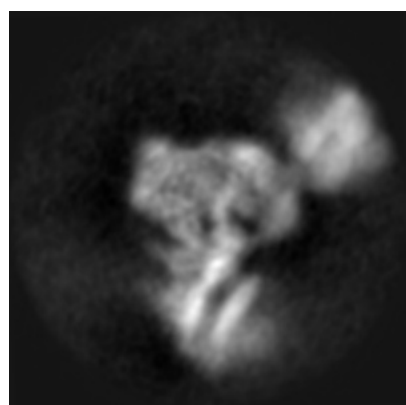
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55759. These allow visual inspection of the internal detail of the map and identification of artifacts.

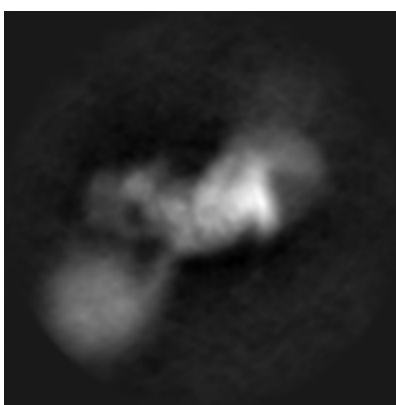
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

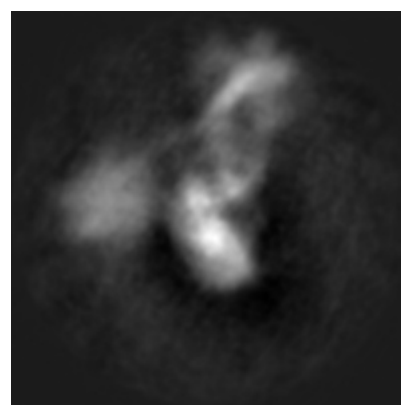
6.1.1 Primary map



X



Y

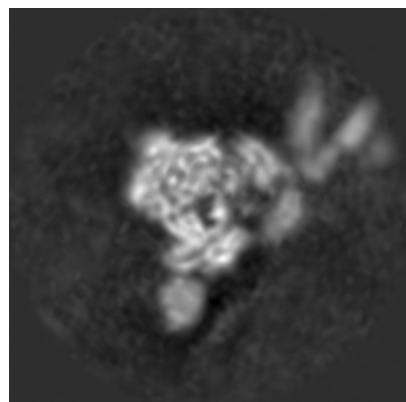


Z

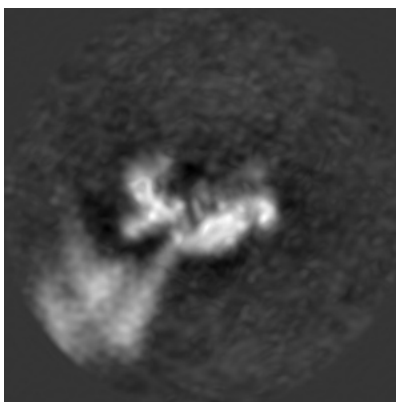
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

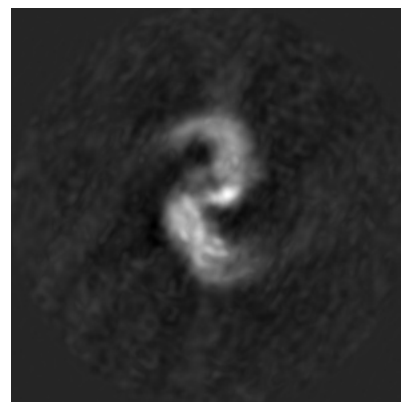
6.2.1 Primary map



X Index: 200



Y Index: 200

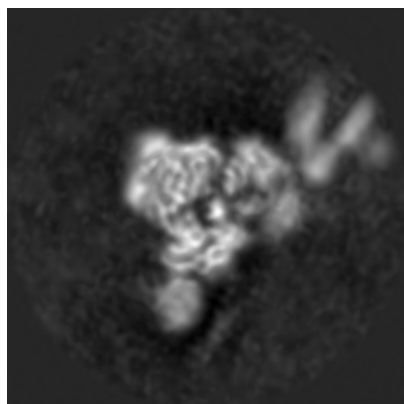


Z Index: 200

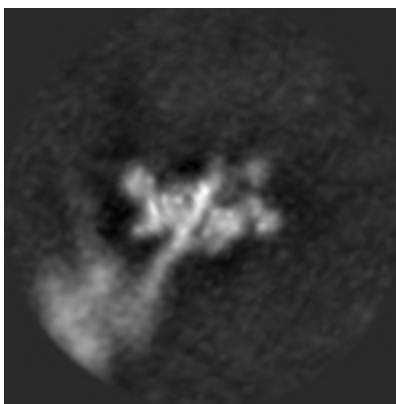
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

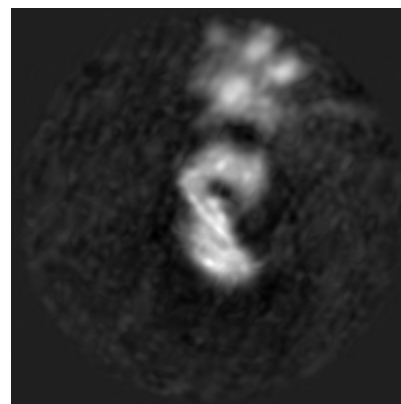
6.3.1 Primary map



X Index: 205



Y Index: 211

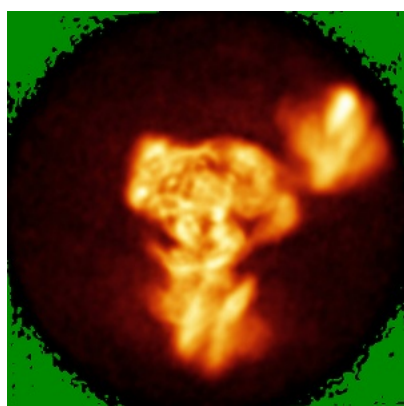


Z Index: 257

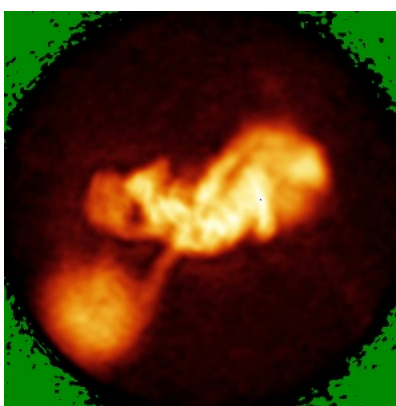
The images above show the largest variance slices of the map in three orthogonal directions.

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

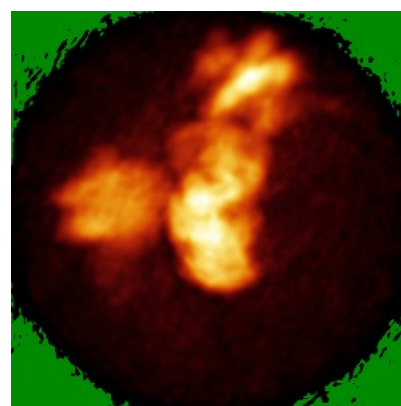
6.4.1 Primary map



X



Y



Z

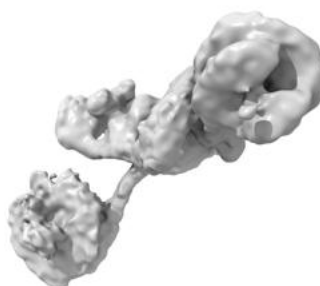
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

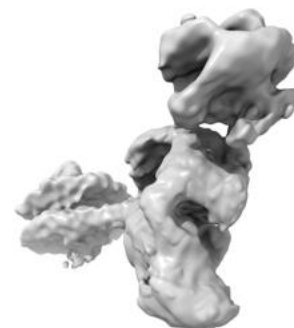
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

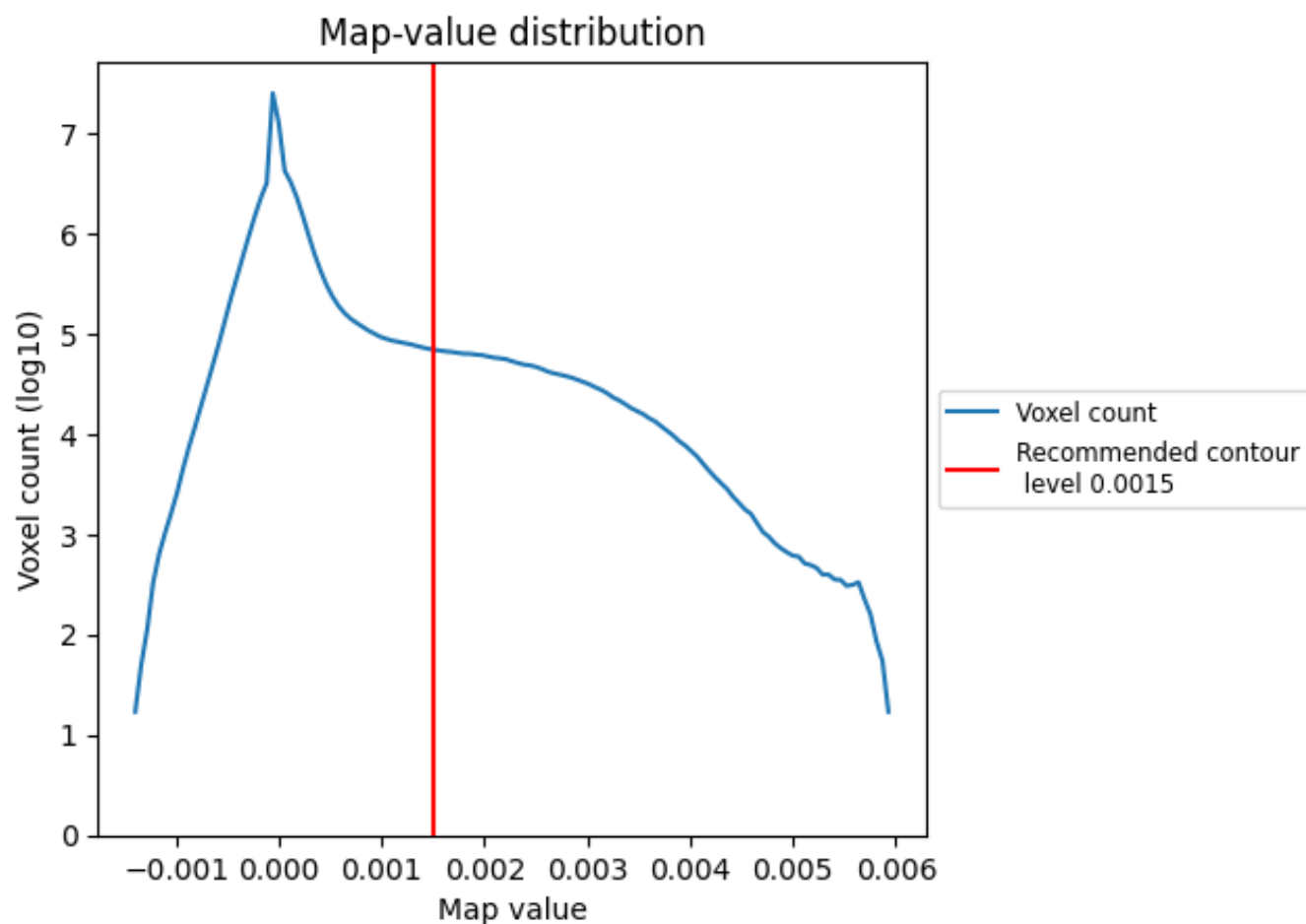
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

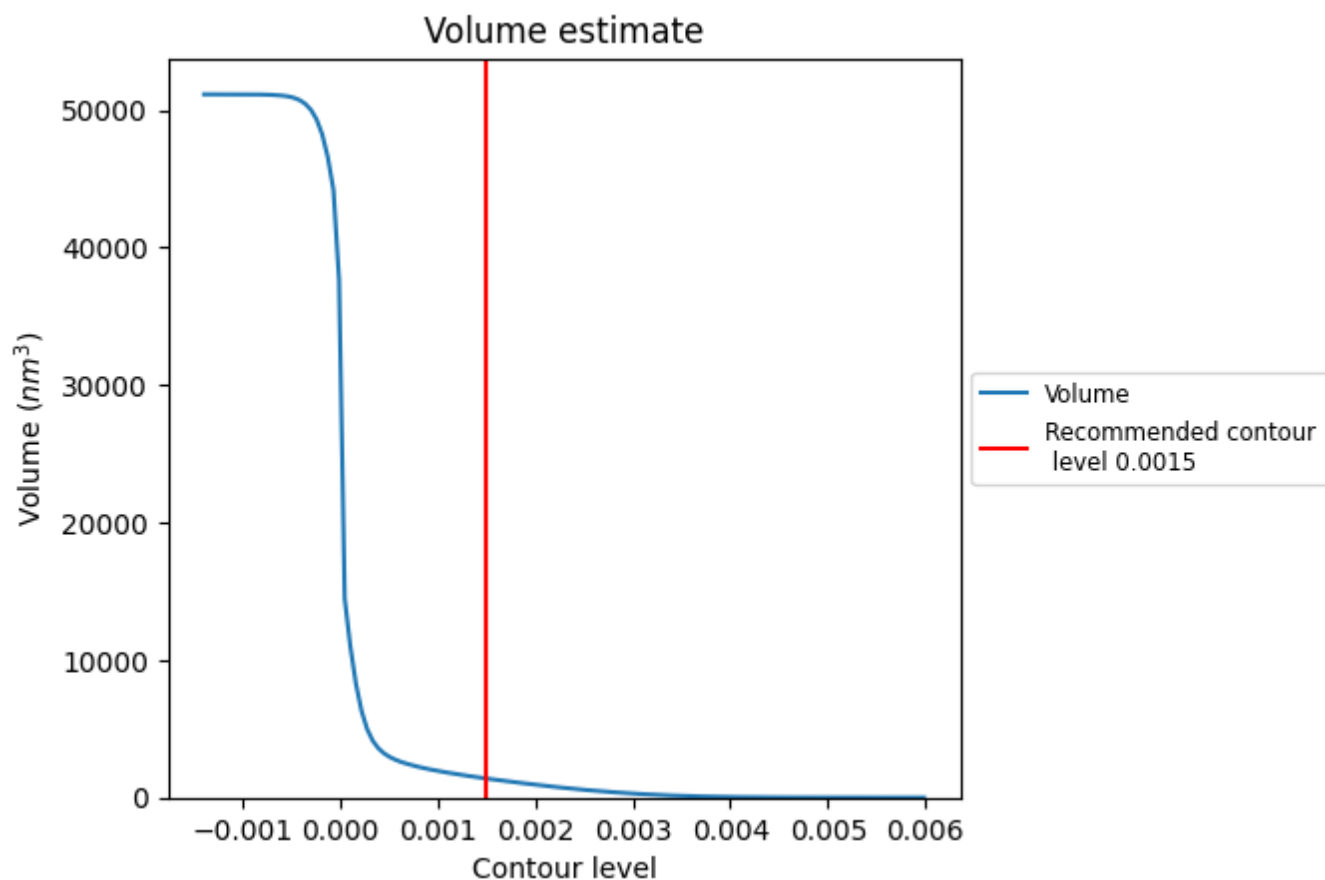
This section contains the results of statistical analysis of the map.

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.

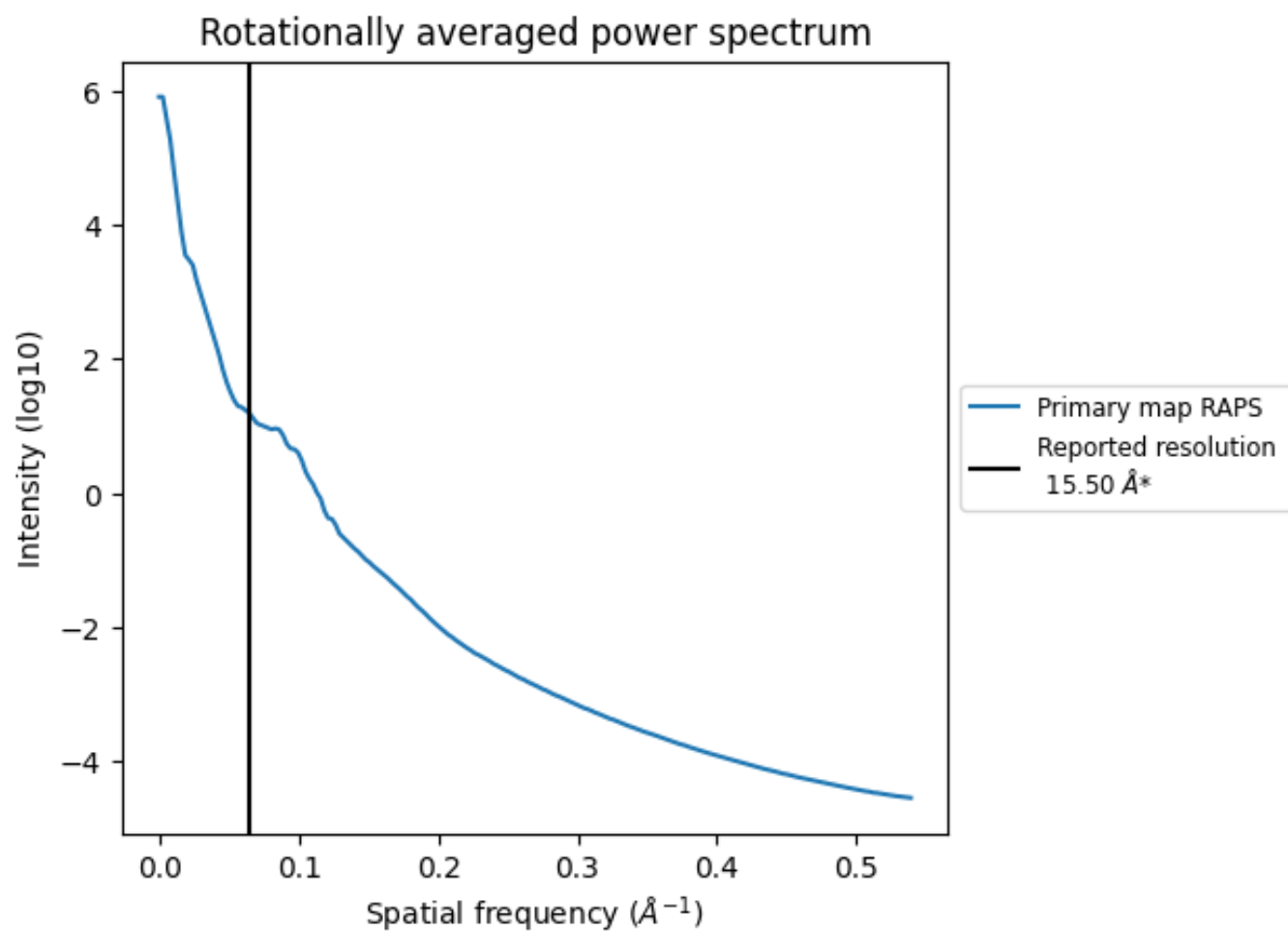
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1384 nm³; this corresponds to an approximate mass of 1250 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.065 Å⁻¹

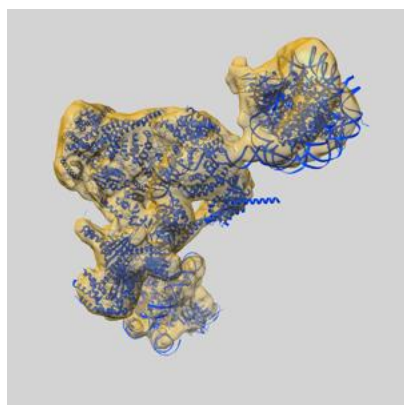
8 Fourier-Shell correlation

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

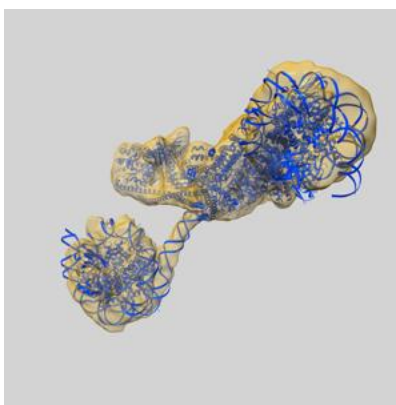
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55759 and PDB model 9TAY. Per-residue inclusion information can be found in section 3 on page 17.

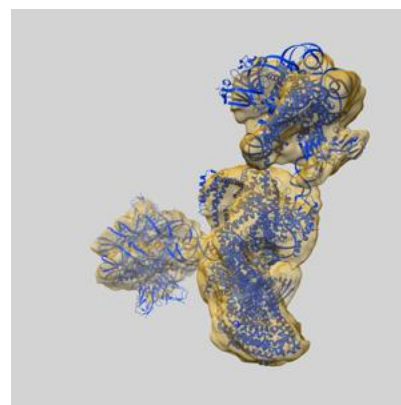
9.1 Map-model overlay [i](#)



X



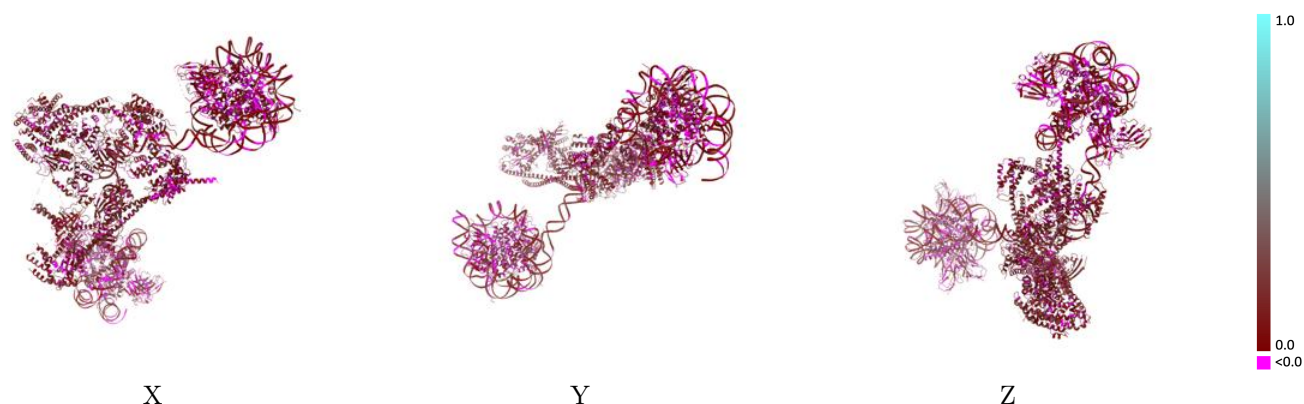
Y



Z

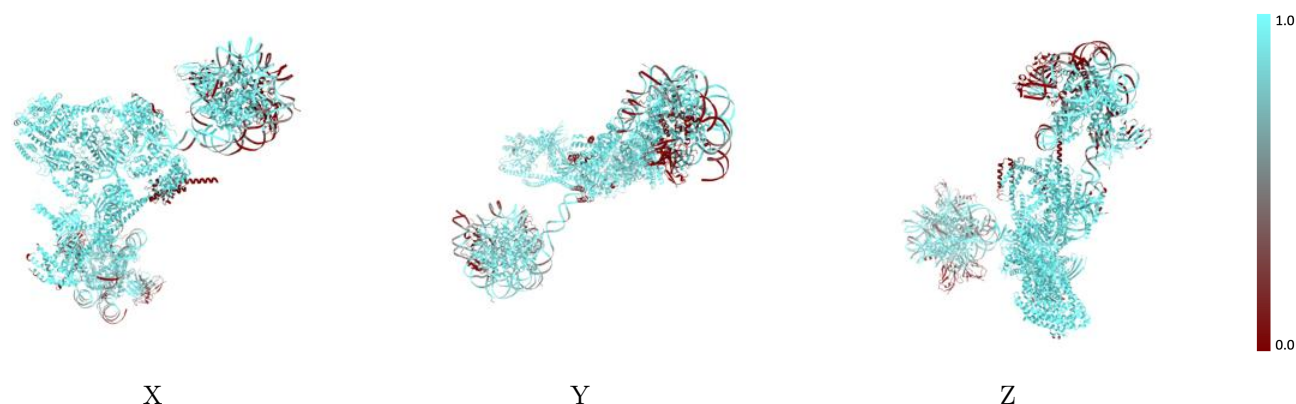
The images above show the 3D surface view of the map at the recommended contour level 0.0015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



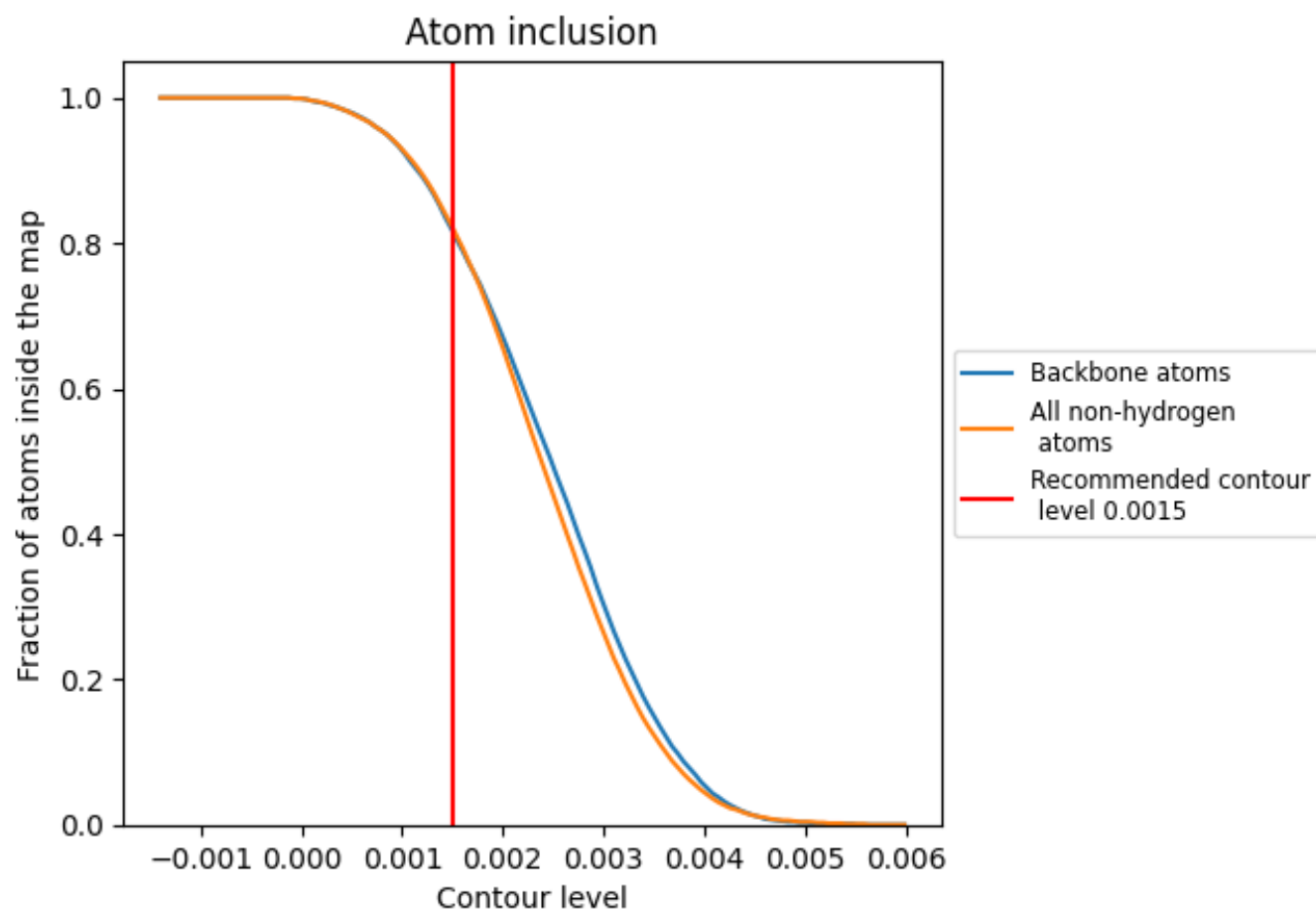
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0015).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (0.0015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8220	 0.0770
A	 0.8090	 0.0420
B	 0.8510	 0.0210
C	 0.9410	 0.0080
D	 0.8750	 -0.0070
E	 0.8960	 0.0590
F	 0.9940	 0.0890
G	 0.6640	 0.0240
H	 0.9930	 0.1230
I	 0.9630	 0.1010
J	 0.5190	 0.0210
K	 0.9680	 0.1230
L	 0.9880	 0.1120
M	 1.0000	 0.1000
N	 0.9990	 0.1370
O	 0.9980	 0.1160
P	 0.9940	 0.1180
Q	 0.8800	 0.1210
R	 0.8170	 0.1090
S	 0.6990	 0.0820
T	 0.9740	 0.1060
U	 0.7670	 0.1110
V	 0.7260	 0.0730
W	 0.9780	 0.0660
X	 0.7410	 0.0700
Y	 0.7340	 0.0760
Z	 0.7720	 0.0430
a	 0.2390	 0.0260
c	 0.8570	 0.0220
d	 0.9770	 0.0830
e	 0.9370	 0.0390
f	 0.9010	 0.0460
g	 0.8610	 0.0470
h	 0.9800	 0.0360
i	 0.8890	 0.0190



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Chain	Atom inclusion	Q-score
j	 0.9070	 0.0380
m	 0.3700	 0.0350
n	 0.5900	 0.0350