



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:39 PM UTC

PDB ID : 9EH0 / pdb_00009eh0
EMDB ID : EMD-48042
Title : RNA polymerase II-DSIF-SPT6-PAF1c-TFIIS-IWS1-SETD2-nucleosome, 30 bp upstream
Authors : Markert, J.; Farnung, L.
Deposited on : 2024-11-21
Resolution : 3.60 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

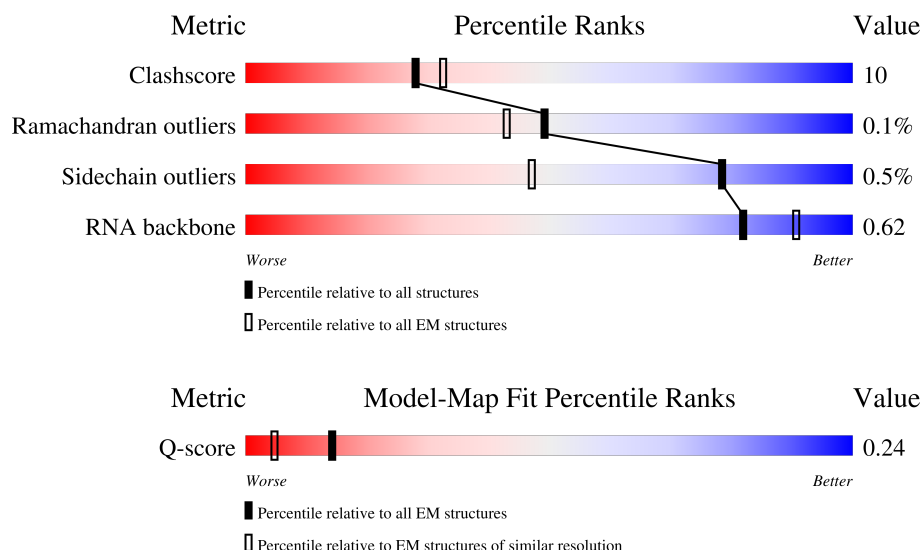
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	A	1984	
2	B	1251	
3	C	275	


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Mol	Chain	Length	Quality of chain
4	D	142	
5	E	210	
6	F	127	
7	G	172	
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	M	1729	
14	N	198	
15	O	821	
16	P	13	
17	Q	1179	
18	R	713	
19	S	304	
20	T	198	
21	U	666	
22	V	531	
23	W	305	
24	X	531	
25	Y	121	
26	Z	1087	
27	a	136	
27	e	136	

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Mol	Chain	Length	Quality of chain
28	b	103	 70% 6% 24%
28	f	103	 75% 0% 24%
29	c	130	 76% 0% 20%
29	g	130	 78% 0% 21%
30	d	123	 72% 0% 25%
30	h	123	 71% 0% 28%
31	l	1133	 32% 0% 64%

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 73438 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1426	Total	C	N	O	P	S	
			11255	7074	2014	2095	2	70	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1122	Total	C	N	O	S		
			8980	5684	1576	1656	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	258	Total	C	N	O	S		
			2072	1300	356	410	6	0	0

- Molecule 4 is a protein called RNA polymerase Rpb4/RPC9 core domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	126	Total	C	N	O	S		
			1004	630	170	200	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S		
			1720	1089	300	323	8	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	78	Total	C	N	O	S		
			626	401	106	114	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1333	866	214	245	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1197	759	195	238	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			942	582	168	181	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			524	339	88	91	6		

- Molecule 11 is a protein called RNA polymerase II subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	47	Total	C	N	O	S	0	0
			397	246	77	68	6		

- Molecule 13 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	1002	Total	C	N	O	S	0	0
			4883	2708	1072	1096	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	SER	-	expression tag	UNP Q7KZ85
M	-1	ASN	-	expression tag	UNP Q7KZ85
M	0	ALA	-	expression tag	UNP Q7KZ85

- Molecule 14 is a DNA chain called Non-template.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	181	Total	C	N	O	P	0	0
			3695	1757	664	1093	181		

- Molecule 15 is a protein called Protein IWS1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	132	Total	C	N	O	S	0	0
			1046	663	181	196	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-1	SER	-	expression tag	UNP Q96ST2
O	0	ASN	-	expression tag	UNP Q96ST2
O	1	ALA	-	expression tag	UNP Q96ST2

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	11	Total	C	N	O	P	0	0
			233	105	42	75	11		

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	890	Total	C	N	O	S	0	0
			7226	4579	1264	1352	31		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 18 is a protein called RNA polymerase-associated protein RTF1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	244	Total	C	N	O	S	0	0
			1836	1152	340	337	7		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	SER	-	expression tag	UNP Q92541
R	-1	ASN	-	expression tag	UNP Q92541
R	0	ALA	-	expression tag	UNP Q92541

- Molecule 19 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	161	Total	C	N	O	0	0
			657	334	161	162		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	-2	SER	-	expression tag	UNP P23193
S	-1	ASN	-	expression tag	UNP P23193
S	0	ALA	-	expression tag	UNP P23193

- Molecule 20 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	192	Total	C	N	O	P	0	0
			3955	1874	745	1144	192		

- Molecule 21 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	125	Total	C	N	O	S	0	0
			856	538	151	166	1		

- Molecule 22 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	244	Total	C	N	O	S	0	0
			1703	1061	305	333	4		

- Molecule 23 is a protein called WDR61.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	300	Total	C	N	O	S	0	0
			2333	1483	392	454	4		

- Molecule 24 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	43	Total	C	N	O	0	0
			353	220	69	64		

- Molecule 25 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	116	Total	C	N	O	S	0	0
			911	570	159	173	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 26 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	510	Total	C	N	O	P	S	0	0
			4025	2552	709	745	1	18		

- Molecule 27 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	101	Total	C	N	O	S	0	0
			823	520	157	142	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	94	Total	C	N	O	S	0	0
			776	491	149	133	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	36	MET	LYS	engineered mutation	UNP A0A310TTQ1
e	36	MET	LYS	engineered mutation	UNP A0A310TTQ1

- Molecule 28 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	78	Total	C	N	O	S	0	0
			622	393	120	108	1		
28	f	78	Total	C	N	O	S	0	0
			622	393	120	108	1		

- Molecule 29 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	104	Total	C	N	O		0	0
			800	504	156	140			
29	g	103	Total	C	N	O		0	0
			795	501	155	139			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	99	ARG	GLY	conflict	UNP P06897
c	123	SER	ALA	conflict	UNP P06897
g	99	ARG	GLY	conflict	UNP P06897
g	123	SER	ALA	conflict	UNP P06897

- Molecule 30 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	92	Total	C	N	O	S	0	0
			721	454	129	136	2		
30	h	89	Total	C	N	O	S	0	0
			694	438	122	132	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	3	MET	-	initiating methionine	UNP P02281
d	32	THR	SER	engineered mutation	UNP P02281
h	3	MET	-	initiating methionine	UNP P02281
h	32	THR	SER	engineered mutation	UNP P02281

- Molecule 31 is a protein called Histone-lysine N-methyltransferase SETD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1	412	Total	C	N	O	S	0	0
			2893	1772	545	555	21		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1432	SER	-	expression tag	UNP Q9BYW2
1	1433	ASN	-	expression tag	UNP Q9BYW2
1	1434	ALA	-	expression tag	UNP Q9BYW2
1	1962	LEU	PRO	conflict	UNP Q9BYW2

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	A	2	Total	Zn	0
			2	2	
32	B	1	Total	Zn	0
			1	1	
32	C	1	Total	Zn	0
			1	1	
32	I	2	Total	Zn	0
			2	2	
32	J	1	Total	Zn	0
			1	1	
32	L	1	Total	Zn	0
			1	1	
32	Y	1	Total	Zn	0
			1	1	

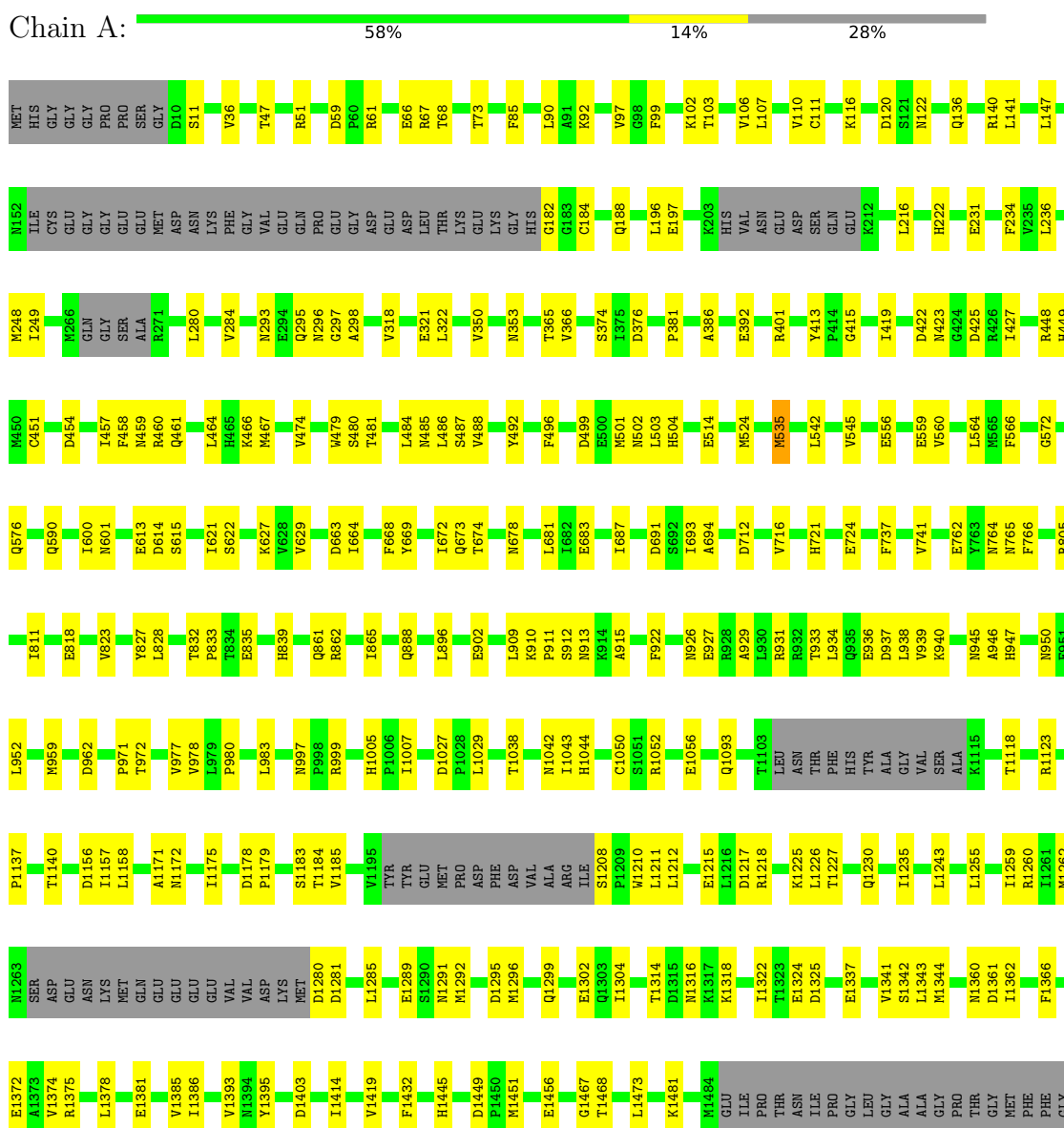
- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

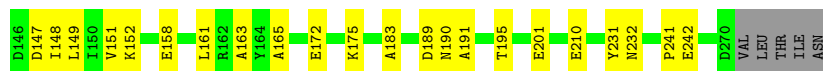
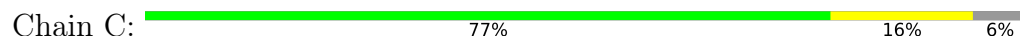
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: DNA-directed RNA polymerase subunit

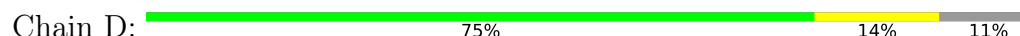




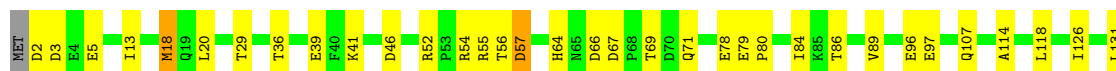
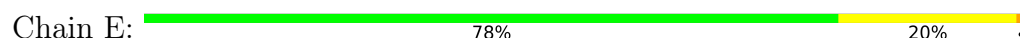
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



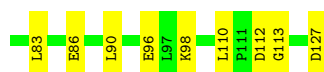
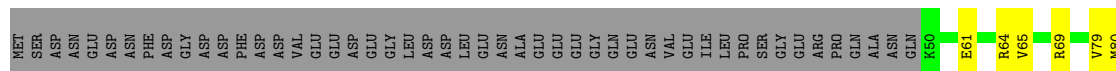
- Molecule 4: RNA polymerase Rpb4/RPC9 core domain-containing protein



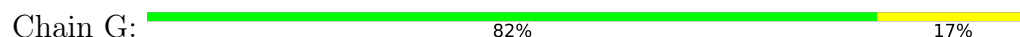
- Molecule 5: DNA-directed RNA polymerase II subunit E



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

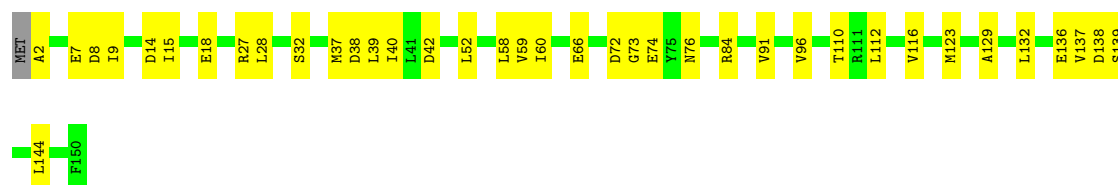


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



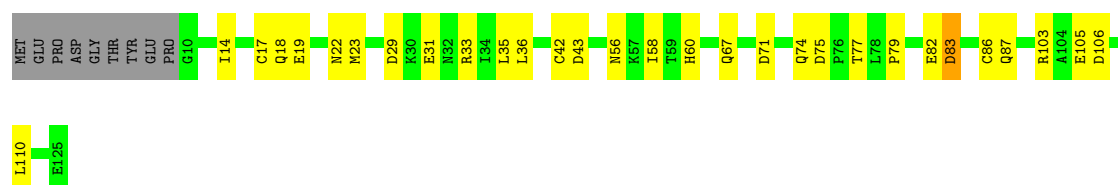
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  74% 25%



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:  69% 23% 7%




- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  73% 25%



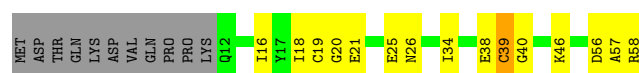
- Molecule 11: RNA polymerase II subunit J

Chain K:  79% 19%



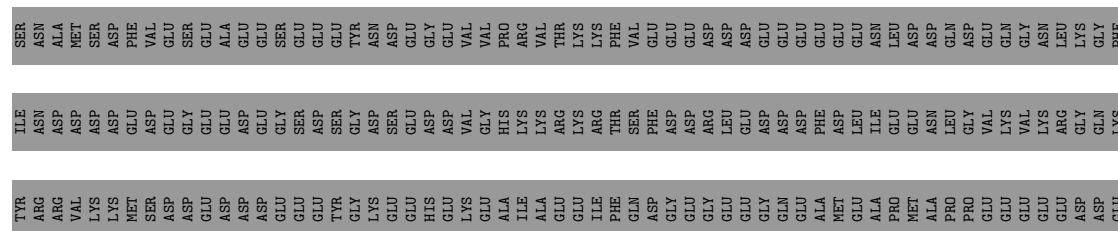
- Molecule 12: RNA polymerase II subunit K

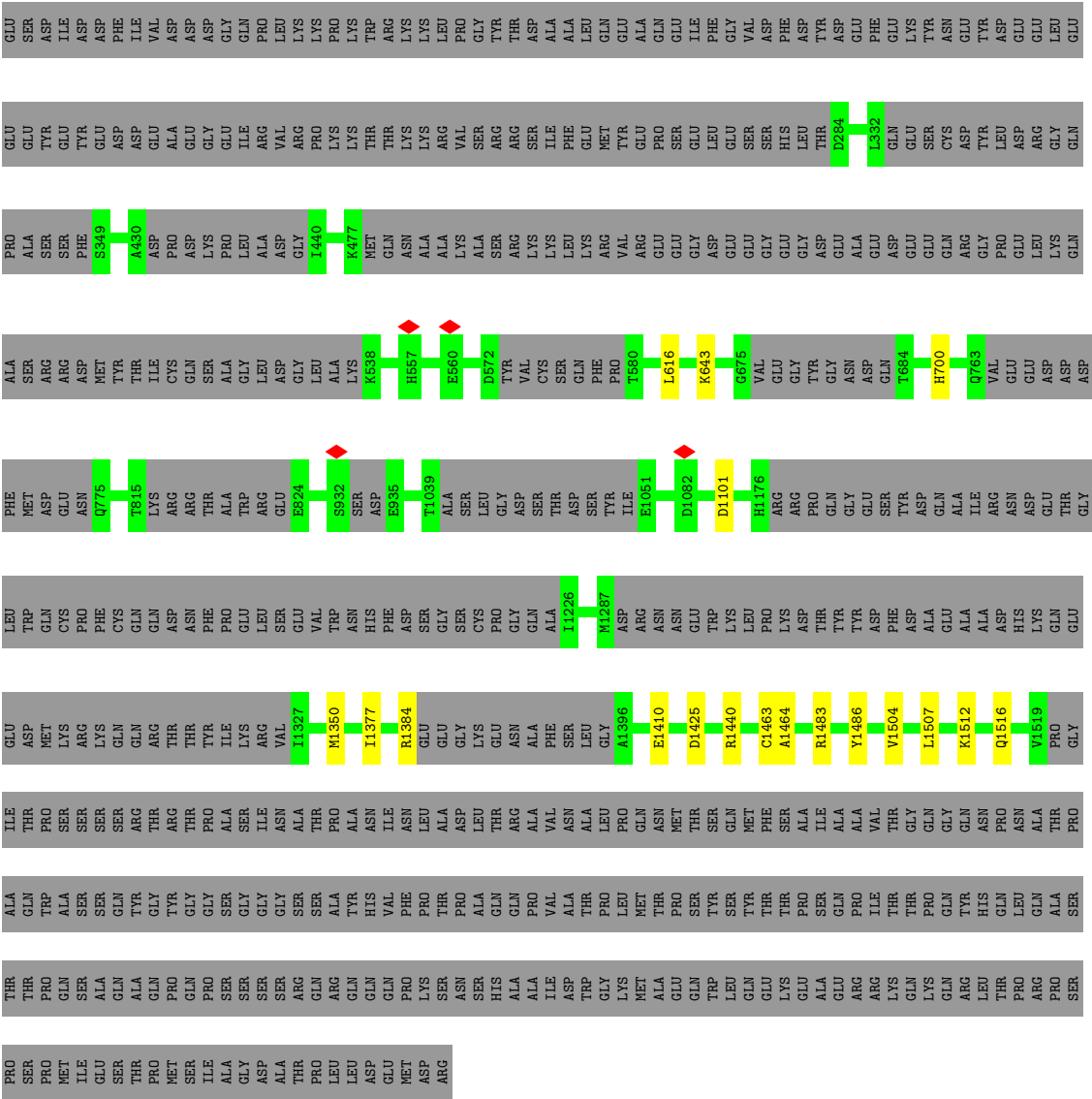
Chain L:  55% 24% 19%



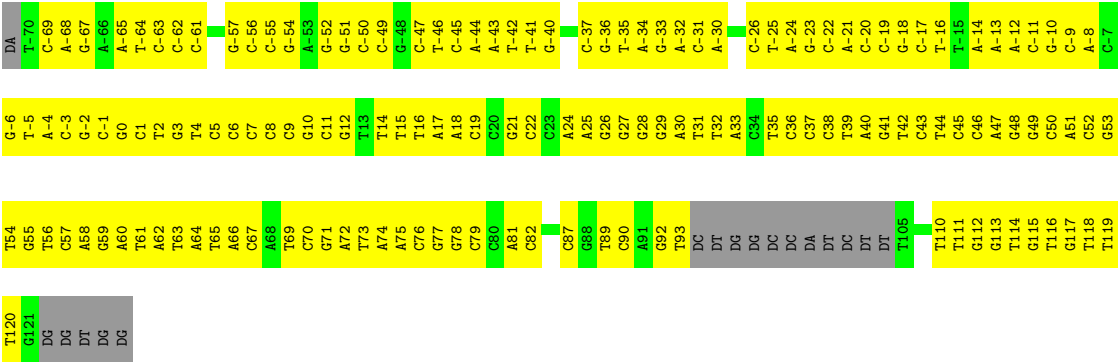
- Molecule 13: Transcription elongation factor SPT6

Chain M:  57% 42%





● Molecule 14: Non-template

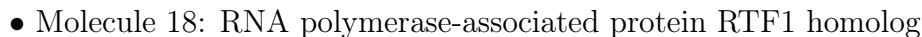


● Molecule 15: Protein IWS1 homolog

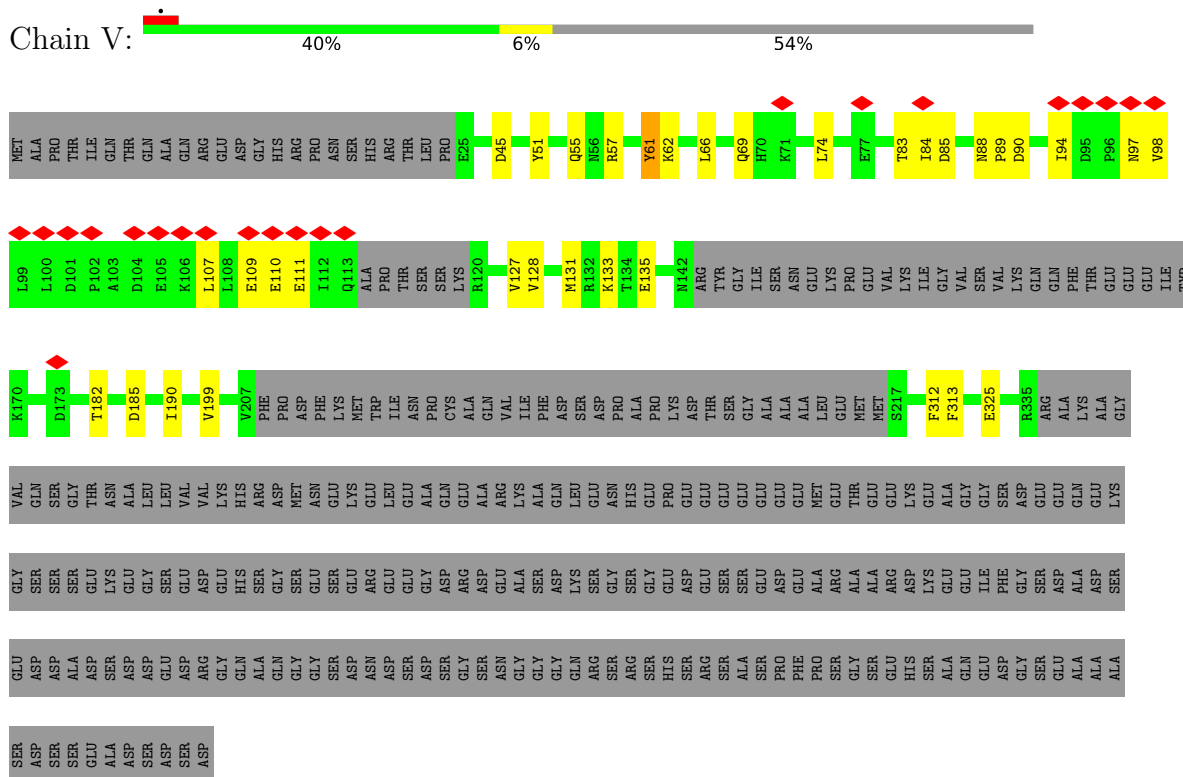
[illegible]

A	A	A16	A17	A18	A19	U20	U21	A22	G23	C24	U25	C26
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[illegible]



- Molecule 22: RNA polymerase II-associated factor 1 homolog

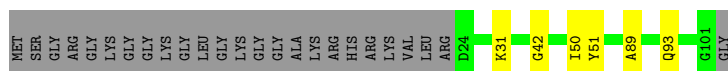


- Molecule 23: WDR61

[illegible][illegible]

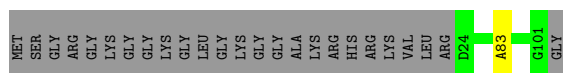
GLY	PRO	GLY	SER	MET	A2	L13	L18	D26	Q27	A38	Y39	L40	Q41	M42	E47	M48	V49	C52	T53	S56	Q75	K81	Y85	A86	T90	R111	D112	T113	K116	T117
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Chain b:  70% 6% 24%



- Molecule 28: Histone H4

Chain f:  75% 0% 24%




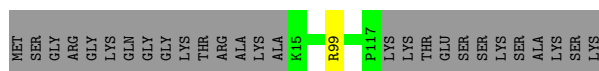
- Molecule 29: Histone H2A type 1

Chain c:  76% 0% 20%



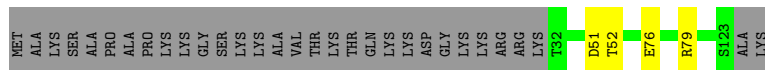
- Molecule 29: Histone H2A type 1

Chain g:  78% 0% 21%



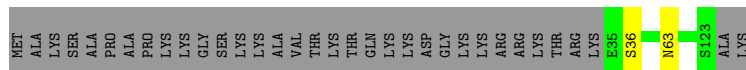
- Molecule 30: Histone H2B 1.1

Chain d:  72% 0% 25%



- Molecule 30: Histone H2B 1.1

Chain h:  71% 0% 28%



- Molecule 31: Histone-lysine N-methyltransferase SETD2

Chain i:  32% 0% 64%



LYS	GLJ	TRP	ALA	TYR	SER	VAL	SER	PRO	GLJ	ASN	PRO	GLJ	ASN	R1670
HIS	MET	ASP	PRO	GLN	GLN	ASP	THR	ASN	GLU	THR	VAL	GLU	THR	Y1671
LYS	SER	PRO	GLY	GLN	GLN	PRO	GLU	GLU	THR	PRO	GLU	GLU	ASP	A1674
THR	PHE	THR	PRO	THR	VAL	ASN	GLU	ARG	SER	PRO	ASP	GLU	ASP	A1675
LYS	TLE	TRP	GLN	CYS	ALA	PRO	ARG	GLU	ARG	SER	GLN	GLU	SER	A1676
TYR	VAL	GLJ	PRO	PRO	GLN	ASN	LYS	ARG	GLU	THR	GLU	GLU	THR	K1677
LYS	CYS	SER	GLN	THR	SER	ALA	LEU	LEU	ASP	LYS	GLN	GLN	LEU	C1678
TYR	LEU	GLY	PRO	TYR	GLY	VAL	GLU	GLU	ASP	SER	GLY	GLY	SER	F1679
MET	PRO	ASP	SER	GLY	VAL	VAL	GLN	LYS	GLN	THR	GLN	GLN	THR	G1681
GLN	TYR	ALA	GLU	VAL	VAL	LEU	VAL	GLN	SER	LEU	LEU	LEU	ALA	M1684
LYS	ARG	SER	VAL	SER	GLN	PRO	ALA	THR	GLU	THR	ASP	ASP	THR	C1685
PHE	LYS	LEU	VAL	PRO	ASP	PRO	GLN	ASN	VAL	PRO	VAL	LEU	THR	R1686
GLY	PRO	GLJ	THR	TYR	SER	PRO	ARG	LYS	GLU	THR	GLN	GLN	ASP	G1687
ALA	ASP	HIS	ASN	SER	SER	MET	ALA	GLU	SER	THR	SER	GLN	THR	Y1688
VAL	CYS	GLJ	ASN	GLN	VAL	VAL	GLN	LYS	GLU	PRO	LEU	LEU	PRO	L1689
TYR	LYS	ALA	LEU	THR	ALA	ASP	GLN	ARG	ARG	PRO	PRO	GLU	LYS	G1690
LYS	VAL	GLJ	LEU	THR	VAL	PRO	LYS	LYS	SER	LYS	GLN	GLN	THR	I1697
PRO	GLY	MET	ASP	PRO	LEU	VAL	GLN	ARG	GLN	CYS	GLN	CYS	LEU	R1698
LYS	ARG	ASP	LEU	PRO	PRO	CYS	GLN	ARG	GLU	LYS	GLN	VAL	MET	A1699
GLJ	TLE	LEU	PRO	TLE	VAL	SER	GLN	SER	GLN	VAL	VAL	PHE	THR	A1700
ASP	THR	GLY	PRO	VAL	PRO	PRO	GLN	SER	PRO	ASP	ASP	ARG	ARG	K1703
THR	THR	PRO	SER	SER	PRO	ALA	MET	LEU	ASP	THR	GLU	SER	ARG	
GLU	GLJ	THR	PRO	TYR	GLY	TYR	GLN	SER	LYS	THR	THR	GLU	LEU	
LEU	GLU	THR	PRO	TYR	GLY	TYR	ASN	PRO	THR	ASN	ASN	ILE	ILE	E1707
GLU	PHE	ASP	LYS	GLN	VAL	HIS	GLY	SER	ASP	TLE	GLU	ILE	ILE	R1708
LYS	LYS	GLJ	PRO	PRO	GLN	ALA	MET	SER	GLU	GLU	GLU	SER	SER	S1709
HIS	HIS	ASN	LYS	SER	GLY	PRO	THR	ALA		ALA	ALA	ASN	ASN	
ALA	LEU	MET	ILE	GLN	GLN	PRO	SER	TYR	GLU	LYS	SER	GLN	GLN	G1927
ARG	ARG	LYS	VAL	TYR	TYR	VAL	PRO	ARG	GLU	LEU	LEU	MET	MET	SER
LYS	LEU	ALA	LEU	TLE	SER	GLY	PRO	GLY	ARG	PRO	PRO	ASP	ASP	GLN
LEU	THR	SER	PRO	GLN	VAL	HIS	TYR	THR	THR	THR	THR	SER	SER	LYS
THR	GLY	LYS	PRO	GLY	TRP	SER	ASP	ASP	LYS	SER	GLU	ILE	ALA	THR
GLY	VAL	PRO	TRP	GLN	SER	THR	SER	LEU	PRO	PRO	PRO	SER	SER	ALA
VAL	MET	THR	LYS	TLE	ASN	PRO	GLY	PRO	T2025	VAL	GLU	SER	VAL	VAL
ASN	ASN	THR	ALA	PHE	GLN	LEU	TYR	ASP	T2031	ALA	GLU	ASP	PRO	PRO
LYS	GLJ	ALA	ARG	THR	GLN	SER	ASN	ARG	T2038	ALA	ASP	ALA	THR	LEU
GLU	GLU	ALA	ASP	HIS	VAL	ALA	PRO	TYR	E2039	ALA	GLU	SER	SER	SER
LEU	LEU	ASP	PRO	PRO	SER	PRO	PRO	ASP	R2040	GLU	GLU	GLU	GLU	GLU
LYS	THR	THR	GLU	GLN	VAL	PRO	HIS	THR	GLY	TLE	GLU	LEU	GLY	GLY
TYR	TYR	SER	GLY	GLY	GLN	VAL	PRO	THR	ASP	GLU	GLU	GLY	GLY	ASP
CYS	CYS	SER	LYS	VAL	GLN	VAL	PHE	SER	ALA	ALA	LYS	LYS	LYS	THR
LYS	LYS	GLJ	ILE	VAL	GLN	VAL	VAL	ALA	T2038	ASP	ASP	ASP	ASP	GLY
ASN	ASN	LEU	ILE	VAL	TYR	VAL	ALA	LYS	E2039	GLY	ILE	GLU	GLY	GLY
LYS	ASN	GLU	TYR	VAL	TYR	VAL	GLY	LYS	R2040	ARG	GLU	GLU	GLY	ASP
ASN	GLU	SER	GLY	VAL	GLN	VAL	GLN	THR	THR	ASP	ALA	LYS	LYS	THR
GLN	TYR	GLU	TYR	VAL	GLN	VAL	ALA	THR	T2038	VAL	ASP	GLU	GLU	GLY
LYS	TYR	LEU	TYR	VAL	TYR	VAL	GLY	LYS	E2039	VAL	GLU	GLU	GLY	GLY
LYS	PRO	ALA	TYR	VAL	TYR	VAL	GLY	LYS	R2040	PHE	GLU	GLU	GLY	GLY
GLY	PRO	LYS	TYR	VAL	SER	VAL	GLY	LYS	E2039	ARG	GLU	GLU	GLY	GLY
GLY	GLU	THR	THR	ALA	SER	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	E2039	GLY	GLU	GLU	GLY	GLY
GLU	GLU	THR	THR	ALA	TYR	VAL	GLY	LYS	R2040	GLY	GLU	GLU	GLY	GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	301837	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.683	Depositor
Minimum map value	-0.193	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	550.0, 550.0, 550.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.18	0/11437	0.32	0/15433
2	B	0.20	0/9158	0.32	0/12360
3	C	0.21	0/2115	0.33	0/2873
4	D	0.15	0/1017	0.27	0/1368
5	E	0.18	0/1751	0.31	0/2366
6	F	0.19	0/636	0.29	0/859
7	G	0.15	0/1364	0.32	0/1853
8	H	0.22	0/1219	0.34	0/1644
9	I	0.18	0/964	0.28	0/1305
10	J	0.25	0/533	0.33	0/719
11	K	0.20	0/939	0.33	0/1271
12	L	0.19	0/403	0.28	0/536
13	M	0.13	0/4944	0.27	0/6387
14	N	0.23	0/4138	0.50	0/6379
15	O	0.12	0/1062	0.23	0/1428
16	P	0.12	0/260	0.42	0/402
17	Q	0.19	1/7365 (0.0%)	0.33	3/9927 (0.0%)
18	R	0.12	0/1866	0.28	0/2519
19	S	0.14	0/659	0.19	0/827
20	T	0.26	0/4443	0.45	0/6859
21	U	0.15	0/870	0.28	0/1183
22	V	0.13	0/1728	0.33	2/2357 (0.1%)
23	W	0.15	0/2392	0.32	0/3257
24	X	0.18	0/356	0.35	0/478
25	Y	0.13	0/927	0.25	0/1250
26	Z	0.11	0/4084	0.23	0/5498
27	a	0.27	0/835	0.40	0/1120
27	e	0.24	0/786	0.37	0/1053
28	b	0.23	0/629	0.35	0/843
28	f	0.23	0/629	0.34	0/843
29	c	0.23	0/810	0.34	0/1095
29	g	0.22	0/805	0.33	0/1088

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	d	0.24	0/732	0.34	0/986
30	h	0.24	0/705	0.35	0/951
31	l	0.18	0/2932	0.40	0/3963
All	All	0.19	1/75493 (0.0%)	0.34	5/103280 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
31	l	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	450	PRO	CA-C	9.63	1.57	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	450	PRO	O-C-N	7.54	124.78	121.31
17	Q	772	GLU	CA-C-N	5.84	132.21	121.70
17	Q	772	GLU	C-N-CA	5.84	132.21	121.70
22	V	61	TYR	CA-C-N	5.34	131.31	121.70
22	V	61	TYR	C-N-CA	5.34	131.31	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	l	2018	ASP	Peptide
31	l	2021	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11255	0	11374	199	0
2	B	8980	0	9019	162	0
3	C	2072	0	2020	40	0
4	D	1004	0	980	16	0
5	E	1720	0	1737	36	0
6	F	626	0	657	10	0
7	G	1333	0	1321	23	0
8	H	1197	0	1156	30	0
9	I	942	0	872	25	0
10	J	524	0	541	14	0
11	K	920	0	942	17	0
12	L	397	0	405	15	0
13	M	4883	0	2550	14	0
14	N	3695	0	2038	226	0
15	O	1046	0	1096	12	0
16	P	233	0	118	16	0
17	Q	7226	0	7169	159	0
18	R	1836	0	1699	27	0
19	S	657	0	199	2	0
20	T	3955	0	2154	145	0
21	U	856	0	680	14	0
22	V	1703	0	1426	30	0
23	W	2333	0	2246	47	0
24	X	353	0	371	9	0
25	Y	911	0	907	15	0
26	Z	4025	0	4041	59	0
27	a	823	0	864	8	0
27	e	776	0	815	3	0
28	b	622	0	660	4	0
28	f	622	0	660	1	0
29	c	800	0	851	4	0
29	g	795	0	846	1	0
30	d	721	0	742	2	0
30	h	694	0	709	1	0
31	l	2893	0	2422	38	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	I	2	0	0	0	0
32	J	1	0	0	0	0
32	L	1	0	0	0	0
32	Y	1	0	0	0	0
33	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	73438	0	66287	1328	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 10.

All (1328) 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)
17:Q:276:ALA:HB1	17:Q:288:VAL:HG23	1.31	1.12
1:A:1172:ASN:N	1:A:1215:GLU:OE2	1.99	0.95
20:T:9:DG:H2''	20:T:10:DC:H5'	1.50	0.94
20:T:67:DC:H2'	20:T:68:DT:H71	1.49	0.93
2:B:790:GLN:O	2:B:968:ASN:ND2	2.01	0.93
20:T:7:DG:H2'	20:T:8:DT:C6	2.03	0.93
1:A:140:ARG:NH2	1:A:234:PHE:O	2.02	0.93
5:E:36:THR:N	5:E:39:GLU:OE2	2.00	0.93
14:N:-47:DC:H2''	14:N:-46:DT:C7	1.98	0.93
31:l:1677:LYS:HA	31:l:1688:TYR:HA	1.49	0.92
2:B:591:ARG:NH2	2:B:663:GLU:OE2	2.03	0.91
1:A:691:ASP:OD2	1:A:765:ASN:ND2	2.06	0.89
3:C:242:GLU:OE1	3:C:242:GLU:N	2.05	0.89
3:C:36:ARG:NH1	11:K:41:THR:OG1	2.06	0.88
14:N:-42:DT:C6	14:N:-41:DT:H72	2.09	0.87
4:D:76:ASN:O	4:D:79:THR:OG1	1.93	0.86
14:N:31:DT:C6	14:N:32:DT:H72	2.12	0.85
20:T:57:DC:H2''	20:T:58:DA:C8	2.11	0.84
14:N:-47:DC:H2''	14:N:-46:DT:H71	1.58	0.84
20:T:-26:DC:H2''	20:T:-25:DT:C7	2.07	0.84
17:Q:94:VAL:HG23	17:Q:140:LEU:HD11	1.59	0.83
5:E:141:GLU:N	5:E:141:GLU:OE1	2.11	0.83
12:L:25:GLU:N	12:L:25:GLU:OE1	2.11	0.83
1:A:1324:GLU:N	1:A:1324:GLU:OE1	2.11	0.83
17:Q:371:TYR:OH	22:V:69:GLN:NE2	2.12	0.82
1:A:818:GLU:OE1	1:A:818:GLU:N	2.12	0.82
2:B:600:GLU:N	2:B:600:GLU:OE1	2.12	0.82
31:l:1698:ARG:HG2	31:l:1703:LYS:HA	1.62	0.82
10:J:31:GLU:OE2	22:V:133:LYS:NZ	2.13	0.81
17:Q:384:LEU:HD13	17:Q:397:ALA:HB2	1.60	0.81
1:A:535:MET:O	1:A:669:TYR:OH	1.97	0.81
14:N:-25:DT:H4'	14:N:-24:DA:OP1	1.79	0.81
31:l:1669:GLN:NE2	31:l:1700:ALA:HA	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:74:GLU:OE2	8:H:76:ASN:ND2	2.14	0.80
14:N:32:DT:H2''	14:N:33:DA:C8	2.17	0.80
17:Q:799:VAL:O	17:Q:802:LYS:NZ	2.14	0.80
1:A:556:GLU:OE1	1:A:556:GLU:N	2.15	0.80
31:I:1671:TYR:OH	31:I:1697:ILE:HG23	1.81	0.80
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.63	0.79
12:L:39:CYS:SG	12:L:40:GLY:N	2.55	0.79
14:N:-26:DC:H2''	14:N:-25:DT:H71	1.64	0.79
17:Q:776:LEU:O	17:Q:779:VAL:HG22	1.83	0.79
1:A:466:LYS:N	1:A:1093:GLN:OE1	2.15	0.79
2:B:1032:PHE:O	3:C:32:ASN:ND2	2.14	0.79
2:B:1040:GLN:OE1	2:B:1040:GLN:N	2.15	0.79
14:N:42:DT:H2''	14:N:43:DC:C6	2.16	0.79
14:N:38:DC:C2'	14:N:39:DT:H71	2.13	0.79
25:Y:38:ALA:O	25:Y:41:GLN:NE2	2.16	0.79
1:A:448:ARG:NH1	1:A:451:CYS:SG	2.55	0.79
14:N:-17:DC:H2'	14:N:-16:DT:H72	1.65	0.79
14:N:17:DA:H1'	14:N:18:DA:N7	1.97	0.79
16:P:16:A:H1'	16:P:17:A:OP2	1.83	0.78
17:Q:333:THR:HG21	17:Q:347:LEU:HD12	1.63	0.78
17:Q:605:LEU:O	17:Q:609:ASN:ND2	2.17	0.78
20:T:19:DG:H4'	20:T:20:DG:OP1	1.84	0.78
14:N:-56:DC:H2''	14:N:-55:DC:C5	2.18	0.78
17:Q:534:TYR:OH	17:Q:556:GLU:OE1	1.99	0.78
20:T:-88:DC:H2''	20:T:-87:DG:C8	2.18	0.78
2:B:100:GLU:N	2:B:100:GLU:OE1	2.17	0.78
20:T:-40:DT:H2''	20:T:-39:DA:C8	2.18	0.78
26:Z:523:GLU:N	26:Z:523:GLU:OE1	2.17	0.78
20:T:-76:DG:H2'	20:T:-75:DT:H72	1.64	0.77
17:Q:65:GLU:OE2	17:Q:93:TYR:OH	2.01	0.77
2:B:765:GLU:OE1	2:B:770:ARG:NE	2.17	0.77
8:H:18:GLU:N	8:H:18:GLU:OE1	2.18	0.77
14:N:46:DC:H2''	14:N:47:DA:C8	2.20	0.77
20:T:-25:DT:H2'	20:T:-24:DT:H72	1.67	0.77
1:A:1302:GLU:OE1	1:A:1302:GLU:N	2.17	0.77
14:N:-33:DG:H1'	14:N:-32:DA:C8	2.19	0.77
9:I:31:GLU:N	9:I:31:GLU:OE1	2.18	0.77
1:A:423:ASN:ND2	1:A:425:ASP:OD1	2.18	0.76
18:R:388:ARG:NH1	18:R:446:GLU:O	2.18	0.76
20:T:36:DC:H2''	20:T:37:DG:C8	2.20	0.76
31:I:1631:CYS:SG	31:I:1685:CYS:HA	2.26	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:GLU:OE1	5:E:78:GLU:N	2.19	0.76
17:Q:768:VAL:HG21	17:Q:778:GLU:HG3	1.68	0.76
14:N:17:DA:H1'	14:N:18:DA:C8	2.21	0.76
12:L:21:GLU:OE1	12:L:21:GLU:N	2.19	0.76
20:T:-26:DC:H2''	20:T:-25:DT:H72	1.64	0.76
1:A:1456:GLU:N	1:A:1456:GLU:OE1	2.20	0.76
11:K:77:THR:OG1	11:K:81:TYR:O	2.04	0.75
2:B:992:ASN:O	10:J:46:ARG:NH1	2.20	0.75
20:T:-25:DT:H2'	20:T:-24:DT:C7	2.17	0.74
14:N:-46:DT:H5''	14:N:-46:DT:H6	1.52	0.74
14:N:-33:DG:H1'	14:N:-32:DA:N7	2.01	0.74
1:A:805:ARG:NH1	9:I:77:THR:OG1	2.21	0.74
14:N:38:DC:H2''	14:N:39:DT:H71	1.68	0.74
26:Z:729:GLU:O	26:Z:747:ARG:NH2	2.20	0.74
23:W:33:GLU:O	23:W:49:TRP:N	2.20	0.74
3:C:210:GLU:N	3:C:210:GLU:OE1	2.21	0.73
1:A:683:GLU:O	2:B:1038:THR:OG1	2.06	0.73
4:D:96:GLU:N	4:D:96:GLU:OE1	2.21	0.73
14:N:41:DG:C8	14:N:42:DT:H72	2.23	0.73
2:B:198:GLU:N	2:B:198:GLU:OE1	2.21	0.73
14:N:-37:DC:H2''	14:N:-36:DG:C8	2.23	0.73
20:T:-10:DC:H2''	20:T:-9:DG:C8	2.24	0.73
1:A:559:GLU:N	1:A:559:GLU:OE1	2.22	0.73
14:N:-6:DG:H2''	14:N:-5:DT:H71	1.71	0.73
2:B:817:GLN:N	2:B:817:GLN:OE1	2.20	0.73
14:N:118:DT:H2'	14:N:119:DT:H71	1.70	0.73
17:Q:286:SER:O	17:Q:290:HIS:ND1	2.21	0.73
2:B:191:GLU:OE1	2:B:191:GLU:N	2.22	0.72
14:N:53:DG:H2'	14:N:54:DT:H72	1.70	0.72
23:W:206:VAL:HG11	23:W:238:VAL:HG21	1.70	0.72
27:a:108:ASN:ND2	28:b:42:GLY:O	2.22	0.72
6:F:112:ASP:OD1	6:F:113:GLY:N	2.22	0.72
17:Q:401:LEU:HD22	17:Q:418:LEU:HG	1.70	0.72
9:I:82:GLU:OE1	9:I:82:GLU:N	2.22	0.72
20:T:9:DG:C2'	20:T:10:DC:H5'	2.20	0.72
26:Z:554:GLU:OE2	26:Z:559:GLN:NE2	2.23	0.72
1:A:487:SER:OG	1:A:673:GLN:OE1	2.07	0.72
1:A:674:THR:O	1:A:678:ASN:ND2	2.23	0.72
1:A:862:ARG:NH1	2:B:1088:GLU:OE1	2.22	0.72
2:B:516:GLU:N	2:B:516:GLU:OE1	2.23	0.72
5:E:79:GLU:N	5:E:79:GLU:OE1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:38:GLU:O	12:L:40:GLY:N	2.23	0.72
14:N:-47:DC:H2''	14:N:-46:DT:H73	1.72	0.72
17:Q:276:ALA:CB	17:Q:288:VAL:HG23	2.17	0.71
20:T:7:DG:H2''	20:T:8:DT:O5'	1.90	0.71
5:E:2:ASP:OD1	5:E:3:ASP:N	2.24	0.71
1:A:946:ALA:O	1:A:950:ASN:ND2	2.24	0.70
5:E:41:LYS:NZ	5:E:46:ASP:OD1	2.24	0.70
23:W:251:SER:OG	23:W:253:ASP:OD1	2.09	0.70
14:N:-41:DT:H2''	14:N:-40:DG:H8	1.57	0.70
31:l:1698:ARG:HG2	31:l:1703:LYS:CB	2.22	0.70
1:A:296:ASN:OD1	1:A:297:GLY:N	2.24	0.70
1:A:1027:ASP:OD1	1:A:1029:LEU:N	2.24	0.70
1:A:1137:PRO:HB2	1:A:1341:VAL:HG23	1.73	0.70
1:A:1217:ASP:OD1	1:A:1218:ARG:N	2.25	0.70
2:B:1004:ASP:OD1	18:R:596:ARG:NH2	2.25	0.69
11:K:17:LYS:O	11:K:36:ASN:ND2	2.25	0.69
17:Q:18:GLU:N	17:Q:18:GLU:OE1	2.25	0.69
8:H:136:GLU:N	8:H:136:GLU:OE1	2.25	0.69
1:A:945:ASN:OD1	1:A:947:HIS:N	2.24	0.69
1:A:1038:THR:O	1:A:1042:ASN:ND2	2.26	0.69
8:H:66:GLU:N	8:H:66:GLU:OE1	2.25	0.69
6:F:86:GLU:N	6:F:86:GLU:OE1	2.26	0.69
7:G:139:GLN:OE1	7:G:139:GLN:N	2.25	0.69
14:N:-43:DA:C2'	14:N:-42:DT:H71	2.23	0.69
14:N:37:DC:H1'	14:N:38:DC:C5	2.28	0.69
14:N:73:DT:H2''	14:N:74:DA:H8	1.57	0.69
20:T:-79:DG:H2''	20:T:-78:DC:C6	2.28	0.69
20:T:57:DC:H2''	20:T:58:DA:H8	1.58	0.69
9:I:87:GLN:OE1	9:I:87:GLN:N	2.26	0.69
16:P:22:A:H2'	16:P:23:G:H8	1.57	0.69
23:W:35:VAL:N	23:W:47:TRP:O	2.25	0.69
1:A:971:PRO:O	1:A:972:THR:OG1	2.04	0.68
2:B:676:ALA:HB2	2:B:693:TYR:CD1	2.28	0.68
17:Q:454:LEU:HD21	17:Q:476:ALA:HB3	1.75	0.68
14:N:-26:DC:H2''	14:N:-25:DT:C7	2.21	0.68
26:Z:541:GLN:NE2	26:Z:543:ASP:O	2.26	0.68
13:M:616:LEU:N	13:M:643:LYS:O	2.26	0.68
18:R:366:ARG:NH2	26:Z:773:SER:OG	2.27	0.68
2:B:19:PRO:O	2:B:21:LEU:N	2.25	0.68
20:T:7:DG:H2'	20:T:8:DT:C5	2.27	0.68
17:Q:708:LEU:HD21	17:Q:719:VAL:HG21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:-106:DC:H2'	20:T:-105:DA:H8	1.58	0.68
1:A:295:GLN:O	15:O:672:ARG:NH1	2.27	0.67
1:A:1342:SER:O	1:A:1344:MET:N	2.25	0.67
2:B:756:LYS:NZ	22:V:135:GLU:O	2.28	0.67
14:N:9:DC:H2''	14:N:10:DG:H8	1.59	0.67
14:N:73:DT:H2''	14:N:74:DA:C8	2.29	0.67
27:e:87:SER:OG	28:f:83:ALA:HB2	1.93	0.67
2:B:849:ASP:OD2	12:L:46:LYS:NZ	2.27	0.67
5:E:5:GLU:N	5:E:5:GLU:OE1	2.27	0.67
5:E:167:GLU:N	5:E:167:GLU:OE1	2.26	0.67
14:N:-11:DC:H2''	14:N:-10:DG:C8	2.30	0.67
17:Q:353:TYR:OH	22:V:57:ARG:O	2.11	0.67
3:C:201:GLU:N	3:C:201:GLU:OE1	2.25	0.67
14:N:62:DA:C8	14:N:63:DT:H72	2.29	0.67
7:G:10:GLU:N	7:G:10:GLU:OE1	2.28	0.67
1:A:116:LYS:NZ	1:A:182:GLY:O	2.27	0.67
26:Z:729:GLU:N	26:Z:729:GLU:OE1	2.28	0.66
1:A:1481:LYS:O	13:M:1384:ARG:NH1	2.27	0.66
14:N:9:DC:H2''	14:N:10:DG:C8	2.30	0.66
2:B:613:ARG:NH1	2:B:615:TYR:OH	2.28	0.66
1:A:184:CYS:SG	15:O:600:LYS:NZ	2.68	0.66
5:E:55:ARG:O	5:E:56:THR:OG1	2.09	0.66
17:Q:768:VAL:HG21	17:Q:778:GLU:CG	2.25	0.66
20:T:-26:DC:C2'	20:T:-25:DT:H72	2.25	0.66
20:T:7:DG:H4'	20:T:8:DT:OP1	1.96	0.66
1:A:1361:ASP:OD1	1:A:1362:ILE:N	2.29	0.66
14:N:7:DC:H4'	14:N:8:DC:OP1	1.95	0.66
5:E:96:GLU:OE1	5:E:96:GLU:N	2.29	0.66
16:P:22:A:H2'	16:P:23:G:C8	2.30	0.66
2:B:23:GLN:N	2:B:23:GLN:OE1	2.29	0.66
14:N:26:DG:H1'	14:N:27:DG:C8	2.31	0.66
20:T:67:DC:C2'	20:T:68:DT:H71	2.24	0.66
1:A:11:SER:O	2:B:1135:TYR:OH	2.12	0.65
2:B:650:ASN:N	2:B:650:ASN:OD1	2.29	0.65
17:Q:750:ASP:OD1	17:Q:752:VAL:N	2.30	0.65
23:W:40:LEU:HD12	23:W:66:GLY:HA3	1.77	0.65
1:A:762:GLU:N	1:A:762:GLU:OE1	2.26	0.65
23:W:258:VAL:O	23:W:267:VAL:HG22	1.96	0.65
31:l:1698:ARG:HG2	31:l:1703:LYS:CA	2.26	0.65
1:A:47:THR:OG1	1:A:51:ARG:O	2.13	0.65
26:Z:589:SER:OG	26:Z:641:ARG:O	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:38:ASP:OD1	8:H:39:LEU:N	2.30	0.64
8:H:137:VAL:HG22	8:H:138:ASP:OD1	1.98	0.64
26:Z:455:GLU:OE1	26:Z:455:GLU:N	2.29	0.64
5:E:97:GLU:N	5:E:97:GLU:OE1	2.29	0.64
14:N:24:DA:H2''	14:N:25:DA:C8	2.33	0.64
20:T:-85:DA:H2'	20:T:-84:DT:H71	1.79	0.64
20:T:-106:DC:H2'	20:T:-105:DA:C8	2.32	0.64
2:B:780:VAL:HG21	2:B:1048:TYR:CE1	2.33	0.64
1:A:1171:ALA:HB3	1:A:1215:GLU:OE2	1.98	0.64
17:Q:500:SER:OG	17:Q:523:ILE:HD11	1.97	0.64
23:W:24:TRP:NE1	23:W:32:SER:O	2.31	0.64
26:Z:602:VAL:HG22	26:Z:643:LEU:CD2	2.28	0.64
1:A:823:VAL:HG22	1:A:835:GLU:HB2	1.78	0.64
2:B:155:MET:O	2:B:158:SER:OG	2.11	0.64
17:Q:620:ARG:NH2	17:Q:629:GLN:OE1	2.31	0.64
17:Q:774:SER:O	17:Q:830:ARG:NH1	2.30	0.64
26:Z:604:ASP:OD1	26:Z:605:GLY:N	2.31	0.64
1:A:936:GLU:N	1:A:936:GLU:OE1	2.31	0.64
2:B:381:GLU:OE1	2:B:381:GLU:N	2.28	0.64
11:K:93:ASP:OD1	11:K:94:LEU:N	2.31	0.64
20:T:-79:DG:H2''	20:T:-78:DC:H6	1.63	0.64
3:C:59:LEU:HD12	3:C:151:VAL:HG12	1.79	0.64
14:N:-1:DC:H2''	14:N:0:DG:C8	2.33	0.64
14:N:28:DG:H1'	14:N:29:DG:C8	2.32	0.64
21:U:372:ASP:OD1	21:U:373:LEU:N	2.30	0.64
1:A:910:LYS:NZ	19:S:264:GLY:O	2.31	0.63
2:B:891:ASP:OD1	2:B:893:SER:OG	2.09	0.63
17:Q:682:ASP:O	17:Q:686:ASN:ND2	2.32	0.63
14:N:-52:DG:H2''	14:N:-51:DG:C8	2.33	0.63
15:O:555:ASP:O	15:O:559:VAL:HG23	1.99	0.63
17:Q:276:ALA:HB1	17:Q:288:VAL:CG2	2.19	0.63
2:B:228:SER:O	2:B:405:ARG:NH1	2.31	0.63
2:B:727:ALA:O	2:B:731:GLN:NE2	2.31	0.63
17:Q:237:GLY:HA2	22:V:74:LEU:HD21	1.80	0.63
20:T:-82:DG:C8	20:T:-81:DT:H72	2.34	0.63
20:T:-10:DC:H2''	20:T:-9:DG:H8	1.63	0.63
1:A:353:ASN:ND2	2:B:1073:GLN:OE1	2.32	0.63
1:A:687:ILE:HD11	1:A:766:PHE:CZ	2.33	0.63
10:J:10:CYS:SG	10:J:42:ARG:NH2	2.72	0.63
20:T:0:DC:H2''	20:T:1:DG:C8	2.34	0.63
27:e:106:ASP:OD2	27:e:131:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:80:MET:N	6:F:96:GLU:OE2	2.29	0.63
17:Q:856:LEU:HD23	17:Q:857:LEU:HD22	1.80	0.63
2:B:347:MET:O	2:B:361:LYS:NZ	2.30	0.62
13:M:1440:ARG:NH1	13:M:1486:TYR:OH	2.31	0.62
1:A:459:ASN:OD1	1:A:460:ARG:N	2.32	0.62
14:N:14:DT:H2'	14:N:15:DT:H72	1.80	0.62
14:N:46:DC:H2''	14:N:47:DA:H8	1.63	0.62
1:A:865:ILE:HG21	2:B:1092:ASP:OD2	1.99	0.62
2:B:998:ASP:OD1	2:B:999:ALA:N	2.32	0.62
2:B:42:GLN:N	2:B:42:GLN:OE1	2.31	0.62
2:B:384:ASP:OD1	2:B:385:ARG:N	2.32	0.62
1:A:1179:PRO:O	9:I:33:ARG:NH2	2.32	0.62
14:N:2:DT:H2''	14:N:3:DG:C8	2.34	0.62
1:A:668:PHE:CE1	1:A:672:ILE:HD11	2.35	0.62
1:A:566:PHE:HB3	1:A:674:THR:HG22	1.80	0.62
14:N:-45:DC:H2''	14:N:-44:DA:C8	2.34	0.62
1:A:1208:SER:O	1:A:1260:ARG:NH1	2.32	0.62
9:I:67:GLN:N	9:I:67:GLN:OE1	2.33	0.62
26:Z:598:ASP:OD1	26:Z:599:ILE:N	2.32	0.62
2:B:30:ILE:HD11	2:B:698:ILE:HG21	1.80	0.61
17:Q:384:LEU:CD1	17:Q:397:ALA:HB2	2.31	0.61
17:Q:41:LEU:HD23	17:Q:81:ASP:HB3	1.81	0.61
1:A:576:GLN:O	1:A:590:GLN:NE2	2.33	0.61
14:N:62:DA:N9	14:N:63:DT:H72	2.15	0.61
25:Y:47:GLU:N	25:Y:47:GLU:OE1	2.32	0.61
2:B:20:ASP:N	2:B:680:ASP:OD2	2.27	0.61
8:H:72:ASP:OD1	8:H:73:GLY:N	2.32	0.61
14:N:26:DG:O3'	14:N:27:DG:H8	1.83	0.61
14:N:64:DA:C2'	14:N:65:DT:H72	2.29	0.61
17:Q:285:TYR:HA	17:Q:288:VAL:HG12	1.82	0.61
23:W:53:ARG:NH1	23:W:54:LEU:O	2.34	0.61
23:W:64:GLN:OE1	23:W:89:ARG:NH2	2.34	0.61
23:W:272:ASP:O	23:W:274:GLN:NE2	2.34	0.61
3:C:190:ASN:ND2	3:C:195:THR:O	2.34	0.60
26:Z:462:GLU:N	26:Z:462:GLU:OE1	2.34	0.60
14:N:38:DC:H2'	14:N:39:DT:H71	1.82	0.60
1:A:231:GLU:OE1	1:A:231:GLU:N	2.33	0.60
17:Q:406:GLU:N	17:Q:406:GLU:OE1	2.34	0.60
25:Y:26:ASP:OD1	25:Y:27:GLN:N	2.34	0.60
27:a:106:ASP:OD2	27:a:131:ARG:NH2	2.25	0.60
31:l:1680:CYS:SG	31:l:1681:GLY:N	2.74	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:ILE:CD1	3:C:151:VAL:HG11	2.32	0.60
14:N:-19:DC:H2''	14:N:-18:DG:C8	2.36	0.60
14:N:7:DC:H1'	14:N:8:DC:C6	2.36	0.60
20:T:-26:DC:H2''	20:T:-25:DT:H73	1.83	0.60
14:N:60:DA:C8	14:N:61:DT:H72	2.36	0.60
14:N:28:DG:H1'	14:N:29:DG:N7	2.16	0.60
17:Q:769:LEU:HD13	17:Q:824:ALA:HB2	1.84	0.60
1:A:1005:HIS:ND1	1:A:1007:ILE:HG22	2.17	0.60
2:B:388:TYR:CE1	2:B:505:LEU:HD21	2.37	0.60
2:B:867:ILE:HG22	2:B:894:THR:HG22	1.82	0.60
2:B:988:LYS:O	2:B:992:ASN:ND2	2.34	0.60
2:B:1040:GLN:NE2	3:C:195:THR:OG1	2.35	0.60
17:Q:743:ALA:O	17:Q:746:VAL:HG22	2.01	0.60
5:E:84:ILE:HD12	14:N:120:DT:H5''	1.84	0.59
11:K:84:GLN:N	11:K:84:GLN:OE1	2.35	0.59
26:Z:613:GLU:N	26:Z:625:HIS:O	2.34	0.59
1:A:627:LYS:O	1:A:629:VAL:HG23	2.02	0.59
14:N:66:DA:H2''	14:N:67:DC:C6	2.37	0.59
16:P:16:A:H1'	16:P:17:A:P	2.42	0.59
21:U:458:ASP:OD1	21:U:459:VAL:N	2.36	0.59
17:Q:776:LEU:HD22	17:Q:831:ALA:HA	1.82	0.59
1:A:454:ASP:O	1:A:474:VAL:HG23	2.02	0.59
1:A:764:ASN:OD1	1:A:765:ASN:N	2.36	0.59
18:R:554:THR:O	18:R:558:SER:OG	2.21	0.59
20:T:9:DG:H2''	20:T:10:DC:C5'	2.30	0.59
4:D:107:THR:HG23	4:D:110:GLU:H	1.67	0.59
2:B:388:TYR:CZ	2:B:505:LEU:HD21	2.37	0.59
2:B:959:GLU:N	2:B:959:GLU:OE1	2.35	0.59
20:T:37:DG:H2''	20:T:38:DA:H8	1.67	0.59
1:A:1280:ASP:OD1	1:A:1281:ASP:N	2.36	0.59
1:A:120:ASP:O	1:A:122:ASN:N	2.36	0.59
2:B:281:ASP:OD1	2:B:285:LEU:HD13	2.02	0.59
14:N:-41:DT:H2''	14:N:-40:DG:C8	2.37	0.59
1:A:280:LEU:O	1:A:284:VAL:HG23	2.03	0.58
7:G:116:GLU:N	7:G:116:GLU:OE1	2.36	0.58
16:P:18:A:O2'	16:P:19:A:P	2.61	0.58
20:T:-95:DT:H2'	20:T:-94:DG:H5''	1.85	0.58
23:W:71:ASP:OD1	23:W:72:ILE:N	2.36	0.58
1:A:492:TYR:CD2	1:A:501:MET:HE1	2.38	0.58
3:C:5:ASN:OD1	3:C:5:ASN:N	2.35	0.58
7:G:110:ARG:NH1	7:G:114:PRO:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-45:DC:H4'	14:N:-44:DA:OP1	2.04	0.58
14:N:71:DG:H2''	14:N:72:DA:C8	2.39	0.58
20:T:-84:DT:C2	20:T:-83:DG:N7	2.71	0.58
14:N:-3:DC:H1'	14:N:-2:DG:C8	2.38	0.58
15:O:634:ARG:NH1	15:O:670:GLU:OE2	2.35	0.58
20:T:-76:DG:C2'	20:T:-75:DT:H72	2.33	0.58
20:T:2:DC:H2''	20:T:3:DG:C8	2.38	0.58
20:T:19:DG:H2''	20:T:20:DG:O5'	2.02	0.58
14:N:-43:DA:H2''	14:N:-42:DT:H71	1.85	0.58
14:N:46:DC:H5''	14:N:46:DC:H6	1.68	0.58
18:R:449:GLU:N	18:R:449:GLU:OE1	2.35	0.58
20:T:-81:DT:C2	20:T:-80:DG:C8	2.91	0.58
20:T:7:DG:H2'	20:T:8:DT:C7	2.33	0.58
20:T:-103:DG:H2'	20:T:-102:DA:O4'	2.02	0.58
26:Z:486:GLU:OE2	26:Z:555:ARG:NH2	2.36	0.58
17:Q:201:ARG:HH12	17:Q:227:LEU:HD13	1.68	0.58
14:N:92:DG:H1'	14:N:93:DT:H5'	1.85	0.58
20:T:15:DA:H1'	20:T:16:DA:C8	2.37	0.58
14:N:-6:DG:H2''	14:N:-5:DT:C7	2.33	0.58
1:A:888:GLN:NE2	1:A:1403:ASP:OD2	2.37	0.58
14:N:31:DT:N1	14:N:32:DT:H72	2.19	0.58
14:N:49:DG:H2''	14:N:50:DC:C5	2.39	0.57
17:Q:86:LEU:HG	17:Q:120:ALA:HB2	1.85	0.57
23:W:95:ASN:O	23:W:97:LYS:NZ	2.35	0.57
23:W:176:ASP:O	23:W:180:GLY:N	2.35	0.57
26:Z:437:GLN:OE1	26:Z:437:GLN:N	2.37	0.57
31:I:1578:GLU:O	31:I:1622:ASN:ND2	2.37	0.57
1:A:479:TRP:HB2	2:B:931:ILE:HD11	1.85	0.57
20:T:-110:DA:H2''	20:T:-109:DA:O5'	2.03	0.57
26:Z:613:GLU:O	26:Z:625:HIS:N	2.37	0.57
2:B:595:ASP:C	2:B:596:ILE:HD12	2.29	0.57
5:E:39:GLU:OE1	5:E:39:GLU:N	2.29	0.57
7:G:151:ARG:NE	7:G:153:ASP:OD1	2.37	0.57
14:N:21:DG:H2''	14:N:22:DC:C6	2.40	0.57
8:H:40:ILE:HG22	8:H:40:ILE:O	2.03	0.57
14:N:75:DA:H2''	14:N:76:DC:C6	2.40	0.57
17:Q:95:GLN:NE2	22:V:84:ILE:O	2.37	0.57
20:T:-24:DT:C2	20:T:-23:DG:C8	2.93	0.57
25:Y:49:VAL:O	25:Y:53:THR:OG1	2.16	0.57
2:B:835:GLU:N	2:B:835:GLU:OE1	2.37	0.57
4:D:70:ARG:NH1	7:G:88:VAL:HG21	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:44:CYS:O	10:J:47:ARG:NH1	2.37	0.57
18:R:402:VAL:O	18:R:430:HIS:ND1	2.38	0.57
26:Z:469:ARG:NH2	26:Z:497:GLU:O	2.38	0.57
2:B:939:HIS:NE2	2:B:983:GLU:OE1	2.37	0.57
17:Q:158:GLN:O	17:Q:159:SER:OG	2.21	0.57
26:Z:466:GLN:OE1	26:Z:466:GLN:N	2.38	0.57
4:D:59:GLU:N	4:D:59:GLU:OE1	2.36	0.56
14:N:38:DC:H2''	14:N:39:DT:C6	2.39	0.56
1:A:1468:THR:O	6:F:64:ARG:NH1	2.38	0.56
2:B:502:HIS:ND1	2:B:504:THR:HG22	2.20	0.56
9:I:19:GLU:N	9:I:19:GLU:OE1	2.38	0.56
14:N:-57:DG:H1'	14:N:-56:DC:C6	2.40	0.56
17:Q:167:LEU:HD21	17:Q:189:ALA:HB2	1.86	0.56
25:Y:112:ASP:OD2	25:Y:116:LYS:NZ	2.37	0.56
1:A:1302:GLU:O	1:A:1304:ILE:N	2.37	0.56
3:C:58:VAL:HG11	10:J:59:LEU:HB3	1.87	0.56
8:H:112:LEU:HB2	8:H:132:LEU:HD12	1.87	0.56
2:B:1142:ASN:ND2	2:B:1145:GLN:O	2.38	0.56
1:A:913:ASN:ND2	1:A:1325:ASP:O	2.38	0.56
2:B:1028:LEU:HD12	2:B:1041:ILE:HG13	1.86	0.56
1:A:1314:THR:OG1	1:A:1316:ASN:OD1	2.21	0.56
2:B:179:LEU:HD22	2:B:768:ARG:HD3	1.87	0.56
14:N:-17:DC:C2'	14:N:-16:DT:H72	2.34	0.56
17:Q:670:PHE:HB3	17:Q:687:LEU:HD21	1.88	0.56
20:T:-54:DA:H2''	20:T:-53:DC:C6	2.41	0.56
26:Z:421:GLN:N	26:Z:421:GLN:OE1	2.39	0.56
1:A:90:LEU:HD21	1:A:92:LYS:O	2.06	0.56
2:B:759:VAL:HG23	2:B:759:VAL:O	2.05	0.56
3:C:109:GLU:OE1	3:C:109:GLU:N	2.33	0.56
20:T:-94:DG:H4'	20:T:-93:DA:OP2	2.04	0.56
20:T:-25:DT:H2''	20:T:-24:DT:C6	2.40	0.56
1:A:321:GLU:C	1:A:322:LEU:HD22	2.30	0.56
3:C:83:GLN:N	3:C:83:GLN:OE1	2.39	0.56
12:L:38:GLU:OE1	12:L:38:GLU:N	2.39	0.56
14:N:-35:DT:O3'	14:N:-34:DA:C8	2.59	0.56
26:Z:426:VAL:HG13	26:Z:440:ILE:HD11	1.87	0.56
1:A:59:ASP:OD1	1:A:61:ARG:N	2.39	0.56
1:A:663:ASP:OD1	1:A:664:ILE:N	2.39	0.56
2:B:1090:GLU:OE1	2:B:1090:GLU:N	2.37	0.56
3:C:161:LEU:HD12	3:C:161:LEU:C	2.31	0.56
11:K:24:ASP:OD1	11:K:25:THR:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-62:DC:H2''	14:N:-61:DC:C6	2.40	0.56
20:T:-50:DG:H2''	20:T:-49:DC:C6	2.41	0.56
1:A:524:MET:HA	1:A:524:MET:HE2	1.88	0.55
9:I:103:ARG:NH2	9:I:105:GLU:OE2	2.39	0.55
15:O:657:ILE:O	15:O:661:VAL:HG23	2.05	0.55
4:D:59:GLU:OE2	4:D:60:VAL:HG23	2.06	0.55
8:H:27:ARG:C	8:H:28:LEU:HD22	2.31	0.55
14:N:110:DT:H2''	14:N:111:DT:H5'	1.89	0.55
16:P:24:C:H2'	16:P:25:U:C6	2.41	0.55
20:T:-25:DT:C6	20:T:-24:DT:H72	2.42	0.55
1:A:427:ILE:N	1:A:427:ILE:HD12	2.21	0.55
13:M:1516:GLN:N	13:M:1516:GLN:OE1	2.39	0.55
20:T:-22:DG:H2''	20:T:-21:DC:C6	2.42	0.55
1:A:67:ARG:O	1:A:68:THR:OG1	2.18	0.55
2:B:937:SER:OG	2:B:938:ARG:N	2.40	0.55
23:W:128:GLY:O	23:W:151:ILE:HD11	2.06	0.55
1:A:197:GLU:N	1:A:197:GLU:OE1	2.39	0.55
1:A:614:ASP:OD1	1:A:615:SER:N	2.40	0.55
2:B:268:PRO:HG2	2:B:271:ILE:HD12	1.89	0.55
14:N:-33:DG:O3'	14:N:-32:DA:H8	1.90	0.55
14:N:2:DT:H2''	14:N:3:DG:H8	1.69	0.55
20:T:-3:DC:H2''	20:T:-2:DA:C8	2.41	0.55
25:Y:18:LEU:O	25:Y:111:ARG:NE	2.39	0.55
25:Y:56:SER:OG	25:Y:90:THR:OG1	2.23	0.55
14:N:41:DG:N9	14:N:42:DT:H72	2.21	0.55
14:N:115:DG:C8	14:N:116:DT:H72	2.42	0.55
3:C:149:LEU:HD21	3:C:152:LYS:NZ	2.22	0.55
26:Z:550:ILE:HD13	26:Z:558:PHE:HB3	1.88	0.55
17:Q:94:VAL:HG21	17:Q:136:CYS:SG	2.47	0.55
1:A:1212:LEU:N	1:A:1212:LEU:HD12	2.23	0.54
2:B:227:ASN:ND2	2:B:227:ASN:O	2.40	0.54
14:N:-5:DT:H1'	14:N:-4:DA:C8	2.42	0.54
17:Q:423:GLU:OE2	24:X:229:ARG:NH2	2.41	0.54
2:B:1085:ARG:NE	20:T:-102:DA:OP1	2.37	0.54
18:R:366:ARG:NH2	26:Z:775:TPO:O2P	2.40	0.54
25:Y:81:LYS:O	25:Y:85:TYR:OH	2.16	0.54
1:A:1262:MET:SD	1:A:1262:MET:N	2.80	0.54
26:Z:504:SER:OG	26:Z:507:THR:O	2.20	0.54
2:B:155:MET:HE2	2:B:183:GLY:HA2	1.88	0.54
13:M:1410:GLU:N	13:M:1410:GLU:OE1	2.40	0.54
14:N:-68:DA:H2''	14:N:-67:DG:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:51:DA:H2''	14:N:52:DC:C6	2.43	0.54
22:V:127:VAL:HG23	22:V:128:VAL:H	1.72	0.54
1:A:827:TYR:HH	1:A:839:HIS:HE2	1.50	0.54
1:A:983:LEU:HD12	1:A:1044:HIS:CE1	2.43	0.54
21:U:445:ASP:OD2	22:V:199:VAL:HG21	2.07	0.54
2:B:775:GLY:N	2:B:1047:TYR:OH	2.40	0.54
20:T:58:DA:H2''	20:T:59:DC:H6	1.72	0.54
26:Z:550:ILE:HD11	26:Z:552:ARG:O	2.06	0.54
26:Z:592:ASN:OD1	26:Z:593:ASN:N	2.40	0.54
5:E:67:ASP:OD1	5:E:69:THR:OG1	2.19	0.54
14:N:-19:DC:H2''	14:N:-18:DG:H8	1.73	0.54
17:Q:341:VAL:HG21	17:Q:367:VAL:HG13	1.90	0.54
20:T:68:DT:H2''	20:T:69:DG:C8	2.43	0.54
1:A:621:ILE:HG23	1:A:621:ILE:O	2.08	0.54
17:Q:423:GLU:OE1	24:X:231:TRP:NE1	2.37	0.54
1:A:724:GLU:OE1	1:A:724:GLU:N	2.41	0.54
7:G:101:ILE:HD12	7:G:101:ILE:N	2.23	0.54
14:N:-46:DT:H2''	14:N:-45:DC:C6	2.43	0.54
18:R:470:ASP:OD1	18:R:471:GLU:N	2.41	0.54
18:R:494:GLU:N	18:R:494:GLU:OE1	2.39	0.53
20:T:37:DG:H2''	20:T:38:DA:C8	2.43	0.53
20:T:51:DC:H2''	20:T:52:DC:O5'	2.07	0.53
1:A:484:LEU:HD21	1:A:496:PHE:CE1	2.43	0.53
26:Z:602:VAL:HG22	26:Z:643:LEU:HD23	1.90	0.53
1:A:1449:ASP:OD1	1:A:1451:MET:N	2.39	0.53
2:B:313:GLU:HG3	2:B:316:VAL:HG12	1.90	0.53
11:K:32:LEU:N	11:K:32:LEU:HD12	2.23	0.53
17:Q:272:LEU:CB	17:Q:295:ALA:HB2	2.38	0.53
1:A:693:ILE:HD13	1:A:828:LEU:HD21	1.90	0.53
2:B:864:ASP:OD1	26:Z:725:LYS:NZ	2.41	0.53
3:C:175:LYS:NZ	12:L:57:ALA:O	2.29	0.53
14:N:81:DA:H2''	14:N:82:DC:C6	2.44	0.53
14:N:89:DT:H2''	14:N:90:DC:C6	2.43	0.53
17:Q:69:ILE:H	17:Q:69:ILE:HD12	1.73	0.53
2:B:265:GLN:N	2:B:265:GLN:OE1	2.42	0.53
14:N:53:DG:H2''	14:N:54:DT:C6	2.44	0.53
1:A:1178:ASP:OD1	1:A:1185:VAL:HG13	2.08	0.53
17:Q:68:ARG:HE	17:Q:89:LEU:HD12	1.74	0.53
17:Q:268:ASN:HB3	17:Q:271:VAL:HG12	1.90	0.53
17:Q:336:ALA:HB1	17:Q:339:SER:OG	2.08	0.53
2:B:474:THR:O	2:B:477:SER:OG	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:-44:DA:C2	20:T:-43:DG:C5	2.97	0.53
20:T:24:DT:O3'	20:T:25:DA:C8	2.62	0.53
1:A:613:GLU:OE2	1:A:622:SER:OG	2.15	0.53
1:A:1372:GLU:OE2	5:E:195:ARG:NH1	2.42	0.53
2:B:814:TYR:OH	2:B:896:LEU:HD12	2.08	0.53
1:A:293:ASN:O	1:A:298:ALA:N	2.42	0.53
7:G:22:LEU:O	7:G:26:VAL:HG23	2.08	0.53
20:T:-72:DT:H2''	20:T:-71:DC:C6	2.44	0.53
17:Q:401:LEU:HD12	17:Q:421:ILE:HD12	1.89	0.53
25:Y:40:LEU:HD23	25:Y:40:LEU:O	2.08	0.53
2:B:898:THR:O	2:B:899:SER:OG	2.23	0.52
3:C:19:VAL:HG23	3:C:241:PRO:CG	2.39	0.52
2:B:484:ARG:C	2:B:485:LEU:HD12	2.34	0.52
5:E:36:THR:OG1	5:E:39:GLU:OE1	2.26	0.52
18:R:410:GLU:OE2	18:R:423:ASN:ND2	2.41	0.52
2:B:139:GLN:OE1	2:B:139:GLN:N	2.42	0.52
8:H:2:ALA:O	8:H:84:ARG:NH2	2.42	0.52
13:M:1101:ASP:O	31:l:2025:ILE:HG22	2.09	0.52
18:R:493:GLU:OE1	18:R:493:GLU:N	2.39	0.52
20:T:-82:DG:H2'	20:T:-81:DT:H72	1.92	0.52
20:T:37:DG:H1'	29:c:42:ARG:NH1	2.24	0.52
1:A:712:ASP:O	1:A:716:VAL:HG23	2.09	0.52
2:B:312:GLN:N	2:B:312:GLN:OE1	2.42	0.52
3:C:91:GLU:N	3:C:91:GLU:OE1	2.42	0.52
20:T:-88:DC:H2''	20:T:-87:DG:H8	1.72	0.52
1:A:484:LEU:N	1:A:484:LEU:HD23	2.24	0.52
7:G:138:GLN:N	7:G:138:GLN:OE1	2.42	0.52
16:P:23:G:H2'	16:P:24:C:C6	2.45	0.52
23:W:248:VAL:HG11	23:W:289:ILE:HD13	1.91	0.52
26:Z:775:TPO:O1P	26:Z:775:TPO:N	2.33	0.52
1:A:66:GLU:N	1:A:66:GLU:OE1	2.40	0.52
1:A:1156:ASP:OD1	1:A:1157:ILE:N	2.43	0.52
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.45	0.52
14:N:-50:DC:H2''	14:N:-49:DC:C6	2.45	0.52
14:N:-26:DC:H1'	14:N:-25:DT:C5	2.45	0.52
17:Q:373:ASN:ND2	22:V:66:LEU:HD12	2.24	0.52
26:Z:554:GLU:OE1	26:Z:557:THR:OG1	2.28	0.52
31:l:1669:GLN:H	31:l:1690:GLY:HA2	1.75	0.52
20:T:28:DG:H2''	20:T:29:DC:H6	1.75	0.52
23:W:237:ASN:OD1	23:W:238:VAL:N	2.42	0.52
2:B:388:TYR:H	2:B:504:THR:HG21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:GLU:N	2:B:609:GLU:OE1	2.43	0.52
2:B:867:ILE:CG2	2:B:894:THR:HG22	2.40	0.52
7:G:101:ILE:N	7:G:104:MET:O	2.42	0.52
14:N:49:DG:H2''	14:N:50:DC:C6	2.45	0.52
17:Q:313:ALA:HB2	17:Q:328:TYR:CB	2.40	0.52
20:T:-33:DT:H2''	20:T:-32:DA:C8	2.44	0.52
14:N:-35:DT:H4'	14:N:-34:DA:OP1	2.10	0.52
14:N:14:DT:C6	14:N:15:DT:H72	2.45	0.52
14:N:32:DT:H2''	14:N:33:DA:H8	1.73	0.52
14:N:64:DA:C2'	14:N:65:DT:C7	2.88	0.52
14:N:119:DT:C6	14:N:120:DT:H72	2.45	0.52
26:Z:184:CYS:SG	26:Z:185:LYS:N	2.83	0.52
1:A:61:ARG:O	1:A:73:THR:OG1	2.28	0.51
14:N:14:DT:C2'	14:N:15:DT:H72	2.40	0.51
14:N:48:DG:C2	14:N:49:DG:C5	2.98	0.51
23:W:14:ALA:N	23:W:296:GLN:O	2.40	0.51
31:l:1669:GLN:HE21	31:l:1700:ALA:HA	1.72	0.51
1:A:1318:LYS:NZ	19:S:292:ASN:O	2.43	0.51
14:N:53:DG:C2'	14:N:54:DT:H72	2.39	0.51
17:Q:272:LEU:HB2	17:Q:295:ALA:HB2	1.92	0.51
20:T:-25:DT:H2''	20:T:-24:DT:H6	1.76	0.51
6:F:90:LEU:HD23	6:F:90:LEU:O	2.11	0.51
9:I:14:ILE:HG23	9:I:23:MET:SD	2.50	0.51
14:N:-62:DC:C2	20:T:63:DG:N2	2.79	0.51
14:N:35:DT:H2''	14:N:36:DC:C6	2.45	0.51
17:Q:386:ALA:HB2	17:Q:393:LYS:CB	2.40	0.51
20:T:7:DG:H2'	20:T:8:DT:H6	1.69	0.51
3:C:7:PRO:O	11:K:104:ARG:NH1	2.43	0.51
14:N:26:DG:H1'	14:N:27:DG:N7	2.24	0.51
14:N:47:DA:H2''	14:N:48:DG:H8	1.74	0.51
20:T:-76:DG:H2'	20:T:-75:DT:C7	2.36	0.51
20:T:28:DG:H2''	20:T:29:DC:C6	2.45	0.51
26:Z:481:ILE:N	26:Z:481:ILE:HD12	2.26	0.51
3:C:86:ARG:NH1	26:Z:716:PRO:O	2.43	0.51
23:W:27:ASN:ND2	23:W:74:HIS:O	2.44	0.51
1:A:1467:GLY:O	1:A:1468:THR:OG1	2.27	0.51
1:A:1525:TPO:O	1:A:1525:TPO:O3P	2.29	0.51
2:B:544:PHE:O	2:B:547:GLU:HG3	2.11	0.51
14:N:-64:DT:H2''	14:N:-63:DC:C6	2.44	0.51
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.83	0.51
4:D:31:THR:HG22	7:G:3:TYR:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-42:DT:C2	14:N:-41:DT:C5	2.99	0.51
14:N:64:DA:H2''	14:N:65:DT:C7	2.40	0.51
17:Q:386:ALA:HB2	17:Q:393:LYS:HB3	1.92	0.51
17:Q:668:ASP:OD1	17:Q:669:VAL:N	2.44	0.51
31:l:1670:ARG:NH1	31:l:1674:GLU:O	2.44	0.51
17:Q:753:LEU:O	17:Q:757:VAL:HG13	2.11	0.51
17:Q:856:LEU:CD2	17:Q:857:LEU:HD22	2.41	0.51
2:B:650:ASN:H	21:U:460:TYR:HH	1.58	0.51
20:T:-80:DG:C2	20:T:-79:DG:C5	2.99	0.51
13:M:1350:MET:HE2	13:M:1350:MET:HA	1.92	0.50
16:P:19:A:O2'	16:P:20:U:H5'	2.10	0.50
2:B:581:GLU:OE1	2:B:581:GLU:N	2.33	0.50
3:C:49:TRP:NE1	26:Z:719:GLY:O	2.44	0.50
20:T:38:DA:H2''	20:T:39:DC:H6	1.77	0.50
26:Z:500:VAL:HG23	26:Z:500:VAL:O	2.10	0.50
1:A:902:GLU:OE1	1:A:902:GLU:N	2.44	0.50
2:B:395:LEU:HD21	2:B:532:ILE:HD13	1.93	0.50
18:R:404:GLU:N	18:R:404:GLU:OE1	2.44	0.50
20:T:-74:DT:H2''	20:T:-73:DA:C8	2.45	0.50
22:V:84:ILE:O	22:V:84:ILE:HG23	2.12	0.50
1:A:693:ILE:HG22	1:A:694:ALA:O	2.11	0.50
14:N:42:DT:H2''	14:N:43:DC:C5	2.45	0.50
14:N:42:DT:H2''	14:N:43:DC:H6	1.67	0.50
17:Q:486:GLU:OE2	17:Q:487:HIS:NE2	2.45	0.50
17:Q:679:ASP:O	17:Q:680:ILE:HD13	2.10	0.50
21:U:392:GLN:OE1	21:U:392:GLN:N	2.44	0.50
26:Z:588:ASP:OD1	26:Z:592:ASN:N	2.40	0.50
2:B:756:LYS:O	10:J:51:ALA:HB1	2.11	0.50
14:N:-31:DC:H2''	14:N:-30:DA:H8	1.76	0.50
20:T:51:DC:H4'	20:T:52:DC:OP1	2.12	0.50
14:N:-50:DC:H2''	14:N:-49:DC:H6	1.76	0.50
14:N:71:DG:H2''	14:N:72:DA:H8	1.76	0.50
16:P:16:A:C1'	16:P:17:A:P	2.98	0.50
17:Q:189:ALA:HB1	17:Q:200:VAL:HG12	1.93	0.50
1:A:827:TYR:OH	1:A:839:HIS:NE2	2.40	0.50
4:D:62:MET:O	4:D:66:ASN:ND2	2.44	0.50
5:E:52:ARG:O	5:E:54:ARG:N	2.44	0.50
14:N:37:DC:H2''	14:N:38:DC:H5	1.77	0.50
14:N:39:DT:O3'	14:N:40:DA:H8	1.95	0.50
14:N:76:DC:C2	14:N:77:DG:N7	2.80	0.50
20:T:61:DG:H2''	20:T:62:DG:C8	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:88:ASN:O	22:V:90:ASP:N	2.45	0.50
23:W:160:GLY:C	23:W:177:ILE:HD11	2.36	0.50
26:Z:189:GLU:N	26:Z:189:GLU:OE1	2.44	0.50
26:Z:746:ASP:OD1	26:Z:747:ARG:N	2.44	0.50
1:A:103:THR:HG22	1:A:248:MET:HE3	1.93	0.50
1:A:488:VAL:O	1:A:488:VAL:HG12	2.11	0.50
6:F:61:GLU:O	6:F:65:VAL:HG23	2.12	0.50
14:N:44:DT:H2''	14:N:45:DC:C6	2.47	0.50
14:N:-56:DC:H4'	14:N:-55:DC:OP1	2.11	0.49
17:Q:386:ALA:HB1	17:Q:394:ARG:CG	2.41	0.49
2:B:85:LEU:HD12	2:B:85:LEU:N	2.27	0.49
17:Q:737:LYS:HZ1	17:Q:764:LEU:HD13	1.77	0.49
20:T:9:DG:OP1	31:I:1639:LYS:NZ	2.42	0.49
22:V:127:VAL:HG23	22:V:128:VAL:N	2.27	0.49
26:Z:341:ASP:OD1	26:Z:342:ALA:N	2.44	0.49
1:A:1210:TRP:CD1	1:A:1285:LEU:HD11	2.47	0.49
14:N:69:DT:C2	14:N:70:DC:C5	3.01	0.49
26:Z:290:ILE:N	26:Z:290:ILE:HD12	2.26	0.49
2:B:633:LEU:HD12	2:B:633:LEU:N	2.28	0.49
2:B:783:ALA:HB2	2:B:1041:ILE:HG23	1.94	0.49
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.38	0.49
14:N:-36:DG:H2'	14:N:-35:DT:H71	1.94	0.49
14:N:61:DT:C2	14:N:62:DA:C8	3.00	0.49
14:N:62:DA:C2'	14:N:63:DT:C7	2.90	0.49
16:P:18:A:O2'	16:P:19:A:OP1	2.30	0.49
17:Q:524:LEU:HD11	17:Q:537:LEU:HD12	1.94	0.49
1:A:1140:THR:HG22	1:A:1337:GLU:OE1	2.13	0.49
14:N:39:DT:H2''	14:N:40:DA:N7	2.28	0.49
14:N:43:DC:H2'	14:N:44:DT:H71	1.94	0.49
14:N:56:DT:H2''	14:N:57:DC:C6	2.47	0.49
17:Q:189:ALA:HB1	17:Q:200:VAL:CG1	2.42	0.49
17:Q:643:ASP:OD2	24:X:239:GLN:NE2	2.45	0.49
20:T:14:DT:H2''	20:T:15:DA:O5'	2.12	0.49
1:A:464:LEU:O	1:A:861:GLN:NE2	2.46	0.49
17:Q:48:ALA:HB2	17:Q:63:LEU:HD11	1.94	0.49
17:Q:493:ASN:O	17:Q:497:VAL:HG23	2.11	0.49
20:T:-22:DG:H2''	20:T:-21:DC:H6	1.77	0.49
2:B:252:ILE:HD12	2:B:252:ILE:N	2.28	0.49
14:N:-24:DA:H2''	14:N:-23:DG:H8	1.78	0.49
14:N:92:DG:H2''	14:N:93:DT:O5'	2.11	0.49
17:Q:386:ALA:HB1	17:Q:394:ARG:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:56:SER:HG	25:Y:90:THR:HG1	1.61	0.49
4:D:115:ILE:N	4:D:115:ILE:HD12	2.28	0.49
5:E:57:ASP:N	5:E:57:ASP:OD1	2.45	0.49
17:Q:237:GLY:CA	22:V:74:LEU:HD21	2.41	0.49
20:T:-109:DA:H2''	20:T:-108:DC:H5'	1.93	0.49
23:W:176:ASP:OD2	23:W:179:THR:HG22	2.12	0.49
31:l:1670:ARG:HH12	31:l:1675:ALA:HB2	1.77	0.49
14:N:31:DT:C2	14:N:32:DT:C5	3.01	0.49
20:T:-33:DT:H6	20:T:-33:DT:H5'	1.78	0.49
2:B:89:GLU:OE1	2:B:89:GLU:N	2.46	0.49
3:C:47:ILE:HD13	3:C:165:ALA:HB2	1.95	0.49
11:K:100:LEU:HD21	11:K:104:ARG:NE	2.28	0.49
14:N:-23:DG:H2''	14:N:-22:DC:H6	1.77	0.49
17:Q:377:THR:O	17:Q:400:HIS:ND1	2.46	0.49
17:Q:852:LEU:HD12	17:Q:852:LEU:C	2.38	0.49
31:l:1593:VAL:HG11	31:l:1671:TYR:OH	2.13	0.49
14:N:35:DT:H2''	14:N:36:DC:C5	2.48	0.48
20:T:8:DT:H5'	27:a:43:PRO:HA	1.93	0.48
23:W:195:SER:OG	23:W:236:LEU:O	2.25	0.48
1:A:392:GLU:OE2	1:A:401:ARG:NH2	2.46	0.48
1:A:896:LEU:HD13	1:A:980:PRO:HG3	1.95	0.48
2:B:567:ILE:N	2:B:567:ILE:HD12	2.28	0.48
15:O:613:MET:HE1	15:O:641:LEU:HD22	1.94	0.48
17:Q:24:LEU:HD11	17:Q:56:LYS:NZ	2.28	0.48
1:A:479:TRP:CB	2:B:931:ILE:HD11	2.42	0.48
2:B:986:GLN:NE2	2:B:998:ASP:O	2.45	0.48
8:H:116:VAL:HG11	8:H:123:MET:HE3	1.94	0.48
8:H:136:GLU:O	8:H:139:SER:OG	2.30	0.48
14:N:-9:DC:H2''	14:N:-8:DA:H8	1.77	0.48
14:N:-5:DT:O3'	14:N:-4:DA:C8	2.66	0.48
14:N:38:DC:H2'	14:N:38:DC:O5'	2.13	0.48
20:T:10:DC:H2''	20:T:11:DG:OP2	2.12	0.48
22:V:94:ILE:HG22	22:V:94:ILE:O	2.14	0.48
25:Y:75:GLN:NE2	25:Y:86:ALA:O	2.45	0.48
1:A:102:LYS:O	1:A:106:VAL:HG23	2.13	0.48
4:D:80:ILE:O	4:D:83:VAL:HG22	2.14	0.48
9:I:86:CYS:SG	9:I:87:GLN:N	2.86	0.48
13:M:1377:ILE:N	13:M:1377:ILE:HD12	2.28	0.48
14:N:-57:DG:H1'	14:N:-56:DC:C5	2.48	0.48
14:N:44:DT:H2''	14:N:45:DC:H6	1.78	0.48
26:Z:448:ILE:O	26:Z:449:THR:OG1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:l:2021:GLU:O	31:l:2023:TYR:N	2.47	0.48
1:A:668:PHE:CZ	1:A:672:ILE:HD11	2.48	0.48
1:A:1547:SEP:O2P	13:M:1512:LYS:NZ	2.45	0.48
14:N:-69:DC:H1'	14:N:-68:DA:C8	2.47	0.48
14:N:75:DA:H2''	14:N:76:DC:H6	1.77	0.48
20:T:-107:DA:C2'	20:T:-106:DC:C6	2.96	0.48
1:A:36:VAL:HG12	1:A:85:PHE:O	2.13	0.48
3:C:11:ILE:N	3:C:11:ILE:HD12	2.29	0.48
5:E:20:LEU:C	5:E:20:LEU:HD23	2.39	0.48
6:F:69:ARG:NE	6:F:96:GLU:OE1	2.44	0.48
7:G:58:VAL:HB	7:G:67:LEU:HD21	1.96	0.48
2:B:1062:ARG:NH1	2:B:1081:ASP:O	2.47	0.48
9:I:17:CYS:SG	9:I:18:GLN:N	2.87	0.48
10:J:8:PHE:H	10:J:48:MET:HE3	1.77	0.48
14:N:43:DC:C6	14:N:44:DT:C7	2.96	0.48
20:T:-26:DC:H1'	20:T:-25:DT:C6	2.48	0.48
20:T:4:DT:H4'	20:T:5:DA:OP1	2.13	0.48
28:b:89:ALA:O	28:b:93:GLN:NE2	2.47	0.48
12:L:25:GLU:O	12:L:26:ASN:ND2	2.47	0.48
14:N:-23:DG:H2''	14:N:-22:DC:C6	2.49	0.48
14:N:-14:DA:H1'	14:N:-13:DA:H5'	1.95	0.48
14:N:21:DG:H2''	14:N:22:DC:H6	1.78	0.48
16:P:16:A:C1'	16:P:17:A:OP2	2.60	0.48
23:W:130:VAL:HG22	23:W:151:ILE:HG13	1.96	0.48
23:W:250:SER:OG	23:W:277:VAL:HG23	2.14	0.48
1:A:99:PHE:O	1:A:103:THR:HG23	2.13	0.48
3:C:23:ILE:HD12	3:C:231:TYR:CE2	2.49	0.48
8:H:32:SER:HB3	8:H:37:MET:H	1.78	0.48
8:H:58:LEU:HD23	8:H:59:VAL:N	2.28	0.48
11:K:36:ASN:OD1	11:K:70:LYS:NZ	2.47	0.48
14:N:-33:DG:C1'	14:N:-32:DA:N7	2.75	0.48
14:N:39:DT:H1'	14:N:40:DA:C8	2.48	0.48
17:Q:182:ALA:O	17:Q:186:TYR:CD2	2.66	0.48
23:W:169:ASP:N	23:W:169:ASP:OD1	2.42	0.48
17:Q:83:MET:HE3	17:Q:124:ILE:HB	1.95	0.48
17:Q:110:ILE:CD1	17:Q:140:LEU:HD13	2.44	0.48
25:Y:52:CYS:SG	25:Y:53:THR:N	2.87	0.48
2:B:581:GLU:O	2:B:585:ASN:ND2	2.47	0.47
5:E:71:GLN:OE1	5:E:71:GLN:N	2.47	0.47
12:L:19:CYS:SG	12:L:20:GLY:N	2.87	0.47
14:N:111:DT:H2''	14:N:112:DG:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:117:DG:H2'	14:N:118:DT:H71	1.96	0.47
20:T:57:DC:C2'	20:T:58:DA:C8	2.91	0.47
1:A:85:PHE:CE1	2:B:1163:MET:HE3	2.50	0.47
4:D:76:ASN:HB3	4:D:79:THR:HG23	1.96	0.47
7:G:101:ILE:HD13	7:G:106:CYS:SG	2.54	0.47
8:H:110:THR:O	8:H:129:ALA:N	2.46	0.47
13:M:1507:LEU:HD23	13:M:1507:LEU:O	2.14	0.47
14:N:-5:DT:O3'	14:N:-4:DA:H8	1.97	0.47
16:P:24:C:H2'	16:P:25:U:H6	1.77	0.47
24:X:233:THR:O	24:X:236:THR:OG1	2.27	0.47
1:A:721:HIS:CG	9:I:110:LEU:HD21	2.49	0.47
17:Q:612:LEU:HD23	17:Q:612:LEU:O	2.13	0.47
17:Q:619:THR:HG22	17:Q:622:ARG:CZ	2.45	0.47
22:V:88:ASN:N	22:V:89:PRO:CD	2.77	0.47
23:W:86:ALA:O	23:W:104:ALA:N	2.47	0.47
31:l:1586:HIS:CD2	31:l:1612:ASP:HB2	2.49	0.47
31:l:1634:ASN:ND2	31:l:1661:GLU:O	2.42	0.47
2:B:414:GLU:HG3	2:B:439:ILE:HD11	1.96	0.47
10:J:7:CYS:HA	10:J:48:MET:HE3	1.96	0.47
14:N:-69:DC:H1'	14:N:-68:DA:N7	2.29	0.47
14:N:59:DG:H2''	14:N:60:DA:H8	1.79	0.47
17:Q:665:GLU:HA	17:Q:668:ASP:OD2	2.14	0.47
20:T:6:DC:H2''	20:T:7:DG:C8	2.50	0.47
27:a:35:VAL:HG21	31:l:1589:PHE:HZ	1.78	0.47
15:O:588:LEU:O	15:O:588:LEU:HD23	2.14	0.47
17:Q:401:LEU:CD1	17:Q:421:ILE:HD12	2.45	0.47
20:T:-69:DA:C2'	20:T:-68:DT:H72	2.44	0.47
23:W:31:ASN:OD1	23:W:32:SER:N	2.48	0.47
26:Z:587:LEU:H	26:Z:587:LEU:HD23	1.79	0.47
1:A:1259:ILE:HD12	1:A:1259:ILE:N	2.28	0.47
2:B:604:ILE:N	2:B:604:ILE:HD12	2.29	0.47
9:I:75:ASP:OD1	9:I:77:THR:HG22	2.14	0.47
15:O:588:LEU:HD23	15:O:588:LEU:C	2.40	0.47
20:T:-101:DG:H2'	20:T:-100:DC:C6	2.50	0.47
23:W:17:ASP:OD1	23:W:18:ALA:N	2.43	0.47
23:W:236:LEU:N	23:W:250:SER:O	2.45	0.47
31:l:1677:LYS:HB2	31:l:1687:GLY:O	2.15	0.47
1:A:147:LEU:HD23	1:A:147:LEU:C	2.40	0.47
1:A:934:LEU:N	1:A:934:LEU:HD12	2.29	0.47
13:M:1425:ASP:OD2	13:M:1504:VAL:HG11	2.15	0.47
14:N:-46:DT:H5''	14:N:-46:DT:C6	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:5:DC:H1'	14:N:6:DC:C5	2.50	0.47
14:N:43:DC:C5	14:N:44:DT:H73	2.49	0.47
14:N:62:DA:H2'	14:N:63:DT:C7	2.44	0.47
17:Q:768:VAL:HG22	17:Q:768:VAL:O	2.14	0.47
18:R:353:VAL:O	18:R:456:LYS:NZ	2.47	0.47
18:R:391:ILE:HD12	18:R:391:ILE:N	2.30	0.47
20:T:-107:DA:H2''	20:T:-106:DC:H6	1.80	0.47
31:l:1589:PHE:O	31:l:1593:VAL:HG12	2.15	0.47
1:A:419:ILE:HG23	1:A:419:ILE:O	2.15	0.47
1:A:912:SER:O	1:A:913:ASN:C	2.58	0.47
14:N:18:DA:C2	14:N:19:DC:C2	3.02	0.47
17:Q:86:LEU:HD23	17:Q:120:ALA:HA	1.97	0.47
23:W:125:THR:CG2	23:W:127:VAL:HG22	2.45	0.47
31:l:1593:VAL:HG21	31:l:1671:TYR:CZ	2.49	0.47
2:B:268:PRO:CG	2:B:271:ILE:HD12	2.45	0.47
2:B:1017:ASP:OD1	2:B:1017:ASP:N	2.46	0.47
14:N:5:DC:H1'	14:N:6:DC:C6	2.50	0.47
20:T:-90:DG:H2''	20:T:-89:DA:C8	2.50	0.47
4:D:87:LEU:O	4:D:87:LEU:HD23	2.15	0.47
9:I:29:ASP:HB2	9:I:36:LEU:HD23	1.97	0.47
1:A:458:PHE:CD2	1:A:501:MET:HE2	2.50	0.46
2:B:1151:MET:HE1	2:B:1171:MET:SD	2.56	0.46
6:F:110:LEU:HD12	6:F:110:LEU:N	2.29	0.46
14:N:64:DA:H2'	14:N:65:DT:H72	1.94	0.46
18:R:553:ARG:CB	18:R:557:ILE:HB	2.45	0.46
20:T:58:DA:C4	20:T:59:DC:C5	3.02	0.46
2:B:626:LEU:N	2:B:626:LEU:HD12	2.30	0.46
2:B:629:GLU:HG2	2:B:634:LEU:HD21	1.97	0.46
14:N:17:DA:O3'	14:N:18:DA:H8	1.97	0.46
14:N:87:DC:H5'	14:N:87:DC:H6	1.81	0.46
18:R:560:ILE:HA	18:R:563:ILE:HG22	1.97	0.46
30:d:51:ASP:O	30:d:52:THR:OG1	2.33	0.46
1:A:222:HIS:ND1	1:A:249:ILE:HD11	2.30	0.46
1:A:1295:ASP:OD1	1:A:1295:ASP:N	2.49	0.46
1:A:1366:PHE:HA	1:A:1374:VAL:CG2	2.44	0.46
3:C:148:ILE:N	3:C:148:ILE:HD12	2.31	0.46
14:N:-6:DG:H2''	14:N:-5:DT:C5	2.50	0.46
14:N:11:DC:H2''	14:N:12:DG:H8	1.80	0.46
17:Q:401:LEU:HA	17:Q:404:VAL:HG22	1.97	0.46
17:Q:538:GLY:O	17:Q:550:ALA:HB2	2.16	0.46
20:T:-118:DA:H2''	20:T:-117:DC:H5'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:395:GLU:N	21:U:395:GLU:OE1	2.49	0.46
21:U:412:LEU:O	21:U:416:VAL:HG12	2.16	0.46
26:Z:192:THR:OG1	26:Z:244:ASN:ND2	2.48	0.46
2:B:497:LYS:N	2:B:498:PRO:CD	2.79	0.46
2:B:646:ARG:C	2:B:648:TYR:H	2.24	0.46
9:I:83:ASP:N	9:I:83:ASP:OD1	2.47	0.46
14:N:-13:DA:H2''	14:N:-12:DA:H8	1.80	0.46
14:N:62:DA:C2'	14:N:63:DT:H72	2.46	0.46
26:Z:178:ASN:OD1	26:Z:179:LEU:N	2.48	0.46
1:A:386:ALA:O	1:A:449:HIS:ND1	2.48	0.46
25:Y:13:LEU:HD23	25:Y:13:LEU:H	1.81	0.46
2:B:30:ILE:CD1	2:B:698:ILE:HG21	2.44	0.46
4:D:92:LEU:N	4:D:92:LEU:HD12	2.30	0.46
20:T:-84:DT:H2''	20:T:-83:DG:H8	1.80	0.46
20:T:33:DC:H2''	20:T:34:DT:C7	2.45	0.46
23:W:160:GLY:CA	23:W:177:ILE:HD11	2.46	0.46
1:A:381:PRO:HB3	1:A:480:SER:HA	1.98	0.46
1:A:1225:LYS:C	1:A:1226:LEU:HD12	2.41	0.46
2:B:615:TYR:HB3	2:B:620:ARG:HD3	1.98	0.46
3:C:118:ARG:NH1	3:C:147:ASP:OD2	2.49	0.46
20:T:19:DG:C4	20:T:20:DG:C8	3.04	0.46
20:T:67:DC:H2''	20:T:68:DT:C6	2.50	0.46
1:A:687:ILE:HD13	2:B:972:ILE:HB	1.97	0.46
3:C:149:LEU:HD21	3:C:152:LYS:HZ2	1.80	0.46
10:J:14:VAL:HG22	10:J:14:VAL:O	2.15	0.46
14:N:78:DG:H2''	14:N:79:DC:C6	2.50	0.46
17:Q:68:ARG:HE	17:Q:86:LEU:HD13	1.80	0.46
17:Q:764:LEU:HD22	17:Q:785:GLU:OE1	2.16	0.46
21:U:459:VAL:HG23	21:U:494:HIS:C	2.41	0.46
1:A:560:VAL:O	1:A:564:LEU:HD23	2.16	0.46
1:A:926:ASN:ND2	1:A:929:ALA:HB2	2.31	0.46
1:A:997:ASN:O	1:A:999:ARG:N	2.45	0.46
2:B:281:ASP:HB3	9:I:22:ASN:HA	1.97	0.46
2:B:529:MET:HG3	2:B:624:PRO:HD2	1.98	0.46
2:B:706:VAL:HG13	2:B:767:LEU:HD11	1.97	0.46
3:C:189:ASP:O	3:C:191:ALA:N	2.46	0.46
9:I:35:LEU:C	9:I:36:LEU:HD22	2.40	0.46
14:N:62:DA:H2'	14:N:63:DT:H72	1.98	0.46
20:T:-75:DT:C5	20:T:-74:DT:H73	2.50	0.46
20:T:34:DT:H4'	20:T:35:DA:OP1	2.16	0.46
1:A:365:THR:HG22	1:A:366:VAL:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:14:DT:C2'	14:N:15:DT:C7	2.94	0.46
14:N:16:DT:H4'	14:N:17:DA:OP1	2.16	0.46
20:T:-76:DG:H2''	20:T:-75:DT:C6	2.51	0.46
1:A:959:MET:HE3	1:A:1050:CYS:SG	2.56	0.45
2:B:431:LEU:HA	2:B:434:ALA:HB3	1.97	0.45
29:c:47:ALA:N	29:c:48:PRO:HD2	2.31	0.45
4:D:44:ARG:NH2	7:G:35:GLU:OE2	2.49	0.45
8:H:58:LEU:HD23	8:H:58:LEU:C	2.40	0.45
14:N:-13:DA:H2''	14:N:-12:DA:C8	2.52	0.45
14:N:38:DC:H2''	14:N:39:DT:C7	2.43	0.45
14:N:63:DT:C2	14:N:64:DA:C8	3.04	0.45
14:N:64:DA:C8	14:N:65:DT:H72	2.50	0.45
17:Q:94:VAL:CG2	17:Q:140:LEU:HD11	2.38	0.45
20:T:39:DC:C2	20:T:40:DC:C5	3.05	0.45
31:l:1476:ILE:HB	31:l:1620:LYS:HB3	1.99	0.45
1:A:1243:LEU:N	1:A:1243:LEU:HD12	2.31	0.45
2:B:433:LEU:HD22	2:B:433:LEU:N	2.30	0.45
2:B:597:ILE:HG23	2:B:601:VAL:HG21	1.98	0.45
16:P:18:A:O2'	16:P:19:A:O5'	2.32	0.45
17:Q:80:LYS:O	17:Q:84:THR:HG23	2.16	0.45
20:T:-91:DT:C2	20:T:-90:DG:N7	2.84	0.45
20:T:45:DG:N2	20:T:46:DA:C2	2.85	0.45
1:A:457:ILE:HG23	1:A:504:HIS:HB2	1.99	0.45
2:B:140:LEU:N	2:B:140:LEU:HD23	2.32	0.45
14:N:-11:DC:H2''	14:N:-10:DG:N7	2.30	0.45
14:N:14:DT:H2'	14:N:15:DT:C7	2.47	0.45
20:T:-95:DT:H3'	20:T:-94:DG:C5'	2.47	0.45
26:Z:424:ASP:HB2	26:Z:440:ILE:HD12	1.97	0.45
26:Z:626:CYS:SG	26:Z:627:LYS:N	2.89	0.45
1:A:484:LEU:HD21	1:A:496:PHE:HE1	1.81	0.45
1:A:485:ASN:OD1	1:A:486:LEU:N	2.50	0.45
1:A:1212:LEU:HD11	1:A:1285:LEU:HD13	1.97	0.45
2:B:867:ILE:O	2:B:893:SER:HB2	2.16	0.45
17:Q:448:ASP:OD1	17:Q:449:VAL:N	2.49	0.45
1:A:392:GLU:OE1	1:A:448:ARG:NE	2.45	0.45
2:B:650:ASN:N	21:U:460:TYR:HH	2.14	0.45
14:N:8:DC:H2''	14:N:9:DC:C6	2.52	0.45
14:N:43:DC:C6	14:N:44:DT:H71	2.52	0.45
18:R:404:GLU:OE2	18:R:455:TRP:NE1	2.49	0.45
18:R:483:LEU:C	18:R:483:LEU:HD23	2.42	0.45
22:V:55:GLN:OE1	22:V:57:ARG:NE	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:182:THR:HA	22:V:185:ASP:OD2	2.16	0.45
31:I:1678:CYS:N	31:I:1687:GLY:O	2.45	0.45
2:B:1041:ILE:HG22	2:B:1042:PHE:N	2.31	0.45
5:E:126:ILE:HD12	5:E:126:ILE:N	2.31	0.45
5:E:131:LEU:O	5:E:134:GLU:N	2.50	0.45
2:B:140:LEU:HD23	2:B:140:LEU:H	1.82	0.45
2:B:910:THR:OG1	2:B:911:LEU:N	2.48	0.45
7:G:60:GLN:NE2	7:G:67:LEU:HD22	2.32	0.45
9:I:110:LEU:N	9:I:110:LEU:HD22	2.31	0.45
17:Q:80:LYS:O	17:Q:83:MET:HG3	2.17	0.45
17:Q:313:ALA:HB2	17:Q:328:TYR:HB2	1.99	0.45
17:Q:835:ASP:OD2	17:Q:839:ARG:NH2	2.50	0.45
1:A:413:TYR:O	1:A:415:GLY:N	2.50	0.45
1:A:503:LEU:C	1:A:503:LEU:HD23	2.41	0.45
1:A:681:LEU:HD23	2:B:785:TYR:O	2.17	0.45
1:A:1366:PHE:HB2	1:A:1374:VAL:HG21	1.99	0.45
2:B:161:CYS:SG	2:B:162:LEU:N	2.90	0.45
7:G:147:ILE:HD12	7:G:147:ILE:N	2.32	0.45
14:N:-42:DT:N1	14:N:-41:DT:H72	2.31	0.45
14:N:-10:DG:C2	14:N:-9:DC:C2	3.05	0.45
14:N:4:DT:H4'	14:N:5:DC:OP1	2.17	0.45
17:Q:249:ASP:O	17:Q:253:ASN:ND2	2.50	0.45
1:A:1227:THR:O	1:A:1230:GLN:HG2	2.17	0.45
2:B:1157:LEU:HD22	2:B:1161:GLU:OE2	2.16	0.45
17:Q:43:ILE:HD12	17:Q:43:ILE:H	1.81	0.45
17:Q:849:LYS:O	17:Q:852:LEU:HG	2.17	0.45
20:T:-83:DG:C2	20:T:-82:DG:C5	3.04	0.45
20:T:55:DG:N2	20:T:56:DG:N2	2.64	0.45
1:A:1322:ILE:N	1:A:1322:ILE:HD12	2.32	0.44
2:B:168:ASP:OD1	2:B:169:ARG:N	2.51	0.44
2:B:756:LYS:N	10:J:51:ALA:O	2.46	0.44
2:B:853:LEU:O	12:L:46:LYS:NZ	2.50	0.44
3:C:56:SER:HG	3:C:158:GLU:H	1.64	0.44
12:L:16:ILE:HD11	12:L:25:GLU:HB3	1.98	0.44
17:Q:858:LYS:HA	17:Q:861:GLU:HG3	1.99	0.44
22:V:97:ASN:ND2	22:V:98:VAL:O	2.50	0.44
1:A:196:LEU:HD12	1:A:196:LEU:N	2.32	0.44
1:A:909:LEU:C	1:A:911:PRO:HD3	2.42	0.44
2:B:207:VAL:HG21	2:B:371:ARG:HG2	1.99	0.44
17:Q:375:TYR:O	17:Q:379:LYS:NZ	2.35	0.44
18:R:505:ALA:N	18:R:506:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:-119:DA:C2	20:T:-118:DA:C6	3.06	0.44
20:T:59:DC:H2''	20:T:60:DC:H6	1.82	0.44
1:A:542:LEU:O	1:A:545:VAL:HG12	2.17	0.44
14:N:-65:DA:H5'	14:N:-65:DA:H8	1.83	0.44
17:Q:401:LEU:HD21	17:Q:417:GLU:HB2	1.99	0.44
17:Q:558:LEU:HD22	17:Q:571:ILE:HG13	2.00	0.44
18:R:577:LYS:HA	18:R:580:VAL:HG22	1.99	0.44
20:T:-91:DT:H6	20:T:-91:DT:H5'	1.83	0.44
1:A:1183:SER:O	1:A:1184:THR:OG1	2.36	0.44
1:A:1366:PHE:HA	1:A:1374:VAL:HG21	2.00	0.44
2:B:166:LEU:HG	2:B:170:ASP:HB2	2.00	0.44
12:L:56:ASP:O	12:L:58:ARG:N	2.50	0.44
14:N:37:DC:H2''	14:N:38:DC:C5	2.52	0.44
17:Q:186:TYR:CE2	17:Q:207:CYS:SG	3.11	0.44
7:G:99:THR:OG1	7:G:100:GLU:N	2.50	0.44
17:Q:190:LEU:O	17:Q:193:ASN:ND2	2.50	0.44
17:Q:326:PHE:HA	17:Q:350:MET:HG2	1.99	0.44
20:T:-91:DT:H5'	20:T:-91:DT:C6	2.53	0.44
1:A:737:PHE:O	1:A:741:VAL:HG23	2.17	0.44
1:A:1395:TYR:CD1	5:E:198:GLU:OE2	2.71	0.44
2:B:82:PRO:HB3	2:B:134:LYS:CB	2.47	0.44
2:B:836:THR:OG1	2:B:889:LYS:NZ	2.40	0.44
2:B:989:VAL:HG12	22:V:131:MET:HE1	1.99	0.44
7:G:108:ILE:N	7:G:108:ILE:HD12	2.33	0.44
9:I:42:CYS:SG	9:I:43:ASP:N	2.91	0.44
14:N:-52:DG:H2''	14:N:-51:DG:H8	1.79	0.44
26:Z:703:ASN:N	26:Z:706:ILE:HD12	2.33	0.44
1:A:136:GLN:OE1	1:A:136:GLN:N	2.51	0.44
14:N:-10:DG:C4	14:N:-9:DC:C5	3.06	0.44
17:Q:511:CYS:O	23:W:229:SER:OG	2.27	0.44
20:T:11:DG:OP1	31:I:1703:LYS:O	2.35	0.44
21:U:441:VAL:HG11	22:V:190:ILE:CD1	2.48	0.44
23:W:206:VAL:HG23	23:W:240:PHE:HZ	1.83	0.44
2:B:759:VAL:HG23	2:B:938:ARG:HH22	1.83	0.44
7:G:30:LEU:O	7:G:34:VAL:HG22	2.17	0.44
7:G:109:SER:CB	26:Z:493:VAL:HG11	2.48	0.44
16:P:23:G:H2'	16:P:24:C:H6	1.82	0.44
17:Q:427:ILE:HG13	17:Q:460:LEU:HD22	2.00	0.44
23:W:8:LEU:HD13	23:W:288:LYS:HE3	2.00	0.44
1:A:1052:ARG:CZ	1:A:1056:GLU:OE2	2.66	0.44
1:A:1378:LEU:O	1:A:1378:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:29:THR:HG23	17:Q:877:GLN:CG	2.48	0.44
14:N:14:DT:H2''	14:N:15:DT:C6	2.52	0.44
17:Q:65:GLU:HA	17:Q:89:LEU:HD11	2.00	0.44
17:Q:81:ASP:O	17:Q:84:THR:OG1	2.32	0.44
17:Q:313:ALA:HB2	17:Q:328:TYR:HB3	1.99	0.44
21:U:450:LEU:HG	21:U:452:LEU:HD23	2.00	0.44
23:W:26:THR:HG23	23:W:284:GLY:HA2	1.98	0.44
30:d:76:GLU:OE1	30:d:79:ARG:NH1	2.51	0.44
1:A:1473:LEU:N	1:A:1473:LEU:HD12	2.33	0.43
2:B:821:LYS:HD2	20:T:-94:DG:H22	1.83	0.43
3:C:59:LEU:HD12	3:C:151:VAL:CG1	2.45	0.43
14:N:37:DC:H1'	14:N:38:DC:C6	2.53	0.43
17:Q:494:ALA:HB2	24:X:223:ASP:OD2	2.18	0.43
18:R:507:PRO:HA	18:R:508:ASN:HA	1.79	0.43
20:T:-107:DA:H2''	20:T:-106:DC:C6	2.52	0.43
23:W:292:VAL:HG12	23:W:298:ILE:HG12	1.98	0.43
1:A:1414:ILE:O	1:A:1414:ILE:HG22	2.19	0.43
14:N:-42:DT:OP2	29:c:17:ARG:NH2	2.47	0.43
14:N:17:DA:C1'	14:N:18:DA:N7	2.78	0.43
14:N:51:DA:H2''	14:N:52:DC:C5	2.53	0.43
14:N:66:DA:H2''	14:N:67:DC:H6	1.82	0.43
18:R:574:GLU:HA	18:R:577:LYS:HG2	2.00	0.43
20:T:-118:DA:H2'	20:T:-117:DC:O4'	2.18	0.43
20:T:-76:DG:C2'	20:T:-75:DT:C7	2.94	0.43
20:T:-69:DA:N9	20:T:-68:DT:H72	2.33	0.43
2:B:297:MET:HE2	2:B:373:LEU:HD12	2.01	0.43
2:B:814:TYR:O	2:B:920:LYS:HA	2.18	0.43
8:H:15:ILE:HG22	8:H:28:LEU:HD13	2.00	0.43
14:N:-35:DT:H2''	14:N:-34:DA:N7	2.33	0.43
17:Q:552:ASP:OD1	17:Q:552:ASP:N	2.51	0.43
20:T:-103:DG:N3	20:T:-102:DA:H1'	2.33	0.43
20:T:-34:DG:C8	20:T:-33:DT:H72	2.53	0.43
23:W:34:THR:HA	23:W:48:LYS:HA	1.99	0.43
24:X:222:ARG:HA	24:X:225:VAL:HG22	2.00	0.43
31:l:2022:VAL:O	31:l:2023:TYR:C	2.60	0.43
1:A:97:VAL:CG1	1:A:318:VAL:HG23	2.48	0.43
9:I:71:ASP:O	9:I:74:GLN:HG2	2.18	0.43
14:N:53:DG:H2'	14:N:54:DT:C7	2.44	0.43
23:W:107:VAL:HG22	23:W:107:VAL:O	2.19	0.43
29:c:99:ARG:NE	29:c:99:ARG:HA	2.33	0.43
1:A:236:LEU:N	1:A:236:LEU:HD22	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:ARG:NH2	3:C:172:GLU:OE2	2.52	0.43
3:C:103:LEU:HD23	3:C:103:LEU:C	2.43	0.43
14:N:-36:DG:C2'	14:N:-35:DT:H71	2.49	0.43
14:N:72:DA:C4	14:N:73:DT:C5	3.06	0.43
18:R:355:LEU:HD12	18:R:355:LEU:N	2.34	0.43
20:T:-52:DG:H2'	20:T:-51:DT:H72	2.01	0.43
20:T:33:DC:H4'	20:T:34:DT:OP1	2.19	0.43
21:U:416:VAL:HG13	21:U:417:GLU:N	2.33	0.43
1:A:499:ASP:OD1	16:P:26:C:H4'	2.19	0.43
3:C:50:VAL:HG22	3:C:163:ALA:HB2	1.99	0.43
5:E:13:ILE:HD11	5:E:132:GLN:HB2	2.00	0.43
5:E:131:LEU:N	5:E:131:LEU:HD12	2.33	0.43
14:N:-41:DT:C2	14:N:-40:DG:N7	2.87	0.43
14:N:54:DT:C2	14:N:55:DG:C8	3.07	0.43
14:N:92:DG:H2''	14:N:93:DT:C5'	2.49	0.43
21:U:440:ILE:HD12	21:U:440:ILE:N	2.34	0.43
26:Z:188:GLU:N	26:Z:188:GLU:OE1	2.51	0.43
31:l:1669:GLN:N	31:l:1690:GLY:HA2	2.33	0.43
1:A:1536:GLY:O	13:M:1483:ARG:NH2	2.51	0.43
2:B:39:LEU:HD12	2:B:39:LEU:N	2.34	0.43
5:E:80:PRO:HA	5:E:107:GLN:HB2	2.00	0.43
7:G:54:ILE:HD13	7:G:70:VAL:HG23	2.01	0.43
14:N:37:DC:C1'	14:N:38:DC:C5	2.98	0.43
14:N:57:DC:C2	14:N:58:DA:C8	3.06	0.43
17:Q:199:GLU:OE2	17:Q:228:ASN:HB3	2.18	0.43
17:Q:764:LEU:C	17:Q:764:LEU:HD23	2.43	0.43
22:V:94:ILE:HD12	22:V:94:ILE:H	1.83	0.43
27:a:124:ILE:HD11	28:b:50:ILE:HG23	2.01	0.43
2:B:529:MET:HB2	2:B:702:MET:CG	2.48	0.43
9:I:106:ASP:N	9:I:106:ASP:OD1	2.50	0.43
10:J:21:TYR:CE2	10:J:25:LEU:HD11	2.54	0.43
14:N:-32:DA:C2	14:N:-31:DC:C2	3.06	0.43
15:O:586:LYS:HA	15:O:589:THR:HG22	2.01	0.43
17:Q:419:ALA:HB2	17:Q:433:ALA:HB3	1.99	0.43
17:Q:869:GLU:O	17:Q:872:LYS:HG2	2.19	0.43
20:T:-15:DA:H2''	20:T:-14:DA:C8	2.53	0.43
23:W:86:ALA:HB1	23:W:104:ALA:O	2.19	0.43
26:Z:511:LEU:C	26:Z:511:LEU:HD23	2.44	0.43
2:B:603:MET:C	2:B:604:ILE:HD12	2.43	0.43
9:I:60:HIS:O	9:I:60:HIS:ND1	2.52	0.43
17:Q:351:TYR:HB2	17:Q:360:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:THR:O	1:A:1123:ARG:HB2	2.18	0.43
2:B:47:PHE:HB2	2:B:155:MET:SD	2.59	0.43
2:B:664:TYR:C	2:B:665:ILE:HD12	2.44	0.43
6:F:79:VAL:HG21	6:F:83:LEU:CD1	2.49	0.43
14:N:-68:DA:C2'	14:N:-67:DG:C8	3.02	0.43
14:N:87:DC:H5'	14:N:87:DC:C6	2.54	0.43
15:O:556:ALA:O	15:O:560:VAL:HG23	2.18	0.43
17:Q:662:TYR:HB3	17:Q:665:GLU:HB2	2.00	0.43
17:Q:837:GLU:O	17:Q:840:GLU:HG3	2.19	0.43
17:Q:858:LYS:O	17:Q:861:GLU:HG3	2.19	0.43
17:Q:879:ALA:O	17:Q:882:VAL:HG12	2.18	0.43
23:W:290:VAL:HG23	23:W:300:ILE:CD1	2.49	0.43
31:l:1684:ASN:O	31:l:1685:CYS:C	2.62	0.43
1:A:832:THR:HG23	1:A:833:PRO:HD2	2.00	0.42
1:A:977:VAL:HG22	1:A:978:VAL:N	2.34	0.42
1:A:1211:LEU:C	1:A:1211:LEU:HD12	2.44	0.42
1:A:1235:ILE:HD12	1:A:1296:MET:HE2	2.01	0.42
2:B:395:LEU:N	2:B:395:LEU:HD22	2.34	0.42
14:N:-64:DT:H2''	14:N:-63:DC:H6	1.84	0.42
14:N:-37:DC:H2''	14:N:-36:DG:H8	1.78	0.42
20:T:36:DC:H2''	20:T:37:DG:H8	1.78	0.42
22:V:313:PHE:H	22:V:325:GLU:HA	1.84	0.42
28:b:31:LYS:HE3	28:b:51:TYR:CZ	2.54	0.42
1:A:1158:LEU:C	1:A:1158:LEU:HD23	2.44	0.42
3:C:88:CYS:SG	3:C:89:THR:N	2.92	0.42
14:N:118:DT:H2'	14:N:119:DT:C6	2.54	0.42
17:Q:118:THR:HG22	17:Q:122:LYS:NZ	2.34	0.42
17:Q:611:TRP:HD1	17:Q:632:ALA:HB2	1.83	0.42
17:Q:772:GLU:N	17:Q:772:GLU:OE1	2.52	0.42
20:T:-69:DA:C8	20:T:-68:DT:H72	2.54	0.42
20:T:59:DC:C2	20:T:60:DC:C5	3.07	0.42
1:A:1255:LEU:N	1:A:1255:LEU:HD12	2.33	0.42
2:B:988:LYS:HD2	2:B:1015:LEU:HD21	2.02	0.42
5:E:185:ILE:HD12	5:E:209:VAL:HG21	2.01	0.42
8:H:7:GLU:HG2	8:H:59:VAL:HG22	2.01	0.42
14:N:-12:DA:C4	14:N:-11:DC:C5	3.07	0.42
14:N:56:DT:H2''	14:N:57:DC:H6	1.84	0.42
20:T:-82:DG:C2'	20:T:-81:DT:H72	2.49	0.42
23:W:272:ASP:OD1	23:W:272:ASP:N	2.50	0.42
1:A:107:LEU:HD23	1:A:107:LEU:O	2.19	0.42
1:A:110:VAL:HG22	1:A:111:CYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ILE:CG2	1:A:504:HIS:HB2	2.49	0.42
5:E:114:ALA:O	5:E:118:LEU:HD13	2.19	0.42
11:K:49:GLN:NE2	11:K:93:ASP:OD2	2.53	0.42
14:N:-55:DC:H4'	14:N:-54:DG:OP1	2.18	0.42
14:N:-47:DC:H4'	14:N:-46:DT:OP1	2.18	0.42
14:N:89:DT:H2''	14:N:90:DC:H6	1.85	0.42
17:Q:454:LEU:HA	17:Q:457:VAL:HG12	2.01	0.42
23:W:25:GLY:N	23:W:72:ILE:HD12	2.34	0.42
1:A:811:ILE:HD11	9:I:79:PRO:N	2.34	0.42
5:E:86:THR:O	5:E:89:VAL:HG12	2.20	0.42
14:N:-51:DG:H2''	14:N:-50:DC:H6	1.83	0.42
15:O:613:MET:HE1	15:O:641:LEU:CD2	2.49	0.42
5:E:66:ASP:OD1	5:E:67:ASP:N	2.52	0.42
8:H:27:ARG:NH1	8:H:42:ASP:OD2	2.53	0.42
17:Q:204:MET:HE1	22:V:107:LEU:HD13	2.01	0.42
20:T:-121:DC:C2	20:T:-120:DA:N7	2.88	0.42
26:Z:245:LEU:HD22	26:Z:245:LEU:N	2.34	0.42
31:I:1707:GLU:O	31:I:1709:SER:N	2.44	0.42
1:A:374:SER:OG	1:A:376:ASP:OD1	2.36	0.42
3:C:23:ILE:HD12	3:C:231:TYR:HE2	1.84	0.42
8:H:27:ARG:O	8:H:28:LEU:HD22	2.20	0.42
14:N:10:DG:H5'	27:e:43:PRO:HA	2.00	0.42
17:Q:454:LEU:HD11	17:Q:473:TYR:CD1	2.54	0.42
17:Q:850:GLU:O	17:Q:854:GLN:NE2	2.53	0.42
17:Q:855:LYS:O	17:Q:858:LYS:HG3	2.19	0.42
20:T:8:DT:C2	20:T:9:DG:C8	3.08	0.42
22:V:61:TYR:N	22:V:62:LYS:HA	2.34	0.42
26:Z:524:THR:HG22	26:Z:525:ALA:N	2.35	0.42
1:A:461:GLN:HE21	20:T:-102:DA:H4'	1.85	0.42
1:A:922:PHE:CD2	1:A:952:LEU:HD23	2.55	0.42
10:J:13:ILE:HD12	10:J:13:ILE:N	2.35	0.42
11:K:100:LEU:HD23	11:K:100:LEU:C	2.44	0.42
14:N:-55:DC:H1'	14:N:-54:DG:C8	2.54	0.42
14:N:30:DA:C8	14:N:31:DT:H71	2.55	0.42
17:Q:68:ARG:NE	17:Q:89:LEU:HD12	2.34	0.42
17:Q:538:GLY:HA3	17:Q:554:PHE:CE1	2.54	0.42
17:Q:776:LEU:HD22	17:Q:831:ALA:CA	2.47	0.42
18:R:369:LEU:C	18:R:369:LEU:HD12	2.45	0.42
20:T:38:DA:C4	20:T:39:DC:C5	3.08	0.42
1:A:600:ILE:HG22	1:A:601:ASN:N	2.35	0.42
2:B:198:GLU:OE2	2:B:487:SER:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:428:ASP:OD1	2:B:429:PHE:N	2.53	0.42
8:H:8:ASP:OD2	8:H:9:ILE:O	2.38	0.42
11:K:78:THR:HB	11:K:79:PRO:HD2	2.01	0.42
11:K:80:ASP:OD1	11:K:80:ASP:N	2.50	0.42
14:N:-63:DC:C2	14:N:-62:DC:C5	3.08	0.42
14:N:27:DG:H2'	14:N:27:DG:O5'	2.20	0.42
14:N:38:DC:C2'	14:N:39:DT:C7	2.90	0.42
22:V:110:GLU:HG3	22:V:111:GLU:H	1.85	0.42
1:A:216:LEU:N	1:A:216:LEU:HD22	2.35	0.42
1:A:1366:PHE:CA	1:A:1374:VAL:HG21	2.50	0.42
2:B:163:LEU:HD22	2:B:163:LEU:N	2.35	0.42
2:B:595:ASP:OD1	2:B:596:ILE:N	2.52	0.42
3:C:123:ASN:OD1	3:C:124:SER:N	2.53	0.42
14:N:42:DT:C2'	14:N:43:DC:C5	3.02	0.42
15:O:591:LEU:O	15:O:594:VAL:HG22	2.19	0.42
17:Q:384:LEU:HD11	17:Q:393:LYS:O	2.20	0.42
17:Q:392:GLU:OE1	17:Q:392:GLU:N	2.52	0.42
17:Q:569:SER:OG	24:X:234:ARG:NH1	2.53	0.42
17:Q:680:ILE:O	17:Q:683:VAL:HG22	2.19	0.42
22:V:45:ASP:HB3	24:X:232:ARG:HE	1.85	0.42
1:A:467:MET:SD	1:A:524:MET:HB3	2.60	0.41
2:B:393:LEU:HD11	2:B:485:LEU:HD23	2.02	0.41
14:N:1:DC:H2'	14:N:2:DT:H71	2.01	0.41
14:N:43:DC:C2	14:N:44:DT:C6	3.08	0.41
17:Q:73:LEU:C	17:Q:73:LEU:HD23	2.45	0.41
20:T:-77:DC:C2	20:T:-76:DG:C8	3.08	0.41
1:A:141:LEU:HD13	1:A:1445:HIS:CE1	2.55	0.41
1:A:912:SER:O	1:A:915:ALA:N	2.53	0.41
1:A:927:GLU:O	1:A:931:ARG:NE	2.48	0.41
2:B:279:VAL:HG13	2:B:280:SER:N	2.34	0.41
8:H:58:LEU:HD21	8:H:60:ILE:CD1	2.50	0.41
8:H:116:VAL:CG1	8:H:123:MET:HE3	2.49	0.41
17:Q:427:ILE:HD13	17:Q:464:LEU:HD21	2.02	0.41
17:Q:772:GLU:HA	17:Q:773:LYS:HB2	2.02	0.41
20:T:-81:DT:N3	20:T:-80:DG:C5	2.88	0.41
20:T:33:DC:H2''	20:T:34:DT:H71	2.01	0.41
22:V:312:PHE:HA	22:V:325:GLU:HA	2.01	0.41
23:W:67:VAL:HG13	23:W:81:SER:OG	2.20	0.41
23:W:248:VAL:HG13	23:W:282:TYR:OH	2.20	0.41
26:Z:360:ILE:HG23	26:Z:364:ASN:HA	2.02	0.41
31:l:1596:TYR:OH	31:l:1601:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:652:SER:N	2:B:655:ASP:OD2	2.43	0.41
5:E:55:ARG:C	5:E:56:THR:HG1	2.19	0.41
5:E:162:ARG:HD3	5:E:162:ARG:C	2.46	0.41
10:J:18:TRP:NE1	10:J:22:LEU:HD11	2.35	0.41
11:K:11:LEU:O	11:K:37:LYS:NZ	2.43	0.41
17:Q:67:ALA:HB3	17:Q:68:ARG:HH12	1.85	0.41
17:Q:532:ASP:O	17:Q:536:ARG:HG2	2.21	0.41
17:Q:691:TYR:CE2	17:Q:703:MET:SD	3.13	0.41
18:R:439:LEU:O	18:R:442:VAL:HG12	2.20	0.41
20:T:-30:DT:H2''	20:T:-29:DC:C6	2.55	0.41
24:X:256:VAL:HG13	24:X:257:LYS:N	2.35	0.41
29:g:99:ARG:NE	29:g:99:ARG:HA	2.35	0.41
2:B:88:PHE:CE2	2:B:128:ILE:HD12	2.55	0.41
2:B:273:PHE:CE1	2:B:365:LEU:HD23	2.55	0.41
5:E:64:HIS:ND1	5:E:66:ASP:OD1	2.53	0.41
8:H:14:ASP:OD1	8:H:15:ILE:N	2.53	0.41
27:a:35:VAL:HG21	31:l:1589:PHE:CZ	2.55	0.41
30:h:36:SER:HB2	30:h:63:ASN:OD1	2.20	0.41
2:B:789:ASN:HB3	2:B:795:ILE:HG13	2.02	0.41
2:B:859:ARG:HB2	26:Z:737:HIS:HD1	1.84	0.41
13:M:1507:LEU:HD23	13:M:1507:LEU:C	2.46	0.41
14:N:-17:DC:H2''	14:N:-16:DT:C6	2.55	0.41
14:N:1:DC:C2'	14:N:2:DT:H71	2.50	0.41
14:N:65:DT:C2	14:N:66:DA:C8	3.08	0.41
17:Q:236:VAL:O	17:Q:240:VAL:HG23	2.20	0.41
17:Q:239:ALA:HB2	17:Q:257:LEU:HB3	2.03	0.41
17:Q:662:TYR:O	17:Q:666:ALA:HB2	2.20	0.41
18:R:493:GLU:O	18:R:496:VAL:HG22	2.20	0.41
20:T:-78:DC:C2	20:T:-77:DC:C5	3.09	0.41
31:l:1640:TRP:O	31:l:1646:LEU:HD12	2.20	0.41
2:B:854:ILE:O	2:B:907:VAL:HG21	2.21	0.41
5:E:154:GLU:O	5:E:157:THR:OG1	2.36	0.41
7:G:12:LEU:N	7:G:12:LEU:HD12	2.36	0.41
8:H:27:ARG:HD3	8:H:42:ASP:OD1	2.21	0.41
8:H:91:VAL:HG13	8:H:144:LEU:HD23	2.01	0.41
12:L:16:ILE:HD11	12:L:25:GLU:CG	2.50	0.41
14:N:-23:DG:C4	14:N:-22:DC:C5	3.09	0.41
14:N:-3:DC:H1'	14:N:-2:DG:N7	2.36	0.41
14:N:4:DT:H2''	14:N:5:DC:C5	2.55	0.41
14:N:113:DG:C2'	14:N:114:DT:H72	2.50	0.41
17:Q:138:CYS:HB3	17:Q:143:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:441:LEU:N	26:Z:441:LEU:HD22	2.36	0.41
1:A:1361:ASP:OD1	1:A:1361:ASP:C	2.64	0.41
2:B:665:ILE:HD12	2:B:665:ILE:N	2.36	0.41
5:E:18:MET:HA	5:E:18:MET:HE2	2.02	0.41
6:F:98:LYS:NZ	6:F:127:ASP:O	2.47	0.41
7:G:85:VAL:HG22	7:G:147:ILE:HD11	2.02	0.41
12:L:18:ILE:N	12:L:18:ILE:HD12	2.35	0.41
17:Q:232:VAL:O	17:Q:232:VAL:HG12	2.21	0.41
17:Q:288:VAL:HG13	17:Q:289:GLN:N	2.36	0.41
17:Q:452:GLU:OE2	22:V:51:TYR:CD1	2.74	0.41
27:a:35:VAL:O	31:l:1669:GLN:HG2	2.20	0.41
31:l:1477:GLU:HG3	31:l:1478:GLU:H	1.86	0.41
1:A:67:ARG:C	1:A:68:THR:HG1	2.21	0.41
1:A:486:LEU:N	1:A:486:LEU:HD12	2.35	0.41
2:B:86:LEU:HD11	2:B:128:ILE:HD11	2.03	0.41
14:N:-26:DC:H4'	14:N:-25:DT:OP1	2.21	0.41
17:Q:554:PHE:CE1	17:Q:570:LEU:HD21	2.55	0.41
20:T:60:DC:C2	20:T:61:DG:C8	3.09	0.41
22:V:83:THR:O	22:V:83:THR:HG23	2.21	0.41
27:a:34:GLY:HA2	31:l:1671:TYR:HB2	2.02	0.41
1:A:1175:ILE:HD11	1:A:1285:LEU:HD12	2.03	0.41
1:A:1360:ASN:HA	1:A:1381:GLU:OE2	2.20	0.41
1:A:1375:ARG:NE	1:A:1403:ASP:OD1	2.39	0.41
2:B:260:LEU:HD12	2:B:260:LEU:N	2.35	0.41
2:B:539:SER:N	2:B:540:PRO:HD2	2.36	0.41
2:B:603:MET:SD	2:B:603:MET:N	2.94	0.41
2:B:1038:THR:HA	3:C:195:THR:HA	2.02	0.41
8:H:52:LEU:N	8:H:52:LEU:HD12	2.36	0.41
14:N:53:DG:C2'	14:N:54:DT:C7	2.99	0.41
17:Q:471:LYS:O	17:Q:475:LEU:HD23	2.20	0.41
18:R:570:TRP:HA	18:R:573:VAL:HG22	2.02	0.41
20:T:-87:DG:C8	20:T:-86:DT:H72	2.55	0.41
20:T:-33:DT:C2'	20:T:-32:DA:C8	3.04	0.41
20:T:-10:DC:C2	20:T:-9:DG:C5	3.08	0.41
22:V:109:GLU:OE1	22:V:109:GLU:N	2.52	0.41
23:W:119:GLN:O	23:W:135:VAL:HG22	2.21	0.41
23:W:186:LEU:HD11	23:W:222:ALA:HB1	2.01	0.41
26:Z:264:LEU:C	26:Z:264:LEU:HD12	2.46	0.41
1:A:480:SER:O	1:A:481:THR:HG23	2.21	0.41
1:A:1386:ILE:HG12	1:A:1393:VAL:HG21	2.03	0.41
2:B:1056:ASP:O	2:B:1078:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:1463:CYS:SG	13:M:1464:ALA:N	2.94	0.41
14:N:-21:DA:C4	14:N:-20:DC:C5	3.08	0.41
17:Q:91:ALA:O	17:Q:94:VAL:HG12	2.21	0.41
20:T:32:DT:H6	20:T:32:DT:H2'	1.78	0.41
26:Z:556:GLU:OE1	26:Z:556:GLU:N	2.54	0.41
2:B:27:TRP:CD1	2:B:762:ARG:HE	2.39	0.40
14:N:73:DT:C2	14:N:74:DA:N7	2.89	0.40
17:Q:437:ALA:O	17:Q:440:ILE:HG22	2.22	0.40
1:A:1123:ARG:CG	1:A:1385:VAL:HG11	2.51	0.40
1:A:1419:VAL:HG21	1:A:1432:PHE:CD2	2.56	0.40
2:B:911:LEU:HD21	12:L:34:ILE:HD13	2.04	0.40
4:D:39:MET:SD	4:D:40:LEU:N	2.94	0.40
8:H:76:ASN:OD1	8:H:76:ASN:N	2.54	0.40
8:H:96:VAL:HA	8:H:116:VAL:HA	2.03	0.40
17:Q:131:LEU:HD13	17:Q:154:PHE:HB2	2.03	0.40
20:T:-91:DT:C2	20:T:-90:DG:C5	3.09	0.40
20:T:15:DA:N3	20:T:16:DA:C5	2.89	0.40
21:U:384:VAL:HG12	21:U:385:GLU:N	2.37	0.40
23:W:134:GLY:HA3	23:W:141:GLU:OE2	2.20	0.40
23:W:152:LEU:HD12	23:W:168:ILE:HA	2.03	0.40
31:l:1494:ILE:HG22	31:l:1494:ILE:O	2.21	0.40
31:l:1685:CYS:C	31:l:1687:GLY:H	2.29	0.40
1:A:422:ASP:OD1	1:A:423:ASN:N	2.54	0.40
1:A:933:THR:OG1	1:A:934:LEU:HD12	2.21	0.40
1:A:937:ASP:C	1:A:938:LEU:HD12	2.46	0.40
2:B:634:LEU:N	2:B:634:LEU:HD22	2.36	0.40
2:B:1003:ASN:OD1	2:B:1006:VAL:HG23	2.20	0.40
4:D:20:LEU:HD12	4:D:20:LEU:N	2.36	0.40
11:K:104:ARG:O	11:K:107:VAL:HG22	2.21	0.40
14:N:-6:DG:H2''	14:N:-5:DT:C6	2.56	0.40
17:Q:384:LEU:HD22	17:Q:397:ALA:CB	2.51	0.40
17:Q:612:LEU:HD23	17:Q:612:LEU:C	2.46	0.40
17:Q:708:LEU:HD11	17:Q:719:VAL:HG21	2.03	0.40
17:Q:716:ASN:OD1	17:Q:717:THR:N	2.54	0.40
17:Q:768:VAL:HG21	17:Q:778:GLU:HG2	2.02	0.40
17:Q:852:LEU:HD12	17:Q:853:ARG:N	2.36	0.40
20:T:-108:DC:C2	20:T:-107:DA:N7	2.90	0.40
26:Z:210:LEU:HD12	26:Z:210:LEU:N	2.36	0.40
1:A:572:GLY:O	11:K:27:VAL:HG11	2.21	0.40
1:A:1226:LEU:HD11	1:A:1299:GLN:OE1	2.21	0.40
1:A:1291:ASN:OD1	1:A:1292:MET:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:-104:DA:C2	20:T:-103:DG:C5	3.09	0.40
20:T:-25:DT:C2'	20:T:-24:DT:C7	2.95	0.40
25:Y:42:MET:CE	25:Y:49:VAL:HG22	2.51	0.40
25:Y:113:THR:O	25:Y:113:THR:HG22	2.21	0.40
26:Z:359:LEU:N	26:Z:359:LEU:HD12	2.36	0.40
1:A:514:GLU:OE2	2:B:1099:ALA:HB1	2.21	0.40
1:A:865:ILE:HG21	2:B:1092:ASP:CG	2.46	0.40
1:A:939:VAL:HG23	1:A:940:LYS:N	2.36	0.40
1:A:962:ASP:HB3	1:A:1043:ILE:HG23	2.03	0.40
2:B:270:ILE:HG13	2:B:305:LEU:HA	2.04	0.40
2:B:565:THR:HA	2:B:610:ARG:HB3	2.04	0.40
3:C:148:ILE:HD12	3:C:148:ILE:H	1.85	0.40
9:I:58:ILE:HD12	9:I:58:ILE:N	2.36	0.40
9:I:105:GLU:OE1	9:I:105:GLU:N	2.43	0.40
14:N:-68:DA:H2''	14:N:-67:DG:H8	1.85	0.40
14:N:36:DC:O5'	14:N:36:DC:H2'	2.21	0.40
14:N:52:DC:C2	14:N:53:DG:C8	3.10	0.40
14:N:116:DT:C2	14:N:117:DG:C8	3.09	0.40
16:P:18:A:H2'	16:P:19:A:C8	2.56	0.40
17:Q:289:GLN:O	17:Q:293:LEU:HD23	2.21	0.40
20:T:-120:DA:H2''	20:T:-119:DA:H8	1.86	0.40
20:T:59:DC:H2''	20:T:60:DC:C6	2.57	0.40
20:T:60:DC:C2	20:T:61:DG:N7	2.89	0.40
26:Z:542:LEU:HD21	26:Z:560:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1408/1984 (71%)	1319 (94%)	88 (6%)	1 (0%)	48 79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1112/1251 (89%)	1024 (92%)	88 (8%)	0	100	100
3	C	254/275 (92%)	229 (90%)	25 (10%)	0	100	100
4	D	124/142 (87%)	120 (97%)	4 (3%)	0	100	100
5	E	207/210 (99%)	198 (96%)	9 (4%)	0	100	100
6	F	76/127 (60%)	74 (97%)	2 (3%)	0	100	100
7	G	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
8	H	147/150 (98%)	134 (91%)	13 (9%)	0	100	100
9	I	114/125 (91%)	103 (90%)	11 (10%)	0	100	100
10	J	64/67 (96%)	57 (89%)	7 (11%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	45/58 (78%)	41 (91%)	3 (7%)	1 (2%)	5	30
13	M	976/1729 (56%)	920 (94%)	55 (6%)	1 (0%)	48	79
15	O	130/821 (16%)	127 (98%)	3 (2%)	0	100	100
17	Q	888/1179 (75%)	847 (95%)	41 (5%)	0	100	100
18	R	240/713 (34%)	231 (96%)	9 (4%)	0	100	100
19	S	157/304 (52%)	154 (98%)	3 (2%)	0	100	100
21	U	117/666 (18%)	106 (91%)	10 (8%)	1 (1%)	14	46
22	V	234/531 (44%)	216 (92%)	18 (8%)	0	100	100
23	W	298/305 (98%)	288 (97%)	10 (3%)	0	100	100
24	X	41/531 (8%)	41 (100%)	0	0	100	100
25	Y	114/121 (94%)	108 (95%)	6 (5%)	0	100	100
26	Z	497/1087 (46%)	479 (96%)	18 (4%)	0	100	100
27	a	99/136 (73%)	96 (97%)	3 (3%)	0	100	100
27	e	90/136 (66%)	89 (99%)	1 (1%)	0	100	100
28	b	76/103 (74%)	76 (100%)	0	0	100	100
28	f	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
29	c	102/130 (78%)	101 (99%)	1 (1%)	0	100	100
29	g	101/130 (78%)	100 (99%)	1 (1%)	0	100	100
30	d	90/123 (73%)	89 (99%)	1 (1%)	0	100	100
30	h	87/123 (71%)	83 (95%)	4 (5%)	0	100	100
31	l	406/1133 (36%)	374 (92%)	30 (7%)	2 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	8652/14782 (58%)	8170 (94%)	476 (6%)	6 (0%)	49 79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	39	CYS
13	M	700	HIS
31	l	2018	ASP
31	l	2022	VAL
1	A	1343	LEU
21	U	510	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	A	1245/1761 (71%)	1241 (100%)	4 (0%)	86 83
2	B	986/1084 (91%)	983 (100%)	3 (0%)	86 83
3	C	235/252 (93%)	234 (100%)	1 (0%)	84 81
4	D	109/126 (86%)	109 (100%)	0	100 100
5	E	191/192 (100%)	189 (99%)	2 (1%)	68 75
6	F	68/111 (61%)	68 (100%)	0	100 100
7	G	146/153 (95%)	146 (100%)	0	100 100
8	H	130/131 (99%)	130 (100%)	0	100 100
9	I	104/112 (93%)	102 (98%)	2 (2%)	50 67
10	J	55/56 (98%)	55 (100%)	0	100 100
11	K	104/106 (98%)	104 (100%)	0	100 100
12	L	44/55 (80%)	44 (100%)	0	100 100
13	M	196/1524 (13%)	196 (100%)	0	100 100
15	O	118/737 (16%)	116 (98%)	2 (2%)	53 69
17	Q	761/1011 (75%)	753 (99%)	8 (1%)	65 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	170/625 (27%)	169 (99%)	1 (1%)	78	79
19	S	4/268 (2%)	4 (100%)	0	100	100
21	U	65/590 (11%)	65 (100%)	0	100	100
22	V	144/462 (31%)	143 (99%)	1 (1%)	76	78
23	W	255/260 (98%)	250 (98%)	5 (2%)	48	66
24	X	40/467 (9%)	40 (100%)	0	100	100
25	Y	102/105 (97%)	102 (100%)	0	100	100
26	Z	435/939 (46%)	435 (100%)	0	100	100
27	a	87/111 (78%)	87 (100%)	0	100	100
27	e	82/111 (74%)	82 (100%)	0	100	100
28	b	64/79 (81%)	64 (100%)	0	100	100
28	f	64/79 (81%)	64 (100%)	0	100	100
29	c	82/102 (80%)	82 (100%)	0	100	100
29	g	82/102 (80%)	82 (100%)	0	100	100
30	d	79/103 (77%)	79 (100%)	0	100	100
30	h	76/103 (74%)	76 (100%)	0	100	100
31	l	237/1017 (23%)	234 (99%)	3 (1%)	61	72
All	All	6560/12934 (51%)	6528 (100%)	32 (0%)	78	80

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	VAL
1	A	502	ASN
1	A	535	MET
1	A	1289	GLU
2	B	650	ASN
2	B	768	ARG
2	B	1017	ASP
3	C	5	ASN
5	E	18	MET
5	E	57	ASP
9	I	56	ASN
9	I	83	ASP
15	O	604	LYS
15	O	652	LEU

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Mol	Chain	Res	Type
17	Q	377	THR
17	Q	552	ASP
17	Q	667	ARG
17	Q	707	CYS
17	Q	780	LEU
17	Q	813	GLU
17	Q	817	CYS
17	Q	820	LEU
18	R	576	GLU
22	V	85	ASP
23	W	35	VAL
23	W	43	LEU
23	W	231	HIS
23	W	250	SER
23	W	272	ASP
31	I	1489	LYS
31	I	2031	THR
31	I	2038	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	122	ASN
1	A	293	ASN
1	A	372	ASN
1	A	449	HIS
1	A	461	GLN
1	A	502	ASN
1	A	529	GLN
1	A	539	GLN
1	A	700	GLN
1	A	711	GLN
1	A	790	GLN
1	A	791	GLN
1	A	1044	HIS
1	A	1417	HIS
2	B	143	GLN
2	B	197	GLN
2	B	227	ASN
2	B	387	HIS
2	B	582	GLN

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Mol	Chain	Res	Type
2	B	649	ASN
2	B	725	GLN
3	C	111	GLN
3	C	217	GLN
5	E	30	GLN
5	E	168	ASN
7	G	9	HIS
9	I	32	ASN
12	L	26	ASN
13	M	1505	ASN
17	Q	38	HIS
17	Q	40	GLN
17	Q	268	ASN
17	Q	278	HIS
17	Q	298	ASN
17	Q	373	ASN
17	Q	391	GLN
17	Q	466	ASN
17	Q	527	HIS
17	Q	546	ASN
17	Q	559	GLN
17	Q	594	GLN
17	Q	616	HIS
17	Q	617	GLN
17	Q	628	HIS
17	Q	714	HIS
17	Q	825	GLN
17	Q	860	GLN
22	V	69	GLN
22	V	72	HIS
22	V	124	HIS
23	W	27	ASN
23	W	268	HIS
23	W	273	HIS
25	Y	12	HIS
26	Z	244	ASN
26	Z	272	ASN
27	a	68	GLN
28	b	93	GLN
30	d	49	HIS
30	d	109	HIS
30	h	49	HIS

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Mol	Chain	Res	Type
31	1	1498	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	11/13 (84%)	2 (18%)	2 (18%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	17	A
16	P	19	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	P	16	A
16	P	18	A

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SEP	A	1547	1	8,9,10	1.61	1 (12%)	7,12,14	1.28	1 (14%)
26	TPO	Z	775	26	8,10,11	1.13	0	10,14,16	1.90	1 (10%)
1	TPO	A	1525	1	8,10,11	1.12	0	10,14,16	2.13	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	1547	1	-	0/6/8/10	-
26	TPO	Z	775	26	-	2/9/11/13	-
1	TPO	A	1525	1	-	0/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1547	SEP	P-O1P	3.51	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1525	TPO	P-OG1-CB	-6.08	106.81	123.33
26	Z	775	TPO	P-OG1-CB	-5.19	109.22	123.33
1	A	1547	SEP	OG-CB-CA	2.76	110.83	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	Z	775	TPO	C-CA-CB-CG2
26	Z	775	TPO	CB-OG1-P-O2P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1547	SEP	1	0
26	Z	775	TPO	2	0
1	A	1525	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	U	1
22	V	1
13	M	1
31	l	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	497:ASP	C	505:SER	N	27.02
1	V	299:GLU	C	310:ASN	N	12.71
1	M	1334:ASN	C	1338:ILE	N	5.60
1	l	1709:SER	C	1710:ARG	N	4.41

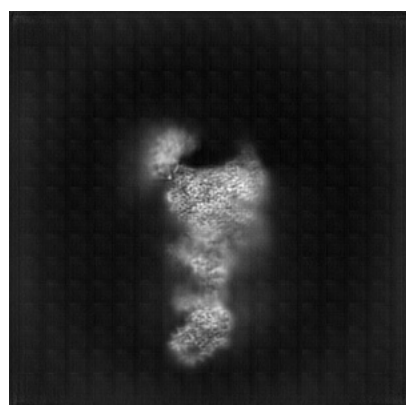
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48042. These allow visual inspection of the internal detail of the map and identification of artifacts.

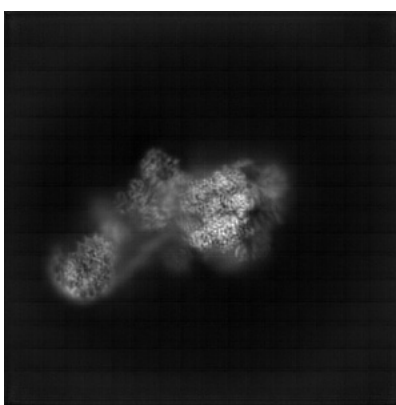
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

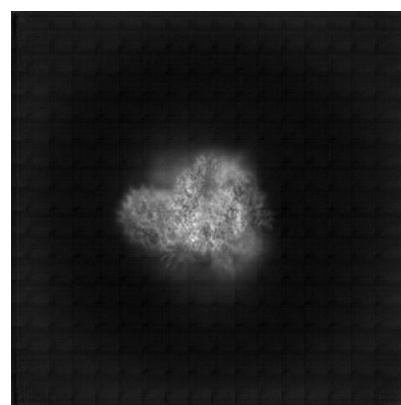
6.1.1 Primary map



X



Y

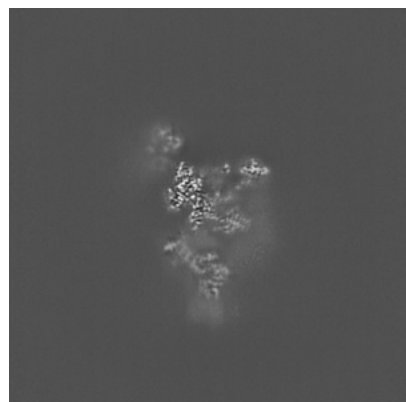


Z

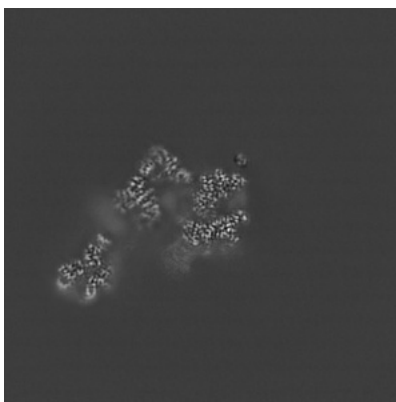
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

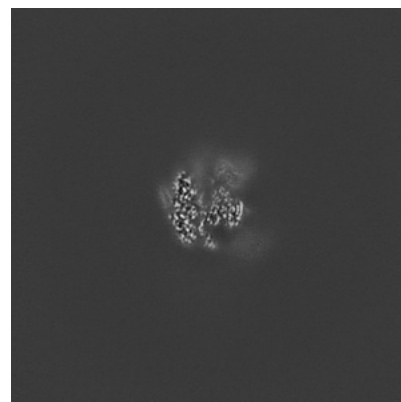
6.2.1 Primary map



X Index: 250



Y Index: 250

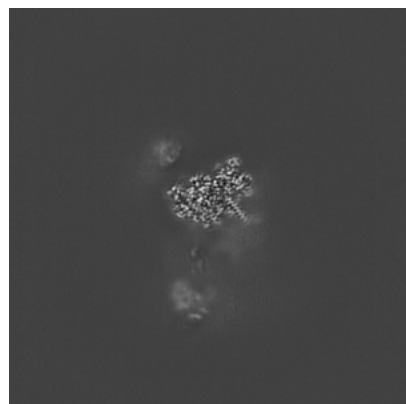


Z Index: 250

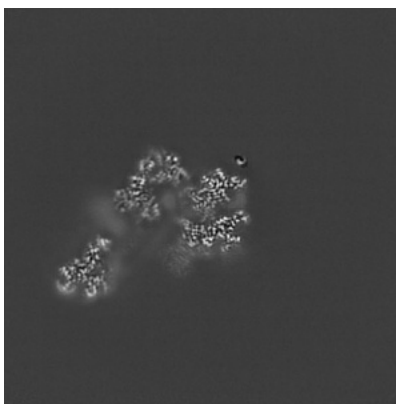
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

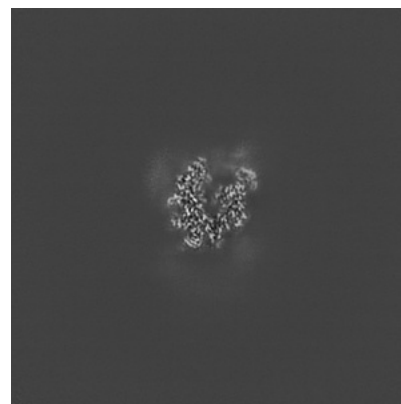
6.3.1 Primary map



X Index: 221



Y Index: 253



Z Index: 275

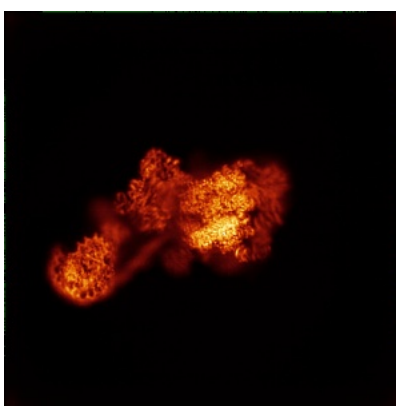
The images above show the largest variance slices of the map in three orthogonal directions.

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

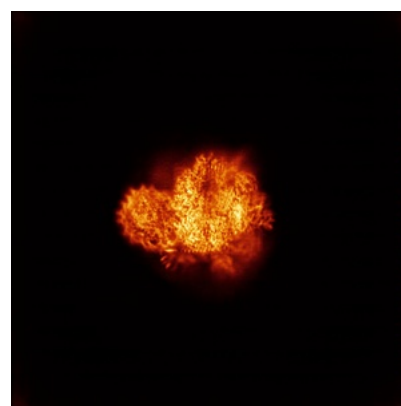
6.4.1 Primary map



X



Y

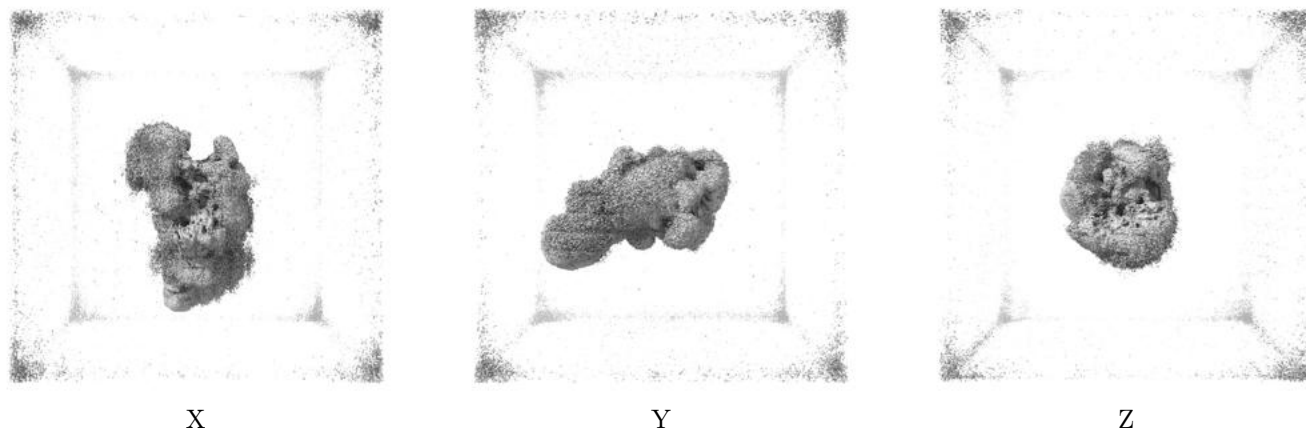


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

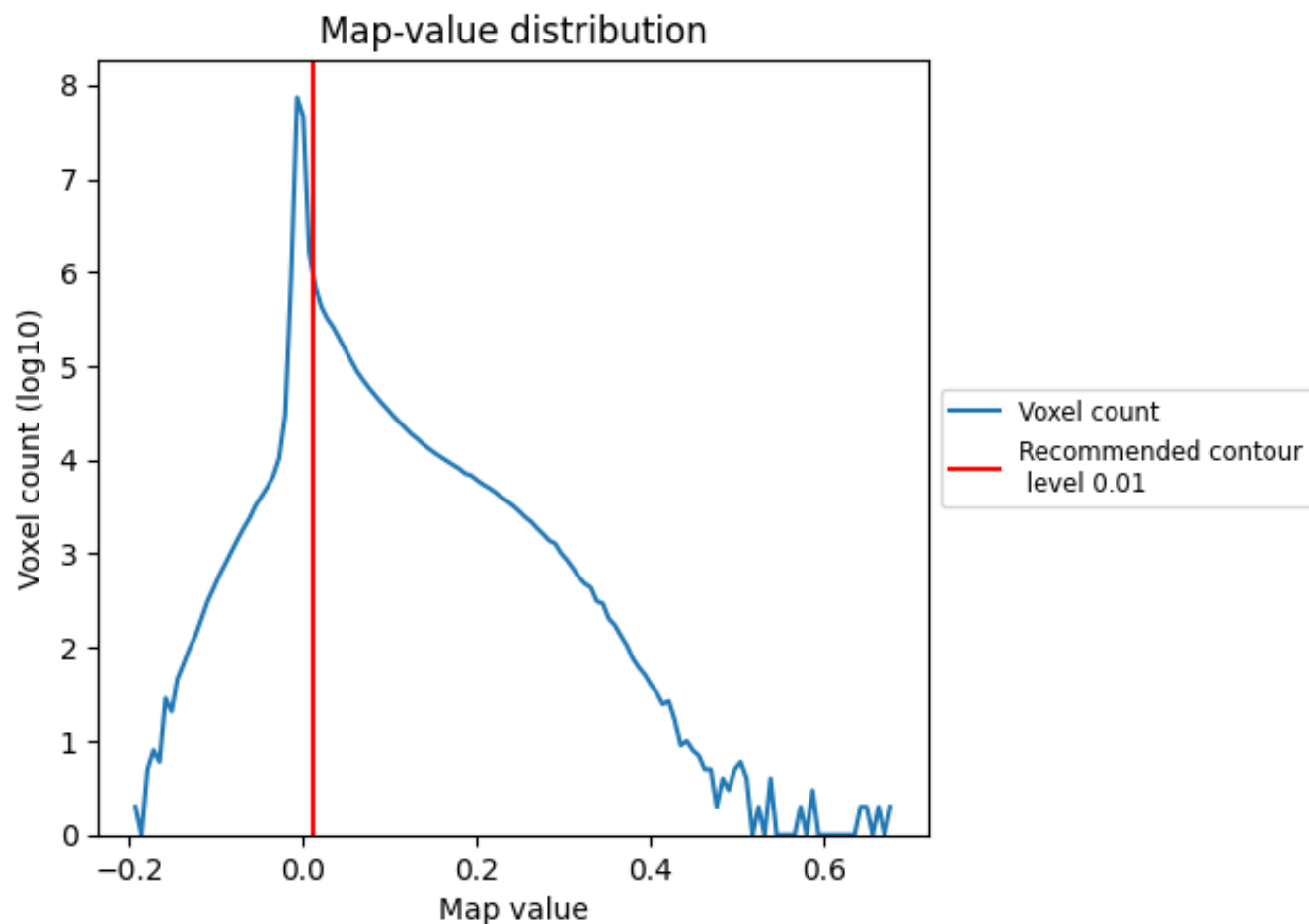
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

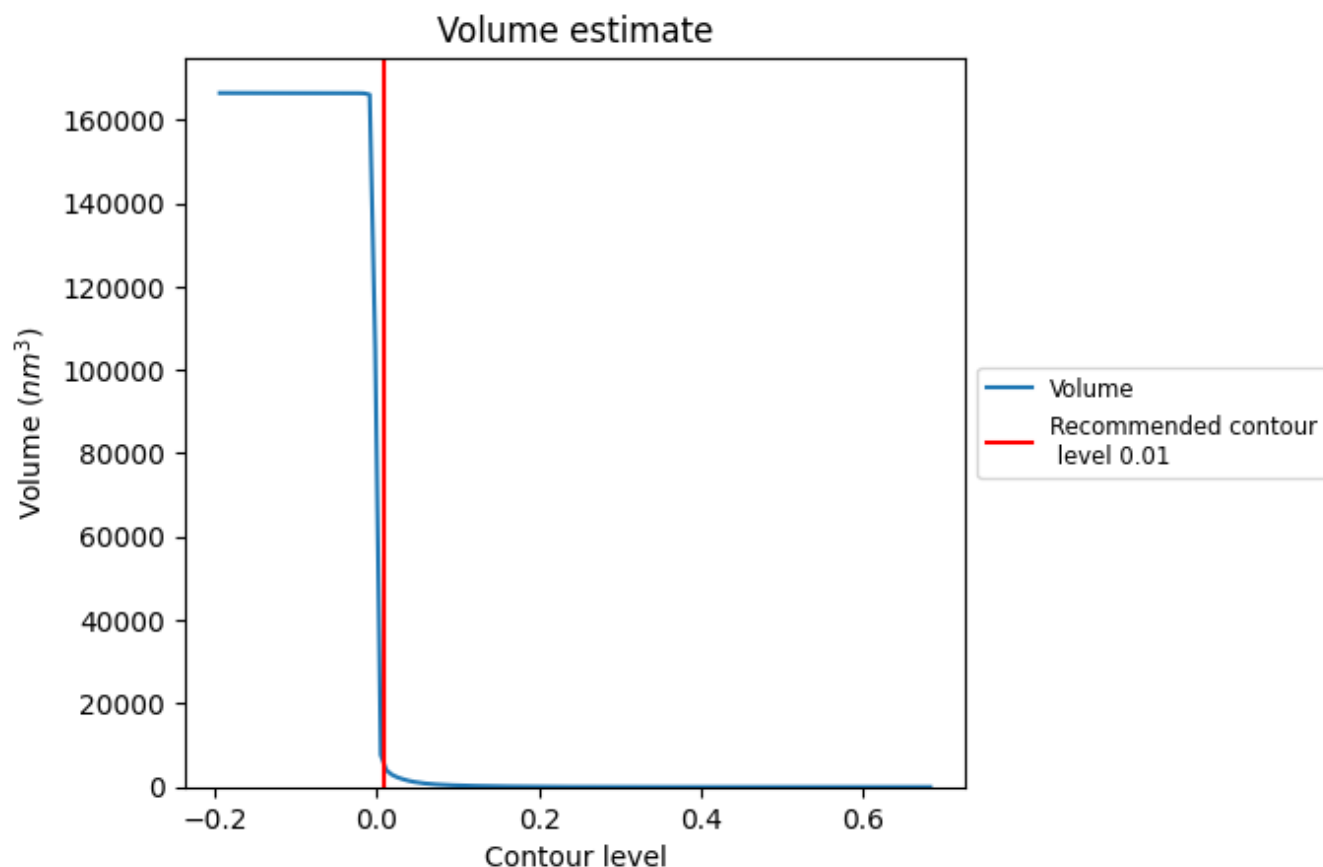
This section contains the results of statistical analysis of the map.

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.

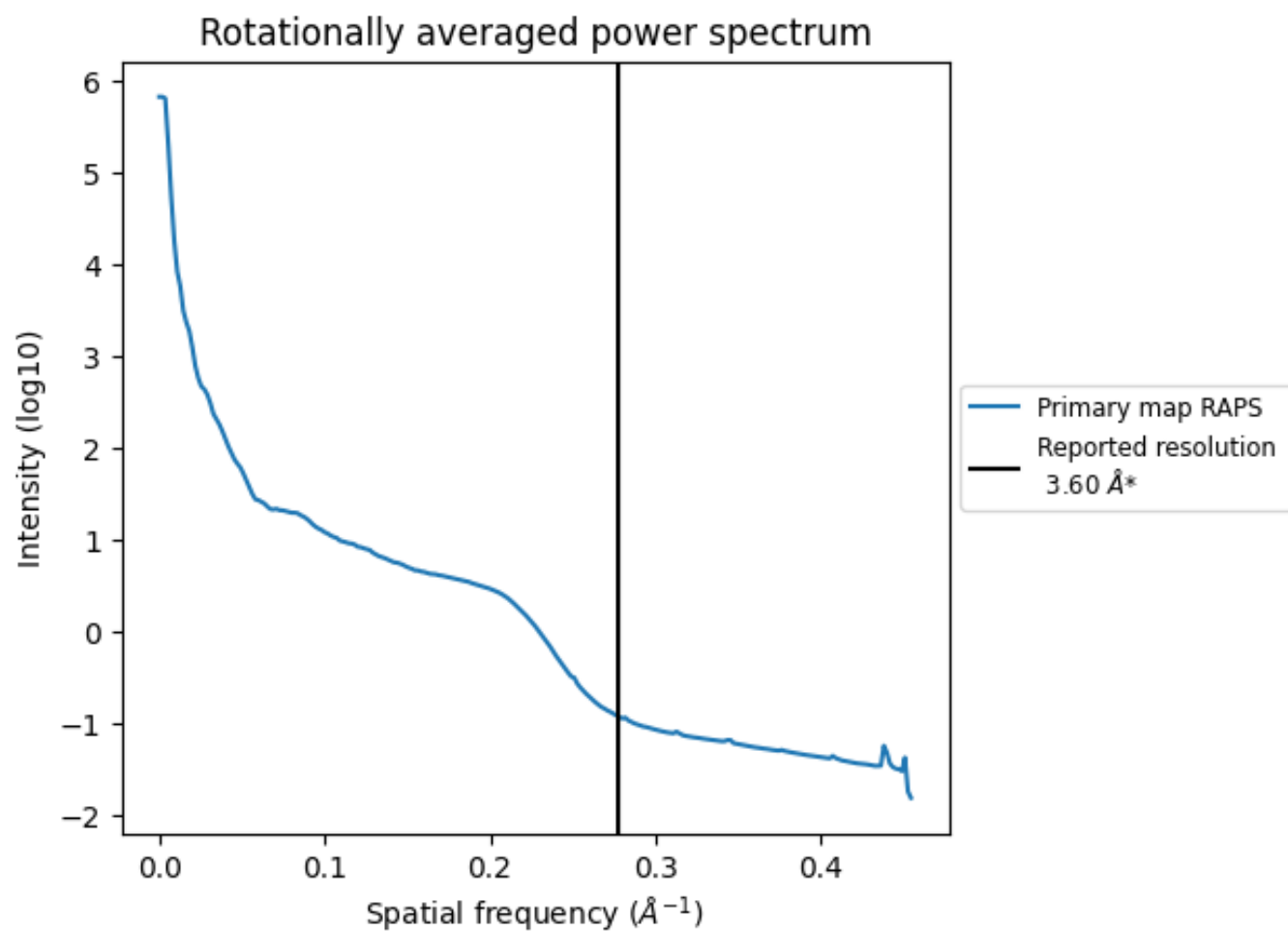
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5148 nm³; this corresponds to an approximate mass of 4651 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 0.278 \AA^{-1}

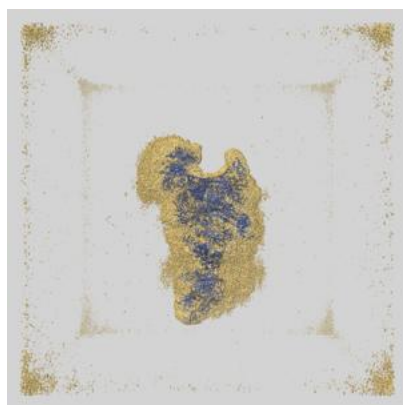
8 Fourier-Shell correlation

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

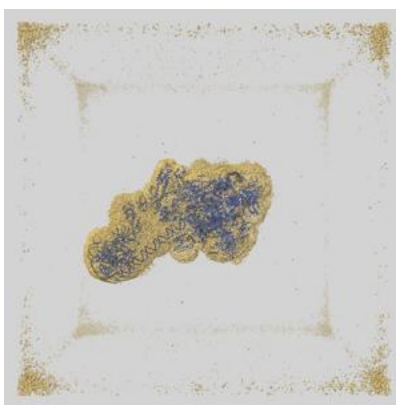
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48042 and PDB model 9EH0. Per-residue inclusion information can be found in section [3](#) on page [12](#).

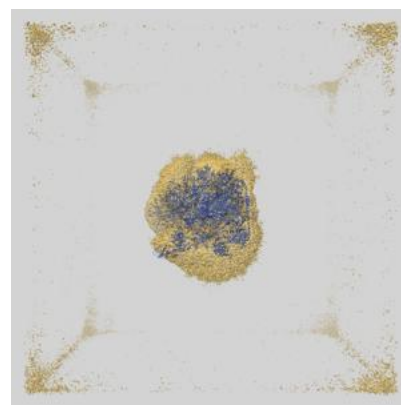
9.1 Map-model overlay [i](#)



X



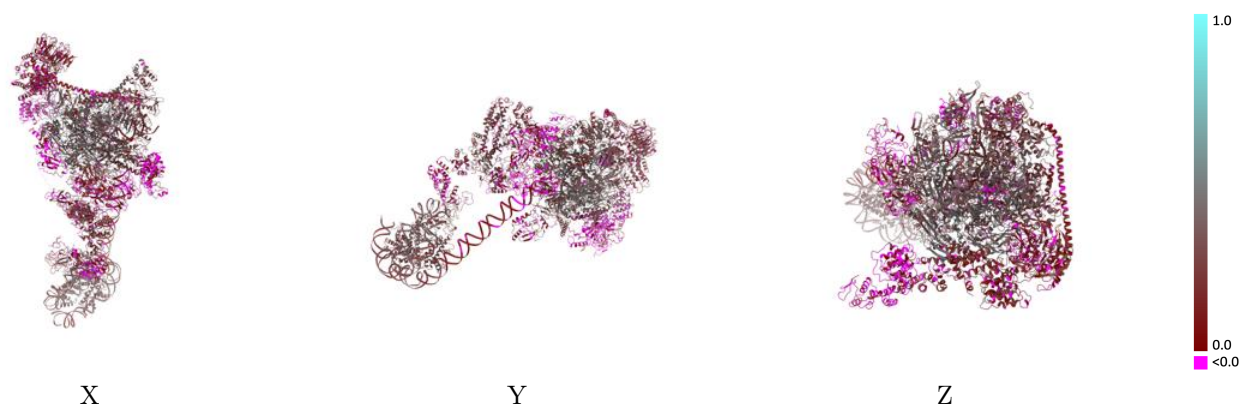
Y



Z

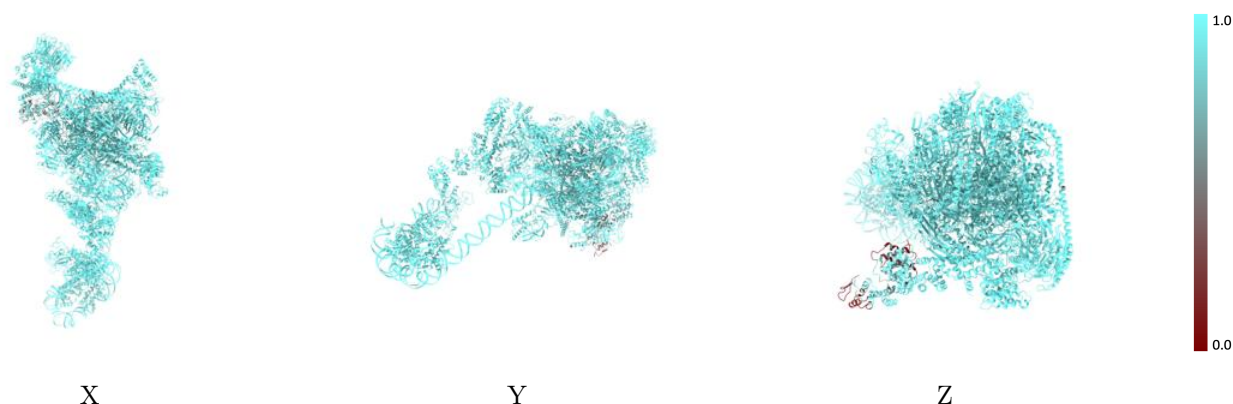
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



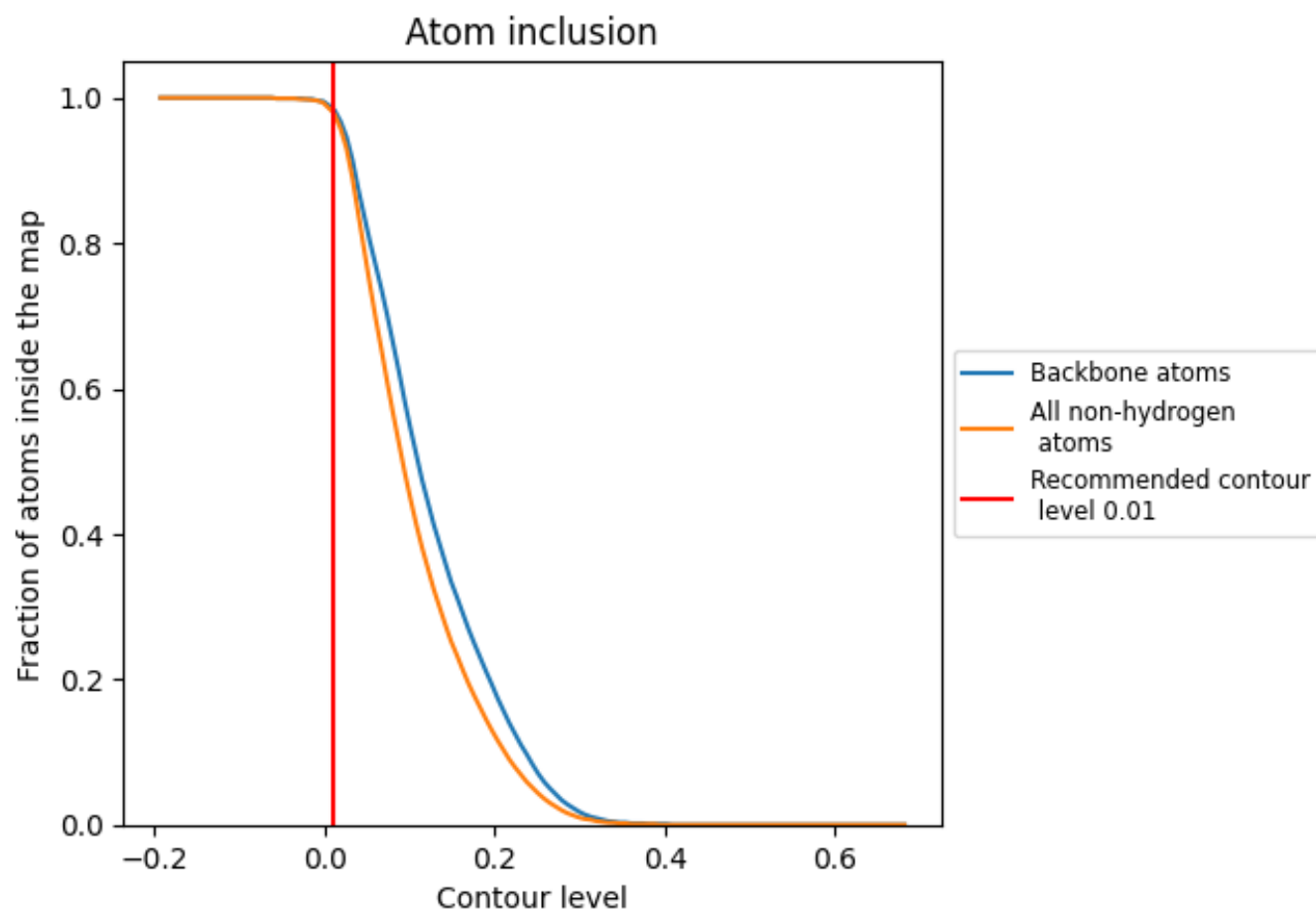
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9800	 0.2400
A	 0.9930	 0.3520
B	 0.9910	 0.3820
C	 0.9970	 0.4190
D	 0.9880	 0.1880
E	 0.9940	 0.3350
F	 0.9870	 0.3930
G	 0.9890	 0.2060
H	 0.9840	 0.3950
I	 0.9890	 0.3460
J	 0.9900	 0.3930
K	 0.9970	 0.4010
L	 1.0000	 0.3580
M	 0.9950	 0.1470
N	 1.0000	 0.2300
O	 1.0000	 0.0150
P	 1.0000	 0.2090
Q	 0.8850	 0.0790
R	 0.9670	 0.0920
S	 1.0000	 0.2400
T	 1.0000	 0.2210
U	 0.9930	 0.0160
V	 0.8710	 0.0570
W	 1.0000	 0.1550
X	 0.9940	 0.1760
Y	 0.9970	 -0.0020
Z	 0.9990	 0.0700
a	 0.9870	 0.3390
b	 0.9980	 0.3680
c	 0.9870	 0.3220
d	 0.9890	 0.3130
e	 0.9810	 0.3320
f	 0.9800	 0.3550
g	 0.9920	 0.3260
h	 0.9880	 0.3260
l	 0.9970	 0.1220

