Full wwPDB EM Validation Report ⓘ

Jul 3, 2023 – 12:36 PM JST

PDB ID	:	8ITY
EMDB ID	:	EMD-35712
Title	:	human RNA polymerase III pre-initiation complex closed DNA 1
Authors	:	Hou, H.; Jin, Q.; Ren, Y.; Wang, Q.; Xu, Y.
Deposited on	:	2023-03-23
Resolution	:	3.90 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:

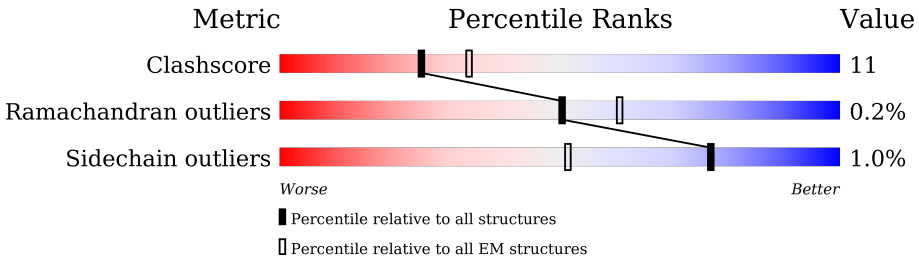
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1	368	25% 36% · 60%
2	3	411	55% 77% 13% 9%
3	4	1469	16% 23% · 75%
4	A	1390	· 70% 28% ·
5	B	1133	· 67% 29% · ·
6	C	346	· 71% 29% ·
7	D	148	14% 57% 25% 18%
8	E	210	· 68% 31%

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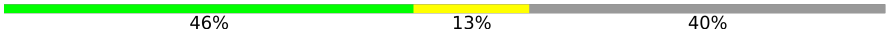
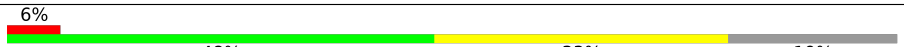
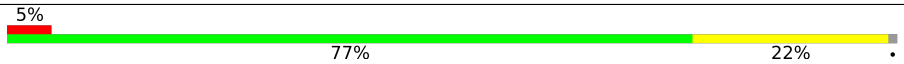
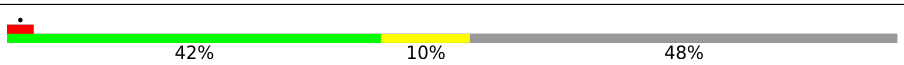
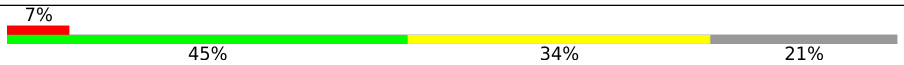
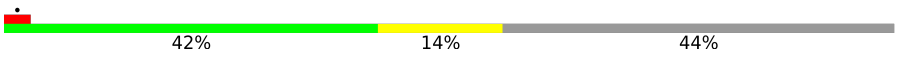
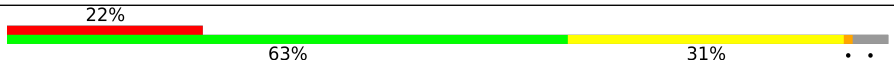
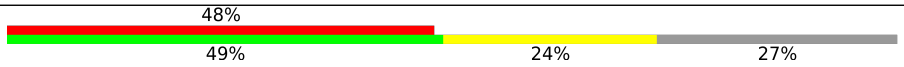
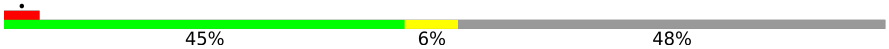
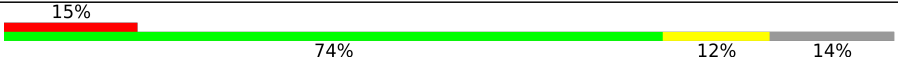
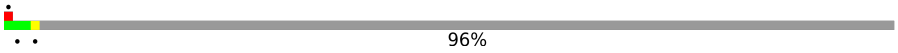
Mol	Chain	Length	Quality of chain
9	F	127	
10	G	204	
11	H	150	
12	I	108	
13	J	67	
14	K	133	
15	L	58	
16	M	708	
17	N	317	
18	O	534	
19	P	316	
20	Q	223	
21	U	339	
22	V	419	
23	W	2624	
24	X	464	
25	Y	464	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 57140 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 snRNA-activating protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	146	1233	804	212	209	8	0	0

- Molecule 2 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	374	3037	1925	521	570	21	0	0

- Molecule 3 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	365	3058	1921	573	555	9	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	1378	10814	6850	1886	2005	73	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	1105	8741	5538	1529	1605	69	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	343	2736	1723	488	514	11	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	122	Total	C	N	O	S	0	0
			985	614	172	196	3		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	209	Total	C	N	O	S	0	0
			1715	1083	300	324	8		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	76	Total	C	N	O	S	0	0
			610	392	103	110	5		

- Molecule 10 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	166	Total	C	N	O	S	0	0
			1337	876	211	245	5		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	56	Total	C	N	O	S	0	0
			435	272	81	76	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	24	ALA	SER	variant	UNP Q9Y2Y1

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	65	Total	C	N	O	S	0	0
			512	331	87	88	6		

- Molecule 14 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	103	Total	C	N	O	S	0	0
			822	513	145	157	7		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	394	Total	C	N	O	S	0	0
			3167	2013	550	584	20		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	146	Total	C	N	O	S	0	0
			1128	710	191	221	6		

- Molecule 18 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	512	Total	C	N	O	S	0	0
			4075	2565	712	774	24		

- Molecule 19 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	232	Total	C	N	O	S	0	0
			1837	1166	305	353	13		

- Molecule 20 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	87	Total	C	N	O	S	0	0
			754	488	126	134	6		

- Molecule 21 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	176	Total	C	N	O	S	1	0
			1396	907	244	238	7		

- Molecule 22 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	361	Total	C	N	O	S	1	0
			2853	1792	507	531	23		

- Molecule 23 is a protein called Transcription factor TFIIIB component B" homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	111	Total	C	N	O	S	0	0
			943	606	163	170	4		

- Molecule 24 is a DNA chain called DNA (82-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	82	Total	C	N	O	P	0	0
			1677	804	291	500	82		

- Molecule 25 is a DNA chain called DNA (82-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	82	Total	C	N	O	P	0	0
			1685	804	315	484	82		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Zn	0
			2	2	
26	B	1	Total	Zn	0
			1	1	

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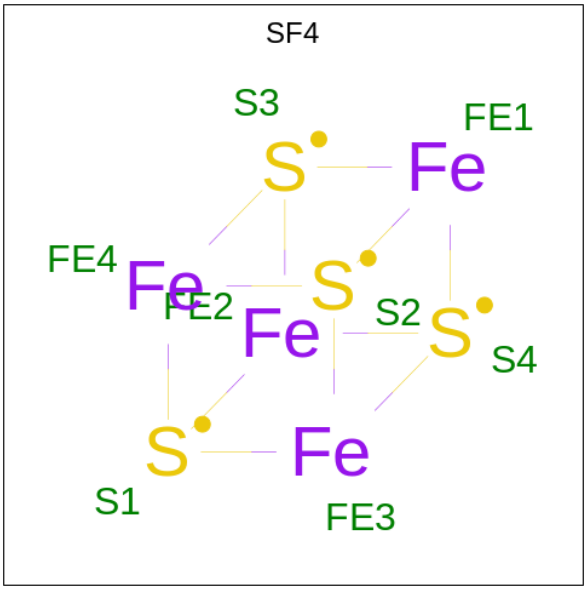
Mol	Chain	Residues	Atoms	AltConf
26	I	1	Total Zn 1 1	0
26	J	1	Total Zn 1 1	0
26	L	1	Total Zn 1 1	0
26	V	1	Total Zn 1 1	0

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



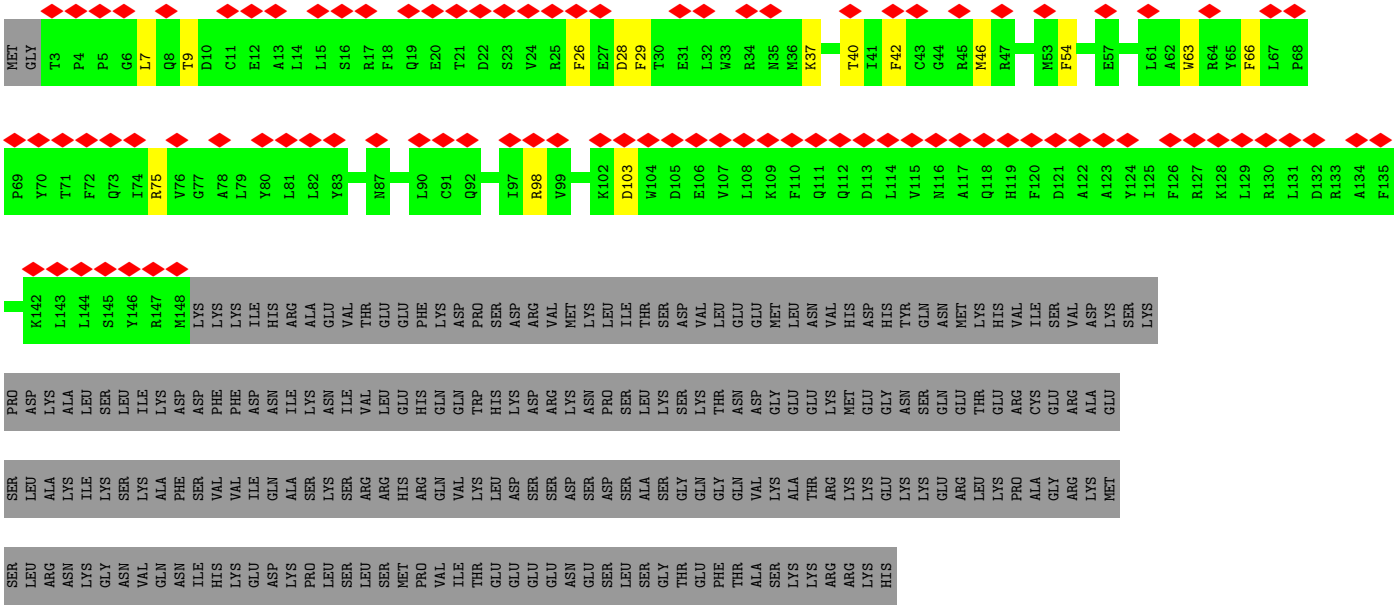
Mol	Chain	Residues	Atoms	AltConf
28	P	1	Total Fe S 8 4 4	0

3 Residue-property plots (i)

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

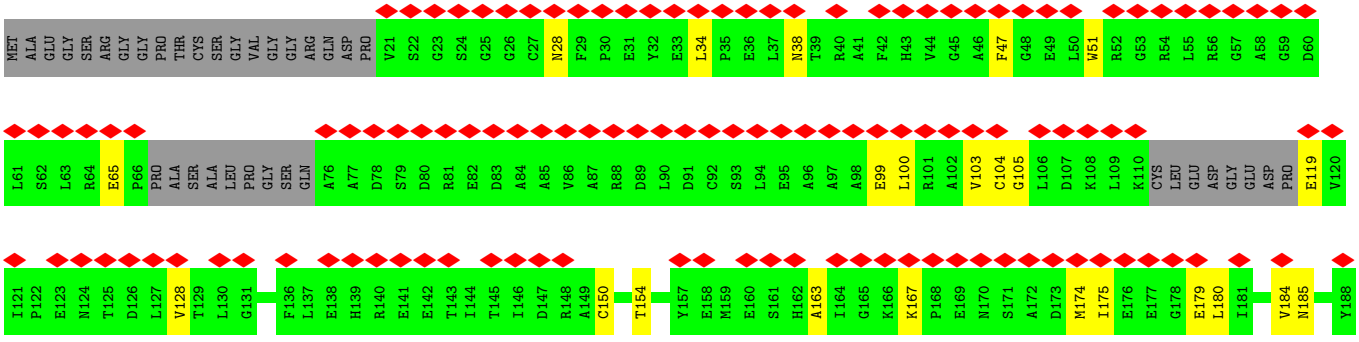
• Molecule 1: snRNA-activating protein complex subunit 1

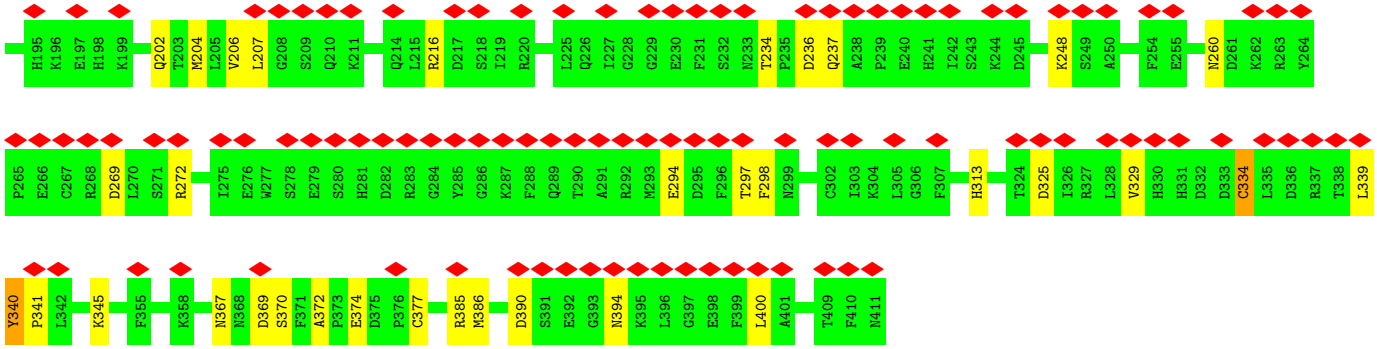
Chain 1:



• Molecule 2: snRNA-activating protein complex subunit 3

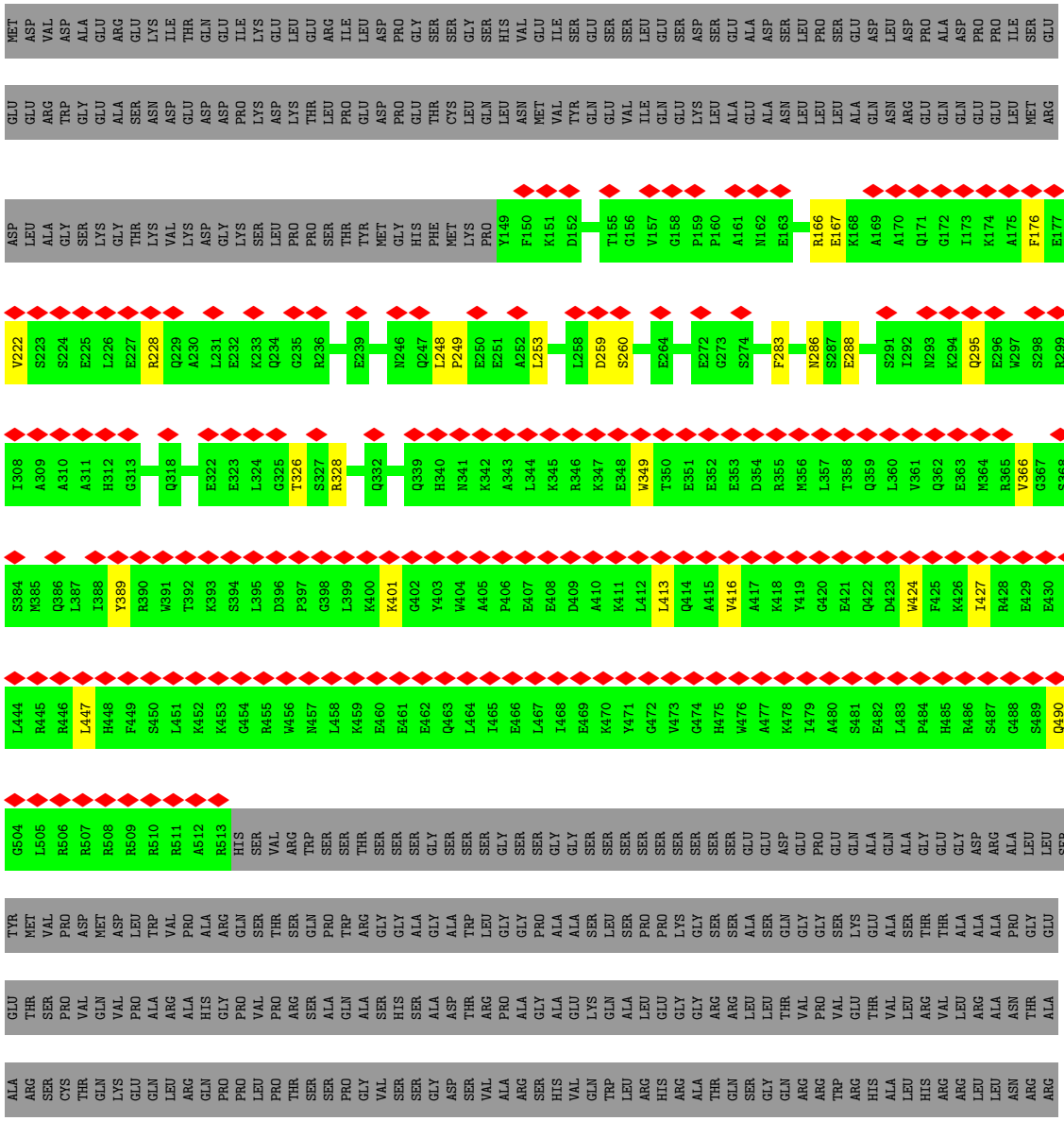
Chain 3:

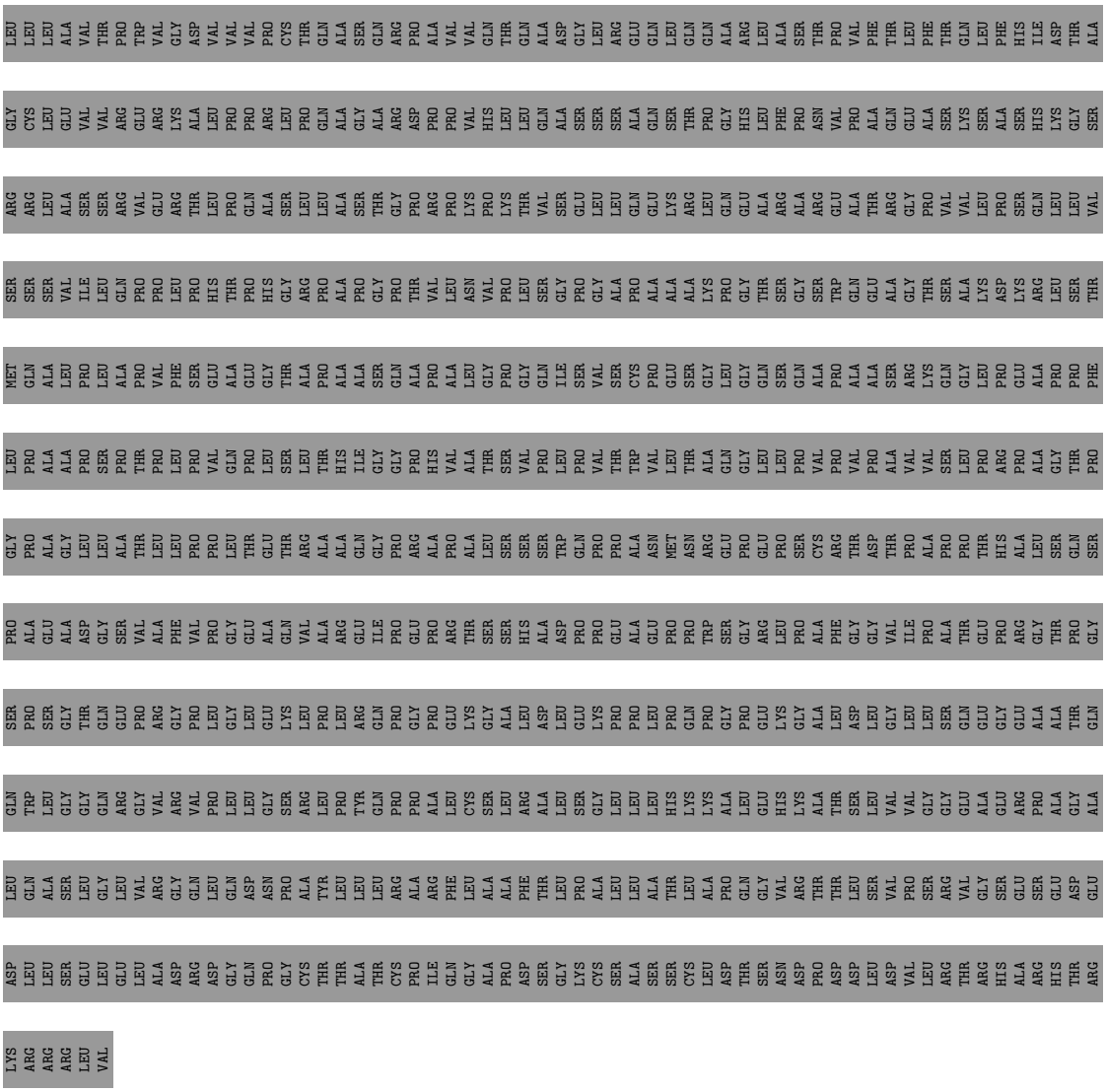




• Molecule 3: snRNA-activating protein complex subunit 4

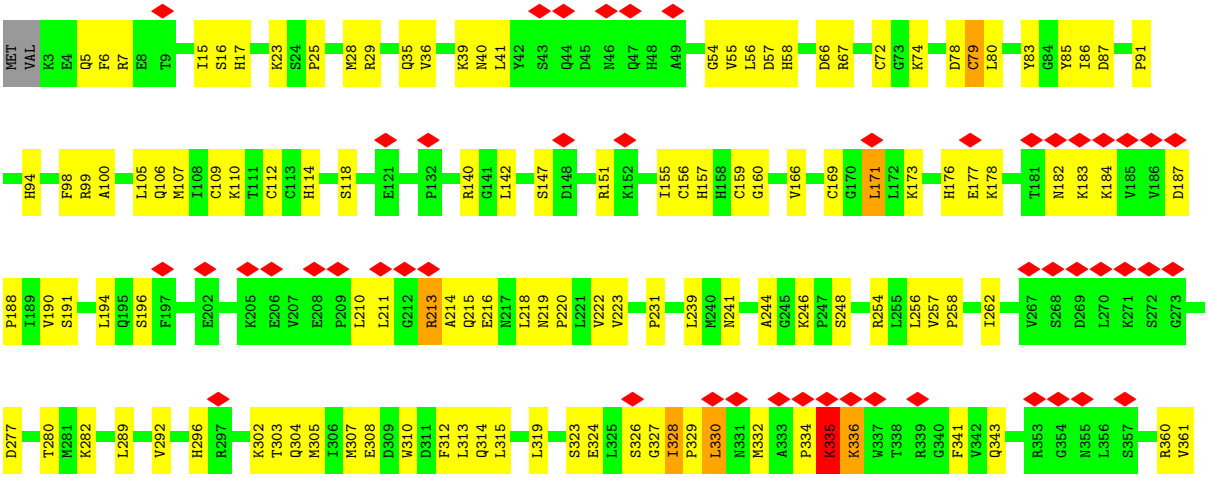
Chain 4:

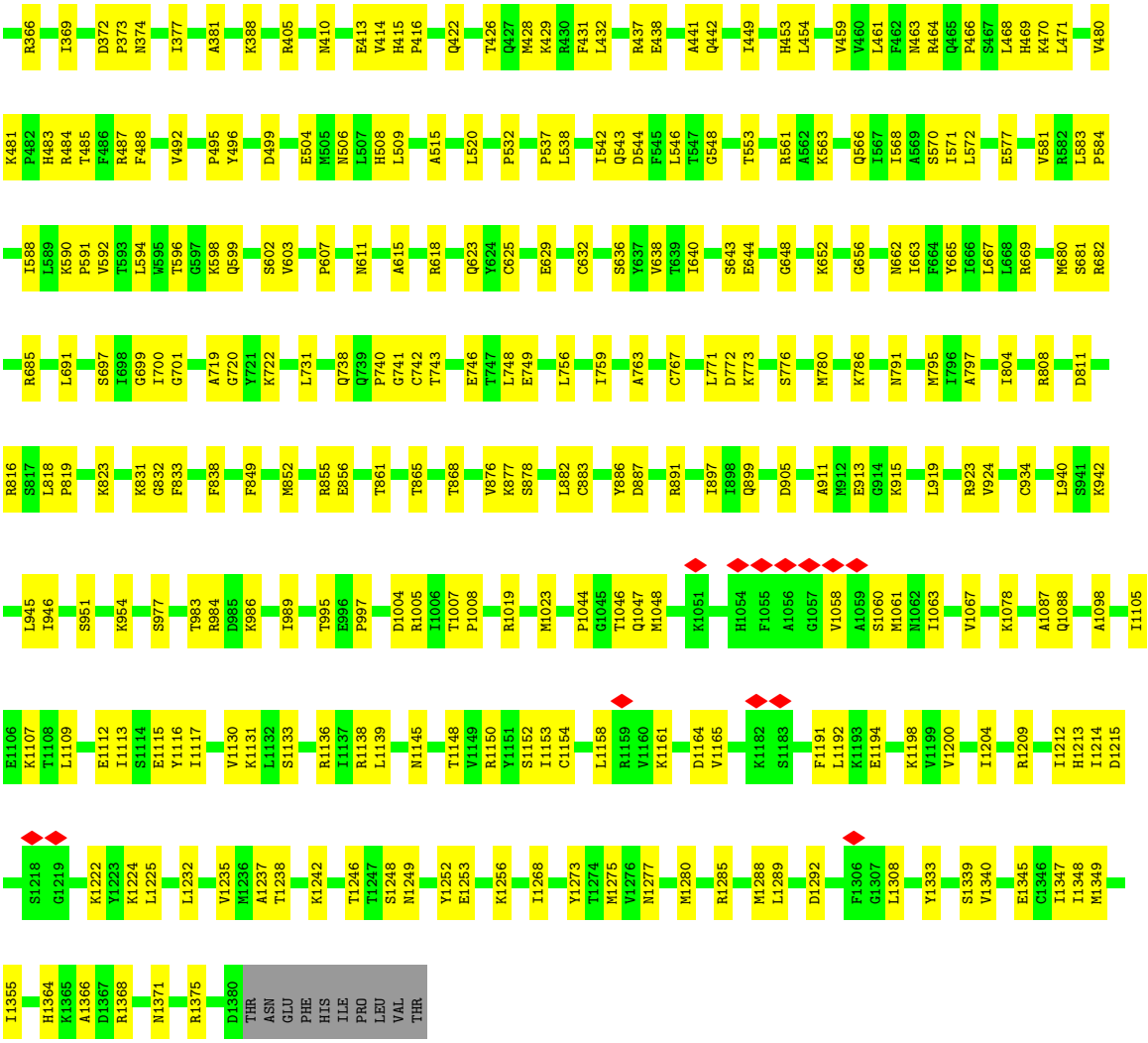




• Molecule 4: DNA-directed RNA polymerase III subunit RPC1

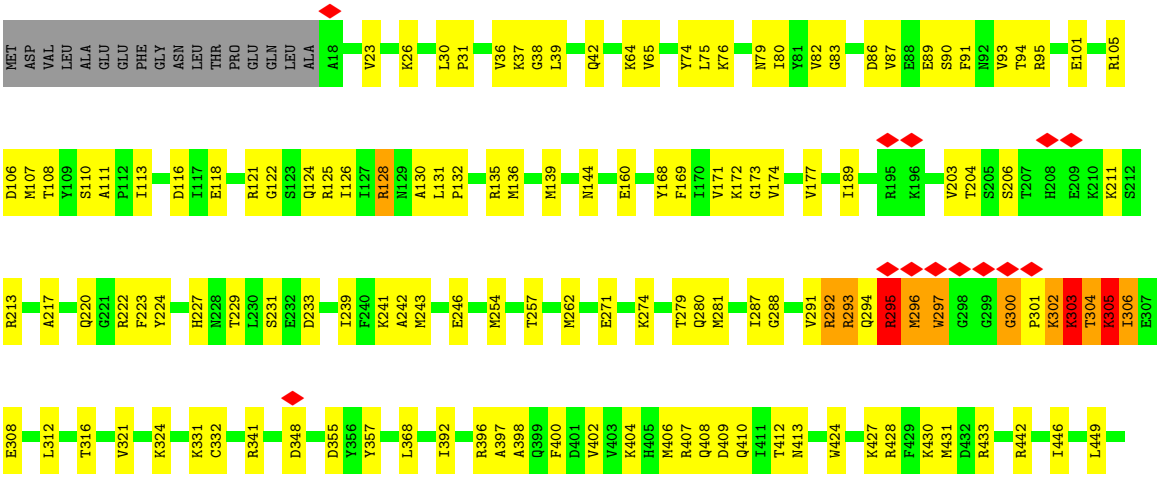
Chain A:

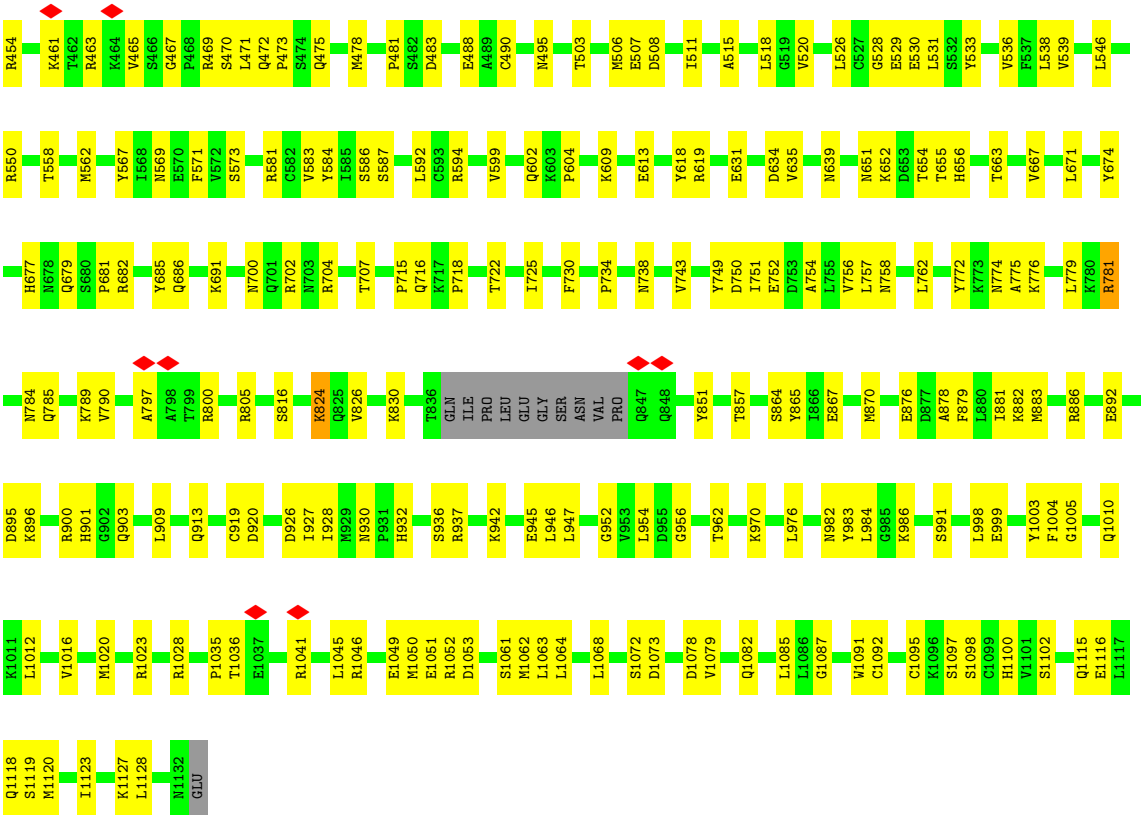




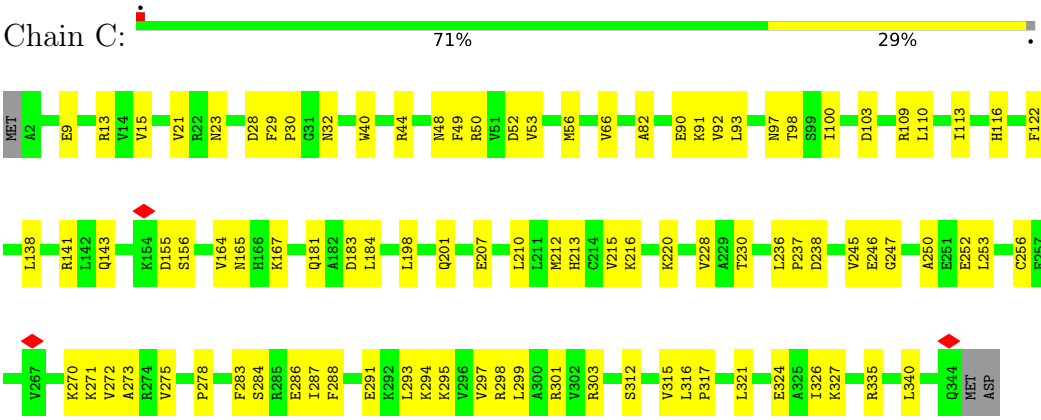
• Molecule 5: DNA-directed RNA polymerase III subunit RPC2

Chain B:

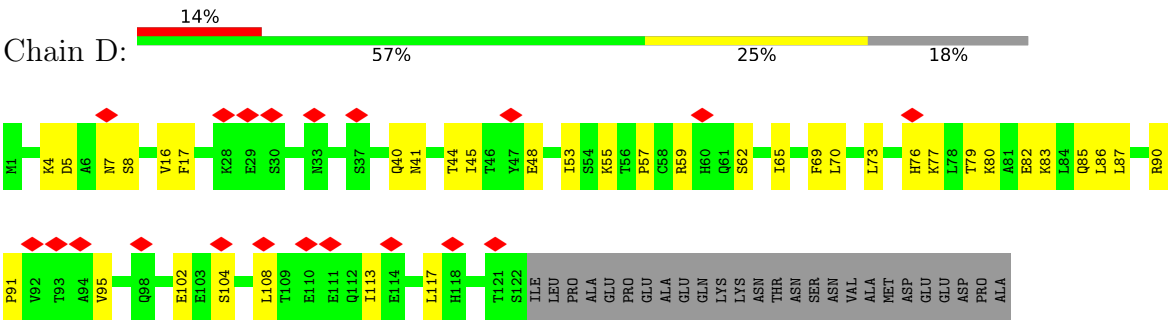




• Molecule 6: DNA-directed RNA polymerases I and III subunit RPAC1

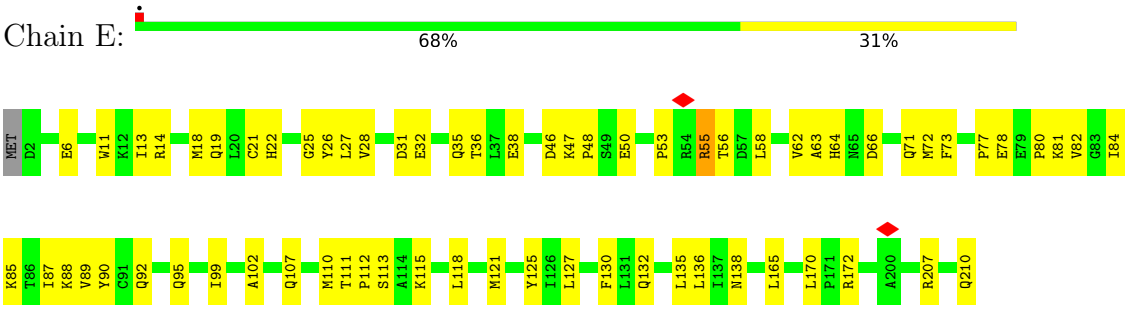


• Molecule 7: DNA-directed RNA polymerase III subunit RPC9



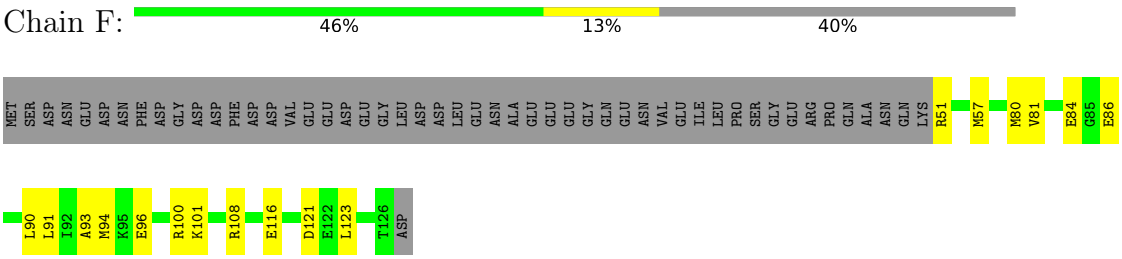
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



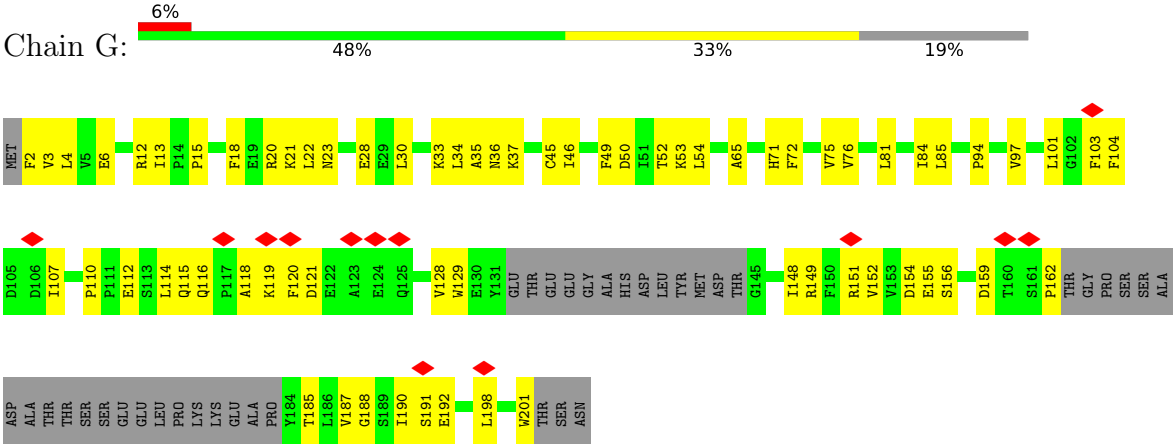
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



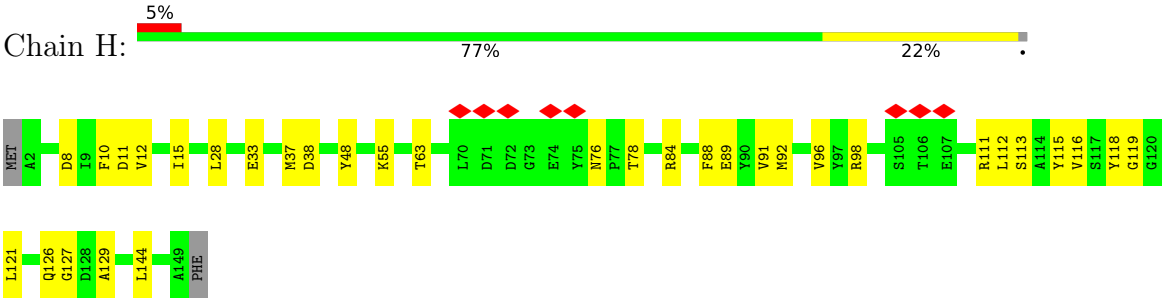
• Molecule 10: DNA-directed RNA polymerase III subunit RPC8

Chain G:



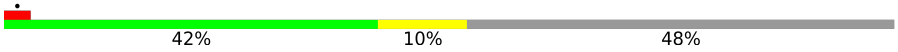
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

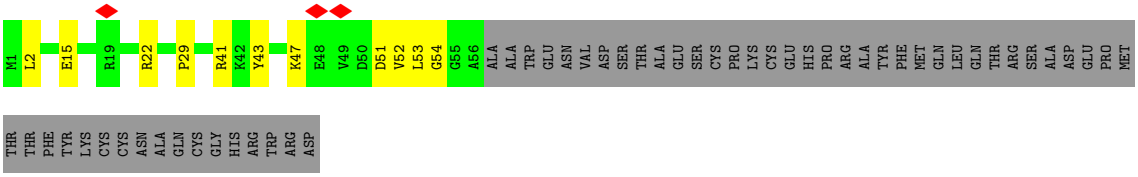
Chain H:



• Molecule 12: DNA-directed RNA polymerase III subunit RPC10

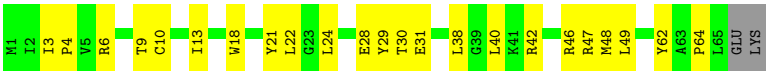
Chain I:





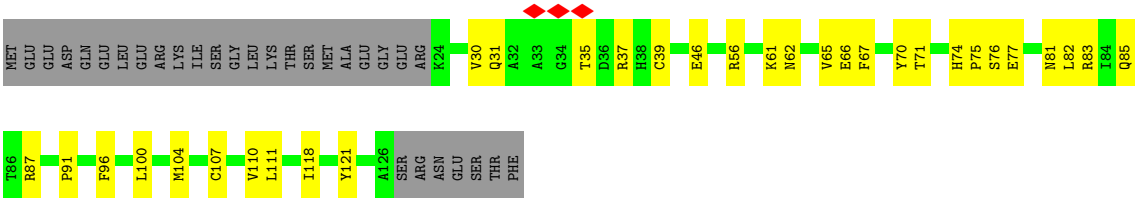
• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



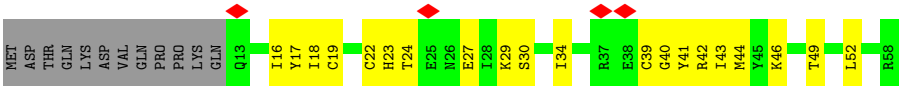
• Molecule 14: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:



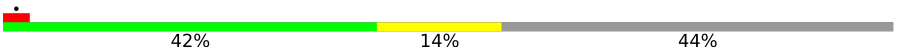
• Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC4

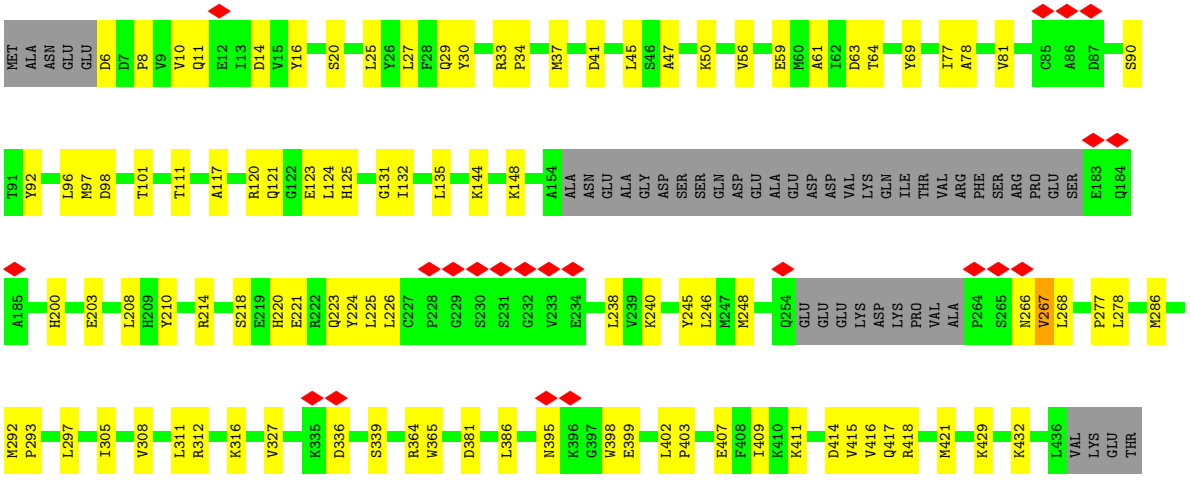
Chain L:

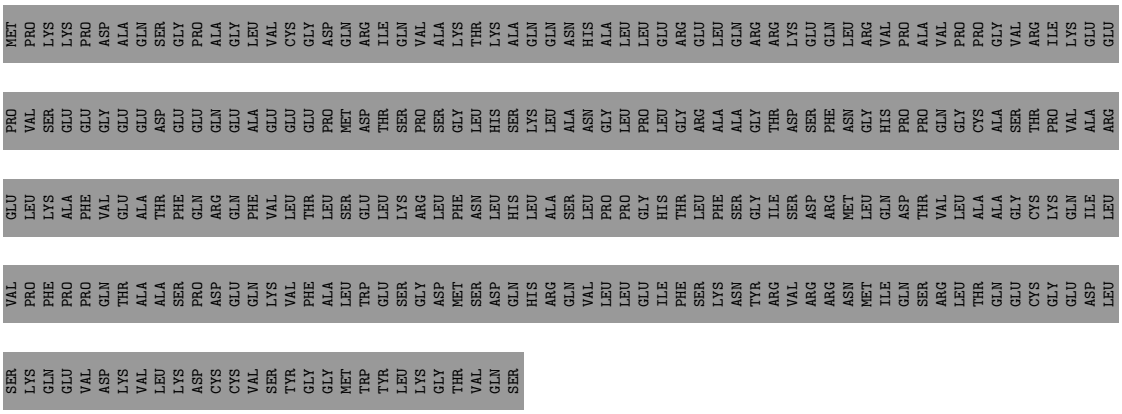


• Molecule 16: DNA-directed RNA polymerase III subunit RPC5

Chain M:

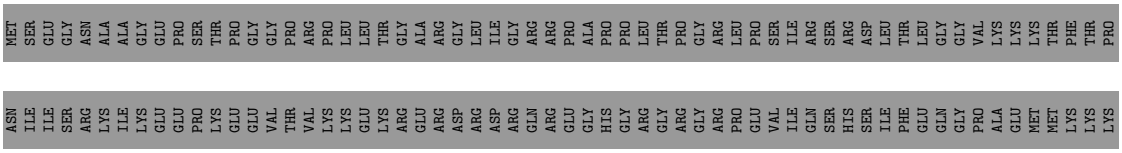


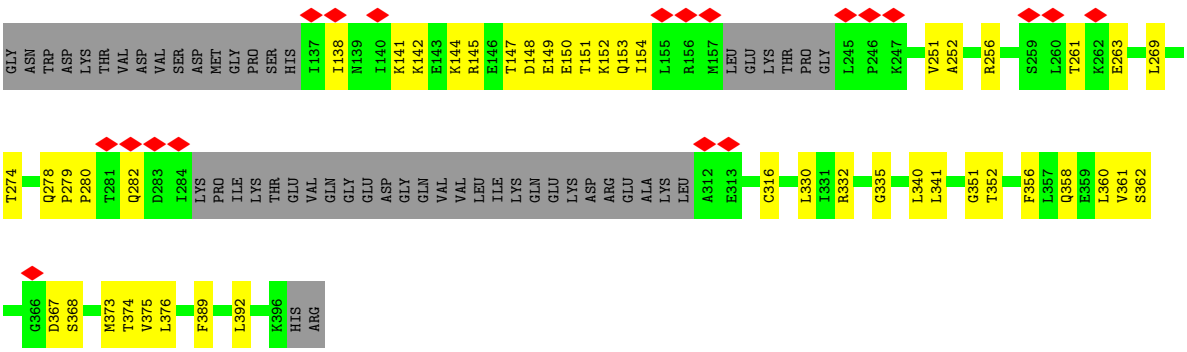




• Molecule 17: DNA-directed RNA polymerase III subunit RPC4

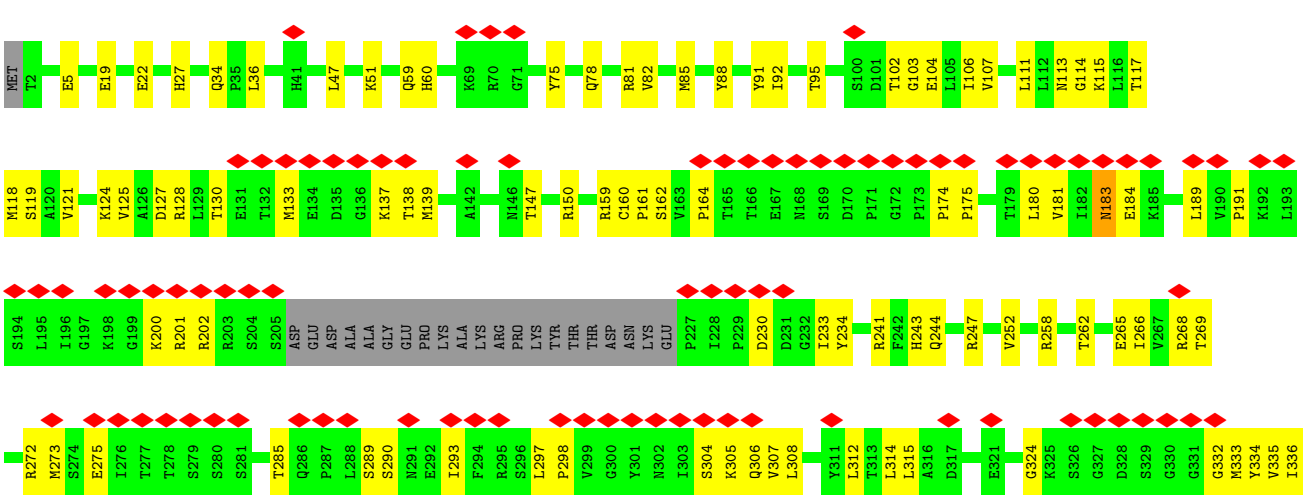
Chain N:

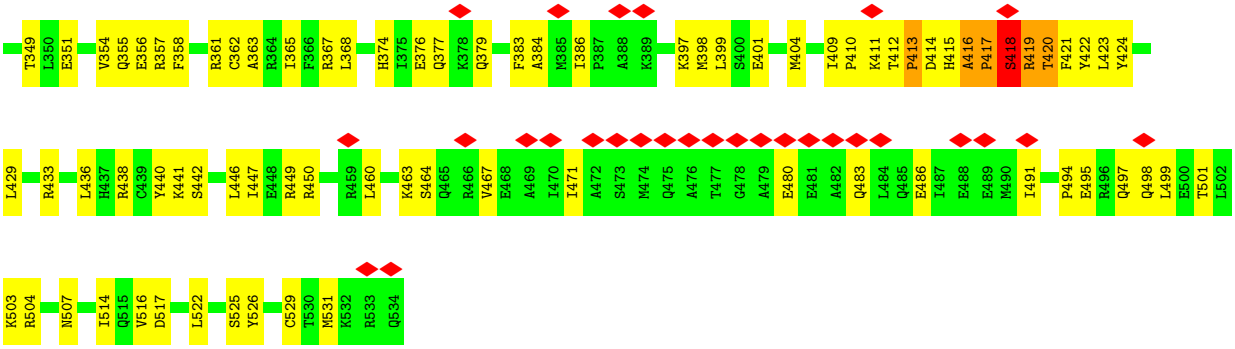




• Molecule 18: DNA-directed RNA polymerase III subunit RPC3

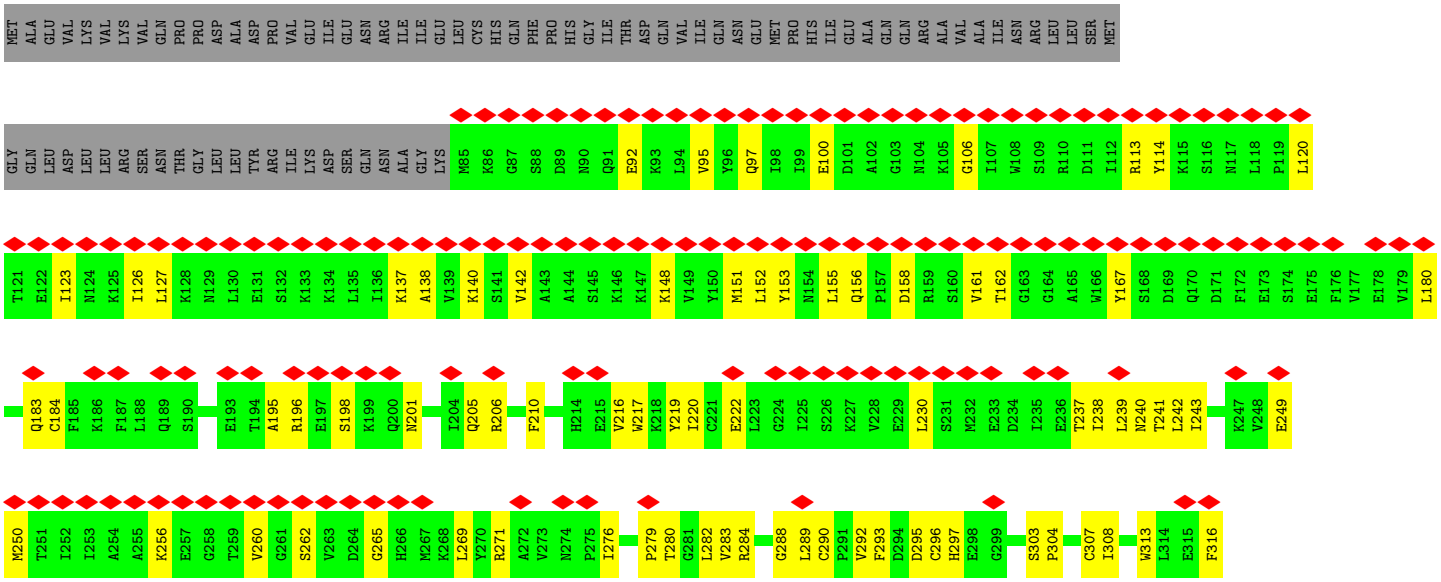
Chain O:





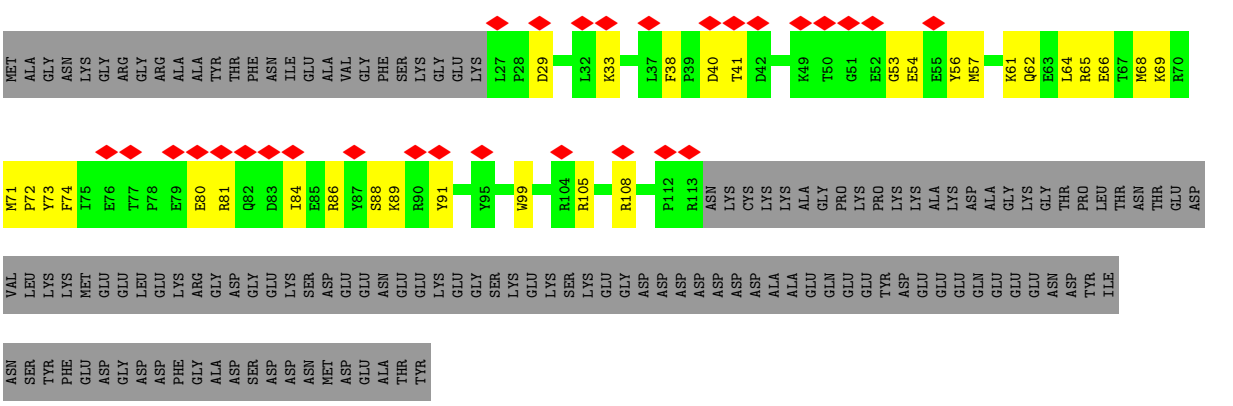
• Molecule 19: DNA-directed RNA polymerase III subunit RPC6

Chain P:



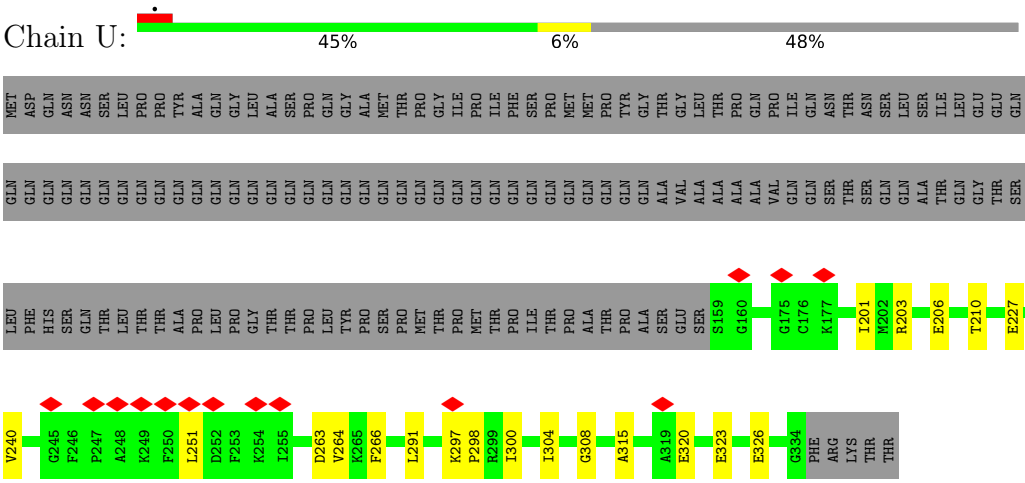
• Molecule 20: DNA-directed RNA polymerase III subunit RPC7

Chain Q:



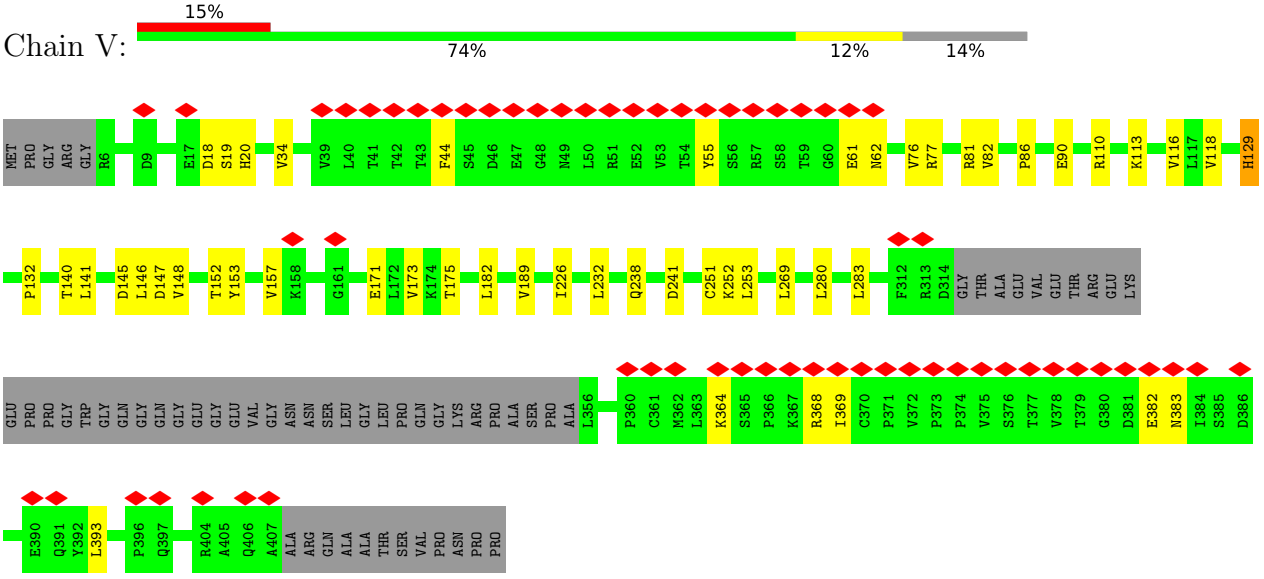
• Molecule 21: TATA-box-binding protein

Chain U:



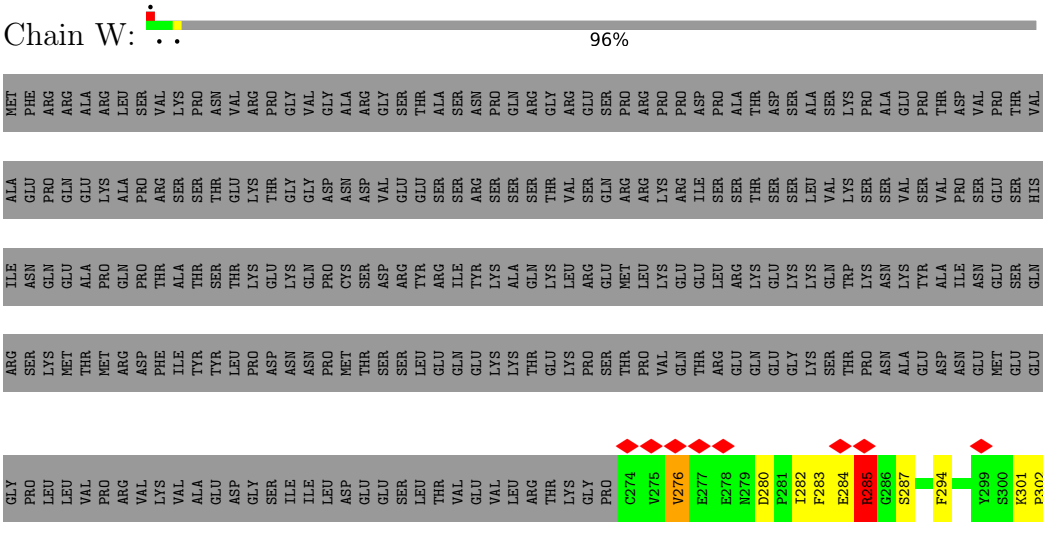
• Molecule 22: Transcription factor IIIB 50 kDa subunit

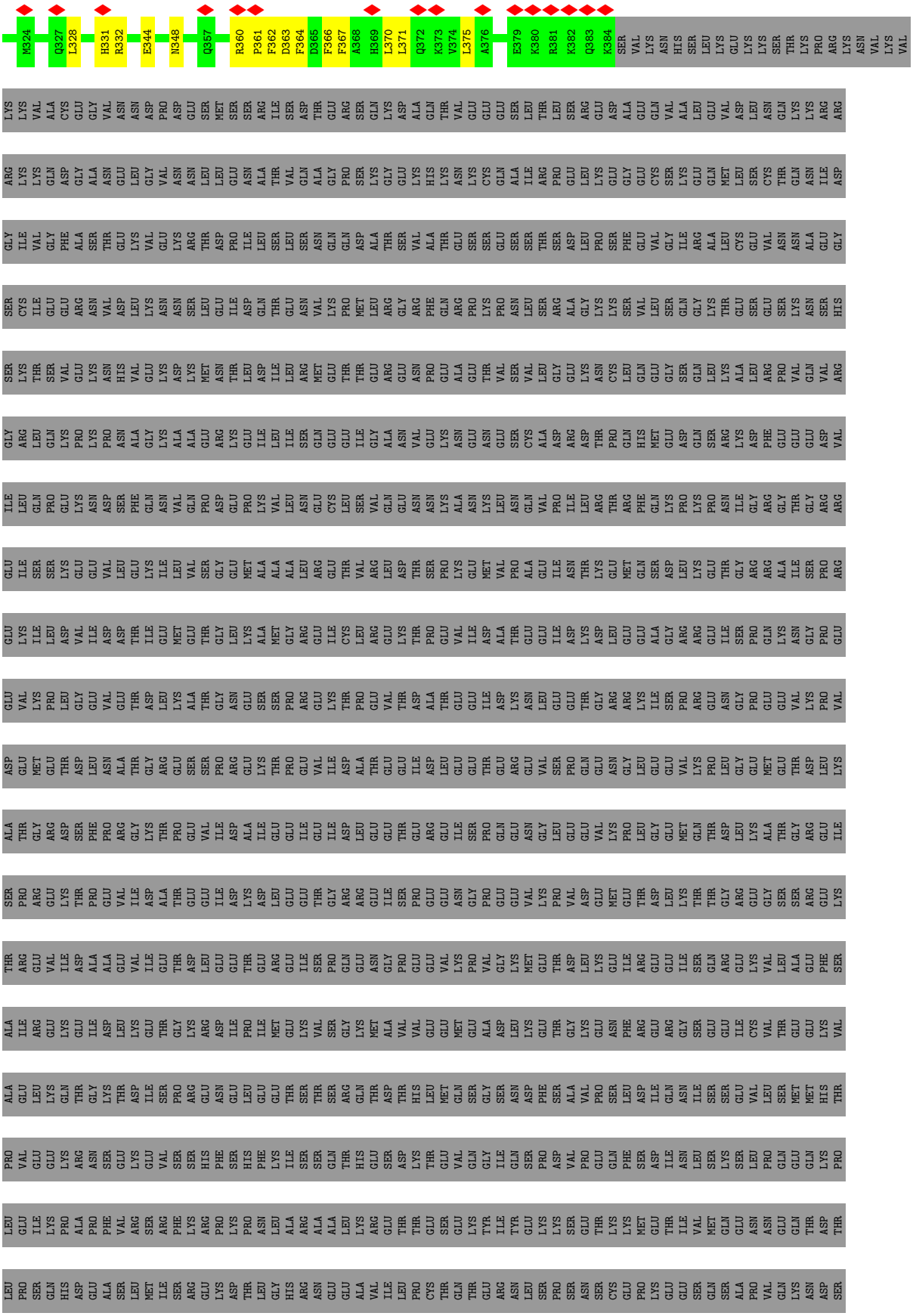
Chain V:

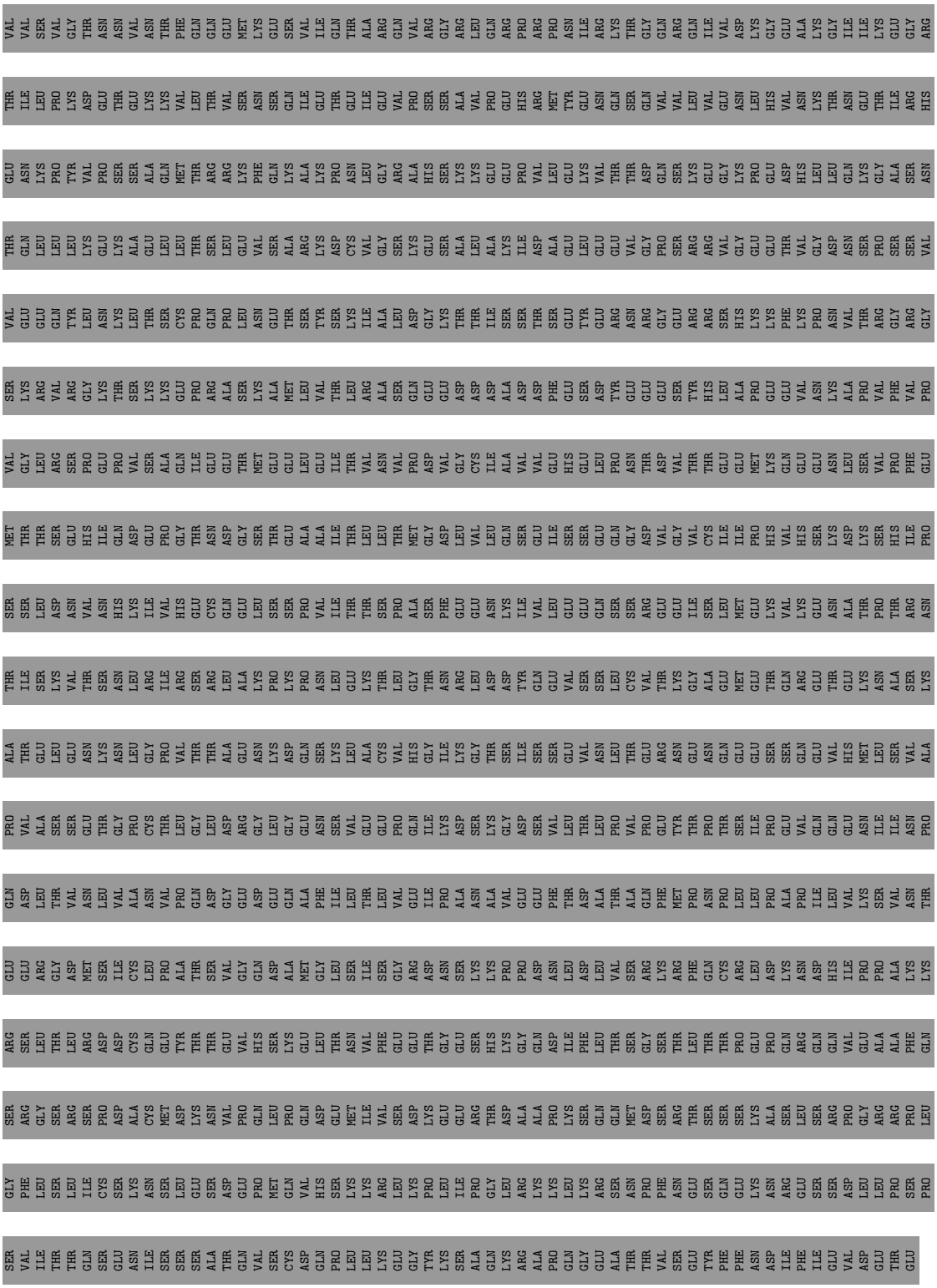


• Molecule 23: Transcription factor TFIIIB component B" homolog

Chain W:

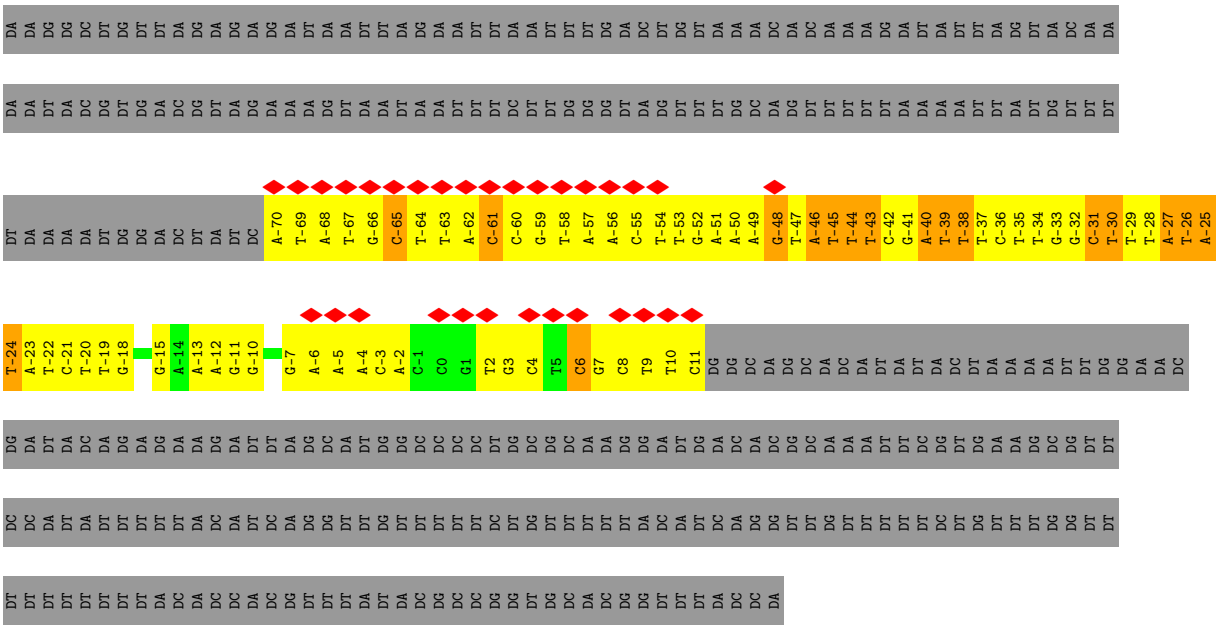



M324
Q327
L328
H331
R332
E344
N348
Q357
R360
P361
F362
D363
F364
D365
F366
F367
A368
H369
L370
L371
Q372
K373
V374
L375
A376
E379
K380
R381
K382
Q383
K384

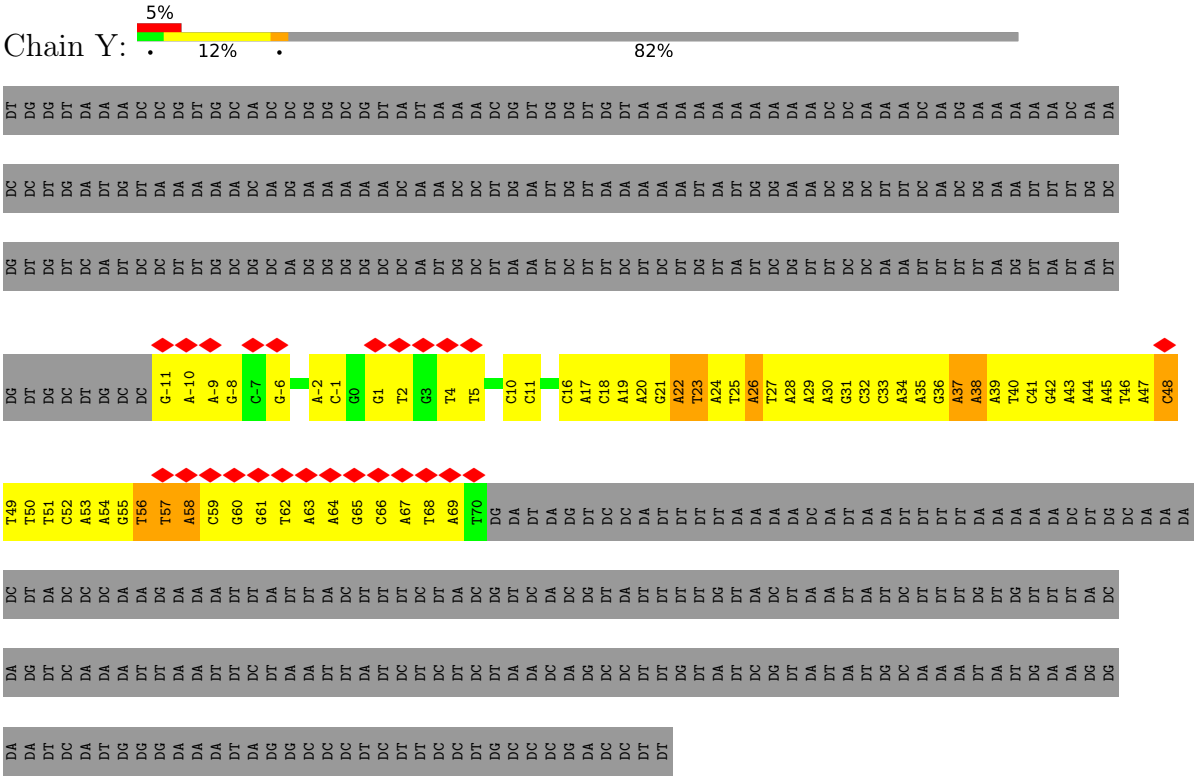


• Molecule 24: DNA (82-MER)

Chain X: 7% 12% 82%



• Molecule 25: DNA (82-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70361	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.020	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, SF4

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	1	0.24	0/1266	0.37	0/1708
2	3	0.23	0/3112	0.40	0/4206
3	4	0.23	0/3121	0.40	1/4181 (0.0%)
4	A	0.27	0/11008	0.49	0/14842
5	B	0.28	0/8910	0.50	2/12018 (0.0%)
6	C	0.27	0/2790	0.51	0/3782
7	D	0.23	0/997	0.46	0/1343
8	E	0.26	0/1745	0.51	0/2358
9	F	0.27	0/620	0.55	0/839
10	G	0.26	0/1374	0.49	0/1868
11	H	0.27	0/1207	0.51	0/1628
12	I	0.28	0/443	0.54	0/596
13	J	0.27	0/521	0.46	0/703
14	K	0.29	0/837	0.52	0/1129
15	L	0.34	0/394	0.69	0/524
16	M	0.25	0/3237	0.46	0/4377
17	N	0.25	0/1137	0.51	0/1530
18	O	0.25	0/4141	0.52	0/5592
19	P	0.25	0/1872	0.45	0/2525
20	Q	0.25	0/777	0.55	0/1050
21	U	0.24	0/1424	0.44	1/1918 (0.1%)
22	V	0.25	0/2904	0.50	3/3941 (0.1%)
23	W	0.26	0/967	0.49	2/1293 (0.2%)
24	X	0.47	0/1877	1.95	91/2895 (3.1%)
25	Y	0.48	0/1893	2.17	88/2919 (3.0%)
All	All	0.28	0/58574	0.73	188/79765 (0.2%)

There are no bond length outliers.

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	49	DT	OP1-P-O3'	-37.68	22.30	105.20
25	Y	67	DA	OP1-P-O3'	-37.60	22.48	105.20
25	Y	69	DA	OP1-P-O3'	-37.59	22.50	105.20
24	X	-70	DA	OP1-P-O3'	-37.54	22.62	105.20
25	Y	50	DT	OP1-P-O3'	-37.37	22.98	105.20
24	X	-45	DT	OP1-P-O3'	-37.13	23.51	105.20
25	Y	39	DA	OP1-P-O3'	-36.96	23.90	105.20
24	X	-44	DT	OP1-P-O3'	-36.45	25.00	105.20
25	Y	48	DC	OP1-P-O3'	-35.84	26.35	105.20
24	X	-46	DA	OP1-P-O3'	-35.02	28.14	105.20
22	V	364	LYS	C-N-CA	11.47	150.37	121.70
22	V	369	ILE	C-N-CA	11.29	149.94	121.70
24	X	-23	DA	OP2-P-O3'	9.08	125.18	105.20
24	X	-61	DC	OP1-P-O3'	8.63	124.19	105.20
24	X	-60	DC	OP1-P-OP2	-8.38	107.02	119.60
25	Y	21	DG	OP1-P-O3'	8.10	123.02	105.20
23	W	276	VAL	C-N-CA	7.91	141.48	121.70
22	V	129	HIS	C-N-CA	7.90	141.45	121.70
25	Y	22	DA	OP1-P-OP2	-7.40	108.50	119.60
24	X	-22	DT	OP1-P-OP2	-7.34	108.59	119.60
25	Y	23	DT	OP1-P-OP2	-7.24	108.74	119.60
24	X	-26	DT	OP1-P-OP2	-7.18	108.84	119.60
25	Y	26	DA	OP1-P-OP2	-6.96	109.16	119.60
24	X	-29	DT	OP1-P-OP2	-6.93	109.20	119.60
25	Y	28	DA	OP1-P-OP2	-6.92	109.23	119.60
24	X	-65	DC	OP1-P-OP2	-6.86	109.31	119.60
25	Y	25	DT	OP1-P-OP2	-6.86	109.32	119.60
25	Y	59	DC	OP1-P-OP2	-6.84	109.33	119.60
25	Y	56	DT	OP1-P-OP2	-6.82	109.36	119.60
24	X	-56	DA	OP1-P-OP2	-6.82	109.37	119.60
25	Y	27	DT	OP1-P-OP2	-6.80	109.39	119.60
25	Y	36	DG	OP1-P-OP2	-6.80	109.39	119.60
25	Y	37	DA	OP1-P-OP2	-6.80	109.39	119.60
24	X	-67	DT	OP1-P-OP2	-6.79	109.41	119.60
25	Y	52	DC	OP1-P-OP2	-6.79	109.41	119.60
24	X	-31	DC	OP1-P-OP2	-6.79	109.41	119.60
24	X	-27	DA	OP1-P-OP2	-6.79	109.42	119.60
25	Y	29	DA	OP1-P-OP2	-6.79	109.42	119.60
25	Y	24	DA	OP1-P-OP2	-6.78	109.43	119.60
24	X	-68	DA	OP1-P-OP2	-6.78	109.43	119.60
24	X	6	DC	C5'-C4'-O4'	6.78	122.18	109.30
24	X	-47	DT	OP1-P-OP2	-6.78	109.44	119.60
25	Y	33	DC	OP1-P-OP2	-6.78	109.44	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	X	-52	DG	OP1-P-OP2	-6.77	109.44	119.60
24	X	-54	DT	OP1-P-OP2	-6.77	109.44	119.60
25	Y	32	DC	OP1-P-OP2	-6.77	109.45	119.60
24	X	-57	DA	OP1-P-OP2	-6.77	109.45	119.60
24	X	-55	DC	OP1-P-OP2	-6.76	109.45	119.60
24	X	-40	DA	OP1-P-OP2	-6.76	109.45	119.60
25	Y	43	DA	OP1-P-OP2	-6.76	109.46	119.60
24	X	-62	DA	OP1-P-OP2	-6.76	109.46	119.60
24	X	-34	DT	OP1-P-OP2	-6.76	109.46	119.60
25	Y	63	DA	OP1-P-OP2	-6.76	109.46	119.60
24	X	-41	DG	OP1-P-OP2	-6.76	109.46	119.60
24	X	-66	DG	OP1-P-OP2	-6.76	109.47	119.60
25	Y	46	DT	OP1-P-OP2	-6.76	109.46	119.60
24	X	-30	DT	OP1-P-OP2	-6.75	109.47	119.60
24	X	-64	DT	OP1-P-OP2	-6.75	109.47	119.60
25	Y	30	DA	OP1-P-OP2	-6.75	109.47	119.60
25	Y	39	DA	OP1-P-OP2	-6.75	109.47	119.60
25	Y	42	DG	OP1-P-OP2	-6.75	109.48	119.60
24	X	-32	DG	OP1-P-OP2	-6.75	109.48	119.60
25	Y	69	DA	OP1-P-OP2	-6.75	109.48	119.60
25	Y	66	DC	OP1-P-OP2	-6.74	109.48	119.60
25	Y	44	DA	OP1-P-OP2	-6.74	109.49	119.60
24	X	-46	DA	OP1-P-OP2	-6.74	109.49	119.60
25	Y	62	DT	OP1-P-OP2	-6.74	109.49	119.60
24	X	-35	DT	OP1-P-OP2	-6.74	109.50	119.60
25	Y	48	DC	OP1-P-OP2	-6.74	109.50	119.60
24	X	-70	DA	OP1-P-OP2	-6.73	109.50	119.60
24	X	-28	DT	OP1-P-OP2	-6.73	109.50	119.60
25	Y	31	DG	OP1-P-OP2	-6.73	109.50	119.60
25	Y	64	DA	OP1-P-OP2	-6.73	109.50	119.60
24	X	-50	DA	OP1-P-OP2	-6.73	109.50	119.60
25	Y	58	DA	OP1-P-OP2	-6.72	109.52	119.60
24	X	-23	DA	OP1-P-OP2	-6.72	109.52	119.60
25	Y	45	DA	OP1-P-OP2	-6.72	109.52	119.60
24	X	-59	DG	OP1-P-OP2	-6.72	109.53	119.60
24	X	-39	DT	OP1-P-OP2	-6.72	109.53	119.60
24	X	-42	DC	OP1-P-OP2	-6.71	109.53	119.60
25	Y	65	DG	OP1-P-OP2	-6.71	109.53	119.60
25	Y	67	DA	OP1-P-OP2	-6.71	109.53	119.60
25	Y	60	DG	OP1-P-OP2	-6.71	109.53	119.60
24	X	-25	DA	OP1-P-OP2	-6.71	109.54	119.60
24	X	-24	DT	OP1-P-OP2	-6.70	109.55	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	55	DG	OP1-P-OP2	-6.70	109.55	119.60
24	X	-38	DT	OP1-P-OP2	-6.69	109.56	119.60
24	X	-51	DA	OP1-P-OP2	-6.69	109.57	119.60
25	Y	41	DC	OP1-P-OP2	-6.69	109.57	119.60
25	Y	57	DT	OP1-P-OP2	-6.69	109.57	119.60
24	X	-49	DA	OP1-P-OP2	-6.68	109.58	119.60
24	X	-58	DT	OP1-P-OP2	-6.67	109.59	119.60
25	Y	38	DA	OP1-P-OP2	-6.67	109.59	119.60
24	X	-37	DT	OP1-P-OP2	-6.67	109.60	119.60
24	X	-48	DG	OP1-P-OP2	-6.66	109.61	119.60
25	Y	35	DA	OP1-P-OP2	-6.65	109.62	119.60
25	Y	47	DA	OP1-P-OP2	-6.65	109.62	119.60
24	X	-63	DT	OP1-P-OP2	-6.64	109.64	119.60
24	X	-36	DC	OP1-P-OP2	-6.62	109.68	119.60
25	Y	53	DA	OP1-P-OP2	-6.61	109.68	119.60
25	Y	34	DA	OP1-P-OP2	-6.58	109.73	119.60
24	X	-33	DG	OP1-P-OP2	-6.57	109.74	119.60
25	Y	61	DG	OP1-P-OP2	-6.51	109.83	119.60
24	X	-27	DA	OP2-P-O3'	6.47	119.44	105.20
25	Y	54	DA	OP1-P-OP2	-6.17	110.34	119.60
24	X	-61	DC	OP1-P-OP2	-6.17	110.34	119.60
24	X	-30	DT	OP2-P-O3'	6.03	118.47	105.20
25	Y	55	DG	OP2-P-O3'	5.92	118.23	105.20
25	Y	26	DA	OP2-P-O3'	5.89	118.15	105.20
25	Y	31	DG	OP1-P-O3'	5.81	117.98	105.20
25	Y	28	DA	OP1-P-O3'	5.80	117.97	105.20
25	Y	35	DA	OP1-P-O3'	5.78	117.92	105.20
25	Y	25	DT	OP1-P-O3'	5.78	117.91	105.20
25	Y	22	DA	OP1-P-O3'	5.74	117.83	105.20
25	Y	43	DA	OP1-P-O3'	5.72	117.79	105.20
25	Y	58	DA	OP1-P-O3'	5.70	117.74	105.20
24	X	-66	DG	OP1-P-O3'	5.69	117.71	105.20
25	Y	32	DC	OP1-P-O3'	5.67	117.67	105.20
24	X	-29	DT	OP1-P-O3'	5.66	117.66	105.20
25	Y	23	DT	OP1-P-O3'	5.64	117.62	105.20
24	X	-33	DG	OP1-P-O3'	5.64	117.60	105.20
24	X	-55	DC	OP1-P-O3'	5.63	117.60	105.20
24	X	-36	DC	OP2-P-O3'	5.62	117.56	105.20
24	X	-40	DA	OP1-P-O3'	5.61	117.54	105.20
25	Y	45	DA	OP1-P-O3'	5.60	117.53	105.20
25	Y	47	DA	OP1-P-O3'	5.59	117.49	105.20
24	X	-42	DC	OP1-P-O3'	5.58	117.48	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	X	-56	DA	OP1-P-O3'	5.58	117.48	105.20
24	X	-69	DT	OP1-P-O3'	5.58	117.47	105.20
24	X	-63	DT	OP1-P-O3'	5.57	117.45	105.20
24	X	-65	DC	OP1-P-O3'	5.56	117.42	105.20
24	X	-24	DT	OP1-P-O3'	5.55	117.41	105.20
25	Y	24	DA	OP1-P-O3'	5.55	117.41	105.20
25	Y	44	DA	OP1-P-O3'	5.54	117.39	105.20
25	Y	57	DT	OP1-P-O3'	5.54	117.38	105.20
25	Y	65	DG	OP1-P-O3'	5.53	117.36	105.20
24	X	-53	DT	OP1-P-O3'	5.52	117.35	105.20
25	Y	29	DA	OP1-P-O3'	5.52	117.35	105.20
25	Y	42	DG	OP1-P-O3'	5.52	117.35	105.20
24	X	-68	DA	OP1-P-O3'	5.52	117.34	105.20
25	Y	36	DG	OP1-P-O3'	5.52	117.34	105.20
24	X	-49	DA	OP1-P-O3'	5.51	117.33	105.20
25	Y	66	DC	OP1-P-O3'	5.51	117.32	105.20
25	Y	59	DC	OP1-P-O3'	5.50	117.30	105.20
24	X	-37	DT	OP1-P-O3'	5.49	117.29	105.20
24	X	-26	DT	OP1-P-O3'	5.49	117.28	105.20
24	X	-48	DG	OP1-P-O3'	5.49	117.28	105.20
25	Y	51	DT	OP1-P-O3'	5.48	117.25	105.20
24	X	-60	DC	OP1-P-O3'	5.45	117.18	105.20
24	X	-57	DA	OP1-P-O3'	5.44	117.18	105.20
24	X	-58	DT	OP1-P-O3'	5.44	117.17	105.20
24	X	-32	DG	OP1-P-O3'	5.44	117.16	105.20
25	Y	41	DC	OP1-P-O3'	5.43	117.15	105.20
25	Y	52	DC	OP1-P-O3'	5.43	117.14	105.20
25	Y	40	DT	OP1-P-O3'	5.42	117.12	105.20
24	X	-39	DT	OP1-P-O3'	5.42	117.12	105.20
25	Y	68	DT	OP1-P-O3'	5.40	117.08	105.20
25	Y	64	DA	OP1-P-O3'	5.39	117.07	105.20
25	Y	61	DG	OP2-P-O3'	5.38	117.05	105.20
24	X	-47	DT	OP1-P-O3'	5.38	117.03	105.20
25	Y	34	DA	OP1-P-O3'	5.38	117.03	105.20
25	Y	54	DA	OP1-P-O3'	5.36	117.00	105.20
25	Y	46	DT	OP1-P-O3'	5.36	116.99	105.20
24	X	-38	DT	OP1-P-O3'	5.35	116.96	105.20
24	X	-35	DT	OP1-P-O3'	5.33	116.92	105.20
24	X	-64	DT	OP1-P-O3'	5.32	116.89	105.20
24	X	-59	DG	OP1-P-O3'	5.31	116.88	105.20
24	X	-67	DT	OP1-P-O3'	5.30	116.87	105.20
24	X	-51	DA	OP1-P-O3'	5.30	116.86	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	295	ARG	CD-NE-CZ	5.30	131.02	123.60
5	B	781	ARG	N-CA-C	-5.30	96.70	111.00
24	X	-52	DG	OP1-P-O3'	5.28	116.82	105.20
25	Y	38	DA	OP1-P-O3'	5.25	116.74	105.20
25	Y	63	DA	OP1-P-O3'	5.24	116.73	105.20
25	Y	27	DT	OP1-P-O3'	5.24	116.72	105.20
23	W	285	ARG	NE-CZ-NH1	5.24	122.92	120.30
24	X	-50	DA	OP1-P-O3'	5.21	116.67	105.20
25	Y	62	DT	OP1-P-O3'	5.21	116.66	105.20
24	X	-53	DT	OP1-P-OP2	-5.19	111.81	119.60
24	X	-31	DC	OP1-P-O3'	5.18	116.59	105.20
24	X	-43	DT	OP1-P-O3'	5.12	116.47	105.20
21	U	251	LEU	C-N-CA	5.12	134.49	121.70
25	Y	37	DA	OP1-P-O3'	5.11	116.43	105.20
3	4	326	THR	C-N-CA	5.09	134.42	121.70
25	Y	60	DG	OP1-P-O3'	5.09	116.39	105.20
24	X	-28	DT	OP1-P-O3'	5.05	116.30	105.20
24	X	-34	DT	OP1-P-O3'	5.03	116.27	105.20
24	X	-25	DA	OP1-P-O3'	5.01	116.22	105.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1233	0	1231	7	0
2	3	3037	0	2911	38	0
3	4	3058	0	3064	19	0
4	A	10814	0	11059	322	0
5	B	8741	0	8867	286	0
6	C	2736	0	2712	68	0
7	D	985	0	1006	37	0
8	E	1715	0	1733	43	0
9	F	610	0	642	9	0
10	G	1337	0	1306	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	H	1186	0	1147	23	0
12	I	435	0	436	10	0
13	J	512	0	526	19	0
14	K	822	0	810	35	0
15	L	388	0	395	13	0
16	M	3167	0	3184	74	0
17	N	1128	0	1181	36	0
18	O	4075	0	4149	137	0
19	P	1837	0	1835	60	0
20	Q	754	0	759	22	0
21	U	1396	0	1490	15	0
22	V	2853	0	2890	39	0
23	W	943	0	924	54	0
24	X	1677	0	932	42	0
25	Y	1685	0	924	34	0
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	I	1	0	0	0	0
26	J	1	0	0	0	0
26	L	1	0	0	0	0
26	V	1	0	0	0	0
27	A	1	0	0	0	0
28	P	8	0	0	0	0
All	All	57140	0	56113	1293	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1293) 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)
23:W:328:LEU:HD13	23:W:367:PHE:CE1	1.56	1.37
8:E:85:LYS:NZ	25:Y:-8:DG:OP2	1.71	1.23
23:W:363:ASP:OD2	23:W:366:PHE:HB3	1.28	1.22
23:W:328:LEU:CD1	23:W:367:PHE:CE1	2.24	1.18
5:B:287:ILE:O	5:B:291:VAL:HG23	1.48	1.13
23:W:363:ASP:CG	23:W:366:PHE:HB3	1.78	1.05
23:W:328:LEU:HD13	23:W:367:PHE:CZ	1.91	1.04
23:W:363:ASP:OD2	23:W:366:PHE:CB	2.06	1.03
5:B:131:LEU:HD13	23:W:287:SER:OG	1.60	1.01
5:B:404:LYS:NZ	22:V:140:THR:O	1.93	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:110:ARG:HB3	24:X:-18:DG:OP1	1.63	0.98
3:4:167:GLU:OE1	16:M:316:LYS:NZ	1.97	0.96
4:A:328:ILE:HB	4:A:329:PRO:HD2	1.48	0.96
4:A:429:LYS:O	22:V:34:VAL:HG22	1.65	0.95
4:A:315:LEU:HD22	4:A:329:PRO:CD	1.96	0.95
5:B:293:ARG:HB2	5:B:295:ARG:HD3	1.49	0.92
23:W:328:LEU:CD1	23:W:367:PHE:CZ	2.50	0.92
4:A:304:GLN:OE1	18:O:418:SER:HA	1.70	0.92
4:A:74:LYS:NZ	4:A:80:LEU:HD12	1.85	0.91
4:A:431:PHE:CE1	22:V:20:HIS:NE2	2.38	0.91
16:M:308:VAL:HG12	16:M:312:ARG:HH21	1.36	0.91
5:B:297:TRP:CE3	5:B:297:TRP:HA	2.05	0.90
11:H:98:ARG:HB3	11:H:115:TYR:HB2	1.57	0.87
2:3:372:ALA:HB1	2:3:377:CYS:SG	2.15	0.87
5:B:124:GLN:NE2	23:W:282:ILE:HB	1.90	0.86
18:O:357:ARG:HG2	19:P:289:LEU:HB3	1.57	0.86
4:A:431:PHE:CZ	22:V:20:HIS:NE2	2.43	0.86
4:A:72:CYS:HA	10:G:162:PRO:HG2	1.59	0.85
5:B:293:ARG:CZ	25:Y:5:DT:H72	2.07	0.85
5:B:302:LYS:HD2	5:B:308:GLU:HG3	1.59	0.84
6:C:49:PHE:HA	6:C:66:VAL:O	1.78	0.84
5:B:297:TRP:HA	5:B:297:TRP:HE3	1.39	0.83
4:A:720:GLY:HA3	4:A:759:ILE:HD11	1.60	0.83
2:3:234:THR:HG23	2:3:237:GLN:HB2	1.59	0.83
2:3:272:ARG:NH1	16:M:277:PRO:HB3	1.95	0.82
4:A:431:PHE:CZ	22:V:20:HIS:CD2	2.68	0.82
4:A:28:MET:HE3	4:A:256:LEU:HG	1.63	0.81
4:A:315:LEU:HD22	4:A:329:PRO:HD3	1.63	0.81
14:K:37:ARG:HB3	14:K:91:PRO:HA	1.63	0.80
4:A:414:VAL:HG12	4:A:416:PRO:HD2	1.63	0.80
23:W:328:LEU:HD12	23:W:367:PHE:CE1	2.18	0.79
5:B:131:LEU:CD1	23:W:287:SER:OG	2.33	0.77
5:B:722:THR:HG23	5:B:962:THR:HA	1.65	0.77
5:B:300:GLY:H	5:B:301:PRO:HD2	1.50	0.77
2:3:234:THR:HG23	2:3:234:THR:O	1.84	0.76
5:B:293:ARG:HD2	5:B:295:ARG:HD3	1.67	0.76
25:Y:-2:DA:H1'	25:Y:-1:DC:H5'	1.66	0.76
23:W:314:ALA:HB2	23:W:367:PHE:CE2	2.21	0.76
4:A:304:GLN:OE1	18:O:418:SER:CA	2.33	0.76
4:A:315:LEU:CD2	4:A:329:PRO:CD	2.64	0.76
14:K:66:GLU:HG2	14:K:87:ARG:HG2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:296:MET:SD	5:B:296:MET:N	2.61	0.74
5:B:302:LYS:CD	5:B:308:GLU:HG3	2.18	0.74
3:4:248:LEU:HD23	3:4:249:PRO:O	1.87	0.73
4:A:570:SER:HA	14:K:71:THR:HG21	1.70	0.73
18:O:361:ARG:HH21	18:O:386:ILE:HG12	1.51	0.73
22:V:110:ARG:HD3	24:X:-19:DT:H4'	1.71	0.73
10:G:114:LEU:HD21	10:G:192:GLU:H	1.54	0.73
4:A:6:PHE:HB2	10:G:37:LYS:HB3	1.70	0.73
5:B:738:ASN:O	13:J:47:ARG:NH1	2.22	0.73
16:M:117:ALA:HB1	16:M:124:LEU:HD11	1.71	0.73
4:A:615:ALA:H	4:A:643:SER:HB3	1.53	0.73
16:M:10:VAL:HG22	16:M:11:GLN:HG2	1.70	0.72
6:C:315:VAL:HG13	6:C:316:LEU:HD23	1.70	0.72
18:O:137:LYS:NZ	18:O:138:THR:O	2.22	0.72
15:L:39:CYS:SG	15:L:40:GLY:N	2.63	0.72
6:C:91:LYS:HB2	6:C:213:HIS:HB2	1.71	0.72
18:O:419:ARG:HG2	18:O:419:ARG:HH11	1.55	0.72
1:1:37:LYS:O	1:1:40:THR:HG23	1.89	0.72
16:M:64:THR:HG21	16:M:96:LEU:HD13	1.70	0.72
4:A:741:GLY:HA3	12:I:53:LEU:HD21	1.72	0.72
23:W:363:ASP:OD1	23:W:367:PHE:N	2.23	0.71
22:V:110:ARG:CB	24:X:-18:DG:OP1	2.38	0.71
16:M:27:LEU:HB3	16:M:132:ILE:HG12	1.73	0.71
18:O:410:PRO:HG3	18:O:415:HIS:CD2	2.25	0.71
14:K:39:CYS:SG	14:K:83:ARG:NH1	2.64	0.71
10:G:115:GLN:HB3	10:G:119:LYS:HD3	1.72	0.71
13:J:30:THR:HG22	13:J:31:GLU:H	1.54	0.71
4:A:214:ALA:HB1	18:O:409:ILE:HG22	1.71	0.70
4:A:583:LEU:HD12	4:A:584:PRO:HD2	1.74	0.70
17:N:362:SER:HB3	17:N:374:THR:HB	1.73	0.70
7:D:48:GLU:HB3	10:G:103:PHE:HB3	1.72	0.70
18:O:410:PRO:HA	18:O:420:THR:HB	1.74	0.70
23:W:317:MET:SD	23:W:363:ASP:HB3	2.30	0.70
3:4:248:LEU:HD22	3:4:253:LEU:HD23	1.72	0.70
4:A:74:LYS:HZ1	4:A:80:LEU:HD12	1.56	0.70
22:V:113:LYS:NZ	25:Y:22:DA:OP2	2.24	0.69
5:B:715:PRO:HB2	5:B:734:PRO:HG2	1.73	0.69
7:D:86:LEU:HD22	7:D:91:PRO:HG3	1.72	0.69
16:M:225:LEU:HD11	17:N:376:LEU:HD13	1.75	0.69
16:M:266:ASN:O	16:M:268:LEU:N	2.25	0.69
4:A:74:LYS:NZ	4:A:80:LEU:CD1	2.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:289:SER:HA	18:O:333:MET:HA	1.75	0.69
5:B:79:ASN:N	5:B:116:ASP:OD1	2.26	0.69
5:B:718:PRO:HB3	5:B:900:ARG:HH12	1.58	0.69
5:B:901:HIS:NE2	5:B:945:GLU:OE1	2.23	0.69
18:O:460:LEU:HB3	18:O:499:LEU:HD21	1.73	0.69
4:A:431:PHE:HE1	22:V:20:HIS:HE2	1.36	0.68
5:B:876:GLU:HG3	22:V:86:PRO:HB3	1.74	0.68
16:M:308:VAL:HG12	16:M:312:ARG:NH2	2.08	0.68
23:W:328:LEU:CD1	23:W:367:PHE:HE1	2.01	0.68
5:B:702:ARG:NH2	5:B:867:GLU:OE2	2.27	0.68
7:D:79:THR:OG1	20:Q:86:ARG:NH1	2.26	0.68
19:P:92:GLU:HG3	19:P:126:ILE:HG23	1.75	0.68
5:B:900:ARG:NH2	5:B:945:GLU:OE2	2.27	0.67
6:C:28:ASP:O	14:K:61:LYS:NZ	2.27	0.67
14:K:30:VAL:HG11	14:K:35:THR:HG23	1.76	0.67
15:L:34:ILE:O	15:L:42:ARG:NH1	2.28	0.67
18:O:503:LYS:HG2	18:O:507:ASN:HD21	1.58	0.67
19:P:217:TRP:NE1	19:P:230:LEU:O	2.21	0.67
4:A:700:ILE:HG21	5:B:947:LEU:HD22	1.77	0.67
5:B:758:ASN:HD21	5:B:913:GLN:HG3	1.60	0.67
6:C:97:ASN:ND2	6:C:103:ASP:OD1	2.28	0.67
4:A:919:LEU:HD23	4:A:924:VAL:HG21	1.76	0.67
7:D:102:GLU:HG2	10:G:149:ARG:HH21	1.59	0.67
5:B:341:ARG:NH2	5:B:584:TYR:OH	2.28	0.67
5:B:919:CYS:SG	5:B:920:ASP:N	2.68	0.67
3:4:494:LYS:NZ	24:X:-65:DC:OP1	2.28	0.67
7:D:73:LEU:HD13	7:D:83:LYS:HB2	1.76	0.67
4:A:786:LYS:HD2	5:B:936:SER:HB2	1.76	0.67
7:D:87:LEU:O	7:D:90:ARG:NH1	2.28	0.67
4:A:381:ALA:HB3	4:A:487:ARG:HB2	1.76	0.66
10:G:115:GLN:HG3	10:G:116:GLN:H	1.60	0.66
13:J:64:PRO:HB3	15:L:23:HIS:CE1	2.30	0.66
10:G:148:ILE:HG23	10:G:190:ILE:HG23	1.77	0.66
5:B:75:LEU:HD22	5:B:402:VAL:HG21	1.77	0.66
18:O:81:ARG:NH2	18:O:88:TYR:OH	2.26	0.66
6:C:326:ILE:HG21	14:K:111:LEU:HB2	1.76	0.66
10:G:114:LEU:HB2	18:O:491:ILE:HG21	1.76	0.66
16:M:111:THR:HG21	16:M:131:GLY:HA2	1.77	0.66
10:G:151:ARG:NH1	10:G:191:SER:OG	2.29	0.66
11:H:91:VAL:HG22	11:H:144:LEU:HG	1.77	0.66
23:W:314:ALA:HB2	23:W:367:PHE:HE2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:816:ARG:HD2	4:A:823:LYS:HG2	1.78	0.65
4:A:984:ARG:HG3	4:A:989:ILE:HB	1.77	0.65
5:B:293:ARG:CZ	25:Y:5:DT:C7	2.74	0.65
16:M:414:ASP:OD2	16:M:418:ARG:NH2	2.29	0.65
6:C:98:THR:HB	6:C:207:GLU:H	1.61	0.65
6:C:9:GLU:OE2	6:C:298:ARG:NH1	2.29	0.65
5:B:124:GLN:HE21	23:W:282:ILE:HB	1.60	0.65
4:A:176:HIS:ND1	4:A:216:GLU:OE1	2.28	0.65
5:B:126:ILE:HD12	23:W:284:GLU:CB	2.26	0.65
19:P:137:LYS:HB3	19:P:153:TYR:HD1	1.61	0.65
4:A:701:GLY:HA3	5:B:984:LEU:HD13	1.79	0.65
5:B:302:LYS:HD2	5:B:308:GLU:CG	2.27	0.65
17:N:274:THR:HG23	17:N:316:CYS:H	1.62	0.65
1:1:66:PHE:O	1:1:75:ARG:NH2	2.30	0.65
4:A:542:ILE:HG13	4:A:543:GLN:H	1.62	0.65
5:B:1036:THR:OG1	5:B:1041:ARG:O	2.12	0.65
5:B:126:ILE:HD12	23:W:284:GLU:HB2	1.77	0.65
16:M:221:GLU:HB3	17:N:374:THR:HG21	1.77	0.64
4:A:566:GLN:OE1	14:K:56:ARG:NH1	2.29	0.64
4:A:590:LYS:HB2	11:H:91:VAL:HB	1.77	0.64
19:P:180:LEU:HD23	19:P:183:GLN:HE21	1.60	0.64
22:V:76:VAL:HG22	22:V:118:VAL:HG13	1.79	0.64
5:B:300:GLY:N	5:B:301:PRO:HD2	2.13	0.64
6:C:141:ARG:NH2	6:C:143:GLN:OE1	2.30	0.64
14:K:67:PHE:HB3	14:K:85:GLN:HB2	1.79	0.64
4:A:74:LYS:HZ2	4:A:80:LEU:HD12	1.59	0.64
4:A:877:LYS:HZ1	5:B:1052:ARG:HH12	1.46	0.64
4:A:934:CYS:O	4:A:1005:ARG:NH1	2.28	0.64
23:W:363:ASP:OD1	23:W:366:PHE:HB3	1.98	0.64
18:O:159:ARG:NH2	18:O:189:LEU:O	2.31	0.64
2:3:99:GLU:N	2:3:99:GLU:OE1	2.31	0.64
10:G:128:VAL:HG21	10:G:201:TRP:HE1	1.63	0.64
5:B:469:ARG:NH1	5:B:490:CYS:O	2.31	0.64
22:V:280:LEU:HD12	22:V:283:LEU:HD12	1.80	0.63
5:B:396:ARG:HD2	5:B:397:ALA:N	2.14	0.63
6:C:291:GLU:OE2	6:C:295:LYS:NZ	2.31	0.63
7:D:57:PRO:HD2	7:D:90:ARG:HH21	1.63	0.63
8:E:19:GLN:OE1	8:E:138:ASN:ND2	2.31	0.63
4:A:464:ARG:HG2	4:A:466:PRO:HD2	1.80	0.63
4:A:681:SER:OG	4:A:685:ARG:NH1	2.31	0.63
5:B:295:ARG:HA	5:B:296:MET:CE	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:750:ASP:HA	5:B:754:ALA:HB3	1.81	0.63
16:M:41:ASP:OD1	16:M:214:ARG:NH2	2.32	0.63
17:N:261:THR:HG22	17:N:263:GLU:H	1.62	0.63
7:D:17:PHE:HB2	7:D:53:ILE:HG21	1.81	0.63
16:M:8:PRO:HB3	17:N:330:LEU:HB3	1.81	0.63
24:X:-10:DG:N2	25:Y:10:DC:N3	2.46	0.63
5:B:686:GLN:HE22	5:B:1010:GLN:HE22	1.46	0.63
16:M:33:ARG:HD2	16:M:37:MET:HB3	1.80	0.63
4:A:366:ARG:NH1	4:A:506:ASN:OD1	2.32	0.63
4:A:899:GLN:NE2	4:A:1292:ASP:OD2	2.28	0.62
5:B:550:ARG:NH2	17:N:351:GLY:O	2.32	0.62
16:M:50:LYS:NZ	16:M:200:HIS:O	2.30	0.62
2:3:374:GLU:O	2:3:377:CYS:SG	2.47	0.62
3:4:401:LYS:NZ	24:X:-61:DC:OP1	2.21	0.62
5:B:526:LEU:HD12	5:B:530:GLU:HG3	1.79	0.62
5:B:1078:ASP:O	5:B:1087:GLY:N	2.31	0.62
8:E:71:GLN:HB3	8:E:99:ILE:HG23	1.80	0.62
4:A:432:LEU:O	4:A:437:ARG:NH1	2.33	0.62
5:B:406:MET:O	22:V:82:VAL:HG12	1.98	0.62
5:B:634:ASP:OD1	5:B:635:VAL:N	2.30	0.62
23:W:317:MET:SD	23:W:363:ASP:N	2.72	0.62
4:A:1340:VAL:HA	4:A:1345:GLU:HG3	1.80	0.62
5:B:781:ARG:HG2	22:V:129:HIS:HE1	1.65	0.62
4:A:324:GLU:HG2	4:A:343:GLN:HE21	1.65	0.62
4:A:374:ASN:O	4:A:685:ARG:NH2	2.32	0.62
4:A:607:PRO:HD2	4:A:611:ASN:HD22	1.65	0.62
10:G:149:ARG:HD3	10:G:151:ARG:HH22	1.65	0.62
18:O:413:PRO:HG2	24:X:-5:DA:H4'	1.80	0.62
19:P:210:PHE:HB3	19:P:269:LEU:HD22	1.82	0.62
4:A:795:MET:HA	4:A:838:PHE:HB2	1.82	0.61
5:B:189:ILE:HA	5:B:203:VAL:HG12	1.81	0.61
8:E:50:GLU:OE2	8:E:56:THR:OG1	2.18	0.61
4:A:315:LEU:CD2	4:A:329:PRO:HD2	2.29	0.61
4:A:372:ASP:HB2	4:A:487:ARG:HB3	1.81	0.61
11:H:118:TYR:HB2	11:H:121:LEU:HB2	1.82	0.61
5:B:91:PHE:O	22:V:175:THR:HG22	2.00	0.61
4:A:107:MET:HE3	4:A:147:SER:HA	1.83	0.61
7:D:41:ASN:HB2	10:G:36:ASN:HD22	1.65	0.61
5:B:631:GLU:OE2	5:B:656:HIS:NE2	2.29	0.61
7:D:5:ASP:HB2	7:D:8:SER:HB3	1.82	0.61
5:B:295:ARG:N	5:B:295:ARG:HE	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:112:LEU:HD13	11:H:129:ALA:HB2	1.82	0.61
18:O:285:THR:HG22	18:O:336:ILE:H	1.65	0.61
5:B:83:GLY:O	5:B:144:ASN:ND2	2.33	0.61
13:J:18:TRP:O	13:J:21:TYR:HB3	2.01	0.61
6:C:109:ARG:NH2	6:C:198:LEU:O	2.33	0.61
18:O:27:HIS:NE2	18:O:34:GLN:OE1	2.28	0.61
19:P:120:LEU:HD22	19:P:123:ILE:HD12	1.81	0.61
5:B:573:SER:OG	5:B:586:SER:OG	2.17	0.61
5:B:679:GLN:HG2	5:B:681:PRO:HD2	1.83	0.61
15:L:18:ILE:HD11	15:L:23:HIS:HB3	1.81	0.61
18:O:404:MET:HE2	18:O:424:TYR:HB3	1.83	0.61
18:O:399:LEU:HA	18:O:404:MET:HB3	1.83	0.60
19:P:279:PRO:HB2	19:P:284:ARG:HH12	1.66	0.60
24:X:-3:DC:N4	25:Y:2:DT:O4	2.34	0.60
10:G:85:LEU:HB2	10:G:148:ILE:HB	1.81	0.60
2:3:369:ASP:OD1	2:3:370:SER:N	2.34	0.60
5:B:1119:SER:OG	5:B:1120:MET:SD	2.59	0.60
18:O:162:SER:N	18:O:181:VAL:O	2.33	0.60
3:4:248:LEU:CD2	3:4:253:LEU:HD23	2.30	0.60
8:E:85:LYS:NZ	25:Y:-8:DG:P	2.75	0.60
23:W:331:HIS:NE2	23:W:375:LEU:HD11	2.16	0.60
4:A:360:ARG:HG2	5:B:1046:ARG:HB2	1.84	0.60
17:N:142:LYS:HE2	17:N:154:ILE:HD11	1.83	0.60
4:A:210:LEU:CD2	18:O:411:LYS:HA	2.31	0.60
16:M:218:SER:HA	17:N:374:THR:HG23	1.83	0.60
4:A:328:ILE:HB	4:A:329:PRO:CD	2.26	0.60
4:A:459:VAL:HG21	4:A:520:LEU:HB2	1.83	0.60
4:A:995:THR:HG22	4:A:997:PRO:HD2	1.82	0.60
5:B:242:ALA:O	5:B:280:GLN:NE2	2.35	0.60
6:C:23:ASN:O	6:C:303:ARG:NH2	2.29	0.60
16:M:308:VAL:CG1	16:M:312:ARG:HH21	2.10	0.60
18:O:507:ASN:OD1	20:Q:62:GLN:NE2	2.35	0.60
2:3:367:ASN:HB2	2:3:400:LEU:HB2	1.83	0.60
4:A:945:LEU:HD23	4:A:977:SER:HB3	1.83	0.60
10:G:53:LYS:HB2	10:G:71:HIS:HB2	1.81	0.60
17:N:252:ALA:O	17:N:256:ARG:HG2	2.02	0.60
18:O:258:ARG:NH2	19:P:249:GLU:OE1	2.35	0.60
18:O:419:ARG:HH11	18:O:419:ARG:CG	2.14	0.60
18:O:516:VAL:HG22	19:P:282:LEU:H	1.67	0.60
18:O:357:ARG:NE	19:P:288:GLY:O	2.34	0.60
22:V:171:GLU:O	22:V:175:THR:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1115:GLU:HB3	4:A:1133:SER:HB3	1.84	0.59
6:C:50:ARG:NH1	6:C:52:ASP:OD2	2.35	0.59
11:H:33:GLU:OE2	11:H:55:LYS:NZ	2.31	0.59
5:B:279:THR:HG22	5:B:281:MET:H	1.68	0.59
23:W:310:MET:HE2	23:W:371:LEU:CD2	2.31	0.59
4:A:1368:ARG:NH1	10:G:54:LEU:O	2.35	0.59
4:A:1117:ILE:HG12	4:A:1130:VAL:HG22	1.84	0.59
5:B:396:ARG:HD2	5:B:397:ALA:H	1.67	0.59
18:O:409:ILE:HG13	18:O:421:PHE:HB2	1.85	0.59
23:W:363:ASP:O	23:W:367:PHE:HB2	2.02	0.59
4:A:481:LYS:HB2	4:A:487:ARG:HH21	1.67	0.59
4:A:336:LYS:H	4:A:336:LYS:HZ2	1.50	0.59
4:A:566:GLN:NE2	14:K:70:TYR:O	2.35	0.59
5:B:241:LYS:NZ	5:B:246:GLU:O	2.35	0.59
4:A:328:ILE:CB	4:A:329:PRO:HD2	2.29	0.59
4:A:471:LEU:HD22	4:A:538:LEU:HD12	1.84	0.59
4:A:1109:LEU:HB2	4:A:1112:GLU:HG3	1.85	0.59
5:B:594:ARG:HH22	5:B:663:THR:HG1	1.49	0.59
22:V:110:ARG:HA	24:X:-18:DG:O5'	2.03	0.59
6:C:335:ARG:NH1	14:K:46:GLU:OE2	2.36	0.59
24:X:-31:DC:C6	24:X:-30:DT:H72	2.37	0.59
2:3:234:THR:CG2	2:3:237:GLN:HB2	2.31	0.58
23:W:310:MET:HE2	23:W:371:LEU:HD21	1.85	0.58
4:A:156:CYS:SG	4:A:159:CYS:N	2.64	0.58
5:B:239:ILE:O	5:B:243:MET:HB2	2.04	0.58
23:W:310:MET:CE	23:W:371:LEU:CD2	2.81	0.58
9:F:100:ARG:NH2	9:F:121:ASP:O	2.36	0.58
4:A:743:THR:HG23	4:A:746:GLU:H	1.67	0.58
5:B:113:ILE:HD11	5:B:136:MET:HB2	1.84	0.58
5:B:991:SER:HB2	5:B:998:LEU:HD21	1.85	0.58
23:W:331:HIS:CD2	23:W:375:LEU:HD21	2.38	0.58
4:A:262:ILE:HD11	5:B:1115:GLN:HB3	1.84	0.58
5:B:131:LEU:HD13	23:W:287:SER:CB	2.34	0.58
18:O:59:GLN:NE2	18:O:113:ASN:O	2.34	0.58
5:B:321:VAL:HB	5:B:331:LYS:HE2	1.85	0.58
5:B:926:ASP:HB2	5:B:927:ILE:HD12	1.86	0.58
10:G:112:GLU:OE1	10:G:119:LYS:NZ	2.32	0.58
4:A:749:GLU:OE1	4:A:808:ARG:NH1	2.37	0.58
14:K:76:SER:OG	14:K:77:GLU:OE1	2.20	0.58
19:P:260:VAL:HG12	19:P:262:SER:H	1.69	0.58
4:A:39:LYS:NZ	4:A:40:ASN:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1105:ILE:HG22	4:A:1238:THR:HG21	1.85	0.58
4:A:1237:ALA:HB1	8:E:136:LEU:HD12	1.85	0.58
16:M:311:LEU:HD21	16:M:415:VAL:HG21	1.86	0.58
4:A:1098:ALA:HB1	4:A:1212:ILE:HD12	1.86	0.57
24:X:8:DC:O2	24:X:8:DC:H2'	2.03	0.57
4:A:15:ILE:HG21	4:A:1349:MET:HG2	1.86	0.57
8:E:13:ILE:HD11	8:E:132:GLN:HG3	1.86	0.57
20:Q:72:PRO:HB2	20:Q:99:TRP:HD1	1.68	0.57
22:V:189:VAL:HG23	22:V:253:LEU:HD11	1.86	0.57
4:A:1145:ASN:N	4:A:1148:THR:OG1	2.27	0.57
5:B:920:ASP:OD2	6:C:301:ARG:NH2	2.36	0.57
16:M:59:GLU:HG2	16:M:101:THR:HG22	1.85	0.57
23:W:328:LEU:HD12	23:W:367:PHE:HE1	1.64	0.57
5:B:38:GLY:O	5:B:42:GLN:NE2	2.33	0.57
8:E:14:ARG:O	8:E:18:MET:HG2	2.03	0.57
10:G:22:LEU:HD23	10:G:54:LEU:HD21	1.87	0.57
14:K:100:LEU:O	14:K:104:MET:HG2	2.05	0.57
6:C:110:LEU:HA	6:C:113:ILE:HD12	1.86	0.57
14:K:70:TYR:HB3	14:K:82:LEU:HD13	1.86	0.57
4:A:905:ASP:OD2	4:A:1285:ARG:NH2	2.37	0.57
5:B:1028:ARG:NH1	5:B:1072:SER:O	2.37	0.57
17:N:361:VAL:HG12	17:N:375:VAL:HG12	1.86	0.57
18:O:241:ARG:NH2	18:O:275:GLU:OE1	2.37	0.57
4:A:74:LYS:HZ1	4:A:80:LEU:CD1	2.16	0.57
4:A:485:THR:HG22	5:B:1016:VAL:HG21	1.84	0.57
8:E:112:PRO:HA	8:E:115:LYS:HD3	1.85	0.57
8:E:172:ARG:O	8:E:207:ARG:NH1	2.37	0.57
18:O:127:ASP:O	18:O:130:THR:OG1	2.20	0.57
4:A:106:GLN:HB3	4:A:151:ARG:HD3	1.87	0.57
4:A:561:ARG:NH2	6:C:30:PRO:O	2.36	0.57
18:O:175:PRO:O	20:Q:108:ARG:NH1	2.29	0.57
2:3:236:ASP:OD1	2:3:385:ARG:NH2	2.37	0.57
4:A:15:ILE:HG23	4:A:1340:VAL:HG21	1.87	0.56
12:I:41:ARG:HD3	12:I:43:TYR:HE1	1.70	0.56
18:O:115:LYS:HB3	18:O:234:TYR:HB3	1.85	0.56
2:3:294:GLU:OE1	2:3:294:GLU:N	2.38	0.56
4:A:109:CYS:SG	4:A:110:LYS:N	2.79	0.56
4:A:142:LEU:HD23	4:A:239:LEU:HD21	1.87	0.56
5:B:132:PRO:O	5:B:408:GLN:NE2	2.30	0.56
5:B:135:ARG:N	5:B:412:THR:OG1	2.36	0.56
6:C:29:PHE:HB2	6:C:32:ASN:ND2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:310:MET:CE	23:W:371:LEU:HD23	2.35	0.56
5:B:407:ARG:HD2	22:V:81:ARG:HD3	1.87	0.56
7:D:80:LYS:HE2	20:Q:84:ILE:HD12	1.86	0.56
18:O:304:SER:OG	18:O:306:GLN:NE2	2.37	0.56
5:B:74:TYR:OH	5:B:125:ARG:NE	2.37	0.56
5:B:533:TYR:O	5:B:581:ARG:NH1	2.38	0.56
7:D:70:LEU:HD11	7:D:80:LYS:HE3	1.87	0.56
23:W:317:MET:SD	23:W:363:ASP:CB	2.94	0.56
4:A:315:LEU:HD22	4:A:329:PRO:CG	2.35	0.56
4:A:405:ARG:NH1	4:A:441:ALA:O	2.39	0.56
4:A:25:PRO:HA	4:A:28:MET:HB2	1.87	0.56
4:A:596:THR:HG21	11:H:119:GLY:HA3	1.86	0.56
16:M:6:ASP:O	17:N:332:ARG:NH1	2.38	0.56
5:B:674:TYR:HB3	5:B:677:HIS:HD2	1.70	0.56
7:D:41:ASN:ND2	10:G:35:ALA:O	2.38	0.56
24:X:-3:DC:H2"	24:X:-2:DA:C8	2.41	0.56
5:B:919:CYS:HB2	5:B:1004:PHE:HE2	1.70	0.56
6:C:287:ILE:HG12	6:C:297:VAL:HG11	1.88	0.56
10:G:116:GLN:HE22	10:G:118:ALA:HB3	1.71	0.56
10:G:118:ALA:HB1	10:G:129:TRP:HE3	1.71	0.56
6:C:116:HIS:ND1	6:C:116:HIS:O	2.40	0.55
18:O:504:ARG:HA	18:O:507:ASN:HD22	1.70	0.55
2:3:119:GLU:N	2:3:119:GLU:OE1	2.39	0.55
16:M:308:VAL:CG1	16:M:312:ARG:NH2	2.69	0.55
18:O:160:CYS:SG	20:Q:105:ARG:NH1	2.78	0.55
4:A:100:ALA:HB1	4:A:1333:TYR:CE1	2.42	0.55
4:A:485:THR:O	4:A:487:ARG:NH1	2.39	0.55
4:A:588:ILE:HG12	11:H:92:MET:HG2	1.88	0.55
5:B:1051:GLU:OE1	5:B:1051:GLU:N	2.34	0.55
9:F:57:MET:HG2	9:F:123:LEU:HD13	1.88	0.55
18:O:324:GLY:N	18:O:335:VAL:O	2.36	0.55
19:P:152:LEU:HB2	19:P:155:LEU:HB2	1.89	0.55
5:B:876:GLU:N	5:B:876:GLU:OE1	2.39	0.55
9:F:81:VAL:HG11	9:F:96:GLU:HA	1.88	0.55
18:O:81:ARG:NH1	18:O:85:MET:SD	2.79	0.55
5:B:896:LYS:HG2	5:B:1012:LEU:HD12	1.87	0.55
7:D:85:GLN:OE1	10:G:84:ILE:N	2.38	0.55
8:E:27:LEU:N	8:E:62:VAL:O	2.37	0.55
4:A:112:CYS:O	4:A:114:HIS:ND1	2.40	0.55
4:A:422:GLN:HB3	4:A:449:ILE:HB	1.88	0.55
4:A:546:LEU:HD22	4:A:652:LYS:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:50:GLU:HG2	8:E:55:ARG:HD2	1.89	0.55
2:3:179:GLU:OE2	2:3:180:LEU:N	2.40	0.55
5:B:876:GLU:HG3	22:V:86:PRO:CB	2.36	0.55
18:O:368:LEU:HD11	18:O:383:PHE:HB2	1.89	0.55
19:P:256:LYS:HA	19:P:265:GLY:HA2	1.89	0.55
2:3:174:MET:SD	2:3:175:ILE:N	2.79	0.55
4:A:36:VAL:HB	4:A:86:ILE:HG12	1.88	0.55
5:B:106:ASP:HA	5:B:173:GLY:HA3	1.87	0.55
10:G:50:ASP:O	10:G:72:PHE:HB2	2.07	0.55
4:A:258:PRO:HB2	4:A:262:ILE:HD12	1.89	0.55
5:B:461:LYS:NZ	5:B:488:GLU:O	2.39	0.55
6:C:134:GLU:O	6:C:181:GLN:NE2	2.40	0.55
23:W:331:HIS:NE2	23:W:375:LEU:HD21	2.22	0.55
6:C:92:VAL:HG13	6:C:210:LEU:HD12	1.89	0.54
4:A:29:ARG:HH21	19:P:297:HIS:CD2	2.25	0.54
4:A:618:ARG:NH2	4:A:629:GLU:OE2	2.40	0.54
8:E:62:VAL:HG12	8:E:71:GLN:HA	1.89	0.54
18:O:449:ARG:NH1	19:P:304:PRO:O	2.39	0.54
24:X:-11:DG:N2	25:Y:11:DC:N3	2.54	0.54
4:A:241:ASN:OD1	4:A:244:ALA:N	2.36	0.54
5:B:296:MET:CE	5:B:296:MET:H	2.19	0.54
16:M:267:VAL:HG13	16:M:268:LEU:HG	1.87	0.54
2:3:234:THR:O	2:3:234:THR:CG2	2.55	0.54
4:A:388:LYS:NZ	4:A:413:GLU:O	2.40	0.54
24:X:-25:DA:C5	24:X:-24:DT:H73	2.43	0.54
5:B:357:TYR:CE2	5:B:475:GLN:HG2	2.42	0.54
5:B:478:MET:HG2	5:B:592:LEU:HB3	1.90	0.54
4:A:35:GLN:HB2	4:A:85:TYR:CZ	2.42	0.54
5:B:702:ARG:NH1	6:C:100:ILE:O	2.38	0.54
6:C:261:VAL:HG23	6:C:278:PRO:HA	1.88	0.54
8:E:84:ILE:HD11	8:E:113:SER:HB2	1.89	0.54
4:A:210:LEU:HD21	18:O:411:LYS:HA	1.88	0.54
4:A:1150:ARG:NH2	4:A:1165:VAL:O	2.40	0.54
5:B:562:MET:HG3	5:B:567:TYR:HB2	1.89	0.54
7:D:4:LYS:HB2	10:G:6:GLU:HB2	1.90	0.54
24:X:-2:DA:N6	25:Y:1:DG:O6	2.41	0.54
2:3:272:ARG:HD2	16:M:277:PRO:HG3	1.90	0.54
5:B:82:VAL:HG23	5:B:144:ASN:HD21	1.73	0.54
16:M:417:GLN:NE2	16:M:421:MET:SD	2.81	0.54
18:O:312:LEU:HB3	18:O:334:TYR:CZ	2.43	0.54
19:P:219:TYR:O	19:P:222:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:263:ASP:OD1	21:U:264:VAL:N	2.40	0.54
10:G:94:PRO:HA	10:G:121:ASP:HB2	1.89	0.54
4:A:16:SER:OG	5:B:1127:LYS:O	2.25	0.53
5:B:892:GLU:N	5:B:895:ASP:OD2	2.35	0.53
11:H:12:VAL:HG22	11:H:28:LEU:HD11	1.90	0.53
13:J:3:ILE:HD12	13:J:4:PRO:HD2	1.89	0.53
4:A:377:ILE:HD13	4:A:680:MET:HG3	1.90	0.53
5:B:304:THR:C	5:B:306:ILE:H	2.11	0.53
5:B:954:LEU:O	13:J:46:ARG:NH2	2.41	0.53
18:O:376:GLU:HB2	18:O:379:GLN:HG3	1.89	0.53
18:O:460:LEU:HD21	18:O:495:GLU:HB3	1.89	0.53
21:U:291:LEU:N	21:U:304:ILE:O	2.40	0.53
6:C:246:GLU:HB3	6:C:270:LYS:NZ	2.24	0.53
8:E:6:GLU:HG2	8:E:47:LYS:HD3	1.89	0.53
10:G:116:GLN:O	10:G:118:ALA:N	2.36	0.53
18:O:438:ARG:HD3	19:P:289:LEU:H	1.73	0.53
5:B:503:THR:HG22	5:B:571:PHE:HB3	1.89	0.53
4:A:304:GLN:OE1	18:O:418:SER:C	2.47	0.53
9:F:51:ARG:N	9:F:116:GLU:OE1	2.42	0.53
17:N:145:ARG:NH2	17:N:152:LYS:O	2.42	0.53
17:N:147:THR:HG22	17:N:150:GLU:H	1.73	0.53
21:U:264:VAL:HG22	21:U:308:GLY:O	2.09	0.53
4:A:543:GLN:HB2	5:B:932:HIS:CD2	2.44	0.53
7:D:7:ASN:HA	10:G:3:VAL:HG21	1.90	0.53
24:X:-7:DG:H2"	24:X:-6:DA:C8	2.43	0.53
2:3:260:ASN:ND2	2:3:269:ASP:OD2	2.42	0.53
4:A:246:LYS:HE2	4:A:248:SER:HB2	1.90	0.53
4:A:315:LEU:CD2	4:A:329:PRO:CG	2.86	0.53
4:A:1347:ILE:HD13	5:B:1052:ARG:HD2	1.89	0.53
16:M:120:ARG:HB2	16:M:123:GLU:HG2	1.90	0.53
18:O:19:GLU:O	18:O:22:GLU:HG3	2.09	0.53
22:V:147:ASP:OD1	22:V:148:VAL:N	2.40	0.53
5:B:296:MET:H	5:B:296:MET:HE2	1.74	0.53
5:B:427:LYS:HD3	5:B:430:LYS:HD3	1.91	0.53
5:B:467:GLY:O	5:B:470:SER:OG	2.23	0.53
5:B:506:MET:SD	5:B:569:ASN:ND2	2.82	0.53
8:E:170:LEU:O	8:E:172:ARG:NH1	2.41	0.53
4:A:1136:ARG:NH2	12:I:47:LYS:O	2.30	0.53
5:B:206:SER:HA	5:B:211:LYS:HA	1.89	0.53
6:C:247:GLY:HA2	6:C:271:LYS:HE2	1.89	0.53
18:O:119:SER:N	18:O:230:ASP:OD2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:303:SER:O	19:P:307:CYS:N	2.41	0.53
4:A:304:GLN:O	4:A:308:GLU:HG2	2.09	0.53
4:A:877:LYS:NZ	5:B:1052:ARG:HH22	2.07	0.53
3:4:366:VAL:HG13	3:4:366:VAL:O	2.09	0.52
4:A:855:ARG:HD2	5:B:471:LEU:HB2	1.91	0.52
4:A:1375:ARG:HH21	10:G:49:PHE:HE1	1.55	0.52
5:B:293:ARG:HB2	5:B:295:ARG:CD	2.32	0.52
18:O:147:THR:HG22	18:O:150:ARG:HH12	1.74	0.52
2:3:216:ARG:NH2	2:3:248:LYS:O	2.39	0.52
7:D:80:LYS:HA	7:D:83:LYS:HG2	1.91	0.52
18:O:36:LEU:HB2	18:O:75:TYR:HE2	1.74	0.52
20:Q:71:MET:SD	20:Q:73:TYR:HD2	2.33	0.52
6:C:56:MET:HB3	14:K:121:TYR:CE2	2.44	0.52
4:A:1212:ILE:HD13	4:A:1225:LEU:HD13	1.91	0.52
5:B:1092:CYS:SG	5:B:1095:CYS:HB2	2.50	0.52
4:A:87:ASP:OD1	4:A:254:ARG:NE	2.42	0.52
5:B:23:VAL:HG23	5:B:26:LYS:HB2	1.91	0.52
16:M:210:TYR:HA	17:N:373:MET:HB2	1.91	0.52
3:4:424:TRP:NE1	25:Y:58:DA:OP2	2.42	0.52
4:A:791:ASN:O	4:A:795:MET:HG3	2.10	0.52
16:M:238:LEU:HD13	17:N:341:LEU:HG	1.92	0.52
17:N:149:GLU:N	17:N:149:GLU:OE1	2.42	0.52
23:W:301:LYS:O	23:W:332:ARG:NH2	2.42	0.52
23:W:302:PRO:O	23:W:332:ARG:NH1	2.42	0.52
8:E:46:ASP:HB3	8:E:48:PRO:HD2	1.91	0.52
15:L:17:TYR:HE1	15:L:46:LYS:HZ3	1.58	0.52
24:X:-39:DT:H2'	24:X:-38:DT:H72	1.92	0.52
4:A:94:HIS:O	4:A:98:PHE:N	2.43	0.52
4:A:304:GLN:HG3	18:O:422:TYR:HE2	1.74	0.52
4:A:307:MET:HG3	18:O:422:TYR:CE1	2.45	0.52
6:C:49:PHE:CZ	14:K:110:VAL:HG23	2.44	0.52
6:C:93:LEU:HD23	15:L:52:LEU:HD21	1.92	0.52
6:C:326:ILE:HG23	14:K:107:CYS:SG	2.50	0.52
19:P:206:ARG:HD2	19:P:271:ARG:HH11	1.75	0.52
5:B:293:ARG:C	5:B:295:ARG:H	2.14	0.52
19:P:220:ILE:HG21	19:P:230:LEU:HD12	1.92	0.52
21:U:206:GLU:OE1	21:U:236:LYS:NZ	2.41	0.52
4:A:315:LEU:HD21	4:A:329:PRO:HD2	1.90	0.51
4:A:326:SER:O	4:A:326:SER:OG	2.21	0.51
25:Y:19:DA:H2"	25:Y:20:DA:C8	2.46	0.51
4:A:492:VAL:O	4:A:495:PRO:HD2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:571:ILE:HD12	4:A:682:ARG:HD3	1.93	0.51
5:B:36:VAL:HG12	5:B:37:LYS:HG3	1.92	0.51
20:Q:88:SER:HA	20:Q:91:TYR:HD2	1.74	0.51
23:W:363:ASP:CG	23:W:366:PHE:CB	2.66	0.51
24:X:-5:DA:N6	25:Y:4:DT:O4	2.43	0.51
4:A:537:PRO:HG3	4:A:665:TYR:HB2	1.92	0.51
4:A:852:MET:HE1	5:B:473:PRO:HG3	1.93	0.51
19:P:308:ILE:HG13	20:Q:38:PHE:CD1	2.45	0.51
4:A:166:VAL:HG22	4:A:176:HIS:HB2	1.92	0.51
15:L:41:TYR:CE2	15:L:43:ILE:HB	2.46	0.51
3:4:389:TYR:OH	25:Y:58:DA:N6	2.43	0.51
5:B:348:ASP:OD1	5:B:348:ASP:N	2.44	0.51
5:B:779:LEU:O	5:B:878:ALA:HA	2.10	0.51
16:M:409:ILE:HG23	16:M:416:VAL:HG21	1.92	0.51
24:X:-44:DT:H2'	24:X:-43:DT:H72	1.93	0.51
4:A:816:ARG:NH1	5:B:639:ASN:O	2.44	0.51
16:M:208:LEU:HD22	17:N:373:MET:HE3	1.92	0.51
18:O:252:VAL:HG11	18:O:268:ARG:HB2	1.91	0.51
19:P:184:CYS:SG	19:P:242:LEU:HD11	2.50	0.51
24:X:-15:DG:N2	25:Y:16:DC:O2	2.44	0.51
25:Y:16:DC:H2"	25:Y:17:DA:H8	1.75	0.51
4:A:553:THR:O	4:A:598:LYS:NZ	2.37	0.51
21:U:210:THR:HG21	25:Y:26:DA:H4'	1.92	0.51
24:X:2:DT:H2"	24:X:3:DG:C8	2.46	0.51
4:A:463:ASN:OD1	4:A:464:ARG:N	2.43	0.51
4:A:640:ILE:HD12	4:A:663:ILE:HD13	1.91	0.51
4:A:855:ARG:NH2	5:B:481:PRO:O	2.44	0.51
16:M:240:LYS:HE3	17:N:278:GLN:HB2	1.91	0.51
20:Q:86:ARG:H	20:Q:89:LYS:NZ	2.09	0.51
4:A:543:GLN:HB2	5:B:932:HIS:HD2	1.75	0.51
8:E:118:LEU:HA	8:E:121:MET:SD	2.51	0.51
4:A:940:LEU:HD21	4:A:1008:PRO:HD3	1.92	0.50
13:J:21:TYR:HB2	13:J:38:LEU:HD11	1.93	0.50
18:O:200:LYS:HG2	18:O:202:ARG:H	1.76	0.50
1:1:9:THR:OG1	2:3:128:VAL:HG11	2.10	0.50
10:G:20:ARG:NH1	10:G:28:GLU:OE1	2.43	0.50
18:O:88:TYR:CE1	18:O:111:LEU:HD22	2.47	0.50
5:B:300:GLY:N	5:B:301:PRO:CD	2.74	0.50
7:D:55:LYS:HZ3	10:G:103:PHE:HE2	1.59	0.50
18:O:183:ASN:HD22	18:O:184:GLU:N	2.09	0.50
18:O:398:MET:SD	18:O:404:MET:HB2	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:296:CYS:O	19:P:297:HIS:ND1	2.45	0.50
3:4:427:ILE:HD12	3:4:427:ILE:H	1.76	0.50
8:E:31:ASP:OD1	8:E:32:GLU:N	2.45	0.50
10:G:114:LEU:HD11	10:G:191:SER:HB2	1.94	0.50
16:M:77:ILE:HG21	16:M:97:MET:HE2	1.93	0.50
16:M:245:TYR:HA	16:M:248:MET:HG2	1.93	0.50
18:O:419:ARG:CG	18:O:419:ARG:NH1	2.73	0.50
4:A:878:SER:HA	4:A:1308:LEU:HD11	1.93	0.50
5:B:508:ASP:OD1	5:B:587:SER:OG	2.23	0.50
5:B:682:ARG:HD2	5:B:937:ARG:HB3	1.92	0.50
6:C:288:PHE:HA	6:C:294:LYS:HG2	1.93	0.50
8:E:22:HIS:HB2	8:E:28:VAL:HG11	1.93	0.50
10:G:120:PHE:HB3	10:G:129:TRP:CZ2	2.46	0.50
16:M:90:SER:OG	16:M:92:TYR:O	2.30	0.50
18:O:88:TYR:CG	18:O:111:LEU:HD13	2.46	0.50
4:A:461:LEU:HB2	4:A:508:HIS:HB2	1.92	0.50
6:C:324:GLU:OE2	6:C:327:LYS:NZ	2.44	0.50
16:M:20:SER:OG	16:M:224:TYR:O	2.22	0.50
3:4:416:VAL:HG22	3:4:443:TYR:CE1	2.47	0.50
4:A:55:VAL:HG11	4:A:280:THR:HG23	1.94	0.50
18:O:272:ARG:HA	18:O:275:GLU:HG3	1.94	0.50
18:O:447:ILE:HA	18:O:450:ARG:HG2	1.94	0.50
4:A:897:ILE:HD12	8:E:165:LEU:HD11	1.94	0.50
4:A:951:SER:HA	4:A:954:LYS:HD2	1.94	0.50
14:K:37:ARG:HD3	14:K:91:PRO:HB3	1.93	0.50
4:A:173:LYS:HE3	18:O:416:ALA:HA	1.94	0.50
4:A:592:VAL:HG13	4:A:594:LEU:HG	1.94	0.50
16:M:29:GLN:OE1	17:N:358:GLN:NE2	2.44	0.50
18:O:106:ILE:HG12	18:O:125:VAL:HG21	1.93	0.50
4:A:289:LEU:HD23	4:A:313:LEU:HA	1.94	0.49
8:E:82:VAL:HB	8:E:110:MET:SD	2.52	0.49
16:M:246:LEU:HB2	17:N:392:LEU:HD13	1.93	0.49
22:V:232:LEU:HD12	22:V:269:LEU:HD23	1.94	0.49
4:A:1161:LYS:N	4:A:1164:ASP:OD2	2.39	0.49
5:B:288:GLY:HA3	5:B:305:LYS:HB3	1.94	0.49
5:B:756:VAL:HG22	5:B:928:ILE:HB	1.94	0.49
16:M:92:TYR:HB3	16:M:98:ASP:H	1.77	0.49
18:O:130:THR:HB	18:O:201:ARG:HG2	1.93	0.49
4:A:169:CYS:O	4:A:173:LYS:HB2	2.13	0.49
4:A:415:HIS:CE1	4:A:480:VAL:HG21	2.48	0.49
5:B:87:VAL:HG22	5:B:89:GLU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:283:PHE:HE1	6:C:299:LEU:HB3	1.76	0.49
4:A:25:PRO:HB3	4:A:254:ARG:HB2	1.94	0.49
5:B:1120:MET:SD	5:B:1120:MET:N	2.84	0.49
8:E:121:MET:HE3	8:E:127:LEU:HB2	1.94	0.49
19:P:250:MET:HE3	19:P:269:LEU:H	1.78	0.49
5:B:64:LYS:HB2	5:B:76:LYS:HE2	1.94	0.49
5:B:1023:ARG:NH1	5:B:1035:PRO:HB3	2.27	0.49
15:L:19:CYS:HG	15:L:24:THR:H	1.60	0.49
16:M:6:ASP:OD1	16:M:6:ASP:N	2.45	0.49
18:O:441:LYS:NZ	19:P:293:PHE:O	2.45	0.49
19:P:140:LYS:HG2	19:P:148:LYS:HG2	1.95	0.49
19:P:195:ALA:O	19:P:205:GLN:NE2	2.42	0.49
23:W:363:ASP:OD1	23:W:366:PHE:N	2.46	0.49
4:A:210:LEU:HD11	18:O:411:LYS:HG2	1.95	0.49
5:B:469:ARG:NH2	5:B:488:GLU:O	2.32	0.49
5:B:999:GLU:O	6:C:21:VAL:N	2.39	0.49
16:M:292:MET:HE1	16:M:297:LEU:HD13	1.94	0.49
5:B:901:HIS:HB2	5:B:942:LYS:HZ1	1.77	0.49
5:B:1049:GLU:OE1	5:B:1049:GLU:N	2.45	0.49
7:D:108:LEU:HB3	7:D:113:ILE:HD11	1.94	0.49
18:O:81:ARG:NH1	18:O:81:ARG:O	2.40	0.49
18:O:92:ILE:HG23	18:O:104:GLU:HG3	1.94	0.49
4:A:366:ARG:NE	4:A:504:GLU:OE1	2.39	0.49
7:D:95:VAL:HG21	10:G:198:LEU:HD23	1.95	0.49
8:E:77:PRO:HG3	8:E:90:TYR:HE2	1.78	0.49
10:G:101:LEU:HB3	10:G:104:PHE:HB3	1.94	0.49
17:N:138:ILE:HG22	17:N:141:LYS:H	1.76	0.49
18:O:463:LYS:O	18:O:467:VAL:HG13	2.12	0.49
4:A:155:ILE:HB	4:A:160:GLY:HA2	1.95	0.49
4:A:1138:ARG:HB2	4:A:1138:ARG:NH1	2.28	0.49
20:Q:68:MET:O	20:Q:74:PHE:HB2	2.13	0.49
22:V:182:LEU:HD11	22:V:253:LEU:HD12	1.95	0.49
10:G:21:LYS:HZ2	10:G:23:ASN:HB2	1.77	0.49
18:O:265:GLU:OE2	18:O:269:THR:OG1	2.30	0.49
4:A:366:ARG:HB2	5:B:1045:LEU:HD21	1.94	0.48
4:A:485:THR:H	4:A:487:ARG:HH12	1.61	0.48
4:A:763:ALA:HB1	4:A:797:ALA:HB1	1.95	0.48
4:A:1088:GLN:HB2	4:A:1242:LYS:HB2	1.94	0.48
4:A:1235:VAL:O	4:A:1238:THR:OG1	2.29	0.48
4:A:1275:MET:HE3	4:A:1280:MET:HB2	1.94	0.48
5:B:79:ASN:OD1	5:B:80:ILE:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:87:VAL:HG23	5:B:107:MET:HE1	1.95	0.48
5:B:303:LYS:HZ1	5:B:306:ILE:HB	1.78	0.48
4:A:289:LEU:HD21	4:A:312:PHE:CD2	2.48	0.48
4:A:515:ALA:HB1	5:B:1063:LEU:HD13	1.93	0.48
5:B:1064:LEU:HD12	5:B:1068:LEU:HD13	1.94	0.48
18:O:503:LYS:HG2	18:O:507:ASN:ND2	2.27	0.48
23:W:310:MET:HB2	23:W:370:LEU:CD2	2.43	0.48
2:3:184:VAL:HG13	2:3:204:MET:HB2	1.94	0.48
4:A:772:ASP:OD1	4:A:773:LYS:N	2.46	0.48
6:C:40:TRP:HE3	14:K:61:LYS:HD3	1.78	0.48
11:H:96:VAL:HG22	11:H:116:VAL:HG22	1.96	0.48
16:M:293:PRO:HG3	16:M:402:LEU:HD13	1.95	0.48
4:A:176:HIS:CE1	4:A:178:LYS:HB2	2.48	0.48
5:B:716:GLN:NE2	13:J:48:MET:SD	2.86	0.48
6:C:340:LEU:HD11	14:K:96:PHE:CD1	2.49	0.48
7:D:95:VAL:HG21	10:G:198:LEU:HB3	1.94	0.48
4:A:105:LEU:HD13	4:A:218:LEU:HD13	1.95	0.48
4:A:590:LYS:HB3	4:A:591:PRO:HD3	1.94	0.48
13:J:28:GLU:CD	16:M:395:ASN:H	2.16	0.48
15:L:19:CYS:SG	15:L:24:THR:N	2.72	0.48
18:O:164:PRO:HD3	18:O:180:LEU:HA	1.95	0.48
18:O:305:LYS:HA	18:O:308:LEU:HD12	1.94	0.48
4:A:499:ASP:OD1	4:A:499:ASP:N	2.42	0.48
4:A:542:ILE:HG13	4:A:543:GLN:N	2.27	0.48
5:B:404:LYS:HD2	22:V:141:LEU:HA	1.96	0.48
9:F:84:GLU:N	9:F:86:GLU:OE1	2.47	0.48
19:P:120:LEU:HD13	19:P:123:ILE:HB	1.95	0.48
4:A:343:GLN:OE1	4:A:343:GLN:N	2.41	0.48
5:B:302:LYS:HZ2	5:B:303:LYS:H	1.61	0.48
5:B:725:ILE:HG23	5:B:730:PHE:HB3	1.96	0.48
4:A:194:LEU:HD22	4:A:211:LEU:HG	1.96	0.48
5:B:790:VAL:HG12	5:B:830:LYS:HA	1.95	0.48
16:M:34:PRO:HA	17:N:356:PHE:HA	1.96	0.48
21:U:320:GLU:HA	21:U:323:GLU:HG2	1.94	0.48
24:X:-21:DC:H2"	24:X:-20:DT:C5	2.48	0.48
2:3:179:GLU:O	2:3:329:VAL:N	2.47	0.48
4:A:548:GLY:HA2	4:A:691:LEU:HD13	1.96	0.48
5:B:91:PHE:O	5:B:93:VAL:HG23	2.14	0.48
5:B:257:THR:HG21	5:B:529:GLU:HG3	1.96	0.48
5:B:1079:VAL:HB	5:B:1128:LEU:HD11	1.96	0.48
8:E:172:ARG:NE	8:E:210:GLN:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:107:ILE:HG13	10:G:187:VAL:HG12	1.96	0.48
18:O:397:LYS:O	18:O:401:GLU:HG2	2.14	0.48
24:X:-27:DA:C8	24:X:-26:DT:H73	2.48	0.48
5:B:775:ALA:HB3	5:B:883:MET:HG2	1.96	0.48
10:G:13:ILE:O	10:G:65:ALA:HB1	2.14	0.48
16:M:121:GLN:H	16:M:121:GLN:CD	2.17	0.48
5:B:562:MET:HE1	17:N:389:PHE:HB3	1.96	0.47
5:B:750:ASP:OD1	5:B:750:ASP:N	2.41	0.47
5:B:1091:TRP:HE3	5:B:1098:SER:HB3	1.78	0.47
18:O:78:GLN:O	18:O:82:VAL:HG23	2.14	0.47
18:O:522:LEU:O	18:O:525:SER:OG	2.16	0.47
22:V:153:TYR:O	22:V:157:VAL:HG22	2.13	0.47
5:B:126:ILE:HD12	23:W:284:GLU:HB3	1.94	0.47
6:C:246:GLU:HG3	6:C:272:VAL:HG12	1.96	0.47
24:X:-18:DG:H1	25:Y:18:DC:H42	1.60	0.47
4:A:804:ILE:HG23	4:A:856:GLU:HG3	1.96	0.47
4:A:1078:LYS:HD3	4:A:1252:TYR:CZ	2.50	0.47
16:M:50:LYS:HD3	16:M:203:GLU:HB2	1.97	0.47
17:N:367:ASP:OD1	17:N:368:SER:N	2.45	0.47
24:X:-11:DG:H2"	24:X:-10:DG:C8	2.49	0.47
2:3:272:ARG:HH12	16:M:277:PRO:HB3	1.78	0.47
4:A:302:LYS:HB2	4:A:305:MET:HG2	1.95	0.47
4:A:341:PHE:HD1	5:B:1116:GLU:HG3	1.79	0.47
5:B:101:GLU:O	5:B:105:ARG:HG3	2.14	0.47
5:B:903:GLN:HG3	5:B:942:LYS:HE3	1.96	0.47
22:V:77:ARG:NH1	22:V:90:GLU:OE2	2.47	0.47
5:B:536:VAL:O	5:B:581:ARG:NH1	2.48	0.47
18:O:526:TYR:HA	18:O:529:CYS:SG	2.54	0.47
20:Q:66:GLU:HA	20:Q:69:LYS:HE2	1.96	0.47
23:W:362:PHE:CZ	23:W:364:PHE:HB2	2.50	0.47
4:A:1058:VAL:HG22	12:I:53:LEU:HD13	1.96	0.47
4:A:1191:PHE:O	4:A:1194:GLU:HB2	2.14	0.47
5:B:254:MET:HA	5:B:528:GLY:HA3	1.95	0.47
5:B:306:ILE:HD13	5:B:306:ILE:HA	1.65	0.47
10:G:81:LEU:HD22	10:G:152:VAL:HA	1.95	0.47
20:Q:80:GLU:O	20:Q:81:ARG:HG2	2.15	0.47
1:1:63:TRP:NE1	1:1:103:ASP:OD1	2.43	0.47
3:4:283:PHE:O	3:4:288:GLU:N	2.41	0.47
4:A:41:LEU:HB3	4:A:56:LEU:HD12	1.95	0.47
4:A:74:LYS:HB3	4:A:78:ASP:HB2	1.95	0.47
4:A:602:SER:HB2	4:A:644:GLU:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:669:ARG:HA	4:A:669:ARG:HD3	1.67	0.47
4:A:741:GLY:HA2	12:I:51:ASP:HB3	1.97	0.47
4:A:1087:ALA:HA	4:A:1246:THR:HG22	1.96	0.47
4:A:1107:LYS:HB2	4:A:1204:ILE:O	2.15	0.47
5:B:431:MET:SD	5:B:433:ARG:HG3	2.53	0.47
5:B:599:VAL:HG22	5:B:604:PRO:HA	1.97	0.47
5:B:700:ASN:HD21	5:B:704:ARG:HH21	1.62	0.47
5:B:1091:TRP:CE3	5:B:1098:SER:HB3	2.50	0.47
6:C:245:VAL:HG21	6:C:253:LEU:HD12	1.96	0.47
6:C:316:LEU:HB2	6:C:317:PRO:HD2	1.97	0.47
7:D:8:SER:OG	10:G:4:LEU:O	2.32	0.47
10:G:114:LEU:CD1	10:G:191:SER:HB2	2.44	0.47
16:M:56:VAL:HG13	16:M:135:LEU:HD21	1.97	0.47
16:M:63:ASP:N	16:M:63:ASP:OD1	2.47	0.47
18:O:464:SER:HA	18:O:467:VAL:HG22	1.96	0.47
23:W:310:MET:HB2	23:W:370:LEU:HD21	1.95	0.47
23:W:310:MET:CB	23:W:370:LEU:HD21	2.45	0.47
5:B:613:GLU:OE1	5:B:619:ARG:NE	2.46	0.47
5:B:946:LEU:HD22	5:B:1003:TYR:CE2	2.49	0.47
6:C:15:VAL:HG12	6:C:23:ASN:HD22	1.79	0.47
9:F:80:MET:HB3	9:F:101:LYS:HE2	1.97	0.47
2:3:390:ASP:OD1	2:3:394:ASN:N	2.42	0.47
4:A:543:GLN:HE21	5:B:752:GLU:HG2	1.80	0.47
4:A:1268:ILE:HD11	4:A:1288:MET:HG3	1.97	0.47
8:E:95:GLN:OE1	8:E:125:TYR:OH	2.32	0.47
16:M:429:LYS:HA	16:M:432:LYS:HE3	1.97	0.47
4:A:1136:ARG:HE	4:A:1139:LEU:HD23	1.79	0.47
5:B:110:SER:OG	5:B:111:ALA:N	2.48	0.47
5:B:304:THR:HB	5:B:305:LYS:H	1.47	0.47
5:B:900:ARG:O	5:B:900:ARG:HG2	2.16	0.47
8:E:14:ARG:HH22	8:E:58:LEU:HD21	1.78	0.47
13:J:40:LEU:HD11	13:J:49:LEU:HD12	1.96	0.47
18:O:107:VAL:O	18:O:111:LEU:HG	2.15	0.47
19:P:180:LEU:HD23	19:P:183:GLN:NE2	2.28	0.47
4:A:83:TYR:HB3	4:A:256:LEU:HD22	1.97	0.46
4:A:373:PRO:HD2	5:B:749:TYR:CZ	2.50	0.46
4:A:934:CYS:HB2	4:A:1007:THR:HG21	1.96	0.46
6:C:228:VAL:HA	6:C:312:SER:HA	1.98	0.46
7:D:104:SER:O	7:D:108:LEU:HG	2.15	0.46
19:P:206:ARG:HD2	19:P:271:ARG:NH1	2.30	0.46
5:B:293:ARG:NE	25:Y:5:DT:C7	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:130:GLU:OE1	6:C:130:GLU:N	2.43	0.46
6:C:183:ASP:OD1	6:C:184:LEU:N	2.47	0.46
10:G:15:PRO:HA	10:G:18:PHE:CE1	2.50	0.46
18:O:47:LEU:HG	18:O:51:LYS:HE3	1.98	0.46
23:W:317:MET:HG2	23:W:362:PHE:HA	1.97	0.46
4:A:330:LEU:HD23	4:A:330:LEU:HA	1.76	0.46
5:B:651:ASN:H	5:B:654:THR:HG21	1.80	0.46
6:C:13:ARG:NE	6:C:238:ASP:OD2	2.43	0.46
6:C:230:THR:HG21	13:J:42:ARG:CZ	2.45	0.46
17:N:145:ARG:NE	17:N:150:GLU:O	2.48	0.46
20:Q:54:GLU:OE1	20:Q:54:GLU:N	2.40	0.46
22:V:18:ASP:OD2	22:V:18:ASP:N	2.49	0.46
24:X:-44:DT:C2'	24:X:-43:DT:H72	2.45	0.46
4:A:1109:LEU:HD12	4:A:1198:LYS:HA	1.96	0.46
5:B:222:ARG:HD3	5:B:271:GLU:HG3	1.97	0.46
5:B:271:GLU:HA	5:B:274:LYS:HD3	1.98	0.46
5:B:312:LEU:HD13	5:B:316:THR:HG21	1.97	0.46
7:D:102:GLU:HG2	10:G:149:ARG:NH2	2.29	0.46
17:N:251:VAL:HG11	17:N:335:GLY:HA2	1.98	0.46
23:W:360:ARG:CG	23:W:361:PRO:HD2	2.45	0.46
4:A:581:VAL:HG21	14:K:67:PHE:CE2	2.51	0.46
5:B:308:GLU:O	5:B:312:LEU:HD23	2.16	0.46
5:B:368:LEU:HB3	5:B:424:TRP:CZ3	2.51	0.46
5:B:946:LEU:HG	5:B:1005:GLY:HA3	1.96	0.46
7:D:57:PRO:HB2	7:D:90:ARG:HE	1.81	0.46
18:O:85:MET:HG3	18:O:88:TYR:CZ	2.50	0.46
18:O:358:PHE:HZ	18:O:401:GLU:HG3	1.80	0.46
23:W:363:ASP:OD1	23:W:366:PHE:CA	2.64	0.46
4:A:177:GLU:HA	4:A:215:GLN:HB3	1.98	0.46
4:A:568:ILE:HG13	4:A:603:VAL:HG11	1.97	0.46
5:B:539:VAL:HG23	5:B:546:LEU:HB2	1.97	0.46
5:B:870:MET:SD	5:B:882:LYS:HB2	2.56	0.46
5:B:1082:GLN:HB2	5:B:1100:HIS:HD2	1.81	0.46
7:D:69:PHE:HD2	7:D:87:LEU:HD12	1.80	0.46
20:Q:53:GLY:O	20:Q:57:MET:HG2	2.16	0.46
21:U:235:ARG:NH1	22:V:382:GLU:O	2.48	0.46
5:B:1085:LEU:HD11	5:B:1118:GLN:NE2	2.30	0.46
18:O:498:GLN:O	18:O:501:THR:OG1	2.25	0.46
4:A:328:ILE:CB	4:A:329:PRO:CD	2.91	0.46
5:B:483:ASP:OD2	5:B:495:ASN:ND2	2.48	0.46
5:B:970:LYS:H	5:B:970:LYS:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:116:GLN:NE2	10:G:118:ALA:HB3	2.31	0.46
11:H:78:THR:H	14:K:87:ARG:HH22	1.63	0.46
5:B:231:SER:HA	5:B:292:ARG:HH21	1.81	0.46
5:B:303:LYS:HB3	5:B:304:THR:H	1.49	0.46
6:C:110:LEU:HD13	6:C:212:MET:SD	2.56	0.46
7:D:62:SER:H	7:D:65:ILE:HB	1.81	0.46
16:M:45:LEU:HD21	16:M:61:ALA:HB2	1.98	0.46
18:O:362:CYS:HA	18:O:365:ILE:HD12	1.98	0.46
3:4:413:LEU:HD22	3:4:447:LEU:HD11	1.98	0.46
4:A:74:LYS:HE3	4:A:79:CYS:HA	1.98	0.46
4:A:114:HIS:CD2	4:A:231:PRO:HG2	2.50	0.46
4:A:159:CYS:HA	18:O:531:MET:SD	2.56	0.46
4:A:861:THR:O	4:A:865:THR:HG23	2.15	0.46
4:A:882:LEU:HD23	4:A:1289:LEU:HD11	1.98	0.46
4:A:1019:ARG:O	4:A:1023:MET:HG2	2.16	0.46
5:B:168:TYR:HB3	5:B:177:VAL:HG22	1.98	0.46
5:B:396:ARG:NH2	5:B:398:ALA:HB2	2.31	0.46
5:B:530:GLU:OE1	17:N:352:THR:HB	2.16	0.46
5:B:539:VAL:HG12	5:B:583:VAL:HB	1.98	0.46
6:C:252:GLU:O	6:C:256:CYS:HB2	2.15	0.46
6:C:340:LEU:HD11	14:K:96:PHE:HD1	1.81	0.46
11:H:88:PHE:CD2	11:H:144:LEU:HB3	2.51	0.46
24:X:-6:DA:H2"	24:X:-5:DA:C8	2.51	0.46
4:A:55:VAL:HG12	4:A:56:LEU:HG	1.98	0.45
4:A:91:PRO:O	4:A:310:TRP:NE1	2.44	0.45
4:A:697:SER:O	4:A:776:SER:OG	2.24	0.45
4:A:1152:SER:OG	4:A:1200:VAL:O	2.34	0.45
10:G:154:ASP:OD1	10:G:154:ASP:N	2.49	0.45
18:O:5:GLU:HG2	18:O:440:TYR:CD2	2.51	0.45
18:O:103:GLY:O	18:O:107:VAL:HG22	2.16	0.45
19:P:97:GLN:O	19:P:100:GLU:HG2	2.16	0.45
25:Y:-9:DA:H2"	25:Y:-8:DG:C8	2.51	0.45
2:3:34:LEU:N	2:3:38:ASN:OD1	2.46	0.45
5:B:224:TYR:HB3	5:B:233:ASP:HB2	1.98	0.45
5:B:602:GLN:HG2	5:B:652:LYS:HA	1.97	0.45
19:P:216:VAL:HG21	19:P:239:LEU:HD11	1.97	0.45
23:W:363:ASP:OD1	23:W:366:PHE:CB	2.63	0.45
25:Y:56:DT:H2'	25:Y:57:DT:H71	1.97	0.45
2:3:185:ASN:ND2	2:3:202:GLN:O	2.50	0.45
4:A:29:ARG:HH12	19:P:295:ASP:HB3	1.80	0.45
4:A:335:LYS:HA	4:A:335:LYS:HD3	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:80:LYS:HD2	7:D:83:LYS:HD2	1.98	0.45
18:O:306:GLN:NE2	18:O:307:VAL:HG23	2.30	0.45
4:A:110:LYS:HD3	4:A:176:HIS:CE1	2.52	0.45
23:W:328:LEU:O	23:W:371:LEU:HD11	2.16	0.45
5:B:206:SER:HB2	5:B:211:LYS:HG2	1.99	0.45
5:B:756:VAL:HG12	5:B:909:LEU:HB3	1.97	0.45
6:C:155:ASP:OD1	6:C:156:SER:N	2.43	0.45
10:G:156:SER:O	10:G:185:THR:OG1	2.23	0.45
11:H:37:MET:SD	11:H:127:GLY:HA3	2.56	0.45
16:M:47:ALA:HB3	16:M:208:LEU:HB2	1.98	0.45
18:O:133:MET:HE2	18:O:139:MET:HG2	1.99	0.45
18:O:160:CYS:SG	18:O:234:TYR:HB2	2.56	0.45
18:O:290:SER:N	18:O:332:GLY:O	2.45	0.45
4:A:667:LEU:HD23	4:A:667:LEU:HA	1.85	0.45
5:B:454:ARG:HH22	5:B:691:LYS:HD3	1.82	0.45
5:B:805:ARG:O	5:B:826:VAL:HG22	2.17	0.45
2:3:163:ALA:O	2:3:334:CYS:N	2.50	0.45
5:B:121:ARG:HG3	5:B:122:GLY:N	2.31	0.45
5:B:472:GLN:OE1	5:B:472:GLN:N	2.34	0.45
5:B:1078:ASP:HA	5:B:1102:SER:O	2.16	0.45
11:H:38:ASP:OD1	11:H:126:GLN:HB3	2.17	0.45
18:O:117:THR:O	18:O:121:VAL:HG12	2.16	0.45
19:P:158:ASP:HB3	19:P:161:VAL:HG12	1.98	0.45
4:A:213:ARG:HE	4:A:213:ARG:HB2	1.47	0.45
4:A:623:GLN:OE1	4:A:623:GLN:N	2.50	0.45
4:A:1113:ILE:O	4:A:1133:SER:OG	2.23	0.45
4:A:1273:TYR:O	4:A:1277:ASN:ND2	2.49	0.45
5:B:227:HIS:ND1	5:B:229:THR:HG22	2.32	0.45
6:C:49:PHE:HZ	14:K:110:VAL:HG23	1.80	0.45
21:U:236:LYS:O	21:U:240:VAL:HG23	2.17	0.45
25:Y:18:DC:H2"	25:Y:19:DA:C8	2.52	0.45
5:B:90:SER:OG	5:B:93:VAL:HB	2.17	0.45
5:B:295:ARG:HE	5:B:295:ARG:H	1.64	0.45
7:D:76:HIS:O	7:D:77:LYS:HG2	2.17	0.45
10:G:116:GLN:NE2	10:G:129:TRP:O	2.50	0.45
24:X:9:DT:OP2	24:X:9:DT:C6	2.70	0.45
4:A:415:HIS:NE2	4:A:480:VAL:HG11	2.32	0.45
4:A:469:HIS:ND1	4:A:471:LEU:HB2	2.32	0.45
10:G:97:VAL:O	10:G:110:PRO:HD2	2.17	0.45
18:O:355:GLN:HB2	18:O:363:ALA:HB2	1.98	0.45
21:U:203:ARG:HG2	21:U:210:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:272:ARG:NH1	16:M:277:PRO:CB	2.75	0.44
4:A:369:ILE:HD11	4:A:488:PHE:CZ	2.52	0.44
4:A:410:ASN:ND2	4:A:416:PRO:O	2.45	0.44
4:A:816:ARG:NH2	4:A:819:PRO:O	2.50	0.44
5:B:407:ARG:NH2	5:B:410:GLN:HB2	2.33	0.44
5:B:1061:SER:OG	5:B:1062:MET:SD	2.75	0.44
5:B:1073:ASP:OD1	5:B:1073:ASP:N	2.49	0.44
9:F:91:LEU:HA	9:F:94:MET:HE3	1.99	0.44
19:P:240:ASN:HA	19:P:243:ILE:HD12	1.98	0.44
4:A:572:LEU:HD13	14:K:83:ARG:HD2	2.00	0.44
4:A:876:VAL:HG11	5:B:1053:ASP:OD2	2.18	0.44
5:B:124:GLN:NE2	23:W:282:ILE:CB	2.71	0.44
15:L:16:ILE:HA	15:L:27:GLU:HA	1.99	0.44
19:P:313:TRP:HA	19:P:316:PHE:CD2	2.52	0.44
21:U:297:LYS:HB3	21:U:298:PRO:HD3	1.99	0.44
24:X:7:DG:C2	25:Y:-6:DG:N2	2.84	0.44
24:X:10:DT:H2"	24:X:11:DC:C6	2.52	0.44
2:3:297:THR:HG22	2:3:298:PHE:N	2.32	0.44
3:4:178:GLU:OE2	3:4:178:GLU:N	2.48	0.44
4:A:913:GLU:OE1	4:A:923:ARG:NH2	2.51	0.44
4:A:1214:ILE:HG12	12:I:54:GLY:HA3	1.99	0.44
5:B:128:ARG:HD2	5:B:128:ARG:HA	1.56	0.44
6:C:250:ALA:HB1	6:C:273:ALA:HB2	1.98	0.44
10:G:21:LYS:NZ	10:G:23:ASN:HB2	2.32	0.44
10:G:149:ARG:HD3	10:G:151:ARG:HH12	1.82	0.44
13:J:9:THR:OG1	13:J:10:CYS:N	2.51	0.44
18:O:161:PRO:O	18:O:180:LEU:HD23	2.17	0.44
19:P:138:ALA:HB1	19:P:148:LYS:HB2	1.99	0.44
20:Q:61:LYS:HE3	20:Q:65:ARG:NH2	2.32	0.44
5:B:288:GLY:HA3	5:B:305:LYS:HA	1.97	0.44
5:B:407:ARG:NH1	5:B:409:ASP:OD1	2.48	0.44
11:H:78:THR:HB	14:K:87:ARG:NH1	2.32	0.44
12:I:15:GLU:OE2	12:I:22:ARG:NE	2.40	0.44
16:M:120:ARG:HH21	16:M:121:GLN:HE22	1.64	0.44
17:N:280:PRO:O	17:N:282:GLN:HG2	2.18	0.44
24:X:-6:DA:N6	25:Y:5:DT:O4	2.50	0.44
4:A:220:PRO:HA	4:A:223:VAL:HG12	1.99	0.44
4:A:818:LEU:HD23	4:A:818:LEU:HA	1.87	0.44
5:B:160:GLU:O	13:J:62:TYR:OH	2.20	0.44
8:E:81:LYS:HE3	8:E:111:THR:HG22	1.99	0.44
17:N:153:GLN:HG3	17:N:154:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:201:ASN:O	19:P:205:GLN:N	2.36	0.44
19:P:256:LYS:HE2	19:P:256:LYS:HB2	1.89	0.44
19:P:280:THR:O	19:P:283:VAL:HG22	2.18	0.44
25:Y:16:DC:H2"	25:Y:17:DA:C8	2.51	0.44
4:A:849:PHE:O	4:A:852:MET:HB2	2.16	0.44
5:B:321:VAL:HG11	5:B:331:LYS:HA	1.99	0.44
14:K:31:GLN:HB3	14:K:39:CYS:HB3	2.00	0.44
18:O:60:HIS:HA	18:O:114:GLY:HA3	2.00	0.44
18:O:429:LEU:HD21	18:O:433:ARG:HE	1.83	0.44
19:P:195:ALA:O	19:P:198:SER:OG	2.30	0.44
19:P:237:THR:O	19:P:241:THR:HG23	2.18	0.44
21:U:300:ILE:HD11	21:U:315:ALA:HB2	2.00	0.44
22:V:251:CYS:SG	22:V:252:LYS:N	2.89	0.44
2:3:340:TYR:N	2:3:341:PRO:CD	2.81	0.44
4:A:468:LEU:HD22	4:A:1046:THR:HG21	1.99	0.44
4:A:632:CYS:SG	4:A:636:SER:N	2.87	0.44
5:B:293:ARG:NH2	25:Y:5:DT:C7	2.80	0.44
7:D:40:GLN:O	7:D:44:THR:HG23	2.17	0.44
10:G:45:CYS:HA	10:G:76:VAL:HG12	2.00	0.44
17:N:279:PRO:HD3	17:N:316:CYS:HB2	2.00	0.44
18:O:85:MET:HA	18:O:88:TYR:CE1	2.53	0.44
18:O:441:LYS:HD3	19:P:293:PHE:CZ	2.52	0.44
19:P:120:LEU:HD23	24:X:-12:DA:OP2	2.18	0.44
20:Q:64:LEU:O	20:Q:68:MET:HE3	2.18	0.44
5:B:515:ALA:O	5:B:520:VAL:HG12	2.18	0.44
5:B:772:TYR:CE1	5:B:886:ARG:HB2	2.53	0.44
7:D:113:ILE:O	7:D:117:LEU:HG	2.18	0.44
16:M:364:ARG:HH22	16:M:403:PRO:HA	1.83	0.44
16:M:407:GLU:HG3	16:M:411:LYS:HE3	1.99	0.44
24:X:7:DG:C2	24:X:8:DC:H1'	2.53	0.44
4:A:23:LYS:HD2	5:B:1123:ILE:HG13	2.00	0.44
4:A:57:ASP:OD1	4:A:58:HIS:N	2.51	0.44
4:A:454:LEU:HD12	4:A:509:LEU:HD22	1.99	0.44
4:A:625:CYS:SG	4:A:632:CYS:HB2	2.58	0.44
4:A:656:GLY:O	4:A:662:ASN:ND2	2.49	0.44
4:A:1345:GLU:HA	4:A:1348:ILE:HB	1.99	0.44
6:C:238:ASP:OD1	6:C:238:ASP:N	2.48	0.44
7:D:82:GLU:O	7:D:86:LEU:HG	2.18	0.44
17:N:330:LEU:HD12	17:N:340:LEU:HD13	2.00	0.44
19:P:113:ARG:HG3	19:P:114:TYR:HD1	1.83	0.44
21:U:235:ARG:NH2	22:V:383:ASN:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:361:VAL:HG12	5:B:1072:SER:HB3	1.98	0.43
4:A:1153:ILE:O	4:A:1154:CYS:HB2	2.18	0.43
4:A:1158:LEU:HD12	4:A:1192:LEU:HD21	1.99	0.43
5:B:128:ARG:CZ	5:B:130:ALA:H	2.31	0.43
5:B:946:LEU:HD21	5:B:1004:PHE:O	2.18	0.43
8:E:80:PRO:HA	8:E:107:GLN:HB2	2.00	0.43
16:M:14:ASP:HB3	16:M:16:TYR:CE1	2.53	0.43
16:M:365:TRP:CZ3	16:M:399:GLU:HB2	2.53	0.43
25:Y:37:DA:H2"	25:Y:38:DA:C8	2.53	0.43
4:A:277:ASP:OD2	4:A:280:THR:N	2.47	0.43
4:A:461:LEU:HD11	5:B:1063:LEU:HD21	2.00	0.43
4:A:868:THR:HG21	4:A:1046:THR:N	2.33	0.43
4:A:1044:PRO:O	4:A:1048:MET:N	2.43	0.43
5:B:30:LEU:HB3	5:B:31:PRO:HD3	2.00	0.43
5:B:743:VAL:HB	5:B:1003:TYR:HB3	2.00	0.43
13:J:30:THR:HG22	13:J:31:GLU:N	2.26	0.43
14:K:70:TYR:HA	14:K:81:ASN:O	2.16	0.43
16:M:364:ARG:HG2	16:M:399:GLU:HG3	2.00	0.43
18:O:81:ARG:HA	18:O:81:ARG:HD2	1.81	0.43
18:O:312:LEU:HB3	18:O:334:TYR:CE1	2.53	0.43
18:O:442:SER:O	18:O:446:LEU:HG	2.17	0.43
19:P:161:VAL:HG13	19:P:162:THR:HG23	2.00	0.43
4:A:177:GLU:HG2	4:A:215:GLN:HG3	2.00	0.43
4:A:187:ASP:HB2	4:A:190:VAL:HG23	2.00	0.43
4:A:887:ASP:OD2	4:A:891:ARG:NH2	2.47	0.43
4:A:1044:PRO:HA	4:A:1047:GLN:HB2	2.01	0.43
8:E:130:PHE:HB3	8:E:135:LEU:HD21	2.00	0.43
17:N:362:SER:N	17:N:374:THR:O	2.48	0.43
18:O:494:PRO:O	18:O:497:GLN:HB3	2.18	0.43
18:O:514:ILE:O	18:O:517:ASP:HB3	2.18	0.43
19:P:95:VAL:HB	19:P:126:ILE:HG21	1.99	0.43
2:3:28:ASN:O	2:3:28:ASN:ND2	2.50	0.43
4:A:942:LYS:O	4:A:946:ILE:HG12	2.18	0.43
5:B:86:ASP:HB3	5:B:94:THR:OG1	2.18	0.43
6:C:91:LYS:HD3	6:C:91:LYS:HA	1.75	0.43
11:H:111:ARG:HA	11:H:127:GLY:O	2.18	0.43
11:H:113:SER:HG	11:H:115:TYR:HE1	1.66	0.43
14:K:107:CYS:HA	14:K:110:VAL:HG12	2.00	0.43
17:N:148:ASP:O	17:N:151:THR:OG1	2.32	0.43
19:P:142:VAL:HG21	19:P:167:TYR:CG	2.53	0.43
3:4:438:GLN:NE2	3:4:439:CYS:SG	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:405:ARG:HH12	4:A:442:GLN:HA	1.83	0.43
4:A:638:VAL:HA	4:A:648:GLY:HA3	2.00	0.43
4:A:767:CYS:O	4:A:771:LEU:HG	2.19	0.43
5:B:124:GLN:NE2	5:B:125:ARG:O	2.51	0.43
5:B:682:ARG:HH21	5:B:685:TYR:HE2	1.65	0.43
6:C:287:ILE:HD11	6:C:293:LEU:HB3	1.98	0.43
18:O:95:THR:HG21	18:O:107:VAL:HG21	2.00	0.43
4:A:17:HIS:HB3	4:A:1339:SER:HA	2.01	0.43
5:B:108:THR:HG22	5:B:172:LYS:H	1.84	0.43
5:B:139:MET:HB2	5:B:169:PHE:CE1	2.53	0.43
5:B:824:LYS:HE2	5:B:824:LYS:HB3	1.65	0.43
10:G:115:GLN:HG3	10:G:116:GLN:N	2.28	0.43
11:H:11:ASP:HB2	11:H:55:LYS:NZ	2.33	0.43
2:3:104:CYS:SG	2:3:105:GLY:N	2.92	0.43
5:B:613:GLU:HB3	5:B:618:TYR:HB2	2.01	0.43
5:B:757:LEU:HD12	5:B:762:LEU:HD11	2.01	0.43
16:M:220:HIS:O	16:M:223:GLN:HG2	2.19	0.43
18:O:349:THR:HG23	19:P:280:THR:HG21	2.01	0.43
19:P:196:ARG:HA	19:P:205:GLN:HE22	1.82	0.43
25:Y:17:DA:H2"	25:Y:18:DC:C5	2.54	0.43
3:4:259:ASP:OD1	3:4:260:SER:N	2.52	0.43
4:A:196:SER:O	18:O:374:HIS:ND1	2.40	0.43
4:A:426:THR:HG23	4:A:428:MET:HG2	2.00	0.43
6:C:82:ALA:HB1	6:C:220:LYS:HB2	2.01	0.43
16:M:278:LEU:HD13	16:M:305:ILE:HD13	2.00	0.43
18:O:436:LEU:HD11	18:O:440:TYR:CZ	2.53	0.43
1:1:98:ARG:NH2	2:3:325:ASP:OD1	2.52	0.43
3:4:490:GLN:OE1	3:4:494:LYS:NZ	2.45	0.43
4:A:719:ALA:HA	4:A:722:LYS:HE2	2.00	0.43
5:B:442:ARG:CZ	5:B:704:ARG:HH12	2.32	0.43
7:D:16:VAL:HG21	10:G:2:PHE:HD2	1.84	0.43
16:M:25:LEU:HD11	17:N:360:LEU:HD11	2.01	0.43
24:X:-48:DG:H22	25:Y:48:DC:H42	1.67	0.43
4:A:699:GLY:HA3	5:B:986:LYS:HE2	2.01	0.43
4:A:1115:GLU:OE2	4:A:1131:LYS:HD2	2.19	0.43
5:B:220:GLN:HB3	5:B:222:ARG:NH1	2.34	0.43
6:C:262:ILE:HD13	6:C:275:VAL:HA	2.00	0.43
8:E:87:ILE:HD12	8:E:118:LEU:HD21	2.01	0.43
14:K:66:GLU:OE2	14:K:87:ARG:NE	2.52	0.43
15:L:29:LYS:HG3	15:L:30:SER:H	1.84	0.43
25:Y:22:DA:C8	25:Y:23:DT:H72	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:832:GLY:HA2	4:A:849:PHE:CD2	2.54	0.42
5:B:204:THR:HG23	5:B:213:ARG:HB3	2.00	0.42
5:B:707:THR:HA	5:B:774:ASN:OD1	2.19	0.42
5:B:903:GLN:OE1	5:B:937:ARG:NH1	2.45	0.42
7:D:41:ASN:O	10:G:36:ASN:ND2	2.52	0.42
8:E:11:TRP:NE1	8:E:35:GLN:O	2.42	0.42
10:G:33:LYS:HG3	10:G:34:LEU:HD22	2.00	0.42
14:K:62:ASN:OD1	14:K:65:VAL:HG23	2.19	0.42
16:M:78:ALA:HA	16:M:81:VAL:HG12	2.00	0.42
18:O:356:GLU:HG3	19:P:279:PRO:HB3	2.01	0.42
22:V:116:VAL:HG21	22:V:152:THR:HG21	1.99	0.42
23:W:344:GLU:O	23:W:348:ASN:N	2.46	0.42
2:3:150:CYS:O	2:3:154:THR:N	2.44	0.42
4:A:5:GLN:OE1	4:A:7:ARG:NH1	2.52	0.42
4:A:36:VAL:HG13	4:A:54:GLY:HA2	2.00	0.42
4:A:756:LEU:HD12	4:A:833:PHE:CE1	2.54	0.42
4:A:811:ASP:OD1	4:A:811:ASP:N	2.52	0.42
5:B:233:ASP:N	5:B:233:ASP:OD1	2.51	0.42
5:B:864:SER:OG	5:B:865:TYR:N	2.52	0.42
5:B:954:LEU:HA	5:B:954:LEU:HD23	1.78	0.42
7:D:69:PHE:CD2	7:D:87:LEU:HD12	2.53	0.42
8:E:26:TYR:HA	8:E:63:ALA:HA	2.01	0.42
11:H:15:ILE:HD13	11:H:15:ILE:HA	1.91	0.42
14:K:74:HIS:CG	14:K:75:PRO:HD2	2.54	0.42
16:M:292:MET:SD	16:M:297:LEU:HB2	2.59	0.42
1:1:7:LEU:HD11	1:1:54:PHE:CZ	2.54	0.42
4:A:66:ASP:N	4:A:66:ASP:OD1	2.53	0.42
5:B:217:ALA:O	5:B:223:PHE:HA	2.20	0.42
5:B:682:ARG:HH11	5:B:937:ARG:HB3	1.85	0.42
5:B:900:ARG:HH21	5:B:945:GLU:CD	2.20	0.42
4:A:182:ASN:HD21	4:A:184:LYS:HD2	1.84	0.42
4:A:310:TRP:O	4:A:314:GLN:HG3	2.20	0.42
4:A:323:SER:H	4:A:343:GLN:HE22	1.68	0.42
4:A:335:LYS:HB3	4:A:336:LYS:H	1.56	0.42
5:B:82:VAL:HG23	5:B:144:ASN:ND2	2.35	0.42
5:B:355:ASP:N	5:B:355:ASP:OD1	2.53	0.42
5:B:392:ILE:HD13	5:B:400:PHE:HB3	2.01	0.42
6:C:258:SER:O	6:C:261:VAL:HG12	2.19	0.42
10:G:128:VAL:HG21	10:G:201:TRP:NE1	2.32	0.42
16:M:336:ASP:OD1	16:M:336:ASP:N	2.51	0.42
18:O:117:THR:HG22	18:O:233:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:374:HIS:HB3	18:O:423:LEU:HD23	2.00	0.42
25:Y:-10:DA:H2"	25:Y:-9:DA:C8	2.54	0.42
2:3:202:GLN:HB2	2:3:345:LYS:O	2.20	0.42
4:A:171:LEU:O	4:A:173:LYS:HG3	2.19	0.42
5:B:409:ASP:O	5:B:413:ASN:HB2	2.18	0.42
5:B:789:LYS:HD2	5:B:851:TYR:CZ	2.55	0.42
6:C:321:LEU:HD23	6:C:321:LEU:HA	1.87	0.42
11:H:63:THR:O	11:H:84:ARG:NH2	2.34	0.42
16:M:120:ARG:HH21	16:M:121:GLN:NE2	2.18	0.42
18:O:314:LEU:HD12	18:O:315:LEU:HD12	2.01	0.42
19:P:238:ILE:O	19:P:241:THR:OG1	2.30	0.42
22:V:145:ASP:OD1	22:V:146:LEU:N	2.52	0.42
4:A:438:GLU:N	4:A:438:GLU:OE1	2.53	0.42
4:A:1138:ARG:HB2	4:A:1138:ARG:HH11	1.84	0.42
4:A:1213:HIS:HB3	4:A:1224:LYS:HG3	2.01	0.42
5:B:220:GLN:HB3	5:B:222:ARG:HH11	1.85	0.42
6:C:53:VAL:HG21	14:K:118:ILE:HD13	2.02	0.42
9:F:90:LEU:HD12	9:F:93:ALA:HB3	2.00	0.42
10:G:187:VAL:HG23	10:G:188:GLY:N	2.34	0.42
11:H:76:ASN:HB3	14:K:87:ARG:NH1	2.35	0.42
18:O:312:LEU:HD22	18:O:334:TYR:CG	2.53	0.42
20:Q:80:GLU:HG2	20:Q:81:ARG:HD3	2.00	0.42
23:W:276:VAL:O	23:W:276:VAL:HG13	2.19	0.42
2:3:339:LEU:O	2:3:339:LEU:HG	2.19	0.42
4:A:740:PRO:HB2	12:I:52:VAL:O	2.19	0.42
5:B:518:LEU:HD21	5:B:558:THR:HG21	2.01	0.42
6:C:284:SER:HB3	6:C:286:GLU:HG2	2.02	0.42
8:E:36:THR:HG22	8:E:38:GLU:H	1.84	0.42
8:E:89:VAL:O	8:E:92:GLN:NE2	2.52	0.42
11:H:8:ASP:HB3	11:H:10:PHE:CE1	2.55	0.42
13:J:6:ARG:HD3	13:J:13:ILE:HD13	2.00	0.42
18:O:104:GLU:OE2	20:Q:56:TYR:OH	2.36	0.42
18:O:368:LEU:HD13	18:O:384:ALA:HB2	2.02	0.42
19:P:292:VAL:O	19:P:296:CYS:N	2.52	0.42
4:A:470:LYS:HE3	4:A:532:PRO:HG3	2.02	0.42
4:A:483:HIS:HB2	4:A:487:ARG:CZ	2.50	0.42
4:A:543:GLN:NE2	5:B:751:ILE:O	2.51	0.42
4:A:544:ASP:OD2	5:B:930:ASN:ND2	2.42	0.42
4:A:1232:LEU:HD22	4:A:1248:SER:HB2	2.02	0.42
5:B:531:LEU:HD11	5:B:538:LEU:HD21	2.01	0.42
5:B:779:LEU:HB2	5:B:879:PHE:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:-46:DA:C4	24:X:-45:DT:H73	2.55	0.42
4:A:563:LYS:HB2	4:A:563:LYS:HE2	1.92	0.42
4:A:691:LEU:HD12	4:A:691:LEU:HA	1.86	0.42
18:O:91:TYR:OH	18:O:243:HIS:NE2	2.46	0.42
22:V:61:GLU:O	22:V:62:ASN:HB2	2.20	0.42
24:X:-13:DA:H2"	24:X:-12:DA:C5	2.54	0.42
4:A:415:HIS:O	4:A:453:HIS:ND1	2.53	0.42
4:A:469:HIS:CE1	4:A:471:LEU:HB2	2.55	0.42
4:A:738:GLN:NE2	4:A:742:CYS:O	2.53	0.42
5:B:446:ILE:HG12	5:B:671:LEU:HD11	2.02	0.42
5:B:463:ARG:CZ	5:B:465:VAL:HG22	2.50	0.42
5:B:749:TYR:CD1	5:B:909:LEU:HD22	2.55	0.42
10:G:30:LEU:HD23	10:G:30:LEU:HA	1.84	0.42
18:O:174:PRO:HB2	20:Q:108:ARG:NH2	2.35	0.42
21:U:264:VAL:HG23	21:U:266:PHE:H	1.85	0.42
22:V:132:PRO:HG2	22:V:175:THR:HG21	2.01	0.42
24:X:9:DT:H2'	24:X:10:DT:H72	2.02	0.42
4:A:7:ARG:CZ	10:G:159:ASP:HB2	2.50	0.41
4:A:289:LEU:HA	4:A:292:VAL:HG12	2.02	0.41
4:A:341:PHE:CD1	5:B:1116:GLU:HG3	2.55	0.41
4:A:883:CYS:HB3	4:A:1355:ILE:HG12	2.02	0.41
4:A:886:TYR:CZ	9:F:108:ARG:HG2	2.55	0.41
4:A:1116:TYR:HE1	4:A:1131:LYS:HE3	1.85	0.41
4:A:1153:ILE:HG22	4:A:1154:CYS:N	2.35	0.41
5:B:507:GLU:OE2	5:B:507:GLU:N	2.43	0.41
5:B:508:ASP:HA	5:B:511:ILE:HD13	2.02	0.41
6:C:164:VAL:HG22	6:C:165:ASN:OD1	2.20	0.41
18:O:486:GLU:N	18:O:486:GLU:OE1	2.53	0.41
4:A:105:LEU:HD21	4:A:223:VAL:HG23	2.02	0.41
4:A:151:ARG:HA	4:A:151:ARG:CZ	2.50	0.41
4:A:471:LEU:HB3	4:A:495:PRO:HB3	2.02	0.41
4:A:596:THR:HG23	4:A:599:GLN:H	1.85	0.41
4:A:1215:ASP:N	4:A:1222:LYS:O	2.49	0.41
5:B:39:LEU:HD13	5:B:449:LEU:HD21	2.02	0.41
8:E:26:TYR:CE2	8:E:72:MET:HB2	2.55	0.41
18:O:258:ARG:HG2	19:P:276:ILE:HG12	2.02	0.41
18:O:262:THR:O	18:O:266:ILE:HG12	2.20	0.41
18:O:351:GLU:HA	18:O:354:VAL:HG12	2.03	0.41
19:P:210:PHE:CG	19:P:269:LEU:HD13	2.55	0.41
22:V:238:GLN:NE2	22:V:241:ASP:OD1	2.53	0.41
24:X:-45:DT:H2"	24:X:-44:DT:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:303:THR:OG1	18:O:377:GLN:OE1	2.27	0.41
4:A:1248:SER:OG	4:A:1249:ASN:N	2.53	0.41
4:A:1253:GLU:O	4:A:1256:LYS:HG2	2.20	0.41
5:B:718:PRO:HB3	5:B:900:ARG:NH1	2.29	0.41
5:B:784:ASN:OD1	5:B:785:GLN:N	2.52	0.41
13:J:24:LEU:O	13:J:29:TYR:HB2	2.20	0.41
18:O:95:THR:HG21	18:O:107:VAL:HG11	2.03	0.41
18:O:147:THR:HA	18:O:150:ARG:NH1	2.35	0.41
18:O:269:THR:O	18:O:273:MET:HG2	2.19	0.41
4:A:915:LYS:HD2	4:A:915:LYS:HA	1.89	0.41
4:A:1364:HIS:CD2	4:A:1366:ALA:HB2	2.54	0.41
5:B:65:VAL:HG23	5:B:75:LEU:HB3	2.01	0.41
5:B:254:MET:HE2	5:B:332:CYS:HB3	2.02	0.41
5:B:655:THR:HG1	5:B:656:HIS:CE1	2.26	0.41
5:B:976:LEU:HD23	5:B:976:LEU:HA	1.90	0.41
6:C:122:PHE:CE1	6:C:138:LEU:HD21	2.56	0.41
18:O:471:ILE:HD13	18:O:483:GLN:HE22	1.85	0.41
23:W:294:PHE:CG	23:W:294:PHE:O	2.71	0.41
24:X:6:DC:H2'	24:X:7:DG:H5"	2.03	0.41
4:A:99:ARG:HD2	4:A:100:ALA:N	2.36	0.41
4:A:464:ARG:HD3	4:A:496:TYR:O	2.21	0.41
4:A:1242:LYS:O	4:A:1246:THR:HG23	2.19	0.41
5:B:797:ALA:HA	5:B:800:ARG:NH2	2.36	0.41
5:B:1049:GLU:HG3	5:B:1052:ARG:HH21	1.85	0.41
8:E:18:MET:HA	8:E:21:CYS:SG	2.60	0.41
8:E:25:GLY:O	8:E:64:HIS:ND1	2.53	0.41
8:E:73:PHE:O	8:E:102:ALA:HA	2.20	0.41
13:J:49:LEU:HA	13:J:49:LEU:HD23	1.79	0.41
15:L:17:TYR:HB3	15:L:44:MET:SD	2.61	0.41
19:P:106:GLY:HA2	19:P:151:MET:HB3	2.01	0.41
2:3:65:GLU:OE1	2:3:65:GLU:N	2.47	0.41
4:A:219:ASN:OD1	4:A:222:VAL:N	2.37	0.41
4:A:484:ARG:HH11	5:B:1020:MET:HE3	1.86	0.41
4:A:577:GLU:O	14:K:83:ARG:NH2	2.53	0.41
4:A:986:LYS:HB3	4:A:986:LYS:HE2	1.83	0.41
5:B:428:ARG:CZ	5:B:428:ARG:HA	2.51	0.41
5:B:776:LYS:HA	5:B:881:ILE:O	2.20	0.41
7:D:69:PHE:CE2	7:D:73:LEU:HD11	2.55	0.41
18:O:289:SER:O	18:O:293:ILE:HG12	2.20	0.41
25:Y:56:DT:C2'	25:Y:57:DT:H71	2.50	0.41
5:B:295:ARG:HA	5:B:296:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:674:TYR:HB3	5:B:677:HIS:CD2	2.54	0.41
5:B:946:LEU:HD22	5:B:1003:TYR:CZ	2.56	0.41
6:C:122:PHE:O	6:C:216:LYS:NZ	2.51	0.41
11:H:48:TYR:OH	11:H:89:GLU:OE1	2.33	0.41
12:I:29:PRO:HG2	16:M:69:TYR:CZ	2.56	0.41
23:W:360:ARG:HG3	23:W:361:PRO:HD2	2.03	0.41
2:3:100:LEU:HA	2:3:103:VAL:HG22	2.01	0.41
3:4:222:VAL:O	3:4:228:ARG:NH2	2.53	0.41
4:A:615:ALA:O	4:A:643:SER:N	2.33	0.41
6:C:236:LEU:HD23	6:C:237:PRO:O	2.21	0.41
13:J:22:LEU:HD23	13:J:22:LEU:HA	1.87	0.41
18:O:124:LYS:O	18:O:128:ARG:HG3	2.21	0.41
22:V:173:VAL:HG22	22:V:226:ILE:HG23	2.03	0.41
25:Y:-11:DG:H2"	25:Y:-10:DA:N7	2.35	0.41
2:3:206:VAL:HG22	2:3:207:LEU:N	2.36	0.41
3:4:295:GLN:O	3:4:328:ARG:NH1	2.54	0.41
4:A:36:VAL:HG21	4:A:257:VAL:HG21	2.03	0.41
4:A:282:LYS:HZ3	4:A:319:LEU:HB3	1.86	0.41
4:A:669:ARG:NH2	4:A:911:ALA:HA	2.36	0.41
5:B:76:LYS:HB3	5:B:118:GLU:CG	2.51	0.41
5:B:171:VAL:O	5:B:174:VAL:HG22	2.20	0.41
5:B:262:MET:HB3	12:I:2:LEU:HD12	2.01	0.41
5:B:609:LYS:HE3	5:B:609:LYS:HB3	1.77	0.41
6:C:90:GLU:HB2	6:C:215:VAL:HG22	2.03	0.41
6:C:167:LYS:NZ	6:C:201:GLN:OE1	2.54	0.41
10:G:155:GLU:HA	10:G:185:THR:O	2.21	0.41
16:M:144:LYS:O	16:M:148:LYS:HG2	2.21	0.41
16:M:386:LEU:HB3	16:M:398:TRP:CE3	2.56	0.41
18:O:102:THR:OG1	18:O:147:THR:HG21	2.21	0.41
23:W:280:ASP:OD2	23:W:280:ASP:N	2.49	0.41
1:1:28:ASP:OD1	1:1:29:PHE:N	2.54	0.41
4:A:983:THR:HG21	4:A:1004:ASP:OD2	2.21	0.41
4:A:1048:MET:HE3	4:A:1067:VAL:HG22	2.02	0.41
5:B:797:ALA:HA	5:B:800:ARG:HH22	1.85	0.41
8:E:85:LYS:HE2	25:Y:-9:DA:H3'	2.02	0.41
16:M:117:ALA:HB2	17:N:269:LEU:HD22	2.03	0.41
20:Q:29:ASP:OD1	20:Q:29:ASP:N	2.52	0.41
23:W:310:MET:HE1	23:W:371:LEU:HG	2.03	0.41
4:A:107:MET:CE	4:A:147:SER:HA	2.50	0.40
4:A:188:PRO:O	4:A:191:SER:OG	2.33	0.40
4:A:289:LEU:HB3	4:A:313:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:292:VAL:HG22	4:A:296:HIS:HD2	1.87	0.40
4:A:776:SER:O	4:A:780:MET:HG3	2.21	0.40
5:B:87:VAL:HG12	5:B:95:ARG:O	2.21	0.40
5:B:826:VAL:HG12	5:B:857:THR:HG22	2.02	0.40
5:B:982:ASN:OD1	5:B:983:TYR:N	2.54	0.40
6:C:262:ILE:HD13	6:C:262:ILE:HA	1.94	0.40
18:O:159:ARG:HD3	18:O:233:ILE:HD12	2.02	0.40
18:O:417:PRO:O	18:O:419:ARG:N	2.55	0.40
19:P:196:ARG:HA	19:P:205:GLN:NE2	2.35	0.40
21:U:201:ILE:N	21:U:201:ILE:HD12	2.36	0.40
21:U:227:GLU:OE1	21:U:227:GLU:N	2.48	0.40
22:V:393:LEU:HD12	22:V:393:LEU:C	2.42	0.40
24:X:-40:DA:H2'	24:X:-39:DT:H71	2.03	0.40
6:C:44:ARG:HG3	6:C:48:ASN:ND2	2.36	0.40
16:M:125:HIS:CE1	16:M:226:LEU:HD22	2.57	0.40
18:O:118:MET:HG3	18:O:191:PRO:HG2	2.03	0.40
18:O:363:ALA:O	18:O:367:ARG:HG3	2.21	0.40
19:P:123:ILE:O	19:P:127:LEU:HG	2.21	0.40
20:Q:40:ASP:OD1	20:Q:41:THR:N	2.54	0.40
4:A:58:HIS:CD2	4:A:67:ARG:HB2	2.57	0.40
4:A:877:LYS:HZ2	5:B:1052:ARG:HH22	1.69	0.40
4:A:1060:SER:HB3	4:A:1209:ARG:HH22	1.86	0.40
5:B:1050:MET:SD	5:B:1050:MET:N	2.89	0.40
8:E:88:LYS:HA	8:E:88:LYS:HD3	1.90	0.40
18:O:410:PRO:HG3	18:O:415:HIS:CG	2.55	0.40
24:X:-5:DA:H2"	24:X:-4:DA:C8	2.57	0.40
4:A:118:SER:HA	4:A:157:HIS:CD2	2.57	0.40
4:A:1058:VAL:HG13	4:A:1060:SER:H	1.86	0.40
4:A:1061:MET:O	4:A:1063:ILE:HG13	2.22	0.40
5:B:23:VAL:HG23	5:B:23:VAL:O	2.22	0.40
5:B:449:LEU:HD23	5:B:667:VAL:HG11	2.03	0.40
5:B:816:SER:OG	15:L:49:THR:HB	2.21	0.40
5:B:952:GLY:O	5:B:956:GLY:N	2.54	0.40
7:D:45:ILE:HB	10:G:36:ASN:HD21	1.86	0.40
13:J:48:MET:HE2	13:J:48:MET:HB2	1.89	0.40
16:M:286:MET:HG3	16:M:327:VAL:HB	2.02	0.40
18:O:480:GLU:O	18:O:483:GLN:HG3	2.22	0.40
19:P:290:CYS:HB3	19:P:293:PHE:HB2	2.03	0.40
22:V:189:VAL:CG2	22:V:253:LEU:HD11	2.50	0.40
4:A:210:LEU:HD22	18:O:411:LYS:HA	2.01	0.40
4:A:731:LEU:HD22	4:A:748:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:831:LYS:HD2	4:A:831:LYS:HA	1.87	0.40
4:A:1371:ASN:HA	10:G:52:THR:O	2.22	0.40
5:B:1097:SER:OG	5:B:1098:SER:N	2.55	0.40
8:E:53:PRO:HD3	8:E:78:GLU:HB2	2.03	0.40
8:E:63:ALA:O	8:E:66:ASP:N	2.53	0.40
10:G:46:ILE:HB	10:G:75:VAL:HG23	2.04	0.40
16:M:30:TYR:HB2	16:M:33:ARG:HB3	2.03	0.40
16:M:339:SER:OG	16:M:381:ASP:OD1	2.39	0.40
18:O:244:GLN:HG3	18:O:247:ARG:HH21	1.86	0.40
18:O:297:LEU:HD12	18:O:298:PRO:HD2	2.04	0.40
23:W:331:HIS:CE1	23:W:371:LEU:HD22	2.57	0.40
24:X:4:DC:H6	24:X:4:DC:OP2	2.05	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	1	144/368 (39%)	144 (100%)	0	0	100	100
2	3	368/411 (90%)	352 (96%)	16 (4%)	0	100	100
3	4	363/1469 (25%)	345 (95%)	18 (5%)	0	100	100
4	A	1376/1390 (99%)	1323 (96%)	50 (4%)	3 (0%)	47	79
5	B	1101/1133 (97%)	1047 (95%)	51 (5%)	3 (0%)	41	75
6	C	341/346 (99%)	337 (99%)	4 (1%)	0	100	100
7	D	120/148 (81%)	112 (93%)	8 (7%)	0	100	100
8	E	207/210 (99%)	199 (96%)	8 (4%)	0	100	100
9	F	74/127 (58%)	71 (96%)	3 (4%)	0	100	100
10	G	160/204 (78%)	137 (86%)	23 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	H	146/150 (97%)	145 (99%)	1 (1%)	0	100	100
12	I	54/108 (50%)	51 (94%)	3 (6%)	0	100	100
13	J	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
14	K	101/133 (76%)	93 (92%)	8 (8%)	0	100	100
15	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
16	M	388/708 (55%)	374 (96%)	13 (3%)	1 (0%)	41	75
17	N	140/317 (44%)	134 (96%)	6 (4%)	0	100	100
18	O	508/534 (95%)	485 (96%)	19 (4%)	4 (1%)	19	57
19	P	230/316 (73%)	223 (97%)	7 (3%)	0	100	100
20	Q	85/223 (38%)	85 (100%)	0	0	100	100
21	U	175/339 (52%)	173 (99%)	2 (1%)	0	100	100
22	V	358/419 (85%)	347 (97%)	11 (3%)	0	100	100
23	W	109/2624 (4%)	106 (97%)	2 (2%)	1 (1%)	17	54
All	All	6655/11802 (56%)	6385 (96%)	258 (4%)	12 (0%)	50	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	O	416	ALA
18	O	418	SER
5	B	305	LYS
16	M	267	VAL
4	A	334	PRO
4	A	335	LYS
18	O	417	PRO
5	B	300	GLY
5	B	303	LYS
18	O	413	PRO
23	W	285	ARG
4	A	327	GLY

5.3.2 Protein sidechains (i)

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	1	130/334 (39%)	127 (98%)	3 (2%)	50 71
2	3	330/356 (93%)	323 (98%)	7 (2%)	53 73
3	4	321/1213 (26%)	317 (99%)	4 (1%)	71 83
4	A	1200/1212 (99%)	1190 (99%)	10 (1%)	81 89
5	B	964/988 (98%)	950 (98%)	14 (2%)	65 80
6	C	299/302 (99%)	299 (100%)	0	100 100
7	D	114/136 (84%)	113 (99%)	1 (1%)	78 87
8	E	191/192 (100%)	190 (100%)	1 (0%)	88 93
9	F	66/111 (60%)	66 (100%)	0	100 100
10	G	149/181 (82%)	148 (99%)	1 (1%)	84 90
11	H	129/131 (98%)	129 (100%)	0	100 100
12	I	48/93 (52%)	48 (100%)	0	100 100
13	J	53/56 (95%)	53 (100%)	0	100 100
14	K	92/119 (77%)	92 (100%)	0	100 100
15	L	43/55 (78%)	42 (98%)	1 (2%)	50 71
16	M	353/622 (57%)	353 (100%)	0	100 100
17	N	131/276 (48%)	130 (99%)	1 (1%)	81 89
18	O	458/476 (96%)	452 (99%)	6 (1%)	69 82
19	P	206/280 (74%)	205 (100%)	1 (0%)	88 93
20	Q	84/195 (43%)	83 (99%)	1 (1%)	71 83
21	U	152/293 (52%)	151 (99%)	1 (1%)	84 90
22	V	325/365 (89%)	321 (99%)	4 (1%)	71 83
23	W	102/2381 (4%)	100 (98%)	2 (2%)	55 74
All	All	5940/10367 (57%)	5882 (99%)	58 (1%)	77 86

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	26	PHE
1	1	42	PHE
1	1	46	MET
2	3	47	PHE
2	3	51	TRP

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Mol	Chain	Res	Type
2	3	167	LYS
2	3	313	HIS
2	3	334	CYS
2	3	340	TYR
2	3	386	MET
3	4	166	ARG
3	4	176	PHE
3	4	286	ASN
3	4	349	TRP
4	A	79	CYS
4	A	140	ARG
4	A	171	LEU
4	A	183	LYS
4	A	213	ARG
4	A	328	ILE
4	A	330	LEU
4	A	332	MET
4	A	335	LYS
4	A	336	LYS
5	B	128	ARG
5	B	292	ARG
5	B	293	ARG
5	B	294	GLN
5	B	295	ARG
5	B	296	MET
5	B	297	TRP
5	B	302	LYS
5	B	303	LYS
5	B	304	THR
5	B	305	LYS
5	B	306	ILE
5	B	324	LYS
5	B	824	LYS
7	D	59	ARG
8	E	55	ARG
10	G	12	ARG
15	L	22	CYS
17	N	144	LYS
18	O	183	ASN
18	O	412	THR
18	O	414	ASP
18	O	418	SER

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Mol	Chain	Res	Type
18	O	419	ARG
18	O	420	THR
19	P	156	GLN
20	Q	33	LYS
21	U	326	GLU
22	V	19	SER
22	V	44	PHE
22	V	55	TYR
22	V	368	ARG
23	W	283	PHE
23	W	285	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	116	ASN
2	3	185	ASN
2	3	210	GLN
2	3	260	ASN
3	4	286	ASN
3	4	438	GLN
3	4	463	GLN
4	A	33	HIS
4	A	48	HIS
4	A	158	HIS
4	A	195	GLN
5	B	124	GLN
5	B	1010	GLN
5	B	1100	HIS
10	G	36	ASN
10	G	116	GLN
18	O	306	GLN
18	O	310	GLN
19	P	156	GLN
22	V	49	ASN
22	V	129	HIS
23	W	279	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
28	SF4	P	401	19	0,12,12	-	-	-		

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
28	SF4	P	401	19	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

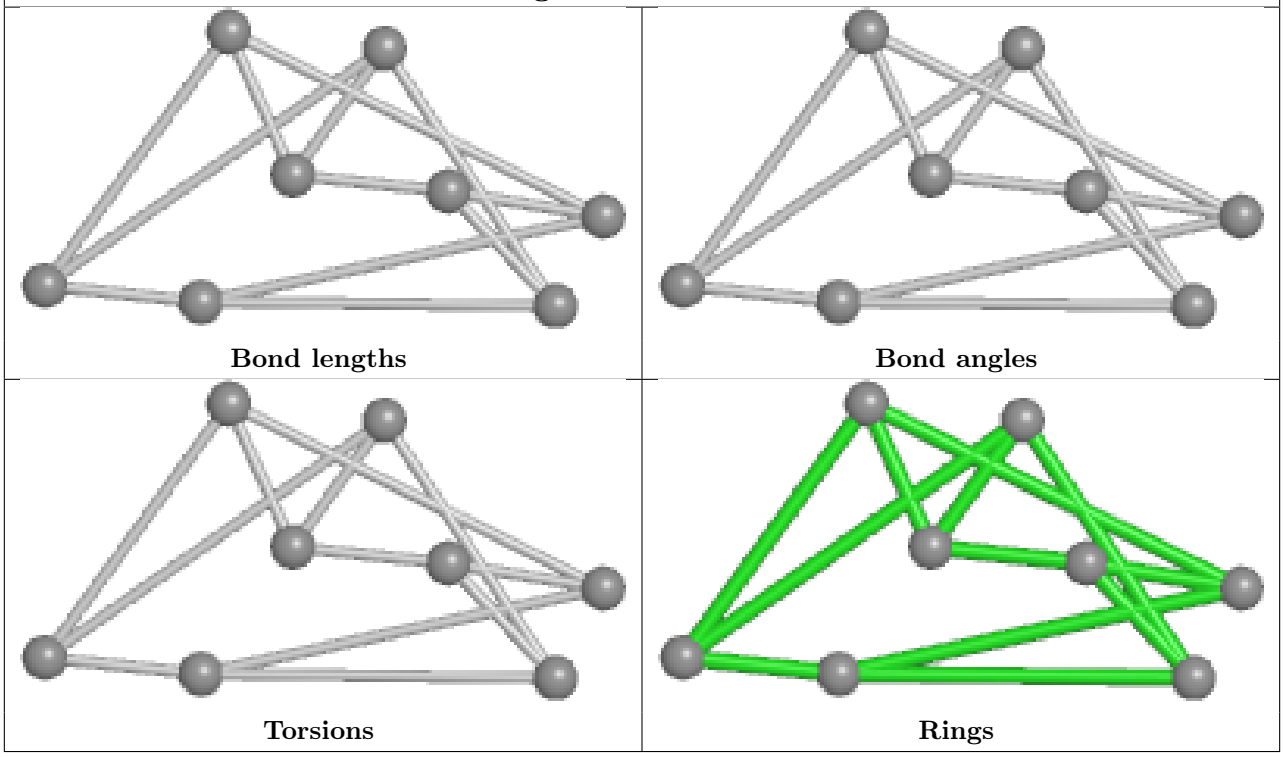
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SF4 P 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

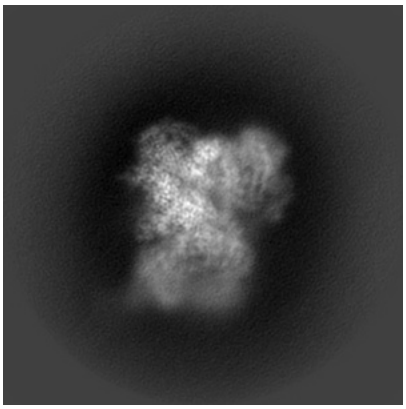
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35712. These allow visual inspection of the internal detail of the map and identification of artifacts.

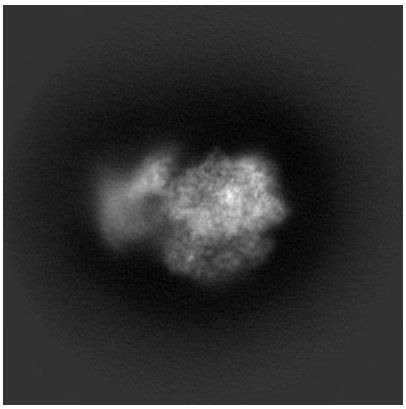
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

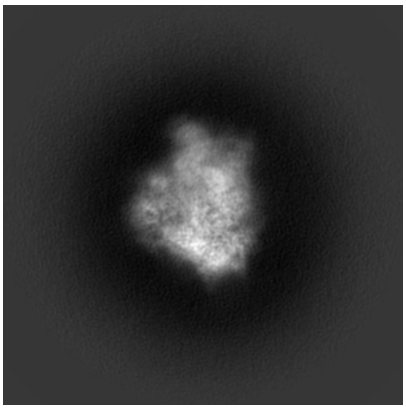
6.1.1 Primary map



X

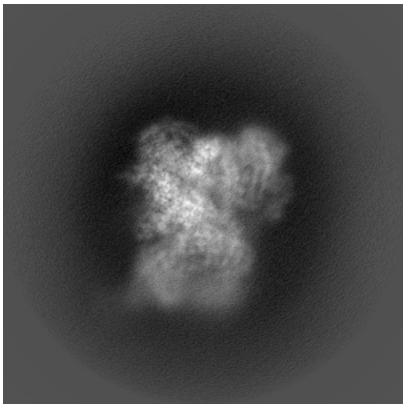


Y

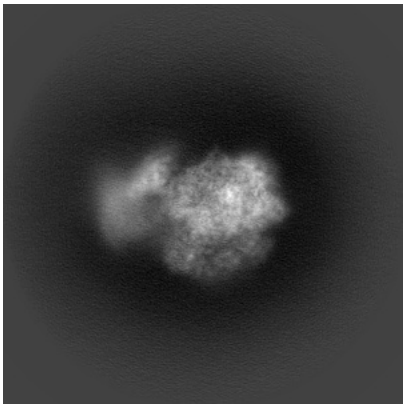


Z

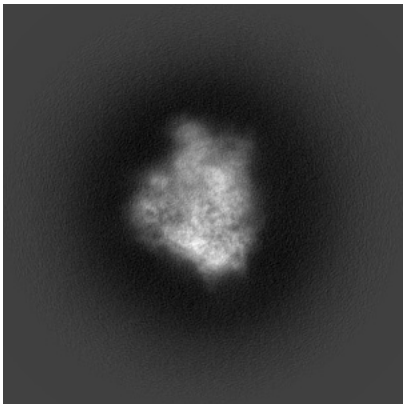
6.1.2 Raw map



X



Y

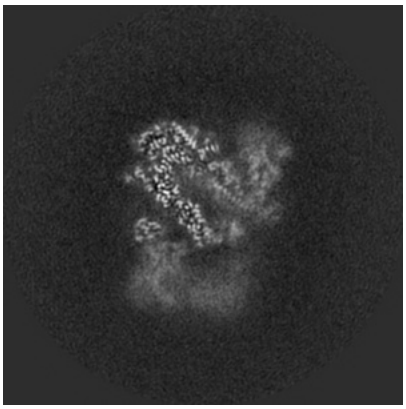


Z

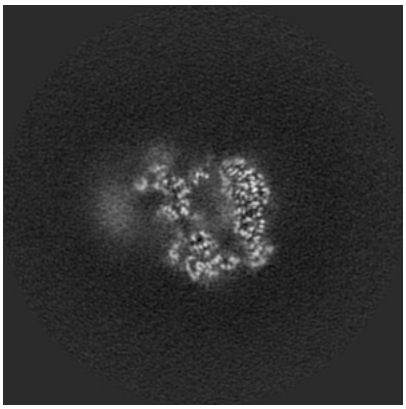
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

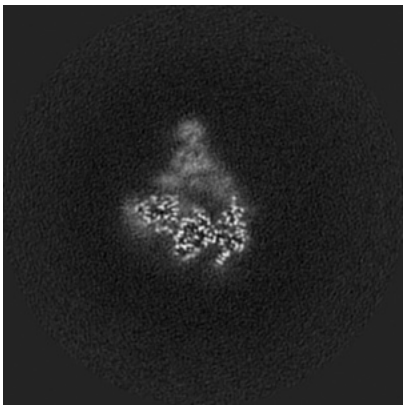
6.2.1 Primary map



X Index: 160

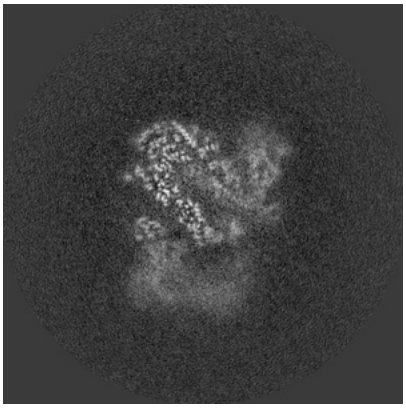


Y Index: 160

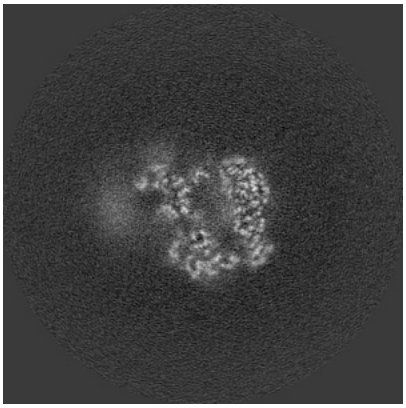


Z Index: 160

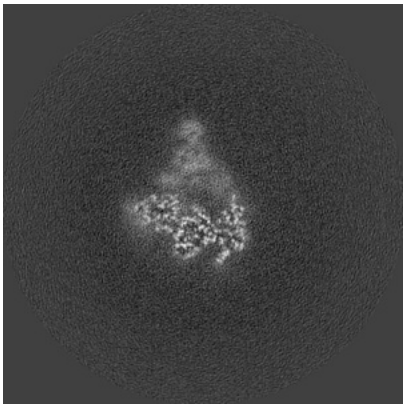
6.2.2 Raw map



X Index: 160



Y Index: 160

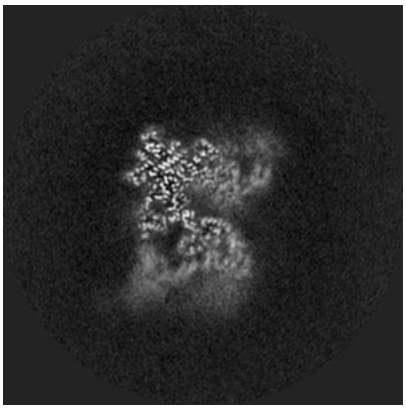


Z Index: 160

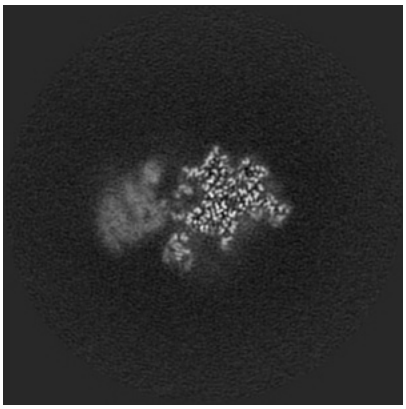
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

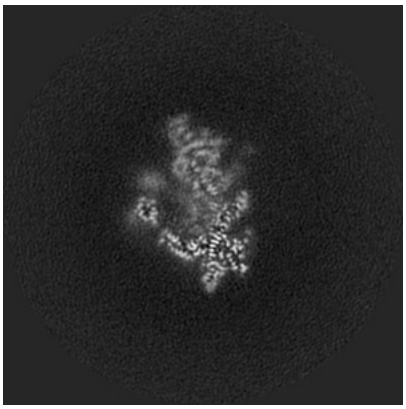
6.3.1 Primary map



X Index: 171

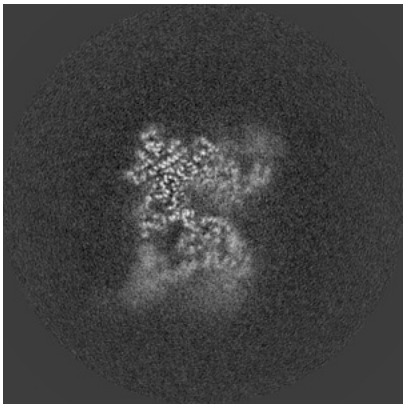


Y Index: 128

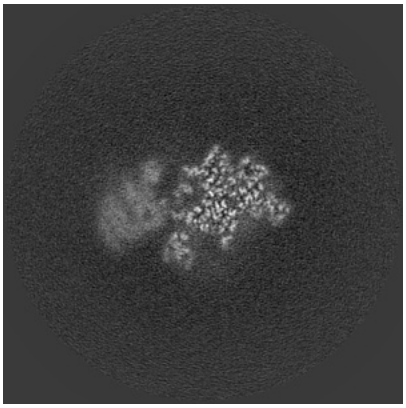


Z Index: 181

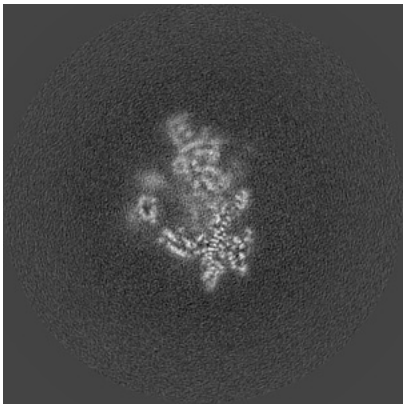
6.3.2 Raw map



X Index: 171



Y Index: 128

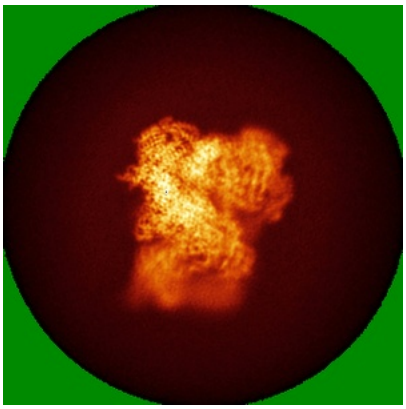


Z Index: 180

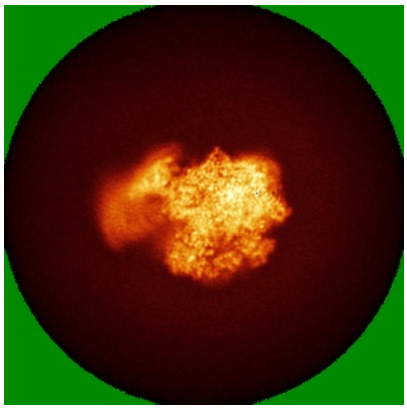
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

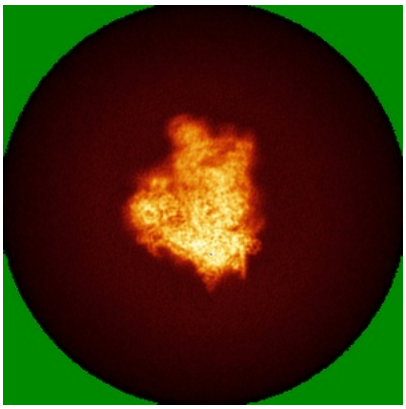
6.4.1 Primary map



X

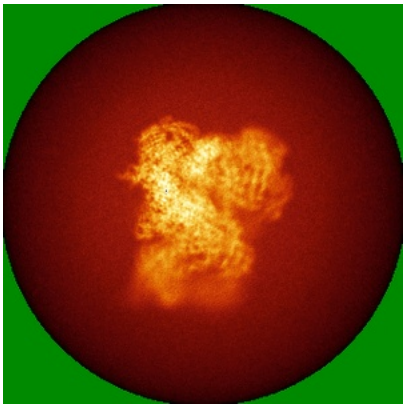


Y

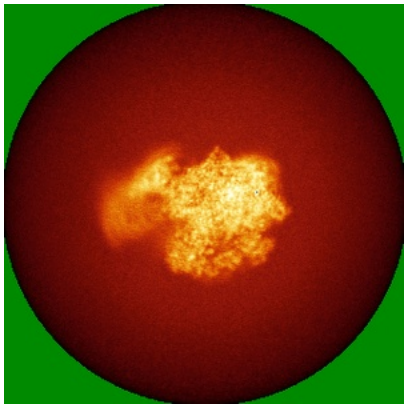


Z

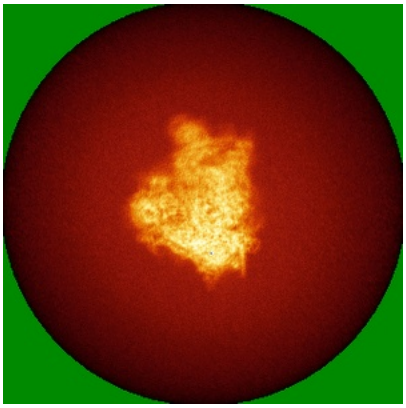
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

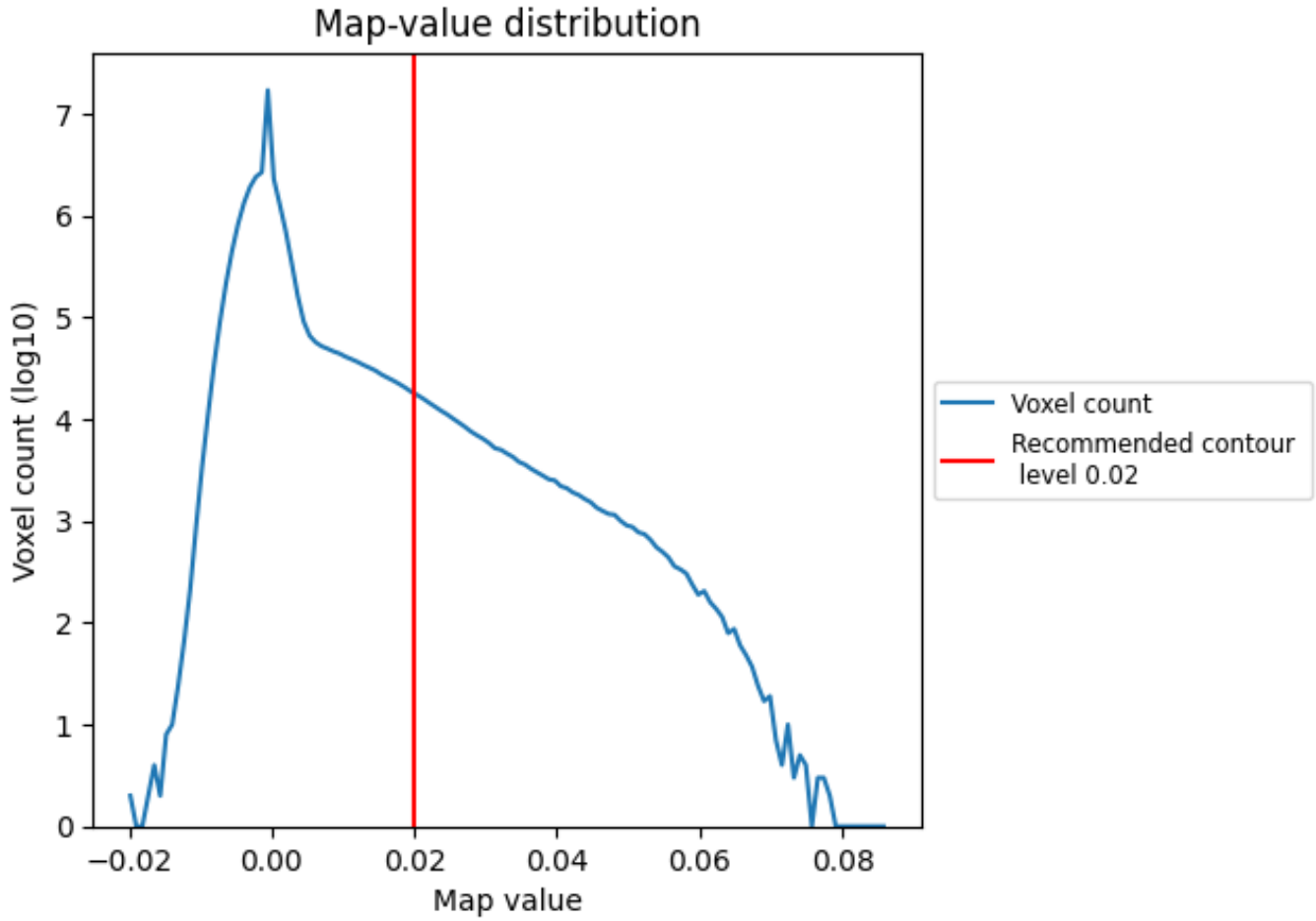
6.6 Mask visualisation (i)

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

7 Map analysis

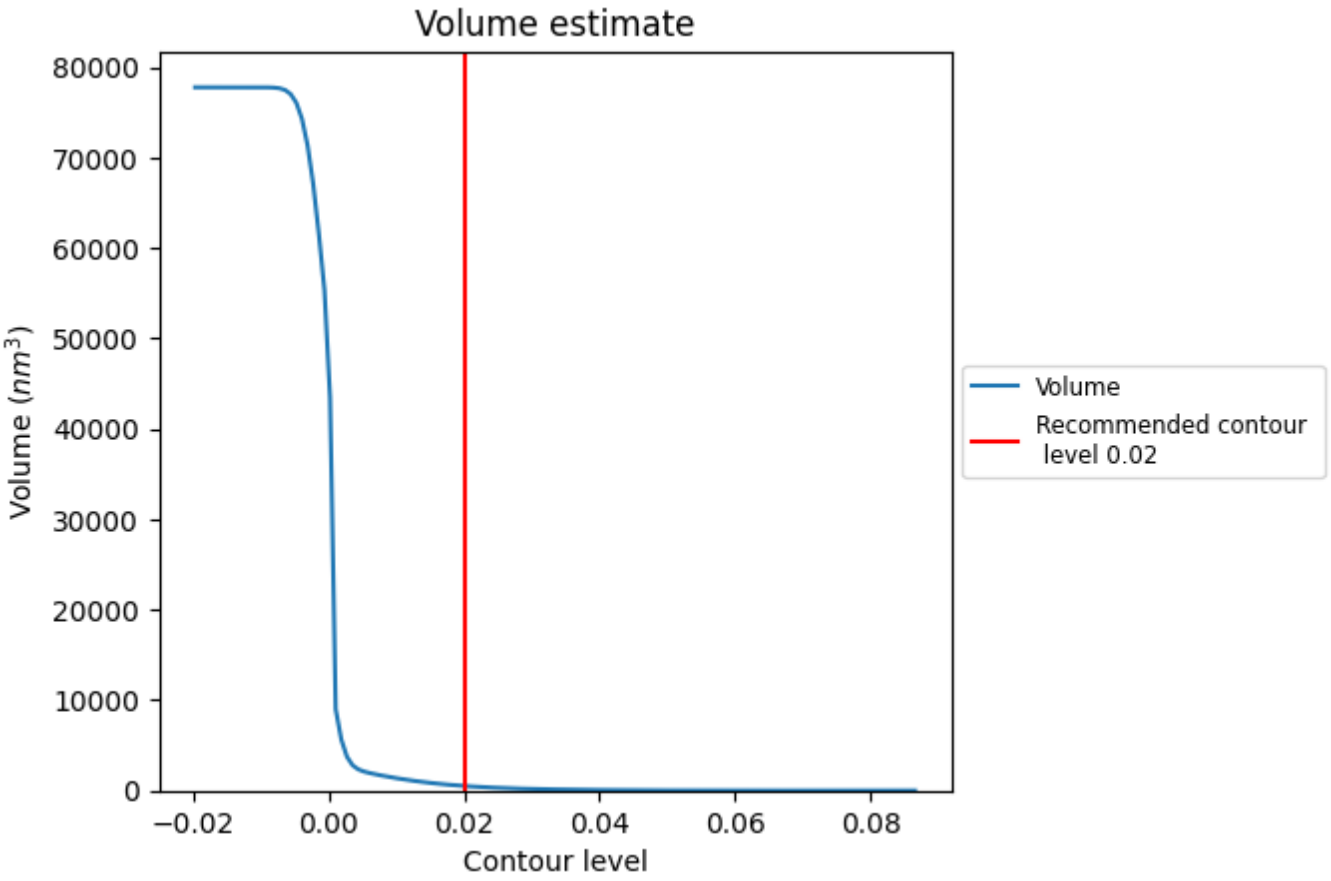
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

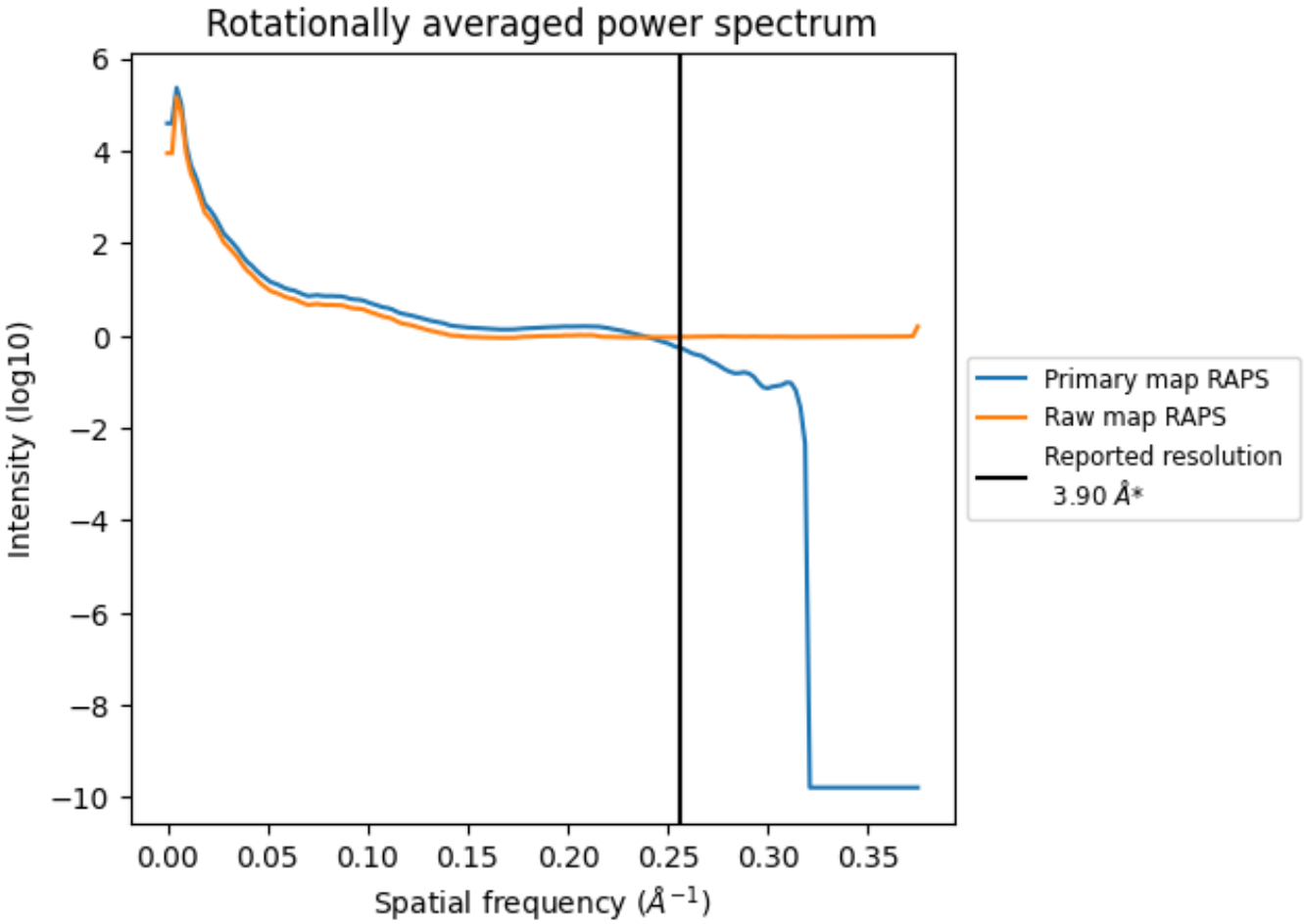
7.2 Volume estimate



The volume at the recommended contour level is 507 nm^3; this corresponds to an approximate mass of 458 kDa.

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

7.3 Rotationally averaged power spectrum (i)

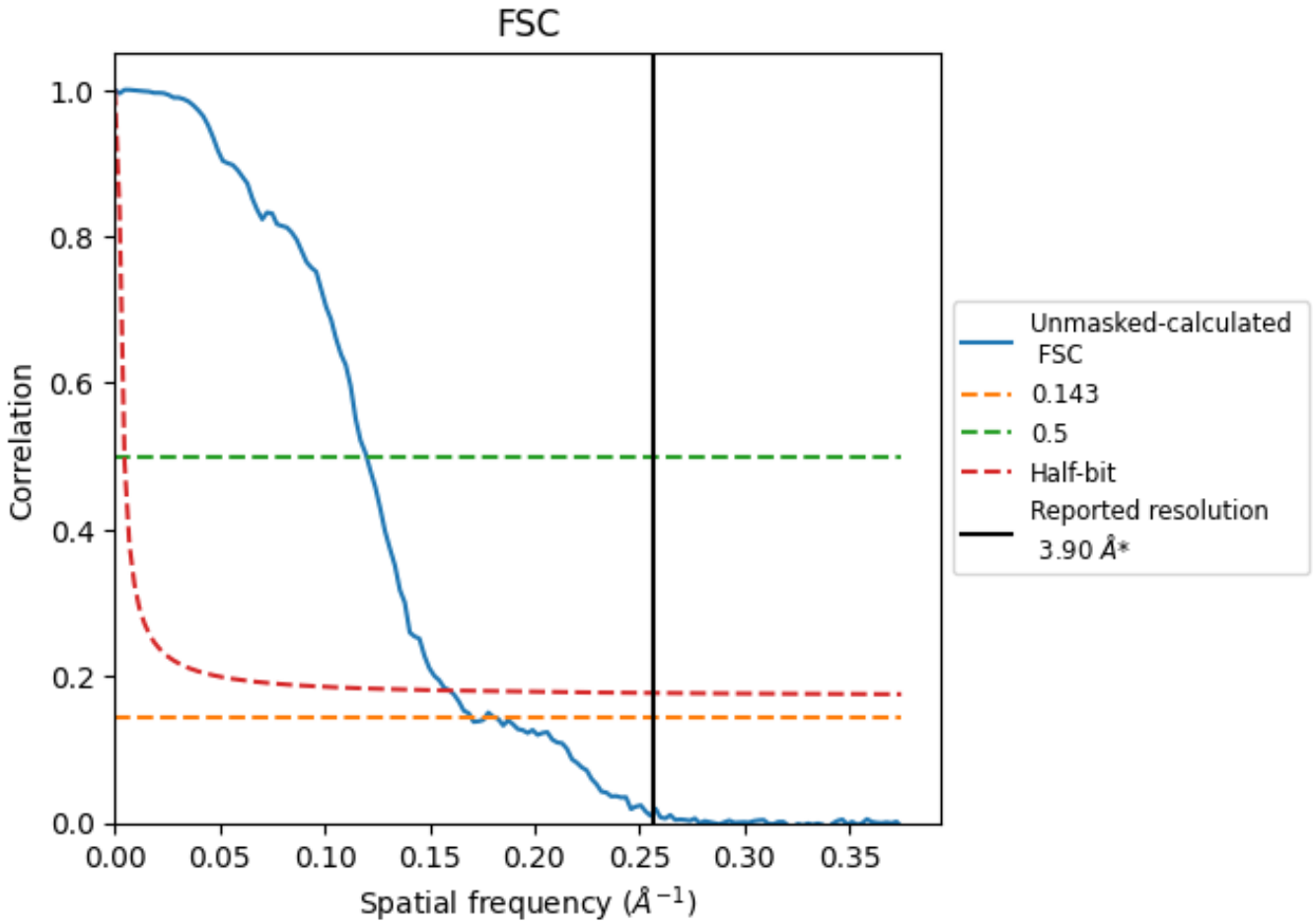


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

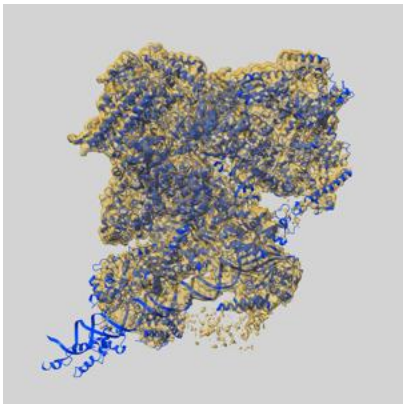
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.89	8.34	6.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.89 differs from the reported value 3.9 by more than 10 %

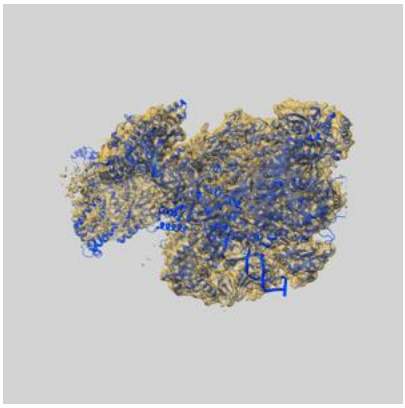
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35712 and PDB model 8ITY. Per-residue inclusion information can be found in section 3 on page 9.

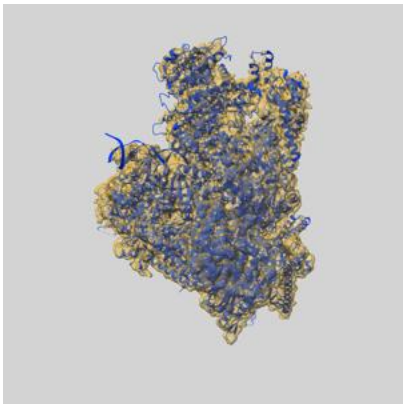
9.1 Map-model overlay



X



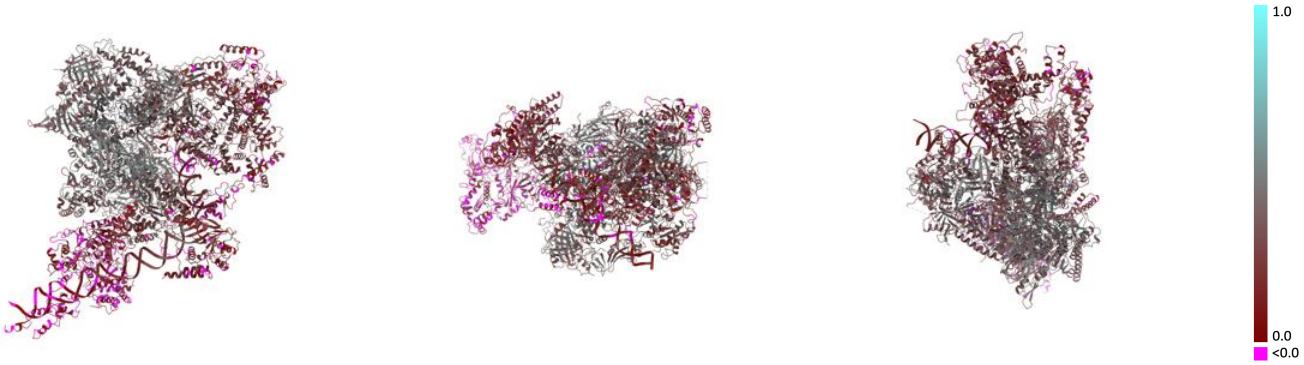
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

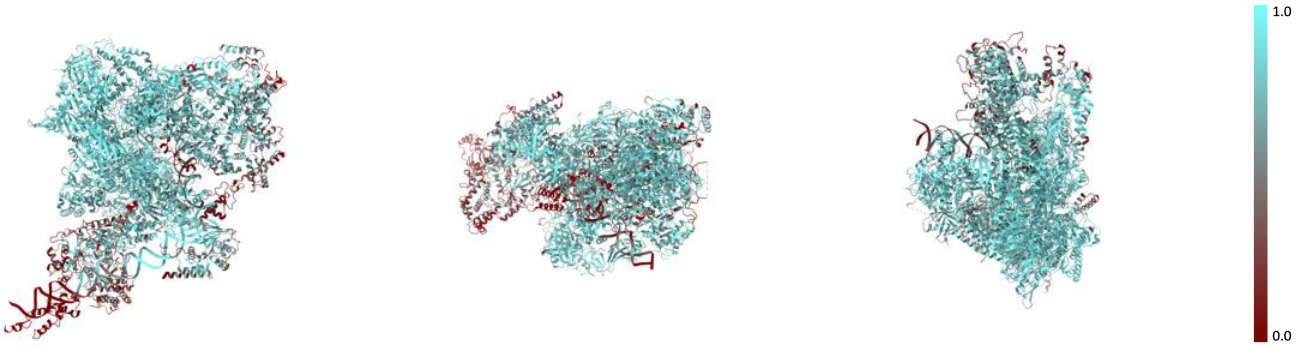
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

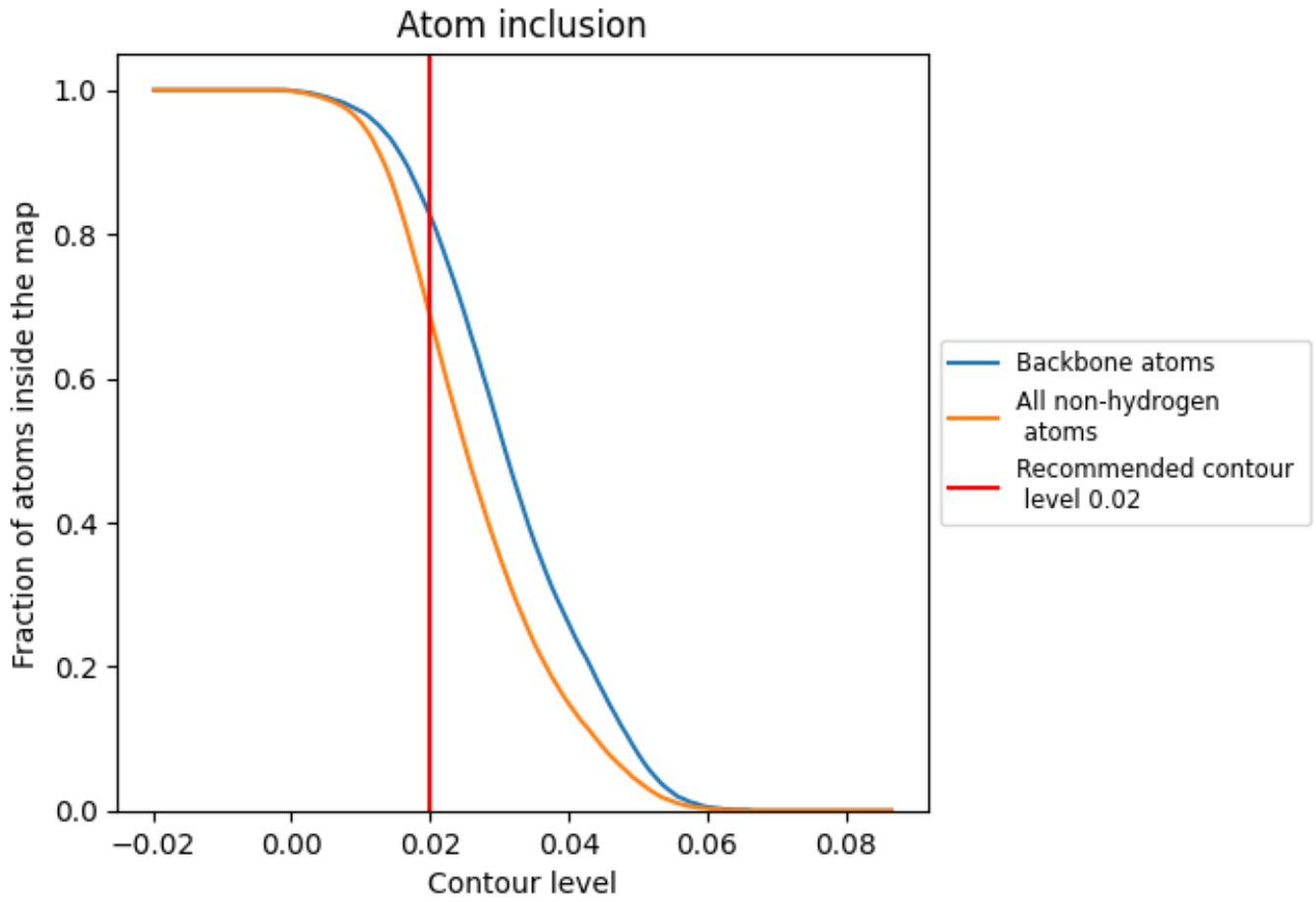
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 69% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6860	0.2910
1	0.3140	0.0520
3	0.3420	0.0470
4	0.2820	0.0900
A	0.8060	0.3660
B	0.8560	0.4260
C	0.8460	0.4350
D	0.6650	0.2070
E	0.8000	0.3420
F	0.8700	0.4210
G	0.7840	0.2740
H	0.7880	0.4100
I	0.8170	0.3700
J	0.8980	0.4530
K	0.8540	0.4170
L	0.8170	0.3780
M	0.7610	0.3630
N	0.7110	0.3530
O	0.6030	0.2180
P	0.3090	0.1460
Q	0.5560	0.2040
U	0.7340	0.2040
V	0.6650	0.2470
W	0.6020	0.1580
X	0.5470	0.1380
Y	0.5640	0.1550