Full wwPDB EM Validation Report

Apr 5, 2026 – 10:13 PM UTC

PDB ID	:	9RZE / pdb_00009rze
EMDB ID	:	EMD-54401
Title	:	State 2 MAP 3 RNA Pol II activated elongation complex with SETD2 bound to proximal upstream H3
Authors	:	Walshe, J.L.; Ochmann, M.; Dienemann, C.; Cramer, P.
Deposited on	:	2025-07-15
Resolution	:	8.53 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

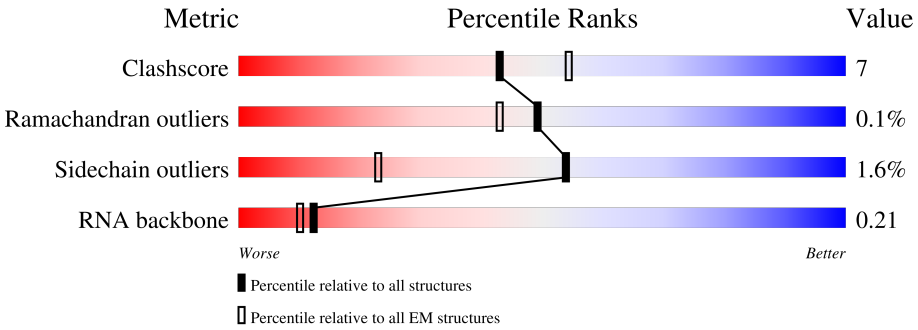
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

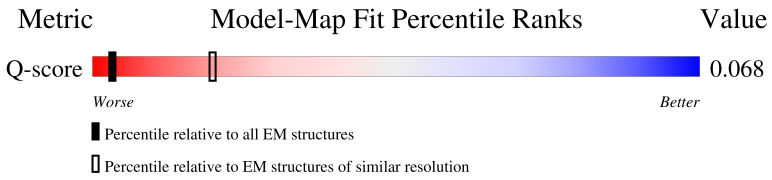
1 Overall quality at a glance

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

The reported resolution of this entry is 8.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	270 (8.04 - 9.02)

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	D	142	60% 25% • 11%
2	E	210	85% 14%
3	F	127	51% 10% 39%

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Mol	Chain	Length	Quality of chain
4	G	172	52% 30% 14%
5	H	150	77% 21%
6	I	125	86% 7% 6%
7	J	67	84% 13%
8	K	117	85% 13%
9	L	58	38% 31% 9% 19%
10	P	46	13% 17% 15% 54%
11	Q	1179	37% 71% 24%
12	T	182	11% 14% 53% 31%
13	W	305	14% 95% 5%
14	X	531	9% 90%
15	Y	121	11% 64% 31%
16	Z	1087	8% 28% 11% 60%
17	a	136	65% 9% 26%
17	e	136	64% 6% 30%
18	b	103	71% 5% 24%
18	f	103	73% 24%
19	c	135	73% 23%
19	g	135	73% 24%
20	d	126	68% 5% 27%
20	h	126	6% 63% 8% 29%
21	j	1049	99%
22	A	1970	62% 9% 29%
23	B	1174	80% 14%
24	C	275	83% 11% 6%

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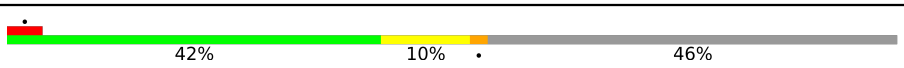
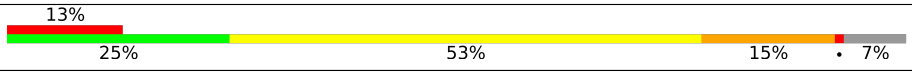
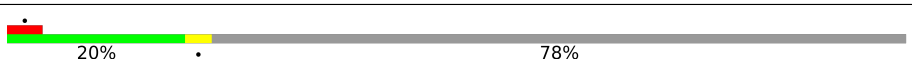
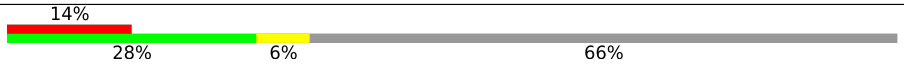
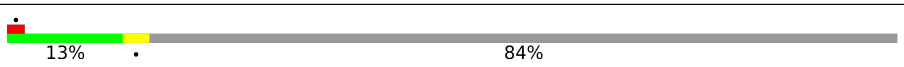
Mol	Chain	Length	Quality of chain
25	M	1729	
26	N	182	
27	O	1133	
28	R	713	
29	U	666	
30	V	531	

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 72793 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 RNA polymerase II subunit D.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	209	1721	1089	300	324	8	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	78	627	401	106	115	5	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	149	1198	759	195	239	5	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	117	950	587	169	183	11	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 9 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	47	Total	C	N	O	S	0	0
			398	246	77	69	6		

- Molecule 10 is a RNA chain called RNA (92-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	21	Total	C	N	O	P	0	0
			452	202	87	142	21		

- Molecule 11 is a protein called RNA polymerase-associated protein CTR9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	892	Total	C	N	O	S	0	0
			7240	4587	1266	1355	32		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1174	GLU	-	expression tag	UNP Q6PD62
Q	1175	ASN	-	expression tag	UNP Q6PD62
Q	1176	LEU	-	expression tag	UNP Q6PD62
Q	1177	TYR	-	expression tag	UNP Q6PD62
Q	1178	PHE	-	expression tag	UNP Q6PD62
Q	1179	GLN	-	expression tag	UNP Q6PD62

- Molecule 12 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	181	Total	C	N	O	P	0	0
			3691	1751	667	1092	181		

- Molecule 13 is a protein called WD repeat-containing protein 61.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	W	305	Total	C	N	O	S	0	0
			2374	1507	399	463	5		

- Molecule 14 is a protein called Parafibromin.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	53	Total	C	N	O	0	0
			434	268	85	81		

- Molecule 15 is a protein called Transcription elongation factor SPT4.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP Q4R941
Y	-2	PRO	-	expression tag	UNP Q4R941
Y	-1	GLY	-	expression tag	UNP Q4R941
Y	0	SER	-	expression tag	UNP Q4R941

- Molecule 16 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	432	Total	C	N	O	S	0	0
			3468	2213	609	630	16		

- Molecule 17 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	101	Total	C	N	O	S	0	0
			821	519	157	142	3		
17	e	95	Total	C	N	O	S	0	0
			782	494	150	136	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	37	MET	LYS	engineered mutation	UNP Q71DI3
a	111	ALA	CYS	engineered mutation	UNP Q71DI3
e	37	MET	LYS	engineered mutation	UNP Q71DI3
e	111	ALA	CYS	engineered mutation	UNP Q71DI3

- Molecule 18 is a protein called Histone H4.

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

- Molecule 19 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	c	104	Total	C	N	O	0	0
			801	505	156	140		
19	g	103	Total	C	N	O	0	0
			796	502	155	139		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-5	SER	-	expression tag	UNP P04908
c	-4	ASN	-	expression tag	UNP P04908
c	-3	ALA	-	expression tag	UNP P04908
c	-2	PRO	-	expression tag	UNP P04908
c	-1	TRP	-	expression tag	UNP P04908
g	-5	SER	-	expression tag	UNP P04908
g	-4	ASN	-	expression tag	UNP P04908
g	-3	ALA	-	expression tag	UNP P04908
g	-2	PRO	-	expression tag	UNP P04908
g	-1	TRP	-	expression tag	UNP P04908

- Molecule 20 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	d	92	Total	C	N	O	S	0	0
			719	452	129	136	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
20	h	89	Total	C	N	O	S	0	0
			693	437	122	132	2		

- Molecule 21 is a protein called FACT complex subunit SPT16.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	j	14	Total	C	N	O	0	0
			111	65	15	31		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	-1	SER	-	expression tag	UNP Q9Y5B9
j	0	ASN	-	expression tag	UNP Q9Y5B9

- Molecule 22 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A	1390	Total	C	N	O	S	0	0
			11015	6932	1976	2038	69		

- Molecule 23 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	1123	Total	C	N	O	S	0	0
			8992	5690	1580	1658	64		

- Molecule 24 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 25 is a protein called Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	M	934	Total	C	N	O	S	0	0
			7638	4822	1325	1455	36		

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 26 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	N	170	Total	C	N	O	P	0	0
			3509	1657	665	1017	170		

- Molecule 27 is a protein called Histone-lysine N-methyltransferase SETD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	O	254	Total	C	N	O	S	0	0
			2071	1285	379	386	21		

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 28 is a protein called RNA polymerase-associated protein RTF1 homolog.

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 29 is a protein called RNA polymerase-associated protein LEO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	104	Total	C	N	O	S	0	0
			751	475	130	145	1		

- Molecule 30 is a protein called RNA polymerase II-associated factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	242	Total	C	N	O	S	0	0
			1687	1055	302	326	4		

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

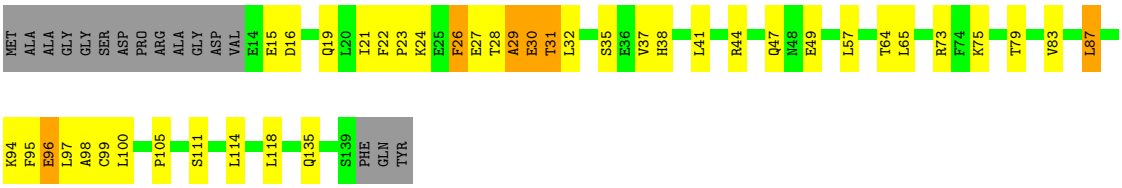
Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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

• Molecule 1: RNA polymerase II subunit D

Chain D:

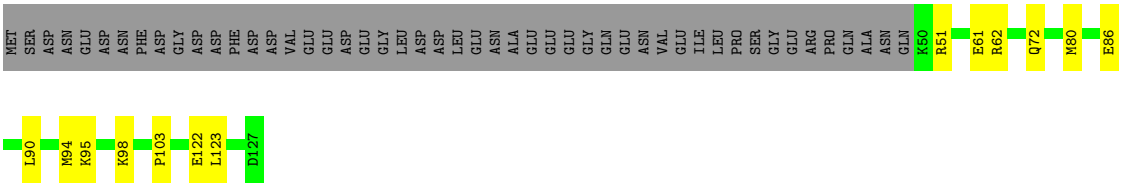


• Molecule 2: DNA-directed RNA polymerase II subunit E

Chain E:

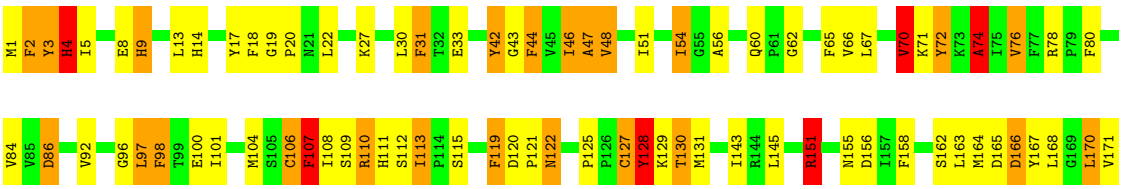
• Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



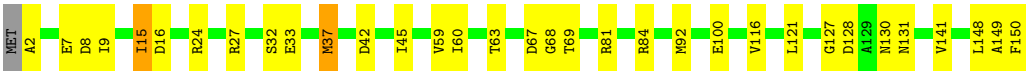
• Molecule 4: DNA-directed RNA polymerase II subunit RPB7

Chain G:



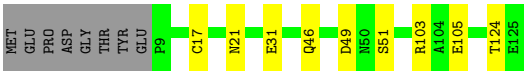
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



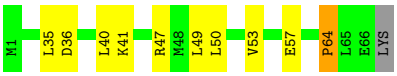
• Molecule 6: DNA-directed RNA polymerase II subunit RPB9

Chain I:



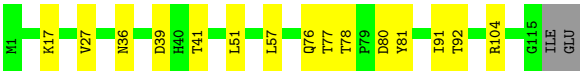
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



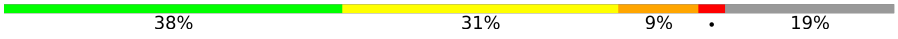
• Molecule 8: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:



• Molecule 9: RNA polymerase II subunit K

Chain L:



• Molecule 10: RNA (92-MER)

Chain P:

• Molecule 11: RNA polymerase-associated protein CTR9 homolog

Chain Q:

M1 S2 R3 G4 S5 I6 E7 I8 P9 L10 R11 D12 T13 D14 E15 V16 I17 E18 L19 D20 F21 D22 Q23 L24 P25 E26 G27 D28 E29 V30 I31 S32 I33 L34 K35 Q36 E37 H38 T39 Q40 L41 H42 I43 W44 I45 A46 L47 A48 L49 E50 Y51 Y52 K53 Q54 G55 K56 T57 E58 E59 F60

V61 K62 L63 L64 E65 A66 A67 R68 I69 D70 G71 N72 L73 D74 Y75 R76 D77 H78 E79 K80 D81 Q82 M83 T84 C85 L86 D87 T88 L89 A90 A91 Y92 Y93 V94 Q95 Q96 A97 R98 K99 E100 K101 N102 K103 D104 N105 K106 K107 D108 L109 I110 T111 Q112 A113 T114 L115 L116 Y117 T118 M119 A120

D121 K122 I123 I124 M125 Y126 D127 Q128 N129 H130 L131 L132 G133 R134 A135 C136 F137 C138 L139 L140 E141 G142 D143 K144 M145 D146 Q147 A148 D149 A150 Q151 F152 H153 F154 V155 L156 N157 Q158 S159 P160 N161 N162 I163 P164 A165 L166 L167 G168 K169 A170 C171 I172 S173 F174 N175 K176 K177 D178 Y179 R180

G181 A182 L183 A184 Y185 Y186 K187 K188 A189 L190 R191 T192 N193 P194 G195 C196 P197 A198 E199 V200 R201 L202 G203 M204 G205 H206 C207 F208 V209 K210 L211 N212 K213 L214 E215 K216 A217 R218 L219 A220 F221 S222 R223 A224 L225 E226 L227 N228 S229 K230 C231 V232 G233 A234 L235 V236 G237 L238 A239 V240

L241 E242 L243 N244 N245 K246 E247 A248 D249 S250 I251 K252 N253 G254 V255 Q256 L257 L258 S259 R260 A261 Y262 T263 I264 D265 P266 S267 N268 P269 M270 V271 L272 N273 H274 L275 A276 N277 H278 F279 F280 F281 K282 K283 D284 Y285 S286 K287 V288 Q289 H290 L291 A292 L293 H294 A295 F296 H297 N298 T299 E300

V301 E302 A303 M304 Q305 A306 E307 S308 C309 Y310 Q311 L312 A313 R314 S315 F316 H317 V318 Q319 E320 D321 Y322 D323 Q324 A325 F326 Q327 Y328 Y329 Y330 Q331 A332 T333 Q334 F335 A336 S337 S338 S339 F340 V341 L342 F345 C363 F364 E365 K366 V367 L368 K369 A370 Y371 P372 N373 N374 Y375 E376 T377

M378 K379 I380 L381 L384 Y385 E392 K393 R394 D395 I396 A397 K398 G399 H400 L401 K402 K403 V404 T405 E406 Q407 Y408 P409 D410 D411 V412 E413 A414 W415 L418 I421 L422 T425 D426 I427 Q428 G429 A430 L431 S432 A433 Y434 G435 T436 A437 T438 R439 I440 L441 Q442 E443 K444 V445 Q446

A447 D448 V449 N456 V457 L460 H461 L464 G465 N466 L467 G468 E469 A470 K471 K472 Y473 A476 S477 L478 D479 R480 E486 H487 D488 E489 I523 L524 V531 D532 C533 L605 R674 W684 I698 P748 Q762 T766 L769 E772 D801 K802 M803

D806 L807 A808 E813 Q816 C817 S818 D819 L820 A824 H827 Y828 A829 R830 K833 Q834 D835 E836 E837 E838 R839 E840 A843 K849 L852 R853 Q854 K855 L856 L857 K858 E859 Q860 E861 R864 Q877 R878 A879 V882 N887 M890 F891 T892 GLY GLU THR

GLU ALA THR LYS GLU LYS LYS ARG GLY GLY GLY GLY GLY ARG ARG SER LYS LYS GLY GLY GLU PHE ASP GLU PHE VAL ASN ASP ASP THR ASP ASP ASP LEU PRO ILE SER LYS LYS LYS ARG ARG LYS GLY SER GLY SER GLU GLN GLU GLY GLU ASP GLU GLU GLY GLY GLU ARG

LYS LYS LYS LYS ARG ARG ARG HIS PRO LYS GLY GLU GLU GLY SER ASP ASP ASP GLU THR GLU ASN GLY PRO LYS PRO LYS LYS ARG ARG PRO PRO LYS ALA GLU LYS LYS LYS ALA PRO LYS PRO GLU ARG LEU PRO PRO SER MET LYS GLY LYS ILE LYS SER LYS ALA ILE ILE SER

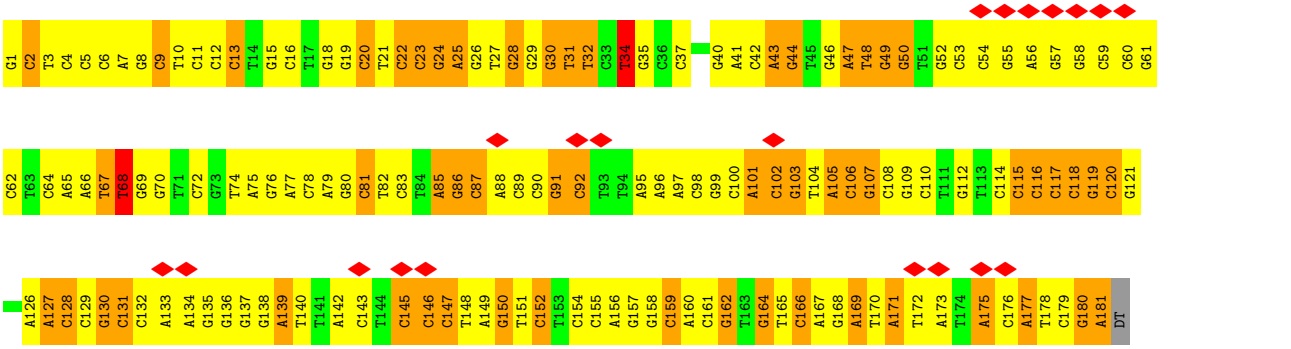
SER SER ASP ASP SER SER ASP GLU ASP LYS LEU LYS ILE ALA ASP GLU GLY HIS PRO ARG ASN SER GLY ASN SER ASN SER ASP SER SER GLU ASP GLU GLN ARG LYS LYS CYS ALA SER SER GLU SER ASP SER ASP GLU ASN GLN ASN LYS SER GLY SER GLU ALA GLU GLY SER ARG ARG

PRO ARG ARG GLN ARG SER ASP GLN ASP SER ASP SER ASP LYS GLN LEU PRO SER ARG LYS ARG ARG PRO SER GLY SER GLU GLN ASP SER VAL GLN SER GLY ARG SER HIS SER GLY VAL SER GLU ASN ASP SER ARG PRO ALA SER PRO SER ALA GLU SER ASP HIS GLU SER GLU

ARG GLY SER ASP ASN GLU GLY SER GLY GLN GLY GLY SER GLY ASN GLU SER GLU PRO GLU GLY SER ASN ASN GLU ALA SER ASP ARG GLY SER GLU HIS GLY SER ASP ASP SER ASP GLU ASN LEU TYR PHE GLN

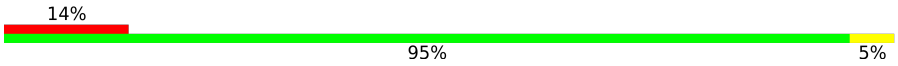
- Molecule 12: Template DNA

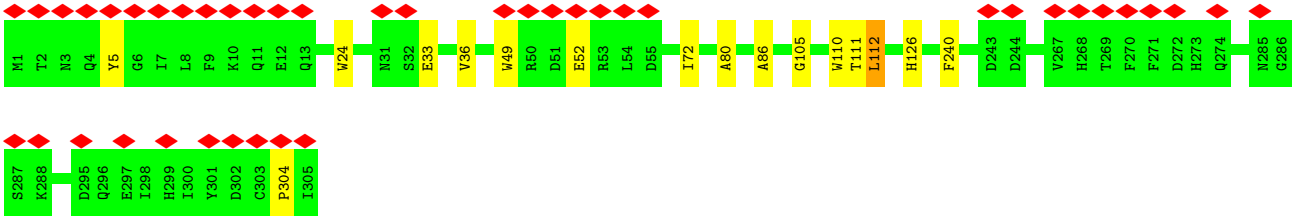
Chain T:



• Molecule 13: WD repeat-containing protein 61

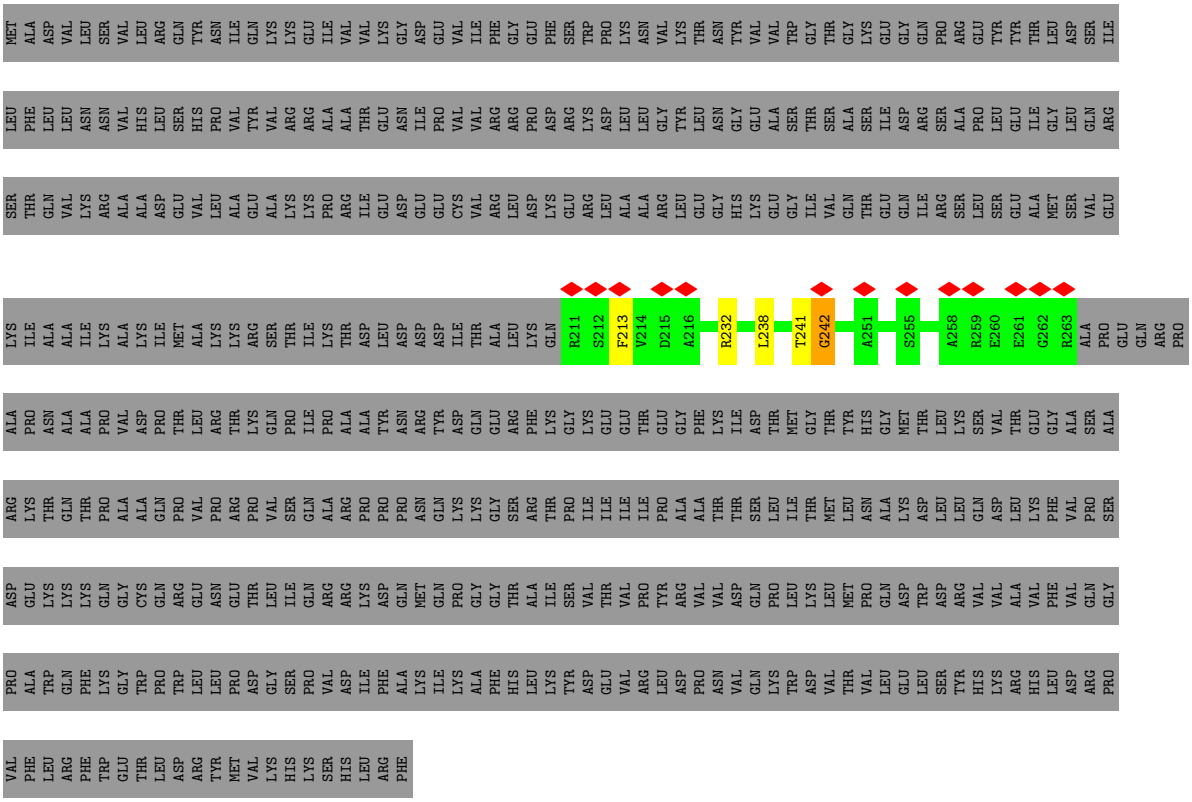
Chain W:



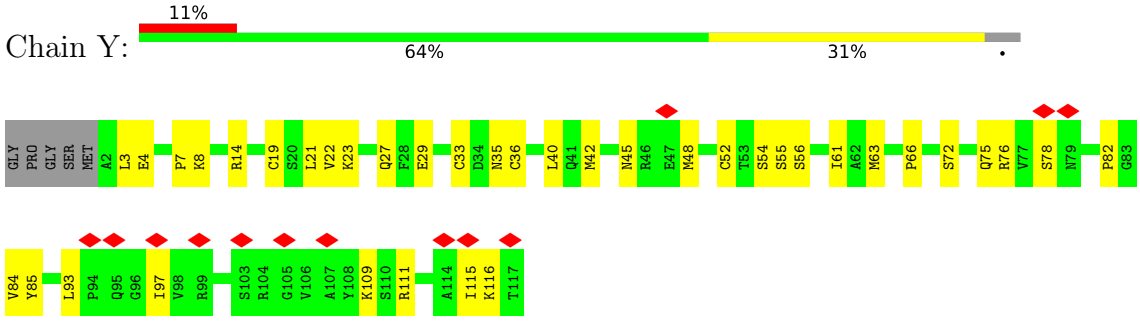


• Molecule 14: Parafibromin

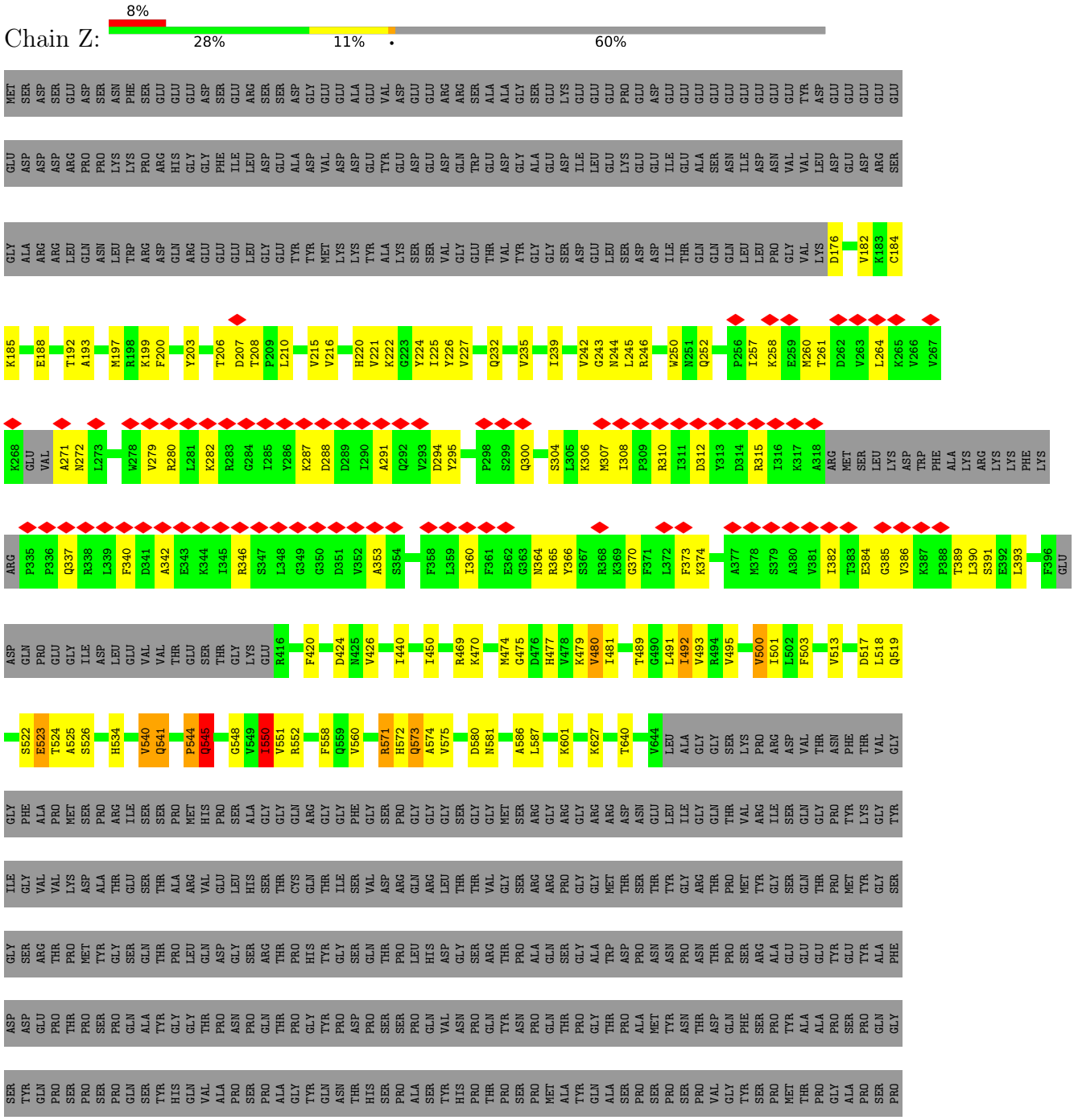
Chain X:

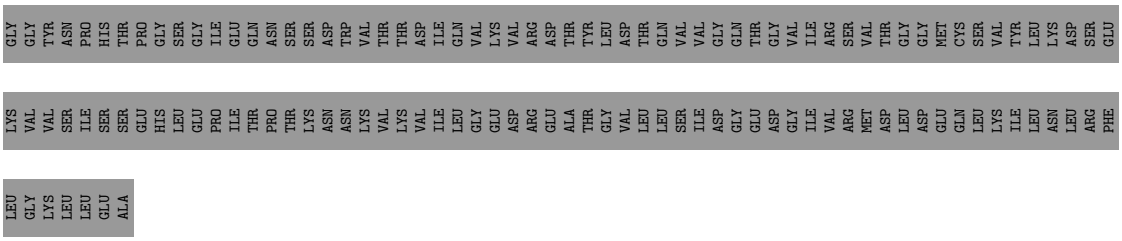


• Molecule 15: Transcription elongation factor SPT4



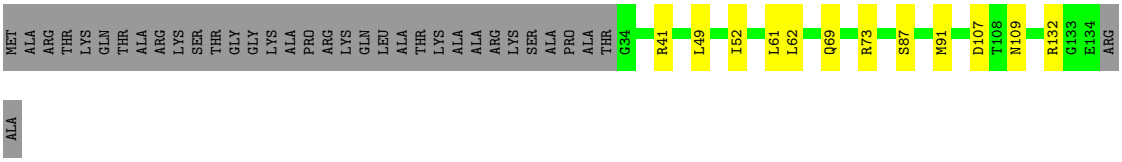
• Molecule 16: Transcription elongation factor SPT5





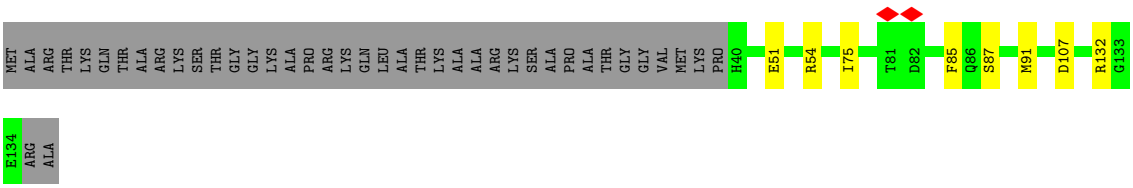
• Molecule 17: Histone H3.2

Chain a:



• Molecule 17: Histone H3.2

Chain e:



• Molecule 18: Histone H4

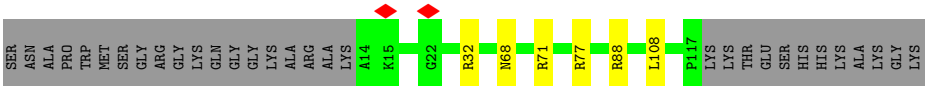
Chain b:

• Molecule 18: Histone H4

Chain f:

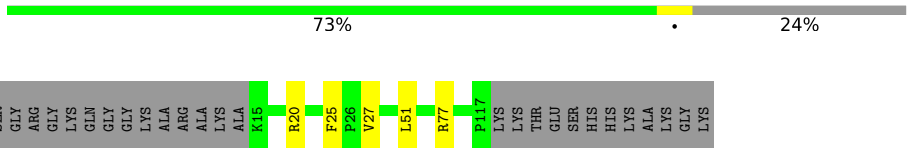
• Molecule 19: Histone H2A type 1-B/E

Chain c:



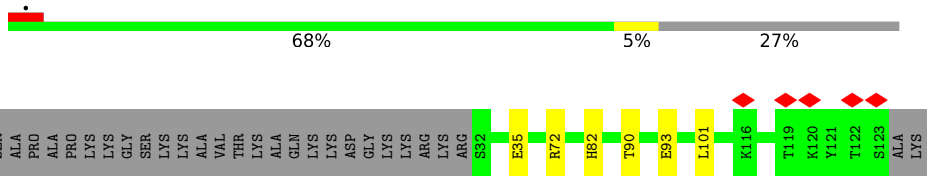
• Molecule 19: Histone H2A type 1-B/E

Chain g:



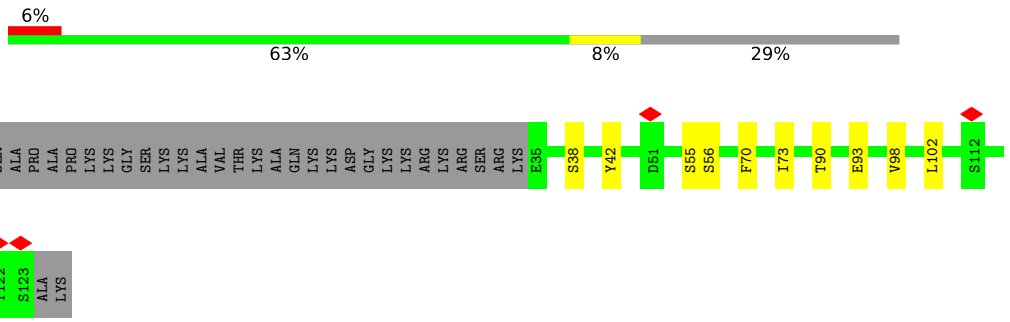
• Molecule 20: Histone H2B type 1-K

Chain d:



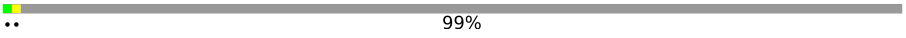
• Molecule 20: Histone H2B type 1-K

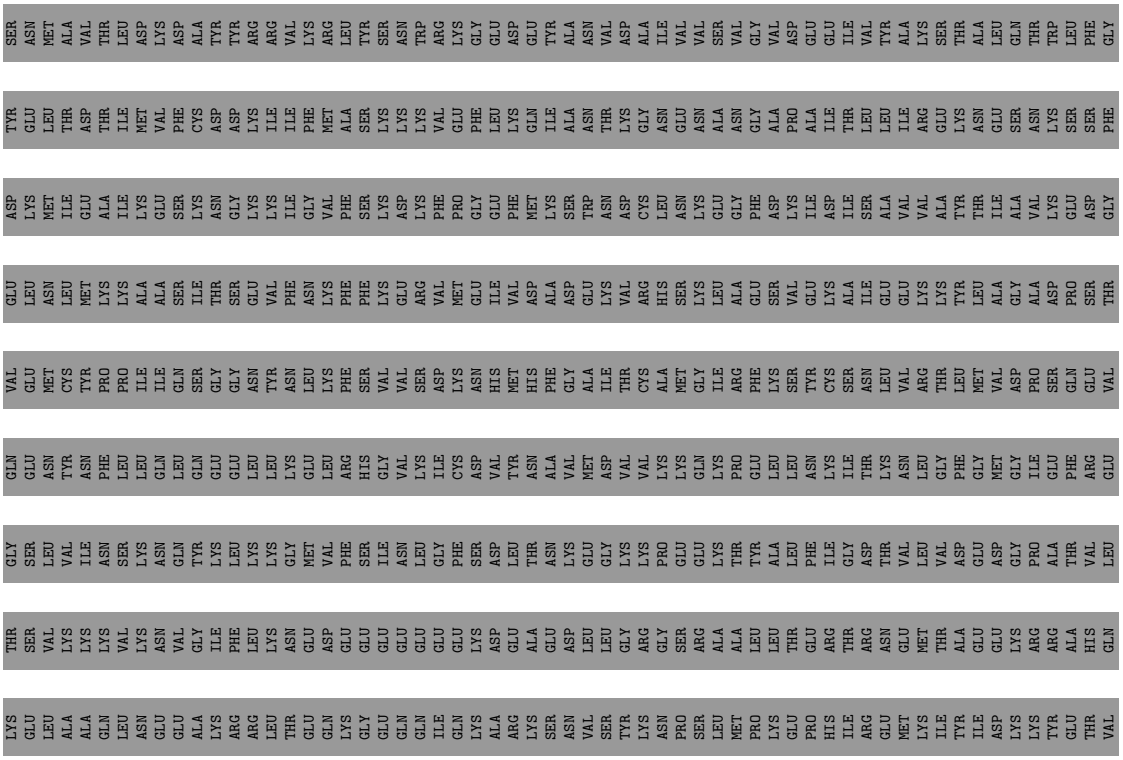
Chain h:

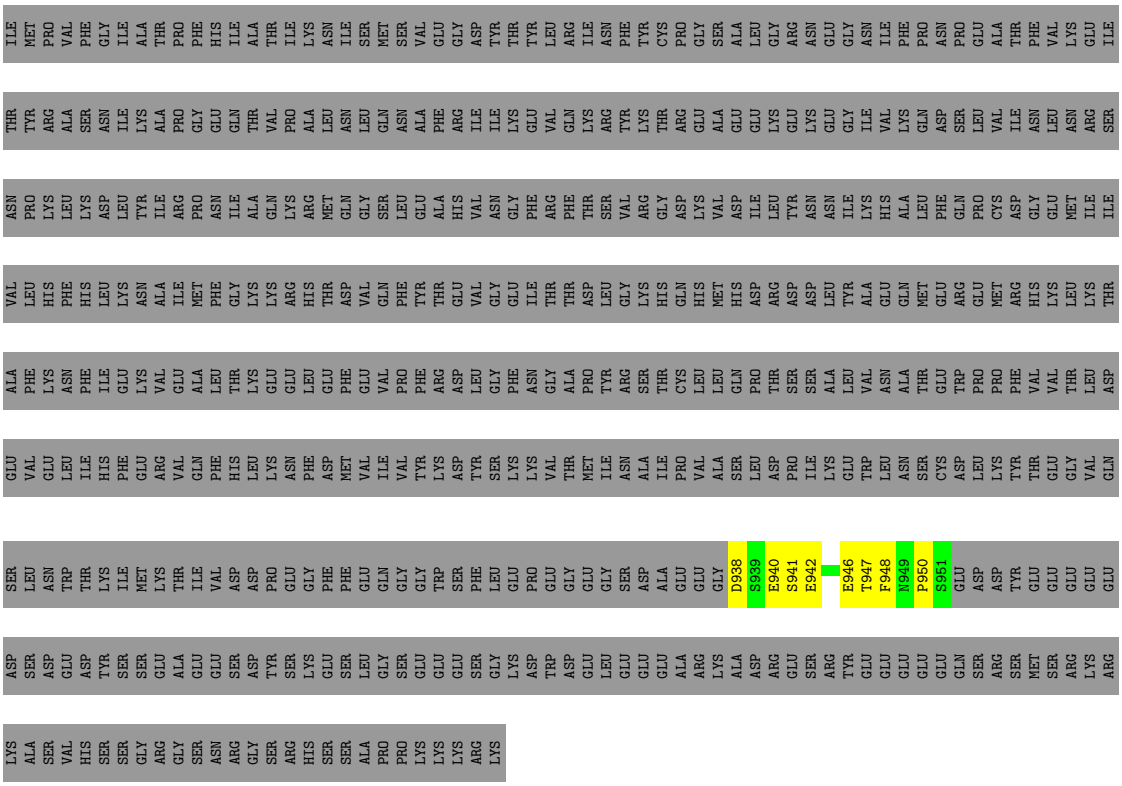


• Molecule 21: FACT complex subunit SPT16

Chain j:

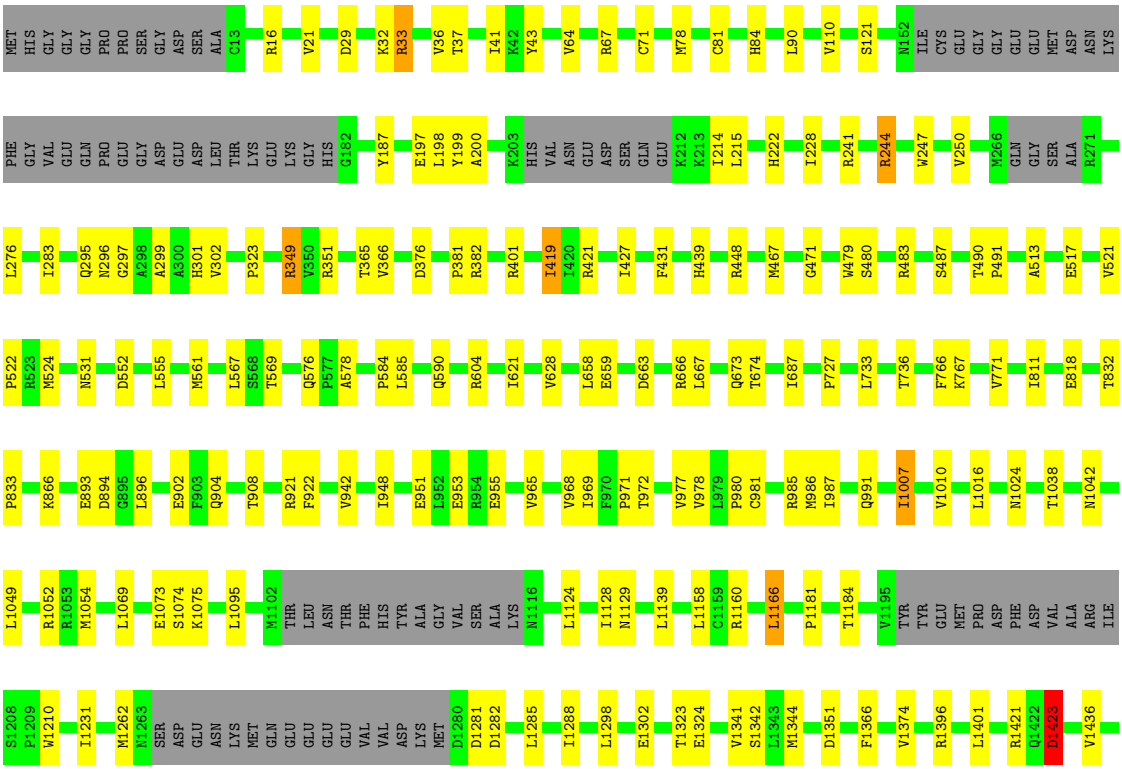


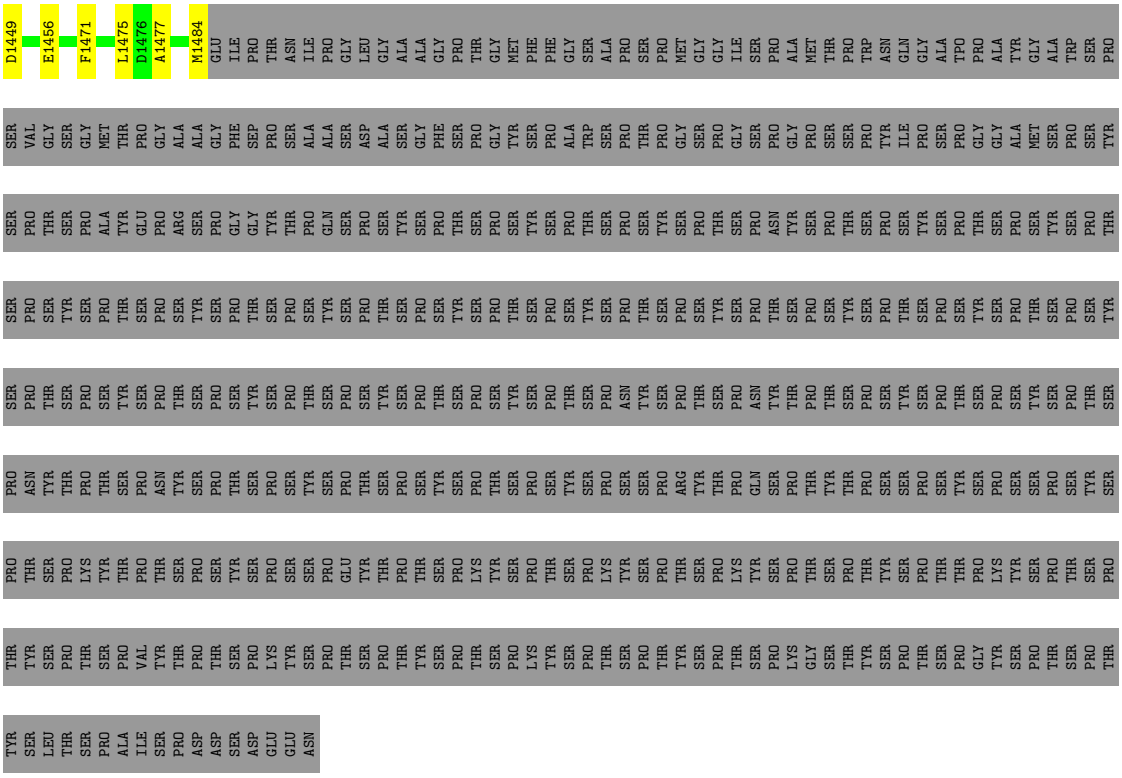




• Molecule 22: DNA-directed RNA polymerase subunit

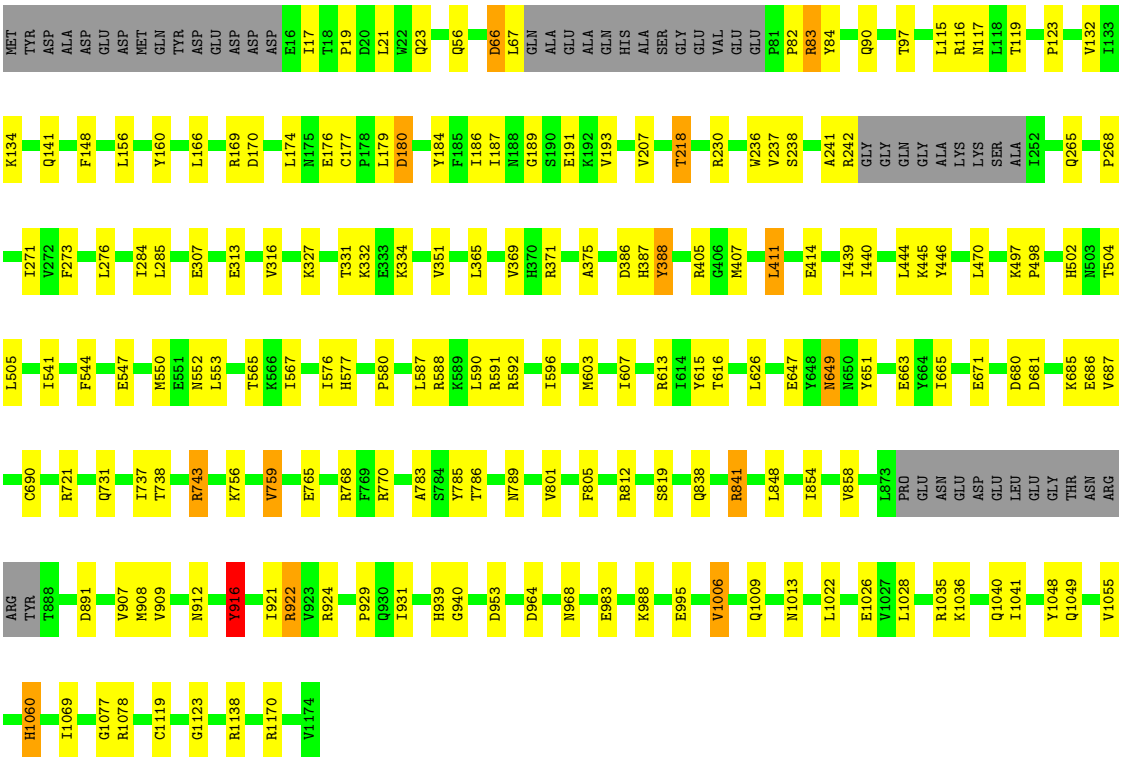
Chain A:





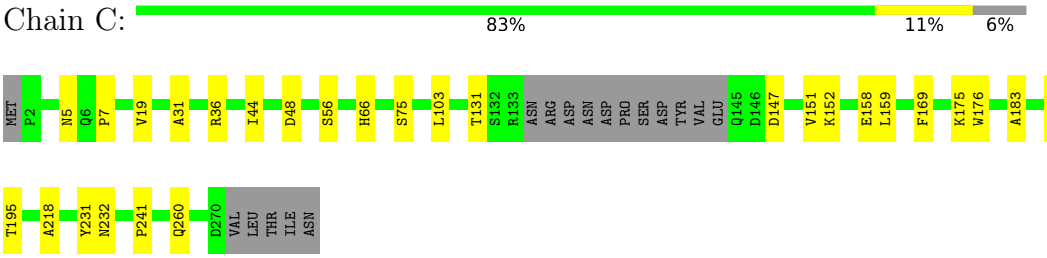
• Molecule 23: DNA-directed RNA polymerase subunit beta

Chain B:



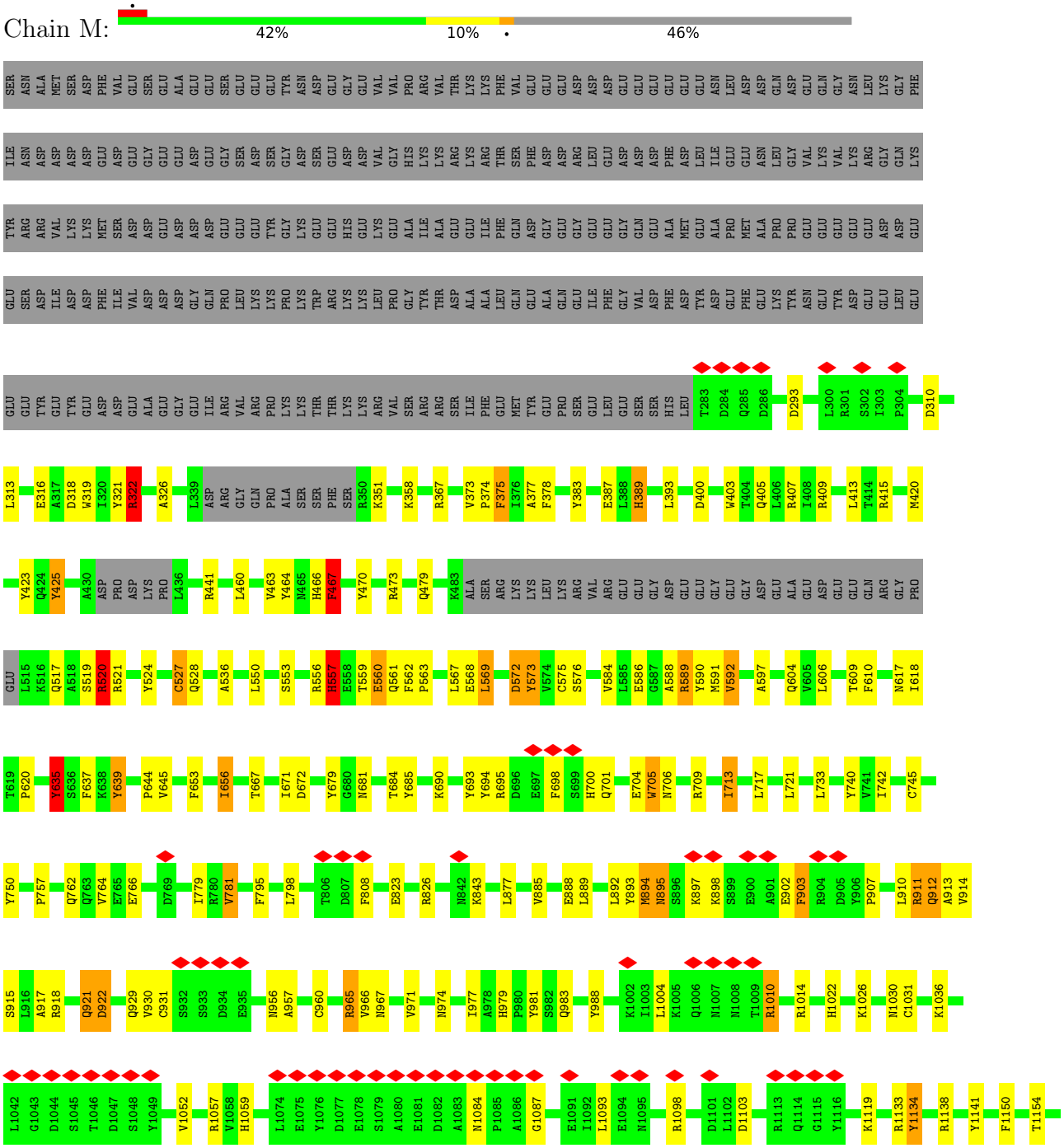
• Molecule 24: DNA-directed RNA polymerase II subunit RPB3

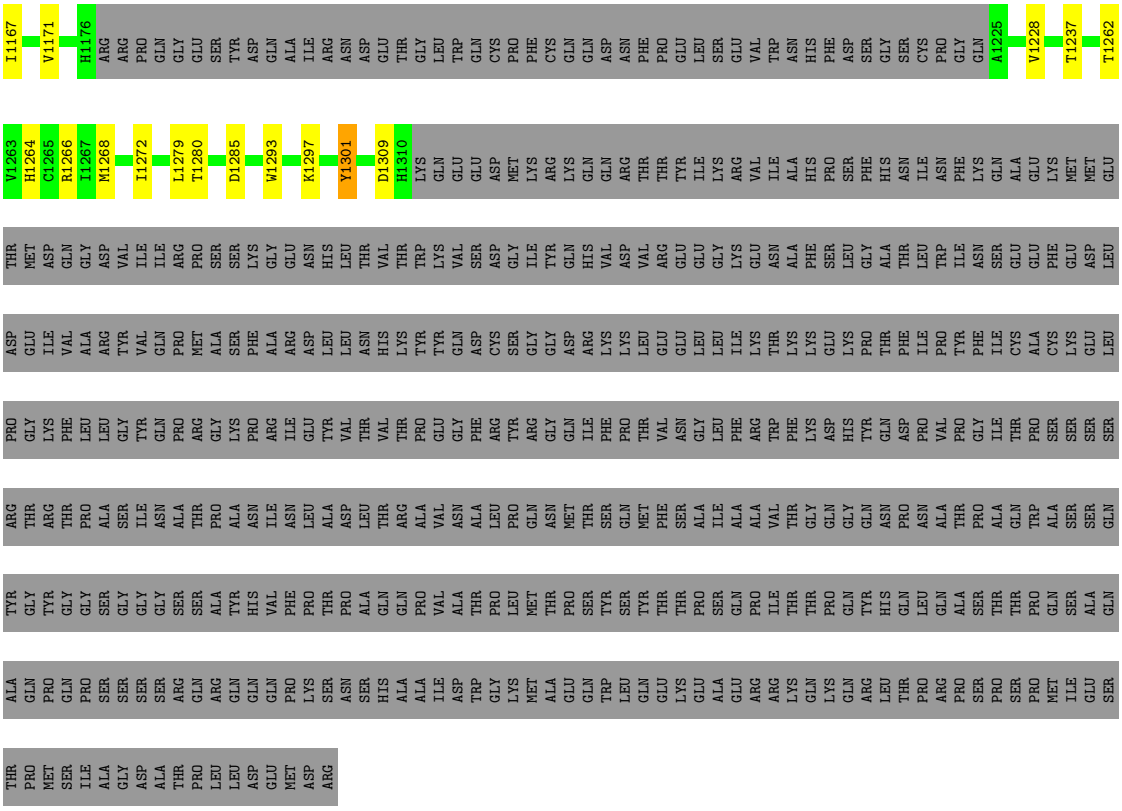
Chain C:



• Molecule 25: Transcription elongation factor SPT6

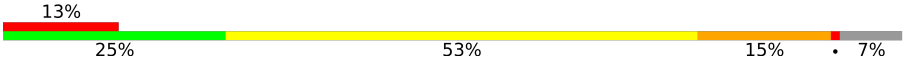
Chain M:

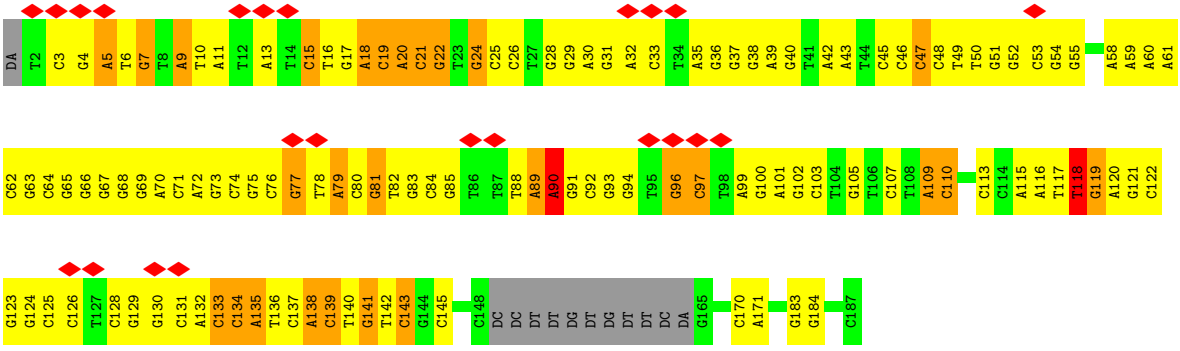




• Molecule 26: Non-template DNA

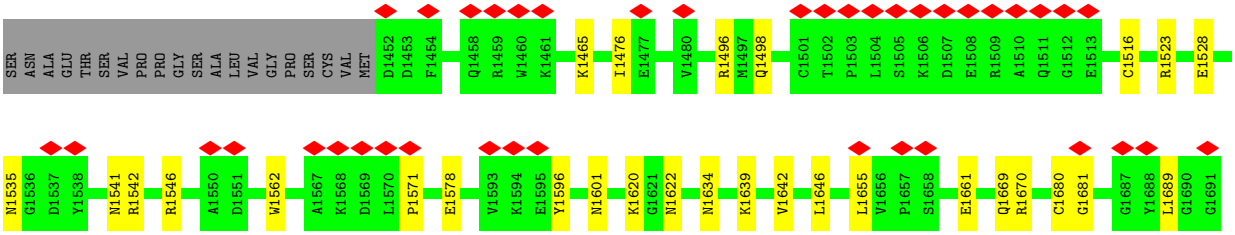
Chain N:

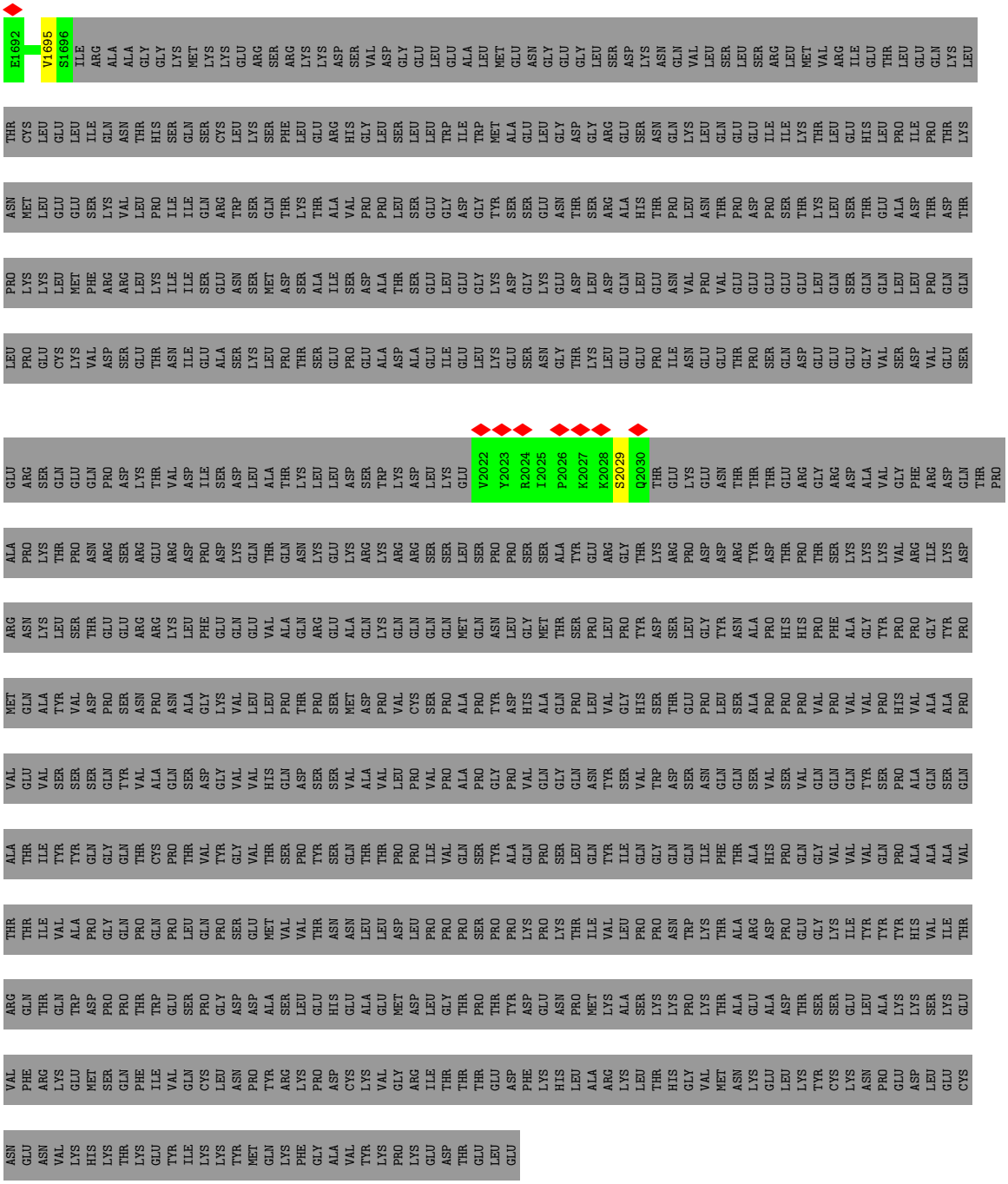




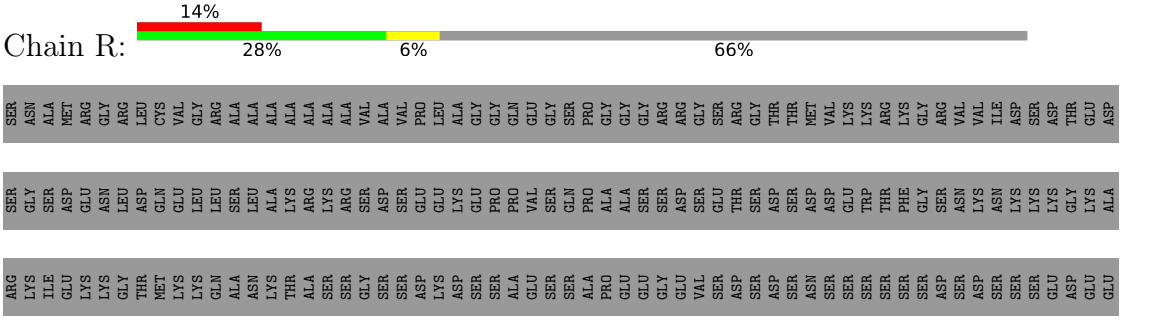
• Molecule 27: Histone-lysine N-methyltransferase SETD2

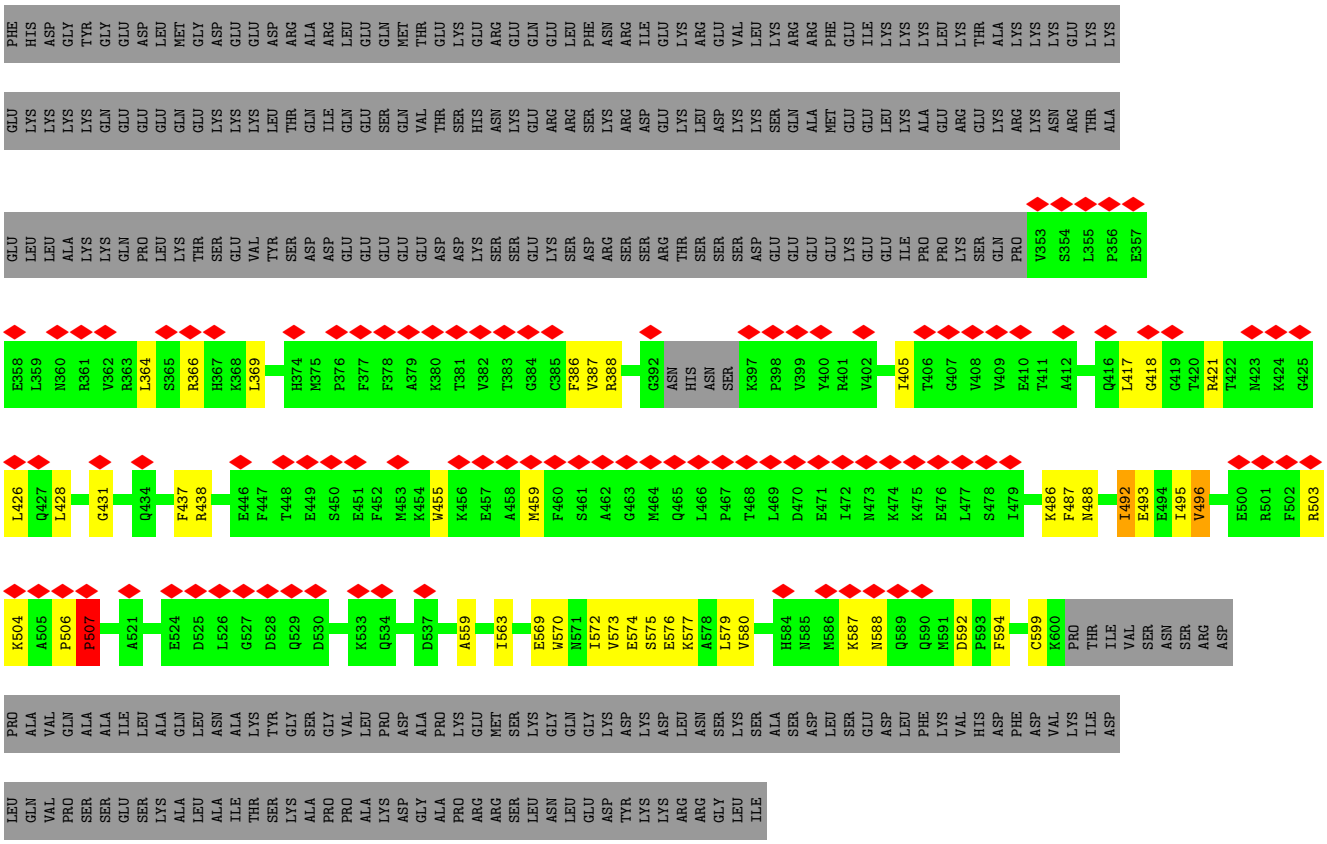
Chain O:





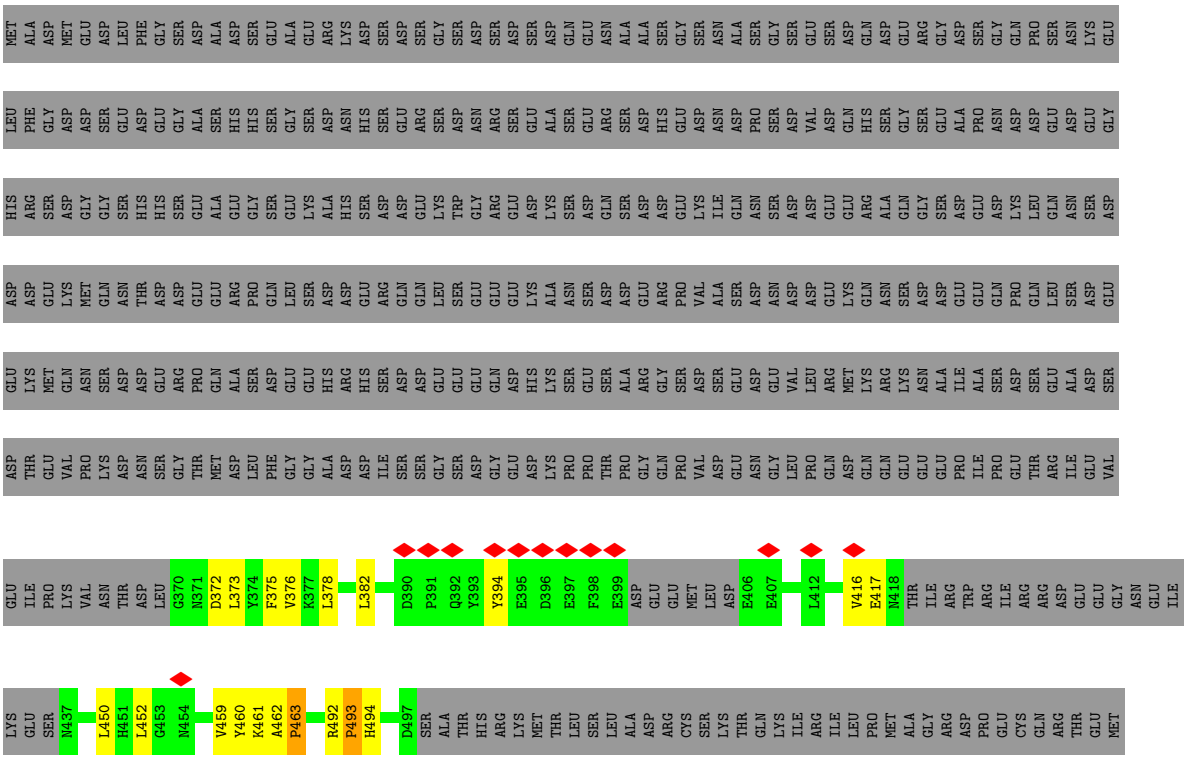
• Molecule 28: RNA polymerase-associated protein RTF1 homolog

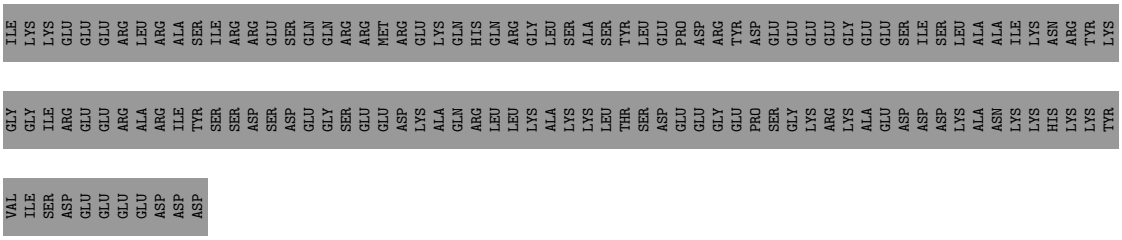




• Molecule 29: RNA polymerase-associated protein LEO1

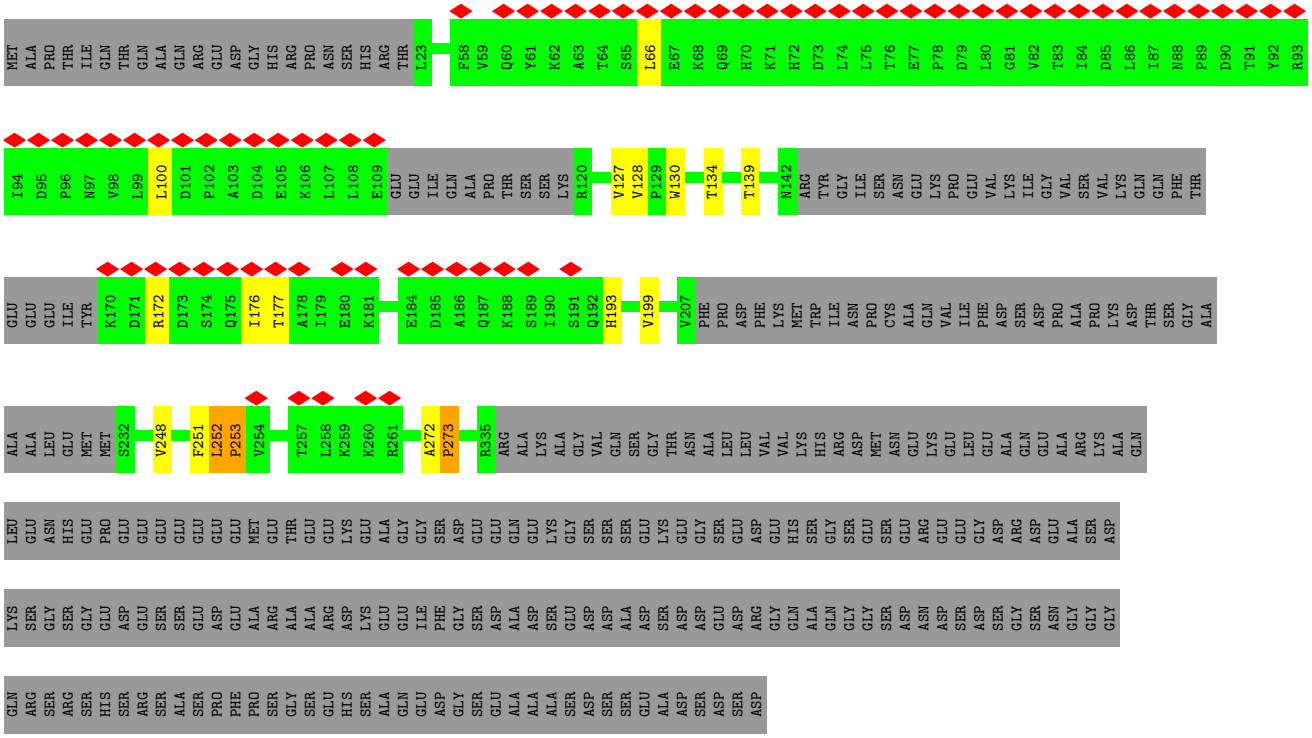
Chain U:





• Molecule 30: RNA polymerase II-associated factor 1 homolog

Chain V:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22642	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39.83	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	537.6, 537.6, 537.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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

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	D	1.15	1/1017 (0.1%)	1.91	18/1368 (1.3%)
2	E	0.27	0/1752	0.56	0/2366
3	F	0.48	0/637	0.78	1/859 (0.1%)
4	G	1.25	2/1364 (0.1%)	2.25	77/1853 (4.2%)
5	H	0.18	0/1220	0.44	0/1644
6	I	0.17	0/973	0.45	0/1316
7	J	0.34	0/533	0.68	0/719
8	K	0.19	0/939	0.37	0/1271
9	L	1.00	0/404	1.75	12/536 (2.2%)
10	P	0.88	0/506	1.43	4/787 (0.5%)
11	Q	0.29	0/7379	0.68	3/9945 (0.0%)
12	T	1.23	125/4134 (3.0%)	1.11	9/6374 (0.1%)
13	W	0.25	0/2433	0.66	1/3311 (0.0%)
14	X	0.29	0/438	0.77	0/587
15	Y	0.17	0/927	0.40	0/1250
16	Z	0.69	1/3533 (0.0%)	1.31	37/4755 (0.8%)
17	a	0.22	0/833	0.48	0/1117
17	e	0.51	0/793	0.84	1/1064 (0.1%)
18	b	0.23	0/629	0.46	0/843
18	f	0.49	0/629	0.73	0/843
19	c	0.26	0/811	0.55	0/1096
19	g	0.64	0/806	0.93	3/1089 (0.3%)
20	d	0.27	0/730	0.55	1/982 (0.1%)
20	h	0.41	0/704	0.73	2/949 (0.2%)
21	j	0.28	0/112	0.88	0/151
22	A	0.50	0/11213	0.87	15/15132 (0.1%)
23	B	0.56	0/9171	0.97	22/12377 (0.2%)
24	C	0.23	0/2115	0.49	1/2873 (0.0%)
25	M	1.37	11/7785 (0.1%)	1.67	123/10503 (1.2%)
26	N	1.14	99/3941 (2.5%)	0.97	10/6084 (0.2%)
27	O	0.24	0/2111	0.52	0/2826
28	R	0.68	0/1866	1.14	7/2519 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	U	0.21	0/766	0.52	4/1039 (0.4%)
30	V	0.28	0/1715	0.60	3/2343 (0.1%)
All	All	0.74	239/74919 (0.3%)	1.04	354/102771 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	3
2	E	0	1
4	G	0	11
7	J	0	1
9	L	0	5
10	P	0	7
12	T	0	9
14	X	0	1
16	Z	0	1
19	g	0	1
22	A	0	7
23	B	0	7
25	M	0	23
26	N	0	8
28	R	0	5
All	All	0	90

All (239) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	M	373	VAL	CA-CB	-10.77	1.48	1.54
1	D	31	THR	CB-OG1	-8.25	1.30	1.43
12	T	53	DC	P-OP1	6.64	1.61	1.48
12	T	28	DG	P-OP1	6.62	1.61	1.48
12	T	117	DC	P-OP1	6.61	1.61	1.48
12	T	64	DC	P-OP1	6.61	1.61	1.48
26	N	4	DG	P-OP1	6.60	1.61	1.48
12	T	29	DG	P-OP1	6.60	1.61	1.48
12	T	157	DG	P-OP1	6.60	1.61	1.48
26	N	83	DG	P-OP1	6.60	1.61	1.48
12	T	22	DC	P-OP1	6.59	1.61	1.48
12	T	59	DC	P-OP1	6.59	1.61	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	23	DC	P-OP1	6.59	1.61	1.48
26	N	96	DG	P-OP1	6.59	1.61	1.48
26	N	68	DG	P-OP1	6.58	1.61	1.48
26	N	107	DC	P-OP1	6.58	1.61	1.48
26	N	121	DG	P-OP1	6.58	1.61	1.48
12	T	41	DA	P-OP1	6.58	1.61	1.48
26	N	74	DC	P-OP1	6.58	1.61	1.48
26	N	134	DC	P-OP1	6.58	1.61	1.48
26	N	35	DA	P-OP1	6.58	1.61	1.48
26	N	64	DC	P-OP1	6.57	1.61	1.48
26	N	119	DG	P-OP1	6.57	1.61	1.48
26	N	131	DC	P-OP1	6.57	1.61	1.48
12	T	52	DG	P-OP1	6.57	1.61	1.48
12	T	76	DG	P-OP1	6.57	1.61	1.48
26	N	55	DG	P-OP1	6.57	1.61	1.48
12	T	103	DG	P-OP1	6.57	1.61	1.48
12	T	120	DC	P-OP1	6.57	1.61	1.48
26	N	102	DG	P-OP1	6.57	1.61	1.48
12	T	40	DG	P-OP1	6.57	1.61	1.48
12	T	43	DA	P-OP1	6.57	1.61	1.48
12	T	101	DA	P-OP1	6.57	1.61	1.48
26	N	37	DG	P-OP1	6.57	1.61	1.48
26	N	58	DA	P-OP1	6.57	1.61	1.48
26	N	73	DG	P-OP1	6.57	1.61	1.48
26	N	63	DG	P-OP1	6.57	1.61	1.48
26	N	70	DA	P-OP1	6.57	1.61	1.48
26	N	84	DC	P-OP1	6.57	1.61	1.48
12	T	24	DG	P-OP1	6.56	1.61	1.48
26	N	77	DG	P-OP1	6.56	1.61	1.48
12	T	9	DC	P-OP1	6.56	1.61	1.48
12	T	49	DG	P-OP2	6.56	1.61	1.48
12	T	60	DC	P-OP1	6.56	1.61	1.48
26	N	122	DC	P-OP1	6.56	1.61	1.48
12	T	50	DG	P-OP1	6.56	1.61	1.48
12	T	118	DC	P-OP1	6.56	1.61	1.48
12	T	175	DA	P-OP1	6.56	1.61	1.48
26	N	60	DA	P-OP1	6.56	1.61	1.48
26	N	92	DC	P-OP1	6.56	1.61	1.48
26	N	125	DC	P-OP1	6.56	1.61	1.48
12	T	99	DG	P-OP1	6.56	1.61	1.48
26	N	29	DG	P-OP1	6.56	1.61	1.48
26	N	39	DA	P-OP1	6.56	1.61	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	8	DG	P-OP1	6.56	1.61	1.48
26	N	21	DC	P-OP1	6.55	1.61	1.48
26	N	93	DG	P-OP1	6.55	1.61	1.48
12	T	107	DG	P-OP1	6.55	1.61	1.48
12	T	156	DA	P-OP1	6.55	1.61	1.48
12	T	137	DG	P-OP1	6.55	1.61	1.48
26	N	139	DC	P-OP1	6.55	1.61	1.48
12	T	132	DC	P-OP1	6.55	1.61	1.48
12	T	26	DG	P-OP1	6.55	1.61	1.48
12	T	112	DG	P-OP1	6.55	1.61	1.48
26	N	105	DG	P-OP1	6.55	1.61	1.48
12	T	57	DG	P-OP1	6.54	1.61	1.48
12	T	46	DG	P-OP1	6.54	1.61	1.48
26	N	80	DC	P-OP1	6.54	1.61	1.48
12	T	135	DG	P-OP1	6.54	1.61	1.48
26	N	24	DG	P-OP1	6.54	1.61	1.48
26	N	120	DA	P-OP1	6.54	1.61	1.48
26	N	143	DC	P-OP1	6.54	1.61	1.48
12	T	19	DG	P-OP1	6.54	1.61	1.48
12	T	77	DA	P-OP1	6.54	1.61	1.48
26	N	17	DG	P-OP1	6.54	1.61	1.48
26	N	138	DA	P-OP1	6.54	1.61	1.48
26	N	67	DG	P-OP1	6.54	1.61	1.48
12	T	85	DA	P-OP1	6.53	1.61	1.48
12	T	167	DA	P-OP1	6.53	1.61	1.48
26	N	46	DC	P-OP1	6.53	1.61	1.48
26	N	141	DG	P-OP1	6.53	1.61	1.48
12	T	47	DA	P-OP1	6.53	1.61	1.48
26	N	65	DG	P-OP1	6.53	1.61	1.48
26	N	132	DA	P-OP1	6.53	1.61	1.48
12	T	11	DC	P-OP1	6.53	1.61	1.48
12	T	119	DG	P-OP1	6.53	1.61	1.48
12	T	138	DG	P-OP1	6.53	1.61	1.48
26	N	62	DC	P-OP1	6.53	1.61	1.48
12	T	181	DA	P-OP1	6.53	1.61	1.48
26	N	94	DG	P-OP1	6.53	1.61	1.48
26	N	128	DC	P-OP1	6.53	1.61	1.48
26	N	130	DG	P-OP1	6.53	1.61	1.48
12	T	180	DG	P-OP1	6.53	1.61	1.48
12	T	95	DA	P-OP1	6.52	1.61	1.48
26	N	85	DG	P-OP1	6.52	1.61	1.48
12	T	1	DG	P-OP1	6.52	1.61	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	12	DC	P-OP1	6.52	1.61	1.48
12	T	79	DA	P-OP1	6.52	1.61	1.48
12	T	128	DC	P-OP1	6.52	1.61	1.48
12	T	146	DC	P-OP1	6.52	1.61	1.48
12	T	169	DA	P-OP1	6.52	1.61	1.48
26	N	71	DC	P-OP1	6.52	1.61	1.48
26	N	26	DC	P-OP1	6.52	1.61	1.48
12	T	121	DG	P-OP1	6.52	1.61	1.48
12	T	152	DC	P-OP1	6.52	1.61	1.48
12	T	158	DG	P-OP1	6.52	1.61	1.48
26	N	22	DG	P-OP1	6.52	1.61	1.48
26	N	33	DC	P-OP1	6.52	1.61	1.48
12	T	42	DC	P-OP1	6.52	1.61	1.48
12	T	61	DG	P-OP1	6.52	1.61	1.48
12	T	155	DC	P-OP1	6.52	1.61	1.48
12	T	106	DC	P-OP1	6.51	1.61	1.48
26	N	5	DA	P-OP1	6.51	1.61	1.48
12	T	147	DC	P-OP1	6.51	1.61	1.48
12	T	54	DC	P-OP1	6.51	1.61	1.48
12	T	134	DA	P-OP1	6.51	1.61	1.48
12	T	176	DC	P-OP1	6.51	1.61	1.48
26	N	28	DG	P-OP1	6.51	1.61	1.48
26	N	53	DC	P-OP1	6.51	1.61	1.48
26	N	59	DA	P-OP1	6.51	1.61	1.48
26	N	7	DG	P-OP1	6.51	1.61	1.48
26	N	36	DG	P-OP1	6.51	1.61	1.48
26	N	123	DG	P-OP1	6.51	1.61	1.48
12	T	92	DC	P-OP1	6.51	1.61	1.48
26	N	40	DG	P-OP1	6.51	1.61	1.48
26	N	66	DG	P-OP1	6.51	1.61	1.48
26	N	76	DC	P-OP1	6.51	1.61	1.48
26	N	99	DA	P-OP1	6.51	1.61	1.48
12	T	88	DA	P-OP1	6.50	1.61	1.48
12	T	105	DA	P-OP1	6.50	1.61	1.48
12	T	136	DG	P-OP1	6.50	1.61	1.48
12	T	149	DA	P-OP1	6.50	1.61	1.48
26	N	11	DA	P-OP1	6.50	1.61	1.48
12	T	115	DC	P-OP1	6.50	1.61	1.48
12	T	164	DG	P-OP1	6.50	1.61	1.48
26	N	52	DG	P-OP1	6.50	1.61	1.48
12	T	7	DA	P-OP1	6.50	1.61	1.48
12	T	44	DG	P-OP1	6.50	1.61	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	97	DC	P-OP1	6.50	1.61	1.48
12	T	2	DC	P-OP1	6.50	1.61	1.48
12	T	80	DG	P-OP1	6.50	1.61	1.48
12	T	97	DA	P-OP1	6.50	1.61	1.48
12	T	5	DC	P-OP1	6.50	1.61	1.48
12	T	25	DA	P-OP1	6.50	1.61	1.48
12	T	160	DA	P-OP1	6.50	1.61	1.48
26	N	45	DC	P-OP1	6.50	1.61	1.48
26	N	72	DA	P-OP1	6.50	1.61	1.48
12	T	161	DC	P-OP1	6.50	1.61	1.48
26	N	124	DG	P-OP1	6.50	1.61	1.48
12	T	58	DG	P-OP1	6.49	1.61	1.48
26	N	19	DC	P-OP1	6.49	1.61	1.48
26	N	129	DG	P-OP1	6.49	1.61	1.48
12	T	90	DC	P-OP1	6.49	1.61	1.48
12	T	139	DA	P-OP1	6.49	1.61	1.48
12	T	129	DC	P-OP1	6.49	1.61	1.48
26	N	91	DG	P-OP1	6.49	1.61	1.48
12	T	62	DC	P-OP1	6.49	1.61	1.48
12	T	142	DA	P-OP1	6.49	1.61	1.48
12	T	145	DC	P-OP1	6.49	1.61	1.48
26	N	100	DG	P-OP1	6.49	1.61	1.48
26	N	126	DC	P-OP1	6.49	1.61	1.48
12	T	18	DG	P-OP1	6.49	1.61	1.48
12	T	83	DC	P-OP1	6.49	1.61	1.48
26	N	25	DC	P-OP1	6.49	1.61	1.48
26	N	54	DG	P-OP1	6.49	1.61	1.48
12	T	102	DC	P-OP1	6.48	1.61	1.48
12	T	13	DC	P-OP1	6.48	1.61	1.48
26	N	69	DG	P-OP1	6.48	1.61	1.48
12	T	98	DC	P-OP1	6.48	1.61	1.48
26	N	31	DG	P-OP1	6.48	1.61	1.48
12	T	171	DA	P-OP1	6.48	1.61	1.48
26	N	101	DA	P-OP1	6.48	1.61	1.48
12	T	81	DC	P-OP1	6.48	1.61	1.48
12	T	114	DC	P-OP1	6.48	1.61	1.48
26	N	75	DG	P-OP1	6.48	1.61	1.48
12	T	4	DC	P-OP1	6.48	1.61	1.48
12	T	6	DC	P-OP1	6.47	1.61	1.48
12	T	162	DG	P-OP1	6.47	1.61	1.48
26	N	42	DA	P-OP1	6.47	1.61	1.48
26	N	61	DA	P-OP1	6.47	1.61	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	15	DG	P-OP1	6.47	1.61	1.48
12	T	55	DG	P-OP1	6.47	1.61	1.48
12	T	109	DG	P-OP1	6.47	1.61	1.48
12	T	127	DA	P-OP1	6.47	1.61	1.48
26	N	20	DA	P-OP1	6.47	1.61	1.48
26	N	38	DG	P-OP1	6.47	1.61	1.48
26	N	51	DG	P-OP1	6.47	1.61	1.48
12	T	131	DC	P-OP1	6.47	1.61	1.48
26	N	135	DA	P-OP1	6.47	1.61	1.48
12	T	108	DC	P-OP1	6.46	1.61	1.48
12	T	126	DA	P-OP1	6.46	1.61	1.48
26	N	13	DA	P-OP1	6.46	1.61	1.48
26	N	103	DC	P-OP1	6.46	1.61	1.48
12	T	130	DG	P-OP1	6.46	1.61	1.48
12	T	91	DG	P-OP1	6.46	1.61	1.48
12	T	166	DC	P-OP1	6.46	1.61	1.48
26	N	3	DC	P-OP1	6.46	1.61	1.48
26	N	9	DA	P-OP1	6.46	1.61	1.48
26	N	47	DC	P-OP1	6.46	1.61	1.48
12	T	168	DG	P-OP1	6.46	1.61	1.48
12	T	16	DC	P-OP1	6.45	1.61	1.48
12	T	20	DC	P-OP1	6.45	1.61	1.48
12	T	173	DA	P-OP1	6.45	1.61	1.48
12	T	96	DA	P-OP1	6.45	1.61	1.48
26	N	30	DA	P-OP1	6.45	1.61	1.48
26	N	81	DG	P-OP1	6.45	1.61	1.48
12	T	150	DG	P-OP1	6.44	1.61	1.48
26	N	133	DC	P-OP1	6.44	1.61	1.48
12	T	56	DA	P-OP1	6.44	1.61	1.48
12	T	78	DC	P-OP1	6.44	1.61	1.48
12	T	100	DC	P-OP1	6.44	1.61	1.48
12	T	110	DC	P-OP1	6.44	1.61	1.48
12	T	89	DC	P-OP1	6.44	1.61	1.48
26	N	137	DC	P-OP1	6.44	1.61	1.48
12	T	30	DG	P-OP1	6.44	1.61	1.48
12	T	159	DC	P-OP1	6.44	1.61	1.48
12	T	154	DC	P-OP1	6.43	1.61	1.48
26	N	32	DA	P-OP1	6.42	1.61	1.48
26	N	79	DA	P-OP1	6.42	1.61	1.48
12	T	177	DA	P-OP1	6.42	1.61	1.48
26	N	18	DA	P-OP1	6.42	1.61	1.48
26	N	43	DA	P-OP1	6.42	1.61	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	133	DA	P-OP1	6.41	1.61	1.48
4	G	4	HIS	N-CA	6.40	1.53	1.46
26	N	15	DC	P-OP1	6.40	1.61	1.48
12	T	179	DC	P-OP1	6.39	1.61	1.48
12	T	116	DC	P-OP1	6.38	1.61	1.48
25	M	1026	LYS	CA-C	-6.22	1.44	1.52
25	M	409	ARG	CA-C	-6.01	1.45	1.52
25	M	885	VAL	CA-CB	-5.89	1.47	1.54
4	G	4	HIS	CA-C	5.74	1.59	1.52
25	M	914	VAL	CA-C	-5.74	1.45	1.52
25	M	706	ASN	CA-C	-5.52	1.45	1.52
25	M	911	ARG	CA-C	-5.28	1.45	1.52
25	M	374	PRO	N-CD	-5.24	1.40	1.47
25	M	1014	ARG	CZ-NH2	-5.24	1.26	1.33
16	Z	526	SER	CA-C	5.16	1.59	1.52
25	M	781	VAL	CA-C	-5.11	1.46	1.52
25	M	592	VAL	CA-C	-5.06	1.46	1.52

All (354) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	48	DT	OP2-P-O3'	-34.28	5.15	108.00
4	G	60	GLN	CA-C-N	13.12	134.00	119.83
4	G	60	GLN	C-N-CA	13.12	134.00	119.83
16	Z	526	SER	N-CA-C	12.50	127.36	111.24
25	M	895	ASN	CA-CB-CG	11.78	124.38	112.60
25	M	520	ARG	N-CA-C	11.66	127.13	110.23
1	D	28	THR	CA-C-N	11.61	140.49	120.87
1	D	28	THR	C-N-CA	11.61	140.49	120.87
4	G	166	ASP	CA-CB-CG	11.13	123.73	112.60
16	Z	541	GLN	CA-C-N	10.97	136.96	121.71
16	Z	541	GLN	C-N-CA	10.97	136.96	121.71
26	N	90	DA	O3'-P-O5'	10.16	119.24	104.00
25	M	967	ASN	CA-CB-CG	-10.10	102.50	112.60
25	M	713	ILE	CB-CA-C	-9.71	99.30	112.02
4	G	129	LYS	CA-C-N	9.43	137.92	121.80
4	G	129	LYS	C-N-CA	9.43	137.92	121.80
4	G	125	PRO	N-CA-C	-9.35	99.29	110.70
1	D	29	ALA	N-CA-C	9.25	122.55	110.43
4	G	113	ILE	CA-C-O	-9.17	113.23	119.19
4	G	48	VAL	N-CA-C	9.06	121.63	108.58
4	G	86	ASP	CA-CB-CG	8.89	121.49	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	87	DC	O3'-P-O5'	8.85	117.28	104.00
1	D	38	HIS	CA-CB-CG	-8.49	105.31	113.80
12	T	30	DG	O3'-P-O5'	-8.46	91.30	104.00
4	G	4	HIS	N-CA-C	8.46	123.44	109.06
30	V	252	LEU	C-N-CD	-8.39	90.62	125.00
4	G	104	MET	N-CA-CB	-8.36	96.16	111.37
16	Z	477	HIS	CA-CB-CG	8.22	122.02	113.80
16	Z	573	GLN	N-CA-C	8.17	123.25	113.28
25	M	375	PHE	CA-CB-CG	-8.15	105.65	113.80
4	G	31	PHE	CA-CB-CG	8.11	121.91	113.80
1	D	31	THR	N-CA-CB	8.11	121.88	109.97
9	L	41	TYR	CA-CB-CG	-7.97	99.55	113.90
25	M	705	TRP	CB-CA-C	-7.97	97.56	110.79
4	G	107	PHE	CA-CB-CG	7.93	121.73	113.80
4	G	121	PRO	CA-C-N	7.88	133.87	120.72
4	G	121	PRO	C-N-CA	7.88	133.87	120.72
4	G	70	VAL	N-CA-C	7.82	119.06	108.11
16	Z	580	ASP	CA-CB-CG	7.77	120.37	112.60
25	M	563	PRO	N-CA-C	7.76	122.75	114.68
25	M	467	PHE	CA-CB-CG	-7.70	106.10	113.80
25	M	576	SER	N-CA-C	7.67	119.64	111.28
4	G	20	PRO	N-CA-C	7.63	124.14	113.53
4	G	3	TYR	CB-CA-C	7.62	130.08	111.95
12	T	75	DA	O3'-P-O5'	7.58	115.37	104.00
10	P	34	G	O5'-C5'-C4'	7.57	123.06	111.70
28	R	496	VAL	CA-CB-CG2	7.52	123.18	110.40
4	G	115	SER	CA-C-N	7.50	130.34	120.28
4	G	115	SER	C-N-CA	7.50	130.34	120.28
25	M	1133	ARG	NE-CZ-NH2	7.50	125.95	119.20
25	M	550	LEU	CB-CA-C	-7.44	99.50	110.96
4	G	2	PHE	N-CA-CB	-7.43	99.04	109.97
4	G	3	TYR	CA-CB-CG	7.40	127.22	113.90
25	M	610	PHE	N-CA-C	-7.36	103.19	111.14
25	M	960	CYS	CA-CB-SG	-7.34	97.51	114.40
25	M	895	ASN	CB-CA-C	-7.32	95.02	110.31
26	N	107	DC	P-O3'-C3'	7.31	131.16	120.20
4	G	98	PHE	CA-CB-CG	7.29	121.09	113.80
25	M	553	SER	N-CA-C	7.22	121.66	112.86
25	M	698	PHE	N-CA-C	7.11	121.97	113.16
16	Z	477	HIS	N-CA-CB	7.09	120.53	109.69
25	M	589	ARG	N-CA-CB	7.08	120.53	110.12
20	h	38	SER	N-CA-C	7.08	118.64	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	241	ARG	NE-CZ-NH2	7.05	125.54	119.20
22	A	33	ARG	CB-CG-CD	7.03	127.47	111.30
25	M	903	PHE	CA-C-N	6.97	129.93	120.38
25	M	903	PHE	C-N-CA	6.97	129.93	120.38
28	R	506	PRO	N-CA-C	6.95	119.17	110.70
4	G	47	ALA	N-CA-C	6.93	119.71	108.76
4	G	119	PHE	N-CA-C	6.91	120.25	110.50
4	G	97	LEU	N-CA-CB	-6.84	99.83	110.57
9	L	31	ARG	NE-CZ-NH1	-6.80	114.70	121.50
25	M	389	HIS	CB-CG-CD2	-6.78	122.39	131.20
25	M	521	ARG	N-CA-C	6.77	119.56	108.52
4	G	167	TYR	N-CA-C	-6.74	103.61	112.24
25	M	694	TYR	CB-CA-C	-6.74	98.13	109.65
26	N	118	DT	P-O3'-C3'	6.72	130.28	120.20
25	M	389	HIS	CA-CB-CG	-6.70	107.10	113.80
25	M	700	HIS	CA-CB-CG	-6.69	107.11	113.80
1	D	87	LEU	N-CA-CB	-6.67	99.84	110.19
10	P	36	G	C2'-C3'-O3'	6.67	119.51	109.50
9	L	33	PRO	N-CA-CB	6.66	108.63	103.30
4	G	54	ILE	CA-CB-CG1	6.64	121.69	110.40
4	G	65	PHE	N-CA-C	6.60	119.94	110.10
25	M	521	ARG	CB-CA-C	-6.59	99.39	110.19
23	B	141	GLN	N-CA-C	6.57	118.33	110.44
4	G	143	ILE	N-CA-CB	-6.54	103.56	111.21
4	G	13	LEU	CA-C-N	6.54	130.61	120.68
4	G	13	LEU	C-N-CA	6.54	130.61	120.68
4	G	19	GLY	O-C-N	-6.54	115.23	121.77
16	Z	534	HIS	CB-CG-CD2	-6.51	122.74	131.20
26	N	88	DT	P-O3'-C3'	6.50	129.96	120.20
4	G	120	ASP	N-CA-CB	6.50	119.24	110.79
9	L	42	ARG	NE-CZ-NH2	6.50	125.05	119.20
25	M	635	TYR	N-CA-C	6.49	118.36	111.28
4	G	2	PHE	O-C-N	-6.48	114.99	122.89
25	M	898	LYS	CA-C-O	-6.47	114.03	120.82
25	M	931	CYS	CB-CA-C	6.45	121.73	111.73
25	M	322	ARG	CB-CA-C	-6.45	100.71	110.90
22	A	1436	VAL	N-CA-C	6.44	116.60	110.74
25	M	617	ASN	CA-CB-CG	-6.38	106.22	112.60
4	G	62	GLY	CA-C-N	6.37	132.58	122.59
4	G	62	GLY	C-N-CA	6.37	132.58	122.59
1	D	30	GLU	CA-C-O	-6.36	113.32	120.32
25	M	310	ASP	CA-CB-CG	-6.36	106.24	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	135	GLN	CA-CB-CG	6.36	126.81	114.10
22	A	448	ARG	NE-CZ-NH2	6.34	124.91	119.20
4	G	43	GLY	CA-C-N	6.32	129.80	120.95
4	G	43	GLY	C-N-CA	6.32	129.80	120.95
26	N	134	DC	P-O3'-C3'	-6.32	110.72	120.20
25	M	912	GLN	N-CA-C	-6.29	105.10	112.89
4	G	9	HIS	N-CA-CB	-6.28	99.77	111.13
26	N	133	DC	P-O3'-C3'	-6.27	110.79	120.20
22	A	84	HIS	CB-CG-CD2	-6.26	123.06	131.20
25	M	562	PHE	CB-CA-C	6.26	118.46	109.26
25	M	779	ILE	N-CA-C	6.26	117.61	108.53
25	M	974	ASN	CA-CB-CG	-6.26	106.34	112.60
4	G	5	ILE	CA-CB-CG1	6.25	121.03	110.40
23	B	123	PRO	CA-C-N	6.25	131.80	122.99
23	B	123	PRO	C-N-CA	6.25	131.80	122.99
25	M	293	ASP	CA-CB-CG	6.25	118.85	112.60
25	M	1309	ASP	N-CA-C	6.25	120.37	112.87
23	B	186	ILE	CB-CA-C	6.23	119.85	111.19
4	G	119	PHE	CA-C-N	6.22	129.70	122.85
4	G	119	PHE	C-N-CA	6.22	129.70	122.85
4	G	130	THR	N-CA-C	-6.22	99.52	108.60
19	g	27	VAL	N-CA-C	-6.22	106.86	111.90
25	M	931	CYS	CA-CB-SG	-6.20	100.13	114.40
25	M	717	LEU	CB-CA-C	-6.19	101.12	110.90
25	M	557	HIS	CA-CB-CG	-6.18	107.62	113.80
4	G	46	ILE	N-CA-C	6.16	122.16	109.34
9	L	34	ILE	CB-CA-C	6.14	118.31	111.80
16	Z	544	PRO	N-CA-C	6.14	121.94	113.65
4	G	127	CYS	N-CA-CB	-6.14	101.67	111.43
4	G	170	LEU	CB-CA-C	6.13	119.78	109.48
25	M	318	ASP	CA-CB-CG	-6.13	106.47	112.60
28	R	507	PRO	CA-N-CD	-6.13	103.42	112.00
4	G	2	PHE	CB-CA-C	6.12	120.11	109.65
28	R	492	ILE	CA-C-N	6.11	128.75	120.44
28	R	492	ILE	C-N-CA	6.11	128.75	120.44
22	A	401	ARG	NE-CZ-NH2	6.11	124.70	119.20
4	G	67	LEU	N-CA-C	6.11	118.90	109.07
16	Z	524	THR	CA-C-N	6.11	130.54	122.30
16	Z	524	THR	C-N-CA	6.11	130.54	122.30
16	Z	601	LYS	CA-C-N	6.10	130.52	122.95
16	Z	601	LYS	C-N-CA	6.10	130.52	122.95
4	G	86	ASP	CB-CA-C	6.09	119.57	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	401	ARG	CD-NE-CZ	6.08	132.92	124.40
25	M	709	ARG	NE-CZ-NH2	6.08	124.67	119.20
25	M	351	LYS	CB-CA-C	6.07	119.37	109.90
25	M	373	VAL	CB-CA-C	-6.07	107.94	113.70
25	M	695	ARG	NE-CZ-NH2	6.07	124.66	119.20
25	M	1134	TYR	N-CA-C	6.07	119.91	111.90
16	Z	540	VAL	N-CA-C	6.07	118.96	108.95
16	Z	480	VAL	CB-CA-C	6.06	118.42	110.91
1	D	75	LYS	N-CA-CB	-6.03	102.29	110.67
25	M	672	ASP	CB-CA-C	-6.03	99.29	109.83
23	B	1069	ILE	N-CA-C	6.02	117.96	111.58
29	U	462	ALA	C-N-CD	-6.01	100.37	125.00
25	M	704	GLU	CB-CA-C	6.00	122.20	110.67
16	Z	575	VAL	N-CA-C	-5.99	99.25	107.99
1	D	64	THR	N-CA-CB	5.99	119.52	110.30
25	M	929	GLN	CB-CA-C	-5.98	100.68	110.85
23	B	97	THR	N-CA-C	5.97	118.85	108.76
4	G	4	HIS	O-C-N	-5.96	116.12	123.33
9	L	31	ARG	NE-CZ-NH2	5.94	124.54	119.20
25	M	917	ALA	N-CA-C	-5.93	104.90	111.36
25	M	466	HIS	CB-CG-CD2	-5.92	123.50	131.20
11	Q	801	ASP	CA-C-N	5.92	132.85	121.54
11	Q	801	ASP	C-N-CA	5.92	132.85	121.54
25	M	560	GLU	CA-C-N	-5.91	115.16	122.84
25	M	560	GLU	C-N-CA	-5.91	115.16	122.84
25	M	586	GLU	CA-C-N	5.89	126.52	119.98
25	M	586	GLU	C-N-CA	5.89	126.52	119.98
25	M	700	HIS	CA-C-N	5.88	130.54	121.19
25	M	700	HIS	C-N-CA	5.88	130.54	121.19
25	M	979	HIS	CA-CB-CG	-5.87	107.93	113.80
16	Z	523	GLU	N-CA-C	5.85	118.10	110.43
16	Z	550	ILE	CB-CA-C	5.84	118.74	111.15
16	Z	469	ARG	NE-CZ-NH2	5.81	124.43	119.20
26	N	118	DT	C4'-C3'-O3'	-5.80	101.29	110.00
25	M	589	ARG	CB-CA-C	-5.79	101.17	110.79
25	M	695	ARG	CA-CB-CG	-5.79	102.51	114.10
25	M	897	LYS	CA-C-N	5.79	127.97	120.44
25	M	897	LYS	C-N-CA	5.79	127.97	120.44
25	M	589	ARG	N-CA-C	-5.78	104.98	111.28
16	Z	540	VAL	N-CA-CB	-5.78	102.73	112.44
25	M	527	CYS	CA-CB-SG	-5.78	101.11	114.40
4	G	3	TYR	O-C-N	-5.77	116.17	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	M	557	HIS	CB-CG-CD2	-5.77	123.70	131.20
16	Z	522	SER	N-CA-C	5.76	120.30	113.16
4	G	143	ILE	N-CA-C	5.75	116.38	107.99
25	M	528	GLN	OE1-CD-NE2	-5.75	116.85	122.60
25	M	701	GLN	CB-CG-CD	-5.74	102.85	112.60
25	M	310	ASP	N-CA-C	5.73	118.30	111.71
25	M	653	PHE	CA-CB-CG	-5.73	108.07	113.80
19	g	20	ARG	NE-CZ-NH2	5.72	124.35	119.20
25	M	519	SER	N-CA-C	5.71	121.28	113.97
25	M	575	CYS	CA-CB-SG	-5.70	101.30	114.40
4	G	128	TYR	CB-CG-CD2	-5.69	112.27	120.80
9	L	42	ARG	CB-CG-CD	5.68	124.37	111.30
4	G	170	LEU	N-CA-C	-5.68	100.44	109.76
16	Z	545	GLN	OE1-CD-NE2	-5.66	116.94	122.60
28	R	418	GLY	O-C-N	-5.66	113.25	122.36
4	G	33	GLU	N-CA-C	-5.65	105.66	113.18
10	P	34	G	C4'-C3'-C2'	5.65	108.25	102.60
16	Z	492	ILE	N-CA-CB	5.65	118.95	110.13
4	G	76	VAL	CG1-CB-CG2	-5.65	98.38	110.80
25	M	415	ARG	NE-CZ-NH2	5.65	124.28	119.20
9	L	42	ARG	CA-CB-CG	5.65	125.39	114.10
16	Z	477	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	D	96	GLU	CA-C-N	5.63	128.39	120.28
1	D	96	GLU	C-N-CA	5.63	128.39	120.28
22	A	866	LYS	CB-CG-CD	5.63	124.25	111.30
25	M	1059	HIS	CA-CB-CG	-5.63	108.17	113.80
25	M	1030	ASN	OD1-CG-ND2	-5.61	116.99	122.60
25	M	373	VAL	N-CA-C	5.61	119.68	112.67
16	Z	525	ALA	N-CA-C	5.60	117.87	108.96
25	M	556	ARG	NE-CZ-NH2	5.59	124.23	119.20
4	G	122	ASN	N-CA-CB	-5.59	101.11	110.39
12	T	34	DT	C2-N1-C1'	-5.59	110.97	119.35
30	V	253	PRO	CA-N-CD	-5.59	104.18	112.00
25	M	921	GLN	OE1-CD-NE2	-5.58	117.02	122.60
30	V	273	PRO	CA-N-CD	-5.57	104.20	112.00
29	U	463	PRO	CA-N-CD	-5.57	104.21	112.00
25	M	409	ARG	CB-CA-C	-5.56	102.14	110.88
4	G	156	ASP	CA-CB-CG	5.55	118.15	112.60
25	M	966	VAL	CB-CA-C	-5.55	104.64	112.14
26	N	116	DA	C2'-C3'-O3'	-5.55	103.18	111.50
29	U	493	PRO	CA-N-CD	-5.55	104.23	112.00
22	A	1484	MET	CB-CA-C	5.55	120.64	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	M	407	ARG	NE-CZ-NH2	5.54	124.19	119.20
25	M	569	LEU	N-CA-CB	-5.54	101.69	110.22
25	M	572	ASP	CA-CB-CG	5.54	118.14	112.60
10	P	34	G	O4'-C1'-N9	5.53	116.49	108.20
17	e	85	PHE	CA-CB-CG	5.53	119.33	113.80
23	B	916	TYR	CA-CB-CG	5.51	123.82	113.90
4	G	106	CYS	CA-CB-SG	-5.50	101.74	114.40
23	B	912	ASN	CA-C-N	5.50	127.92	120.38
23	B	912	ASN	C-N-CA	5.50	127.92	120.38
13	W	126	HIS	CB-CG-CD2	-5.50	124.05	131.20
23	B	1049	GLN	OE1-CD-NE2	-5.50	117.10	122.60
9	L	33	PRO	N-CA-C	-5.49	101.88	110.50
4	G	163	LEU	N-CA-CB	-5.49	101.11	111.43
25	M	894	MET	CB-CA-C	5.49	121.11	110.46
16	Z	551	VAL	N-CA-C	5.49	118.91	113.53
4	G	18	PHE	CA-CB-CG	5.46	119.26	113.80
25	M	568	GLU	CA-C-N	5.46	128.14	120.28
25	M	568	GLU	C-N-CA	5.46	128.14	120.28
25	M	1031	CYS	N-CA-C	5.46	120.95	113.97
4	G	74	ALA	O-C-N	-5.45	116.62	123.27
25	M	520	ARG	CA-C-N	5.44	130.67	123.05
25	M	520	ARG	C-N-CA	5.44	130.67	123.05
16	Z	581	ASN	CA-CB-CG	5.43	118.03	112.60
23	B	1060	HIS	CB-CG-CD2	-5.43	124.14	131.20
25	M	672	ASP	N-CA-C	5.43	118.56	110.52
16	Z	575	VAL	CA-CB-CG1	5.42	119.62	110.40
25	M	709	ARG	NE-CZ-NH1	-5.42	116.08	121.50
25	M	560	GLU	CB-CA-C	-5.41	101.47	109.90
3	F	72	GLN	OE1-CD-NE2	-5.40	117.20	122.60
25	M	584	VAL	CB-CA-C	-5.40	105.06	111.97
20	h	70	PHE	CA-CB-CG	-5.40	108.40	113.80
4	G	9	HIS	O-C-N	-5.39	117.11	123.41
22	A	1423	ASP	CA-CB-CG	5.38	117.98	112.60
25	M	956	ASN	CA-CB-CG	-5.36	107.24	112.60
23	B	174	LEU	CB-CA-C	5.36	120.08	110.81
23	B	116	ARG	NE-CZ-NH2	5.35	124.01	119.20
25	M	701	GLN	N-CA-CB	-5.34	100.64	109.72
19	g	20	ARG	CD-NE-CZ	5.33	131.87	124.40
23	B	841	ARG	NE-CZ-NH2	5.33	124.00	119.20
16	Z	572	HIS	N-CA-C	5.33	119.71	112.04
16	Z	551	VAL	CB-CA-C	-5.33	105.43	110.65
25	M	1264	HIS	CB-CG-CD2	-5.32	124.28	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	M	517	GLN	N-CA-CB	-5.32	101.50	110.49
24	C	66	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	D	98	ALA	CB-CA-C	5.31	118.32	109.56
4	G	47	ALA	CA-C-N	5.30	129.21	122.37
4	G	47	ALA	C-N-CA	5.30	129.21	122.37
4	G	155	ASN	CA-C-N	5.29	129.75	121.76
4	G	155	ASN	C-N-CA	5.29	129.75	121.76
4	G	66	VAL	N-CA-C	5.29	115.47	107.80
29	U	492	ARG	C-N-CD	-5.28	103.34	125.00
20	d	82	HIS	CB-CG-CD2	-5.28	124.34	131.20
25	M	519	SER	N-CA-CB	-5.26	103.35	110.67
23	B	148	PHE	CA-CB-CG	5.25	119.05	113.80
1	D	49	GLU	N-CA-C	-5.25	105.73	111.82
25	M	1022	HIS	CB-CG-CD2	-5.25	124.38	131.20
16	Z	518	LEU	N-CA-C	5.25	118.62	110.17
26	N	109	DA	C2'-C3'-O3'	-5.24	103.64	111.50
4	G	100	GLU	N-CA-CB	-5.24	102.70	110.71
12	T	32	DT	O5'-C5'-C4'	5.23	118.65	110.80
9	L	38	GLU	CA-C-N	5.23	131.53	121.54
9	L	38	GLU	C-N-CA	5.23	131.53	121.54
12	T	31	DT	C5'-C4'-C3'	-5.23	107.06	114.90
23	B	405	ARG	NE-CZ-NH2	5.22	123.90	119.20
25	M	971	VAL	N-CA-C	5.22	115.36	107.80
28	R	388	ARG	NE-CZ-NH2	5.21	123.89	119.20
16	Z	541	GLN	OE1-CD-NE2	-5.21	117.39	122.60
25	M	922	ASP	CA-CB-CG	-5.21	107.39	112.60
25	M	713	ILE	CA-CB-CG1	5.21	119.26	110.40
22	A	421	ARG	NE-CZ-NH2	5.21	123.88	119.20
4	G	3	TYR	CA-C-O	-5.20	115.84	121.36
16	Z	627	LYS	CA-C-N	5.20	127.51	120.44
16	Z	627	LYS	C-N-CA	5.20	127.51	120.44
23	B	922	ARG	NE-CZ-NH2	5.20	123.88	119.20
4	G	44	PHE	CA-CB-CG	-5.19	108.61	113.80
25	M	409	ARG	N-CA-CB	5.19	117.53	110.01
25	M	604	GLN	CA-C-O	-5.18	115.38	120.82
25	M	1036	LYS	CB-CA-C	-5.18	101.30	109.80
1	D	35	SER	N-CA-CB	-5.18	102.51	110.12
25	M	378	PHE	CA-CB-CG	-5.17	108.63	113.80
25	M	701	GLN	OE1-CD-NE2	-5.17	117.43	122.60
23	B	924	ARG	NE-CZ-NH1	-5.16	116.34	121.50
22	A	349	ARG	NE-CZ-NH2	5.16	123.84	119.20
22	A	16	ARG	NE-CZ-NH2	5.15	123.84	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	M	367	ARG	NE-CZ-NH2	5.15	123.83	119.20
4	G	151	ARG	NE-CZ-NH2	5.15	123.83	119.20
25	M	479	GLN	OE1-CD-NE2	-5.14	117.46	122.60
25	M	561	GLN	OE1-CD-NE2	-5.14	117.45	122.60
4	G	3	TYR	N-CA-CB	-5.13	102.65	111.21
4	G	31	PHE	N-CA-C	-5.12	104.96	111.11
4	G	56	ALA	N-CA-C	5.12	117.86	110.28
23	B	97	THR	CA-C-N	5.11	129.66	122.09
23	B	97	THR	C-N-CA	5.11	129.66	122.09
25	M	1057	ARG	CB-CG-CD	5.11	123.05	111.30
25	M	589	ARG	NE-CZ-NH2	5.11	123.80	119.20
25	M	745	CYS	CB-CA-C	-5.11	102.83	110.90
25	M	1285	ASP	CA-CB-CG	5.09	117.69	112.60
25	M	656	ILE	CA-C-O	-5.08	115.41	121.05
25	M	983	GLN	OE1-CD-NE2	-5.08	117.52	122.60
12	T	68	DT	C2'-C3'-O3'	-5.08	103.88	111.50
23	B	924	ARG	NE-CZ-NH2	5.08	123.77	119.20
25	M	888	GLU	CB-CA-C	5.08	118.85	110.88
9	L	26	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	D	24	LYS	CA-C-N	5.07	130.42	120.99
1	D	24	LYS	C-N-CA	5.07	130.42	120.99
25	M	965	ARG	NE-CZ-NH2	5.07	123.76	119.20
25	M	322	ARG	CB-CG-CD	-5.07	99.65	111.30
25	M	897	LYS	N-CA-C	-5.07	105.88	111.71
25	M	903	PHE	N-CA-C	5.07	116.48	109.54
22	A	1421	ARG	NE-CZ-NH2	5.06	123.76	119.20
11	Q	808	ALA	N-CA-C	5.04	118.69	112.54
22	A	244	ARG	NE-CZ-NH2	5.04	123.73	119.20
26	N	118	DT	C2'-C3'-O3'	5.03	119.05	111.50
16	Z	518	LEU	N-CA-CB	-5.03	102.43	110.63
25	M	1103	ASP	N-CA-C	5.02	116.83	107.99
12	T	67	DT	C2'-C3'-O3'	-5.02	103.97	111.50
16	Z	500	VAL	CA-CB-CG2	5.02	118.94	110.40
16	Z	552	ARG	CB-CA-C	5.02	117.57	110.24
23	B	66	ASP	CA-CB-CG	5.01	117.61	112.60
25	M	1010	ARG	N-CA-C	-5.01	103.44	110.50
25	M	644	PRO	CA-C-O	-5.00	115.31	121.31
1	D	47	GLN	N-CA-C	5.00	116.54	111.14
4	G	158	PHE	O-C-N	-5.00	117.75	123.40

There are no chirality outliers.

All (90) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A	187	TYR	Sidechain
22	A	222	HIS	Sidechain
22	A	33	ARG	Sidechain
22	A	349	ARG	Sidechain
22	A	43	TYR	Sidechain
22	A	431	PHE	Sidechain
22	A	439	HIS	Sidechain
23	B	1060	HIS	Sidechain
23	B	1170	ARG	Sidechain
23	B	160	TYR	Sidechain
23	B	230	ARG	Sidechain
23	B	446	TYR	Sidechain
23	B	83	ARG	Sidechain
23	B	916	TYR	Sidechain
1	D	26	PHE	Sidechain
1	D	44	ARG	Sidechain
1	D	73	ARG	Sidechain
2	E	187	ARG	Sidechain
4	G	107	PHE	Sidechain
4	G	110	ARG	Sidechain
4	G	128	TYR	Sidechain
4	G	151	ARG	Sidechain
4	G	2	PHE	Mainchain
4	G	4	HIS	Sidechain
4	G	42	TYR	Sidechain
4	G	44	PHE	Sidechain
4	G	72	TYR	Sidechain
4	G	74	ALA	Mainchain
4	G	98	PHE	Sidechain
7	J	47	ARG	Sidechain
9	L	31	ARG	Sidechain
9	L	40	GLY	Mainchain
9	L	41	TYR	Sidechain
9	L	42	ARG	Sidechain
9	L	45	TYR	Sidechain
25	M	1010	ARG	Sidechain
25	M	1098	ARG	Sidechain
25	M	1301	TYR	Sidechain
25	M	321	TYR	Sidechain
25	M	322	ARG	Sidechain
25	M	383	TYR	Sidechain
25	M	389	HIS	Sidechain
25	M	423	TYR	Sidechain

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Mol	Chain	Res	Type	Group
25	M	425	TYR	Sidechain
25	M	441	ARG	Sidechain
25	M	464	TYR	Sidechain
25	M	467	PHE	Sidechain
25	M	470	TYR	Sidechain
25	M	473	ARG	Sidechain
25	M	520	ARG	Sidechain
25	M	557	HIS	Sidechain
25	M	573	TYR	Sidechain
25	M	590	TYR	Sidechain
25	M	635	TYR	Sidechain
25	M	639	TYR	Sidechain
25	M	679	TYR	Sidechain
25	M	685	TYR	Sidechain
25	M	988	TYR	Sidechain
26	N	110	DC	Sidechain
26	N	113	DC	Sidechain
26	N	115	DA	Sidechain
26	N	117	DT	Sidechain
26	N	118	DT	Sidechain
26	N	145	DC	Sidechain
26	N	89	DA	Sidechain
26	N	90	DA	Sidechain
10	P	28	A	Sidechain
10	P	29	C	Sidechain
10	P	31	G	Sidechain
10	P	32	G	Sidechain
10	P	35	A	Sidechain
10	P	40	A	Sidechain
10	P	42	C	Sidechain
28	R	366	ARG	Sidechain
28	R	386	PHE	Sidechain
28	R	421	ARG	Sidechain
28	R	438	ARG	Sidechain
28	R	503	ARG	Sidechain
12	T	34	DT	Sidechain
12	T	35	DG	Sidechain
12	T	37	DC	Sidechain
12	T	68	DT	Sidechain
12	T	70	DG	Sidechain
12	T	72	DC	Sidechain
12	T	74	DT	Sidechain

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Mol	Chain	Res	Type	Group
12	T	86	DG	Sidechain
12	T	87	DC	Sidechain
14	X	232	ARG	Sidechain
16	Z	571	ARG	Sidechain
19	g	25	PHE	Sidechain

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	D	1004	0	980	25	0
2	E	1721	0	1737	21	0
3	F	627	0	657	8	0
4	G	1333	0	1321	51	0
5	H	1198	0	1156	34	0
6	I	950	0	880	5	0
7	J	524	0	541	6	0
8	K	920	0	942	10	0
9	L	398	0	404	31	0
10	P	452	0	230	2	0
11	Q	7240	0	7186	41	0
12	T	3691	0	2030	115	0
13	W	2374	0	2290	9	0
14	X	434	0	443	12	0
15	Y	911	0	908	26	0
16	Z	3468	0	3522	135	0
17	a	821	0	862	8	0
17	e	782	0	818	4	0
18	b	622	0	660	4	0
18	f	622	0	660	2	0
19	c	801	0	853	4	0
19	g	796	0	848	14	0
20	d	719	0	738	3	0
20	h	693	0	707	28	0
21	j	111	0	86	41	0
22	A	11015	0	11171	124	0
23	B	8992	0	9036	98	0
24	C	2072	0	2019	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	M	7638	0	7529	86	0
26	N	3509	0	1905	84	0
27	O	2071	0	2016	16	0
28	R	1836	0	1699	38	0
29	U	751	0	633	15	0
30	V	1687	0	1425	19	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	Y	1	0	0	0	0
32	A	1	0	0	0	0
All	All	72793	0	68892	930	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 7.

All (930) 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)
12:T:47:DA:C2'	12:T:48:DT:H71	1.27	1.62
16:Z:250:TRP:CZ3	23:B:327:LYS:HE3	1.07	1.60
26:N:139:DC:C2'	26:N:140:DT:H71	1.35	1.54
16:Z:250:TRP:CH2	23:B:327:LYS:NZ	1.71	1.54
16:Z:250:TRP:CZ3	23:B:327:LYS:CE	1.91	1.52
12:T:47:DA:C2'	12:T:48:DT:C7	1.84	1.44
16:Z:250:TRP:CH2	23:B:327:LYS:CE	1.97	1.43
5:H:150:PHE:C	14:X:241:THR:OG1	1.64	1.40
12:T:47:DA:H2"	12:T:48:DT:C7	0.95	1.40
30:V:251:PHE:C	30:V:253:PRO:HD2	1.50	1.34
26:N:48:DC:C2'	26:N:49:DT:H71	1.61	1.30
12:T:20:DC:OP1	22:A:323:PRO:HG3	1.30	1.30
16:Z:250:TRP:HH2	23:B:327:LYS:NZ	0.80	1.30
16:Z:224:TYR:OH	22:A:301:HIS:HB3	1.31	1.29
16:Z:226:TYR:OH	22:A:301:HIS:CD2	1.85	1.29
12:T:48:DT:C7	12:T:48:DT:OP2	1.81	1.28
19:g:77:ARG:HD3	21:j:947:THR:OG1	1.19	1.28
26:N:139:DC:H2"	26:N:140:DT:C7	1.64	1.28
12:T:48:DT:OP2	12:T:48:DT:H72	1.32	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:139:DC:C2'	26:N:140:DT:C7	2.13	1.25
16:Z:220:HIS:HB2	22:A:297:GLY:O	1.19	1.24
16:Z:220:HIS:HB2	22:A:297:GLY:C	1.68	1.18
20:h:42:TYR:OH	21:j:948:PHE:HD2	1.28	1.16
16:Z:220:HIS:CB	22:A:297:GLY:O	1.94	1.14
12:T:47:DA:H2"	12:T:48:DT:H73	1.19	1.14
19:g:77:ARG:CD	21:j:947:THR:OG1	1.97	1.13
12:T:48:DT:H3'	12:T:49:DG:H4'	1.30	1.10
26:N:5:DA:H2"	26:N:6:DT:H71	1.14	1.10
16:Z:250:TRP:CH2	23:B:327:LYS:HE3	1.69	1.08
20:h:55:SER:HA	21:j:948:PHE:H	1.11	1.08
26:N:5:DA:H2"	26:N:6:DT:C7	1.82	1.07
5:H:150:PHE:O	14:X:241:THR:OG1	1.74	1.06
25:M:889:LEU:HD11	25:M:930:VAL:HG21	1.38	1.06
11:Q:772:GLU:HG2	11:Q:827:HIS:ND1	1.70	1.05
26:N:48:DC:H2"	26:N:49:DT:C7	1.85	1.05
11:Q:762:GLN:NE2	11:Q:813:GLU:HG3	1.72	1.04
12:T:49:DG:N2	26:N:135:DA:N1	2.07	1.02
20:h:56:SER:N	21:j:948:PHE:HB2	1.73	1.02
11:Q:762:GLN:HE22	11:Q:813:GLU:HG3	1.25	1.02
26:N:15:DC:H2"	26:N:16:DT:H71	1.42	1.02
16:Z:224:TYR:OH	22:A:301:HIS:CB	2.08	1.01
20:h:42:TYR:CE2	21:j:950:PRO:HB3	1.97	0.98
26:N:48:DC:H2"	26:N:49:DT:H71	0.98	0.98
20:h:55:SER:C	21:j:948:PHE:HB2	1.89	0.98
30:V:251:PHE:C	30:V:253:PRO:CD	2.37	0.97
29:U:461:LYS:O	29:U:463:PRO:CD	2.12	0.97
26:N:139:DC:H2'	26:N:140:DT:C7	1.90	0.96
12:T:49:DG:N2	26:N:135:DA:C2	2.34	0.96
29:U:461:LYS:O	29:U:463:PRO:HD3	1.65	0.96
16:Z:224:TYR:CZ	22:A:301:HIS:HB3	2.00	0.95
26:N:139:DC:H2'	26:N:140:DT:H71	1.42	0.94
26:N:81:DG:H2"	26:N:82:DT:H71	1.49	0.93
16:Z:220:HIS:C	22:A:299:ALA:HB2	1.94	0.93
19:g:77:ARG:HD3	21:j:947:THR:HG1	1.13	0.93
20:h:56:SER:CB	21:j:948:PHE:HD1	1.81	0.93
12:T:81:DC:H2"	12:T:82:DT:H71	1.48	0.93
30:V:272:ALA:HB3	30:V:273:PRO:HD2	1.52	0.92
26:N:5:DA:C2'	26:N:6:DT:H71	1.99	0.92
5:H:150:PHE:OXT	14:X:241:THR:OG1	1.88	0.91
8:K:77:THR:OG1	8:K:81:TYR:O	1.89	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:48:DC:C2'	26:N:49:DT:C7	2.46	0.90
12:T:48:DT:C3'	12:T:49:DG:H4'	2.01	0.90
12:T:48:DT:H71	12:T:48:DT:OP2	1.72	0.90
16:Z:221:VAL:N	22:A:299:ALA:HB2	1.86	0.89
15:Y:7:PRO:HG3	15:Y:23:LYS:HA	1.53	0.89
12:T:47:DA:C2'	12:T:48:DT:H73	1.74	0.89
16:Z:226:TYR:OH	22:A:301:HIS:CG	2.24	0.89
26:N:135:DA:H2"	26:N:136:DT:H5'	1.55	0.89
16:Z:250:TRP:HZ3	23:B:327:LYS:CE	1.47	0.88
12:T:43:DA:C2	26:N:141:DG:C2	2.61	0.87
23:B:953:ASP:OD1	24:C:36:ARG:NH1	2.08	0.86
20:h:56:SER:CA	21:j:948:PHE:HB2	2.05	0.86
12:T:47:DA:H2"	12:T:48:DT:H72	1.54	0.86
12:T:47:DA:C3'	12:T:48:DT:H71	2.05	0.86
20:h:55:SER:HA	21:j:948:PHE:N	1.88	0.86
26:N:138:DA:H2"	26:N:139:DC:H5	1.39	0.86
12:T:47:DA:C1'	12:T:48:DT:C7	2.52	0.86
26:N:81:DG:H2"	26:N:82:DT:C7	2.06	0.85
16:Z:250:TRP:CZ3	23:B:327:LYS:CD	2.60	0.85
30:V:252:LEU:N	30:V:253:PRO:HD2	1.91	0.85
15:Y:75:GLN:O	15:Y:111:ARG:NH1	2.09	0.85
11:Q:769:LEU:HD22	11:Q:824:ALA:HB2	1.60	0.83
26:N:133:DC:H4'	26:N:134:DC:H5'	1.58	0.83
15:Y:3:LEU:O	15:Y:8:LYS:NZ	2.13	0.82
23:B:765:GLU:OE1	23:B:770:ARG:NE	2.13	0.82
29:U:450:LEU:HD21	29:U:452:LEU:HD23	1.62	0.82
2:E:55:ARG:O	2:E:56:THR:OG1	1.98	0.81
26:N:18:DA:H2"	26:N:19:DC:C5	2.15	0.81
23:B:613:ARG:NH2	23:B:615:TYR:OH	2.14	0.81
12:T:48:DT:H3'	12:T:49:DG:C4'	2.11	0.81
12:T:175:DA:C2	26:N:9:DA:C2	2.70	0.80
23:B:387:HIS:NE2	23:B:671:GLU:OE2	2.14	0.80
25:M:889:LEU:CD1	25:M:930:VAL:HG21	2.10	0.80
12:T:164:DG:C2	26:N:20:DA:C2	2.70	0.80
12:T:47:DA:C1'	12:T:48:DT:H71	2.11	0.79
29:U:461:LYS:O	29:U:463:PRO:HD2	1.82	0.79
30:V:251:PHE:O	30:V:253:PRO:HD2	1.82	0.79
5:H:8:ASP:OD2	5:H:32:SER:OG	2.00	0.79
11:Q:769:LEU:HD22	11:Q:824:ALA:CB	2.13	0.78
26:N:48:DC:H2'	26:N:49:DT:H71	1.64	0.78
16:Z:424:ASP:HB2	16:Z:440:ILE:HD12	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:V:251:PHE:O	30:V:253:PRO:CD	2.31	0.78
12:T:48:DT:H71	12:T:48:DT:P	2.24	0.78
1:D:29:ALA:HB1	4:G:4:HIS:H	1.49	0.78
16:Z:221:VAL:HB	22:A:299:ALA:HB1	1.65	0.78
23:B:169:ARG:NH1	30:V:139:THR:O	2.16	0.77
26:N:138:DA:H2"	26:N:139:DC:C5	2.18	0.77
16:Z:216:VAL:HB	16:Z:226:TYR:HB2	1.65	0.77
16:Z:385:GLY:HA2	22:A:295:GLN:HE21	1.48	0.77
5:H:33:GLU:HB3	11:Q:674:ARG:HH12	1.50	0.76
5:H:37:MET:HE2	5:H:127:GLY:HA3	1.67	0.76
11:Q:772:GLU:CG	11:Q:827:HIS:CE1	2.68	0.76
12:T:177:DA:C2	26:N:7:DG:C2	2.75	0.75
26:N:139:DC:H2"	26:N:140:DT:H71	0.77	0.75
11:Q:772:GLU:HG2	11:Q:827:HIS:CE1	2.22	0.75
26:N:142:DT:H2"	26:N:143:DC:C5	2.21	0.75
16:Z:353:ALA:HB3	16:Z:360:ILE:HB	1.69	0.75
12:T:147:DC:H2"	12:T:148:DT:H71	1.69	0.75
8:K:41:THR:OG1	24:C:36:ARG:NH2	2.21	0.74
20:h:56:SER:HA	21:j:948:PHE:CD1	2.23	0.74
2:E:162:ARG:NH1	22:A:1024:ASN:O	2.20	0.74
26:N:81:DG:C2'	26:N:82:DT:H71	2.18	0.74
16:Z:257:ILE:HA	16:Z:260:MET:HE2	1.68	0.73
5:H:128:ASP:OD1	5:H:131:ASN:ND2	2.21	0.73
28:R:405:ILE:HG23	28:R:426:LEU:HD11	1.71	0.73
16:Z:226:TYR:OH	22:A:301:HIS:HD2	1.64	0.73
20:h:56:SER:HA	21:j:948:PHE:HB2	1.69	0.73
19:g:77:ARG:CZ	21:j:942:GLU:OE2	2.36	0.73
16:Z:226:TYR:CZ	22:A:301:HIS:CD2	2.76	0.72
15:Y:93:LEU:HD22	15:Y:97:ILE:HD11	1.70	0.72
26:N:139:DC:H2'	26:N:140:DT:H73	1.71	0.72
16:Z:295:TYR:N	16:Z:304:SER:OG	2.17	0.72
29:U:376:VAL:HG13	29:U:493:PRO:HB2	1.70	0.72
16:Z:188:GLU:O	16:Z:192:THR:OG1	2.05	0.72
16:Z:426:VAL:HG13	16:Z:440:ILE:HD11	1.72	0.72
26:N:135:DA:C2'	26:N:136:DT:H5'	2.19	0.72
26:N:77:DG:H2"	26:N:78:DT:H71	1.72	0.71
9:L:35:ARG:HD2	28:R:493:GLU:OE2	1.90	0.71
25:M:907:PRO:HG2	25:M:910:LEU:HB3	1.71	0.71
26:N:15:DC:H2"	26:N:16:DT:C7	2.18	0.70
12:T:117:DC:H2"	12:T:118:DC:C5	2.26	0.70
16:Z:221:VAL:CA	22:A:299:ALA:HB2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:224:TYR:OH	22:A:301:HIS:CA	2.38	0.70
30:V:272:ALA:HB3	30:V:273:PRO:CD	2.20	0.70
19:g:77:ARG:NH2	21:j:942:GLU:CD	2.50	0.70
9:L:57:ALA:O	24:C:175:LYS:NZ	2.18	0.69
26:N:5:DA:C2'	26:N:6:DT:C7	2.64	0.69
12:T:164:DG:N2	26:N:20:DA:N3	2.41	0.69
22:A:1038:THR:O	22:A:1042:ASN:ND2	2.25	0.69
27:O:1542:ARG:HH12	27:O:1546:ARG:HH11	1.38	0.69
20:h:55:SER:CA	21:j:948:PHE:H	1.97	0.69
23:B:783:ALA:O	23:B:789:ASN:ND2	2.26	0.69
28:R:387:VAL:HG13	28:R:405:ILE:HD11	1.75	0.69
19:g:77:ARG:NH2	21:j:947:THR:OG1	2.26	0.69
24:C:193:ARG:NH1	24:C:218:ALA:O	2.26	0.68
12:T:49:DG:C2	26:N:135:DA:N1	2.60	0.68
16:Z:307:MET:HE3	16:Z:308:ILE:H	1.57	0.68
16:Z:221:VAL:CA	22:A:299:ALA:CB	2.71	0.68
4:G:30:LEU:HD22	4:G:70:VAL:HG13	1.75	0.68
12:T:159:DC:H42	26:N:24:DG:H1	1.40	0.68
19:g:77:ARG:NH2	21:j:942:GLU:HG2	2.09	0.68
23:B:756:LYS:NZ	30:V:134:THR:OG1	2.27	0.68
26:N:77:DG:H2"	26:N:78:DT:C7	2.24	0.68
26:N:139:DC:H2"	26:N:140:DT:C5	2.29	0.67
9:L:37:ARG:HE	28:R:492:ILE:HG23	1.58	0.67
4:G:22:LEU:HD21	22:A:1475:LEU:HD23	1.77	0.67
16:Z:250:TRP:CH2	23:B:327:LYS:CD	2.76	0.67
23:B:591:ARG:HE	23:B:603:MET:HE1	1.60	0.67
9:L:35:ARG:O	28:R:492:ILE:HG21	1.94	0.67
28:R:492:ILE:O	28:R:496:VAL:HG13	1.94	0.67
23:B:565:THR:HG21	23:B:580:PRO:HB3	1.77	0.67
3:F:86:GLU:OE2	3:F:95:LYS:NZ	2.25	0.67
5:H:150:PHE:HD1	14:X:241:THR:OG1	1.77	0.67
11:Q:856:LEU:HD23	11:Q:857:LEU:HD22	1.76	0.66
4:G:22:LEU:HD23	22:A:1477:ALA:HA	1.77	0.66
5:H:2:ALA:O	5:H:84:ARG:NH1	2.28	0.66
20:h:42:TYR:OH	21:j:948:PHE:CD2	2.17	0.66
26:N:81:DG:H2"	26:N:82:DT:C5	2.30	0.66
23:B:237:VAL:HG11	23:B:369:VAL:HG22	1.76	0.66
25:M:808:PHE:HB2	25:M:910:LEU:HD21	1.77	0.66
15:Y:14:ARG:HH21	15:Y:54:SER:HA	1.61	0.65
16:Z:282:LYS:O	16:Z:287:LYS:NZ	2.28	0.65
12:T:103:DG:H2"	12:T:104:DT:C5	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:175:DA:C2	26:N:9:DA:N1	2.65	0.65
15:Y:4:GLU:O	15:Y:27:GLN:NE2	2.30	0.65
16:Z:184:CYS:SG	16:Z:185:LYS:N	2.68	0.65
26:N:81:DG:C2'	26:N:82:DT:C7	2.75	0.65
12:T:48:DT:C5'	12:T:48:DT:H6	2.10	0.65
29:U:378:LEU:HD23	29:U:382:LEU:O	1.95	0.65
26:N:5:DA:H2"	26:N:6:DT:C5	2.31	0.64
5:H:9:ILE:HD12	5:H:148:LEU:HD11	1.80	0.64
26:N:18:DA:H2"	26:N:19:DC:H5	1.59	0.64
16:Z:221:VAL:HG23	22:A:302:VAL:HB	1.79	0.64
30:V:251:PHE:O	30:V:253:PRO:HD3	1.98	0.64
2:E:96:GLU:OE1	2:E:96:GLU:N	2.31	0.64
12:T:115:DC:H2"	12:T:116:DC:C5	2.33	0.64
11:Q:674:ARG:HG2	11:Q:674:ARG:HH21	1.63	0.64
12:T:20:DC:H2"	12:T:21:DT:H71	1.79	0.64
11:Q:766:THR:OG1	11:Q:820:LEU:HD21	1.98	0.64
16:Z:295:TYR:H	16:Z:304:SER:HG	1.45	0.63
2:E:2:ASP:OD1	2:E:3:ASP:N	2.30	0.63
12:T:47:DA:H2"	12:T:48:DT:OP2	1.98	0.63
20:h:56:SER:CB	21:j:948:PHE:CD1	2.74	0.63
24:C:131:THR:HG22	24:C:147:ASP:OD1	1.98	0.63
5:H:69:THR:OG1	5:H:81:ARG:NH1	2.32	0.63
20:h:56:SER:HB3	21:j:948:PHE:HD1	1.62	0.63
22:A:767:LYS:O	22:A:771:VAL:HG22	1.98	0.63
12:T:164:DG:N2	26:N:20:DA:C2	2.67	0.62
16:Z:366:TYR:O	16:Z:373:PHE:N	2.28	0.62
24:C:31:ALA:O	24:C:231:TYR:OH	2.12	0.62
16:Z:221:VAL:HA	22:A:299:ALA:CB	2.29	0.62
16:Z:574:ALA:N	25:M:895:ASN:HA	2.15	0.62
21:j:938:ASP:C	21:j:940:GLU:H	2.06	0.62
12:T:130:DG:H2'	12:T:131:DC:C6	2.34	0.62
17:a:61:LEU:HD11	17:a:91:MET:HE1	1.81	0.61
4:G:107:PHE:CZ	16:Z:503:PHE:CE1	2.89	0.61
5:H:150:PHE:O	14:X:242:GLY:N	2.33	0.61
12:T:119:DG:N3	17:a:41:ARG:NH1	2.48	0.61
15:Y:66:PRO:HB2	15:Y:78:SER:HA	1.82	0.61
16:Z:224:TYR:OH	22:A:301:HIS:C	2.43	0.61
23:B:179:LEU:HD22	23:B:768:ARG:HD3	1.82	0.61
22:A:487:SER:OG	22:A:673:GLN:NE2	2.34	0.61
16:Z:390:LEU:HD12	16:Z:393:LEU:HD12	1.82	0.61
12:T:47:DA:H2"	12:T:48:DT:H71	0.61	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:LEU:HB2	1:D:65:LEU:HD21	1.82	0.61
11:Q:772:GLU:CG	11:Q:827:HIS:ND1	2.55	0.61
1:D:29:ALA:CB	4:G:4:HIS:H	2.13	0.60
5:H:150:PHE:CD1	14:X:241:THR:OG1	2.54	0.60
12:T:28:DG:OP1	23:B:1078:ARG:N	2.34	0.60
24:C:56:SER:OG	24:C:158:GLU:N	2.34	0.60
20:h:56:SER:N	21:j:948:PHE:CB	2.58	0.60
23:B:854:ILE:HD11	23:B:858:VAL:HG11	1.84	0.60
15:Y:19:CYS:SG	15:Y:21:LEU:HB2	2.42	0.60
6:I:103:ARG:NH1	6:I:105:GLU:OE2	2.35	0.59
20:h:56:SER:CA	21:j:948:PHE:HD1	2.15	0.59
25:M:889:LEU:HD11	25:M:930:VAL:CG2	2.24	0.59
29:U:375:PHE:O	29:U:493:PRO:HG2	2.02	0.59
23:B:1009:GLN:NE2	23:B:1013:ASN:OD1	2.35	0.59
28:R:455:TRP:CD1	28:R:459:MET:HE3	2.38	0.59
13:W:80:ALA:HB1	13:W:112:LEU:HD21	1.84	0.59
28:R:569:GLU:O	28:R:573:VAL:HG23	2.02	0.59
12:T:101:DA:H2"	12:T:102:DC:C5	2.38	0.59
13:W:36:VAL:HG23	13:W:72:ILE:HD11	1.85	0.59
23:B:177:CYS:SG	23:B:737:ILE:HD11	2.43	0.59
5:H:150:PHE:HD1	14:X:241:THR:CB	2.16	0.59
12:T:147:DC:C2'	12:T:148:DT:H71	2.33	0.59
22:A:199:TYR:CZ	22:A:215:LEU:HD13	2.38	0.59
23:B:207:VAL:HG11	23:B:375:ALA:CB	2.33	0.59
12:T:81:DC:H2"	12:T:82:DT:C7	2.26	0.58
16:Z:481:ILE:HD11	16:Z:519:GLN:HB3	1.85	0.58
16:Z:222:LYS:HG3	22:A:302:VAL:HG21	1.86	0.58
6:I:31:GLU:N	6:I:31:GLU:OE1	2.37	0.58
16:Z:192:THR:HG23	16:Z:245:LEU:HD21	1.85	0.58
12:T:9:DC:H2'	12:T:10:DT:H71	1.85	0.58
22:A:955:GLU:OE1	22:A:1010:VAL:HG22	2.03	0.58
7:J:36:ASP:OD1	7:J:41:LYS:NZ	2.34	0.58
12:T:117:DC:H2"	12:T:118:DC:H5	1.66	0.58
12:T:177:DA:H2"	12:T:178:DT:H72	1.85	0.58
17:e:87:SER:O	17:e:91:MET:HG2	2.04	0.58
20:h:56:SER:CA	21:j:948:PHE:CD1	2.86	0.58
22:A:197:GLU:HB2	22:A:215:LEU:HD11	1.84	0.58
20:h:42:TYR:OH	21:j:950:PRO:HD3	2.04	0.58
5:H:7:GLU:HG2	5:H:59:VAL:HG22	1.84	0.58
16:Z:365:ARG:HD3	16:Z:374:LYS:HD2	1.85	0.57
30:V:272:ALA:CB	30:V:273:PRO:CD	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:388:TYR:CE1	23:B:505:LEU:HD21	2.39	0.57
28:R:577:LYS:O	28:R:580:VAL:HG22	2.04	0.57
9:L:37:ARG:C	28:R:496:VAL:HG12	2.29	0.57
25:M:420:MET:HE3	25:M:467:PHE:CZ	2.39	0.57
26:N:47:DC:H2"	26:N:48:DC:C5	2.40	0.57
12:T:47:DA:H1'	12:T:48:DT:C5	2.39	0.57
23:B:177:CYS:SG	23:B:180:ASP:N	2.77	0.57
12:T:49:DG:H2'	12:T:50:DG:C8	2.40	0.57
12:T:165:DT:H2"	12:T:166:DC:C5	2.39	0.57
21:j:938:ASP:C	21:j:940:GLU:N	2.62	0.57
22:A:971:PRO:O	22:A:972:THR:OG1	2.19	0.57
1:D:26:PHE:CE2	4:G:42:TYR:CE2	2.92	0.57
12:T:28:DG:OP1	23:B:1077:GLY:HA2	2.04	0.57
16:Z:280:ARG:HH21	16:Z:288:ASP:HB3	1.69	0.57
22:A:200:ALA:HB3	22:A:214:ILE:HG12	1.86	0.56
27:O:1465:LYS:HE2	27:O:1562:TRP:HE1	1.69	0.56
29:U:450:LEU:CD2	29:U:452:LEU:HD23	2.32	0.56
19:g:77:ARG:NH2	21:j:942:GLU:CG	2.68	0.56
19:g:77:ARG:HH21	21:j:942:GLU:HG2	1.70	0.56
22:A:110:VAL:HG11	22:A:228:ILE:HD11	1.87	0.56
25:M:1150:PHE:CD2	25:M:1272:ILE:HG23	2.41	0.56
25:M:375:PHE:CD2	25:M:375:PHE:C	2.83	0.56
28:R:575:SER:O	28:R:579:LEU:HD13	2.04	0.56
7:J:57:GLU:OE2	24:C:152:LYS:NZ	2.22	0.56
23:B:565:THR:HG22	23:B:577:HIS:O	2.06	0.56
25:M:618:ILE:HG12	25:M:667:THR:HG22	1.88	0.56
15:Y:14:ARG:NH1	15:Y:55:SER:OG	2.39	0.56
24:C:190:ASN:ND2	24:C:195:THR:O	2.34	0.56
1:D:27:GLU:C	1:D:29:ALA:H	2.14	0.56
2:E:55:ARG:C	2:E:56:THR:HG1	2.08	0.56
12:T:30:DG:H2'	12:T:31:DT:C6	2.41	0.56
12:T:43:DA:N1	26:N:141:DG:N1	2.54	0.56
30:V:127:VAL:HG23	30:V:128:VAL:H	1.70	0.56
16:Z:226:TYR:OH	22:A:301:HIS:CB	2.54	0.56
16:Z:586:ALA:HB1	16:Z:640:THR:HG21	1.88	0.56
22:A:198:LEU:O	22:A:215:LEU:HD12	2.07	0.55
12:T:43:DA:C2	26:N:141:DG:N1	2.73	0.55
12:T:65:DA:H1'	12:T:66:DA:C5	2.41	0.55
23:B:907:VAL:HG22	23:B:921:ILE:HG23	1.88	0.55
23:B:939:HIS:NE2	23:B:983:GLU:OE1	2.30	0.55
27:O:1578:GLU:O	27:O:1622:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:364:ASN:O	16:Z:374:LYS:NZ	2.39	0.55
16:Z:541:GLN:HE21	16:Z:544:PRO:HA	1.72	0.55
22:A:687:ILE:HD11	22:A:766:PHE:CZ	2.42	0.55
25:M:681:ASN:HA	25:M:684:THR:HG23	1.88	0.55
25:M:910:LEU:HD12	25:M:913:ALA:HB3	1.88	0.55
3:F:62:ARG:NH2	22:A:517:GLU:OE1	2.39	0.55
25:M:907:PRO:HG2	25:M:910:LEU:CB	2.37	0.55
12:T:150:DG:C2'	12:T:151:DT:H71	2.36	0.55
27:O:1496:ARG:HB2	27:O:1498:GLN:HE21	1.71	0.55
12:T:162:DG:C2	26:N:22:DG:C2	2.94	0.55
16:Z:221:VAL:CG2	22:A:302:VAL:HB	2.37	0.55
26:N:134:DC:H2"	26:N:135:DA:O4'	2.07	0.55
27:O:1680:CYS:SG	27:O:1681:GLY:N	2.79	0.54
4:G:31:PHE:HB3	4:G:48:VAL:HG11	1.88	0.54
26:N:133:DC:H1'	26:N:134:DC:C6	2.42	0.54
27:O:1516:CYS:SG	27:O:1535:ASN:ND2	2.80	0.54
23:B:502:HIS:ND1	23:B:504:THR:HG22	2.22	0.54
12:T:130:DG:H2'	12:T:131:DC:H6	1.72	0.54
16:Z:279:VAL:HA	16:Z:386:VAL:HG21	1.90	0.54
19:g:77:ARG:NH2	21:j:942:GLU:OE2	2.40	0.54
20:h:55:SER:C	21:j:948:PHE:CB	2.71	0.54
26:N:48:DC:H2"	26:N:49:DT:C5	2.43	0.54
19:c:32:ARG:NH1	20:d:35:GLU:OE2	2.41	0.54
25:M:645:VAL:HG11	25:M:733:LEU:HD11	1.90	0.54
12:T:169:DA:C8	12:T:170:DT:H72	2.43	0.54
16:Z:244:ASN:HB3	16:Z:245:LEU:HD22	1.90	0.54
15:Y:40:LEU:HD22	15:Y:42:MET:HB3	1.89	0.54
16:Z:224:TYR:HH	22:A:301:HIS:C	2.15	0.54
16:Z:550:ILE:HD13	16:Z:558:PHE:HB3	1.89	0.54
22:A:299:ALA:HB3	22:A:302:VAL:HG12	1.89	0.54
12:T:44:DG:N2	26:N:140:DT:C2	2.75	0.54
16:Z:235:VAL:O	16:Z:239:ILE:HG12	2.07	0.54
1:D:23:PRO:HB2	1:D:26:PHE:CD1	2.43	0.53
2:E:153:LYS:O	2:E:157:THR:HG23	2.08	0.53
23:B:414:GLU:HG3	23:B:439:ILE:HD11	1.89	0.53
24:C:48:ASP:OD1	24:C:175:LYS:NZ	2.37	0.53
27:O:1634:ASN:ND2	27:O:1661:GLU:O	2.38	0.53
9:L:29:LYS:HB2	28:R:486:LYS:HZ2	1.73	0.53
17:e:107:ASP:OD2	17:e:132:ARG:NH1	2.41	0.53
12:T:105:DA:C2	26:N:79:DA:C2	2.97	0.53
12:T:139:DA:C8	12:T:140:DT:H72	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:M:808:PHE:CB	25:M:910:LEU:HD21	2.38	0.53
20:h:56:SER:HB2	21:j:948:PHE:HD1	1.69	0.53
2:E:185:ILE:HD12	2:E:209:VAL:HG21	1.90	0.53
12:T:9:DC:C2'	12:T:10:DT:H71	2.39	0.53
12:T:47:DA:C1'	12:T:48:DT:C5	2.92	0.53
18:b:89:ALA:O	18:b:93:GLN:NE2	2.42	0.53
22:A:733:LEU:O	22:A:736:THR:HG22	2.08	0.53
23:B:591:ARG:NE	23:B:603:MET:HE1	2.22	0.53
23:B:785:TYR:O	23:B:786:THR:HG22	2.09	0.53
12:T:117:DC:H4'	18:b:45:ARG:HE	1.73	0.53
23:B:407:MET:SD	23:B:444:LEU:HD22	2.49	0.53
27:O:1596:TYR:OH	27:O:1601:ASN:ND2	2.42	0.53
12:T:48:DT:H6	12:T:48:DT:O5'	1.91	0.52
23:B:789:ASN:OD1	23:B:968:ASN:N	2.42	0.52
23:B:854:ILE:O	23:B:907:VAL:HG21	2.08	0.52
26:N:134:DC:H2'	26:N:135:DA:C8	2.44	0.52
30:V:193:HIS:HB2	30:V:199:VAL:HG12	1.92	0.52
8:K:51:LEU:HD22	22:A:561:MET:HE1	1.92	0.52
25:M:536:ALA:HB1	25:M:592:VAL:HG23	1.92	0.52
4:G:4:HIS:CD2	4:G:74:ALA:O	2.63	0.52
4:G:92:VAL:HG11	4:G:128:TYR:CZ	2.45	0.52
12:T:43:DA:N1	26:N:141:DG:C6	2.77	0.52
25:M:1266:ARG:HD3	25:M:1293:TRP:CG	2.44	0.52
15:Y:45:ASN:HD21	15:Y:48:MET:HB2	1.75	0.52
22:A:576:GLN:O	22:A:590:GLN:NE2	2.42	0.52
22:A:896:LEU:HD13	22:A:980:PRO:HG3	1.90	0.52
26:N:49:DT:C6	26:N:50:DT:H72	2.44	0.52
30:V:248:VAL:CB	30:V:253:PRO:HB2	2.39	0.52
23:B:191:GLU:OE2	23:B:743:ARG:NH1	2.43	0.52
4:G:4:HIS:HA	4:G:76:VAL:HG12	1.92	0.52
4:G:109:SER:HB3	16:Z:493:VAL:HG21	1.91	0.52
12:T:20:DC:C2'	12:T:21:DT:H71	2.40	0.52
24:C:183:ALA:HB3	24:C:232:ASN:HB3	1.92	0.52
2:E:189:GLN:O	2:E:209:VAL:HG23	2.10	0.52
5:H:33:GLU:CB	11:Q:674:ARG:HH12	2.22	0.52
9:L:32:ASP:O	9:L:34:ILE:HD12	2.09	0.52
16:Z:206:THR:OG1	16:Z:207:ASP:N	2.43	0.52
16:Z:193:ALA:O	16:Z:197:MET:HG3	2.10	0.52
26:N:109:DA:H1'	26:N:110:DC:C6	2.45	0.52
16:Z:574:ALA:CB	25:M:895:ASN:CG	2.83	0.51
22:A:894:ASP:OD2	22:A:1396:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:63:THR:HG21	5:H:68:GLY:HA2	1.91	0.51
16:Z:573:GLN:C	25:M:895:ASN:HA	2.35	0.51
1:D:22:PHE:CE2	1:D:94:LYS:HE3	2.45	0.51
5:H:33:GLU:HB3	11:Q:674:ARG:NH1	2.22	0.51
25:M:524:TYR:CE1	25:M:591:MET:HG3	2.45	0.51
9:L:45:TYR:CE2	23:B:908:MET:HB3	2.46	0.51
16:Z:224:TYR:CE2	22:A:301:HIS:HB3	2.44	0.51
22:A:110:VAL:HG11	22:A:228:ILE:CD1	2.41	0.51
22:A:951:GLU:HB3	22:A:1007:ILE:HD11	1.91	0.51
27:O:1476:ILE:HB	27:O:1620:LYS:HB3	1.91	0.51
27:O:1639:LYS:HB3	27:O:1646:LEU:HD11	1.92	0.51
12:T:177:DA:C2'	12:T:178:DT:H72	2.40	0.51
1:D:105:PRO:CG	1:D:111:SER:HB3	2.40	0.51
4:G:47:ALA:C	4:G:74:ALA:HB1	2.36	0.51
15:Y:40:LEU:HD21	15:Y:52:CYS:SG	2.51	0.51
5:H:130:ASN:HD22	11:Q:698:ILE:HD13	1.76	0.51
16:Z:475:GLY:H	16:Z:492:ILE:HG13	1.76	0.51
19:g:77:ARG:HD3	21:j:947:THR:CB	2.32	0.51
26:N:135:DA:C8	26:N:136:DT:C5	2.99	0.51
15:Y:63:MET:SD	15:Y:72:SER:HB2	2.51	0.50
16:Z:232:GLN:HE21	16:Z:252:GLN:HB2	1.75	0.50
5:H:150:PHE:OXT	14:X:241:THR:CB	2.59	0.50
12:T:44:DG:N2	26:N:140:DT:O2	2.44	0.50
25:M:903:PHE:CB	25:M:911:ARG:HD3	2.41	0.50
11:Q:856:LEU:CD2	11:Q:857:LEU:HD22	2.42	0.50
26:N:133:DC:H1'	26:N:134:DC:C5	2.45	0.50
1:D:57:LEU:HD12	1:D:57:LEU:H	1.76	0.50
9:L:21:GLU:CG	9:L:41:TYR:CG	2.94	0.50
25:M:1150:PHE:CG	25:M:1272:ILE:HG23	2.47	0.50
1:D:22:PHE:CE2	1:D:94:LYS:CE	2.95	0.50
17:a:87:SER:O	17:a:91:MET:HG2	2.12	0.50
12:T:127:DA:H2"	12:T:128:DC:H5"	1.93	0.50
16:Z:420:PHE:HA	16:Z:470:LYS:HE3	1.93	0.50
16:Z:312:ASP:O	16:Z:315:ARG:HG2	2.11	0.50
23:B:351:VAL:HG12	23:B:351:VAL:O	2.11	0.50
28:R:492:ILE:HD12	28:R:492:ILE:H	1.77	0.50
29:U:459:VAL:HG23	29:U:494:HIS:C	2.36	0.50
2:E:173:ILE:O	2:E:173:ILE:HG23	2.12	0.50
4:G:96:GLY:HA3	4:G:109:SER:HA	1.92	0.50
9:L:39:CYS:SG	9:L:41:TYR:CE2	3.05	0.50
12:T:20:DC:P	22:A:323:PRO:HG3	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:g:77:ARG:CZ	21:j:947:THR:OG1	2.60	0.50
8:K:78:THR:OG1	8:K:80:ASP:OD1	2.27	0.50
20:h:56:SER:HB3	21:j:948:PHE:CD1	2.41	0.50
25:M:903:PHE:CD2	25:M:911:ARG:CZ	2.95	0.50
1:D:29:ALA:HA	4:G:4:HIS:HB3	1.94	0.49
22:A:381:PRO:HB3	22:A:480:SER:HA	1.93	0.49
22:A:948:ILE:HG23	22:A:1007:ILE:HD13	1.94	0.49
16:Z:199:LYS:HG2	16:Z:210:LEU:HD21	1.93	0.49
23:B:313:GLU:OE1	23:B:316:VAL:N	2.44	0.49
23:B:591:ARG:NH1	23:B:663:GLU:OE2	2.45	0.49
4:G:78:ARG:HD3	4:G:80:PHE:CZ	2.47	0.49
15:Y:33:CYS:SG	15:Y:36:CYS:N	2.85	0.49
23:B:84:TYR:HA	23:B:132:VAL:HA	1.94	0.49
22:A:1342:SER:O	22:A:1344:MET:N	2.45	0.49
25:M:425:TYR:C	25:M:425:TYR:CD2	2.90	0.49
25:M:781:VAL:HG21	25:M:921:GLN:HG3	1.94	0.49
23:B:686:GLU:N	23:B:686:GLU:OE1	2.45	0.49
25:M:757:PRO:HD3	25:M:1138:ARG:CZ	2.42	0.49
26:N:20:DA:H2"	26:N:21:DC:C5	2.47	0.49
5:H:15:ILE:O	5:H:16:ASP:C	2.55	0.49
16:Z:215:VAL:HG12	16:Z:227:VAL:HG23	1.94	0.49
25:M:358:LYS:HE3	25:M:387:GLU:OE1	2.12	0.49
16:Z:342:ALA:HB1	16:Z:346:ARG:NH2	2.28	0.49
23:B:218:THR:HG23	23:B:238:SER:HB3	1.94	0.49
28:R:569:GLU:O	28:R:572:ILE:HG22	2.12	0.49
4:G:9:HIS:HB3	4:G:30:LEU:HD13	1.95	0.49
16:Z:220:HIS:HB2	22:A:297:GLY:CA	2.40	0.49
22:A:832:THR:HG23	22:A:833:PRO:HD2	1.95	0.49
22:A:987:ILE:O	22:A:991:GLN:HG3	2.13	0.49
9:L:33:PRO:O	28:R:492:ILE:HD13	2.13	0.49
25:M:463:VAL:HG12	25:M:463:VAL:O	2.11	0.49
4:G:27:LYS:HG2	4:G:54:ILE:HD11	1.94	0.49
4:G:97:LEU:HB3	4:G:113:ILE:HD11	1.95	0.49
16:Z:366:TYR:HB2	16:Z:374:LYS:HA	1.95	0.49
23:B:1028:LEU:HD12	23:B:1041:ILE:HG13	1.94	0.49
16:Z:257:ILE:O	16:Z:260:MET:HG2	2.13	0.48
16:Z:221:VAL:CB	22:A:299:ALA:HB1	2.38	0.48
16:Z:206:THR:HG23	16:Z:208:THR:H	1.79	0.48
20:h:56:SER:CA	21:j:948:PHE:CB	2.87	0.48
25:M:569:LEU:CD2	25:M:705:TRP:CZ2	2.96	0.48
29:U:416:VAL:HG13	29:U:417:GLU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:145:DC:H2"	12:T:146:DC:C5	2.49	0.48
12:T:48:DT:C7	12:T:48:DT:P	2.86	0.48
22:A:621:ILE:HG23	22:A:621:ILE:O	2.14	0.48
1:D:32:LEU:HB3	1:D:37:VAL:HG13	1.94	0.48
6:I:17:CYS:O	6:I:21:ASN:N	2.41	0.48
22:A:965:VAL:O	22:A:968:VAL:HG22	2.14	0.48
28:R:574:GLU:HA	28:R:577:LYS:HG2	1.94	0.48
4:G:46:ILE:H	4:G:76:VAL:HA	1.78	0.48
12:T:119:DG:C5	12:T:120:DC:C4	3.02	0.48
15:Y:56:SER:HA	16:Z:271:ALA:HA	1.96	0.48
12:T:151:DT:C2	12:T:152:DC:C4	3.01	0.48
21:j:938:ASP:O	21:j:941:SER:N	2.42	0.48
22:A:727:PRO:HA	22:A:736:THR:HG21	1.96	0.48
29:U:372:ASP:OD1	29:U:373:LEU:N	2.46	0.48
5:H:27:ARG:NH2	5:H:42:ASP:OD2	2.46	0.48
9:L:34:ILE:HG23	9:L:44:MET:SD	2.54	0.48
10:P:38:G:H2'	10:P:39:A:C8	2.48	0.48
23:B:907:VAL:HG13	23:B:921:ILE:HG12	1.95	0.48
1:D:16:ASP:H	1:D:21:ILE:HG23	1.78	0.48
5:H:92:MET:HE1	5:H:121:LEU:HD22	1.96	0.48
9:L:21:GLU:HG3	9:L:41:TYR:CG	2.49	0.48
9:L:36:CYS:O	28:R:492:ILE:HG22	2.13	0.48
12:T:177:DA:H2"	12:T:178:DT:C7	2.44	0.48
16:Z:573:GLN:O	25:M:894:MET:HG2	2.13	0.48
17:a:109:ASN:ND2	18:b:42:GLY:O	2.46	0.48
22:A:1166:LEU:HD13	22:A:1166:LEU:O	2.14	0.48
12:T:147:DC:H2"	12:T:148:DT:C7	2.40	0.47
19:g:77:ARG:NE	21:j:947:THR:OG1	2.46	0.47
22:A:1049:LEU:HG	22:A:1054:MET:HE3	1.96	0.47
22:A:818:GLU:OE2	28:R:599:CYS:N	2.48	0.47
2:E:185:ILE:HD12	2:E:209:VAL:CG2	2.44	0.47
8:K:39:ASP:OD1	8:K:39:ASP:N	2.47	0.47
11:Q:772:GLU:HG3	11:Q:827:HIS:CE1	2.46	0.47
22:A:1016:LEU:HD22	22:A:1069:LEU:HD22	1.96	0.47
24:C:19:VAL:HG23	24:C:241:PRO:HB2	1.95	0.47
27:O:1465:LYS:HB3	27:O:1562:TRP:HE1	1.79	0.47
4:G:170:LEU:HD12	25:M:520:ARG:HD3	1.97	0.47
20:d:72:ARG:HB3	20:d:101:LEU:HD11	1.96	0.47
22:A:902:GLU:OE1	22:A:985:ARG:NH1	2.46	0.47
11:Q:835:ASP:OD1	11:Q:839:ARG:NE	2.47	0.47
11:Q:849:LYS:O	11:Q:852:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:M:740:TYR:CD2	25:M:740:TYR:C	2.90	0.47
1:D:30:GLU:H	4:G:4:HIS:CB	2.28	0.47
2:E:29:THR:HG23	11:Q:877:GLN:HG2	1.97	0.47
4:G:127:CYS:C	4:G:128:TYR:CZ	2.92	0.47
11:Q:762:GLN:HE22	11:Q:813:GLU:CG	2.11	0.47
16:Z:182:VAL:O	16:Z:224:TYR:HB2	2.14	0.47
16:Z:221:VAL:CB	22:A:299:ALA:CB	2.92	0.47
16:Z:310:ARG:CZ	16:Z:337:GLN:HB2	2.44	0.47
4:G:54:ILE:HD13	4:G:70:VAL:CG2	2.45	0.47
16:Z:540:VAL:HG22	16:Z:548:GLY:O	2.15	0.47
17:e:51:GLU:HA	17:e:54:ARG:HG2	1.96	0.47
20:h:56:SER:HA	21:j:948:PHE:CB	2.40	0.47
26:N:133:DC:H1'	26:N:134:DC:C4	2.50	0.47
16:Z:239:ILE:O	16:Z:242:VAL:HG22	2.15	0.47
16:Z:574:ALA:HB2	25:M:895:ASN:CG	2.40	0.47
23:B:1006:VAL:HG22	30:V:130:TRP:CB	2.45	0.47
23:B:17:ILE:HG23	23:B:19:PRO:HD3	1.96	0.47
25:M:524:TYR:CD1	25:M:591:MET:HG3	2.50	0.47
23:B:273:PHE:CD2	23:B:284:ILE:HG23	2.50	0.46
9:L:30:SER:O	28:R:486:LYS:NZ	2.46	0.46
12:T:66:DA:C5	12:T:67:DT:C4	3.03	0.46
23:B:241:ALA:O	23:B:242:ARG:C	2.57	0.46
25:M:795:PHE:HB3	25:M:910:LEU:HD13	1.98	0.46
25:M:823:GLU:HA	25:M:826:ARG:NE	2.30	0.46
12:T:105:DA:H2"	12:T:106:DC:C6	2.50	0.46
16:Z:221:VAL:HA	22:A:299:ALA:HB2	1.94	0.46
25:M:922:ASP:OD1	25:M:922:ASP:C	2.57	0.46
12:T:48:DT:H72	12:T:49:DG:C8	2.50	0.46
22:A:199:TYR:CE2	22:A:215:LEU:HD13	2.51	0.46
22:A:1262:MET:HE2	22:A:1262:MET:HA	1.98	0.46
23:B:82:PRO:HB3	23:B:134:LYS:CB	2.46	0.46
23:B:365:LEU:O	23:B:369:VAL:HG23	2.15	0.46
3:F:86:GLU:N	3:F:86:GLU:OE1	2.48	0.46
4:G:47:ALA:O	4:G:74:ALA:HA	2.15	0.46
11:Q:163:ILE:HB	11:Q:164:PRO:HD3	1.98	0.46
16:Z:221:VAL:N	22:A:299:ALA:CB	2.70	0.46
16:Z:222:LYS:CG	22:A:302:VAL:HG21	2.44	0.46
23:B:119:THR:HG21	23:B:445:LYS:HE2	1.98	0.46
23:B:388:TYR:H	23:B:504:THR:HG21	1.80	0.46
25:M:527:CYS:HB3	25:M:591:MET:SD	2.55	0.46
2:E:58:LEU:HD23	2:E:58:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:h:90:THR:H	20:h:93:GLU:CG	2.29	0.46
22:A:467:MET:SD	22:A:524:MET:HE3	2.55	0.46
23:B:411:LEU:HD12	23:B:411:LEU:C	2.40	0.46
26:N:6:DT:H2"	26:N:7:DG:H5"	1.97	0.46
30:V:127:VAL:HG23	30:V:128:VAL:N	2.29	0.46
4:G:107:PHE:CZ	16:Z:503:PHE:CD1	3.03	0.46
19:c:77:ARG:HE	26:N:19:DC:H4'	1.81	0.46
22:A:471:GLY:O	22:A:521:VAL:HG23	2.14	0.46
22:A:951:GLU:HG2	22:A:1007:ILE:HD11	1.97	0.46
22:A:1281:ASP:OD1	22:A:1281:ASP:N	2.49	0.46
25:M:467:PHE:CD2	25:M:467:PHE:C	2.94	0.46
2:E:115:LYS:O	2:E:119:VAL:HG22	2.16	0.46
9:L:21:GLU:HG3	9:L:41:TYR:CZ	2.51	0.46
9:L:29:LYS:HB2	28:R:486:LYS:NZ	2.31	0.46
11:Q:772:GLU:HB3	11:Q:830:ARG:NE	2.31	0.46
16:Z:224:TYR:CZ	22:A:301:HIS:CB	2.86	0.46
19:c:68:ASN:OD1	19:c:71:ARG:NH1	2.41	0.46
22:A:419:ILE:HG23	22:A:427:ILE:HB	1.98	0.46
4:G:8:GLU:HA	4:G:71:LYS:HA	1.97	0.46
4:G:27:LYS:HA	4:G:51:ILE:CD1	2.46	0.46
15:Y:35:ASN:ND2	15:Y:85:TYR:OH	2.49	0.46
15:Y:66:PRO:HD3	15:Y:82:PRO:HG3	1.98	0.46
20:h:56:SER:HA	21:j:948:PHE:CG	2.51	0.46
22:A:986:MET:HE2	22:A:1075:LYS:HG3	1.98	0.46
23:B:268:PRO:HG2	23:B:271:ILE:HD12	1.98	0.46
25:M:637:PHE:CE1	25:M:656:ILE:CG1	2.99	0.46
25:M:903:PHE:HB2	25:M:911:ARG:HD3	1.97	0.46
3:F:51:ARG:NH2	3:F:122:GLU:OE1	2.46	0.45
9:L:21:GLU:HG3	9:L:41:TYR:CE2	2.51	0.45
9:L:37:ARG:HD3	28:R:495:ILE:HG21	1.99	0.45
11:Q:887:ASN:HA	11:Q:890:MET:HG2	1.98	0.45
15:Y:22:VAL:HB	15:Y:84:VAL:HG12	1.97	0.45
23:B:67:LEU:H	23:B:83:ARG:HB2	1.82	0.45
3:F:80:MET:HE3	3:F:103:PRO:HG3	1.97	0.45
24:C:151:VAL:HG21	24:C:159:LEU:HD22	1.98	0.45
25:M:742:ILE:HG23	25:M:957:ALA:HB3	1.98	0.45
22:A:64:VAL:HG11	22:A:78:MET:HA	1.99	0.45
25:M:750:TYR:CE1	25:M:965:ARG:NH1	2.84	0.45
3:F:94:MET:HE3	3:F:98:LYS:HE3	1.99	0.45
4:G:14:HIS:HB3	4:G:17:TYR:CD2	2.52	0.45
4:G:127:CYS:O	4:G:128:TYR:CE1	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:38:G:H1	12:T:34:DT:H3	1.63	0.45
25:M:1084:ASN:CG	25:M:1087:GLY:H	2.24	0.45
25:M:1119:LYS:HA	25:M:1119:LYS:HD3	1.77	0.45
9:L:37:ARG:HH11	28:R:492:ILE:HG12	1.82	0.45
11:Q:855:LYS:O	11:Q:858:LYS:HG3	2.16	0.45
25:M:911:ARG:HD2	25:M:911:ARG:HA	1.69	0.45
25:M:918:ARG:HD3	25:M:981:TYR:CE1	2.52	0.45
28:R:369:LEU:HD11	28:R:417:LEU:HD23	1.99	0.45
2:E:41:LYS:NZ	2:E:46:ASP:OD1	2.41	0.45
12:T:171:DA:C8	12:T:172:DT:C7	3.00	0.45
16:Z:280:ARG:HG3	16:Z:386:VAL:HG13	1.98	0.45
16:Z:294:ASP:HB2	16:Z:306:LYS:HE2	1.98	0.45
17:a:107:ASP:OD2	17:a:132:ARG:NH1	2.38	0.45
22:A:480:SER:O	23:B:1055:VAL:HG21	2.16	0.45
22:A:1366:PHE:HB2	22:A:1374:VAL:HG21	1.99	0.45
23:B:721:ARG:NH2	23:B:940:GLY:O	2.48	0.45
23:B:801:VAL:HG13	23:B:929:PRO:HD2	1.97	0.45
25:M:420:MET:HE3	25:M:467:PHE:HZ	1.81	0.45
25:M:893:TYR:CD2	25:M:915:SER:HB2	2.51	0.45
28:R:486:LYS:HE2	28:R:488:ASN:HD21	1.81	0.45
5:H:149:ALA:O	5:H:150:PHE:OXT	2.34	0.45
6:I:49:ASP:OD1	6:I:49:ASP:N	2.49	0.45
11:Q:524:LEU:HD21	11:Q:533:CYS:HB2	1.98	0.45
12:T:24:DG:H2'	12:T:25:DA:H8	1.82	0.45
16:Z:272:ASN:ND2	16:Z:384:GLU:HB2	2.32	0.45
22:A:1095:LEU:HD23	22:A:1401:LEU:HD22	1.97	0.45
23:B:119:THR:HG23	23:B:187:ILE:HA	1.99	0.45
23:B:841:ARG:HH11	23:B:891:ASP:CG	2.25	0.45
25:M:319:TRP:CZ3	25:M:403:TRP:HB2	2.52	0.45
26:N:89:DA:H1'	26:N:90:DA:C8	2.51	0.45
1:D:95:PHE:CD1	4:G:1:MET:HE1	2.52	0.45
9:L:16:ILE:HD11	9:L:25:GLU:HB3	1.98	0.45
22:A:490:THR:HB	22:A:491:PRO:HD3	1.99	0.45
25:M:377:ALA:HB2	25:M:393:LEU:HD12	1.98	0.45
16:Z:243:GLY:O	16:Z:246:ARG:HG2	2.17	0.45
17:e:75:ILE:HG21	18:f:63:GLU:HA	1.98	0.45
20:h:42:TYR:HE2	21:j:950:PRO:HB3	1.74	0.45
22:A:479:TRP:O	22:A:483:ARG:NH1	2.46	0.45
2:E:126:ILE:HD12	2:E:126:ILE:H	1.81	0.44
4:G:145:LEU:HD12	4:G:145:LEU:C	2.42	0.44
11:Q:523:ILE:HG21	11:Q:533:CYS:SG	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:91:DG:H2"	12:T:92:DC:C6	2.52	0.44
22:A:663:ASP:OD1	22:A:666:ARG:NH1	2.50	0.44
22:A:921:ARG:NH1	22:A:953:GLU:OE2	2.43	0.44
22:A:1181:PRO:O	22:A:1184:THR:HG23	2.17	0.44
5:H:150:PHE:C	14:X:242:GLY:N	2.76	0.44
16:Z:340:PHE:HD2	16:Z:370:GLY:HA2	1.81	0.44
16:Z:384:GLU:HG3	22:A:296:ASN:HA	1.99	0.44
22:A:1302:GLU:OE1	22:A:1302:GLU:N	2.44	0.44
25:M:572:ASP:HB2	25:M:573:TYR:CD2	2.52	0.44
16:Z:481:ILE:HD12	16:Z:517:ASP:O	2.17	0.44
24:C:103:LEU:HD23	24:C:103:LEU:C	2.41	0.44
28:R:486:LYS:HB3	28:R:486:LYS:HE3	1.72	0.44
28:R:486:LYS:CE	28:R:488:ASN:HD21	2.30	0.44
4:G:54:ILE:HD13	4:G:70:VAL:HG21	1.99	0.44
5:H:60:ILE:HG23	5:H:141:VAL:CG2	2.47	0.44
5:H:150:PHE:O	14:X:241:THR:N	2.49	0.44
9:L:21:GLU:HG3	9:L:41:TYR:CD1	2.52	0.44
12:T:47:DA:O3'	12:T:48:DT:H71	2.15	0.44
16:Z:182:VAL:HG23	16:Z:225:ILE:HG13	1.98	0.44
16:Z:188:GLU:N	16:Z:188:GLU:OE1	2.51	0.44
22:A:604:ARG:O	22:A:628:VAL:N	2.50	0.44
23:B:988:LYS:NZ	23:B:1026:GLU:OE2	2.50	0.44
30:V:252:LEU:N	30:V:253:PRO:CD	2.61	0.44
4:G:127:CYS:C	4:G:128:TYR:CE2	2.96	0.44
12:T:81:DC:C2'	12:T:82:DT:H71	2.35	0.44
15:Y:116:LYS:HA	15:Y:116:LYS:HD3	1.74	0.44
16:Z:540:VAL:HG21	16:Z:560:VAL:HG21	2.00	0.44
24:C:44:ILE:HG23	24:C:176:TRP:HD1	1.82	0.44
3:F:61:GLU:HA	22:A:1471:PHE:CZ	2.52	0.44
4:G:97:LEU:CB	4:G:113:ILE:HD11	2.47	0.44
12:T:171:DA:C5	12:T:172:DT:C4	3.05	0.44
16:Z:479:LYS:HE2	16:Z:523:GLU:HB2	1.98	0.44
20:d:90:THR:OG1	20:d:93:GLU:OE1	2.31	0.44
23:B:550:MET:CE	23:B:567:ILE:HG21	2.48	0.44
23:B:1119:CYS:HB3	23:B:1123:GLY:O	2.17	0.44
25:M:762:GLN:C	25:M:764:VAL:H	2.26	0.44
12:T:151:DT:H2"	12:T:152:DC:C5	2.53	0.44
12:T:171:DA:H2'	12:T:172:DT:H71	2.00	0.44
22:A:569:THR:CG2	22:A:667:LEU:HD13	2.47	0.44
22:A:578:ALA:N	22:A:590:GLN:OE1	2.51	0.44
23:B:166:LEU:HG	23:B:170:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:135:DA:H2"	26:N:136:DT:H2'	1.98	0.44
4:G:72:TYR:O	4:G:72:TYR:CG	2.71	0.44
11:Q:674:ARG:HH21	11:Q:674:ARG:CG	2.26	0.44
15:Y:8:LYS:HE2	15:Y:27:GLN:NE2	2.32	0.44
9:L:19:CYS:SG	9:L:36:CYS:HB2	2.57	0.44
22:A:1158:LEU:C	22:A:1158:LEU:HD23	2.43	0.44
23:B:541:ILE:HD12	23:B:616:THR:CG2	2.48	0.44
26:N:81:DG:H2"	26:N:82:DT:C6	2.52	0.44
26:N:139:DC:C2'	26:N:140:DT:H73	2.25	0.44
12:T:48:DT:OP2	12:T:48:DT:C5	2.65	0.43
23:B:1035:ARG:NH2	23:B:1036:LYS:O	2.50	0.43
9:L:19:CYS:SG	9:L:20:GLY:N	2.90	0.43
9:L:40:GLY:C	9:L:41:TYR:CG	2.97	0.43
12:T:47:DA:C1'	12:T:48:DT:H73	2.38	0.43
17:a:69:GLN:HE21	17:a:73:ARG:HH11	1.65	0.43
23:B:785:TYR:C	23:B:786:THR:HG22	2.43	0.43
25:M:1141:TYR:CD1	25:M:1141:TYR:C	2.96	0.43
1:D:114:LEU:HD12	4:G:84:VAL:HG21	1.99	0.43
3:F:90:LEU:HD21	22:A:513:ALA:HB2	1.99	0.43
8:K:92:THR:OG1	24:C:260:GLN:NE2	2.39	0.43
13:W:24:TRP:HE1	13:W:33:GLU:HB3	1.82	0.43
15:Y:76:ARG:HH11	15:Y:109:LYS:HD3	1.83	0.43
23:B:84:TYR:HB3	23:B:132:VAL:HG23	2.00	0.43
23:B:552:ASN:OD1	23:B:553:LEU:N	2.52	0.43
13:W:49:TRP:CZ2	13:W:52:GLU:HA	2.52	0.43
13:W:86:ALA:HB1	13:W:105:GLY:O	2.18	0.43
15:Y:29:GLU:HG3	15:Y:45:ASN:O	2.19	0.43
15:Y:61:ILE:HD12	15:Y:63:MET:HE2	2.00	0.43
16:Z:389:THR:O	16:Z:393:LEU:HG	2.18	0.43
26:N:133:DC:H1'	26:N:134:DC:C2	2.54	0.43
26:N:134:DC:C2'	26:N:135:DA:C8	3.02	0.43
27:O:1670:ARG:HH11	27:O:1689:LEU:HB2	1.82	0.43
4:G:165:ASP:O	4:G:168:LEU:HD12	2.18	0.43
12:T:164:DG:N1	26:N:20:DA:N1	2.66	0.43
16:Z:250:TRP:CH2	23:B:327:LYS:HD3	2.52	0.43
22:A:904:GLN:NE2	22:A:981:CYS:O	2.47	0.43
25:M:316:GLU:CD	25:M:403:TRP:CD1	2.97	0.43
7:J:35:LEU:HD11	7:J:50:LEU:HG	2.00	0.43
7:J:64:PRO:O	9:L:23:HIS:CE1	2.70	0.43
12:T:107:DG:C2	26:N:77:DG:N2	2.86	0.43
13:W:36:VAL:CG2	13:W:72:ILE:HD11	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:261:THR:O	16:Z:264:LEU:HG	2.18	0.43
22:A:1285:LEU:HA	22:A:1288:ILE:HG12	2.01	0.43
25:M:413:LEU:HD23	25:M:460:LEU:HD11	1.99	0.43
25:M:637:PHE:CE1	25:M:656:ILE:HG12	2.53	0.43
25:M:1167:ILE:HD11	25:M:1279:LEU:HD22	1.99	0.43
16:Z:280:ARG:HB2	16:Z:382:ILE:HG23	2.00	0.43
22:A:584:PRO:O	22:A:585:LEU:HD12	2.18	0.43
22:A:1323:THR:HG22	22:A:1324:GLU:N	2.34	0.43
23:B:265:GLN:N	23:B:265:GLN:OE1	2.51	0.43
25:M:1268:MET:SD	25:M:1280:THR:HB	2.59	0.43
26:N:170:DC:H2"	26:N:171:DA:C8	2.54	0.43
1:D:27:GLU:O	1:D:27:GLU:HG3	2.19	0.43
2:E:24:ARG:NH2	2:E:128:GLU:OE2	2.48	0.43
22:A:1139:LEU:HD21	22:A:1341:VAL:HG13	2.01	0.43
25:M:977:ILE:HD11	25:M:1004:LEU:HD12	2.01	0.43
25:M:1171:VAL:HG13	25:M:1228:VAL:CG1	2.48	0.43
28:R:587:LYS:O	28:R:588:ASN:ND2	2.51	0.43
2:E:20:LEU:C	2:E:20:LEU:HD23	2.44	0.43
5:H:24:ARG:NH2	22:A:552:ASP:O	2.50	0.43
5:H:150:PHE:OXT	14:X:242:GLY:N	2.51	0.43
12:T:31:DT:H2"	12:T:32:DT:C6	2.54	0.43
15:Y:19:CYS:SG	15:Y:35:ASN:ND2	2.84	0.43
26:N:9:DA:H2'	26:N:10:DT:H71	2.01	0.43
1:D:29:ALA:CA	4:G:4:HIS:O	2.67	0.43
23:B:596:ILE:N	23:B:596:ILE:HD12	2.34	0.43
4:G:108:ILE:HG23	4:G:162:SER:HA	2.00	0.42
5:H:33:GLU:O	11:Q:684:TRP:HH2	2.02	0.42
16:Z:291:ALA:HB2	16:Z:307:MET:HG2	2.00	0.42
23:B:156:LEU:HD22	23:B:184:TYR:CE1	2.55	0.42
25:M:635:TYR:OH	25:M:1297:LYS:HE3	2.18	0.42
27:O:1523:ARG:HB2	27:O:1541:ASN:HD21	1.84	0.42
12:T:171:DA:C8	12:T:172:DT:H73	2.54	0.42
16:Z:586:ALA:CB	16:Z:640:THR:HG21	2.48	0.42
23:B:812:ARG:O	23:B:922:ARG:HA	2.20	0.42
28:R:428:LEU:HB2	28:R:437:PHE:CD1	2.54	0.42
1:D:96:GLU:HG2	1:D:118:LEU:CD2	2.50	0.42
11:Q:858:LYS:HA	11:Q:861:GLU:HG3	2.00	0.42
16:Z:200:PHE:HA	16:Z:210:LEU:HD13	2.00	0.42
17:a:49:LEU:HD23	17:a:52:ILE:HD12	2.00	0.42
23:B:541:ILE:HD12	23:B:616:THR:HG21	2.01	0.42
28:R:364:LEU:HB2	28:R:387:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2:ASP:OD1	2:E:4:GLU:N	2.52	0.42
23:B:1040:GLN:NE2	24:C:195:THR:OG1	2.49	0.42
25:M:637:PHE:CE1	25:M:656:ILE:HG13	2.55	0.42
25:M:742:ILE:HG23	25:M:957:ALA:CB	2.50	0.42
4:G:110:ARG:NH1	4:G:128:TYR:CG	2.87	0.42
8:K:17:LYS:O	8:K:36:ASN:ND2	2.42	0.42
9:L:29:LYS:NZ	28:R:487:PHE:CE2	2.87	0.42
12:T:27:DT:H2'	12:T:28:DG:H8	1.83	0.42
16:Z:242:VAL:HG23	16:Z:245:LEU:HB2	2.00	0.42
16:Z:540:VAL:HG22	16:Z:548:GLY:C	2.44	0.42
22:A:37:THR:HG21	22:A:41:ILE:HD11	2.01	0.42
25:M:559:THR:O	25:M:560:GLU:C	2.63	0.42
26:N:118:DT:H2"	26:N:119:DG:C8	2.54	0.42
4:G:27:LYS:HA	4:G:51:ILE:HD13	2.01	0.42
12:T:164:DG:N1	26:N:20:DA:C2	2.88	0.42
16:Z:226:TYR:OH	22:A:301:HIS:HB2	2.19	0.42
16:Z:479:LYS:HE3	16:Z:489:THR:OG1	2.20	0.42
25:M:588:ALA:O	25:M:589:ARG:C	2.62	0.42
28:R:576:GLU:O	28:R:580:VAL:HG13	2.19	0.42
28:R:592:ASP:O	28:R:594:PHE:N	2.47	0.42
9:L:35:ARG:HA	9:L:41:TYR:O	2.19	0.42
26:N:96:DG:H2"	26:N:97:DC:C5	2.54	0.42
26:N:139:DC:H2"	26:N:140:DT:C6	2.54	0.42
29:U:373:LEU:HD23	29:U:375:PHE:H	1.84	0.42
2:E:112:PRO:HG2	12:T:13:DC:H5'	2.02	0.42
9:L:29:LYS:CB	28:R:486:LYS:NZ	2.83	0.42
11:Q:833:LYS:O	11:Q:836:GLU:HG3	2.19	0.42
16:Z:258:LYS:HE2	16:Z:258:LYS:HB3	1.73	0.42
16:Z:545:GLN:HG2	25:M:1154:THR:HA	2.01	0.42
16:Z:574:ALA:N	25:M:895:ASN:CA	2.81	0.42
20:h:98:VAL:HG13	20:h:102:LEU:HD12	2.01	0.42
28:R:431:GLY:N	28:R:459:MET:HE1	2.35	0.42
11:Q:748:PRO:HB3	13:W:110:TRP:CH2	2.55	0.42
11:Q:766:THR:OG1	11:Q:820:LEU:CD2	2.67	0.42
22:A:29:ASP:HA	22:A:32:LYS:HE3	2.02	0.42
22:A:71:CYS:HB2	22:A:81:CYS:SG	2.59	0.42
23:B:497:LYS:CG	23:B:498:PRO:HD3	2.50	0.42
25:M:557:HIS:CD2	25:M:557:HIS:N	2.87	0.42
13:W:110:TRP:CD1	13:W:111:THR:H	2.38	0.42
16:Z:199:LYS:HG3	16:Z:203:TYR:HD2	1.84	0.42
18:f:78:ARG:NH2	18:f:80:THR:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:244:ARG:HB2	22:A:247:TRP:CD2	2.55	0.42
22:A:922:PHE:H	22:A:1052:ARG:HD2	1.85	0.42
22:A:965:VAL:O	22:A:969:ILE:HG12	2.19	0.42
23:B:588:ARG:O	23:B:592:ARG:HD3	2.20	0.42
25:M:609:THR:HG22	25:M:671:ILE:HD11	2.02	0.42
1:D:19:GLN:HG3	1:D:21:ILE:HG22	2.01	0.41
1:D:96:GLU:HG2	1:D:118:LEU:HD21	2.01	0.41
1:D:99:CYS:SG	1:D:100:LEU:N	2.92	0.41
16:Z:220:HIS:CG	22:A:297:GLY:O	2.69	0.41
25:M:322:ARG:HA	25:M:326:ALA:HB3	2.02	0.41
1:D:87:LEU:CD2	1:D:97:LEU:HG	2.51	0.41
9:L:35:ARG:C	28:R:492:ILE:HG21	2.46	0.41
12:T:22:DC:H2'	12:T:23:DC:C6	2.56	0.41
12:T:105:DA:H2"	12:T:106:DC:C5	2.55	0.41
15:Y:14:ARG:NH1	16:Z:300:GLN:OE1	2.53	0.41
15:Y:72:SER:HG	15:Y:78:SER:HG	1.62	0.41
27:O:1669:GLN:NE2	27:O:1695:VAL:O	2.50	0.41
28:R:486:LYS:HE3	28:R:486:LYS:CA	2.46	0.41
5:H:121:LEU:HD12	5:H:121:LEU:N	2.35	0.41
12:T:2:DC:H2'	12:T:3:DT:H72	2.02	0.41
12:T:130:DG:C6	12:T:131:DC:N4	2.88	0.41
12:T:169:DA:C2'	12:T:170:DT:H72	2.50	0.41
16:Z:424:ASP:OD1	16:Z:519:GLN:HB2	2.19	0.41
22:A:365:THR:HG22	22:A:366:VAL:N	2.35	0.41
23:B:117:ASN:HA	23:B:189:GLY:HA3	2.01	0.41
23:B:207:VAL:HG11	23:B:375:ALA:HB3	2.02	0.41
23:B:587:LEU:HB3	23:B:603:MET:HE3	2.01	0.41
29:U:394:TYR:O	30:V:172:ARG:NH1	2.50	0.41
5:H:24:ARG:O	5:H:45:ILE:N	2.48	0.41
11:Q:837:GLU:O	11:Q:840:GLU:HG3	2.20	0.41
12:T:21:DT:H2"	12:T:22:DC:C6	2.56	0.41
16:Z:200:PHE:HB2	16:Z:210:LEU:HD22	2.02	0.41
16:Z:500:VAL:HG22	16:Z:513:VAL:O	2.20	0.41
25:M:313:LEU:HD23	25:M:313:LEU:HA	1.89	0.41
25:M:567:LEU:HD12	25:M:567:LEU:HA	1.92	0.41
28:R:504:LYS:HG3	28:R:507:PRO:CD	2.51	0.41
4:G:101:ILE:CD1	4:G:106:CYS:HB2	2.50	0.41
8:K:104:ARG:NH2	24:C:7:PRO:O	2.48	0.41
12:T:27:DT:H2'	12:T:28:DG:C8	2.56	0.41
12:T:150:DG:H2"	12:T:151:DT:H71	2.00	0.41
12:T:150:DG:C8	12:T:151:DT:H73	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:244:ARG:HB2	22:A:247:TRP:CE2	2.54	0.41
23:B:805:PHE:CZ	23:B:964:ASP:HB3	2.55	0.41
23:B:1022:LEU:HD23	23:B:1022:LEU:H	1.84	0.41
25:M:639:TYR:O	25:M:1301:TYR:HA	2.20	0.41
5:H:37:MET:HE1	5:H:131:ASN:HB2	2.02	0.41
8:K:91:ILE:HG21	24:C:260:GLN:HB2	2.03	0.41
11:Q:605:LEU:HD12	14:X:238:LEU:HD13	2.03	0.41
11:Q:816:GLN:HA	11:Q:819:ASP:OD2	2.19	0.41
16:Z:250:TRP:HZ3	23:B:327:LYS:HE3	0.62	0.41
16:Z:440:ILE:HA	16:Z:450:ILE:HD11	2.02	0.41
19:g:51:LEU:HD13	20:h:73:ILE:HG21	2.02	0.41
30:V:176:ILE:HG23	30:V:177:THR:N	2.35	0.41
6:I:103:ARG:O	6:I:103:ARG:HG2	2.21	0.41
11:Q:879:ALA:O	11:Q:882:VAL:HG12	2.21	0.41
16:Z:475:GLY:H	16:Z:492:ILE:CG1	2.32	0.41
23:B:680:ASP:OD1	23:B:681:ASP:N	2.54	0.41
25:M:597:ALA:HA	25:M:721:LEU:HD11	2.01	0.41
26:N:139:DC:C2	26:N:140:DT:C4	3.09	0.41
2:E:73:PHE:CD2	2:E:99:ILE:HD12	2.54	0.41
5:H:67:ASP:OD1	5:H:67:ASP:N	2.50	0.41
12:T:165:DT:H2"	12:T:166:DC:C6	2.56	0.41
16:Z:192:THR:OG1	16:Z:244:ASN:ND2	2.54	0.41
22:A:951:GLU:CB	22:A:1007:ILE:HD11	2.51	0.41
22:A:977:VAL:HG22	22:A:978:VAL:N	2.36	0.41
23:B:331:THR:HG23	23:B:334:LYS:HB2	2.02	0.41
23:B:651:TYR:HB2	29:U:460:TYR:CZ	2.56	0.41
26:N:183:DG:H2"	26:N:184:DG:C8	2.56	0.41
4:G:48:VAL:HA	4:G:74:ALA:HA	2.02	0.41
4:G:111:HIS:CE1	16:Z:501:ILE:HG21	2.56	0.41
4:G:151:ARG:HD2	16:Z:491:LEU:HD11	2.02	0.41
7:J:40:LEU:HD11	7:J:49:LEU:HD12	2.03	0.41
9:L:22:CYS:HG	9:L:41:TYR:HD2	1.65	0.41
12:T:25:DA:OP1	22:A:351:ARG:NH1	2.44	0.41
16:Z:176:ASP:OD2	16:Z:176:ASP:N	2.53	0.41
16:Z:389:THR:HG23	16:Z:391:SER:H	1.86	0.41
19:c:88:ARG:HB3	19:c:108:LEU:HD11	2.01	0.41
22:A:21:VAL:HG22	22:A:1449:ASP:HB3	2.03	0.41
22:A:658:LEU:HD13	22:A:902:GLU:CD	2.46	0.41
22:A:659:GLU:OE2	22:A:985:ARG:NH2	2.49	0.41
23:B:649:ASN:HB2	29:U:460:TYR:OH	2.21	0.41
23:B:759:VAL:O	23:B:759:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:M:690:LYS:HA	25:M:713:ILE:CD1	2.51	0.41
25:M:902:GLU:HG2	25:M:903:PHE:CE2	2.56	0.41
26:N:135:DA:H1'	26:N:136:DT:H5'	2.03	0.41
28:R:559:ALA:O	28:R:563:ILE:HG23	2.20	0.41
4:G:109:SER:CB	16:Z:493:VAL:HG21	2.51	0.41
4:G:128:TYR:CD2	4:G:128:TYR:N	2.89	0.41
11:Q:829:ALA:O	11:Q:833:LYS:HG3	2.21	0.41
12:T:143:DC:H6	12:T:143:DC:H2'	1.75	0.41
16:Z:571:ARG:HB2	25:M:895:ASN:CG	2.45	0.41
16:Z:587:LEU:HD22	25:M:1262:THR:HG21	2.03	0.41
22:A:376:ASP:HB3	22:A:522:PRO:HD3	2.02	0.41
23:B:218:THR:HG22	23:B:236:TRP:HD1	1.86	0.41
8:K:57:LEU:N	8:K:76:GLN:O	2.54	0.40
11:Q:769:LEU:HD22	11:Q:824:ALA:HB1	2.00	0.40
12:T:147:DC:H2"	12:T:148:DT:C6	2.56	0.40
16:Z:260:MET:N	16:Z:260:MET:SD	2.94	0.40
23:B:193:VAL:HG11	23:B:470:LEU:HD13	2.03	0.40
23:B:819:SER:HA	23:B:916:TYR:CE1	2.56	0.40
26:N:138:DA:C2'	26:N:139:DC:C5	2.95	0.40
1:D:22:PHE:CZ	1:D:94:LYS:HE3	2.56	0.40
4:G:112:SER:HA	4:G:164:MET:HE3	2.03	0.40
4:G:122:ASN:C	25:M:405:GLN:HE22	2.28	0.40
12:T:150:DG:H2'	12:T:151:DT:H71	2.03	0.40
12:T:180:DG:H2"	12:T:181:DA:C8	2.56	0.40
22:A:1073:GLU:HG3	22:A:1074:SER:N	2.36	0.40
25:M:798:LEU:HD22	25:M:843:LYS:HB3	2.03	0.40
4:G:130:THR:O	4:G:131:MET:C	2.65	0.40
13:W:5:TYR:CE1	13:W:304:PRO:HD2	2.56	0.40
22:A:1231:ILE:HD12	22:A:1298:LEU:HD13	2.02	0.40
25:M:420:MET:HE3	25:M:467:PHE:CE1	2.56	0.40
25:M:892:LEU:HD12	25:M:895:ASN:HD22	1.85	0.40
12:T:85:DA:C4	12:T:86:DG:C6	3.10	0.40
16:Z:495:VAL:HA	16:Z:500:VAL:HG12	2.03	0.40
22:A:36:VAL:HA	23:B:1138:ARG:NH2	2.37	0.40
22:A:1282:ASP:OD1	22:A:1282:ASP:N	2.54	0.40
25:M:524:TYR:CE1	25:M:591:MET:CG	3.03	0.40
25:M:1052:VAL:HG11	25:M:1093:LEU:HD13	2.03	0.40
27:O:1528:GLU:HB2	27:O:1642:VAL:HG22	2.03	0.40
1:D:83:VAL:O	1:D:87:LEU:HB2	2.20	0.40
2:E:197:SER:OG	22:A:893:GLU:OE1	2.32	0.40
7:J:53:VAL:HG13	7:J:53:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:441:LEU:O	11:Q:446:GLN:N	2.55	0.40
11:Q:803:MET:C	11:Q:803:MET:SD	3.04	0.40
12:T:68:DT:H1'	12:T:69:DG:C8	2.56	0.40
16:Z:474:MET:HA	16:Z:492:ILE:HD11	2.04	0.40
17:a:62:LEU:HD11	18:b:40:ARG:HH11	1.85	0.40
22:A:531:ASN:OD1	22:A:531:ASN:C	2.64	0.40
23:B:544:PHE:CE1	23:B:590:LEU:HD21	2.57	0.40
25:M:620:PRO:HD2	25:M:639:TYR:CE1	2.57	0.40
27:O:1571:PRO:HA	27:O:1655:LEU:HD13	2.04	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	D	124/142 (87%)	117 (94%)	6 (5%)	1 (1%)	16 54
2	E	207/210 (99%)	199 (96%)	7 (3%)	1 (0%)	24 63
3	F	76/127 (60%)	72 (95%)	4 (5%)	0	100 100
4	G	169/172 (98%)	153 (90%)	16 (10%)	0	100 100
5	H	147/150 (98%)	137 (93%)	10 (7%)	0	100 100
6	I	115/125 (92%)	106 (92%)	9 (8%)	0	100 100
7	J	64/67 (96%)	60 (94%)	3 (5%)	1 (2%)	7 38
8	K	113/117 (97%)	110 (97%)	3 (3%)	0	100 100
9	L	45/58 (78%)	39 (87%)	6 (13%)	0	100 100
11	Q	890/1179 (76%)	874 (98%)	14 (2%)	2 (0%)	43 78
13	W	303/305 (99%)	296 (98%)	7 (2%)	0	100 100
14	X	51/531 (10%)	50 (98%)	0	1 (2%)	6 31
15	Y	114/121 (94%)	108 (95%)	6 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Z	424/1087 (39%)	400 (94%)	24 (6%)	0	100	100
17	a	99/136 (73%)	97 (98%)	2 (2%)	0	100	100
17	e	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
18	b	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
18	f	76/103 (74%)	74 (97%)	2 (3%)	0	100	100
19	c	102/135 (76%)	100 (98%)	2 (2%)	0	100	100
19	g	101/135 (75%)	100 (99%)	1 (1%)	0	100	100
20	d	90/126 (71%)	90 (100%)	0	0	100	100
20	h	87/126 (69%)	84 (97%)	3 (3%)	0	100	100
21	j	12/1049 (1%)	11 (92%)	1 (8%)	0	100	100
22	A	1376/1970 (70%)	1322 (96%)	52 (4%)	2 (0%)	48	83
23	B	1115/1174 (95%)	1052 (94%)	63 (6%)	0	100	100
24	C	254/275 (92%)	246 (97%)	8 (3%)	0	100	100
25	M	924/1729 (53%)	899 (97%)	24 (3%)	1 (0%)	48	83
27	O	250/1133 (22%)	224 (90%)	26 (10%)	0	100	100
28	R	240/713 (34%)	232 (97%)	8 (3%)	0	100	100
29	U	98/666 (15%)	88 (90%)	10 (10%)	0	100	100
30	V	232/531 (44%)	213 (92%)	19 (8%)	0	100	100
All	All	8067/14631 (55%)	7720 (96%)	338 (4%)	9 (0%)	49	83

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	A	1423	ASP
25	M	766	GLU
1	D	15	GLU
11	Q	802	LYS
11	Q	806	ASP
22	A	121	SER
14	X	242	GLY
2	E	45	GLY
7	J	64	PRO

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	D	109/126 (86%)	107 (98%)	2 (2%)	51 68
2	E	191/192 (100%)	188 (98%)	3 (2%)	55 70
3	F	68/111 (61%)	67 (98%)	1 (2%)	57 72
4	G	146/153 (95%)	140 (96%)	6 (4%)	27 49
5	H	130/131 (99%)	126 (97%)	4 (3%)	35 56
6	I	105/112 (94%)	102 (97%)	3 (3%)	37 58
7	J	55/56 (98%)	55 (100%)	0	100 100
8	K	104/106 (98%)	103 (99%)	1 (1%)	68 78
9	L	44/55 (80%)	43 (98%)	1 (2%)	44 64
11	Q	763/1011 (76%)	756 (99%)	7 (1%)	70 79
13	W	260/260 (100%)	258 (99%)	2 (1%)	73 80
14	X	48/467 (10%)	47 (98%)	1 (2%)	47 65
15	Y	102/105 (97%)	101 (99%)	1 (1%)	68 78
16	Z	381/940 (40%)	378 (99%)	3 (1%)	73 80
17	a	86/110 (78%)	86 (100%)	0	100 100
17	e	82/110 (74%)	82 (100%)	0	100 100
18	b	64/79 (81%)	64 (100%)	0	100 100
18	f	64/79 (81%)	64 (100%)	0	100 100
19	c	82/104 (79%)	82 (100%)	0	100 100
19	g	82/104 (79%)	82 (100%)	0	100 100
20	d	79/105 (75%)	79 (100%)	0	100 100
20	h	76/105 (72%)	76 (100%)	0	100 100
21	j	14/929 (2%)	13 (93%)	1 (7%)	13 35
22	A	1225/1747 (70%)	1202 (98%)	23 (2%)	50 67
23	B	987/1027 (96%)	948 (96%)	39 (4%)	28 49
24	C	235/252 (93%)	232 (99%)	3 (1%)	61 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	M	826/1524 (54%)	819 (99%)	7 (1%)	73 80
27	O	226/1017 (22%)	225 (100%)	1 (0%)	84 84
28	R	170/625 (27%)	168 (99%)	2 (1%)	63 75
29	U	65/590 (11%)	65 (100%)	0	100 100
30	V	144/462 (31%)	142 (99%)	2 (1%)	59 72
All	All	7013/12794 (55%)	6900 (98%)	113 (2%)	54 70

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	31	THR
1	D	79	THR
2	E	36	THR
2	E	73	PHE
2	E	129	GLN
3	F	123	LEU
4	G	3	TYR
4	G	70	VAL
4	G	86	ASP
4	G	119	PHE
4	G	166	ASP
4	G	171	VAL
5	H	15	ILE
5	H	37	MET
5	H	100	GLU
5	H	116	VAL
6	I	46	GLN
6	I	51	SER
6	I	124	THR
8	K	27	VAL
9	L	34	ILE
11	Q	263	THR
11	Q	293	LEU
11	Q	531	VAL
11	Q	674	ARG
11	Q	698	ILE
11	Q	817	CYS
11	Q	820	LEU
13	W	112	LEU
13	W	240	PHE

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Mol	Chain	Res	Type
14	X	213	PHE
15	Y	115	ILE
16	Z	480	VAL
16	Z	545	GLN
16	Z	550	ILE
21	j	946	GLU
22	A	67	ARG
22	A	90	LEU
22	A	250	VAL
22	A	276	LEU
22	A	283	ILE
22	A	382	ARG
22	A	419	ILE
22	A	555	LEU
22	A	567	LEU
22	A	674	THR
22	A	811	ILE
22	A	908	THR
22	A	942	VAL
22	A	1007	ILE
22	A	1124	LEU
22	A	1128	ILE
22	A	1129	ASN
22	A	1160	ARG
22	A	1166	LEU
22	A	1210	TRP
22	A	1351	ASP
22	A	1423	ASP
22	A	1456	GLU
23	B	21	LEU
23	B	23	GLN
23	B	56	GLN
23	B	66	ASP
23	B	90	GLN
23	B	115	LEU
23	B	176	GLU
23	B	180	ASP
23	B	218	THR
23	B	276	LEU
23	B	285	LEU
23	B	307	GLU
23	B	332	LYS

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Mol	Chain	Res	Type
23	B	371	ARG
23	B	386	ASP
23	B	388	TYR
23	B	411	LEU
23	B	440	ILE
23	B	547	GLU
23	B	576	ILE
23	B	607	ILE
23	B	626	LEU
23	B	647	GLU
23	B	649	ASN
23	B	665	ILE
23	B	685	LYS
23	B	687	VAL
23	B	690	CYS
23	B	731	GLN
23	B	738	THR
23	B	743	ARG
23	B	759	VAL
23	B	838	GLN
23	B	848	LEU
23	B	909	VAL
23	B	931	ILE
23	B	995	GLU
23	B	1006	VAL
23	B	1048	TYR
24	C	5	ASN
24	C	75	SER
24	C	169	PHE
25	M	400	ASP
25	M	606	LEU
25	M	693	TYR
25	M	877	LEU
25	M	912	GLN
25	M	1134	TYR
25	M	1237	THR
27	O	2029	SER
28	R	507	PRO
28	R	570	TRP
30	V	66	LEU
30	V	100	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87)

such sidechains are listed below:

Mol	Chain	Res	Type
1	D	102	ASN
2	E	30	GLN
2	E	133	GLN
4	G	24	ASN
5	H	46	GLN
5	H	130	ASN
5	H	133	HIS
8	K	29	ASN
8	K	69	HIS
11	Q	151	GLN
11	Q	278	HIS
11	Q	373	ASN
11	Q	564	HIS
11	Q	762	GLN
11	Q	860	GLN
13	W	173	ASN
13	W	184	HIS
15	Y	27	GLN
15	Y	35	ASN
16	Z	232	GLN
16	Z	425	ASN
16	Z	477	HIS
16	Z	541	GLN
16	Z	545	GLN
16	Z	559	GLN
16	Z	581	ASN
16	Z	625	HIS
17	a	69	GLN
20	d	49	HIS
20	d	109	HIS
17	e	69	GLN
20	h	49	HIS
22	A	96	HIS
22	A	143	HIS
22	A	289	GLN
22	A	295	GLN
22	A	301	HIS
22	A	320	ASN
22	A	341	GLN
22	A	423	ASN
22	A	742	ASN
22	A	791	GLN

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Mol	Chain	Res	Type
22	A	804	HIS
22	A	1005	HIS
22	A	1032	GLN
22	A	1044	HIS
22	A	1101	GLN
22	A	1422	GLN
23	B	52	GLN
23	B	117	ASN
23	B	175	ASN
23	B	188	ASN
23	B	254	GLN
23	B	642	GLN
23	B	649	ASN
23	B	654	GLN
23	B	725	GLN
23	B	825	GLN
23	B	930	GLN
23	B	1021	HIS
23	B	1030	ASN
23	B	1040	GLN
23	B	1049	GLN
23	B	1053	HIS
23	B	1060	HIS
23	B	1117	HIS
24	C	6	GLN
24	C	32	ASN
24	C	111	GLN
24	C	260	GLN
24	C	262	GLN
25	M	323	ASN
25	M	389	HIS
25	M	517	GLN
25	M	683	GLN
25	M	751	ASN
25	M	762	GLN
25	M	792	HIS
25	M	876	GLN
25	M	929	GLN
25	M	1151	ASN
27	O	1498	GLN
27	O	1535	ASN
27	O	1541	ASN

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Mol	Chain	Res	Type
27	O	1667	GLN
28	R	488	ASN
28	R	588	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	P	21/46 (45%)	9 (42%)	5 (23%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	P	27	A
10	P	28	A
10	P	29	C
10	P	30	C
10	P	34	G
10	P	35	A
10	P	36	G
10	P	37	G
10	P	39	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	P	26	U
10	P	34	G
10	P	35	A
10	P	36	G
10	P	38	G

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	299:GLU	C	310:ASN	N	12.62

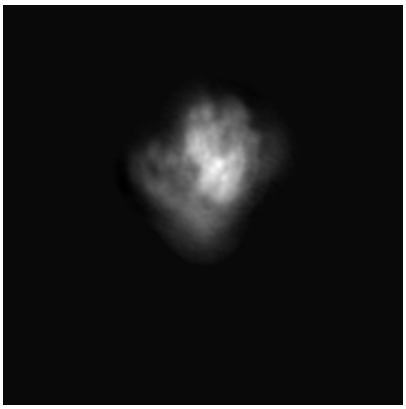
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-54401. These allow visual inspection of the internal detail of the map and identification of artifacts.

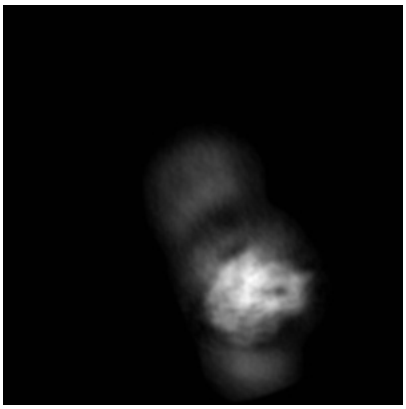
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

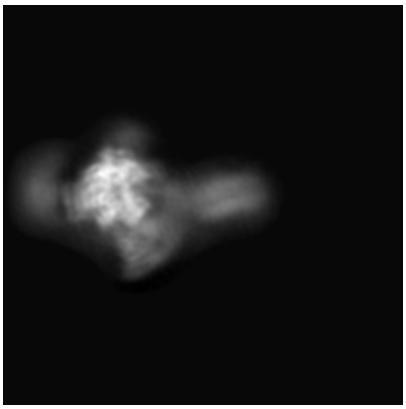
6.1.1 Primary map



X

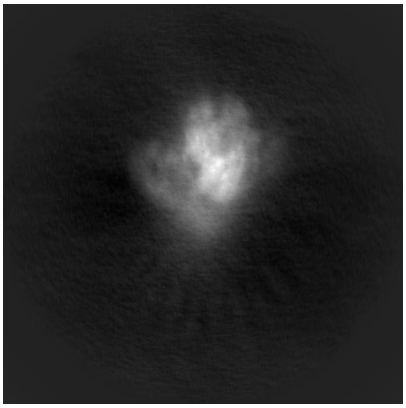


Y

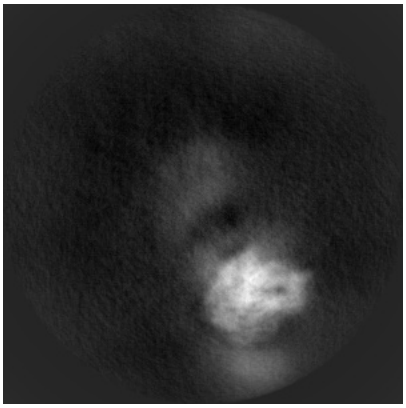


Z

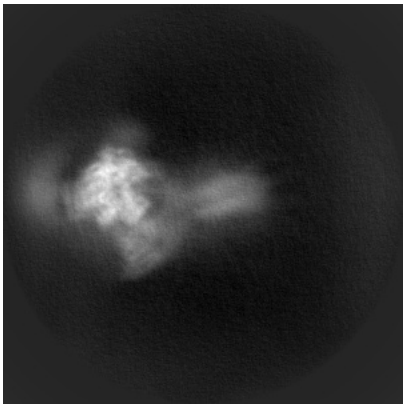
6.1.2 Raw map



X



Y

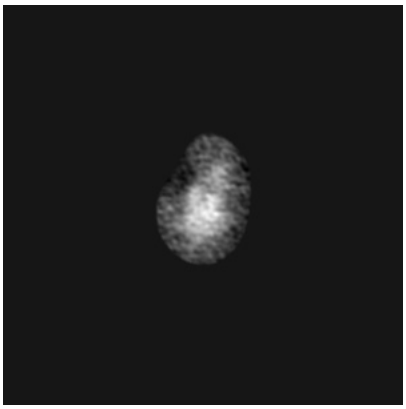


Z

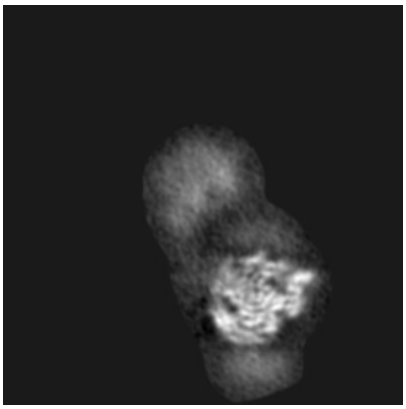
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

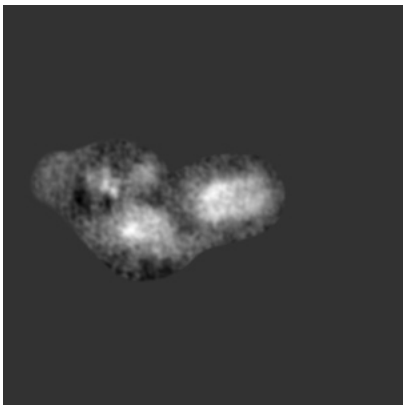
6.2.1 Primary map



X Index: 256

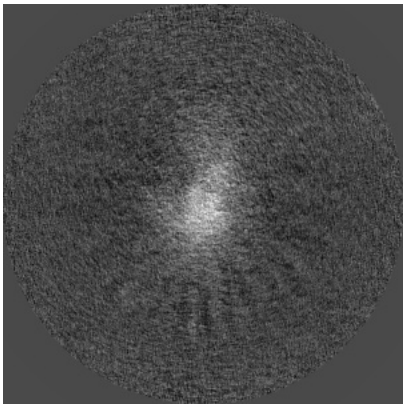


Y Index: 256

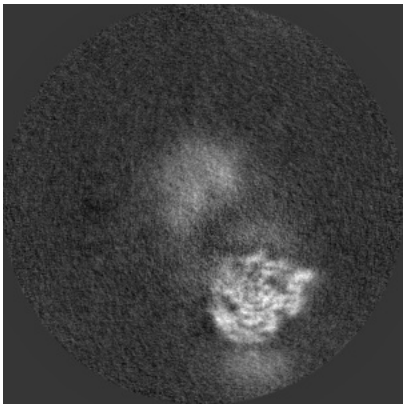


Z Index: 256

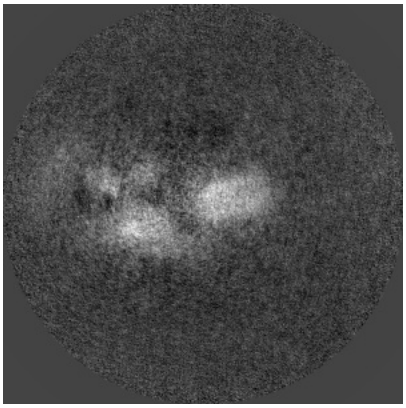
6.2.2 Raw map



X Index: 256



Y Index: 256

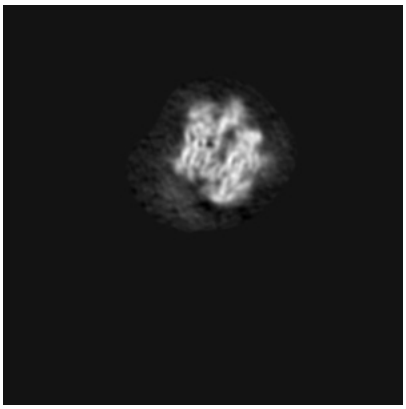


Z Index: 256

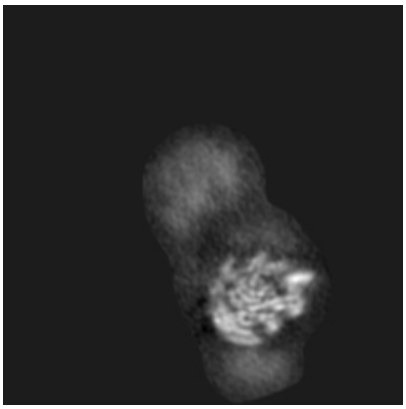
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

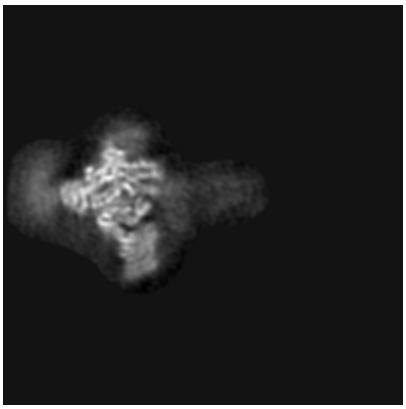
6.3.1 Primary map



X Index: 134

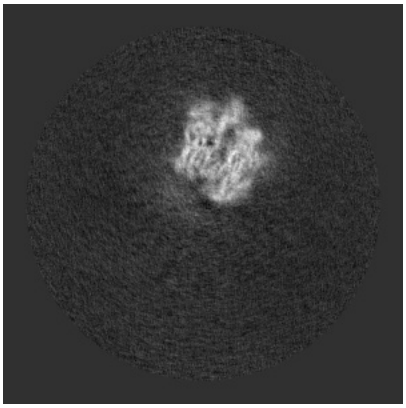


Y Index: 260

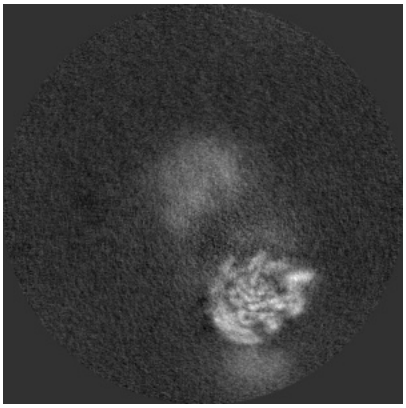


Z Index: 313

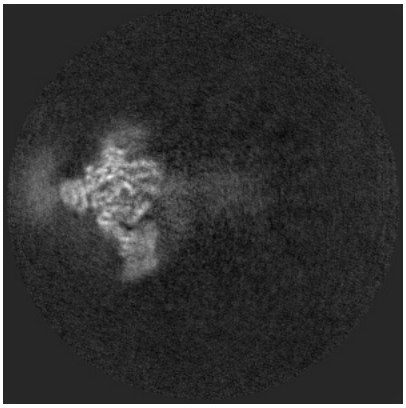
6.3.2 Raw map



X Index: 134



Y Index: 260

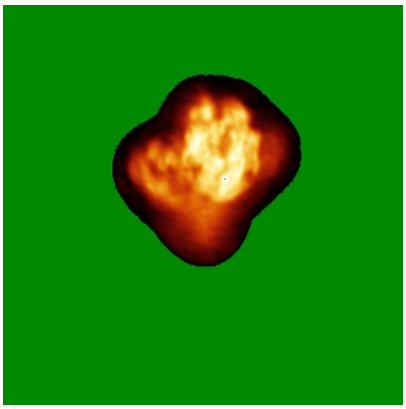


Z Index: 312

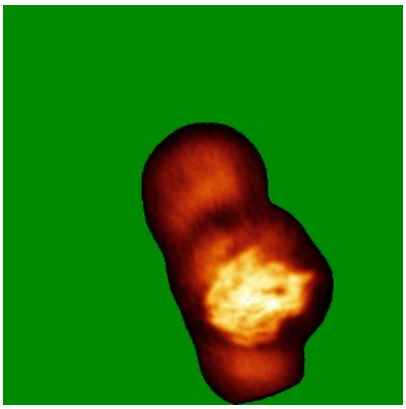
The images above show the largest variance slices of the map in three orthogonal directions.

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

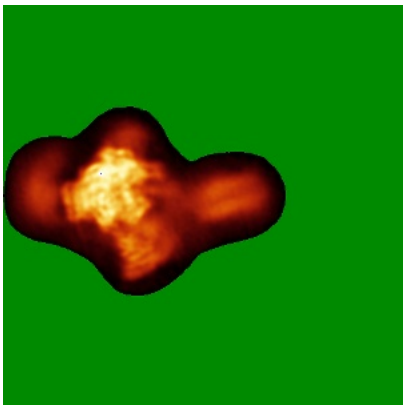
6.4.1 Primary map



X

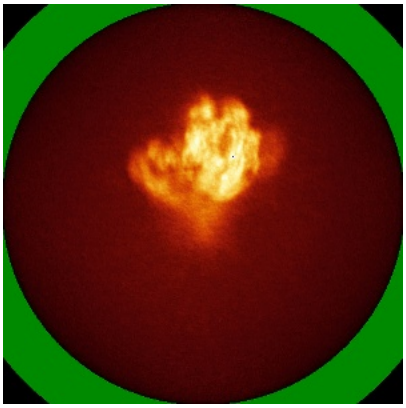


Y

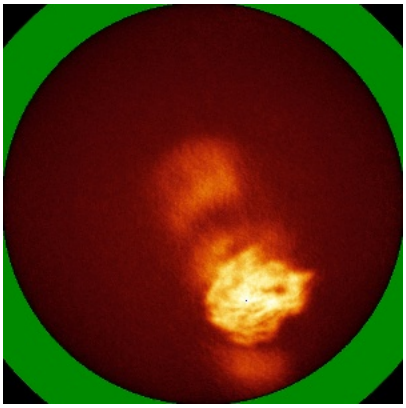


Z

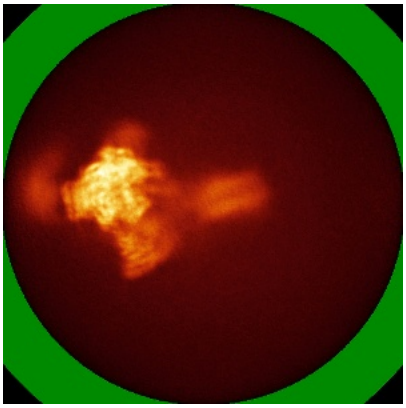
6.4.2 Raw map



X



Y

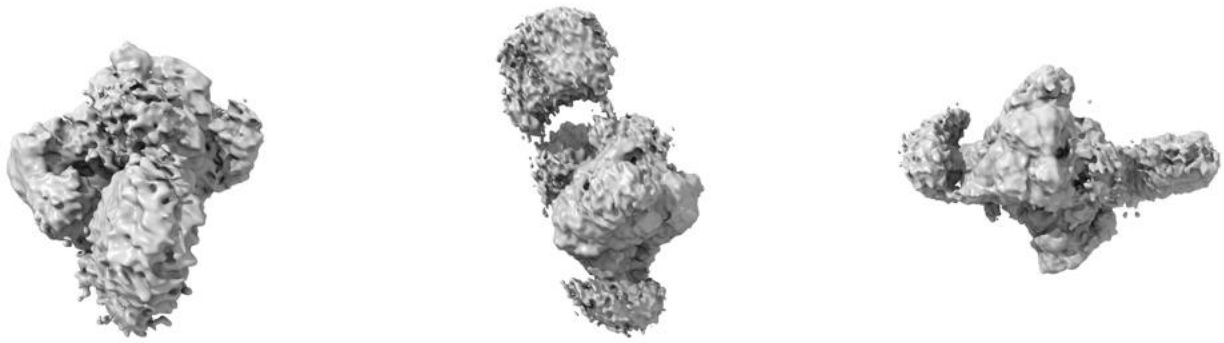


Z

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 0.008. 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.

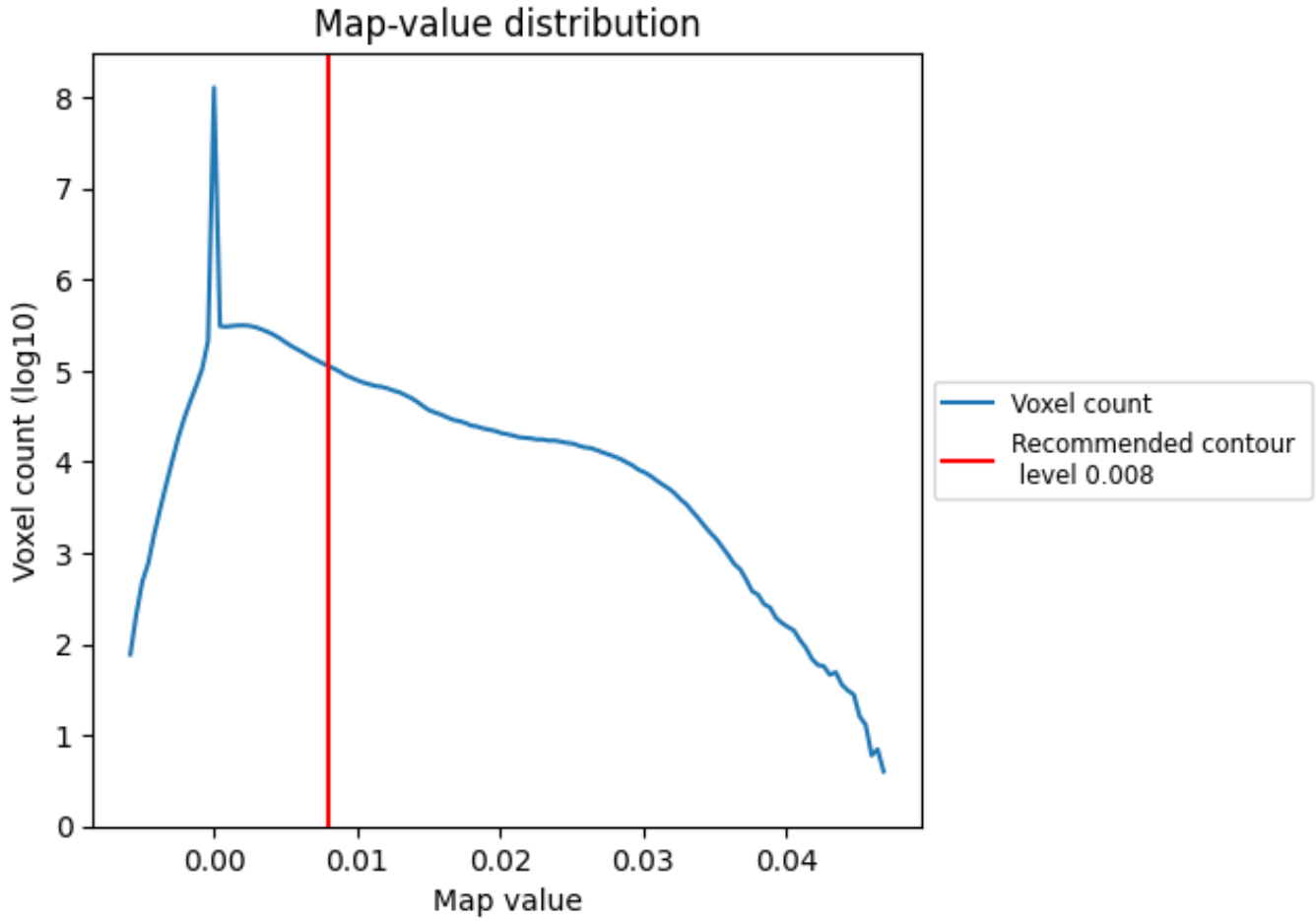
6.6 Mask visualisation (i)

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

7 Map analysis

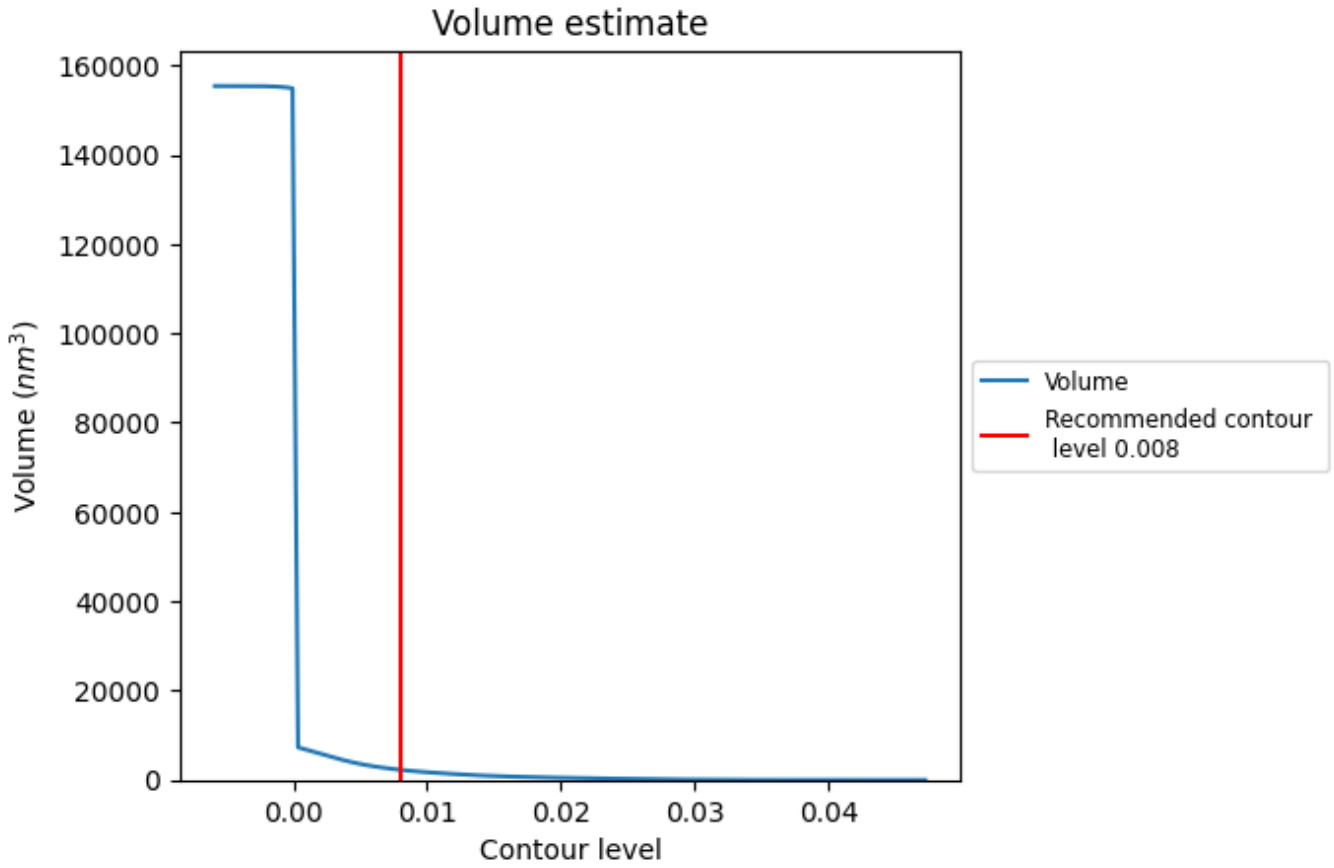
This section contains the results of statistical analysis of the map.

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.

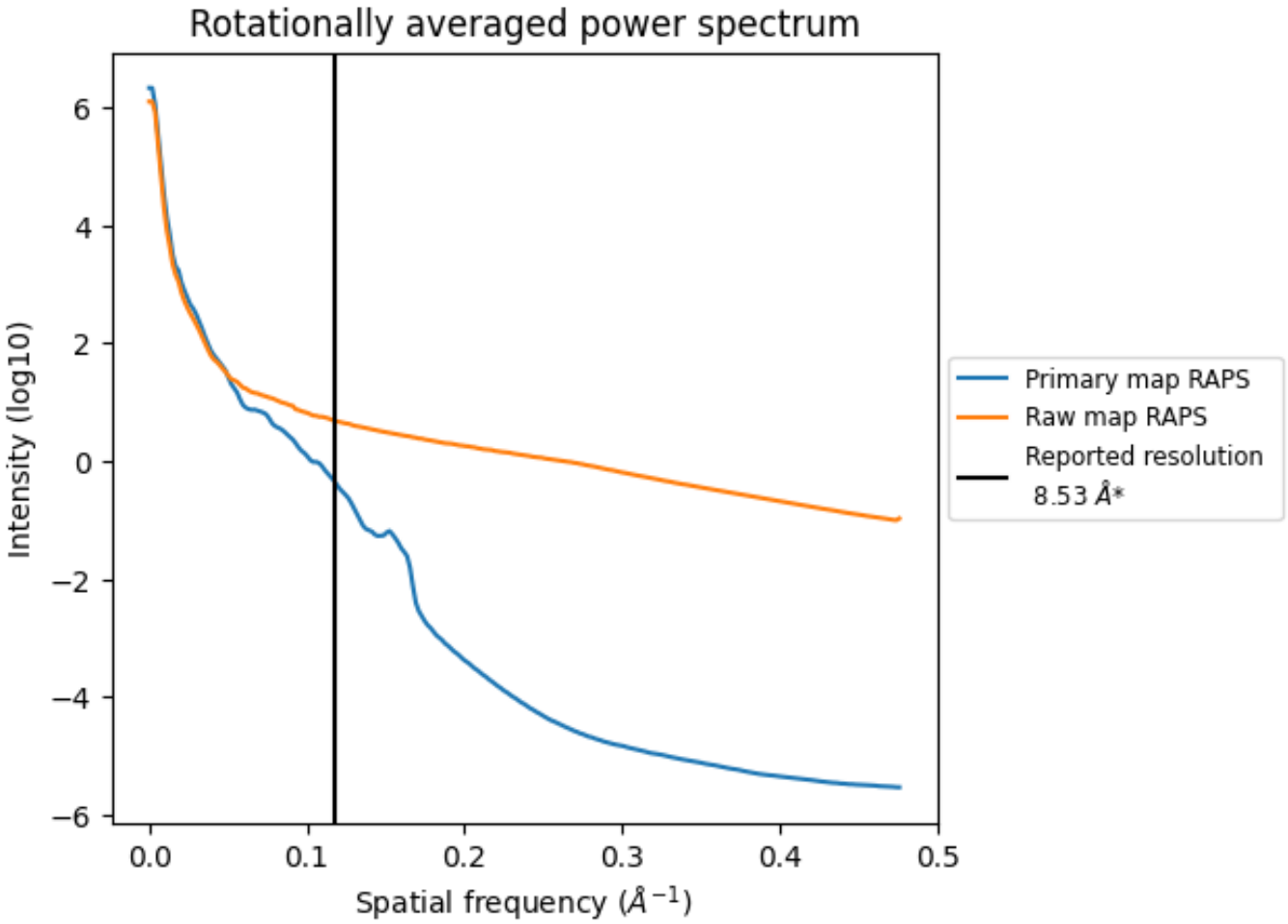
7.2 Volume estimate



The volume at the recommended contour level is 2269 nm^3; this corresponds to an approximate mass of 2049 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)

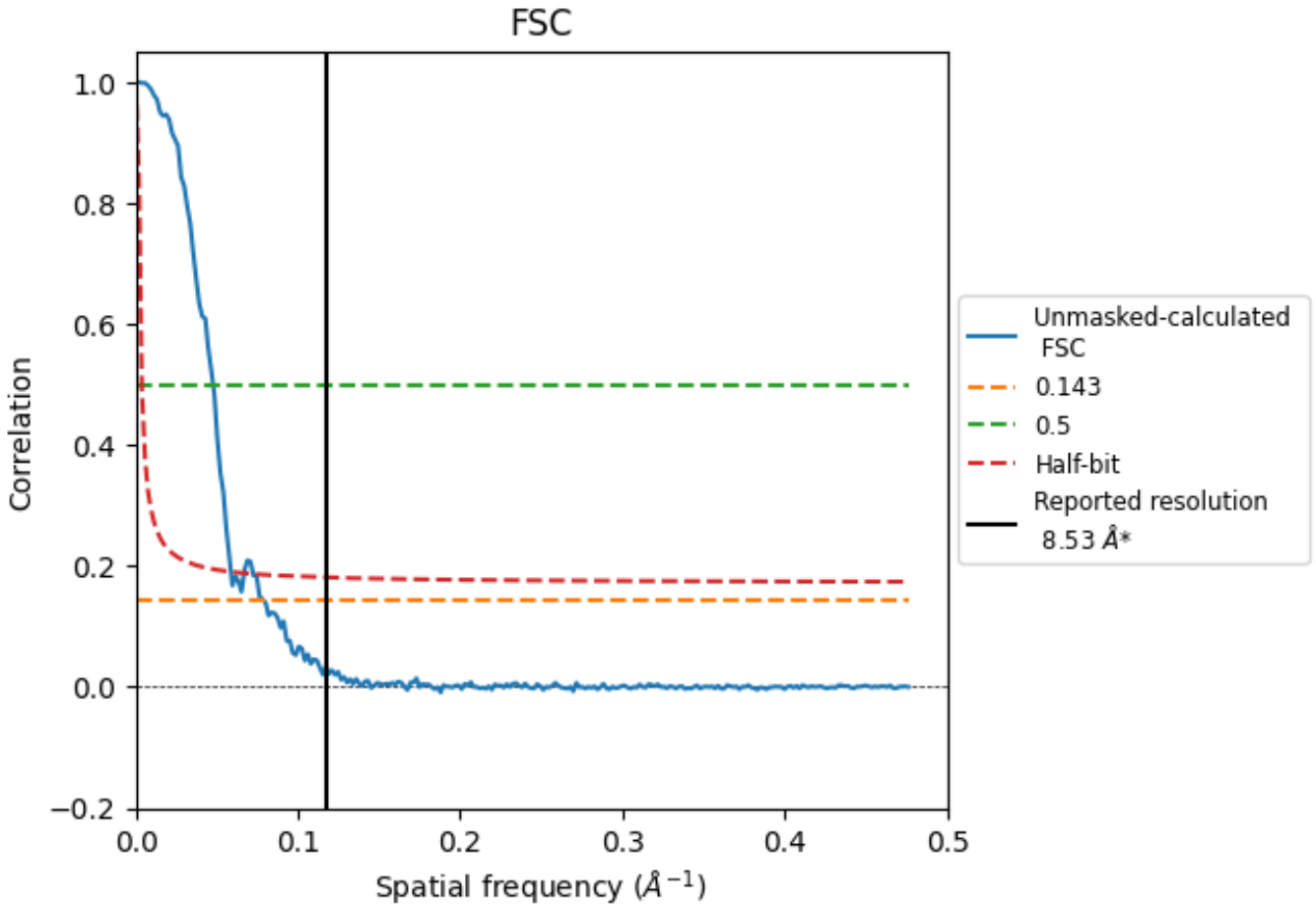


*Reported resolution corresponds to spatial frequency of 0.117 Å^{-1}

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 0.117 Å^{-1}

8.2 Resolution estimates (i)

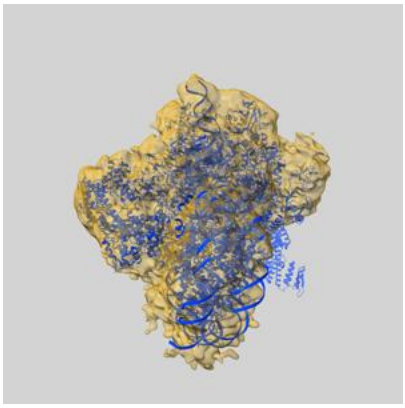
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	12.71	21.01	17.06

*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 12.71 differs from the reported value 8.53 by more than 10 %

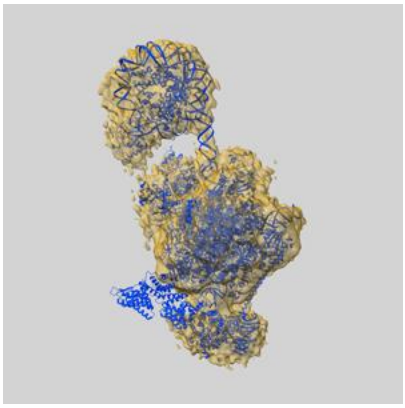
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-54401 and PDB model 9RZE. Per-residue inclusion information can be found in section 3 on page 12.

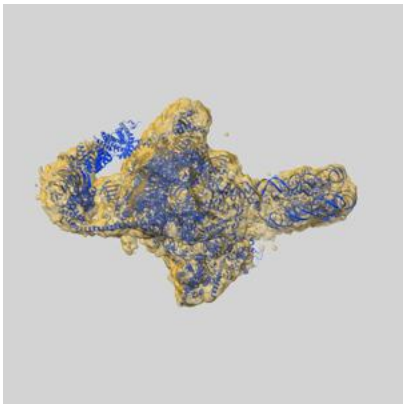
9.1 Map-model overlay



X



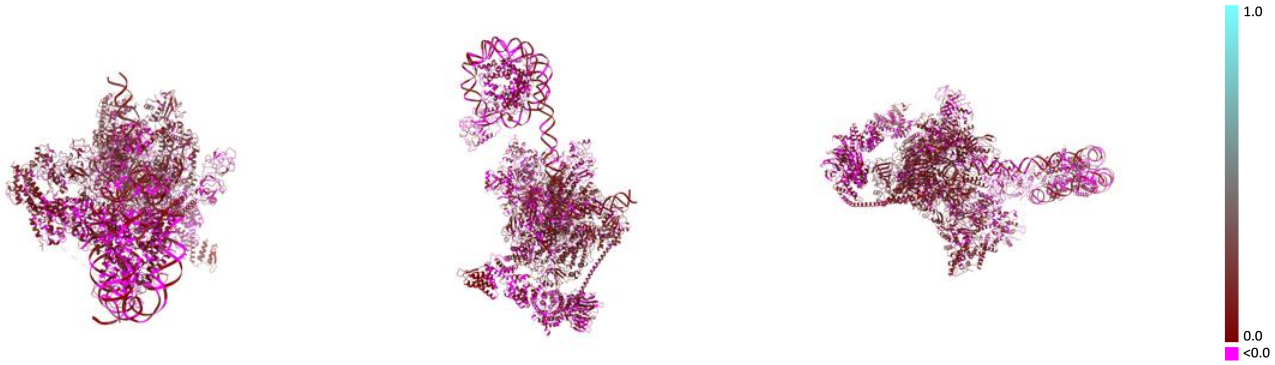
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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.

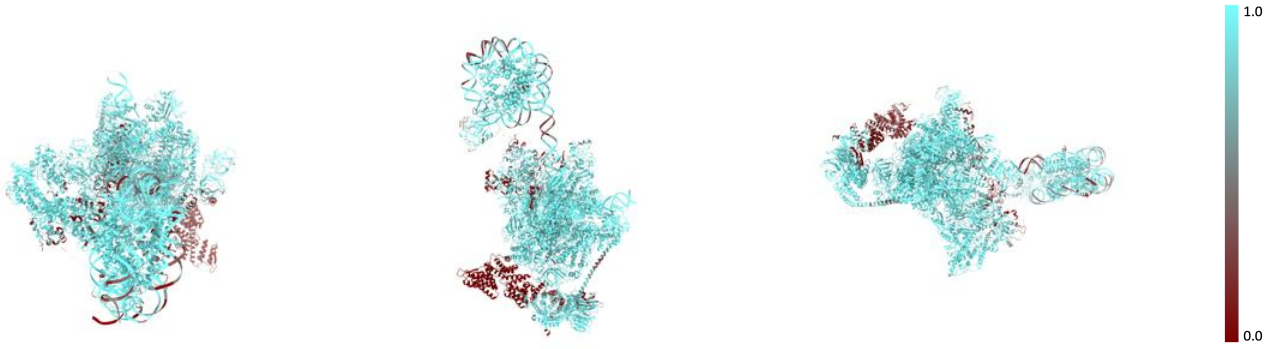
9.2 Q-score mapped to coordinate model



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.

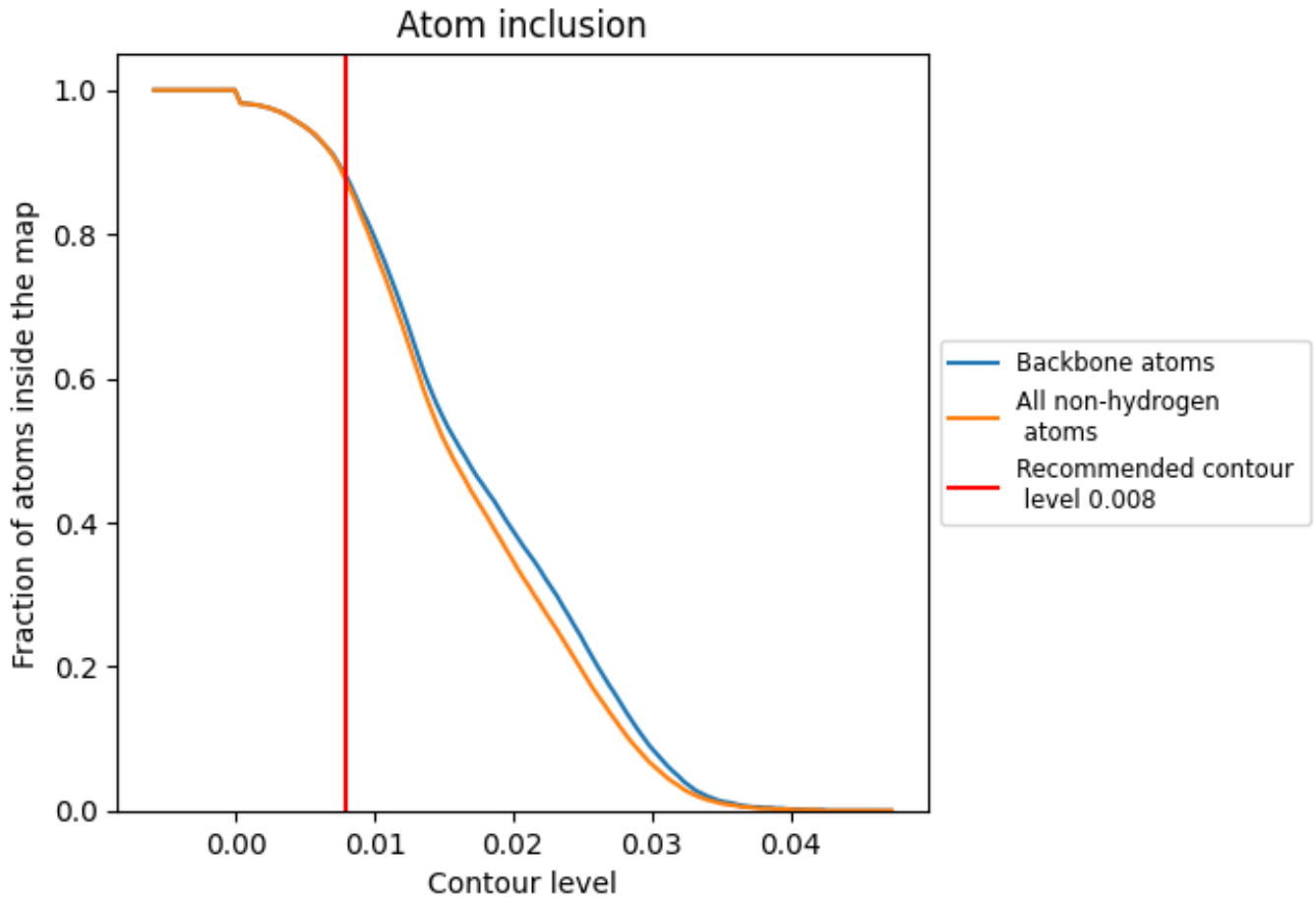
9.3 Atom inclusion mapped to coordinate model



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 (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8730	0.0680
A	0.9990	0.1200
B	0.9990	0.1010
C	0.9920	0.0810
D	0.9940	0.0950
E	1.0000	0.1270
F	0.9930	0.1350
G	0.9980	0.0970
H	0.9960	0.0940
I	0.9950	0.1020
J	1.0000	0.1090
K	0.9930	0.1030
L	1.0000	0.0670
M	0.9140	0.0580
N	0.8080	0.0570
O	0.7950	0.0160
P	1.0000	0.1410
Q	0.4950	0.0300
R	0.5560	0.0270
T	0.8270	0.0610
U	0.8200	0.0220
V	0.6460	-0.0010
W	0.8290	0.0290
X	0.7410	0.0030
Y	0.8700	0.0180
Z	0.7910	0.0380
a	0.9950	0.0040
b	1.0000	0.0260
c	0.9730	0.0380
d	0.9290	0.0070
e	0.9480	0.0200
f	0.9970	0.0480
g	0.9960	0.0510
h	0.9230	0.0270
j	1.0000	0.0740