Full wwPDB EM Validation Report ⓘ

Jan 7, 2025 – 12:47 pm GMT

PDB ID	:	9FSP
EMDB ID	:	EMD-50731
Title	:	RNA Polymerase III Class III Open Pre-initation Complex 2 (OC2)
Authors	:	Shah, S.Z.; Ramsay, E.P.; Cecatiello, V.; Perry, T.N.; Vannini, A.
Deposited on	:	2024-06-21
Resolution	:	3.39 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:

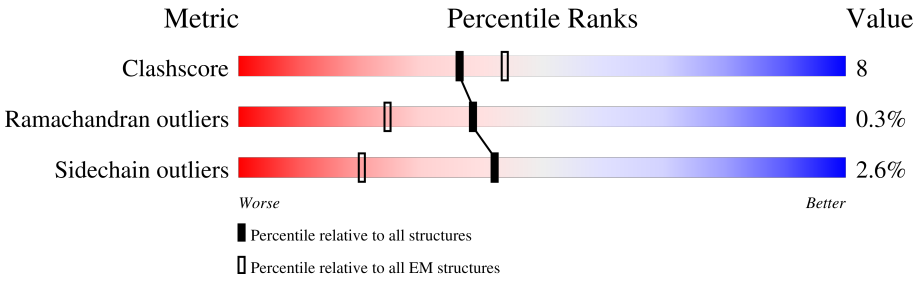
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.39 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	1390	82% 16%
2	B	1133	85% 11%
3	C	534	79% 16%
4	D	398	5% 39% 6% 53%
5	E	708	6% 47% 9% 44%
6	F	316	6% 56% 30% 8%
7	G	223	24% 12% 63%
8	H	204	82% 11% 7%

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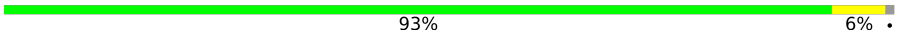
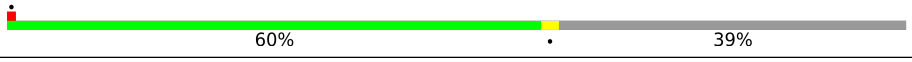
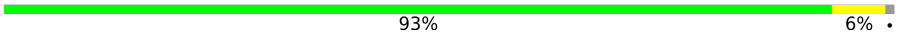
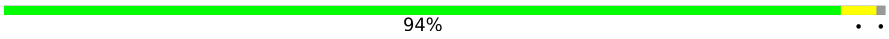
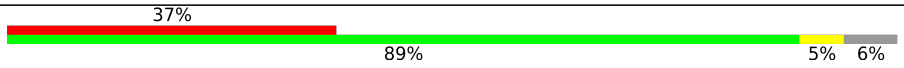
Mol	Chain	Length	Quality of chain
9	I	148	
10	J	108	
11	K	346	
12	L	133	
13	M	210	
14	N	127	
15	O	150	
16	P	58	
17	Q	67	
18	R	200	
19	S	419	
20	T	484	
21	U	368	
22	W	1519	
23	X	98	
24	Y	98	
25	Z	411	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	SF4	F	401	-	-	X	-

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 56808 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1381	10848	6876	1891	2008	73	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1097	8680	5499	1516	1597	68	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase III subunit RPC3.

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

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	186	1448	907	251	281	9	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	400	3211	2038	557	596	20	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	302	2395	1512	410	457	16	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	82	Total	C	N	O	S	0	0
			717	463	121	127	6		

- Molecule 8 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	189	Total	C	N	O	S	0	0
			1509	979	237	286	7		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	124	Total	C	N	O	S	0	0
			1001	626	174	198	3		

- Molecule 10 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	107	Total	C	N	O	S	0	0
			849	525	157	154	13		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	107	Total	C	N	O	S	0	0
			856	531	153	165	7		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	78	Total	C	N	O	S	0	0
			627	402	106	114	5		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 17 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 18 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	178	Total	C	N	O	S	0	0
			1402	909	246	240	7		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	140	MET	-	initiating methionine	UNP P20226
R	141	ALA	-	expression tag	UNP P20226
R	142	HIS	-	expression tag	UNP P20226
R	143	HIS	-	expression tag	UNP P20226
R	144	HIS	-	expression tag	UNP P20226
R	145	HIS	-	expression tag	UNP P20226
R	146	HIS	-	expression tag	UNP P20226
R	147	HIS	-	expression tag	UNP P20226
R	148	VAL	-	expression tag	UNP P20226
R	149	GLY	-	expression tag	UNP P20226
R	150	THR	-	expression tag	UNP P20226
R	151	LEU	-	expression tag	UNP P20226

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Chain	Residue	Modelled	Actual	Comment	Reference
R	152	GLU	-	expression tag	UNP P20226
R	153	VAL	-	expression tag	UNP P20226
R	154	LEU	-	expression tag	UNP P20226
R	155	PHE	-	expression tag	UNP P20226
R	156	GLN	-	expression tag	UNP P20226
R	157	GLY	-	expression tag	UNP P20226
R	158	PRO	-	expression tag	UNP P20226

- Molecule 19 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	361	Total	C	N	O	S	0	0
			2847	1789	506	530	22		

- Molecule 20 is a protein called Transcription factor TFIIIB component B" homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	78	Total	C	N	O	S	0	0
			665	430	117	115	3		

- Molecule 21 is a protein called snRNA-activating protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	141	Total	C	N	O	S	0	0
			1183	770	203	202	8		

- Molecule 22 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	242	Total	C	N	O	S	0	0
			2018	1264	370	378	6		

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-38	MET	-	initiating methionine	UNP Q5SXM2
W	-37	ALA	-	expression tag	UNP Q5SXM2
W	-36	SER	-	expression tag	UNP Q5SXM2
W	-35	TRP	-	expression tag	UNP Q5SXM2
W	-34	SER	-	expression tag	UNP Q5SXM2
W	-33	HIS	-	expression tag	UNP Q5SXM2

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Chain	Residue	Modelled	Actual	Comment	Reference
W	-32	PRO	-	expression tag	UNP Q5SXM2
W	-31	GLN	-	expression tag	UNP Q5SXM2
W	-30	PHE	-	expression tag	UNP Q5SXM2
W	-29	GLU	-	expression tag	UNP Q5SXM2
W	-28	LYS	-	expression tag	UNP Q5SXM2
W	-27	GLY	-	expression tag	UNP Q5SXM2
W	-26	GLY	-	expression tag	UNP Q5SXM2
W	-25	GLY	-	expression tag	UNP Q5SXM2
W	-24	SER	-	expression tag	UNP Q5SXM2
W	-23	GLY	-	expression tag	UNP Q5SXM2
W	-22	GLY	-	expression tag	UNP Q5SXM2
W	-21	GLY	-	expression tag	UNP Q5SXM2
W	-20	SER	-	expression tag	UNP Q5SXM2
W	-19	TRP	-	expression tag	UNP Q5SXM2
W	-18	SER	-	expression tag	UNP Q5SXM2
W	-17	HIS	-	expression tag	UNP Q5SXM2
W	-16	PRO	-	expression tag	UNP Q5SXM2
W	-15	GLN	-	expression tag	UNP Q5SXM2
W	-14	PHE	-	expression tag	UNP Q5SXM2
W	-13	GLU	-	expression tag	UNP Q5SXM2
W	-12	LYS	-	expression tag	UNP Q5SXM2
W	-11	GLY	-	expression tag	UNP Q5SXM2
W	-10	GLY	-	expression tag	UNP Q5SXM2
W	-9	GLY	-	expression tag	UNP Q5SXM2
W	-8	SER	-	expression tag	UNP Q5SXM2
W	-7	GLU	-	expression tag	UNP Q5SXM2
W	-6	ASN	-	expression tag	UNP Q5SXM2
W	-5	LEU	-	expression tag	UNP Q5SXM2
W	-4	TYR	-	expression tag	UNP Q5SXM2
W	-3	PHE	-	expression tag	UNP Q5SXM2
W	-2	GLN	-	expression tag	UNP Q5SXM2
W	-1	GLY	-	expression tag	UNP Q5SXM2
W	0	SER	-	expression tag	UNP Q5SXM2
W	1	ALA	-	expression tag	UNP Q5SXM2
W	1470	ALA	-	expression tag	UNP Q5SXM2
W	1471	HIS	-	expression tag	UNP Q5SXM2
W	1472	HIS	-	expression tag	UNP Q5SXM2
W	1473	HIS	-	expression tag	UNP Q5SXM2
W	1474	HIS	-	expression tag	UNP Q5SXM2
W	1475	HIS	-	expression tag	UNP Q5SXM2
W	1476	HIS	-	expression tag	UNP Q5SXM2
W	1477	HIS	-	expression tag	UNP Q5SXM2

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Chain	Residue	Modelled	Actual	Comment	Reference
W	1478	HIS	-	expression tag	UNP Q5SXM2
W	1479	HIS	-	expression tag	UNP Q5SXM2
W	1480	HIS	-	expression tag	UNP Q5SXM2

- Molecule 23 is a DNA chain called U6_2_Template.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	69	Total	C	N	O	P	0	0
			1403	672	246	416	69		

- Molecule 24 is a DNA chain called U6_2_Non template.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	67	Total	C	N	O	P	0	0
			1384	659	259	399	67		

- Molecule 25 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	385	Total	C	N	O	S	0	0
			3123	1977	533	591	22		

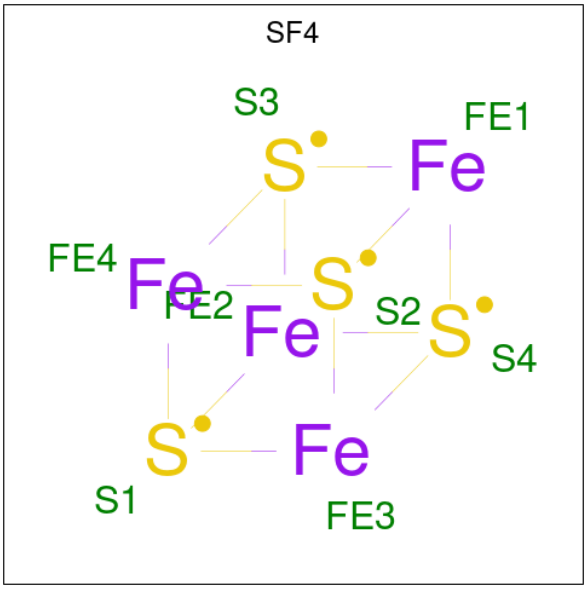
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Zn	0
			2	2	
26	B	1	Total	Zn	0
			1	1	
26	J	1	Total	Zn	0
			1	1	
26	P	1	Total	Zn	0
			1	1	
26	Q	1	Total	Zn	0
			1	1	
26	S	1	Total	Zn	0
			1	1	
26	Z	2	Total	Zn	0
			2	2	

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



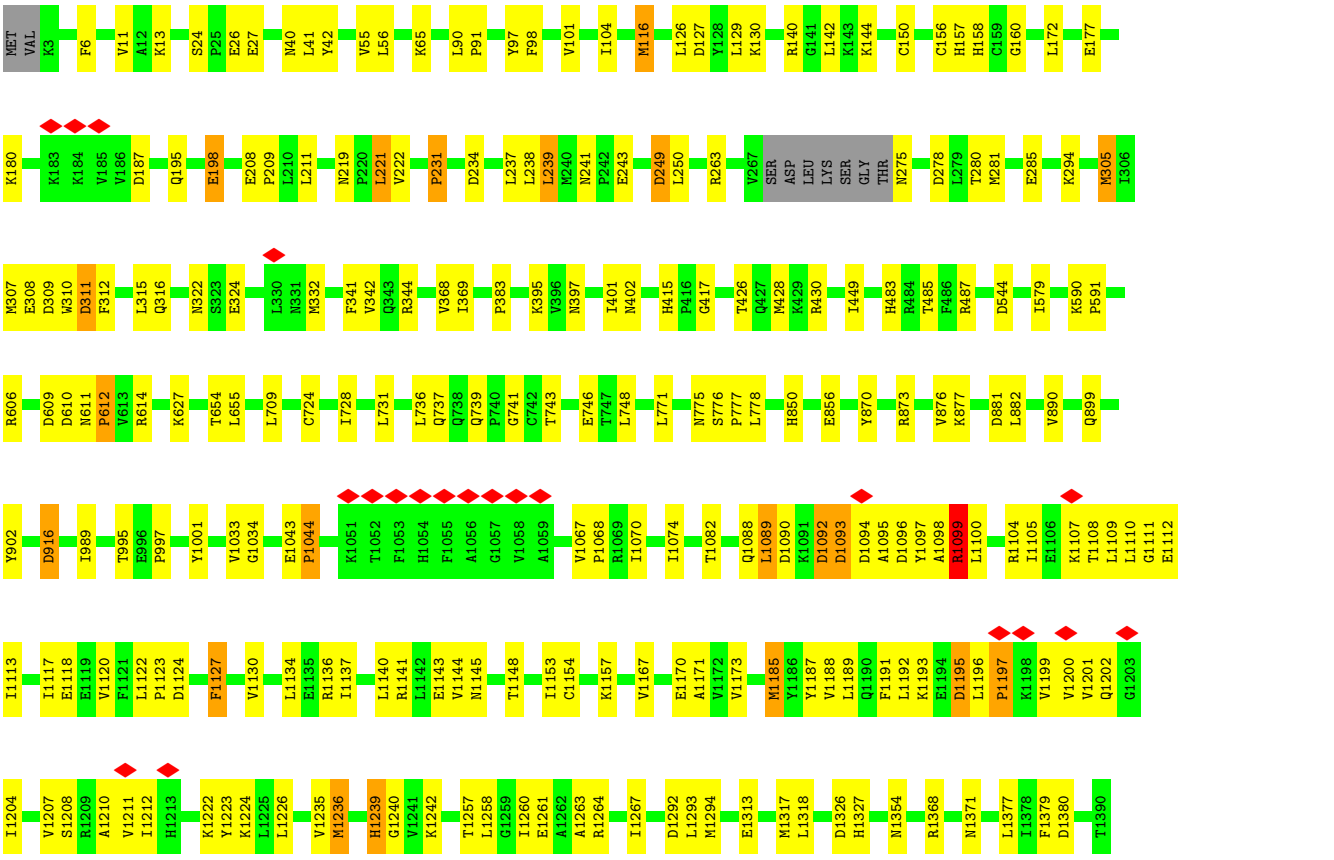
Mol	Chain	Residues	Atoms	AltConf
28	F	1	Total Fe S 8 4 4	0

3 Residue-property plots (i)

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

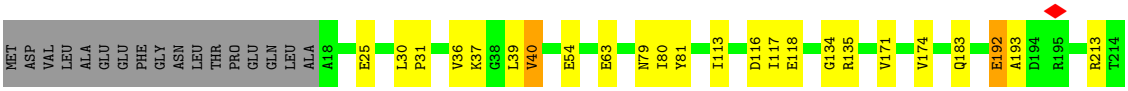
• Molecule 1: DNA-directed RNA polymerase III subunit RPC1

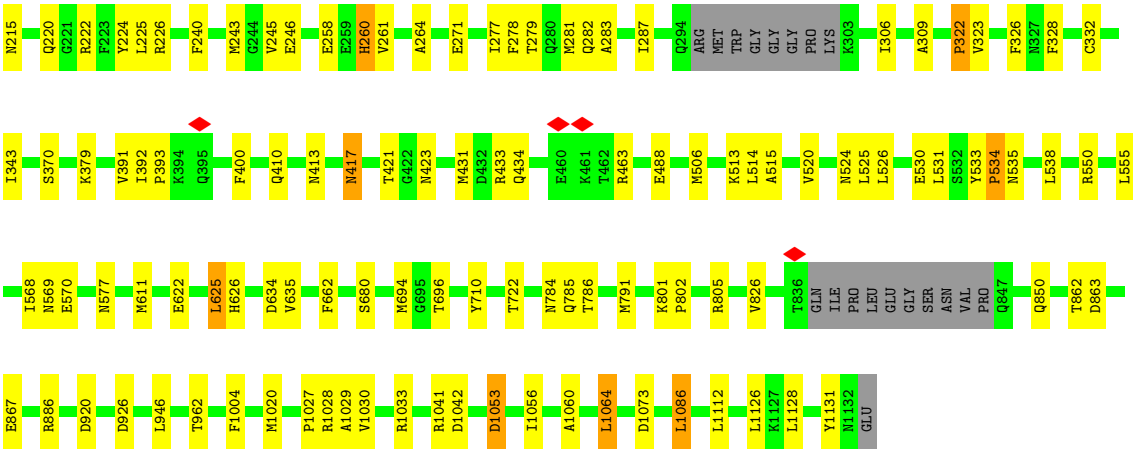
Chain A:



• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

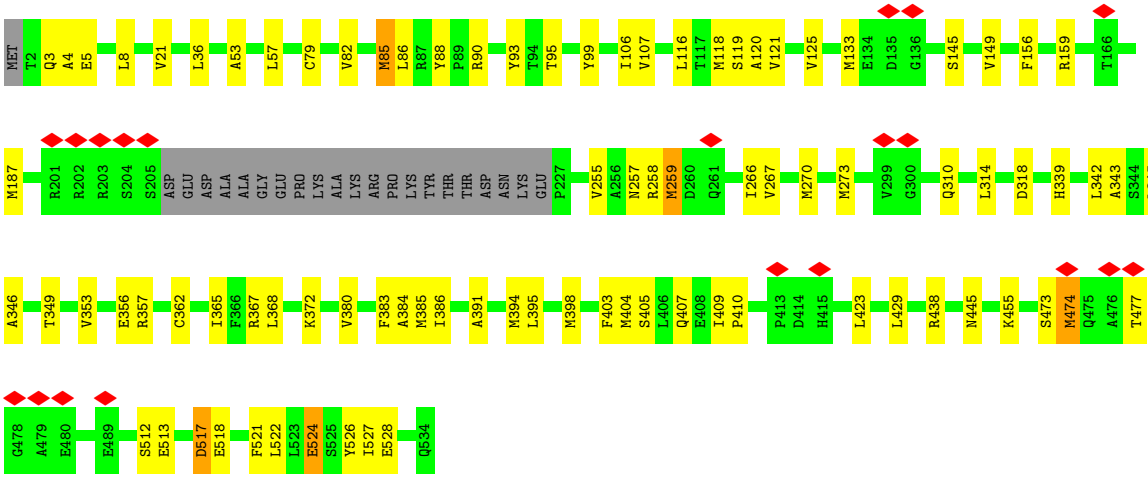
Chain B:





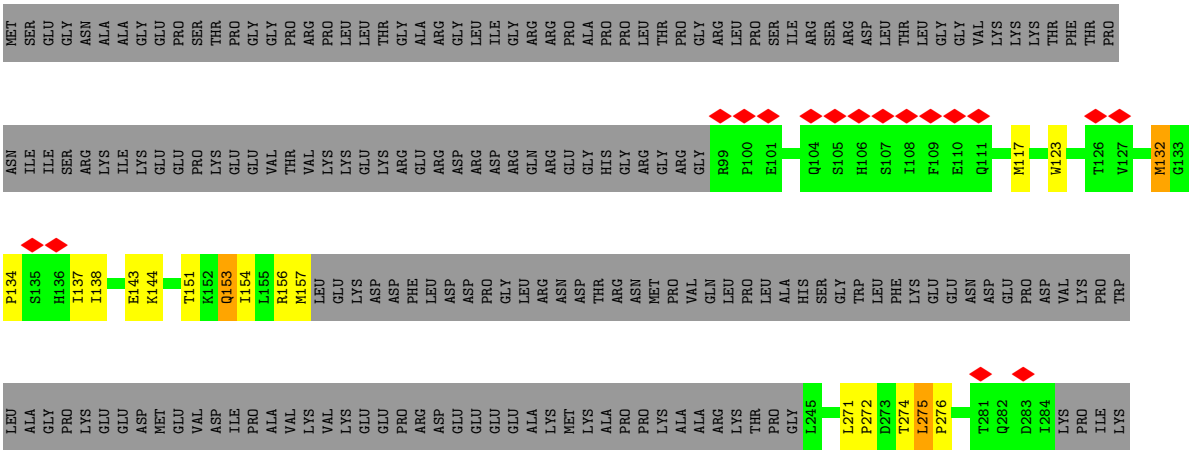
• Molecule 3: DNA-directed RNA polymerase III subunit RPC3

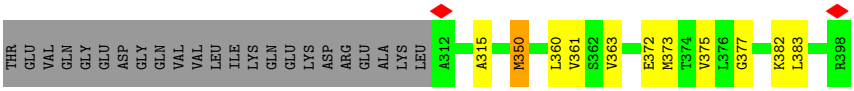
Chain C:



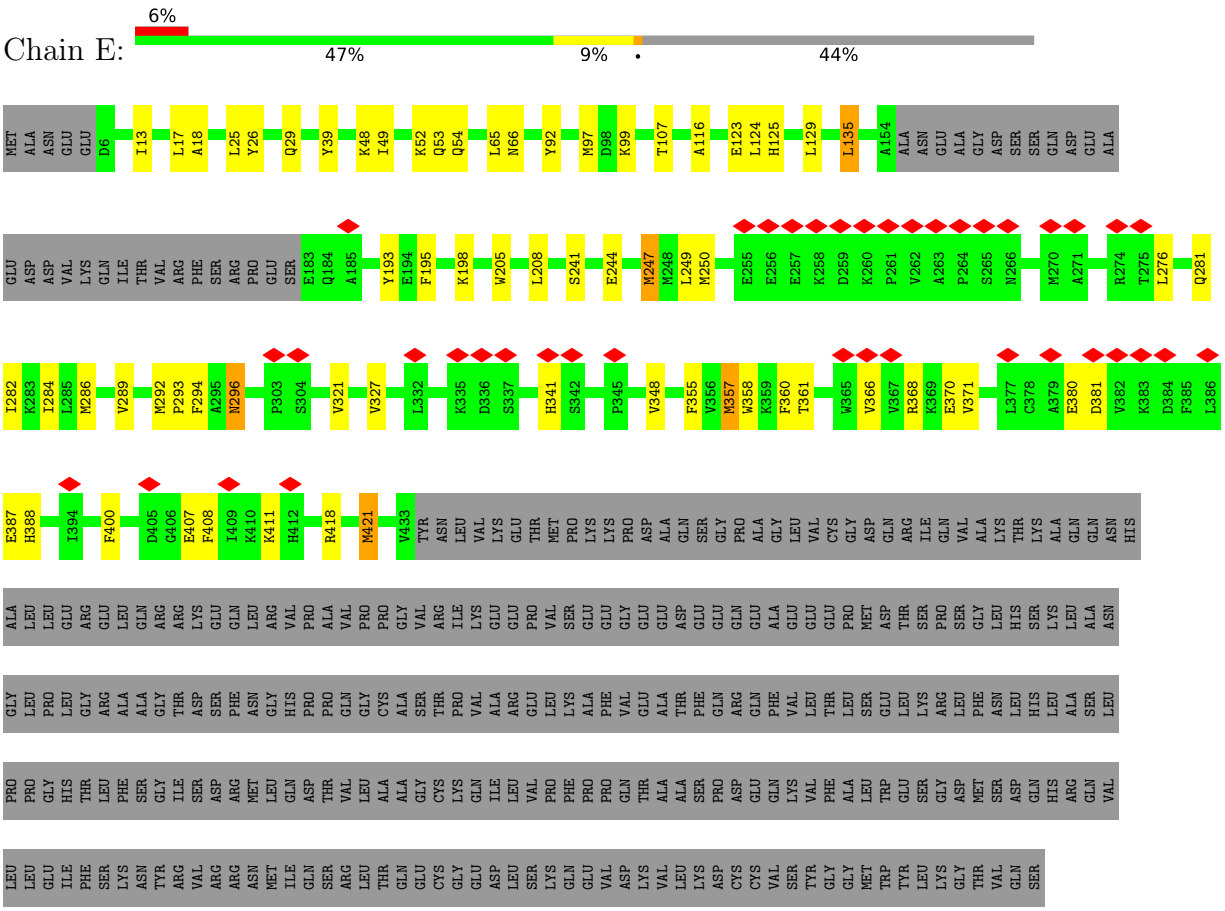
• Molecule 4: DNA-directed RNA polymerase III subunit RPC4

Chain D:

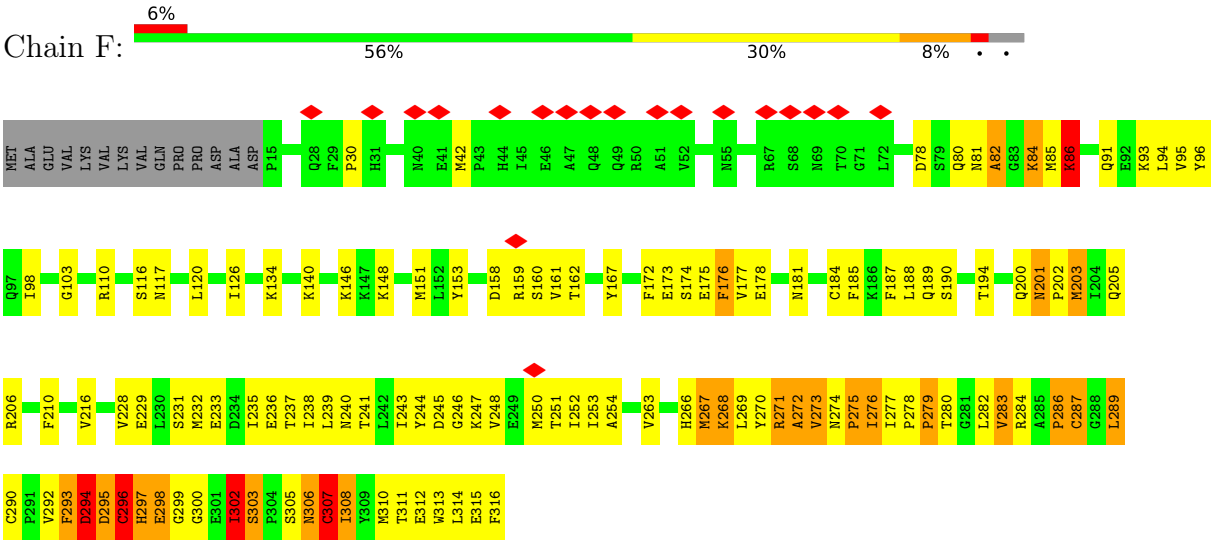




• Molecule 5: DNA-directed RNA polymerase III subunit RPC5

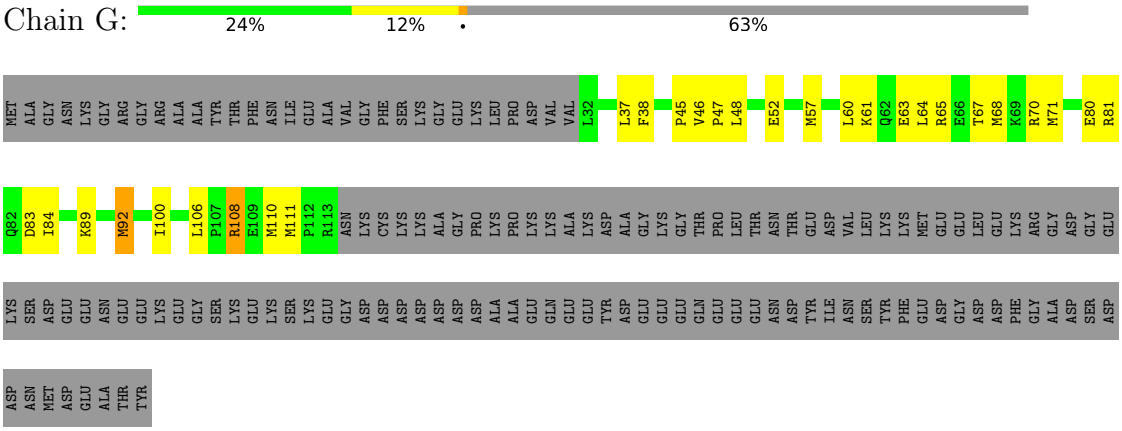


• Molecule 6: DNA-directed RNA polymerase III subunit RPC6



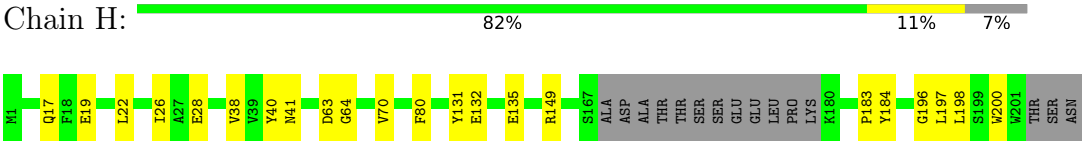
• Molecule 7: DNA-directed RNA polymerase III subunit RPC7

Chain G:



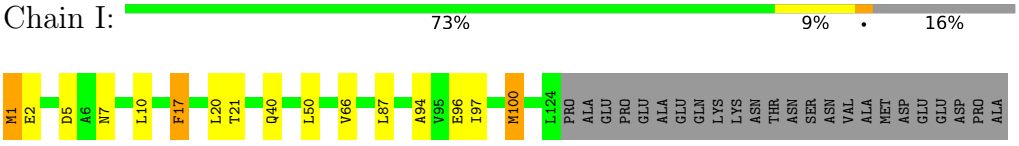
• Molecule 8: DNA-directed RNA polymerase III subunit RPC8

Chain H:



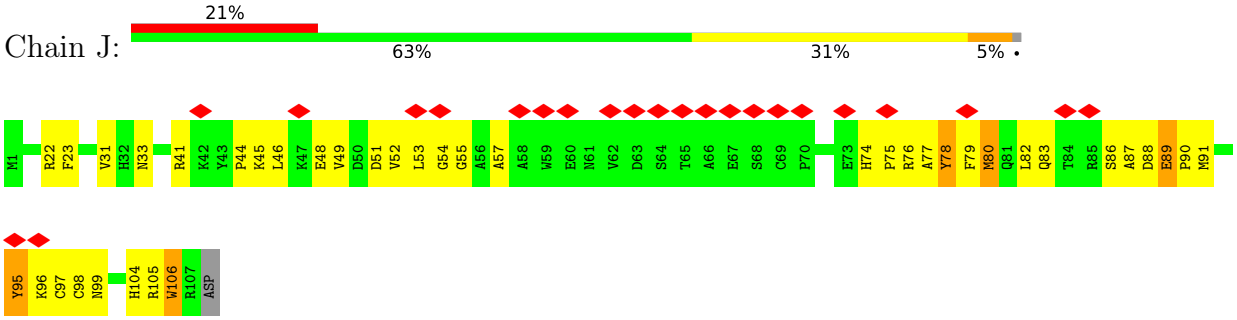
• Molecule 9: DNA-directed RNA polymerase III subunit RPC9

Chain I:



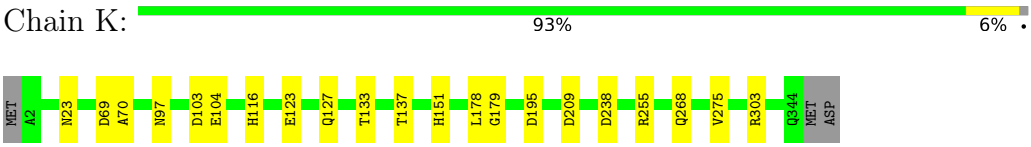
• Molecule 10: DNA-directed RNA polymerase III subunit RPC10

Chain J:



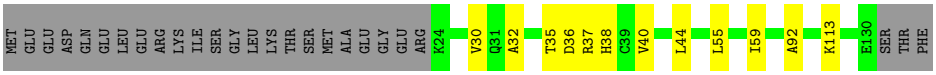
• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC1

Chain K:



• Molecule 12: DNA-directed RNA polymerases I and III subunit RPAC2

Chain L:

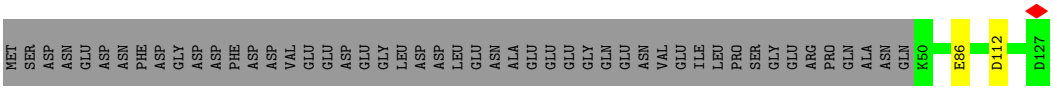


• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain M:

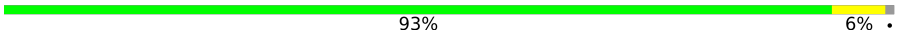
• Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC2

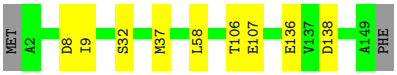
Chain N:



• Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain O:



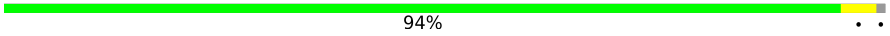


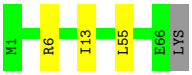
• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain P:

• Molecule 17: DNA-directed RNA polymerases I, II, and III subunit RPABC5

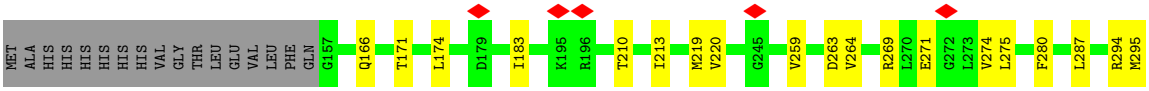
Chain Q:

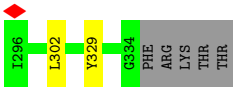




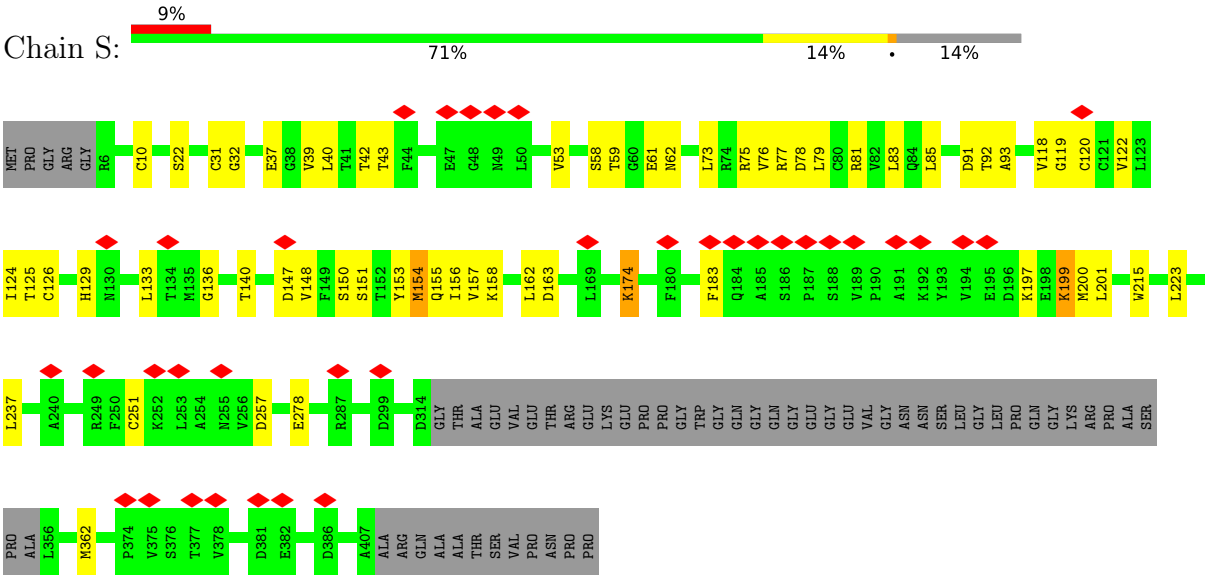
• Molecule 18: TATA-box-binding protein

Chain R:

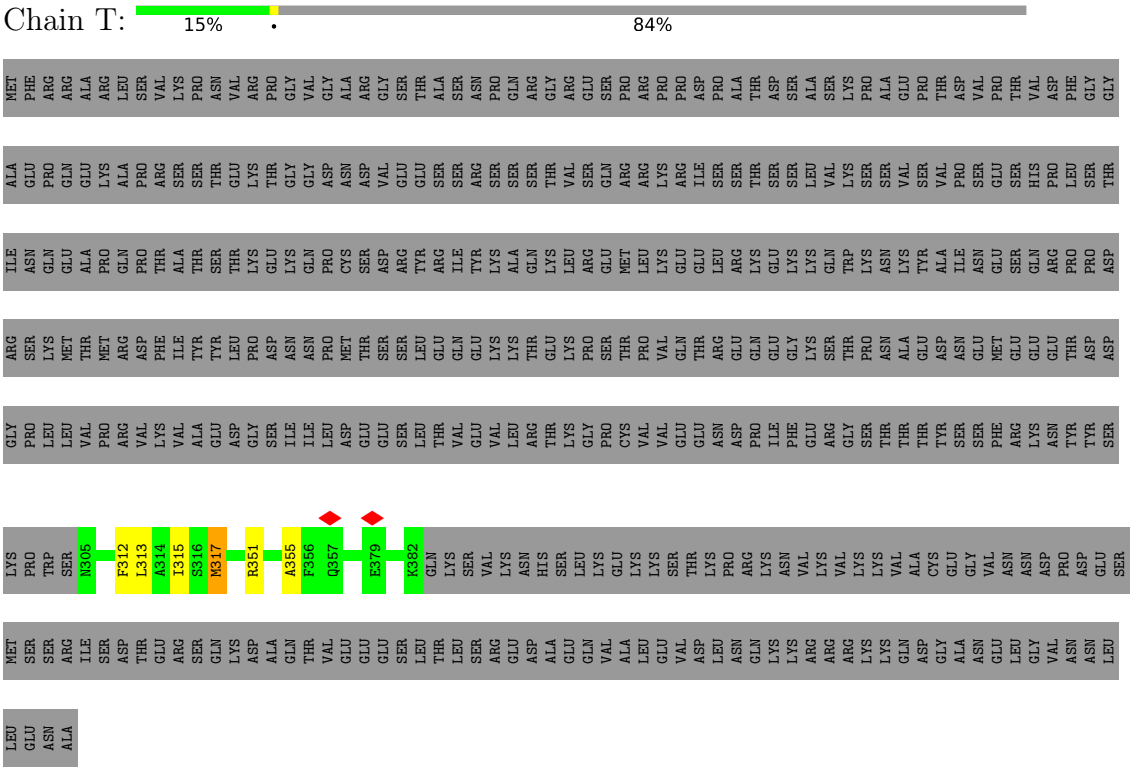




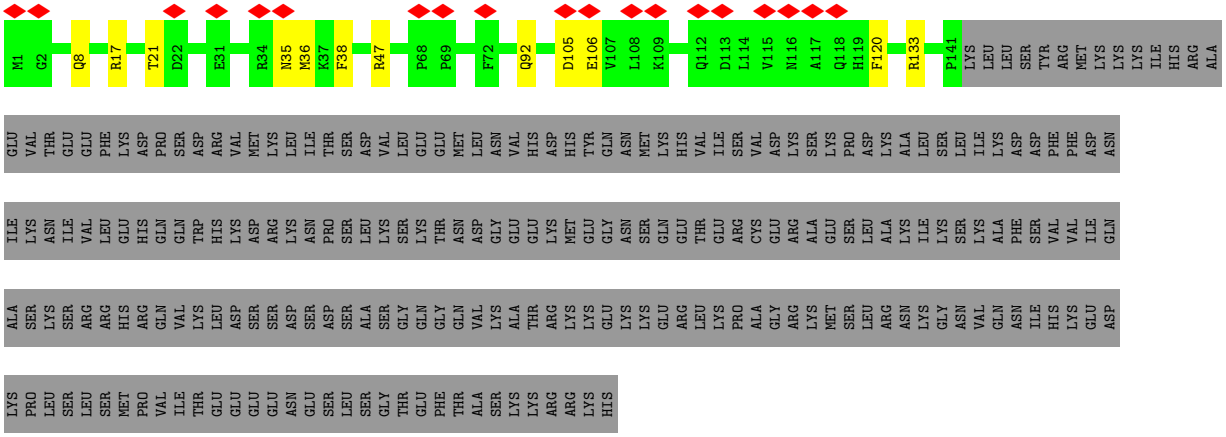
• Molecule 19: Transcription factor IIIB 50 kDa subunit



• Molecule 20: Transcription factor TFIIIB component B" homolog

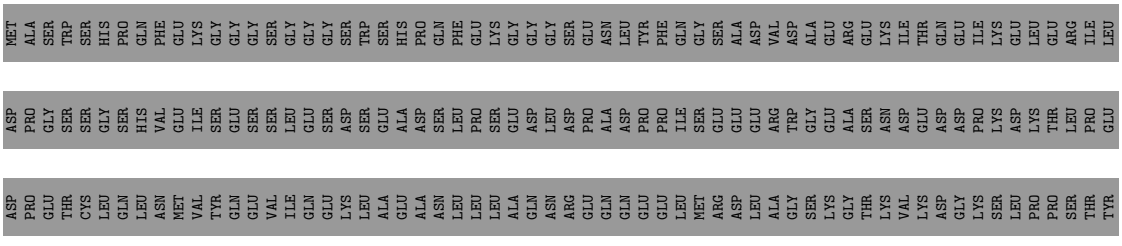


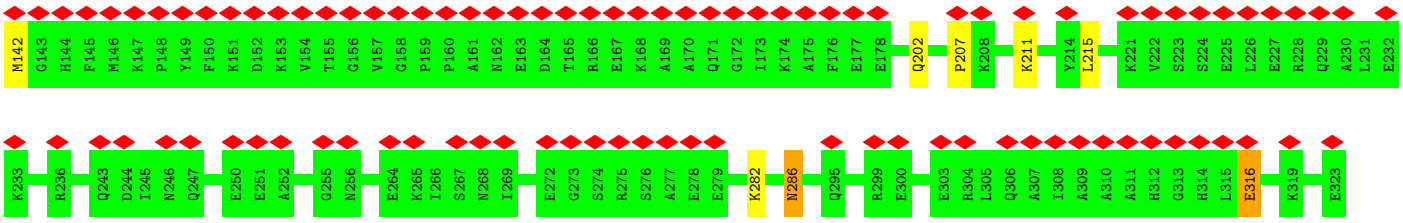
• Molecule 21: snRNA-activating protein complex subunit 1

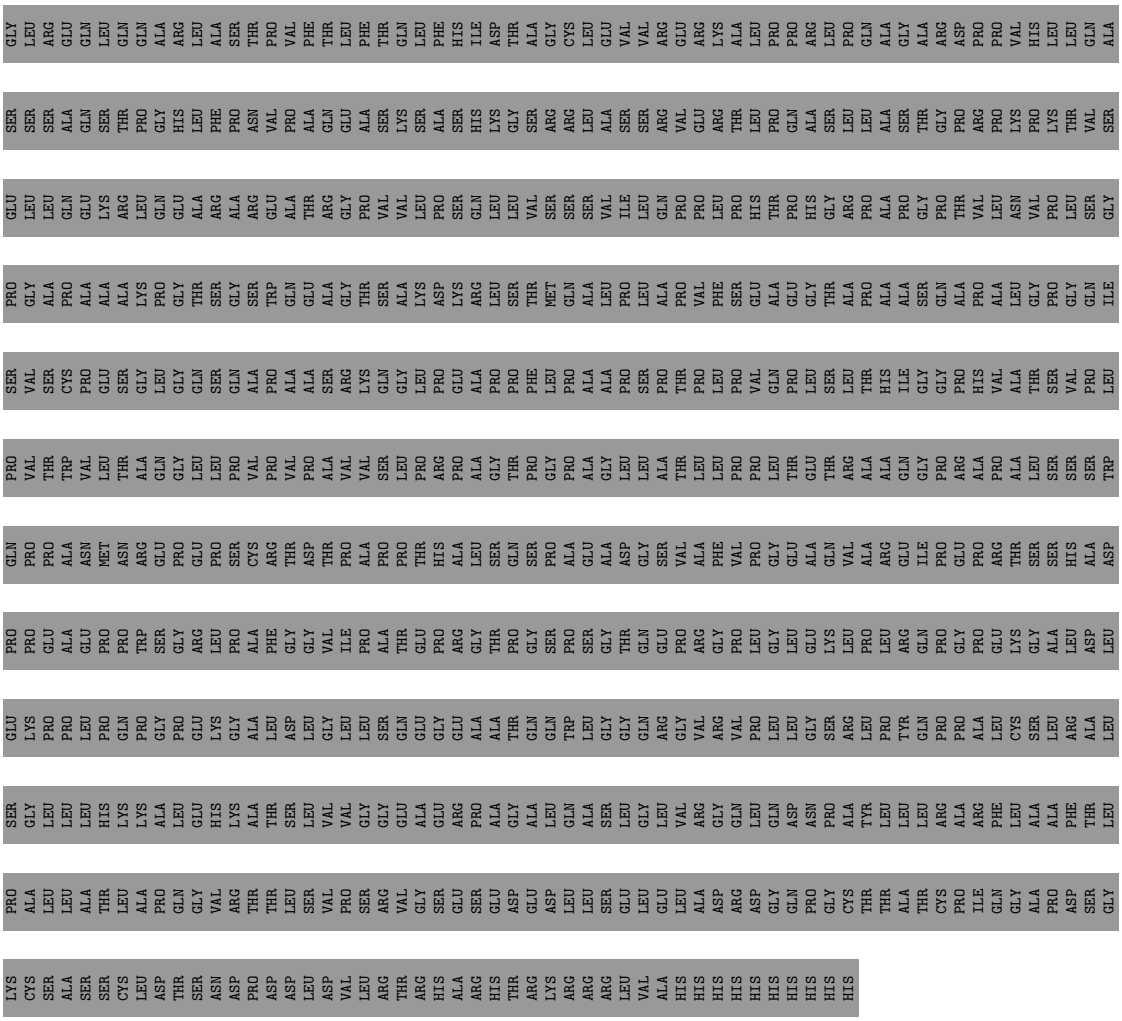


• Molecule 22: snRNA-activating protein complex subunit 4

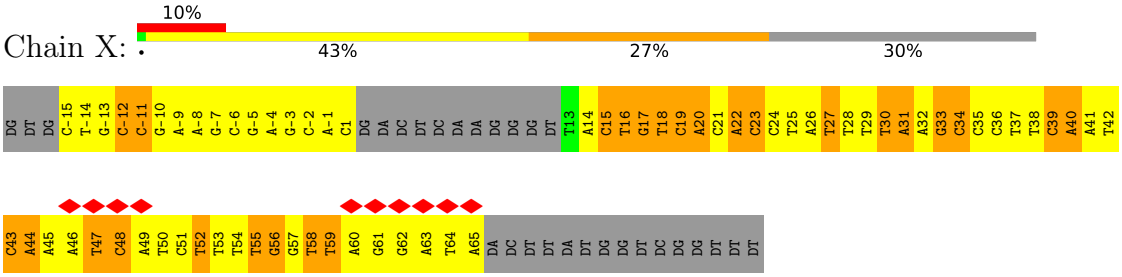
Chain W:



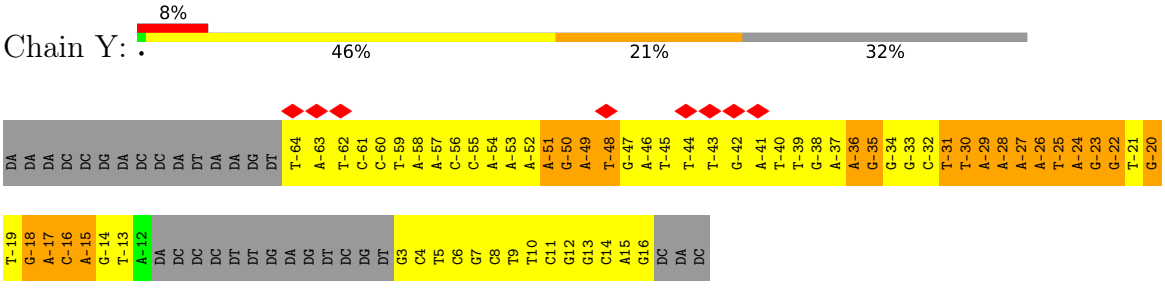




• Molecule 23: U6_2_Template

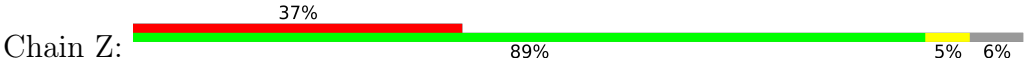


• Molecule 24: U6_2_Non template



• Molecule 25: snRNA-activating protein complex subunit 3

Chain Z:


37%
89%
5%
6%


MET ALA GLU GLY SER ARG GLY GLY PRO THR CYS SER GLY VAL GLY GLY ARG GLN ASP PRO VAL SER GLY SER GLY GLY
C27 N28 F29 P30 E31 Y32 E33 L34 P35 E36 L37 N38 T39 R40 A41 F42 H43 V44 G45 A46
L50 W51 R52 G53 R54 L55 R56 G57 A58 G59 D60 L61 S62
L63 R64 E65 P66 P67 A68 P72 G73 S74 Q75 A76 A77 D78 S79 D80 R81 E82 D83 A84 A85 V86 A87 R88 D89 L90 D91 C92 S93 L94 E95 A96 A97 A98 E99 L100 R101 A102 V103 D107 G115 E116 D117 V120 E123 R151 V156 M159 K166 K167 P168 E169
N170 S171 A172 D173 M174 I175 E176 E177 G178 E179 L180 P189 V190 I191 F192 H193 K194 H195 Q202 T203 M204 T213 R216 G228 G229 N233 T234 P235 D236 Q237 A238 P239 E240 H241 L246 G256 K262 R263 Y264 P265 R268 R272 T273 I274 I275 E276 W277 S278 E279
S280 H281 D282 R283 G284 Y285 G286 K287 F288 Q289 T290 A291 R292 M293 E294 D295 F296 T297 F298 N299 D300 L301 C302 G315 D316 C317 T324 D325 L328 D336 R337 T338 I344 W350 N367 N368 D375 V382 C383 M386 D390 S391 E392 G393 N394 K395 L396 G397 E398
F399 L400 N411

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11036	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.687	Depositor
Minimum map value	-1.299	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	401.1, 401.1, 401.1	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95500004, 0.95500004, 0.95500004	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, SF4, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.38	1/11044 (0.0%)	0.59	4/14893 (0.0%)
2	B	0.40	0/8845	0.58	2/11930 (0.0%)
3	C	0.26	0/4141	0.56	0/5592
4	D	0.26	0/1466	0.55	0/1972
5	E	0.26	0/3282	0.53	0/4439
6	F	0.41	1/2438 (0.0%)	0.68	3/3289 (0.1%)
7	G	0.28	0/739	0.68	0/996
8	H	0.32	0/1551	0.51	0/2110
9	I	0.25	0/1013	0.51	0/1365
10	J	0.31	0/870	0.67	0/1175
11	K	0.42	0/2790	0.57	0/3782
12	L	0.44	0/871	0.55	0/1174
13	M	0.31	0/1745	0.58	0/2358
14	N	0.44	0/637	0.59	0/861
15	O	0.41	0/1207	0.56	0/1628
16	P	0.41	0/394	0.62	0/524
17	Q	0.50	0/533	0.56	0/719
18	R	0.26	0/1428	0.56	0/1924
19	S	0.27	0/2898	0.57	0/3933
20	T	0.27	0/680	0.54	0/904
21	U	0.26	0/1215	0.53	0/1640
22	W	0.24	0/2058	0.52	0/2760
23	X	0.57	0/1569	1.66	106/2414 (4.4%)
24	Y	0.57	0/1554	1.65	101/2396 (4.2%)
25	Z	0.25	0/3203	0.52	0/4335
All	All	0.36	2/58171 (0.0%)	0.69	216/79113 (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	A	0	3
6	F	0	5
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	30	PRO	CG-CD	-7.56	1.25	1.50
1	A	1044	PRO	CG-CD	-5.27	1.33	1.50

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	30	PRO	CA-N-CD	-12.08	94.58	111.50
1	A	231	PRO	CA-N-CD	-9.22	98.59	111.50
6	F	30	PRO	N-CD-CG	-9.12	89.52	103.20
24	Y	-30	DT	O4'-C1'-N1	8.94	114.26	108.00
1	A	1044	PRO	CA-N-CD	-8.61	99.44	111.50
23	X	19	DC	OP1-P-OP2	-7.94	107.69	119.60
24	Y	-30	DT	OP1-P-OP2	-7.89	107.76	119.60
24	Y	-20	DG	OP1-P-OP2	-7.63	108.16	119.60
23	X	18	DT	OP1-P-O3'	7.54	121.79	105.20
24	Y	-31	DT	OP1-P-O3'	7.52	121.73	105.20
24	Y	-19	DT	OP1-P-OP2	-7.51	108.34	119.60
23	X	26	DA	OP1-P-OP2	-7.36	108.57	119.60
23	X	18	DT	OP1-P-OP2	-7.35	108.57	119.60
24	Y	-33	DG	OP1-P-O3'	7.32	121.30	105.20
24	Y	-18	DG	OP1-P-OP2	-7.31	108.64	119.60
24	Y	-27	DA	OP1-P-OP2	-7.29	108.66	119.60
24	Y	-50	DG	OP1-P-OP2	-7.28	108.68	119.60
23	X	34	DC	OP1-P-OP2	-7.27	108.70	119.60
24	Y	-33	DG	OP1-P-OP2	-7.27	108.70	119.60
23	X	27	DT	OP1-P-OP2	-7.23	108.76	119.60
24	Y	-38	DG	OP1-P-OP2	-7.23	108.76	119.60
23	X	29	DT	OP1-P-OP2	-7.22	108.77	119.60
24	Y	-21	DT	OP1-P-O3'	7.20	121.04	105.20
23	X	1	DC	OP1-P-OP2	-7.19	108.81	119.60
23	X	-1	DA	OP1-P-OP2	-7.16	108.87	119.60
23	X	28	DT	OP1-P-OP2	-7.15	108.88	119.60
24	Y	-58	DA	OP1-P-OP2	-7.15	108.88	119.60
24	Y	-32	DC	OP1-P-OP2	-7.13	108.90	119.60
24	Y	-41	DA	OP1-P-OP2	-7.08	108.98	119.60
23	X	63	DA	OP1-P-OP2	-7.08	108.98	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	X	58	DT	OP1-P-OP2	-7.07	108.99	119.60
1	A	1044	PRO	N-CD-CG	-7.05	92.63	103.20
24	Y	-35	DG	OP1-P-OP2	-7.04	109.03	119.60
24	Y	-14	DG	OP1-P-OP2	-7.04	109.04	119.60
23	X	20	DA	OP1-P-OP2	-7.04	109.04	119.60
24	Y	-39	DT	OP1-P-O3'	7.04	120.68	105.20
24	Y	-17	DA	OP1-P-OP2	-7.03	109.05	119.60
23	X	21	DC	OP1-P-OP2	-7.01	109.08	119.60
24	Y	-26	DA	OP1-P-OP2	-7.01	109.09	119.60
24	Y	-28	DA	OP1-P-OP2	-6.95	109.17	119.60
24	Y	-62	DT	OP1-P-OP2	-6.92	109.22	119.60
24	Y	-24	DA	OP1-P-OP2	-6.91	109.23	119.60
24	Y	-37	DA	OP1-P-OP2	-6.90	109.24	119.60
23	X	51	DC	OP1-P-OP2	-6.90	109.26	119.60
24	Y	-46	DA	OP1-P-OP2	-6.89	109.26	119.60
23	X	17	DG	OP1-P-O3'	6.89	120.36	105.20
24	Y	13	DG	OP1-P-OP2	-6.88	109.28	119.60
23	X	65	DA	OP1-P-OP2	-6.88	109.28	119.60
23	X	62	DG	OP1-P-OP2	-6.86	109.31	119.60
24	Y	11	DC	OP1-P-OP2	-6.84	109.33	119.60
23	X	64	DT	OP1-P-OP2	-6.84	109.34	119.60
23	X	43	DC	OP1-P-OP2	-6.83	109.35	119.60
24	Y	-49	DA	OP1-P-OP2	-6.83	109.35	119.60
24	Y	-60	DC	OP1-P-OP2	-6.81	109.38	119.60
23	X	42	DT	OP1-P-OP2	-6.81	109.39	119.60
24	Y	-25	DT	OP1-P-OP2	-6.80	109.39	119.60
23	X	59	DT	OP1-P-OP2	-6.80	109.40	119.60
24	Y	3	DG	OP1-P-OP2	-6.80	109.40	119.60
24	Y	-57	DA	OP1-P-OP2	-6.80	109.41	119.60
23	X	22	DA	OP1-P-OP2	-6.79	109.42	119.60
24	Y	-55	DC	OP1-P-OP2	-6.79	109.42	119.60
24	Y	-52	DA	OP1-P-OP2	-6.79	109.42	119.60
23	X	-10	DG	OP1-P-OP2	-6.78	109.43	119.60
24	Y	-40	DT	OP1-P-OP2	-6.78	109.43	119.60
23	X	-5	DG	OP1-P-OP2	-6.77	109.44	119.60
23	X	50	DT	OP1-P-OP2	-6.77	109.45	119.60
24	Y	-22	DG	OP1-P-OP2	-6.76	109.45	119.60
24	Y	-42	DG	OP1-P-OP2	-6.76	109.46	119.60
24	Y	-47	DG	OP1-P-OP2	-6.76	109.47	119.60
23	X	-13	DG	OP1-P-OP2	-6.75	109.47	119.60
24	Y	16	DG	OP1-P-OP2	-6.75	109.47	119.60
24	Y	-36	DA	OP1-P-OP2	-6.75	109.48	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	-29	DA	OP1-P-O3'	6.74	120.02	105.20
24	Y	-44	DT	OP1-P-OP2	-6.73	109.51	119.60
24	Y	-63	DA	OP1-P-OP2	-6.72	109.52	119.60
23	X	-2	DC	OP1-P-OP2	-6.71	109.54	119.60
23	X	37	DT	OP1-P-OP2	-6.71	109.54	119.60
23	X	61	DG	OP1-P-OP2	-6.71	109.54	119.60
23	X	47	DT	OP1-P-OP2	-6.70	109.55	119.60
23	X	48	DC	OP1-P-OP2	-6.70	109.56	119.60
23	X	30	DT	OP1-P-OP2	-6.69	109.56	119.60
23	X	-12	DC	OP1-P-OP2	-6.69	109.57	119.60
23	X	24	DC	OP1-P-OP2	-6.68	109.58	119.60
24	Y	-20	DG	OP1-P-O3'	6.68	119.89	105.20
24	Y	9	DT	OP1-P-OP2	-6.67	109.60	119.60
24	Y	-64	DT	OP1-P-OP2	-6.67	109.60	119.60
23	X	-8	DA	OP1-P-OP2	-6.66	109.61	119.60
24	Y	-48	DT	OP1-P-OP2	-6.66	109.61	119.60
24	Y	-45	DT	OP1-P-OP2	-6.66	109.61	119.60
24	Y	-39	DT	OP1-P-OP2	-6.65	109.62	119.60
23	X	-14	DT	OP1-P-OP2	-6.64	109.63	119.60
23	X	40	DA	OP1-P-OP2	-6.64	109.63	119.60
23	X	46	DA	OP1-P-OP2	-6.64	109.63	119.60
24	Y	-34	DG	OP1-P-OP2	-6.64	109.64	119.60
23	X	35	DC	OP1-P-OP2	-6.64	109.64	119.60
23	X	33	DG	OP1-P-OP2	-6.62	109.66	119.60
23	X	52	DT	OP1-P-OP2	-6.61	109.68	119.60
23	X	25	DT	OP1-P-O3'	6.61	119.74	105.20
23	X	44	DA	OP1-P-OP2	-6.61	109.69	119.60
23	X	55	DT	OP1-P-OP2	-6.61	109.69	119.60
24	Y	12	DG	OP1-P-OP2	-6.60	109.69	119.60
24	Y	-56	DC	OP1-P-OP2	-6.59	109.72	119.60
24	Y	8	DC	OP1-P-OP2	-6.59	109.72	119.60
24	Y	14	DC	OP1-P-OP2	-6.58	109.72	119.60
24	Y	-21	DT	OP1-P-OP2	-6.58	109.72	119.60
24	Y	-54	DA	OP1-P-OP2	-6.58	109.73	119.60
24	Y	-28	DA	OP1-P-O3'	6.58	119.67	105.20
2	B	534	PRO	CA-N-CD	-6.57	102.30	111.50
23	X	-15	DC	OP1-P-OP2	-6.57	109.75	119.60
23	X	-9	DA	OP1-P-OP2	-6.57	109.74	119.60
23	X	-4	DA	OP1-P-OP2	-6.57	109.75	119.60
23	X	45	DA	OP1-P-OP2	-6.56	109.77	119.60
24	Y	7	DG	OP1-P-OP2	-6.54	109.78	119.60
23	X	-7	DG	OP1-P-OP2	-6.54	109.80	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	-43	DT	OP1-P-OP2	-6.54	109.80	119.60
24	Y	15	DA	OP1-P-OP2	-6.53	109.81	119.60
23	X	49	DA	OP1-P-OP2	-6.52	109.82	119.60
23	X	39	DC	OP1-P-OP2	-6.51	109.83	119.60
23	X	-11	DC	OP1-P-OP2	-6.50	109.85	119.60
24	Y	5	DT	OP1-P-OP2	-6.50	109.85	119.60
24	Y	-53	DA	OP1-P-OP2	-6.50	109.86	119.60
23	X	23	DC	OP1-P-OP2	-6.49	109.86	119.60
24	Y	-15	DA	OP1-P-O3'	6.47	119.44	105.20
23	X	36	DC	OP1-P-OP2	-6.47	109.89	119.60
23	X	41	DA	OP1-P-OP2	-6.44	109.94	119.60
23	X	57	DG	OP1-P-OP2	-6.42	109.97	119.60
23	X	31	DA	OP1-P-OP2	-6.41	109.98	119.60
23	X	-3	DG	OP1-P-OP2	-6.41	109.99	119.60
23	X	35	DC	OP1-P-O3'	6.41	119.29	105.20
23	X	60	DA	OP1-P-OP2	-6.39	110.01	119.60
23	X	-6	DC	OP1-P-OP2	-6.39	110.02	119.60
24	Y	-61	DC	OP1-P-OP2	-6.38	110.02	119.60
23	X	32	DA	OP1-P-O3'	6.38	119.24	105.20
24	Y	10	DT	OP1-P-OP2	-6.37	110.04	119.60
24	Y	-16	DC	OP1-P-OP2	-6.35	110.07	119.60
24	Y	4	DC	OP1-P-OP2	-6.34	110.09	119.60
23	X	56	DG	OP1-P-OP2	-6.33	110.11	119.60
24	Y	6	DC	OP1-P-OP2	-6.32	110.12	119.60
24	Y	-31	DT	OP1-P-OP2	-6.31	110.13	119.60
24	Y	-23	DG	OP1-P-OP2	-6.31	110.13	119.60
23	X	32	DA	OP1-P-OP2	-6.30	110.14	119.60
23	X	34	DC	OP1-P-O3'	6.29	119.03	105.20
23	X	25	DT	OP1-P-OP2	-6.27	110.19	119.60
23	X	17	DG	OP1-P-OP2	-6.23	110.26	119.60
24	Y	-59	DT	OP1-P-OP2	-6.20	110.30	119.60
24	Y	-19	DT	OP1-P-O3'	6.19	118.83	105.20
23	X	38	DT	OP1-P-OP2	-6.18	110.33	119.60
23	X	23	DC	OP1-P-O3'	6.16	118.75	105.20
23	X	54	DT	OP1-P-OP2	-6.15	110.38	119.60
24	Y	-26	DA	OP2-P-O3'	6.15	118.72	105.20
24	Y	-25	DT	OP1-P-O3'	6.13	118.69	105.20
23	X	16	DT	OP1-P-OP2	-6.13	110.41	119.60
24	Y	-34	DG	OP1-P-O3'	6.08	118.58	105.20
23	X	-6	DC	OP1-P-O3'	6.04	118.49	105.20
23	X	-2	DC	OP1-P-O3'	5.95	118.29	105.20
24	Y	-32	DC	OP1-P-O3'	5.95	118.28	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	X	-1	DA	OP1-P-O3'	5.92	118.23	105.20
23	X	-11	DC	OP1-P-O3'	5.92	118.21	105.20
24	Y	-51	DA	OP1-P-OP2	-5.91	110.74	119.60
23	X	36	DC	OP2-P-O3'	5.88	118.14	105.20
24	Y	-27	DA	OP1-P-O3'	5.88	118.13	105.20
24	Y	-59	DT	OP1-P-O3'	5.86	118.09	105.20
23	X	42	DT	OP1-P-O3'	5.73	117.81	105.20
23	X	-5	DG	OP1-P-O3'	5.71	117.75	105.20
24	Y	-42	DG	OP1-P-O3'	5.66	117.64	105.20
23	X	20	DA	OP1-P-O3'	5.64	117.61	105.20
23	X	29	DT	OP1-P-O3'	5.64	117.61	105.20
23	X	63	DA	OP1-P-O3'	5.63	117.58	105.20
23	X	-15	DC	OP2-P-O3'	5.62	117.57	105.20
23	X	19	DC	OP1-P-O3'	5.61	117.53	105.20
24	Y	10	DT	OP1-P-O3'	5.60	117.53	105.20
24	Y	-18	DG	OP1-P-O3'	5.56	117.44	105.20
24	Y	-64	DT	OP1-P-O3'	5.55	117.42	105.20
23	X	64	DT	OP1-P-O3'	5.55	117.41	105.20
23	X	-14	DT	OP1-P-O3'	5.55	117.40	105.20
23	X	41	DA	OP1-P-O3'	5.53	117.37	105.20
23	X	-8	DA	OP1-P-O3'	5.48	117.26	105.20
23	X	28	DT	OP2-P-O3'	5.47	117.24	105.20
23	X	57	DG	OP1-P-O3'	5.44	117.17	105.20
24	Y	8	DC	OP1-P-O3'	5.44	117.17	105.20
23	X	22	DA	OP1-P-O3'	5.41	117.11	105.20
24	Y	-36	DA	OP1-P-O3'	5.40	117.08	105.20
23	X	46	DA	OP1-P-O3'	5.38	117.03	105.20
23	X	49	DA	OP1-P-O3'	5.34	116.95	105.20
24	Y	-63	DA	OP1-P-O3'	5.34	116.95	105.20
24	Y	13	DG	OP1-P-O3'	5.33	116.92	105.20
24	Y	-37	DA	OP1-P-O3'	5.31	116.89	105.20
24	Y	14	DC	OP1-P-O3'	5.31	116.88	105.20
23	X	54	DT	OP1-P-O3'	5.29	116.84	105.20
24	Y	-47	DG	OP1-P-O3'	5.29	116.83	105.20
24	Y	-40	DT	OP1-P-O3'	5.28	116.81	105.20
23	X	50	DT	OP1-P-O3'	5.28	116.81	105.20
24	Y	-56	DC	OP1-P-O3'	5.27	116.80	105.20
23	X	-7	DG	OP1-P-O3'	5.27	116.79	105.20
24	Y	-41	DA	OP1-P-O3'	5.27	116.79	105.20
23	X	-3	DG	OP1-P-O3'	5.26	116.76	105.20
23	X	38	DT	OP1-P-O3'	5.25	116.75	105.20
23	X	26	DA	OP2-P-O3'	5.23	116.70	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	-35	DG	OP1-P-O3'	5.23	116.70	105.20
23	X	62	DG	OP1-P-O3'	5.21	116.66	105.20
24	Y	-46	DA	OP1-P-O3'	5.21	116.66	105.20
23	X	58	DT	OP1-P-O3'	5.19	116.62	105.20
23	X	48	DC	OP1-P-O3'	5.17	116.57	105.20
24	Y	-45	DT	OP1-P-O3'	5.13	116.50	105.20
24	Y	-58	DA	OP1-P-O3'	5.12	116.47	105.20
2	B	322	PRO	CA-N-CD	-5.12	104.34	111.50
24	Y	5	DT	OP1-P-O3'	5.11	116.45	105.20
23	X	51	DC	OP1-P-O3'	5.11	116.44	105.20
23	X	27	DT	OP2-P-O3'	5.09	116.40	105.20
23	X	15	DC	OP1-P-O3'	5.08	116.39	105.20
6	F	30	PRO	CA-CB-CG	-5.07	94.37	104.00
24	Y	-60	DC	OP1-P-O3'	5.07	116.35	105.20
24	Y	4	DC	OP1-P-O3'	5.07	116.35	105.20
24	Y	-48	DT	OP1-P-O3'	5.06	116.34	105.20
1	A	231	PRO	N-CD-CG	-5.05	95.63	103.20
23	X	37	DT	OP1-P-O3'	5.01	116.23	105.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1092	ASP	Peptide
1	A	1093	ASP	Peptide
1	A	1099	ARG	Sidechain
6	F	201	ASN	Peptide
6	F	272	ALA	Peptide
6	F	84	LYS	Peptide
6	F	85	MET	Peptide
6	F	86	LYS	Peptide

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	A	10848	0	11089	218	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8680	0	8805	132	0
3	C	4075	0	4149	83	0
4	D	1448	0	1489	26	0
5	E	3211	0	3227	41	0
6	F	2395	0	2405	151	0
7	G	717	0	719	23	0
8	H	1509	0	1461	15	0
9	I	1001	0	1028	10	0
10	J	849	0	813	70	0
11	K	2736	0	2712	15	0
12	L	856	0	840	8	0
13	M	1715	0	1733	26	0
14	N	627	0	659	2	0
15	O	1186	0	1147	6	0
16	P	388	0	393	3	0
17	Q	524	0	540	2	0
18	R	1402	0	1489	14	0
19	S	2847	0	2886	63	0
20	T	665	0	665	5	0
21	U	1183	0	1175	6	0
22	W	2018	0	1997	9	0
23	X	1403	0	782	43	0
24	Y	1384	0	757	20	0
25	Z	3123	0	2983	13	0
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	J	1	0	0	0	0
26	P	1	0	0	0	0
26	Q	1	0	0	0	0
26	S	1	0	0	0	0
26	Z	2	0	0	0	0
27	A	1	0	0	0	0
28	F	8	0	0	9	0
All	All	56808	0	55943	845	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 8.

All (845) 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)
6:F:297:HIS:CE1	6:F:299:GLY:O	1.72	1.42
6:F:110:ARG:HH22	23:X:15:DC:C1'	1.50	1.22
6:F:110:ARG:NH2	23:X:15:DC:H1'	1.53	1.21
6:F:110:ARG:NH2	23:X:15:DC:C1'	2.12	1.11
2:B:1028:ARG:O	19:S:40:LEU:HA	1.50	1.09
6:F:110:ARG:NH2	23:X:15:DC:C2'	2.21	1.04
2:B:1041:ARG:NH1	19:S:42:THR:O	1.97	0.97
6:F:297:HIS:HE1	6:F:299:GLY:O	1.33	0.96
2:B:1042:ASP:OD2	19:S:22:SER:HB2	1.66	0.95
1:A:285:GLU:OE1	1:A:316:GLN:NE2	2.02	0.93
6:F:110:ARG:HH22	23:X:15:DC:H1'	0.77	0.92
6:F:110:ARG:NH2	23:X:15:DC:H2"	1.85	0.90
2:B:1041:ARG:CZ	19:S:42:THR:O	2.18	0.89
6:F:297:HIS:CE1	6:F:299:GLY:C	2.44	0.89
1:A:1099:ARG:NH1	10:J:80:MET:SD	2.47	0.87
20:T:351:ARG:HH12	20:T:355:ALA:HB2	1.41	0.85
15:O:136:GLU:N	15:O:136:GLU:OE2	2.09	0.85
15:O:8:ASP:OD1	15:O:9:ILE:N	2.10	0.85
4:D:143:GLU:OE2	4:D:153:GLN:NE2	2.10	0.84
6:F:120:LEU:CD2	23:X:15:DC:O5'	2.25	0.84
13:M:130:PHE:HB3	13:M:135:LEU:HD11	1.59	0.84
1:A:324:GLU:N	1:A:324:GLU:OE1	2.10	0.84
1:A:1094:ASP:OD1	1:A:1095:ALA:N	2.11	0.83
1:A:1108:THR:OG1	10:J:49:VAL:O	1.99	0.81
19:S:126:CYS:SG	19:S:133:LEU:HD13	2.21	0.81
1:A:1313:GLU:OE1	1:A:1313:GLU:N	2.15	0.80
6:F:297:HIS:NE2	6:F:299:GLY:O	2.15	0.80
6:F:307:CYS:SG	28:F:401:SF4:FE2	1.73	0.80
1:A:41:LEU:HB2	19:S:58:SER:O	1.82	0.79
2:B:850:GLN:N	2:B:850:GLN:OE1	2.16	0.79
4:D:373:MET:SD	5:E:208:LEU:HD13	2.21	0.79
1:A:104:ILE:HD11	1:A:238:LEU:HD13	1.65	0.78
2:B:1028:ARG:O	19:S:40:LEU:CA	2.29	0.78
1:A:1099:ARG:HG2	10:J:77:ALA:HB1	1.65	0.78
2:B:1027:PRO:HB3	19:S:39:VAL:HG23	1.66	0.77
6:F:110:ARG:HH21	23:X:15:DC:H2"	1.47	0.77
1:A:1144:VAL:HG22	10:J:52:VAL:HG21	1.65	0.76
6:F:287:CYS:HA	28:F:401:SF4:S3	2.25	0.76
2:B:1029:ALA:O	19:S:40:LEU:HD23	1.85	0.76
1:A:1137:ILE:HD13	1:A:1140:LEU:HD12	1.66	0.76
1:A:1099:ARG:CG	10:J:77:ALA:HB1	2.17	0.75
2:B:1042:ASP:OD2	19:S:22:SER:CB	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1041:ARG:NE	19:S:43:THR:HA	2.02	0.74
15:O:106:THR:HG23	15:O:107:GLU:OE2	1.87	0.74
1:A:24:SER:OG	1:A:27:GLU:OE1	2.05	0.74
3:C:357:ARG:HD2	6:F:289:LEU:HD22	1.68	0.74
2:B:79:ASN:OD1	2:B:80:ILE:N	2.21	0.73
8:H:22:LEU:HG	8:H:26:ILE:HD11	1.70	0.72
1:A:1196:LEU:HB3	1:A:1197:PRO:HD3	1.71	0.72
24:Y:-30:DT:H2"	24:Y:-29:DA:H5'	1.72	0.72
6:F:110:ARG:HH22	23:X:15:DC:C2'	1.95	0.72
1:A:1117:ILE:HG22	10:J:41:ARG:HD2	1.70	0.71
11:K:255:ARG:O	11:K:255:ARG:NE	2.22	0.71
2:B:525:LEU:HD23	2:B:525:LEU:O	1.90	0.70
5:E:241:SER:OG	5:E:244:GLU:OE1	2.08	0.70
1:A:40:ASN:OD1	19:S:59:THR:HA	1.91	0.70
6:F:239:LEU:HD22	6:F:266:HIS:CE1	2.26	0.70
1:A:989:ILE:HD11	1:A:1001:TYR:CZ	2.27	0.70
6:F:302:ILE:HG23	7:G:37:LEU:HD21	1.73	0.70
2:B:281:MET:HE1	2:B:306:ILE:HD12	1.73	0.70
2:B:622:GLU:OE1	2:B:626:HIS:NE2	2.25	0.69
3:C:258:ARG:HB3	3:C:259:MET:SD	2.32	0.69
6:F:296:CYS:SG	28:F:401:SF4:S1	2.90	0.69
8:H:22:LEU:O	8:H:26:ILE:HD12	1.91	0.69
3:C:266:ILE:HG22	3:C:270:MET:HE3	1.74	0.68
2:B:634:ASP:OD1	2:B:635:VAL:N	2.27	0.68
1:A:1118:GLU:O	10:J:41:ARG:NE	2.27	0.68
1:A:485:THR:O	1:A:487:ARG:NH1	2.26	0.68
1:A:415:HIS:O	1:A:417:GLY:N	2.27	0.68
9:I:1:MET:SD	9:I:2:GLU:N	2.67	0.68
2:B:1027:PRO:HA	19:S:39:VAL:O	1.94	0.67
6:F:120:LEU:HD21	23:X:15:DC:H5'	1.74	0.67
3:C:79:CYS:O	3:C:82:VAL:HG22	1.95	0.67
1:A:1093:ASP:O	10:J:77:ALA:HB3	1.94	0.67
1:A:1317:MET:CE	1:A:1318:LEU:HD12	2.25	0.67
25:Z:51:TRP:HB3	25:Z:328:LEU:HD11	1.75	0.67
6:F:267:MET:SD	6:F:268:LYS:N	2.68	0.67
6:F:290:CYS:SG	28:F:401:SF4:S4	2.93	0.67
6:F:308:ILE:HB	7:G:38:PHE:CD2	2.30	0.67
6:F:284:ARG:HG2	7:G:46:VAL:HB	1.77	0.66
2:B:1060:ALA:O	2:B:1064:LEU:HD23	1.96	0.66
10:J:88:ASP:N	10:J:89:GLU:OE1	2.28	0.66
6:F:245:ASP:OD1	6:F:247:LYS:HG2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:363:VAL:HA	4:D:373:MET:HE1	1.78	0.65
1:A:1211:VAL:HG22	1:A:1212:ILE:H	1.60	0.65
3:C:409:ILE:HD13	3:C:423:LEU:HD22	1.77	0.65
18:R:287:LEU:HD13	19:S:150:SER:HB2	1.78	0.65
2:B:1027:PRO:CA	19:S:39:VAL:O	2.45	0.65
19:S:154:MET:SD	19:S:155:GLN:N	2.69	0.65
13:M:167:GLU:OE1	13:M:167:GLU:N	2.30	0.65
18:R:174:LEU:HD21	18:R:219:MET:SD	2.37	0.65
21:U:17:ARG:O	21:U:21:THR:HG23	1.97	0.64
6:F:146:LYS:O	23:X:16:DT:H4'	1.96	0.64
3:C:386:ILE:HG21	3:C:391:ALA:HB2	1.80	0.64
2:B:1027:PRO:HB3	19:S:39:VAL:CG2	2.28	0.64
2:B:417:ASN:O	2:B:421:THR:HG22	1.97	0.63
1:A:876:VAL:HG21	2:B:1053:ASP:OD1	1.98	0.63
1:A:231:PRO:HD2	1:A:231:PRO:O	1.98	0.63
10:J:86:SER:OG	10:J:87:ALA:N	2.31	0.63
3:C:255:VAL:HG13	3:C:259:MET:HE1	1.81	0.63
2:B:1030:VAL:HA	19:S:40:LEU:HD23	1.80	0.63
2:B:514:LEU:HD23	2:B:568:ILE:HD11	1.80	0.63
6:F:120:LEU:HD22	23:X:15:DC:O5'	1.98	0.62
6:F:140:LYS:HE2	23:X:17:DG:H5"	1.81	0.62
1:A:590:LYS:HB3	1:A:591:PRO:HD3	1.81	0.62
1:A:1317:MET:HE3	1:A:1318:LEU:HD12	1.81	0.62
2:B:326:PHE:HA	2:B:328:PHE:CE1	2.34	0.62
6:F:251:THR:HG22	6:F:251:THR:O	2.00	0.62
4:D:373:MET:SD	5:E:208:LEU:HB3	2.39	0.62
1:A:1089:LEU:HD13	10:J:98:CYS:SG	2.40	0.61
1:A:1144:VAL:CG2	10:J:52:VAL:HG11	2.30	0.61
6:F:110:ARG:HH21	23:X:15:DC:C2'	2.04	0.61
10:J:89:GLU:OE1	10:J:89:GLU:N	2.33	0.61
10:J:95:TYR:N	10:J:106:TRP:O	2.32	0.61
13:M:61:LEU:HD23	13:M:61:LEU:H	1.65	0.61
19:S:158:LYS:NZ	24:Y:-29:DA:OP1	2.32	0.61
2:B:570:GLU:OE1	2:B:625:LEU:HD13	2.00	0.61
3:C:391:ALA:O	3:C:395:LEU:HD22	2.00	0.61
6:F:78:ASP:O	6:F:81:ASN:N	2.32	0.61
2:B:513:LYS:NZ	5:E:249:LEU:O	2.33	0.61
6:F:295:ASP:O	6:F:296:CYS:C	2.39	0.61
20:T:351:ARG:NH1	20:T:355:ALA:HB2	2.13	0.61
6:F:294:ASP:O	6:F:295:ASP:C	2.39	0.60
6:F:120:LEU:HD21	23:X:15:DC:C5'	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:438:ARG:HG3	6:F:293:PHE:CZ	2.35	0.60
4:D:361:VAL:HG12	4:D:375:VAL:HA	1.83	0.60
19:S:91:ASP:OD1	19:S:92:THR:N	2.34	0.60
2:B:277:ILE:HG23	2:B:277:ILE:O	2.01	0.60
3:C:445:ASN:ND2	28:F:401:SF4:S1	2.75	0.60
1:A:1201:VAL:HG11	10:J:48:GLU:O	2.02	0.60
1:A:606:ARG:HG3	1:A:611:ASN:HD22	1.67	0.60
16:P:15:MET:H	16:P:15:MET:CE	2.14	0.60
1:A:1120:VAL:HG11	1:A:1127:PHE:CD1	2.37	0.59
1:A:263:ARG:HH11	1:A:280:THR:HG22	1.66	0.59
5:E:387:GLU:OE2	5:E:388:HIS:ND1	2.35	0.59
3:C:512:SER:OG	6:F:313:TRP:CH2	2.49	0.59
8:H:26:ILE:HG21	8:H:70:VAL:HG21	1.85	0.59
12:L:38:HIS:O	12:L:38:HIS:ND1	2.33	0.59
1:A:1110:LEU:HG	1:A:1113:ILE:HD11	1.84	0.59
3:C:95:THR:HG21	3:C:107:VAL:HG21	1.84	0.59
1:A:90:LEU:HD12	1:A:310:TRP:CZ2	2.38	0.59
3:C:99:TYR:HH	3:C:156:PHE:HE2	1.51	0.58
3:C:93:TYR:HB2	7:G:57:MET:HE2	1.84	0.58
3:C:409:ILE:HD12	3:C:409:ILE:H	1.68	0.58
12:L:32:ALA:HB3	12:L:35:THR:OG1	2.03	0.58
19:S:75:ARG:HE	19:S:118:VAL:HG21	1.69	0.58
24:Y:-26:DA:H2'	24:Y:-25:DT:C6	2.39	0.58
1:A:1096:ASP:H	10:J:77:ALA:N	2.01	0.58
2:B:434:GLN:OE1	2:B:434:GLN:N	2.36	0.58
1:A:1109:LEU:HA	10:J:48:GLU:HA	1.86	0.57
1:A:1195:ASP:O	10:J:46:LEU:HB3	2.04	0.57
6:F:84:LYS:NZ	6:F:95:VAL:HG23	2.18	0.57
11:K:195:ASP:OD1	11:K:195:ASP:O	2.21	0.57
1:A:1120:VAL:HG11	1:A:1127:PHE:CE1	2.40	0.57
2:B:722:THR:HG23	2:B:962:THR:HA	1.87	0.57
7:G:48:LEU:HD23	7:G:48:LEU:H	1.69	0.57
1:A:1137:ILE:O	1:A:1141:ARG:N	2.37	0.57
20:T:312:PHE:HA	20:T:315:ILE:HG22	1.87	0.57
2:B:514:LEU:HD13	5:E:250:MET:HE1	1.87	0.57
2:B:1028:ARG:HB2	19:S:40:LEU:HG	1.86	0.57
2:B:40:VAL:O	2:B:40:VAL:HG22	2.05	0.56
6:F:293:PHE:O	6:F:294:ASP:C	2.43	0.56
18:R:263:ASP:OD1	18:R:264:VAL:N	2.38	0.56
1:A:11:VAL:O	1:A:13:LYS:HG3	2.05	0.56
2:B:1041:ARG:HH22	19:S:42:THR:HG23	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:250:MET:O	6:F:250:MET:SD	2.64	0.56
1:A:989:ILE:HD11	1:A:1001:TYR:CE1	2.40	0.56
2:B:867:GLU:OE1	2:B:886:ARG:NH1	2.39	0.56
4:D:153:GLN:OE1	4:D:154:ILE:N	2.36	0.56
2:B:530:GLU:OE1	2:B:530:GLU:N	2.38	0.56
2:B:1028:ARG:N	19:S:39:VAL:O	2.37	0.56
19:S:76:VAL:HG22	19:S:118:VAL:HG13	1.87	0.56
3:C:85:MET:SD	3:C:85:MET:N	2.79	0.56
7:G:64:LEU:O	7:G:68:MET:SD	2.64	0.56
13:M:116:GLN:O	13:M:119:VAL:HG12	2.05	0.56
13:M:131:LEU:O	13:M:135:LEU:HD12	2.05	0.56
5:E:116:ALA:HB2	5:E:129:LEU:HD21	1.86	0.56
2:B:413:ASN:O	2:B:417:ASN:OD1	2.24	0.56
6:F:120:LEU:CD2	23:X:15:DC:C5'	2.84	0.56
5:E:25:LEU:HD23	5:E:26:TYR:N	2.21	0.56
2:B:946:LEU:HD23	2:B:946:LEU:O	2.06	0.55
11:K:69:ASP:OD1	11:K:70:ALA:N	2.39	0.55
11:K:127:GLN:OE1	11:K:127:GLN:N	2.36	0.55
3:C:4:ALA:O	3:C:8:LEU:HD22	2.06	0.55
15:O:106:THR:HG23	15:O:107:GLU:CD	2.27	0.55
1:A:776:SER:HB2	1:A:777:PRO:HD3	1.89	0.55
1:A:1113:ILE:CG2	1:A:1137:ILE:HD11	2.37	0.55
3:C:429:LEU:H	3:C:429:LEU:HD23	1.71	0.55
6:F:306:ASN:O	6:F:308:ILE:N	2.40	0.55
13:M:135:LEU:HD12	13:M:135:LEU:H	1.71	0.55
1:A:1108:THR:O	10:J:49:VAL:N	2.39	0.54
3:C:404:MET:SD	3:C:405:SER:N	2.79	0.54
11:K:123:GLU:N	11:K:123:GLU:OE1	2.40	0.54
19:S:37:GLU:N	19:S:37:GLU:OE1	2.40	0.54
3:C:512:SER:CB	6:F:313:TRP:HH2	2.21	0.54
6:F:300:GLY:H	6:F:303:SER:HB2	1.72	0.54
7:G:108:ARG:HA	7:G:111:MET:HE1	1.89	0.54
17:Q:6:ARG:HG2	17:Q:13:ILE:HD13	1.89	0.54
1:A:1195:ASP:HA	10:J:46:LEU:HB2	1.89	0.54
2:B:81:TYR:O	2:B:113:ILE:HD12	2.08	0.54
6:F:269:LEU:O	6:F:273:VAL:HG12	2.07	0.54
23:X:22:DA:N3	24:Y:-20:DG:N2	2.54	0.54
2:B:79:ASN:N	2:B:116:ASP:OD1	2.41	0.54
1:A:1089:LEU:CD1	10:J:98:CYS:SG	2.96	0.54
5:E:348:VAL:HG13	5:E:348:VAL:O	2.08	0.54
3:C:383:PHE:HB3	6:F:244:TYR:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:138:ILE:HD12	4:D:138:ILE:H	1.73	0.54
6:F:297:HIS:O	6:F:298:GLU:C	2.45	0.54
1:A:1144:VAL:HG23	10:J:52:VAL:HG11	1.89	0.54
3:C:133:MET:SD	3:C:133:MET:N	2.81	0.54
5:E:25:LEU:HD22	5:E:129:LEU:HD22	1.90	0.54
6:F:148:LYS:HE3	23:X:17:DG:OP2	2.08	0.54
3:C:255:VAL:HG11	3:C:267:VAL:HG21	1.89	0.54
3:C:438:ARG:HG3	6:F:293:PHE:CE1	2.42	0.54
3:C:512:SER:CB	6:F:313:TRP:CH2	2.91	0.53
3:C:513:GLU:O	3:C:517:ASP:OD2	2.26	0.53
4:D:372:GLU:N	4:D:372:GLU:OE1	2.41	0.53
6:F:110:ARG:CZ	23:X:15:DC:H1'	2.32	0.53
10:J:89:GLU:HB2	10:J:90:PRO:HD2	1.89	0.53
2:B:287:ILE:CD1	2:B:309:ALA:HB1	2.38	0.53
3:C:145:SER:O	3:C:149:VAL:HG13	2.08	0.53
3:C:367:ARG:HD2	6:F:246:GLY:H	1.73	0.53
4:D:151:THR:HG23	4:D:151:THR:O	2.09	0.53
4:D:363:VAL:HG13	4:D:363:VAL:O	2.08	0.53
6:F:160:SER:O	6:F:162:THR:N	2.41	0.53
16:P:15:MET:SD	16:P:15:MET:N	2.80	0.53
1:A:1197:PRO:HD2	10:J:45:LYS:HA	1.90	0.53
1:A:1141:ARG:HD3	10:J:79:PHE:O	2.09	0.53
4:D:360:LEU:HD11	5:E:25:LEU:HD21	1.90	0.53
6:F:293:PHE:HA	28:F:401:SF4:S2	2.49	0.53
18:R:271:GLU:O	18:R:275:LEU:HG	2.08	0.53
6:F:306:ASN:O	6:F:307:CYS:C	2.47	0.53
7:G:61:LYS:O	7:G:65:ARG:HG3	2.09	0.53
10:J:95:TYR:O	10:J:106:TRP:N	2.40	0.53
2:B:1028:ARG:O	19:S:40:LEU:CB	2.56	0.53
3:C:346:ALA:O	3:C:349:THR:HG22	2.09	0.53
11:K:178:LEU:HD23	11:K:179:GLY:N	2.24	0.53
2:B:514:LEU:CD2	2:B:568:ILE:HD11	2.39	0.53
8:H:26:ILE:HD12	8:H:26:ILE:H	1.74	0.53
10:J:55:GLY:O	10:J:57:ALA:N	2.42	0.53
13:M:27:LEU:HD13	13:M:64:HIS:CG	2.44	0.53
2:B:379:LYS:HA	2:B:379:LYS:HE2	1.90	0.52
6:F:158:ASP:O	6:F:160:SER:N	2.42	0.52
2:B:271:GLU:N	2:B:271:GLU:OE1	2.42	0.52
6:F:82:ALA:HA	6:F:94:LEU:HD13	1.92	0.52
2:B:277:ILE:HD11	2:B:283:ALA:N	2.25	0.52
3:C:512:SER:OG	6:F:313:TRP:CZ2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:380:VAL:O	3:C:384:ALA:N	2.41	0.52
4:D:360:LEU:CD1	5:E:25:LEU:HD21	2.40	0.52
6:F:296:CYS:SG	28:F:401:SF4:S4	3.08	0.52
11:K:23:ASN:O	11:K:303:ARG:NH2	2.43	0.52
19:S:83:LEU:HB2	19:S:85:LEU:CD2	2.40	0.52
1:A:1377:LEU:HD23	1:A:1377:LEU:H	1.73	0.52
6:F:201:ASN:O	6:F:203:MET:N	2.43	0.52
6:F:251:THR:H	6:F:268:LYS:HG2	1.74	0.52
7:G:46:VAL:HG13	7:G:47:PRO:HD2	1.91	0.52
2:B:287:ILE:HD12	2:B:309:ALA:HB1	1.91	0.52
10:J:96:LYS:HA	10:J:105:ARG:HA	1.91	0.52
11:K:275:VAL:HG13	11:K:275:VAL:O	2.10	0.52
1:A:1140:LEU:HD22	10:J:82:LEU:HA	1.91	0.52
6:F:252:ILE:HG23	6:F:254:ALA:H	1.74	0.52
23:X:33:DG:H3'	23:X:34:DC:H5"	1.91	0.52
1:A:1110:LEU:O	1:A:1113:ILE:HG12	2.10	0.52
1:A:1199:VAL:HG13	1:A:1200:VAL:N	2.25	0.52
2:B:277:ILE:HD11	2:B:283:ALA:CA	2.40	0.52
3:C:5:GLU:HA	3:C:8:LEU:HD23	1.91	0.52
3:C:356:GLU:HB2	6:F:283:VAL:HG11	1.91	0.52
1:A:116:MET:HE1	1:A:150:CYS:HB2	1.93	0.51
1:A:237:LEU:HD12	1:A:237:LEU:O	2.10	0.51
3:C:53:ALA:O	3:C:57:LEU:HD13	2.10	0.51
3:C:398:MET:N	3:C:398:MET:SD	2.83	0.51
6:F:84:LYS:HB2	6:F:94:LEU:HD23	1.91	0.51
1:A:322:ASN:OD1	1:A:324:GLU:OE1	2.28	0.51
1:A:1371:ASN:O	1:A:1371:ASN:ND2	2.41	0.51
2:B:36:VAL:HG23	2:B:37:LYS:HG3	1.92	0.51
2:B:488:GLU:OE1	2:B:488:GLU:N	2.43	0.51
3:C:512:SER:HG	6:F:313:TRP:HH2	1.46	0.51
2:B:279:THR:HG22	2:B:282:GLN:NE2	2.25	0.51
3:C:255:VAL:HG11	3:C:267:VAL:CG2	2.40	0.51
5:E:276:LEU:HD21	5:E:284:ILE:HD12	1.92	0.51
12:L:36:ASP:O	12:L:36:ASP:OD2	2.28	0.51
1:A:1113:ILE:HG22	1:A:1137:ILE:HD11	1.91	0.51
2:B:531:LEU:HD21	2:B:538:LEU:HD21	1.93	0.51
3:C:473:SER:O	3:C:474:MET:SD	2.69	0.51
2:B:696:THR:HG21	17:Q:55:LEU:HD11	1.91	0.51
6:F:173:GLU:HG2	6:F:176:PHE:HB3	1.91	0.51
2:B:421:THR:HG23	2:B:423:ASN:H	1.75	0.51
2:B:1041:ARG:CZ	19:S:43:THR:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:23:PHE:O	10:J:31:VAL:HG13	2.11	0.51
15:O:138:ASP:OD1	15:O:138:ASP:O	2.28	0.51
1:A:430:ARG:HG3	19:S:32:GLY:O	2.10	0.51
1:A:322:ASN:ND2	1:A:342:VAL:HG21	2.25	0.51
1:A:1143:GLU:HB3	10:J:53:LEU:HD13	1.92	0.51
2:B:243:MET:HG3	2:B:332:CYS:SG	2.51	0.51
2:B:1028:ARG:O	19:S:40:LEU:HG	2.10	0.51
3:C:310:GLN:O	3:C:314:LEU:HD22	2.11	0.51
6:F:187:PHE:HE2	6:F:216:VAL:HG22	1.76	0.51
1:A:1067:VAL:HG23	1:A:1068:PRO:HD3	1.93	0.51
1:A:1098:ALA:HB3	10:J:77:ALA:HA	1.93	0.51
2:B:277:ILE:HD12	2:B:282:GLN:HB2	1.93	0.51
2:B:886:ARG:NH2	11:K:104:GLU:OE1	2.42	0.51
3:C:258:ARG:NH2	3:C:318:ASP:OD2	2.43	0.51
6:F:140:LYS:CE	23:X:17:DG:H5”	2.40	0.51
7:G:68:MET:SD	7:G:68:MET:N	2.84	0.51
1:A:1104:ARG:HB3	10:J:54:GLY:HA2	1.93	0.50
6:F:231:SER:O	6:F:233:GLU:N	2.44	0.50
1:A:1260:ILE:O	1:A:1263:ALA:N	2.44	0.50
8:H:149:ARG:NH1	8:H:196:GLY:O	2.44	0.50
11:K:97:ASN:ND2	11:K:103:ASP:OD1	2.41	0.50
1:A:1187:TYR:CG	1:A:1187:TYR:O	2.63	0.50
2:B:240:PHE:O	2:B:243:MET:HB3	2.11	0.50
5:E:418:ARG:HA	5:E:421:MET:SD	2.51	0.50
1:A:1210:ALA:HB3	10:J:105:ARG:CZ	2.42	0.50
3:C:93:TYR:HB2	7:G:57:MET:CE	2.41	0.50
5:E:52:LYS:O	5:E:53:GLN:NE2	2.40	0.50
1:A:1195:ASP:H	10:J:44:PRO:HB2	1.75	0.50
6:F:110:ARG:NH2	23:X:15:DC:C3’	2.74	0.50
24:Y:-36:DA:C2	24:Y:-35:DG:C5	3.00	0.50
1:A:140:ARG:O	1:A:144:LYS:HD2	2.11	0.50
2:B:39:LEU:O	2:B:40:VAL:HG12	2.11	0.50
3:C:409:ILE:CD1	3:C:423:LEU:HD22	2.41	0.50
13:M:4:GLU:N	13:M:4:GLU:OE1	2.45	0.50
1:A:309:ASP:HA	1:A:312:PHE:CD2	2.47	0.50
1:A:1089:LEU:HD12	1:A:1089:LEU:N	2.27	0.50
2:B:920:ASP:OD1	2:B:920:ASP:N	2.45	0.50
1:A:739:GLN:OE1	1:A:741:GLY:N	2.45	0.50
6:F:200:GLN:O	6:F:201:ASN:C	2.50	0.50
7:G:60:LEU:C	7:G:60:LEU:HD23	2.32	0.50
16:P:15:MET:H	16:P:15:MET:HE3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:-25:DT:H2'	24:Y:-24:DA:O4'	2.12	0.50
1:A:307:MET:O	1:A:311:ASP:OD2	2.29	0.49
1:A:1185:MET:SD	1:A:1185:MET:N	2.84	0.49
13:M:18:MET:HE1	13:M:33:LEU:HA	1.94	0.49
19:S:133:LEU:HD12	19:S:133:LEU:N	2.26	0.49
1:A:395:LYS:HG2	1:A:449:ILE:HG22	1.94	0.49
1:A:1267:ILE:HD13	1:A:1294:MET:HE3	1.92	0.49
6:F:140:LYS:NZ	23:X:17:DG:H5"	2.28	0.49
9:I:17:PHE:O	9:I:21:THR:HG23	2.12	0.49
3:C:266:ILE:HG22	3:C:270:MET:CE	2.41	0.49
3:C:367:ARG:HD2	6:F:246:GLY:N	2.27	0.49
8:H:40:TYR:CD2	8:H:41:ASN:OD1	2.65	0.49
2:B:192:GLU:OE2	2:B:193:ALA:N	2.45	0.49
6:F:243:ILE:N	6:F:270:TYR:OH	2.45	0.49
4:D:275:LEU:H	4:D:275:LEU:HD12	1.77	0.49
1:A:579:ILE:HD12	1:A:579:ILE:O	2.13	0.49
2:B:80:ILE:HG12	2:B:113:ILE:HD11	1.94	0.49
6:F:78:ASP:O	6:F:80:GLN:N	2.46	0.49
13:M:199:THR:HG23	13:M:201:GLY:H	1.77	0.49
19:S:154:MET:O	19:S:158:LYS:HG2	2.11	0.49
6:F:86:LYS:HE3	6:F:91:GLN:HG3	1.94	0.49
22:W:356:MET:HE2	22:W:378:TYR:HB3	1.95	0.49
24:Y:-27:DA:H2'	24:Y:-26:DA:C8	2.48	0.49
1:A:90:LEU:HD12	1:A:310:TRP:CE2	2.47	0.49
1:A:1143:GLU:CB	10:J:53:LEU:HD13	2.43	0.49
6:F:188:LEU:HD11	6:F:270:TYR:HB3	1.95	0.49
6:F:307:CYS:SG	28:F:401:SF4:S3	3.04	0.49
10:J:74:HIS:HB3	10:J:75:PRO:HD2	1.94	0.49
23:X:22:DA:H2'	23:X:23:DC:H6	1.78	0.49
2:B:391:VAL:HG23	2:B:392:ILE:N	2.28	0.49
1:A:275:ASN:N	19:S:53:VAL:HG22	2.27	0.48
6:F:78:ASP:O	6:F:81:ASN:HB2	2.13	0.48
7:G:57:MET:HE3	7:G:57:MET:HA	1.95	0.48
10:J:95:TYR:CD2	10:J:106:TRP:CZ3	3.01	0.48
14:N:112:ASP:OD2	14:N:112:ASP:C	2.52	0.48
19:S:75:ARG:HA	19:S:78:ASP:OD1	2.12	0.48
24:Y:-18:DG:H1'	24:Y:-17:DA:C8	2.47	0.48
1:A:654:THR:O	1:A:655:LEU:HD12	2.13	0.48
18:R:271:GLU:O	18:R:274:VAL:HG12	2.13	0.48
19:S:124:ILE:HD11	19:S:163:ASP:O	2.13	0.48
22:W:282:LYS:O	22:W:286:ASN:OD1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:LEU:HA	1:A:1192:LEU:HD12	1.94	0.48
1:A:1223:TYR:C	10:J:98:CYS:HA	2.34	0.48
21:U:36:MET:O	21:U:36:MET:SD	2.71	0.48
1:A:1201:VAL:HG22	1:A:1202:GLN:N	2.27	0.48
1:A:1099:ARG:HD3	10:J:78:TYR:C	2.33	0.48
2:B:323:VAL:HG21	2:B:328:PHE:HD1	1.79	0.48
2:B:534:PRO:HD2	2:B:535:ASN:N	2.27	0.48
4:D:271:LEU:HB3	4:D:272:PRO:HD2	1.95	0.48
20:T:313:LEU:O	20:T:317:MET:HG2	2.12	0.48
25:Z:382:VAL:O	25:Z:386:MET:HG3	2.13	0.48
1:A:1113:ILE:HG23	10:J:83:GLN:OE1	2.14	0.48
2:B:550:ARG:NH2	4:D:350:MET:O	2.47	0.48
6:F:296:CYS:SG	6:F:302:ILE:O	2.71	0.48
18:R:269:ARG:HA	19:S:215:TRP:CH2	2.49	0.48
1:A:6:PHE:CD1	1:A:6:PHE:C	2.87	0.48
1:A:995:THR:HG22	1:A:997:PRO:HD2	1.95	0.48
2:B:258:GLU:O	2:B:261:VAL:HG22	2.13	0.48
6:F:251:THR:HB	6:F:268:LYS:HA	1.95	0.48
25:Z:159:MET:HE1	25:Z:344:ILE:HG13	1.96	0.48
25:Z:202:GLN:HG3	25:Z:204:MET:HE1	1.94	0.48
1:A:208:GLU:HB3	1:A:209:PRO:HD3	1.96	0.48
5:E:124:LEU:HD12	5:E:125:HIS:N	2.28	0.48
7:G:63:GLU:O	7:G:67:THR:HG23	2.13	0.48
1:A:142:LEU:HD23	1:A:142:LEU:O	2.13	0.48
3:C:357:ARG:HG3	6:F:289:LEU:HD13	1.96	0.48
4:D:275:LEU:HB3	4:D:276:PRO:HD2	1.96	0.48
1:A:27:GLU:CD	1:A:27:GLU:H	2.17	0.48
1:A:1094:ASP:O	10:J:77:ALA:O	2.32	0.48
1:A:1099:ARG:HH11	1:A:1099:ARG:HB2	1.79	0.47
8:H:197:LEU:HD13	8:H:200:TRP:CZ2	2.49	0.47
13:M:6:GLU:O	13:M:10:LEU:HD23	2.14	0.47
21:U:133:ARG:NH1	25:Z:64:ARG:O	2.46	0.47
1:A:916:ASP:OD1	1:A:916:ASP:N	2.47	0.47
2:B:1030:VAL:HA	19:S:40:LEU:CD2	2.43	0.47
5:E:17:LEU:HD23	5:E:18:ALA:N	2.29	0.47
14:N:86:GLU:H	14:N:86:GLU:CD	2.16	0.47
18:R:183:ILE:HD13	18:R:213:ILE:HG21	1.97	0.47
19:S:119:GLY:O	19:S:122:VAL:HG12	2.14	0.47
23:X:43:DC:H2"	23:X:44:DA:C8	2.49	0.47
1:A:1195:ASP:H	10:J:45:LYS:N	2.12	0.47
2:B:63:GLU:OE1	2:B:63:GLU:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:577:ASN:C	2:B:577:ASN:OD1	2.52	0.47
4:D:132:MET:HG2	4:D:134:PRO:HD2	1.96	0.47
1:A:332:MET:SD	1:A:332:MET:N	2.88	0.47
6:F:84:LYS:HD3	6:F:86:LYS:HD3	1.95	0.47
19:S:136:GLY:O	19:S:140:THR:HG23	2.14	0.47
1:A:238:LEU:C	1:A:239:LEU:HD12	2.35	0.47
4:D:360:LEU:N	4:D:377:GLY:O	2.43	0.47
6:F:310:MET:O	6:F:311:THR:C	2.52	0.47
23:X:14:DA:H61	24:Y:-13:DT:H3	1.61	0.47
2:B:524:ASN:OD1	2:B:524:ASN:C	2.52	0.47
5:E:341:HIS:NE2	5:E:381:ASP:OD1	2.48	0.47
6:F:82:ALA:N	6:F:94:LEU:HD13	2.30	0.47
6:F:269:LEU:HD12	6:F:273:VAL:H	1.78	0.47
13:M:18:MET:CE	13:M:33:LEU:HA	2.45	0.47
1:A:116:MET:HE1	1:A:116:MET:O	2.15	0.47
3:C:86:LEU:HD12	3:C:86:LEU:H	1.79	0.47
3:C:368:LEU:C	3:C:368:LEU:HD23	2.35	0.47
5:E:276:LEU:HD23	5:E:281:GLN:HG2	1.96	0.47
6:F:84:LYS:HD3	6:F:86:LYS:CD	2.44	0.47
6:F:184:CYS:O	6:F:188:LEU:HG	2.14	0.47
13:M:110:MET:SD	13:M:115:LYS:HG3	2.55	0.47
15:O:32:SER:OG	15:O:37:MET:N	2.48	0.47
23:X:15:DC:H2'	23:X:16:DT:C6	2.49	0.47
24:Y:-31:DT:H3'	24:Y:-30:DT:H71	1.96	0.47
1:A:579:ILE:HD12	1:A:579:ILE:C	2.34	0.47
1:A:1264:ARG:NH1	1:A:1292:ASP:OD1	2.47	0.47
2:B:1126:LEU:HD12	2:B:1126:LEU:O	2.15	0.47
6:F:237:THR:O	6:F:241:THR:HG23	2.15	0.47
9:I:20:LEU:HD23	9:I:20:LEU:O	2.15	0.47
9:I:66:VAL:HG13	9:I:87:LEU:HD21	1.97	0.47
6:F:81:ASN:O	6:F:82:ALA:O	2.33	0.47
6:F:280:THR:O	6:F:283:VAL:HG23	2.15	0.47
23:X:39:DC:H2"	23:X:40:DA:C8	2.50	0.47
1:A:156:CYS:O	1:A:160:GLY:N	2.47	0.47
1:A:1157:LYS:HE3	1:A:1157:LYS:HA	1.96	0.47
2:B:1041:ARG:NH2	19:S:42:THR:HG23	2.29	0.47
2:B:1073:ASP:OD1	2:B:1073:ASP:N	2.48	0.47
11:K:209:ASP:OD2	11:K:209:ASP:C	2.54	0.46
23:X:18:DT:H2"	23:X:19:DC:C6	2.50	0.46
2:B:1112:LEU:HD23	2:B:1112:LEU:O	2.16	0.46
6:F:239:LEU:O	6:F:243:ILE:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:240:ASN:O	6:F:243:ILE:HG12	2.15	0.46
24:Y:-51:DA:H4'	24:Y:-50:DG:OP1	2.15	0.46
1:A:42:TYR:HB2	19:S:59:THR:HG22	1.98	0.46
23:X:53:DT:C6	23:X:53:DT:OP2	2.69	0.46
3:C:383:PHE:HB3	6:F:244:TYR:CD2	2.50	0.46
6:F:270:TYR:O	6:F:271:ARG:C	2.54	0.46
19:S:120:CYS:SG	19:S:156:ILE:HG21	2.55	0.46
1:A:850:HIS:CD2	2:B:680:SER:OG	2.69	0.46
2:B:791:MET:SD	2:B:791:MET:N	2.89	0.46
10:J:83:GLN:HA	10:J:91:MET:HG2	1.98	0.46
13:M:104:ILE:HD11	13:M:127:LEU:HD12	1.98	0.46
13:M:163:TYR:HB3	13:M:165:LEU:HD13	1.97	0.46
1:A:771:LEU:HD21	1:A:775:ASN:ND2	2.31	0.46
1:A:1153:ILE:HG22	1:A:1154:CYS:N	2.30	0.46
1:A:1204:ILE:H	10:J:51:ASP:HB2	1.81	0.46
5:E:244:GLU:O	5:E:247:MET:SD	2.74	0.46
6:F:286:PRO:O	6:F:287:CYS:C	2.53	0.46
1:A:1193:LYS:HA	10:J:44:PRO:HB3	1.97	0.46
2:B:1056:ILE:HG22	2:B:1056:ILE:O	2.16	0.46
6:F:275:PRO:O	6:F:276:ILE:C	2.54	0.46
23:X:52:DT:C2'	23:X:53:DT:H72	2.46	0.46
23:X:52:DT:H1'	23:X:53:DT:OP2	2.16	0.46
1:A:308:GLU:HA	1:A:311:ASP:OD2	2.16	0.46
1:A:724:CYS:O	1:A:728:ILE:HG22	2.16	0.46
1:A:736:LEU:HD12	1:A:737:GLN:N	2.31	0.46
1:A:856:GLU:OE1	1:A:856:GLU:HA	2.15	0.46
1:A:882:LEU:HD11	1:A:1293:LEU:HD12	1.98	0.46
1:A:1099:ARG:HD3	10:J:79:PHE:HA	1.96	0.46
3:C:349:THR:O	3:C:353:VAL:HG13	2.15	0.46
3:C:357:ARG:NE	6:F:289:LEU:HA	2.31	0.46
6:F:93:LYS:HA	6:F:96:TYR:HB3	1.98	0.46
6:F:167:TYR:HA	6:F:172:PHE:HA	1.98	0.46
6:F:266:HIS:CG	6:F:266:HIS:O	2.69	0.46
12:L:37:ARG:O	12:L:37:ARG:HG2	2.16	0.46
24:Y:-49:DA:H2'	24:Y:-48:DT:H72	1.98	0.46
1:A:1104:ARG:CD	10:J:55:GLY:O	2.64	0.45
2:B:433:ARG:C	2:B:434:GLN:OE1	2.54	0.45
2:B:1027:PRO:CB	19:S:39:VAL:O	2.63	0.45
3:C:36:LEU:HD23	3:C:36:LEU:C	2.37	0.45
4:D:117:MET:C	4:D:117:MET:SD	2.94	0.45
6:F:268:LYS:O	6:F:269:LEU:HD22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:86:SER:HB3	10:J:89:GLU:OE2	2.17	0.45
19:S:73:LEU:O	19:S:77:ARG:HG3	2.16	0.45
5:E:366:VAL:HG13	5:E:366:VAL:O	2.16	0.45
19:S:158:LYS:CE	24:Y:-29:DA:OP1	2.64	0.45
1:A:612:PRO:HA	1:A:614:ARG:HH12	1.81	0.45
1:A:877:LYS:HE3	1:A:1317:MET:SD	2.57	0.45
7:G:84:ILE:HD13	8:H:80:PHE:CE2	2.52	0.45
9:I:10:LEU:N	9:I:10:LEU:HD22	2.31	0.45
24:Y:-23:DG:H2'	24:Y:-22:DG:C8	2.52	0.45
1:A:709:LEU:O	1:A:709:LEU:HD23	2.16	0.45
1:A:1067:VAL:CG2	1:A:1068:PRO:HD3	2.46	0.45
2:B:322:PRO:HD2	2:B:322:PRO:O	2.16	0.45
6:F:303:SER:O	6:F:305:SER:N	2.49	0.45
7:G:48:LEU:H	7:G:48:LEU:CD2	2.28	0.45
24:Y:-30:DT:C2	24:Y:-29:DA:C8	3.05	0.45
3:C:257:ASN:O	6:F:274:ASN:ND2	2.50	0.45
6:F:103:GLY:O	6:F:151:MET:SD	2.74	0.45
6:F:134:LYS:HA	6:F:153:TYR:CE1	2.52	0.45
2:B:243:MET:SD	2:B:328:PHE:HB3	2.57	0.45
3:C:384:ALA:O	3:C:385:MET:HG2	2.16	0.45
6:F:190:SER:O	6:F:194:THR:HG23	2.17	0.45
19:S:151:SER:O	19:S:154:MET:HG3	2.16	0.45
1:A:654:THR:O	1:A:654:THR:HG22	2.17	0.45
1:A:1043:GLU:HB3	1:A:1044:PRO:HD2	1.98	0.45
2:B:277:ILE:HD11	2:B:283:ALA:HA	1.99	0.45
7:G:80:GLU:OE1	7:G:80:GLU:N	2.50	0.45
8:H:63:ASP:OD1	8:H:64:GLY:N	2.50	0.45
19:S:147:ASP:OD1	19:S:148:VAL:N	2.49	0.45
19:S:199:LYS:NZ	19:S:237:LEU:HD13	2.31	0.45
1:A:1105:ILE:HA	10:J:51:ASP:OD2	2.16	0.45
2:B:25:GLU:O	2:B:611:MET:HE2	2.16	0.45
2:B:410:GLN:HA	2:B:410:GLN:OE1	2.17	0.45
2:B:1128:LEU:H	2:B:1128:LEU:HD23	1.82	0.45
25:Z:383:CYS:HA	25:Z:386:MET:SD	2.57	0.45
1:A:1082:THR:O	1:A:1082:THR:HG23	2.17	0.45
1:A:1099:ARG:NH2	10:J:95:TYR:HA	2.32	0.45
2:B:801:LYS:HE3	2:B:802:PRO:HD2	1.99	0.45
6:F:283:VAL:HA	6:F:289:LEU:HD21	1.98	0.45
1:A:97:TYR:HB2	1:A:250:LEU:HD21	1.99	0.45
1:A:144:LYS:HD2	1:A:144:LYS:N	2.32	0.45
2:B:524:ASN:ND2	5:E:107:THR:O	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:200:GLN:O	6:F:205:GLN:N	2.50	0.45
1:A:1379:PHE:CD2	1:A:1380:ASP:OD1	2.71	0.44
6:F:277:ILE:HB	6:F:278:PRO:HD2	2.00	0.44
11:K:133:THR:O	11:K:137:THR:HG22	2.17	0.44
23:X:47:DT:H2"	23:X:48:DC:C6	2.52	0.44
1:A:1070:ILE:O	1:A:1074:ILE:HD12	2.17	0.44
3:C:3:GLN:CD	3:C:3:GLN:H	2.20	0.44
3:C:372:LYS:HE3	6:F:244:TYR:CZ	2.52	0.44
6:F:295:ASP:O	6:F:297:HIS:N	2.51	0.44
8:H:28:GLU:C	8:H:28:GLU:OE2	2.56	0.44
19:S:10:CYS:SG	19:S:31:CYS:HB3	2.57	0.44
5:E:289:VAL:HG21	5:E:292:MET:HE3	1.99	0.44
6:F:310:MET:O	6:F:314:LEU:HG	2.18	0.44
1:A:195:GLN:O	1:A:198:GLU:OE2	2.36	0.44
1:A:1204:ILE:HD12	10:J:51:ASP:CB	2.47	0.44
3:C:85:MET:CE	3:C:85:MET:H	2.31	0.44
3:C:365:ILE:HG21	3:C:395:LEU:HD11	1.98	0.44
6:F:228:VAL:HG12	6:F:229:GLU:N	2.32	0.44
6:F:308:ILE:HD12	6:F:308:ILE:HA	1.87	0.44
1:A:241:ASN:OD1	1:A:243:GLU:OE1	2.35	0.44
1:A:1223:TYR:CD2	10:J:104:HIS:CG	3.06	0.44
6:F:84:LYS:HA	6:F:86:LYS:HD2	1.98	0.44
6:F:243:ILE:O	6:F:248:VAL:HG11	2.17	0.44
6:F:302:ILE:O	6:F:303:SER:C	2.55	0.44
11:K:238:ASP:CG	11:K:238:ASP:O	2.54	0.44
22:W:356:MET:SD	22:W:356:MET:C	2.96	0.44
25:Z:156:VAL:O	25:Z:159:MET:HE3	2.18	0.44
1:A:383:PRO:HB3	1:A:483:HIS:O	2.18	0.44
1:A:1207:VAL:HG12	1:A:1208:SER:N	2.32	0.44
3:C:159:ARG:N	3:C:187:MET:SD	2.90	0.44
9:I:5:ASP:OD1	9:I:7:ASN:N	2.45	0.44
19:S:78:ASP:HA	19:S:81:ARG:HG2	2.00	0.44
21:U:8:GLN:OE1	21:U:8:GLN:N	2.46	0.44
1:A:1097:TYR:O	1:A:1097:TYR:CG	2.71	0.44
2:B:1086:LEU:H	2:B:1086:LEU:CD2	2.31	0.44
3:C:386:ILE:CG2	3:C:391:ALA:HB2	2.47	0.44
4:D:363:VAL:HA	4:D:373:MET:CE	2.46	0.44
4:D:373:MET:SD	5:E:208:LEU:CB	3.06	0.44
6:F:110:ARG:NH2	23:X:15:DC:C4'	2.81	0.44
2:B:555:LEU:C	2:B:555:LEU:HD23	2.39	0.44
5:E:293:PRO:HD2	5:E:296:ASN:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:370:GLU:OE1	5:E:370:GLU:N	2.50	0.44
22:W:316:GLU:OE2	25:Z:396:LEU:HD22	2.18	0.44
1:A:26:GLU:OE2	6:F:295:ASP:HA	2.18	0.44
1:A:1033:VAL:HG13	1:A:1034:GLY:N	2.33	0.44
1:A:1197:PRO:CD	10:J:45:LYS:HA	2.48	0.44
3:C:116:LEU:HD11	3:C:120:ALA:HB3	2.00	0.44
9:I:94:ALA:HA	9:I:97:ILE:HG12	1.99	0.44
1:A:401:ILE:HG23	1:A:402:ASN:N	2.32	0.43
1:A:1261:GLU:OE2	13:M:207:ARG:NH1	2.51	0.43
6:F:245:ASP:OD1	6:F:245:ASP:C	2.56	0.43
23:X:19:DC:H1'	23:X:20:DA:C5	2.53	0.43
5:E:65:LEU:N	5:E:65:LEU:HD22	2.33	0.43
9:I:96:GLU:O	9:I:100:MET:SD	2.76	0.43
13:M:18:MET:CE	13:M:33:LEU:HD23	2.48	0.43
21:U:105:ASP:OD1	21:U:106:GLU:N	2.51	0.43
1:A:1120:VAL:HG12	1:A:1127:PHE:O	2.18	0.43
2:B:785:GLN:HE22	19:S:129:HIS:CD2	2.35	0.43
3:C:21:VAL:HG13	3:C:57:LEU:HD11	2.00	0.43
11:K:116:HIS:CG	11:K:116:HIS:O	2.71	0.43
13:M:92:GLN:O	13:M:96:GLU:HG2	2.18	0.43
19:S:75:ARG:O	19:S:79:LEU:HG	2.18	0.43
1:A:116:MET:O	1:A:116:MET:CE	2.66	0.43
1:A:1222:LYS:C	1:A:1223:TYR:CD1	2.92	0.43
2:B:533:TYR:N	2:B:533:TYR:CD1	2.85	0.43
2:B:785:GLN:HA	2:B:785:GLN:OE1	2.18	0.43
2:B:805:ARG:O	2:B:826:VAL:HG12	2.19	0.43
1:A:1088:GLN:O	1:A:1242:LYS:N	2.48	0.43
1:A:1318:LEU:HD23	1:A:1327:HIS:CD2	2.53	0.43
2:B:243:MET:SD	2:B:328:PHE:CB	3.06	0.43
6:F:270:TYR:O	6:F:272:ALA:N	2.51	0.43
12:L:55:LEU:O	12:L:59:ILE:HG12	2.18	0.43
18:R:171:THR:HG22	18:R:220:VAL:HG12	2.00	0.43
1:A:130:LYS:HE3	1:A:130:LYS:HA	2.01	0.43
2:B:515:ALA:O	2:B:520:VAL:HG12	2.18	0.43
18:R:210:THR:HG21	23:X:27:DT:H4'	2.00	0.43
23:X:-12:DC:H2"	23:X:-11:DC:C6	2.54	0.43
1:A:55:VAL:O	1:A:56:LEU:HB2	2.19	0.43
1:A:1099:ARG:HG3	10:J:77:ALA:HB1	1.95	0.43
1:A:1224:LYS:N	10:J:98:CYS:HA	2.33	0.43
3:C:255:VAL:HG13	3:C:259:MET:CE	2.48	0.43
13:M:61:LEU:HD23	13:M:61:LEU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LYS:HD2	1:A:130:LYS:N	2.34	0.43
1:A:1099:ARG:HD3	10:J:78:TYR:O	2.19	0.43
1:A:1143:GLU:HG3	10:J:53:LEU:HD13	2.01	0.43
3:C:343:ALA:HA	3:C:526:TYR:CE1	2.54	0.43
5:E:282:ILE:O	5:E:286:MET:HG2	2.17	0.43
9:I:1:MET:SD	9:I:1:MET:C	2.97	0.43
13:M:89:VAL:O	13:M:92:GLN:HG3	2.19	0.43
24:Y:-16:DC:H2'	24:Y:-15:DA:C8	2.53	0.43
25:Z:99:GLU:OE1	25:Z:99:GLU:HA	2.19	0.43
1:A:1143:GLU:HG3	1:A:1143:GLU:O	2.19	0.43
1:A:1167:VAL:O	1:A:1167:VAL:HG13	2.19	0.43
1:A:1188:VAL:HG23	1:A:1191:PHE:HD1	1.83	0.43
1:A:1199:VAL:CG1	1:A:1200:VAL:N	2.82	0.43
2:B:54:GLU:OE1	2:B:370:SER:HB2	2.19	0.43
3:C:106:ILE:HD13	3:C:125:VAL:HG21	2.00	0.43
6:F:84:LYS:CB	6:F:94:LEU:HD23	2.49	0.43
6:F:176:PHE:CD2	6:F:176:PHE:O	2.72	0.43
6:F:187:PHE:CE2	6:F:216:VAL:HG22	2.53	0.43
7:G:81:ARG:HG3	7:G:81:ARG:O	2.18	0.43
7:G:100:ILE:O	7:G:100:ILE:HG13	2.19	0.43
1:A:177:GLU:HG3	1:A:180:LYS:HB3	2.01	0.43
1:A:221:LEU:HD12	1:A:221:LEU:H	1.82	0.43
1:A:1170:GLU:OE1	1:A:1170:GLU:N	2.48	0.43
1:A:1226:LEU:N	1:A:1226:LEU:HD12	2.34	0.43
2:B:622:GLU:OE2	2:B:622:GLU:C	2.57	0.43
6:F:286:PRO:O	6:F:289:LEU:N	2.51	0.43
7:G:48:LEU:HD23	7:G:48:LEU:N	2.33	0.43
21:U:36:MET:HE1	21:U:38:PHE:HA	2.01	0.43
1:A:1090:ASP:OD2	10:J:76:ARG:NH2	2.50	0.42
1:A:1107:LYS:O	1:A:1108:THR:HG23	2.19	0.42
9:I:20:LEU:HD22	9:I:50:LEU:HD13	2.01	0.42
19:S:362:MET:SD	19:S:362:MET:C	2.98	0.42
1:A:1257:THR:HB	1:A:1258:LEU:HD12	2.01	0.42
2:B:1029:ALA:C	19:S:40:LEU:HD23	2.39	0.42
1:A:315:LEU:C	1:A:315:LEU:HD23	2.40	0.42
1:A:1210:ALA:H	10:J:105:ARG:NH2	2.17	0.42
2:B:117:ILE:HD12	2:B:118:GLU:H	1.85	0.42
5:E:49:ILE:CG2	5:E:208:LEU:HD11	2.50	0.42
5:E:92:TYR:CE2	5:E:97:MET:SD	3.12	0.42
7:G:89:LYS:HA	7:G:92:MET:SD	2.60	0.42
18:R:166:GLN:OE1	18:R:259:VAL:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:30:DT:H2'	23:X:31:DA:N7	2.35	0.42
1:A:341:PHE:O	1:A:344:ARG:HG2	2.19	0.42
1:A:873:ARG:HG3	1:A:873:ARG:HH11	1.84	0.42
1:A:1100:LEU:HA	10:J:80:MET:HG2	2.01	0.42
2:B:225:LEU:HD23	2:B:226:ARG:N	2.34	0.42
2:B:514:LEU:HD13	5:E:250:MET:CE	2.50	0.42
3:C:409:ILE:CD1	3:C:423:LEU:HB2	2.49	0.42
3:C:521:PHE:O	3:C:524:GLU:HG3	2.20	0.42
4:D:274:THR:HB	4:D:315:ALA:HB1	2.00	0.42
5:E:48:LYS:HB3	5:E:205:TRP:CE3	2.54	0.42
6:F:176:PHE:CD2	6:F:176:PHE:C	2.93	0.42
8:H:149:ARG:HG3	8:H:149:ARG:HH11	1.83	0.42
1:A:1067:VAL:N	1:A:1068:PRO:CD	2.83	0.42
1:A:1111:GLY:O	1:A:1113:ILE:N	2.52	0.42
2:B:171:VAL:O	2:B:174:VAL:HG12	2.19	0.42
2:B:220:GLN:OE1	2:B:222:ARG:HG3	2.19	0.42
2:B:277:ILE:O	2:B:277:ILE:CG2	2.67	0.42
3:C:385:MET:SD	6:F:181:ASN:ND2	2.92	0.42
5:E:29:GLN:O	5:E:135:LEU:HD12	2.19	0.42
6:F:94:LEU:O	6:F:98:ILE:HG12	2.19	0.42
6:F:173:GLU:CG	6:F:176:PHE:HB3	2.49	0.42
6:F:278:PRO:HB2	6:F:279:PRO:CD	2.50	0.42
8:H:131:TYR:CG	8:H:132:GLU:N	2.87	0.42
10:J:22:ARG:NH1	10:J:31:VAL:HG11	2.34	0.42
1:A:1223:TYR:HB3	10:J:97:CYS:O	2.20	0.42
2:B:213:ARG:NH2	2:B:215:ASN:OD1	2.52	0.42
3:C:512:SER:OG	6:F:313:TRP:HH2	1.98	0.42
24:Y:-24:DA:H2'	24:Y:-23:DG:O4'	2.19	0.42
1:A:771:LEU:HD21	1:A:775:ASN:HD22	1.84	0.42
5:E:13:ILE:HD11	5:E:123:GLU:N	2.34	0.42
6:F:174:SER:HA	6:F:177:VAL:HG22	2.02	0.42
12:L:40:VAL:HG12	12:L:92:ALA:HB3	2.02	0.42
19:S:257:ASP:OD1	19:S:257:ASP:O	2.38	0.42
22:W:356:MET:CE	22:W:378:TYR:HB3	2.50	0.42
1:A:249:ASP:C	1:A:249:ASP:OD1	2.57	0.42
2:B:243:MET:SD	2:B:243:MET:O	2.77	0.42
6:F:316:PHE:HE2	7:G:45:PRO:HG2	1.84	0.42
12:L:30:VAL:HG23	12:L:30:VAL:O	2.19	0.42
13:M:110:MET:HG2	13:M:114:ALA:HB3	2.01	0.42
1:A:368:VAL:HG12	1:A:369:ILE:N	2.34	0.42
1:A:1236:MET:SD	1:A:1236:MET:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:253:ILE:O	6:F:253:ILE:HG22	2.20	0.42
10:J:48:GLU:O	10:J:48:GLU:HG2	2.18	0.42
13:M:27:LEU:HD13	13:M:64:HIS:CB	2.49	0.42
19:S:153:TYR:O	19:S:157:VAL:HG13	2.20	0.42
1:A:97:TYR:O	1:A:101:VAL:HG23	2.20	0.42
1:A:129:LEU:HD22	1:A:142:LEU:HD11	2.02	0.42
1:A:278:ASP:OD1	1:A:278:ASP:N	2.53	0.42
1:A:305:MET:SD	1:A:305:MET:N	2.87	0.42
1:A:1136:ARG:O	1:A:1140:LEU:HG	2.19	0.42
2:B:392:ILE:CG2	2:B:393:PRO:HD3	2.50	0.42
2:B:526:LEU:C	2:B:526:LEU:HD12	2.40	0.42
2:B:694:MET:SD	2:B:710:TYR:HB3	2.60	0.42
3:C:85:MET:HA	3:C:88:TYR:CD1	2.55	0.42
3:C:118:MET:O	3:C:121:VAL:HG12	2.19	0.42
5:E:341:HIS:CD2	5:E:380:GLU:OE2	2.73	0.42
6:F:91:GLN:HB3	6:F:126:ILE:HG13	2.01	0.42
6:F:175:GLU:O	6:F:178:GLU:HG2	2.20	0.42
6:F:181:ASN:OD1	6:F:238:ILE:HG12	2.20	0.42
8:H:38:VAL:HG11	8:H:183:PRO:HG2	2.02	0.42
11:K:268:GLN:OE1	11:K:268:GLN:N	2.53	0.42
23:X:58:DT:C6	23:X:59:DT:H72	2.55	0.42
1:A:55:VAL:HG22	1:A:56:LEU:H	1.85	0.41
3:C:391:ALA:O	3:C:394:MET:N	2.51	0.41
3:C:395:LEU:HD22	3:C:395:LEU:H	1.85	0.41
5:E:286:MET:HB3	5:E:327:VAL:HG12	2.02	0.41
6:F:116:SER:O	6:F:117:ASN:HB2	2.19	0.41
12:L:44:LEU:N	12:L:44:LEU:HD12	2.35	0.41
20:T:312:PHE:HA	20:T:315:ILE:CG2	2.50	0.41
23:X:52:DT:H2"	23:X:53:DT:H72	2.02	0.41
1:A:322:ASN:ND2	1:A:342:VAL:HG11	2.35	0.41
1:A:322:ASN:HD21	1:A:342:VAL:HG21	1.84	0.41
1:A:775:ASN:OD1	1:A:776:SER:N	2.53	0.41
1:A:1122:LEU:HD22	1:A:1124:ASP:OD1	2.20	0.41
1:A:1130:VAL:HB	1:A:1173:VAL:HG13	2.01	0.41
1:A:1235:VAL:HG13	1:A:1236:MET:N	2.35	0.41
2:B:801:LYS:HB3	2:B:802:PRO:HD2	2.02	0.41
2:B:862:THR:HG22	2:B:863:ASP:N	2.34	0.41
3:C:342:LEU:HA	3:C:345:LEU:HD23	2.02	0.41
3:C:362:CYS:HA	3:C:394:MET:SD	2.60	0.41
3:C:407:GLN:OE1	3:C:409:ILE:HG13	2.19	0.41
3:C:409:ILE:HG22	3:C:410:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:522:LEU:HD12	3:C:522:LEU:O	2.20	0.41
4:D:363:VAL:HG23	4:D:373:MET:HE2	2.00	0.41
5:E:368:ARG:NH1	5:E:370:GLU:OE2	2.51	0.41
6:F:188:LEU:HD12	6:F:189:GLN:N	2.35	0.41
6:F:235:ILE:CG2	6:F:236:GLU:N	2.82	0.41
23:X:34:DC:H4'	23:X:34:DC:OP1	2.20	0.41
24:Y:-36:DA:N3	24:Y:-35:DG:N7	2.68	0.41
25:Z:180:LEU:HD23	25:Z:328:LEU:HD23	2.01	0.41
1:A:144:LYS:HD2	1:A:144:LYS:H	1.85	0.41
1:A:250:LEU:O	1:A:250:LEU:HD23	2.19	0.41
1:A:876:VAL:HG11	2:B:1053:ASP:OD1	2.20	0.41
1:A:1092:ASP:HB3	10:J:99:ASN:N	2.35	0.41
6:F:160:SER:C	6:F:162:THR:N	2.74	0.41
6:F:267:MET:O	6:F:268:LYS:C	2.58	0.41
1:A:55:VAL:HG13	1:A:56:LEU:HD13	2.01	0.41
2:B:264:ALA:HB3	2:B:343:ILE:HD11	2.02	0.41
2:B:506:MET:SD	2:B:569:ASN:ND2	2.94	0.41
3:C:90:ARG:NH1	3:C:518:GLU:OE1	2.50	0.41
23:X:55:DT:H2"	23:X:56:DG:H5'	2.02	0.41
1:A:90:LEU:HD13	1:A:91:PRO:HD2	2.02	0.41
1:A:278:ASP:HA	1:A:281:MET:HG2	2.03	0.41
1:A:731:LEU:HD22	1:A:748:LEU:HD22	2.01	0.41
1:A:771:LEU:HD22	1:A:778:LEU:HD22	2.02	0.41
1:A:876:VAL:CG2	2:B:1053:ASP:OD1	2.67	0.41
1:A:890:VAL:HG22	1:A:899:GLN:HB2	2.02	0.41
1:A:1122:LEU:HD23	1:A:1123:PRO:CD	2.51	0.41
2:B:135:ARG:HG2	2:B:135:ARG:HH11	1.84	0.41
2:B:226:ARG:HD3	2:B:226:ARG:HA	1.97	0.41
3:C:528:GLU:HA	3:C:528:GLU:OE1	2.20	0.41
18:R:294:ARG:NH2	24:Y:-28:DA:OP1	2.53	0.41
22:W:211:LYS:O	22:W:215:LEU:HD23	2.21	0.41
2:B:79:ASN:OD1	2:B:79:ASN:C	2.57	0.41
2:B:113:ILE:HG22	2:B:134:GLY:C	2.41	0.41
2:B:243:MET:CG	2:B:332:CYS:SG	3.08	0.41
2:B:431:MET:SD	2:B:431:MET:C	2.99	0.41
19:S:197:LYS:HD3	19:S:201:LEU:HD13	2.03	0.41
24:Y:-31:DT:H2'	24:Y:-30:DT:C6	2.55	0.41
25:Z:151:ARG:HD3	25:Z:151:ARG:N	2.35	0.41
25:Z:213:THR:HG21	25:Z:294:GLU:CD	2.41	0.41
1:A:126:LEU:HD12	1:A:130:LYS:HD3	2.02	0.41
1:A:1134:LEU:HD11	1:A:1171:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:622:GLU:OE2	2:B:622:GLU:O	2.38	0.41
6:F:82:ALA:CA	6:F:94:LEU:HD13	2.51	0.41
18:R:295:MET:HE1	18:R:302:LEU:HD11	2.02	0.41
1:A:397:ASN:OD1	1:A:397:ASN:C	2.59	0.41
1:A:743:THR:HG22	1:A:746:GLU:OE1	2.21	0.41
3:C:118:MET:HG3	3:C:119:SER:N	2.36	0.41
3:C:524:GLU:HA	3:C:527:ILE:HG22	2.01	0.41
4:D:137:ILE:HD11	10:J:33:ASN:H	1.85	0.41
6:F:293:PHE:CD1	28:F:401:SF4:S2	3.14	0.41
19:S:61:GLU:O	19:S:62:ASN:CG	2.59	0.41
1:A:211:LEU:HD12	1:A:211:LEU:C	2.41	0.41
2:B:30:LEU:HB3	2:B:31:PRO:HD3	2.01	0.41
2:B:245:VAL:O	2:B:245:VAL:HG23	2.21	0.41
2:B:258:GLU:HG3	2:B:260:HIS:ND1	2.36	0.41
2:B:662:PHE:CD1	2:B:662:PHE:C	2.94	0.41
6:F:86:LYS:HE3	6:F:91:GLN:HA	2.01	0.41
19:S:183:PHE:CE1	19:S:200:MET:HG2	2.56	0.41
19:S:223:LEU:HD12	19:S:223:LEU:H	1.85	0.41
22:W:207:PRO:O	22:W:211:LYS:HG2	2.21	0.41
1:A:1112:GLU:OE1	10:J:83:GLN:NE2	2.54	0.41
1:A:1212:ILE:CD1	10:J:106:TRP:HA	2.49	0.41
1:A:1236:MET:SD	1:A:1236:MET:O	2.79	0.41
4:D:382:LYS:C	4:D:383:LEU:HD22	2.42	0.41
6:F:244:TYR:O	6:F:245:ASP:HB3	2.21	0.41
18:R:213:ILE:HD13	18:R:219:MET:HG3	2.02	0.41
22:W:334:LEU:HD12	22:W:337:PHE:HD2	1.85	0.41
1:A:219:ASN:O	1:A:222:VAL:HG12	2.21	0.40
3:C:477:THR:O	3:C:477:THR:HG22	2.21	0.40
6:F:206:ARG:O	6:F:210:PHE:CD1	2.74	0.40
1:A:98:PHE:CE1	1:A:172:LEU:HD12	2.56	0.40
1:A:1096:ASP:H	10:J:77:ALA:H	1.68	0.40
1:A:1157:LYS:HA	1:A:1157:LYS:CE	2.52	0.40
2:B:784:ASN:O	2:B:786:THR:N	2.54	0.40
2:B:1029:ALA:O	2:B:1033:ARG:HA	2.20	0.40
6:F:303:SER:C	6:F:305:SER:H	2.25	0.40
19:S:174:LYS:HD2	19:S:174:LYS:O	2.20	0.40
23:X:22:DA:H2'	23:X:23:DC:C6	2.55	0.40
25:Z:202:GLN:HG3	25:Z:204:MET:CE	2.52	0.40
1:A:126:LEU:CD1	1:A:130:LYS:HD3	2.51	0.40
1:A:902:TYR:CE1	1:A:1033:VAL:HG21	2.55	0.40
5:E:368:ARG:HG2	5:E:371:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:94:LEU:HD12	6:F:94:LEU:HA	1.99	0.40
8:H:198:LEU:H	8:H:198:LEU:HD12	1.86	0.40
10:J:86:SER:C	10:J:89:GLU:OE1	2.60	0.40
13:M:18:MET:HE2	13:M:33:LEU:HD23	2.03	0.40
13:M:31:ASP:N	13:M:31:ASP:OD2	2.54	0.40
13:M:167:GLU:CD	13:M:168:ASN:N	2.75	0.40
18:R:166:GLN:OE1	18:R:166:GLN:N	2.47	0.40
19:S:93:ALA:HA	19:S:125:THR:HG21	2.02	0.40
22:W:356:MET:CE	22:W:379:MET:HB3	2.51	0.40
1:A:1145:ASN:OD1	1:A:1148:THR:HG23	2.21	0.40
2:B:570:GLU:OE1	2:B:625:LEU:CD1	2.67	0.40
3:C:21:VAL:CG1	3:C:57:LEU:HD11	2.51	0.40
6:F:245:ASP:CG	6:F:247:LYS:HG2	2.41	0.40
13:M:193:ILE:HD12	13:M:193:ILE:N	2.36	0.40
1:A:198:GLU:H	1:A:198:GLU:CD	2.24	0.40
1:A:426:THR:HB	1:A:428:MET:CE	2.51	0.40
1:A:1239:HIS:ND1	1:A:1240:GLY:N	2.68	0.40
4:D:153:GLN:CD	4:D:154:ILE:HG12	2.42	0.40
5:E:293:PRO:O	5:E:296:ASN:OD1	2.40	0.40
5:E:321:VAL:HG13	5:E:361:THR:HG22	2.02	0.40
5:E:357:MET:O	5:E:361:THR:HG23	2.22	0.40
6:F:247:LYS:HA	6:F:247:LYS:HE2	2.04	0.40
7:G:83:ASP:OD1	7:G:84:ILE:N	2.48	0.40
8:H:17:GLN:O	8:H:19:GLU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1377/1390 (99%)	1292 (94%)	83 (6%)	2 (0%)	48 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	1091/1133 (96%)	1039 (95%)	51 (5%)	1 (0%)	48 78
3	C	508/534 (95%)	496 (98%)	12 (2%)	0	100 100
4	D	180/398 (45%)	177 (98%)	3 (2%)	0	100 100
5	E	396/708 (56%)	378 (96%)	18 (4%)	0	100 100
6	F	300/316 (95%)	230 (77%)	50 (17%)	20 (7%)	1 7
7	G	80/223 (36%)	76 (95%)	4 (5%)	0	100 100
8	H	185/204 (91%)	175 (95%)	10 (5%)	0	100 100
9	I	122/148 (82%)	121 (99%)	1 (1%)	0	100 100
10	J	105/108 (97%)	85 (81%)	20 (19%)	0	100 100
11	K	341/346 (99%)	329 (96%)	12 (4%)	0	100 100
12	L	105/133 (79%)	97 (92%)	8 (8%)	0	100 100
13	M	207/210 (99%)	203 (98%)	4 (2%)	0	100 100
14	N	76/127 (60%)	71 (93%)	5 (7%)	0	100 100
15	O	146/150 (97%)	142 (97%)	4 (3%)	0	100 100
16	P	44/58 (76%)	41 (93%)	3 (7%)	0	100 100
17	Q	64/67 (96%)	63 (98%)	1 (2%)	0	100 100
18	R	176/200 (88%)	176 (100%)	0	0	100 100
19	S	357/419 (85%)	345 (97%)	12 (3%)	0	100 100
20	T	76/484 (16%)	74 (97%)	2 (3%)	0	100 100
21	U	139/368 (38%)	136 (98%)	3 (2%)	0	100 100
22	W	240/1519 (16%)	234 (98%)	6 (2%)	0	100 100
25	Z	383/411 (93%)	375 (98%)	8 (2%)	0	100 100
All	All	6698/9654 (69%)	6355 (95%)	320 (5%)	23 (0%)	38 66

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	82	ALA
6	F	161	VAL
6	F	268	LYS
6	F	273	VAL
6	F	295	ASP
6	F	296	CYS
6	F	86	LYS

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Mol	Chain	Res	Type
6	F	232	MET
6	F	263	VAL
6	F	298	GLU
6	F	307	CYS
6	F	159	ARG
6	F	294	ASP
6	F	306	ASN
1	A	1197	PRO
2	B	40	VAL
6	F	275	PRO
6	F	286	PRO
1	A	612	PRO
6	F	276	ILE
6	F	202	PRO
6	F	279	PRO
6	F	302	ILE

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	A	1204/1212 (99%)	1173 (97%)	31 (3%)	41 64
2	B	959/988 (97%)	942 (98%)	17 (2%)	54 73
3	C	458/476 (96%)	449 (98%)	9 (2%)	50 70
4	D	167/347 (48%)	159 (95%)	8 (5%)	21 48
5	E	358/622 (58%)	338 (94%)	20 (6%)	17 43
6	F	268/280 (96%)	246 (92%)	22 (8%)	9 31
7	G	79/195 (40%)	72 (91%)	7 (9%)	8 27
8	H	168/181 (93%)	166 (99%)	2 (1%)	67 80
9	I	116/136 (85%)	112 (97%)	4 (3%)	32 57
10	J	93/94 (99%)	88 (95%)	5 (5%)	18 44
11	K	299/302 (99%)	298 (100%)	1 (0%)	91 95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	L	96/119 (81%)	95 (99%)	1 (1%)	73 83
13	M	191/192 (100%)	189 (99%)	2 (1%)	73 83
14	N	68/111 (61%)	68 (100%)	0	100 100
15	O	129/131 (98%)	128 (99%)	1 (1%)	79 87
16	P	43/55 (78%)	40 (93%)	3 (7%)	12 37
17	Q	55/56 (98%)	55 (100%)	0	100 100
18	R	152/172 (88%)	150 (99%)	2 (1%)	65 78
19	S	324/365 (89%)	318 (98%)	6 (2%)	52 71
20	T	70/440 (16%)	69 (99%)	1 (1%)	62 77
21	U	124/334 (37%)	120 (97%)	4 (3%)	34 59
22	W	215/1250 (17%)	210 (98%)	5 (2%)	45 67
25	Z	340/356 (96%)	335 (98%)	5 (2%)	60 76
All	All	5976/8414 (71%)	5820 (97%)	156 (3%)	42 64

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	116	MET
1	A	127	ASP
1	A	157	HIS
1	A	158	HIS
1	A	187	ASP
1	A	198	GLU
1	A	221	LEU
1	A	234	ASP
1	A	239	LEU
1	A	249	ASP
1	A	294	LYS
1	A	305	MET
1	A	311	ASP
1	A	544	ASP
1	A	609	ASP
1	A	610	ASP
1	A	627	LYS
1	A	870	TYR
1	A	881	ASP
1	A	916	ASP

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Mol	Chain	Res	Type
1	A	1089	LEU
1	A	1099	ARG
1	A	1127	PHE
1	A	1185	MET
1	A	1195	ASP
1	A	1236	MET
1	A	1239	HIS
1	A	1326	ASP
1	A	1354	ASN
1	A	1368	ARG
2	B	183	GLN
2	B	192	GLU
2	B	224	TYR
2	B	246	GLU
2	B	260	HIS
2	B	278	PHE
2	B	400	PHE
2	B	417	ASN
2	B	463	ARG
2	B	625	LEU
2	B	926	ASP
2	B	1004	PHE
2	B	1020	MET
2	B	1053	ASP
2	B	1064	LEU
2	B	1086	LEU
2	B	1131	TYR
3	C	85	MET
3	C	259	MET
3	C	273	MET
3	C	339	HIS
3	C	403	PHE
3	C	455	LYS
3	C	474	MET
3	C	517	ASP
3	C	524	GLU
4	D	123	TRP
4	D	132	MET
4	D	144	LYS
4	D	153	GLN
4	D	156	ARG
4	D	157	MET

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Mol	Chain	Res	Type
4	D	275	LEU
4	D	350	MET
5	E	39	TYR
5	E	54	GLN
5	E	66	ASN
5	E	99	LYS
5	E	135	LEU
5	E	193	TYR
5	E	195	PHE
5	E	198	LYS
5	E	247	MET
5	E	294	PHE
5	E	296	ASN
5	E	355	PHE
5	E	357	MET
5	E	358	TRP
5	E	360	PHE
5	E	400	PHE
5	E	407	GLU
5	E	408	PHE
5	E	411	LYS
5	E	421	MET
6	F	42	MET
6	F	86	LYS
6	F	176	PHE
6	F	185	PHE
6	F	203	MET
6	F	267	MET
6	F	271	ARG
6	F	282	LEU
6	F	283	VAL
6	F	287	CYS
6	F	289	LEU
6	F	292	VAL
6	F	293	PHE
6	F	294	ASP
6	F	296	CYS
6	F	297	HIS
6	F	302	ILE
6	F	303	SER
6	F	307	CYS
6	F	308	ILE

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Mol	Chain	Res	Type
6	F	312	GLU
6	F	315	GLU
7	G	52	GLU
7	G	70	ARG
7	G	71	MET
7	G	92	MET
7	G	106	LEU
7	G	108	ARG
7	G	110	MET
8	H	135	GLU
8	H	184	TYR
9	I	1	MET
9	I	17	PHE
9	I	40	GLN
9	I	100	MET
10	J	78	TYR
10	J	80	MET
10	J	89	GLU
10	J	95	TYR
10	J	106	TRP
11	K	151	HIS
12	L	113	LYS
13	M	91	CYS
13	M	110	MET
15	O	58	LEU
16	P	15	MET
16	P	41	TYR
16	P	50	LYS
18	R	280	PHE
18	R	329	TYR
19	S	154	MET
19	S	162	LEU
19	S	174	LYS
19	S	199	LYS
19	S	251	CYS
19	S	278	GLU
20	T	317	MET
21	U	35	ASN
21	U	47	ARG
21	U	92	GLN
21	U	120	PHE
22	W	142	MET

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Mol	Chain	Res	Type
22	W	202	GLN
22	W	286	ASN
22	W	316	GLU
22	W	337	PHE
25	Z	151	ARG
25	Z	174	MET
25	Z	216	ARG
25	Z	264	TYR
25	Z	350	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	HIS
1	A	611	ASN
2	B	227	HIS
6	F	297	HIS
10	J	74	HIS
18	R	277	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
28	SF4	F	401	6	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SF4	F	401	6	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	F	401	SF4	9	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

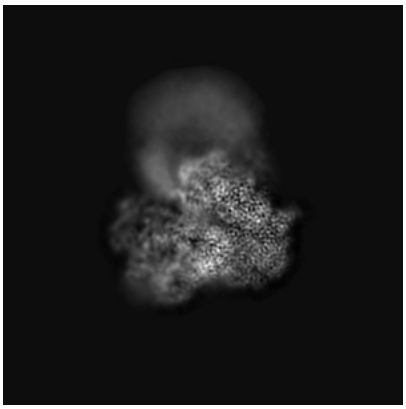
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50731. These allow visual inspection of the internal detail of the map and identification of artifacts.

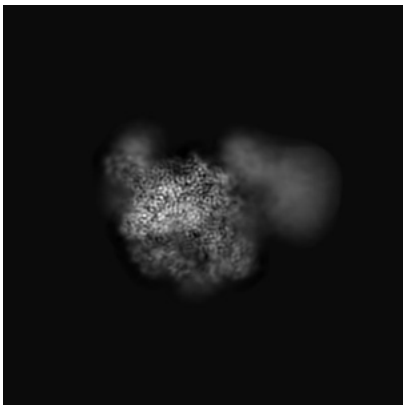
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

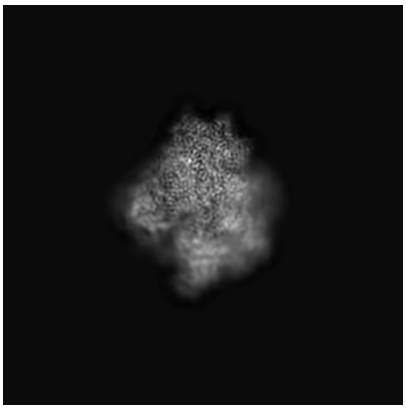
6.1.1 Primary map



X

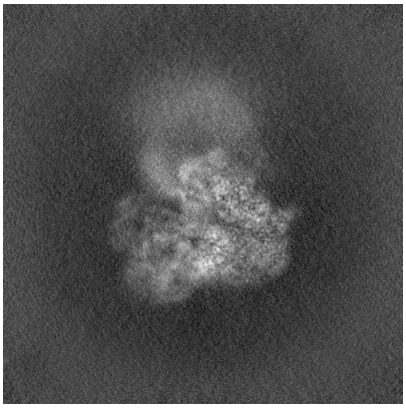


Y

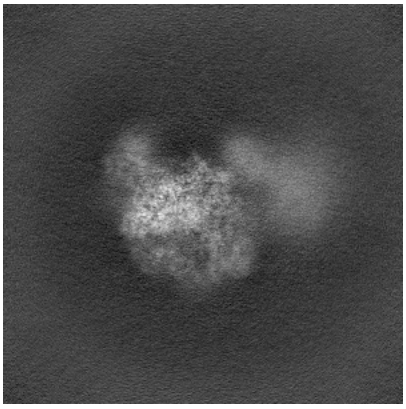


Z

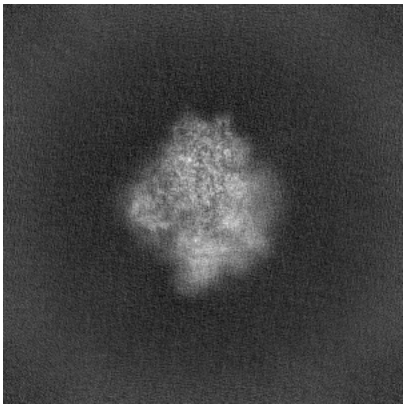
6.1.2 Raw map



X



Y

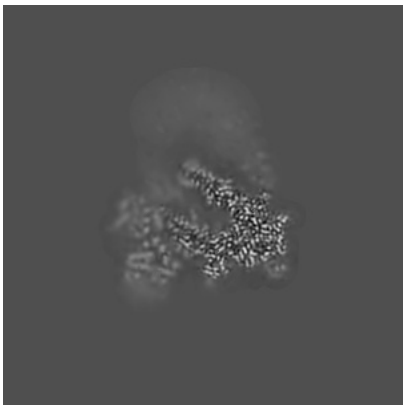


Z

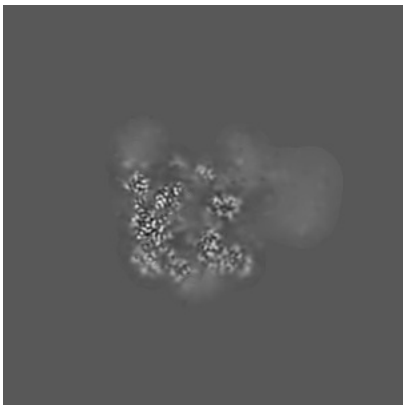
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

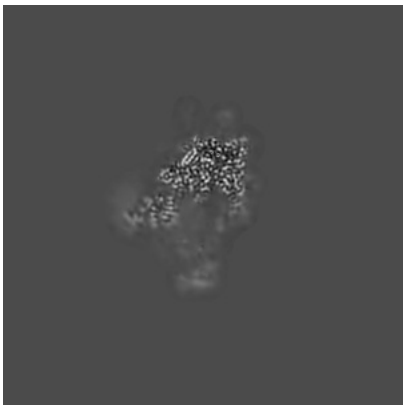
6.2.1 Primary map



X Index: 210

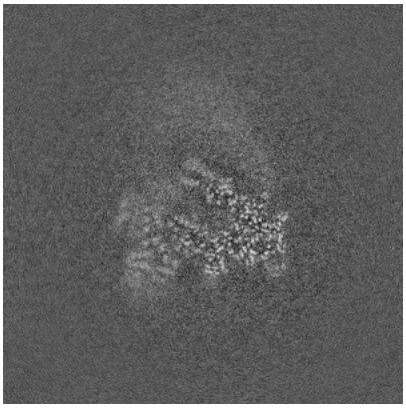


Y Index: 210

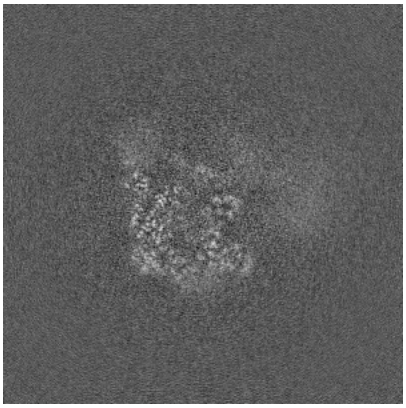


Z Index: 210

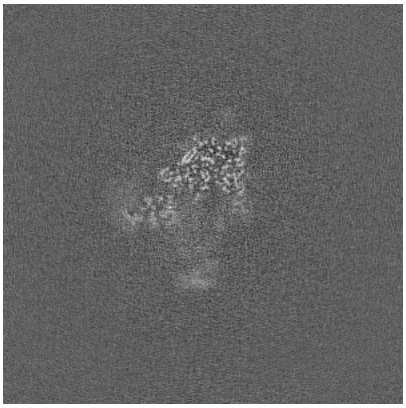
6.2.2 Raw map



X Index: 210



Y Index: 210

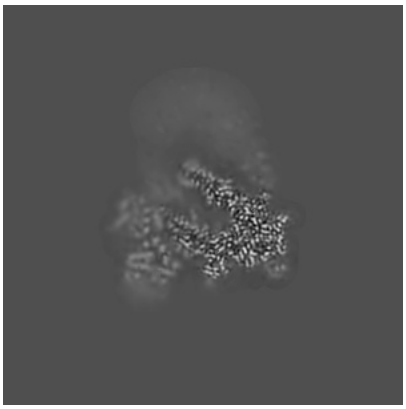


Z Index: 210

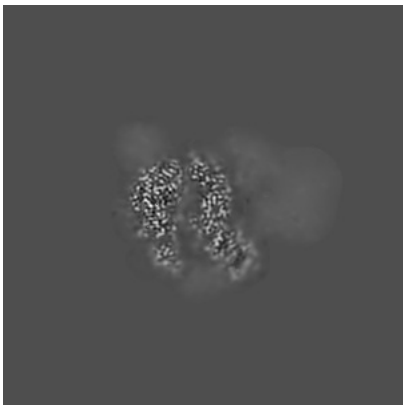
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



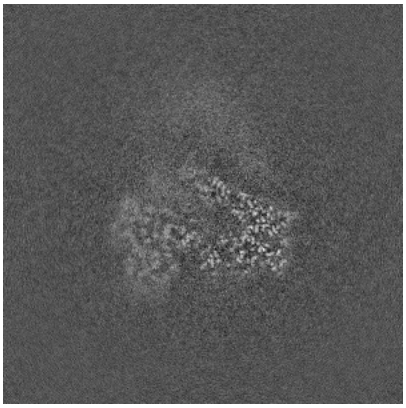
X Index: 210



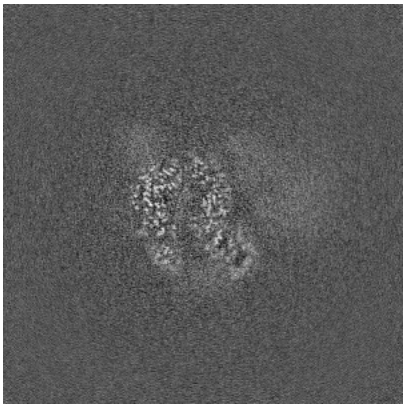
Y Index: 226

Z Index: 167

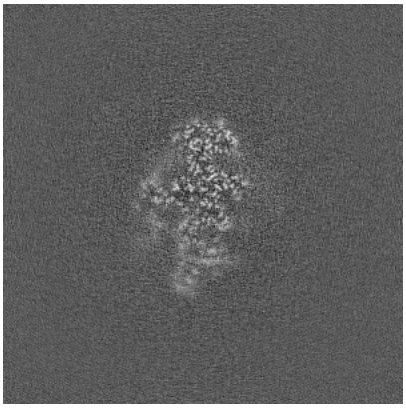
6.3.2 Raw map



X Index: 203



Y Index: 226

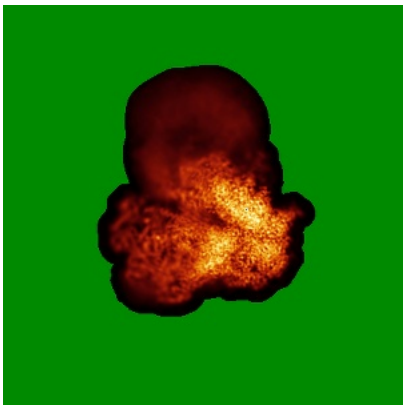


Z Index: 167

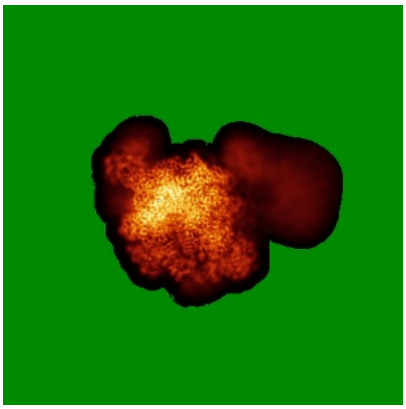
The images above show the largest variance slices of the map in three orthogonal directions.

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

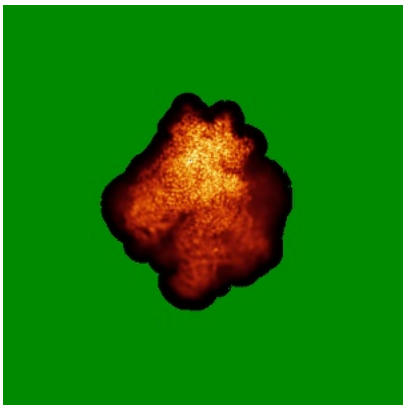
6.4.1 Primary map



X

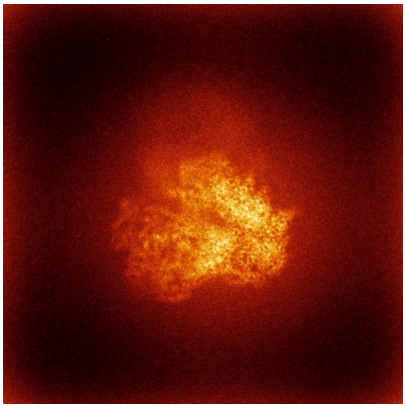


Y

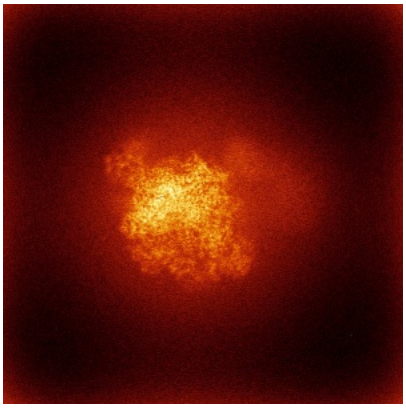


Z

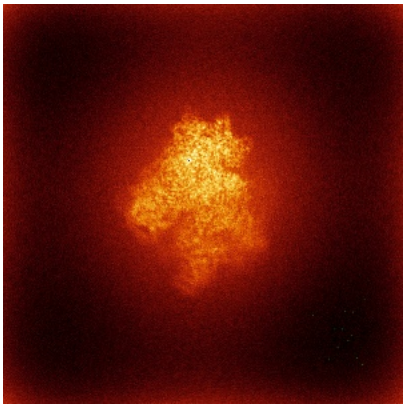
6.4.2 Raw map



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.

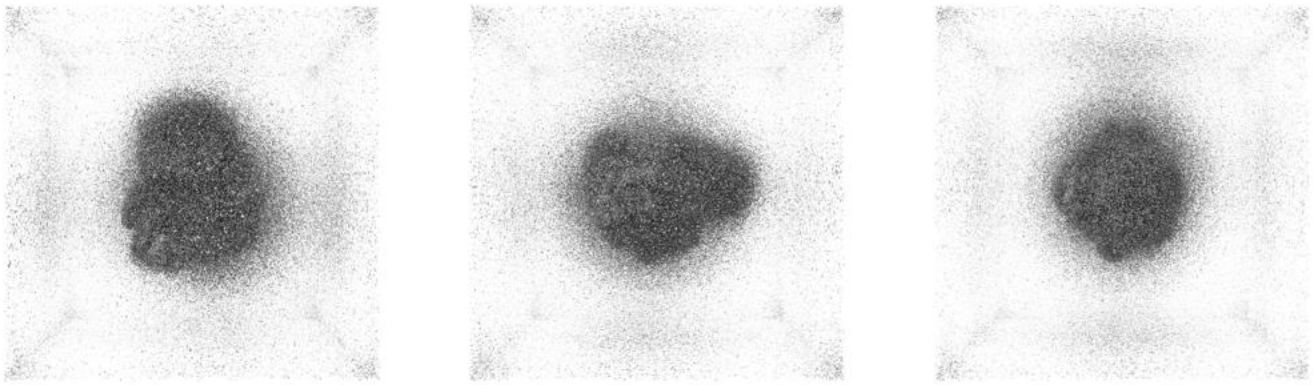
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

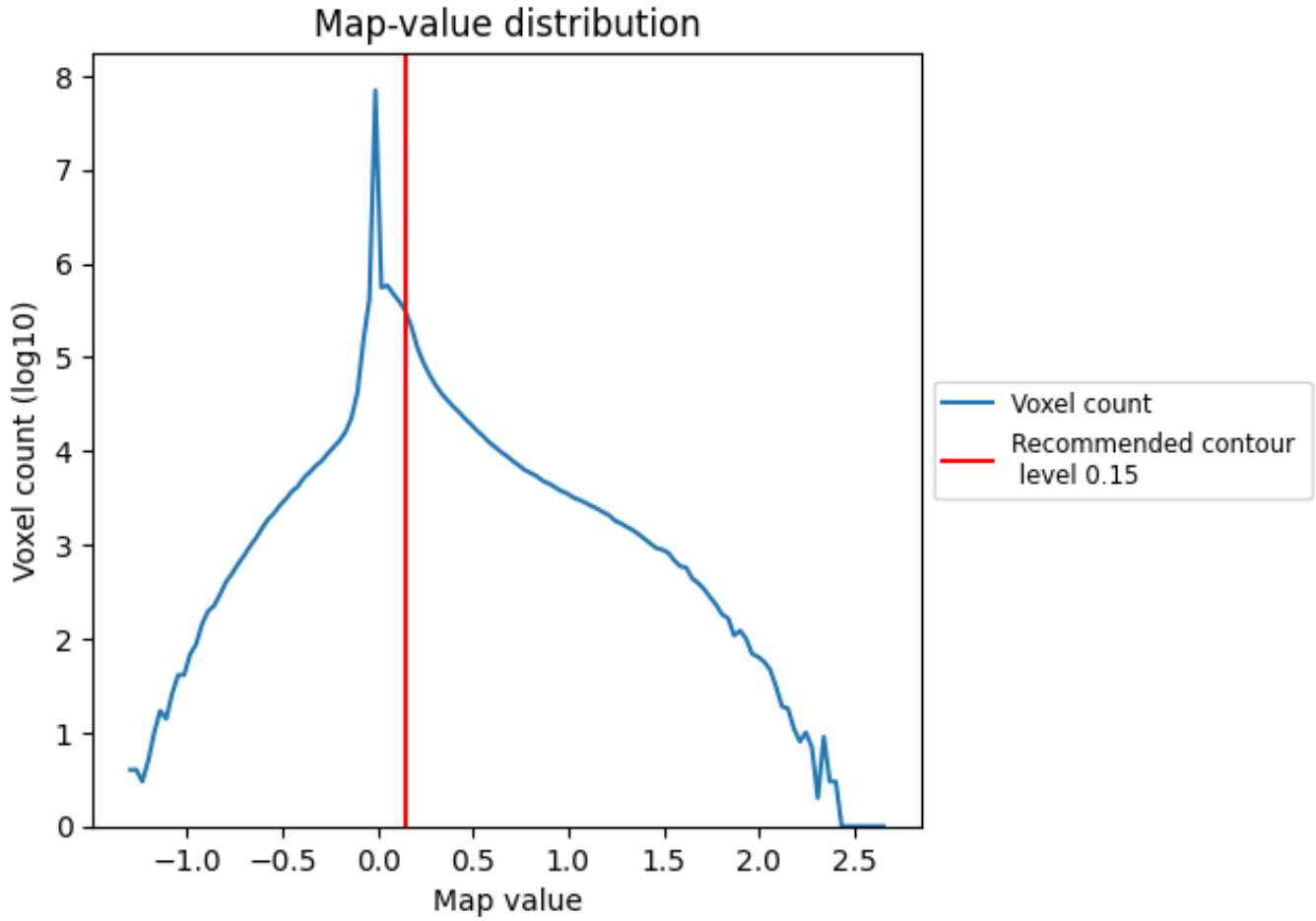
6.6 Mask visualisation (i)

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

7 Map analysis

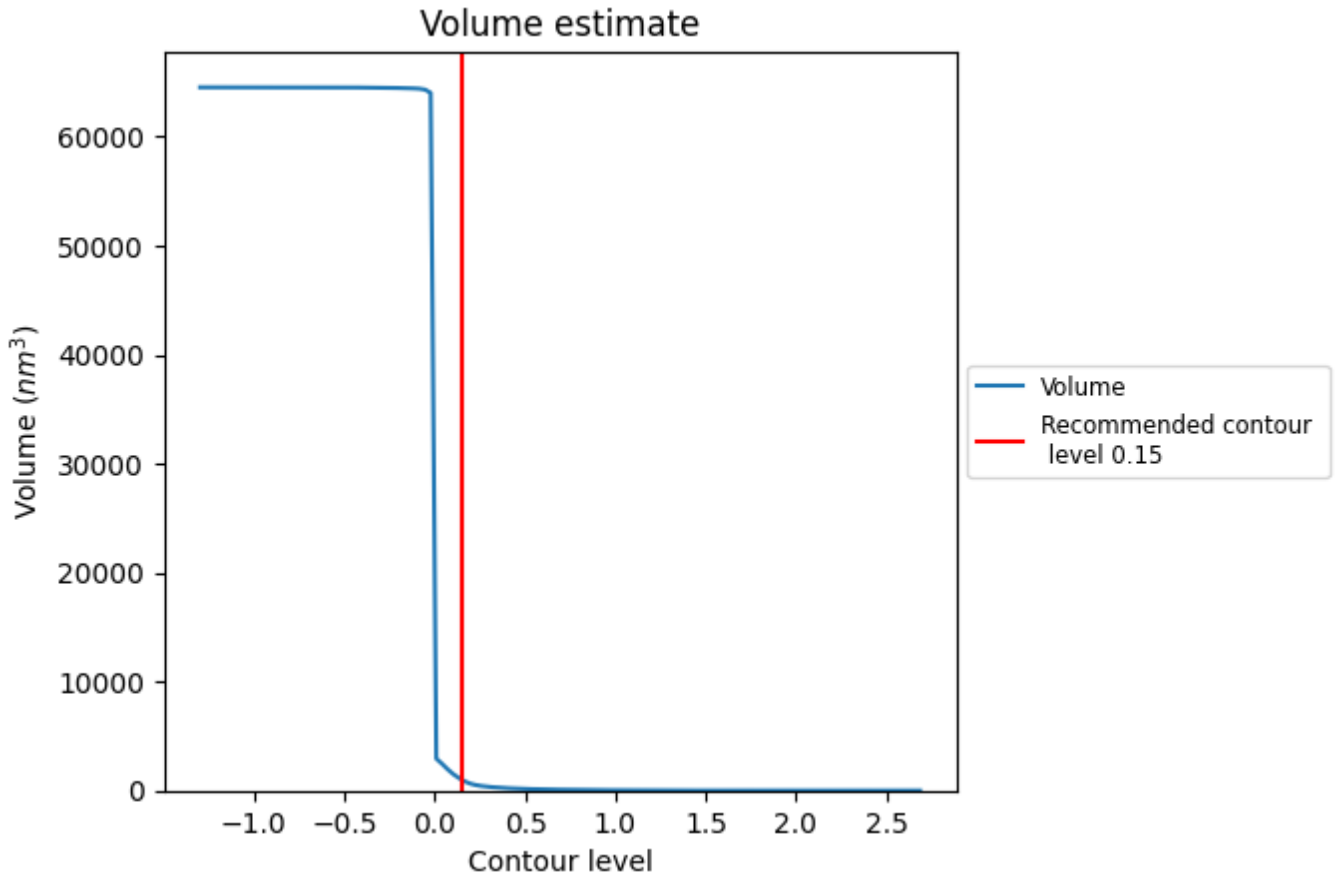
This section contains the results of statistical analysis of the map.

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.

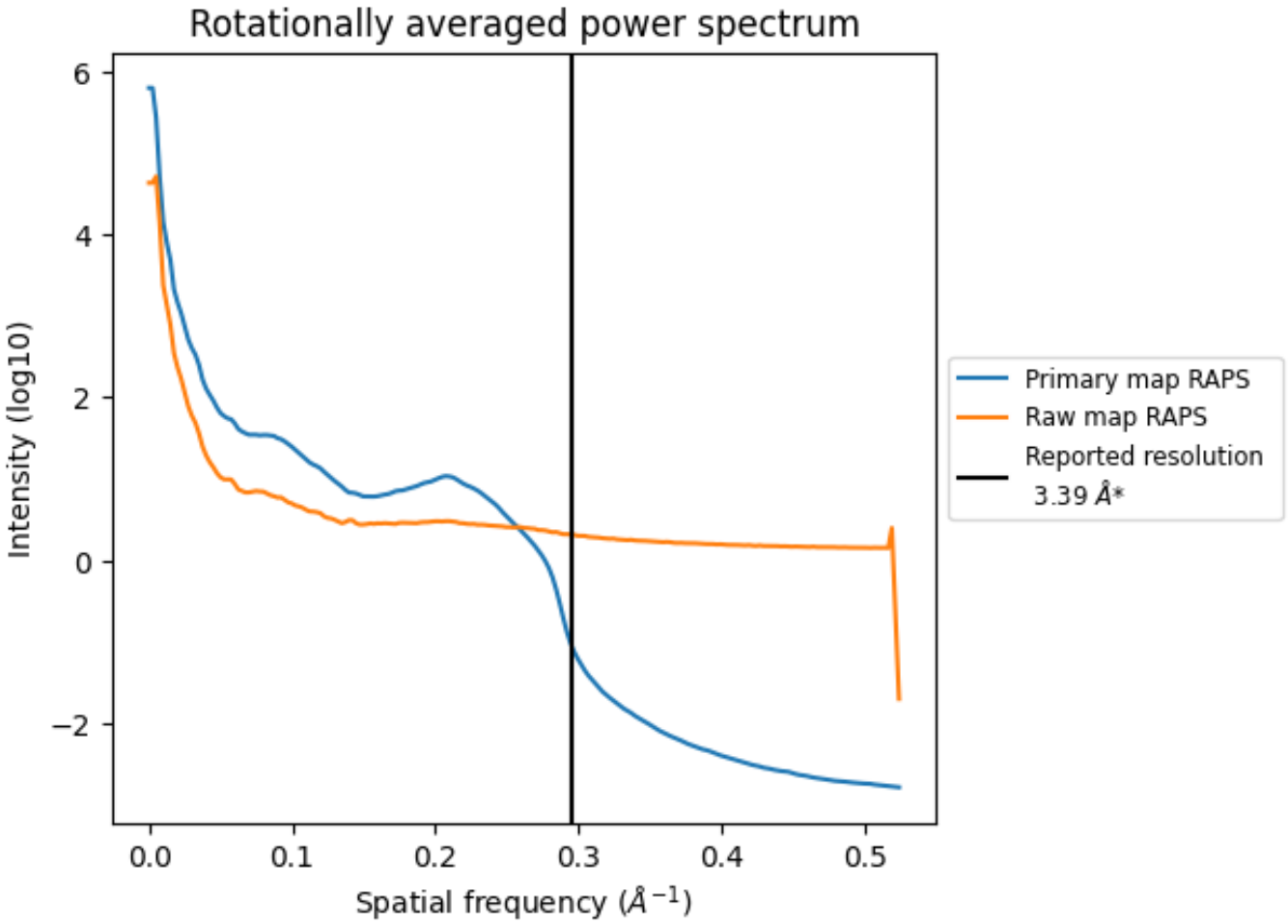
7.2 Volume estimate



The volume at the recommended contour level is 999 nm^3; this corresponds to an approximate mass of 902 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)

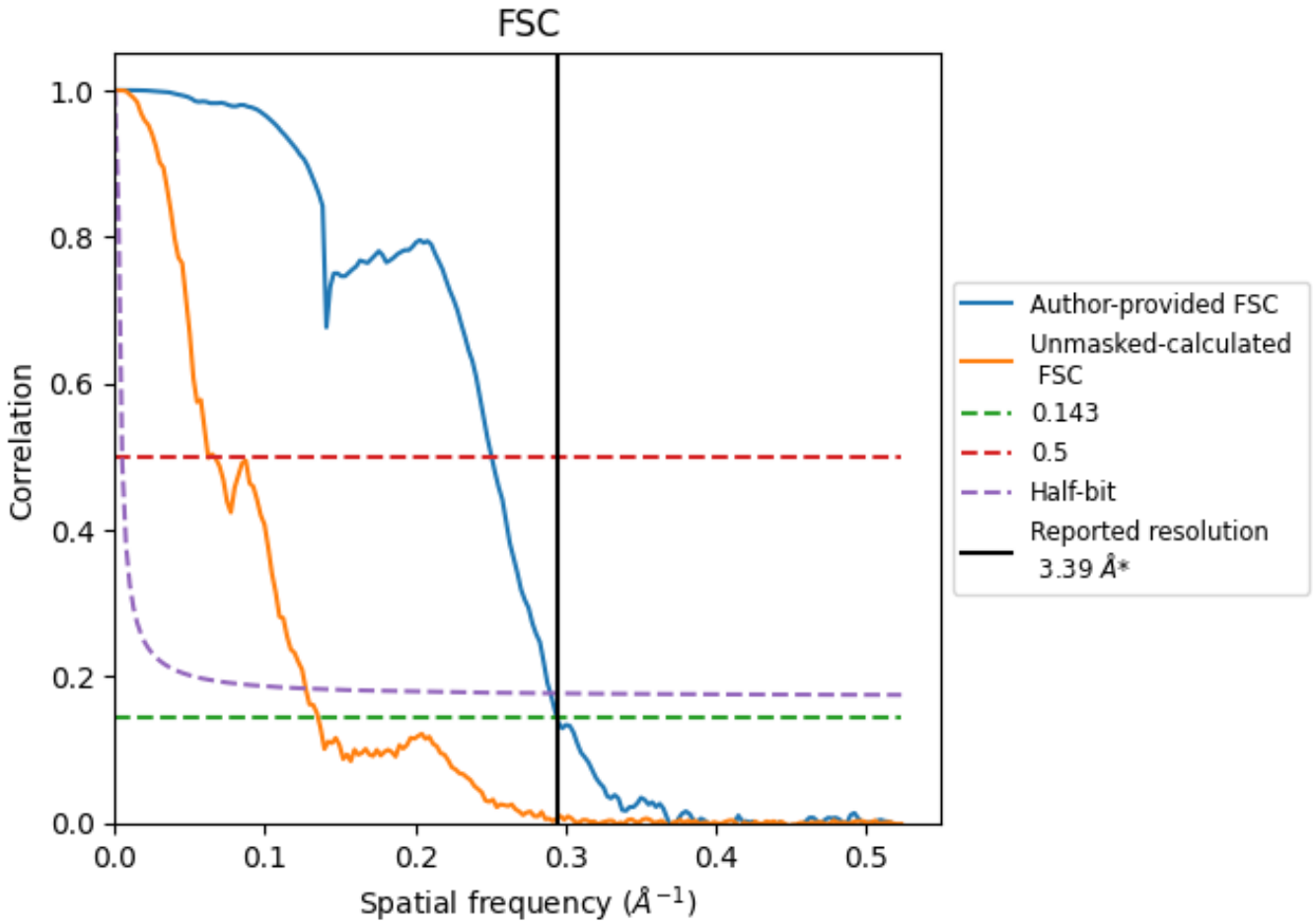


*Reported resolution corresponds to spatial frequency of 0.295 Å^{-1}

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 0.295 $Å^{-1}$

8.2 Resolution estimates (i)

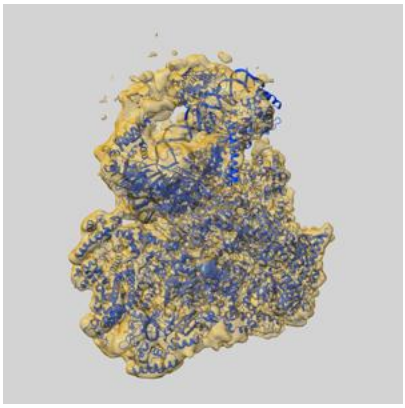
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.39	-	-
Author-provided FSC curve	3.40	3.99	3.45
Unmasked-calculated*	7.39	16.08	7.87

*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 7.39 differs from the reported value 3.39 by more than 10 %

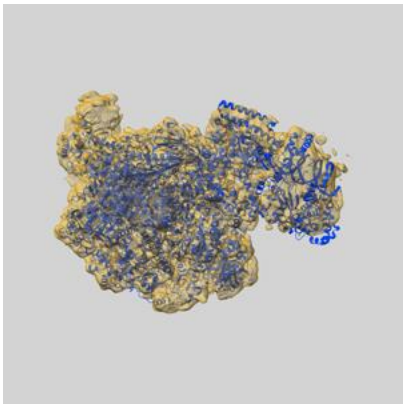
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50731 and PDB model 9FSP. Per-residue inclusion information can be found in section 3 on page 11.

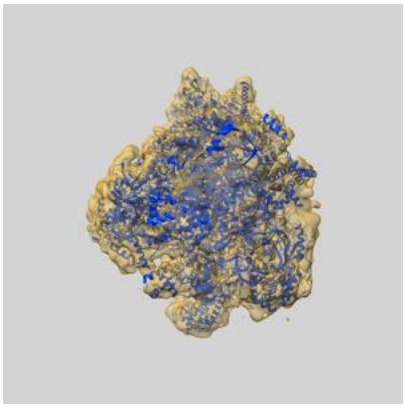
9.1 Map-model overlay



X



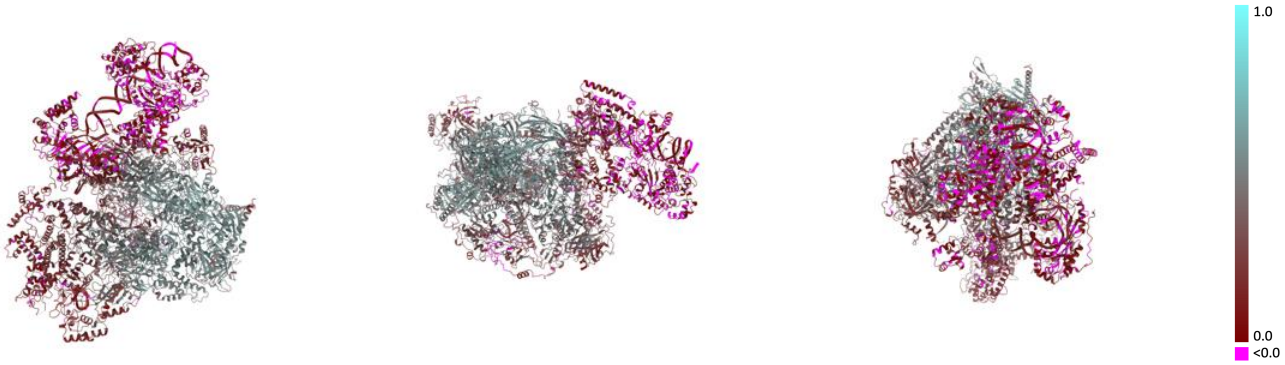
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

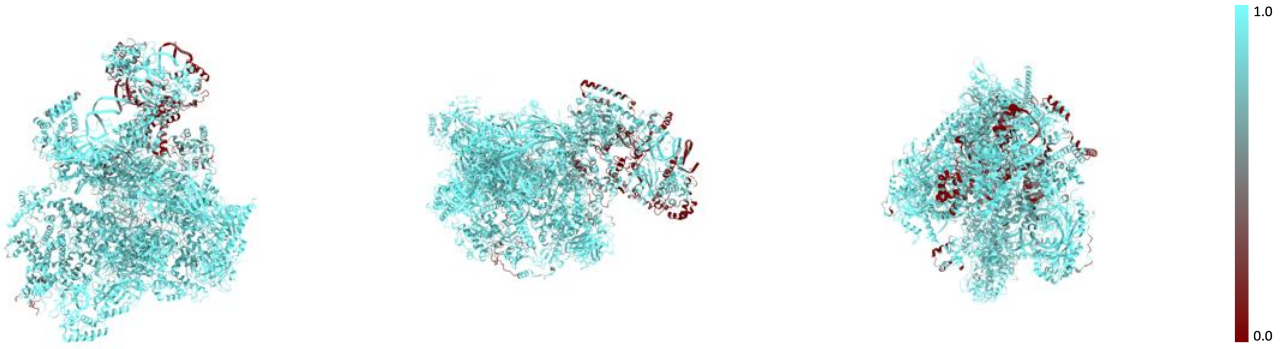
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

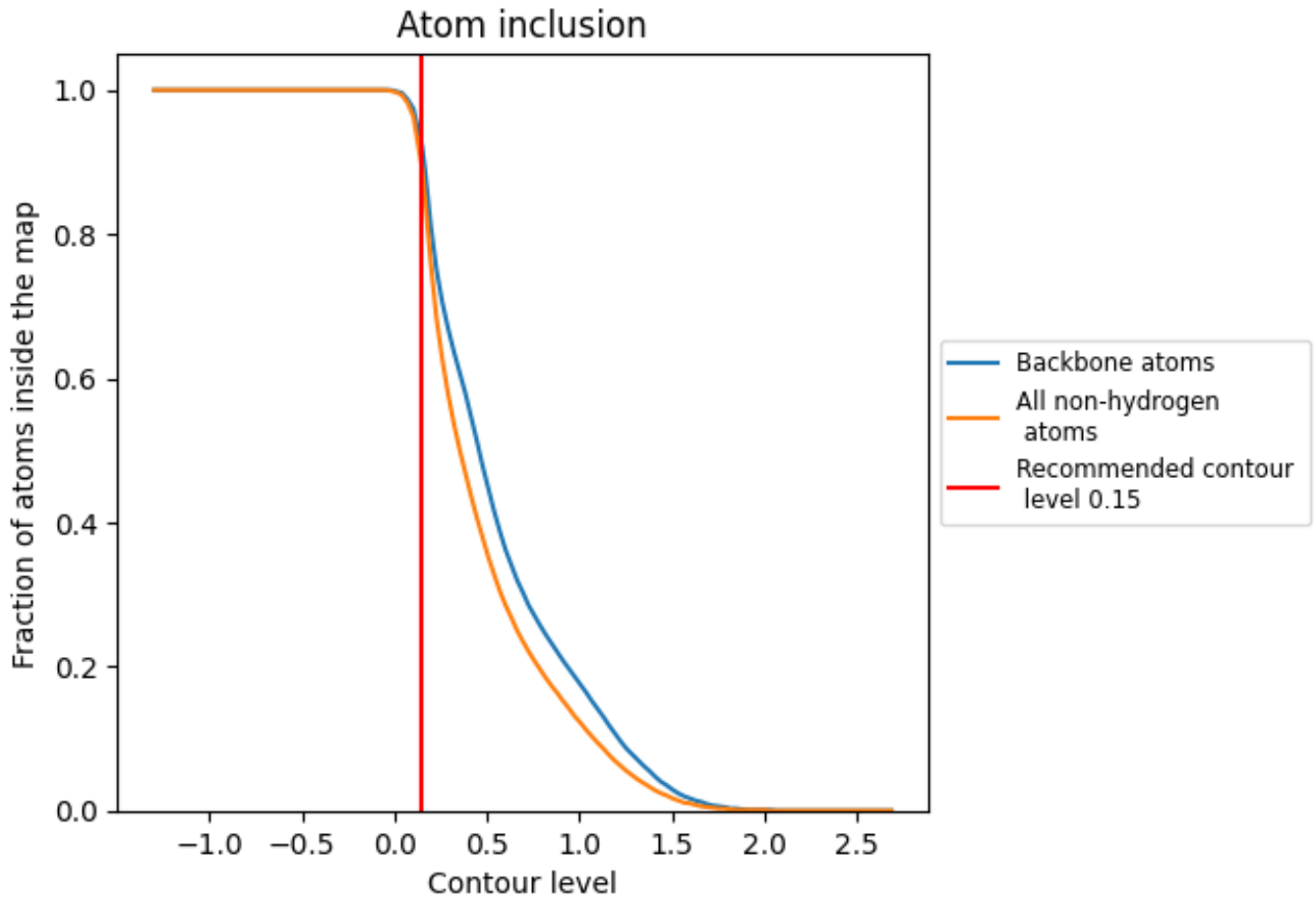
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8900	0.3010
A	0.9610	0.4330
B	0.9700	0.4780
C	0.8960	0.1800
D	0.8740	0.2650
E	0.8090	0.2410
F	0.8850	0.1470
G	0.9570	0.2280
H	0.9790	0.3290
I	0.9840	0.2510
J	0.7230	0.1610
K	0.9940	0.5220
L	0.9980	0.5080
M	0.9820	0.3500
N	0.9850	0.5230
O	0.9910	0.4940
P	0.9970	0.4840
Q	1.0000	0.5560
R	0.9290	0.0630
S	0.8110	0.1330
T	0.9480	0.0760
U	0.8170	0.0660
W	0.5140	0.0380
X	0.8030	0.1280
Y	0.8400	0.1090
Z	0.5820	0.0350