Full wwPDB EM Validation Report ⓘ

Jan 7, 2025 – 12:45 pm GMT

PDB ID	:	9FSO
EMDB ID	:	EMD-50730
Title	:	Human RNA Polymerase III Class III Open Pre-initiation Complex 1 (OC1)
Authors	:	Shah, S.Z.; Ramsay, E.P.; Cecatiello, V.; Perry, T.N.; Vannini, A.
Deposited on	:	2024-06-21
Resolution	:	3.28 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:

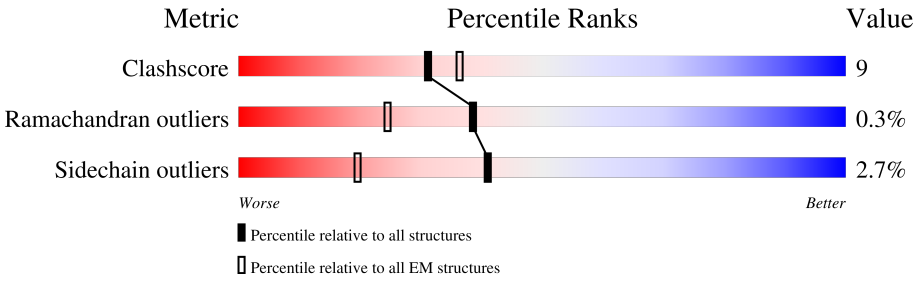
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.28 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	84% 14%
2	B	1133	85% 11%
3	C	534	78% 16%
4	D	398	42% 53%
5	E	666	52% 6% 40%
6	F	316	51% 36% 7%
7	G	223	20% 15% 63%
8	H	204	78% 13% 7%

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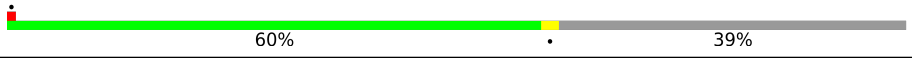
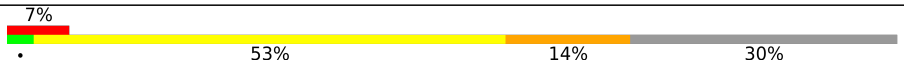
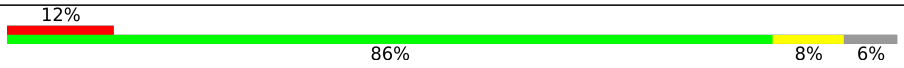
Mol	Chain	Length	Quality of chain
9	I	148	
10	J	108	
11	K	346	
12	L	133	
13	M	210	
14	N	127	
15	O	150	
16	P	58	
17	Q	67	
18	R	200	
19	S	419	
20	T	484	
21	U	368	
22	W	1519	
23	X	98	
24	Y	98	
25	Z	411	

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 56873 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	10849	6876	1891	2009	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	4076	2565	712	775	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	1449	907	251	282	9	0	0

- Molecule 5 is a protein called Isoform 2 of 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
			1716	1083	300	325	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
			628	402	106	115	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
			389	241	75	67	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	70	Total	C	N	O	P	0	0
			1443	687	270	416	70		

- 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) (labeled as "Ligand of Interest" by depositor).

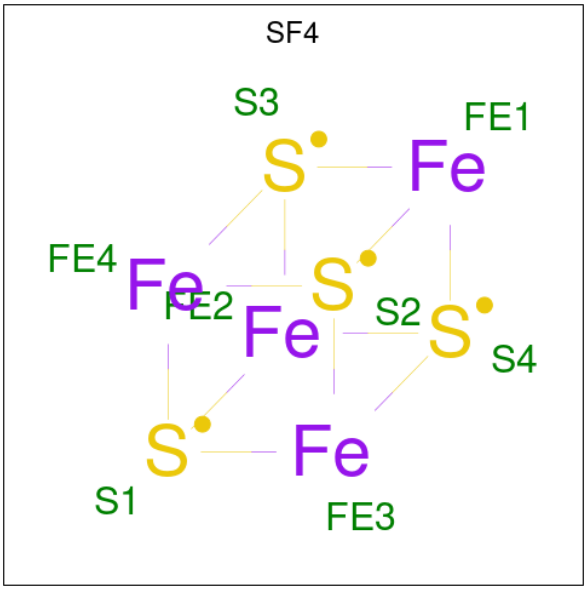
Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Zn	0
			2	2	
26	B	1	Total	Zn	0
			1	1	
26	J	1	Total	Zn	0
			1	1	
26	P	1	Total	Zn	0
			1	1	
26	Q	1	Total	Zn	0
			1	1	
26	S	1	Total	Zn	0
			1	1	
26	Z	2	Total	Zn	0
			2	2	

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Lig-

and of Interest" by depositor).

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

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



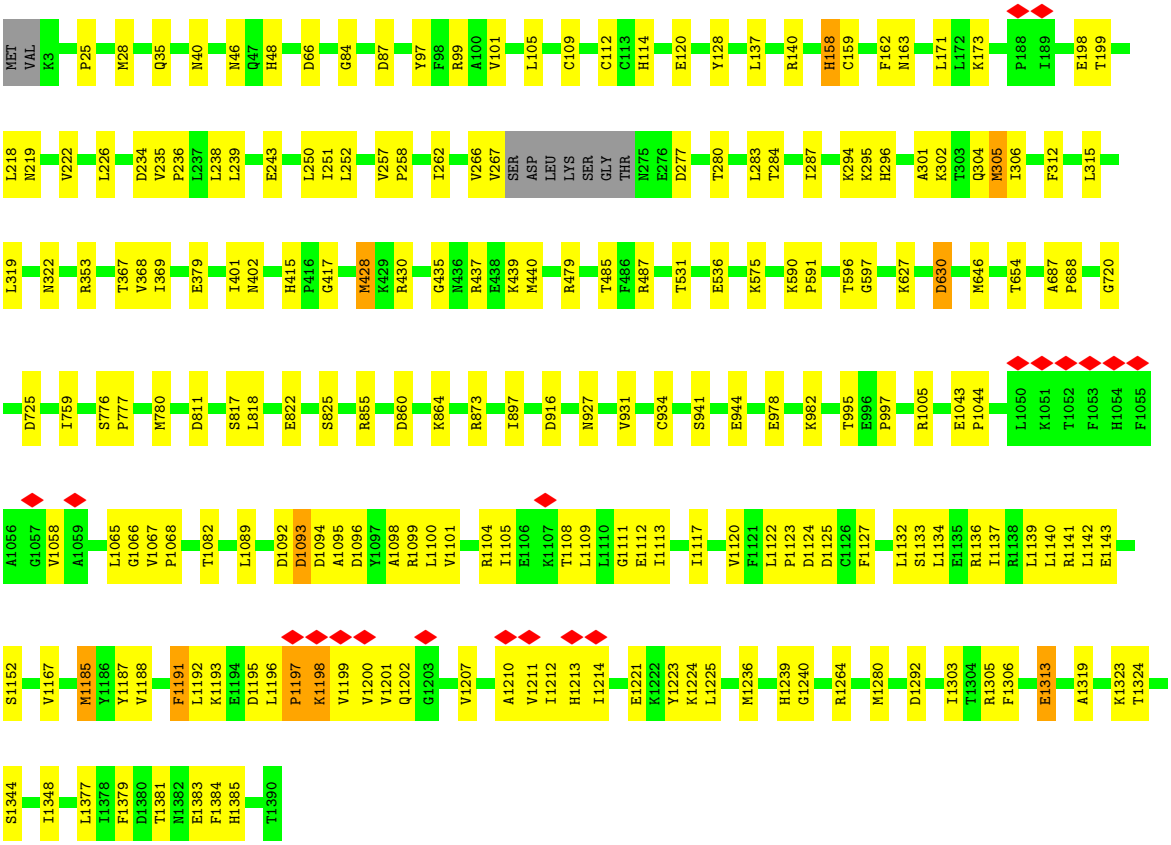
Mol	Chain	Residues	Atoms	AltConf
28	F	1	Total Fe S 8 4 4	0

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.

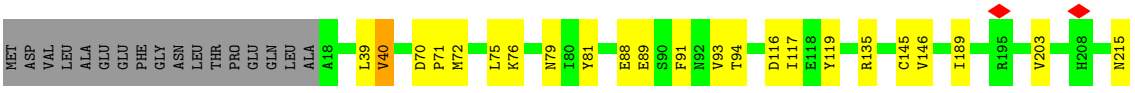
• Molecule 1: DNA-directed RNA polymerase III subunit RPC1

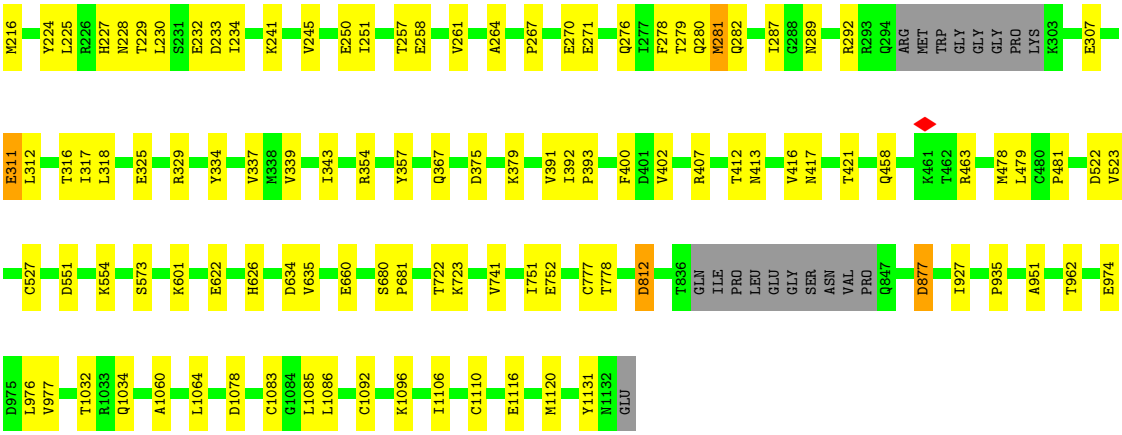
Chain A:



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

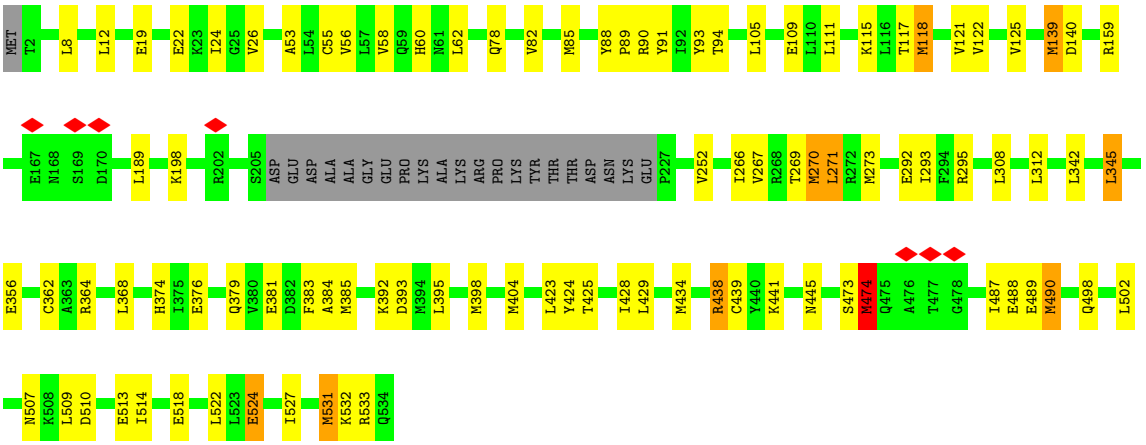
Chain B:





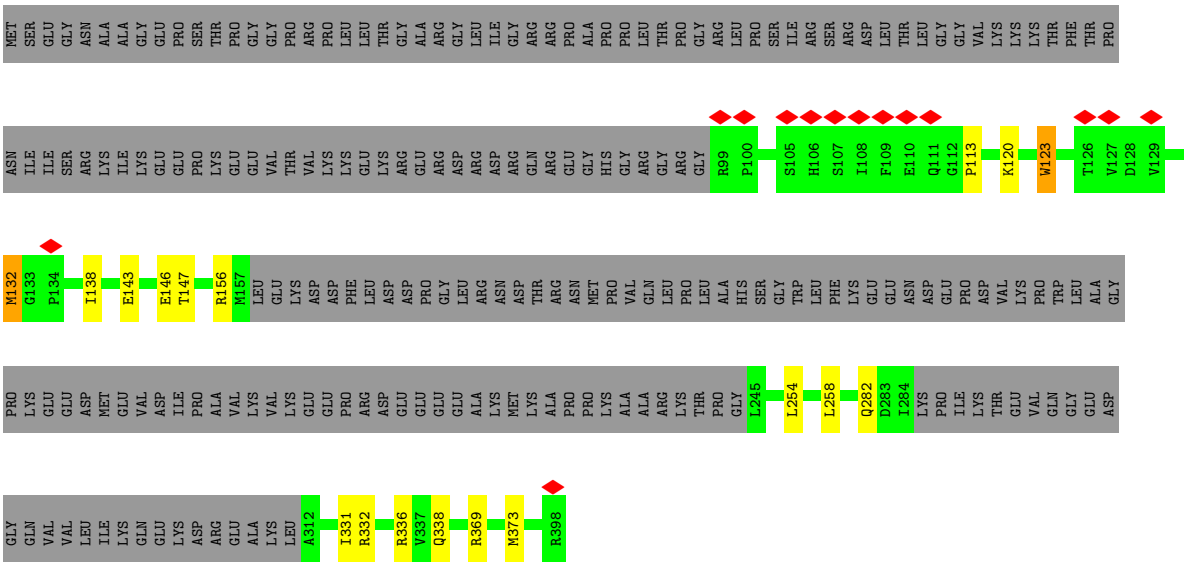
• Molecule 3: DNA-directed RNA polymerase III subunit RPC3

Chain C:



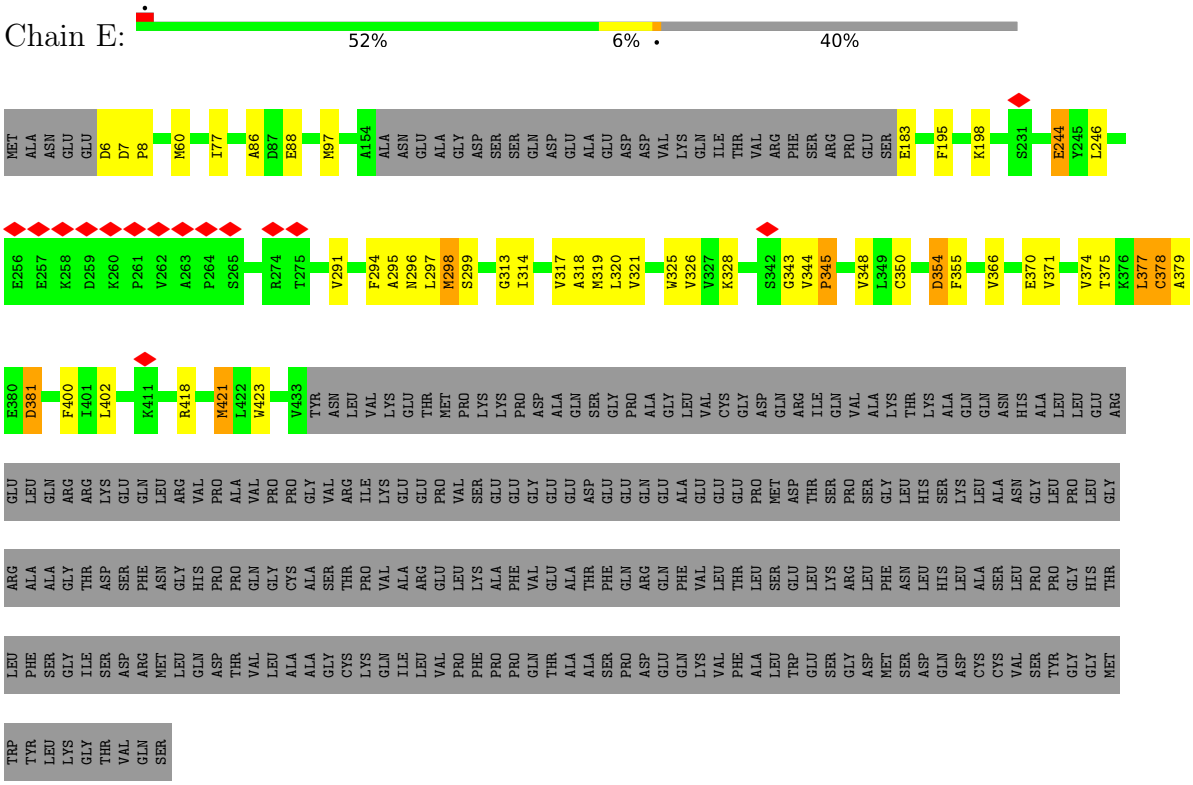
• Molecule 4: DNA-directed RNA polymerase III subunit RPC4

Chain D:



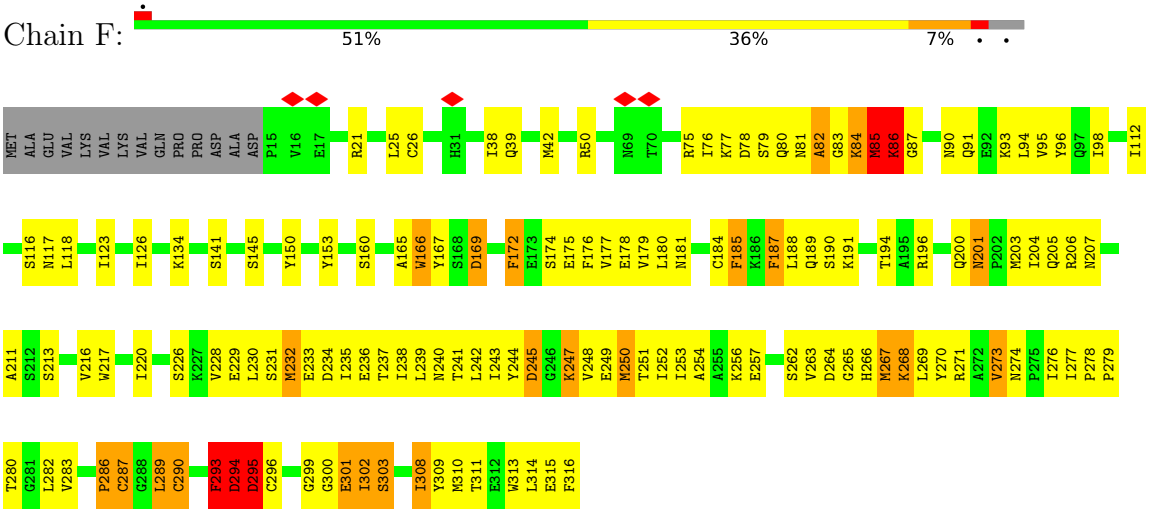
• Molecule 5: Isoform 2 of DNA-directed RNA polymerase III subunit RPC5

Chain E:



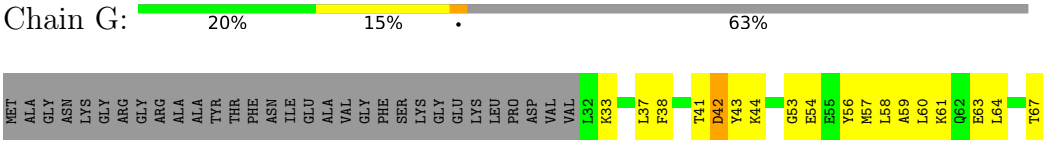
• Molecule 6: DNA-directed RNA polymerase III subunit RPC6

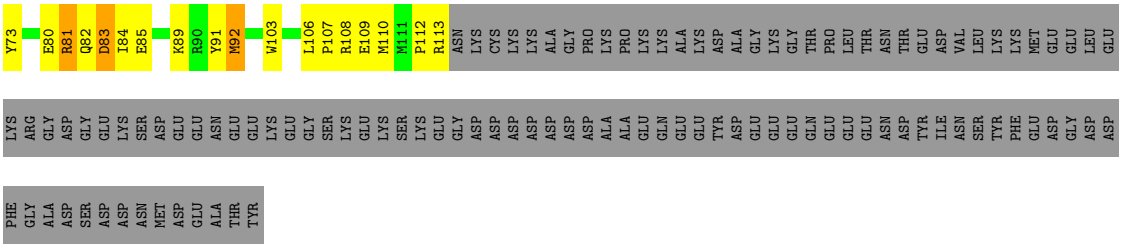
Chain F:



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

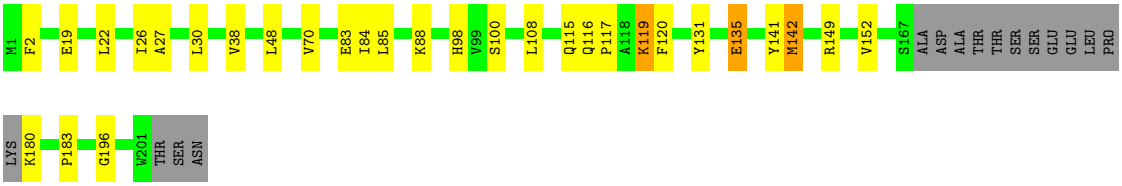
Chain G:





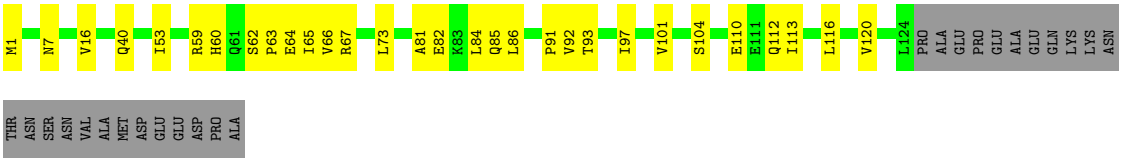
• Molecule 8: DNA-directed RNA polymerase III subunit RPC8

Chain H:



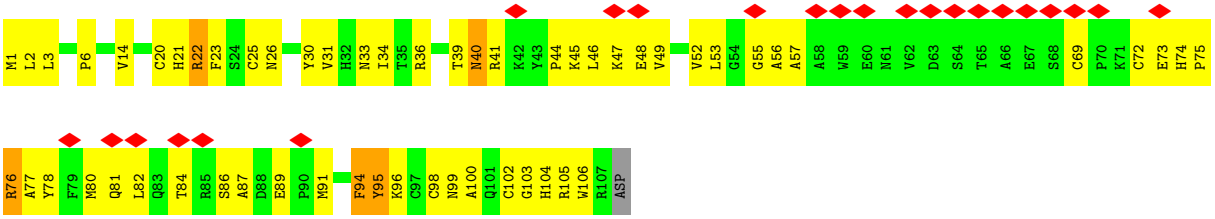
• Molecule 9: DNA-directed RNA polymerase III subunit RPC9

Chain I:



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

Chain J:



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

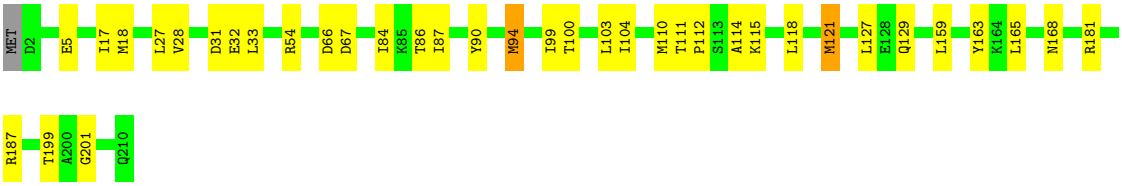
Chain K:

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

Chain L:

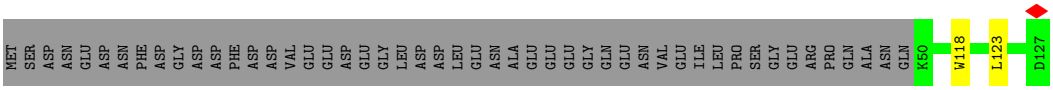
• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain M:



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

Chain N:

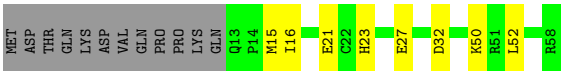


• Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain O:

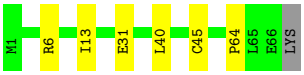
• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain P:



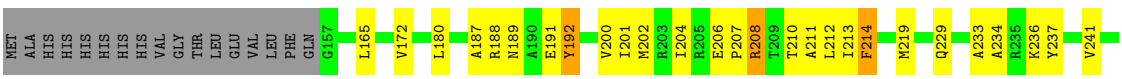
• Molecule 17: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain Q:

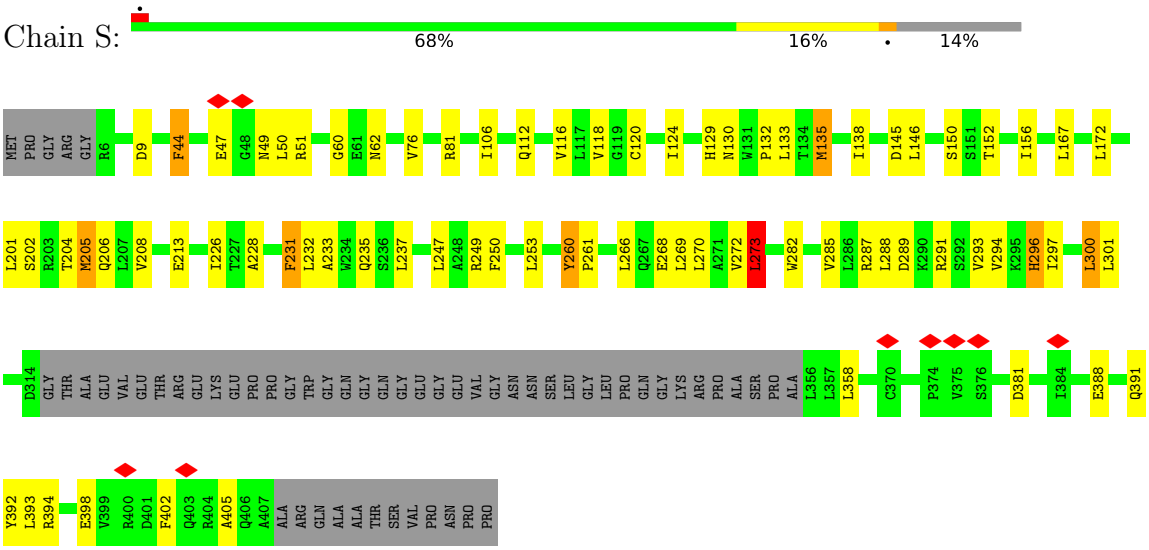


• Molecule 18: TATA-box-binding protein

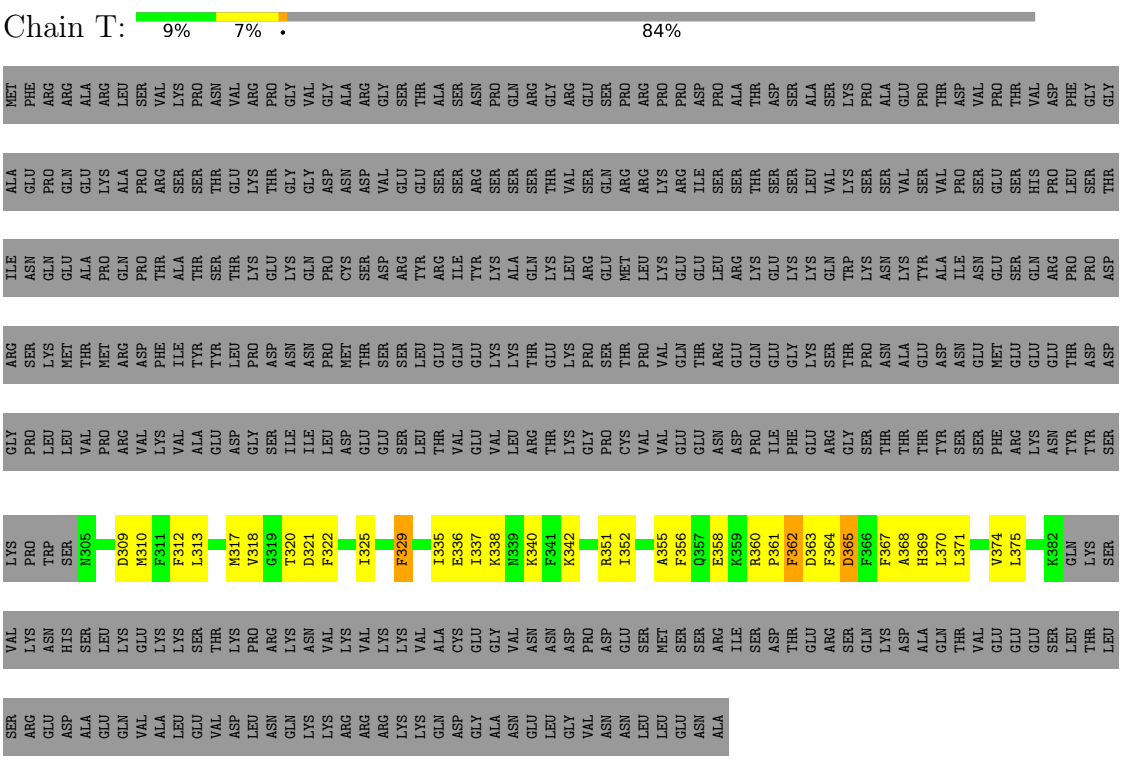
Chain R:



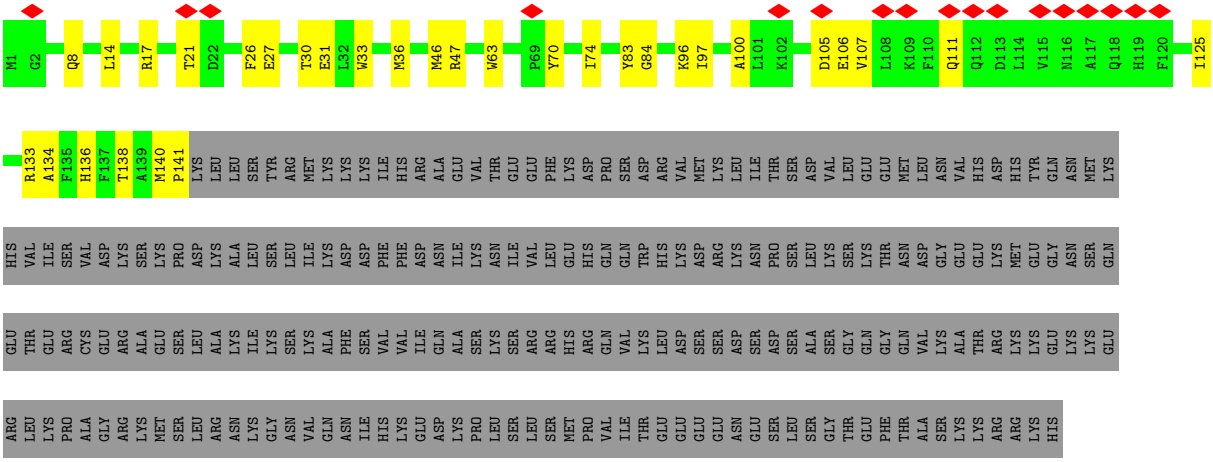
• Molecule 19: Transcription factor IIIB 50 kDa subunit



• Molecule 20: Transcription factor TFIIIB component B" homolog

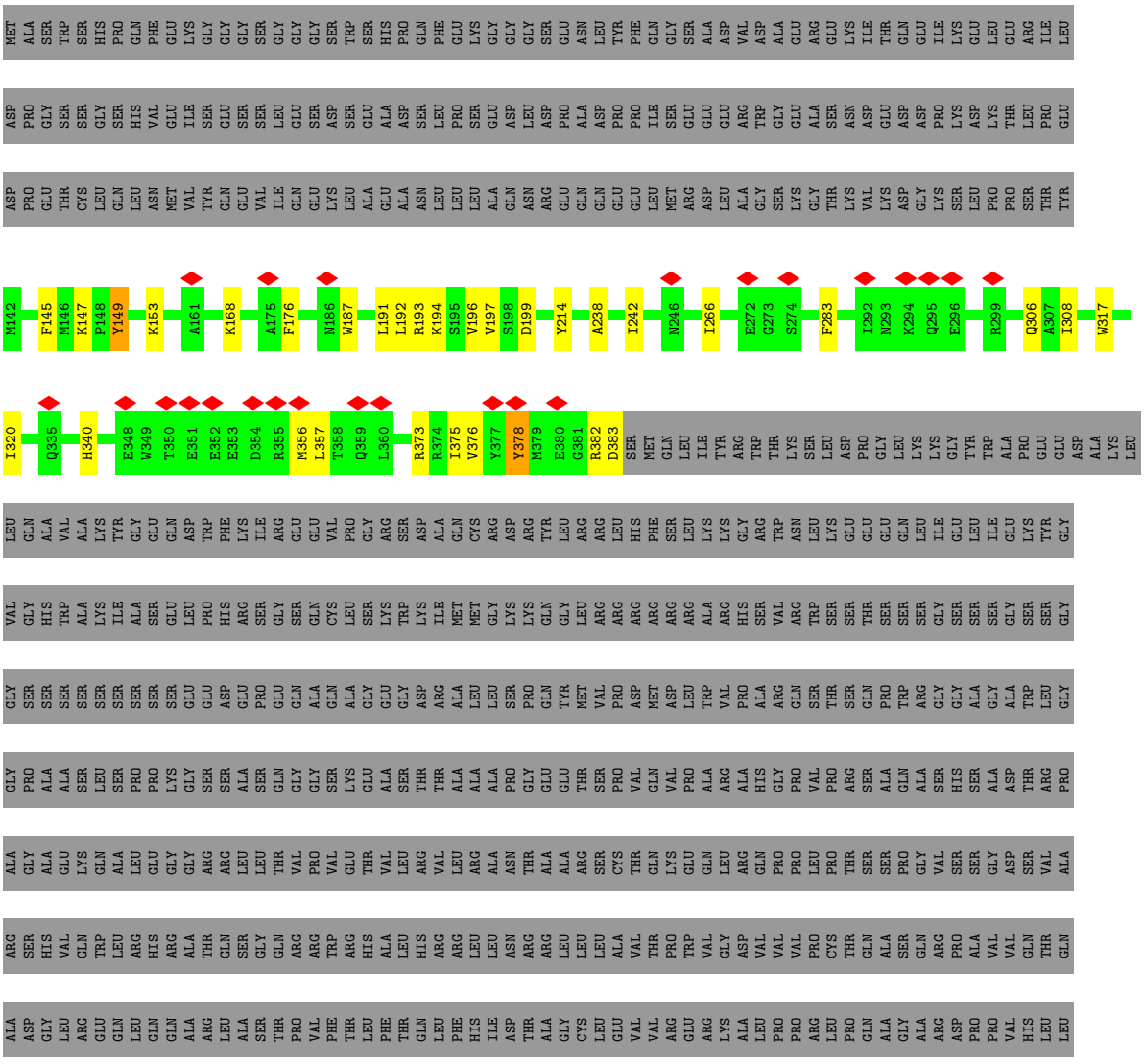


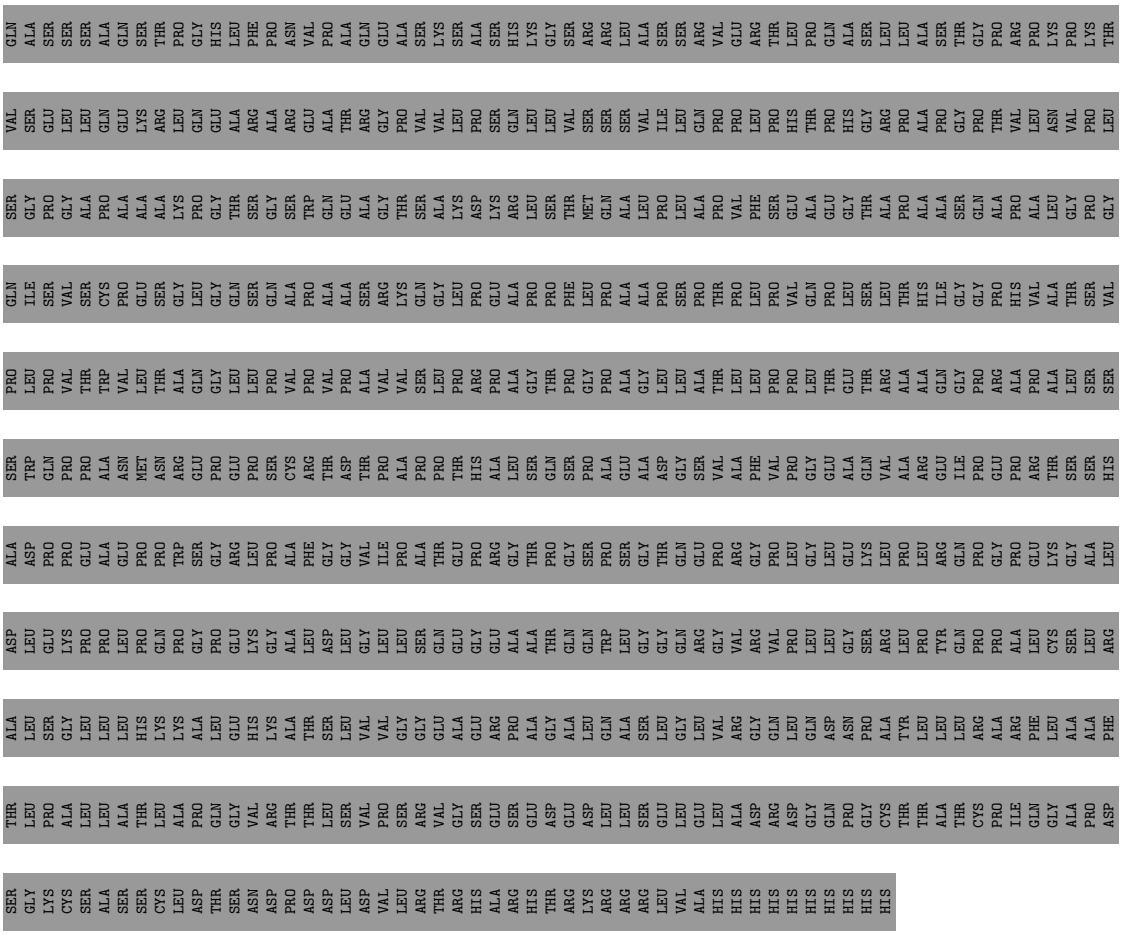
• Molecule 21: snRNA-activating protein complex subunit 1



• Molecule 22: snRNA-activating protein complex subunit 4

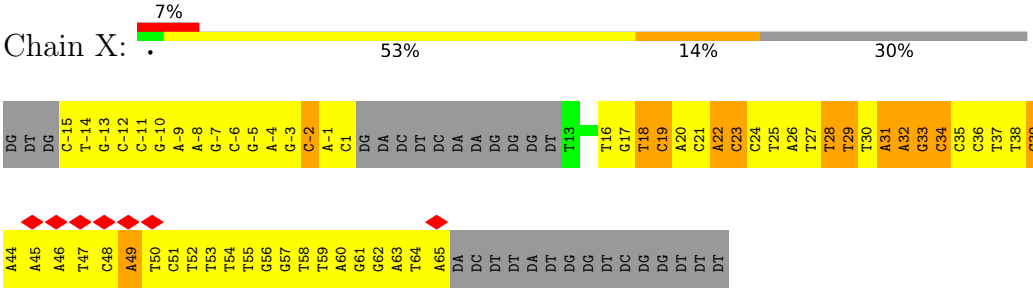
Chain W:





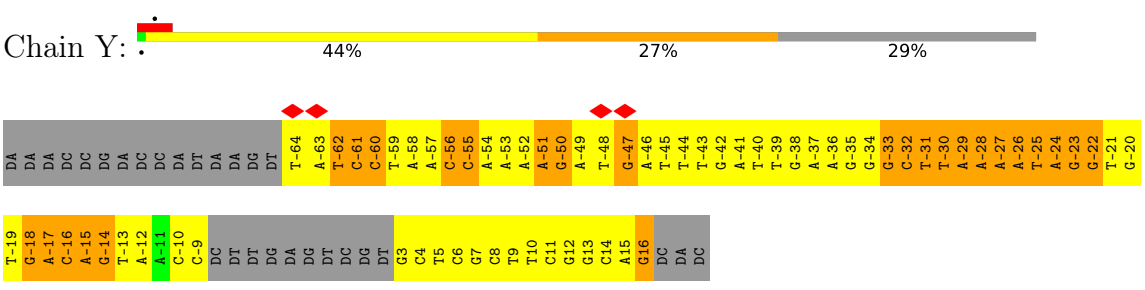
• Molecule 23: U6_2_Template

Chain X:



• Molecule 24: U6_2_Non template

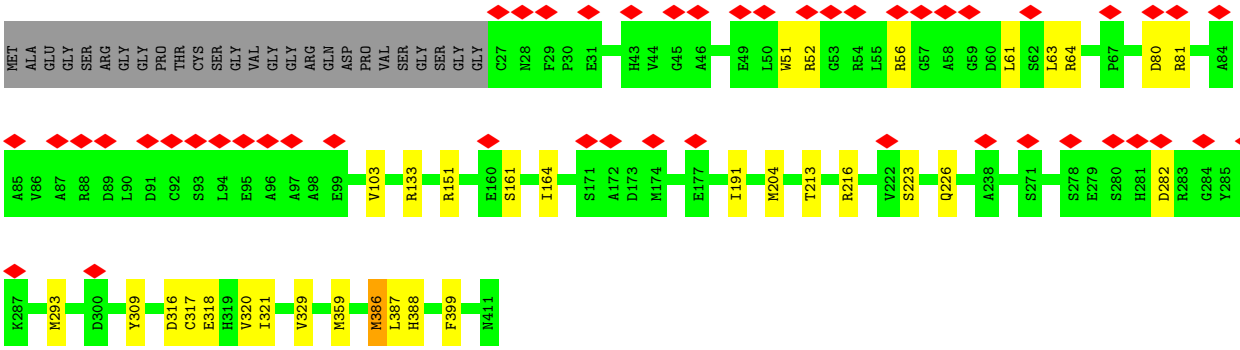
Chain Y:



• Molecule 25: snRNA-activating protein complex subunit 3

Chain Z:


12%
86%
8%
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 H43 V44 G45 A46 E49 L50 W51 R52 G53 R54 L55 R56 G57 A58 G59 D60 L61 S62 L63 R64 P67 D80 R81 A84
A85 V86 A87 R88 D89 L90 D91 C92 S93 L94 E95 A96 A97 A98 E99 V103 R133 R151 E160 S161 I164 S171 A172 D173 M174 E177 I191 M204 T213 R216 V222 S223 Q226 A238 S271 S278 E279 S280 H281 D282 R283 G284 Y285 G286
K287 M293 D300 Y309 D316 C317 E318 H319 V320 I321 V329 M359 M386 L387 H388 F399 N411

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15661	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	2.786	Depositor
Minimum map value	-1.639	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.059	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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.28	0/11045	0.54	0/14893
2	B	0.30	0/8845	0.54	0/11930
3	C	0.25	0/4142	0.57	2/5592 (0.0%)
4	D	0.34	1/1467 (0.1%)	0.66	2/1972 (0.1%)
5	E	0.25	0/3282	0.53	1/4439 (0.0%)
6	F	0.40	0/2438	0.64	1/3289 (0.0%)
7	G	0.30	0/739	0.76	0/996
8	H	0.27	0/1551	0.49	0/2110
9	I	0.25	0/1013	0.54	0/1365
10	J	0.29	0/870	0.67	0/1175
11	K	0.30	0/2790	0.55	0/3782
12	L	0.30	0/871	0.53	0/1174
13	M	0.27	0/1746	0.57	0/2358
14	N	0.31	0/638	0.56	0/861
15	O	0.30	0/1207	0.54	0/1628
16	P	0.32	0/395	0.62	0/524
17	Q	0.35	0/533	0.52	0/719
18	R	0.28	0/1428	0.57	0/1924
19	S	0.26	0/2898	0.59	1/3933 (0.0%)
20	T	0.28	0/680	0.68	0/904
21	U	0.25	0/1215	0.51	0/1640
22	W	0.24	0/2058	0.50	0/2760
23	X	0.53	0/1569	1.67	114/2414 (4.7%)
24	Y	0.54	0/1620	1.64	111/2497 (4.4%)
25	Z	0.24	0/3203	0.51	0/4335
All	All	0.30	1/58243 (0.0%)	0.68	232/79214 (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	3
10	J	0	1
20	T	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	113	PRO	CG-CD	-7.12	1.27	1.50

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	113	PRO	CA-N-CD	-11.22	95.80	111.50
4	D	113	PRO	N-CD-CG	-9.14	89.50	103.20
24	Y	-21	DT	OP1-P-O3'	8.78	124.51	105.20
24	Y	-20	DG	OP1-P-OP2	-8.25	107.22	119.60
23	X	19	DC	OP1-P-OP2	-7.91	107.73	119.60
23	X	18	DT	OP1-P-O3'	7.84	122.46	105.20
23	X	34	DC	OP1-P-OP2	-7.75	107.98	119.60
24	Y	-19	DT	OP1-P-OP2	-7.58	108.22	119.60
24	Y	-18	DG	OP1-P-OP2	-7.48	108.38	119.60
24	Y	-49	DA	OP1-P-OP2	-7.43	108.45	119.60
24	Y	-27	DA	OP1-P-OP2	-7.39	108.52	119.60
23	X	18	DT	OP1-P-OP2	-7.38	108.53	119.60
24	Y	-50	DG	OP1-P-OP2	-7.27	108.69	119.60
23	X	26	DA	OP1-P-OP2	-7.23	108.75	119.60
24	Y	-58	DA	OP1-P-OP2	-7.22	108.77	119.60
24	Y	-60	DC	OP1-P-OP2	-7.21	108.79	119.60
24	Y	-61	DC	OP1-P-OP2	-7.19	108.81	119.60
23	X	33	DG	OP1-P-OP2	-7.17	108.85	119.60
24	Y	-33	DG	OP1-P-OP2	-7.15	108.88	119.60
23	X	63	DA	OP1-P-OP2	-7.14	108.89	119.60
23	X	43	DC	OP1-P-OP2	-7.10	108.95	119.60
23	X	21	DC	OP1-P-OP2	-7.10	108.95	119.60
23	X	-1	DA	OP1-P-OP2	-7.09	108.96	119.60
24	Y	-29	DA	OP1-P-OP2	-7.08	108.98	119.60
23	X	32	DA	OP1-P-OP2	-7.07	109.00	119.60
24	Y	-59	DT	OP1-P-OP2	-7.05	109.03	119.60
23	X	28	DT	OP1-P-OP2	-7.04	109.04	119.60
24	Y	-52	DA	OP1-P-OP2	-7.04	109.04	119.60
24	Y	-35	DG	OP1-P-OP2	-7.04	109.05	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	-41	DA	OP1-P-OP2	-7.03	109.05	119.60
23	X	51	DC	OP1-P-OP2	-7.03	109.06	119.60
24	Y	-22	DG	OP1-P-OP2	-7.01	109.09	119.60
23	X	58	DT	OP1-P-OP2	-7.00	109.11	119.60
23	X	35	DC	OP1-P-OP2	-6.99	109.12	119.60
23	X	-6	DC	OP1-P-OP2	-6.98	109.13	119.60
23	X	37	DT	OP1-P-OP2	-6.97	109.14	119.60
23	X	-9	DA	OP1-P-OP2	-6.97	109.15	119.60
24	Y	-37	DA	OP1-P-OP2	-6.96	109.16	119.60
24	Y	-32	DC	OP1-P-OP2	-6.96	109.16	119.60
23	X	24	DC	OP1-P-OP2	-6.95	109.18	119.60
24	Y	-48	DT	OP1-P-OP2	-6.95	109.18	119.60
24	Y	-25	DT	OP1-P-OP2	-6.95	109.18	119.60
24	Y	-20	DG	OP1-P-O3'	6.95	120.48	105.20
24	Y	-36	DA	OP1-P-OP2	-6.94	109.19	119.60
24	Y	-14	DG	OP1-P-OP2	-6.94	109.19	119.60
23	X	-8	DA	OP1-P-OP2	-6.94	109.19	119.60
24	Y	-40	DT	OP1-P-OP2	-6.94	109.19	119.60
24	Y	-28	DA	OP1-P-OP2	-6.92	109.22	119.60
24	Y	3	DG	OP1-P-OP2	-6.91	109.23	119.60
24	Y	-38	DG	OP1-P-OP2	-6.91	109.23	119.60
23	X	44	DA	OP1-P-OP2	-6.91	109.24	119.60
24	Y	-26	DA	OP1-P-OP2	-6.91	109.24	119.60
24	Y	5	DT	OP1-P-OP2	-6.90	109.25	119.60
23	X	-7	DG	OP1-P-OP2	-6.90	109.25	119.60
23	X	20	DA	OP1-P-OP2	-6.88	109.28	119.60
23	X	65	DA	OP1-P-OP2	-6.88	109.28	119.60
24	Y	-47	DG	OP1-P-OP2	-6.86	109.31	119.60
24	Y	-53	DA	OP1-P-OP2	-6.86	109.31	119.60
23	X	42	DT	OP1-P-OP2	-6.84	109.33	119.60
24	Y	14	DC	OP1-P-OP2	-6.84	109.33	119.60
24	Y	9	DT	OP1-P-OP2	-6.84	109.34	119.60
23	X	29	DT	OP1-P-OP2	-6.84	109.34	119.60
24	Y	-42	DG	OP1-P-OP2	-6.84	109.34	119.60
24	Y	-39	DT	OP1-P-OP2	-6.83	109.36	119.60
24	Y	12	DG	OP1-P-OP2	-6.83	109.36	119.60
24	Y	8	DC	OP1-P-OP2	-6.83	109.36	119.60
24	Y	-24	DA	OP1-P-OP2	-6.82	109.38	119.60
23	X	61	DG	OP1-P-OP2	-6.81	109.38	119.60
24	Y	-62	DT	OP1-P-OP2	-6.81	109.38	119.60
23	X	22	DA	OP1-P-OP2	-6.81	109.39	119.60
24	Y	-19	DT	OP1-P-O3'	6.80	120.17	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	15	DA	OP1-P-OP2	-6.80	109.39	119.60
23	X	45	DA	OP1-P-OP2	-6.80	109.40	119.60
24	Y	-31	DT	OP1-P-OP2	-6.80	109.41	119.60
23	X	57	DG	OP1-P-OP2	-6.79	109.41	119.60
5	E	345	PRO	CA-N-CD	-6.79	101.99	111.50
23	X	17	DG	OP1-P-O3'	6.79	120.14	105.20
23	X	-15	DC	OP1-P-OP2	-6.79	109.42	119.60
23	X	-10	DG	OP1-P-OP2	-6.78	109.42	119.60
24	Y	-64	DT	OP1-P-OP2	-6.78	109.43	119.60
24	Y	11	DC	OP1-P-OP2	-6.77	109.44	119.60
23	X	-14	DT	OP1-P-OP2	-6.77	109.45	119.60
23	X	34	DC	OP1-P-O3'	6.77	120.08	105.20
23	X	62	DG	OP1-P-OP2	-6.76	109.45	119.60
24	Y	10	DT	OP1-P-OP2	-6.76	109.45	119.60
23	X	36	DC	OP1-P-OP2	-6.74	109.49	119.60
23	X	46	DA	OP1-P-OP2	-6.74	109.49	119.60
23	X	1	DC	OP1-P-OP2	-6.74	109.50	119.60
24	Y	-28	DA	OP1-P-O3'	6.73	120.02	105.20
24	Y	7	DG	OP1-P-OP2	-6.73	109.50	119.60
24	Y	-44	DT	OP1-P-OP2	-6.72	109.52	119.60
24	Y	4	DC	OP1-P-OP2	-6.72	109.53	119.60
24	Y	-33	DG	OP1-P-O3'	6.71	119.96	105.20
23	X	50	DT	OP1-P-OP2	-6.69	109.57	119.60
23	X	39	DC	OP1-P-OP2	-6.68	109.59	119.60
23	X	-3	DG	OP1-P-OP2	-6.67	109.59	119.60
24	Y	-56	DC	OP1-P-OP2	-6.67	109.59	119.60
24	Y	13	DG	OP1-P-OP2	-6.67	109.59	119.60
23	X	41	DA	OP1-P-OP2	-6.67	109.60	119.60
23	X	-4	DA	OP1-P-OP2	-6.67	109.60	119.60
23	X	-13	DG	OP1-P-OP2	-6.66	109.61	119.60
23	X	-5	DG	OP1-P-OP2	-6.66	109.61	119.60
24	Y	-46	DA	OP1-P-OP2	-6.66	109.61	119.60
23	X	23	DC	OP1-P-O3'	6.66	119.85	105.20
23	X	30	DT	OP1-P-OP2	-6.65	109.63	119.60
24	Y	-23	DG	OP1-P-OP2	-6.65	109.63	119.60
23	X	49	DA	OP1-P-OP2	-6.64	109.64	119.60
23	X	55	DT	OP1-P-OP2	-6.64	109.64	119.60
24	Y	-57	DA	OP1-P-OP2	-6.64	109.64	119.60
23	X	31	DA	OP1-P-OP2	-6.64	109.64	119.60
24	Y	-17	DA	OP1-P-OP2	-6.62	109.66	119.60
23	X	48	DC	OP1-P-OP2	-6.62	109.67	119.60
23	X	52	DT	OP1-P-OP2	-6.62	109.67	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	-43	DT	OP1-P-OP2	-6.61	109.69	119.60
24	Y	-30	DT	OP1-P-OP2	-6.61	109.69	119.60
23	X	23	DC	OP1-P-OP2	-6.60	109.70	119.60
24	Y	-54	DA	OP1-P-OP2	-6.59	109.72	119.60
24	Y	-45	DT	OP1-P-OP2	-6.58	109.72	119.60
23	X	47	DT	OP1-P-OP2	-6.57	109.75	119.60
23	X	56	DG	OP1-P-OP2	-6.55	109.77	119.60
23	X	-11	DC	OP1-P-OP2	-6.55	109.78	119.60
23	X	40	DA	OP1-P-OP2	-6.55	109.78	119.60
24	Y	-34	DG	OP1-P-OP2	-6.54	109.79	119.60
24	Y	6	DC	OP1-P-OP2	-6.54	109.80	119.60
24	Y	-55	DC	OP1-P-OP2	-6.53	109.80	119.60
23	X	27	DT	OP1-P-OP2	-6.52	109.83	119.60
24	Y	-63	DA	OP1-P-OP2	-6.50	109.84	119.60
24	Y	-50	DG	OP1-P-O3'	6.49	119.48	105.20
24	Y	16	DG	OP1-P-OP2	-6.47	109.90	119.60
23	X	64	DT	OP1-P-OP2	-6.46	109.91	119.60
24	Y	-16	DC	OP1-P-OP2	-6.46	109.91	119.60
23	X	38	DT	OP1-P-OP2	-6.44	109.94	119.60
23	X	59	DT	OP1-P-OP2	-6.43	109.95	119.60
23	X	25	DT	OP1-P-OP2	-6.43	109.95	119.60
23	X	-12	DC	OP1-P-OP2	-6.42	109.97	119.60
24	Y	-60	DC	OP1-P-O3'	6.42	119.32	105.20
23	X	16	DT	OP1-P-OP2	-6.42	109.97	119.60
23	X	54	DT	OP1-P-OP2	-6.40	110.00	119.60
24	Y	-21	DT	OP1-P-OP2	-6.39	110.02	119.60
23	X	60	DA	OP1-P-OP2	-6.32	110.12	119.60
23	X	25	DT	OP1-P-O3'	6.22	118.88	105.20
23	X	17	DG	OP1-P-OP2	-6.21	110.29	119.60
23	X	-7	DG	OP1-P-O3'	6.19	118.81	105.20
24	Y	-61	DC	OP1-P-O3'	6.17	118.78	105.20
23	X	31	DA	OP1-P-O3'	6.05	118.52	105.20
24	Y	-30	DT	O4'-C1'-N1	6.04	112.23	108.00
23	X	20	DA	OP1-P-O3'	6.02	118.45	105.20
23	X	35	DC	OP1-P-O3'	6.01	118.42	105.20
23	X	42	DT	OP1-P-O3'	5.99	118.37	105.20
24	Y	-27	DA	OP1-P-O3'	5.98	118.37	105.20
24	Y	-59	DT	OP1-P-O3'	5.95	118.29	105.20
23	X	-11	DC	OP1-P-O3'	5.92	118.22	105.20
24	Y	-32	DC	OP1-P-O3'	5.92	118.22	105.20
3	C	474	MET	CA-CB-CG	5.91	123.34	113.30
24	Y	-37	DA	OP1-P-O3'	5.86	118.08	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	-39	DT	OP1-P-O3'	5.83	118.04	105.20
23	X	36	DC	OP2-P-O3'	5.82	118.01	105.20
24	Y	-24	DA	OP1-P-O3'	5.82	117.99	105.20
23	X	41	DA	OP1-P-O3'	5.77	117.89	105.20
24	Y	-36	DA	OP1-P-O3'	5.76	117.88	105.20
23	X	32	DA	OP1-P-O3'	5.76	117.88	105.20
23	X	43	DC	OP1-P-O3'	5.76	117.88	105.20
23	X	19	DC	OP1-P-O3'	5.76	117.87	105.20
24	Y	-62	DT	OP1-P-O3'	5.74	117.83	105.20
23	X	33	DG	OP1-P-O3'	5.73	117.80	105.20
23	X	-6	DC	OP1-P-O3'	5.70	117.74	105.20
23	X	-8	DA	OP1-P-O3'	5.69	117.72	105.20
24	Y	-26	DA	OP2-P-O3'	5.69	117.72	105.20
24	Y	-15	DA	OP1-P-O3'	5.69	117.72	105.20
24	Y	-29	DA	OP1-P-O3'	5.68	117.69	105.20
24	Y	-41	DA	OP1-P-O3'	5.67	117.68	105.20
23	X	-2	DC	OP1-P-OP2	-5.64	111.13	119.60
24	Y	4	DC	OP1-P-O3'	5.64	117.60	105.20
24	Y	-40	DT	OP1-P-O3'	5.63	117.59	105.20
23	X	22	DA	OP1-P-O3'	5.63	117.58	105.20
24	Y	-31	DT	OP1-P-O3'	5.62	117.56	105.20
24	Y	-34	DG	OP1-P-O3'	5.61	117.55	105.20
23	X	60	DA	OP1-P-O3'	5.60	117.52	105.20
24	Y	-42	DG	OP1-P-O3'	5.60	117.51	105.20
24	Y	3	DG	OP1-P-O3'	5.59	117.50	105.20
24	Y	-25	DT	OP1-P-O3'	5.58	117.47	105.20
23	X	-5	DG	OP1-P-O3'	5.57	117.44	105.20
3	C	271	LEU	CA-CB-CG	5.56	128.09	115.30
24	Y	-38	DG	OP1-P-O3'	5.56	117.43	105.20
23	X	29	DT	OP1-P-O3'	5.55	117.41	105.20
23	X	56	DG	OP1-P-O3'	5.55	117.42	105.20
24	Y	-53	DA	OP1-P-O3'	5.53	117.37	105.20
24	Y	6	DC	OP1-P-O3'	5.52	117.34	105.20
24	Y	9	DT	OP1-P-O3'	5.50	117.30	105.20
23	X	-2	DC	OP1-P-O3'	5.49	117.27	105.20
23	X	30	DT	OP1-P-O3'	5.48	117.26	105.20
24	Y	14	DC	OP1-P-O3'	5.46	117.22	105.20
24	Y	-63	DA	OP1-P-O3'	5.46	117.21	105.20
24	Y	-54	DA	OP1-P-O3'	5.46	117.20	105.20
24	Y	8	DC	OP1-P-O3'	5.46	117.20	105.20
23	X	-1	DA	OP1-P-O3'	5.45	117.18	105.20
23	X	37	DT	OP1-P-O3'	5.45	117.18	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	X	-15	DC	OP2-P-O3'	5.43	117.16	105.20
23	X	53	DT	OP1-P-OP2	-5.43	111.45	119.60
23	X	50	DT	OP1-P-O3'	5.43	117.14	105.20
23	X	48	DC	OP1-P-O3'	5.41	117.09	105.20
6	F	86	LYS	N-CA-C	5.40	125.59	111.00
23	X	-9	DA	OP1-P-O3'	5.39	117.05	105.20
24	Y	-64	DT	OP1-P-O3'	5.37	117.01	105.20
24	Y	7	DG	OP1-P-O3'	5.36	116.99	105.20
23	X	62	DG	OP1-P-O3'	5.36	116.99	105.20
23	X	64	DT	OP1-P-O3'	5.34	116.94	105.20
23	X	57	DG	OP1-P-O3'	5.30	116.87	105.20
23	X	21	DC	OP1-P-O3'	5.30	116.86	105.20
23	X	24	DC	OP2-P-O3'	5.29	116.85	105.20
23	X	40	DA	OP1-P-O3'	5.29	116.84	105.20
23	X	38	DT	OP1-P-O3'	5.29	116.84	105.20
24	Y	-43	DT	OP1-P-O3'	5.29	116.83	105.20
23	X	-4	DA	OP1-P-O3'	5.27	116.80	105.20
24	Y	-51	DA	OP1-P-OP2	-5.26	111.71	119.60
24	Y	13	DG	OP1-P-O3'	5.24	116.73	105.20
23	X	-10	DG	OP1-P-O3'	5.22	116.69	105.20
23	X	-14	DT	OP1-P-O3'	5.21	116.67	105.20
23	X	49	DA	OP1-P-O3'	5.20	116.65	105.20
24	Y	-23	DG	OP1-P-O3'	5.20	116.63	105.20
24	Y	-44	DT	OP1-P-O3'	5.19	116.62	105.20
24	Y	-45	DT	OP1-P-O3'	5.18	116.61	105.20
24	Y	-48	DT	OP1-P-O3'	5.17	116.58	105.20
23	X	61	DG	OP1-P-O3'	5.11	116.44	105.20
23	X	44	DA	OP1-P-O3'	5.09	116.40	105.20
19	S	273	LEU	CA-CB-CG	5.09	127.00	115.30
23	X	45	DA	OP1-P-O3'	5.08	116.39	105.20
24	Y	-30	DT	OP1-P-O3'	5.08	116.37	105.20
24	Y	-18	DG	OP1-P-O3'	5.06	116.34	105.20
24	Y	-46	DA	OP1-P-O3'	5.02	116.25	105.20
23	X	51	DC	OP1-P-O3'	5.01	116.22	105.20
23	X	-12	DC	OP1-P-O3'	5.00	116.21	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

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Mol	Chain	Res	Type	Group
1	A	1198	LYS	Peptide
6	F	201	ASN	Peptide
6	F	84	LYS	Peptide
6	F	85	MET	Peptide
10	J	76	ARG	Peptide
20	T	363	ASP	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	10849	0	11089	200	0
2	B	8680	0	8805	86	0
3	C	4076	0	4149	91	0
4	D	1449	0	1489	15	0
5	E	3211	0	3227	39	0
6	F	2395	0	2405	175	0
7	G	717	0	719	42	0
8	H	1509	0	1461	20	0
9	I	1001	0	1028	22	0
10	J	849	0	814	97	0
11	K	2736	0	2712	15	0
12	L	856	0	840	5	0
13	M	1716	0	1733	29	0
14	N	628	0	659	1	0
15	O	1186	0	1147	8	0
16	P	389	0	393	7	0
17	Q	524	0	540	4	0
18	R	1402	0	1489	44	0
19	S	2847	0	2887	62	0
20	T	665	0	665	34	0
21	U	1183	0	1175	20	0
22	W	2018	0	1997	28	0
23	X	1403	0	782	17	0
24	Y	1443	0	790	26	0
25	Z	3123	0	2983	19	0
26	A	2	0	0	0	0
26	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	56873	0	55978	961	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 9.

All (961) 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:287:CYS:SG	28:F:401:SF4:FE4	1.24	1.29
6:F:296:CYS:SG	28:F:401:SF4:FE3	1.41	1.12
3:C:445:ASN:ND2	28:F:401:SF4:S1	2.37	0.96
7:G:106:LEU:HD12	7:G:107:PRO:HD2	1.49	0.91
6:F:252:ILE:HG23	6:F:254:ALA:H	1.36	0.90
6:F:287:CYS:HG	28:F:401:SF4:FE4	0.55	0.85
1:A:1137:ILE:O	1:A:1141:ARG:N	2.11	0.83
2:B:279:THR:OG1	2:B:281:MET:SD	2.37	0.83
2:B:89:GLU:OE1	2:B:93:VAL:HG13	1.79	0.82
3:C:438:ARG:HD3	6:F:293:PHE:CE2	2.15	0.81
1:A:1223:TYR:O	10:J:100:ALA:N	2.14	0.80
19:S:112:GLN:N	19:S:112:GLN:OE1	2.15	0.80
1:A:1224:LYS:N	10:J:102:CYS:SG	2.54	0.80
6:F:85:MET:SD	6:F:85:MET:N	2.54	0.80
22:W:199:ASP:OD1	22:W:266:ILE:HD11	1.83	0.79
1:A:1211:VAL:HG22	1:A:1212:ILE:H	1.47	0.79
6:F:84:LYS:HA	6:F:86:LYS:HD2	1.62	0.79
19:S:249:ARG:O	19:S:253:LEU:HD22	1.83	0.79
1:A:280:THR:O	1:A:284:THR:HG23	1.84	0.78
4:D:143:GLU:HG3	10:J:3:LEU:HD23	1.65	0.78
8:H:30:LEU:HD11	8:H:48:LEU:HD12	1.65	0.78
6:F:239:LEU:HD22	6:F:266:HIS:CE1	2.20	0.76
1:A:941:SER:OG	1:A:944:GLU:OE1	2.04	0.76
19:S:296:HIS:O	19:S:300:LEU:HD12	1.87	0.75
7:G:57:MET:SD	7:G:57:MET:N	2.60	0.74
6:F:287:CYS:SG	28:F:401:SF4:S3	2.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:21:HIS:HB2	10:J:34:ILE:HD11	1.69	0.74
1:A:266:VAL:HG12	19:S:50:LEU:HD22	1.69	0.74
9:I:91:PRO:HD2	9:I:120:VAL:HG21	1.70	0.73
6:F:187:PHE:HE2	6:F:216:VAL:HG22	1.51	0.73
6:F:251:THR:HG22	6:F:251:THR:O	1.89	0.73
3:C:438:ARG:NH1	6:F:293:PHE:CD2	2.57	0.73
6:F:308:ILE:HG23	7:G:38:PHE:HE2	1.53	0.72
5:E:375:THR:HG23	5:E:377:LEU:HD12	1.70	0.72
2:B:417:ASN:O	2:B:421:THR:HG22	1.89	0.71
3:C:438:ARG:NH1	6:F:293:PHE:CE2	2.56	0.71
1:A:1100:LEU:HD12	10:J:80:MET:SD	2.29	0.71
1:A:1196:LEU:HB3	1:A:1197:PRO:HD3	1.72	0.71
6:F:187:PHE:CE2	6:F:216:VAL:HG22	2.26	0.71
6:F:248:VAL:CG2	6:F:268:LYS:HB2	2.21	0.71
18:R:259:VAL:HG21	23:X:29:DT:O2	1.91	0.71
2:B:215:ASN:OD1	2:B:216:MET:N	2.24	0.71
3:C:441:LYS:CE	6:F:293:PHE:CE2	2.73	0.71
6:F:268:LYS:O	6:F:269:LEU:HD22	1.91	0.70
11:K:287:ILE:HD13	11:K:297:VAL:HG21	1.74	0.70
18:R:187:ALA:O	19:S:394:ARG:NH2	2.24	0.70
18:R:189:ASN:ND2	18:R:202:MET:SD	2.65	0.70
1:A:97:TYR:O	1:A:101:VAL:HG23	1.92	0.70
2:B:339:VAL:O	2:B:343:ILE:HG22	1.91	0.70
3:C:374:HIS:HB3	3:C:423:LEU:HD12	1.71	0.69
3:C:441:LYS:HE3	6:F:293:PHE:CE2	2.27	0.69
10:J:82:LEU:HD21	10:J:94:PHE:CE1	2.28	0.68
21:U:27:GLU:OE2	25:Z:103:VAL:HG13	1.94	0.68
10:J:20:CYS:O	10:J:22:ARG:NH2	2.27	0.67
10:J:102:CYS:SG	10:J:103:GLY:N	2.67	0.67
24:Y:-30:DT:C2	24:Y:-29:DA:C8	2.82	0.67
21:U:26:PHE:O	21:U:30:THR:HG23	1.94	0.67
1:A:1212:ILE:HD11	10:J:106:TRP:CG	2.28	0.67
18:R:295:MET:SD	18:R:297:LYS:N	2.68	0.67
7:G:82:GLN:OE1	7:G:82:GLN:N	2.19	0.67
13:M:27:LEU:HD12	13:M:28:VAL:N	2.11	0.66
6:F:91:GLN:OE1	6:F:126:ILE:HD11	1.96	0.66
19:S:205:MET:SD	19:S:206:GLN:N	2.68	0.66
1:A:1201:VAL:HG11	10:J:48:GLU:O	1.96	0.66
3:C:117:THR:O	3:C:121:VAL:HG12	1.96	0.66
11:K:238:ASP:O	11:K:238:ASP:OD2	2.14	0.66
1:A:855:ARG:NH2	2:B:481:PRO:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:83:GLY:O	6:F:86:LYS:NZ	2.28	0.65
7:G:110:MET:SD	7:G:110:MET:N	2.70	0.65
10:J:14:VAL:HG22	10:J:23:PHE:CE1	2.32	0.65
19:S:120:CYS:O	19:S:124:ILE:HG22	1.96	0.65
20:T:313:LEU:O	20:T:317:MET:HE2	1.96	0.65
10:J:82:LEU:HD21	10:J:94:PHE:CD1	2.32	0.64
6:F:243:ILE:HB	6:F:248:VAL:HG11	1.79	0.64
3:C:531:MET:SD	3:C:532:LYS:N	2.70	0.64
1:A:1095:ALA:HB3	10:J:75:PRO:O	1.97	0.64
6:F:267:MET:SD	6:F:268:LYS:N	2.70	0.64
19:S:233:ALA:O	19:S:237:LEU:HD22	1.98	0.64
6:F:83:GLY:O	6:F:86:LYS:HA	1.98	0.63
19:S:268:GLU:O	19:S:272:VAL:HG23	1.98	0.63
13:M:5:GLU:OE1	13:M:5:GLU:N	2.32	0.63
6:F:78:ASP:O	6:F:81:ASN:N	2.32	0.63
19:S:145:ASP:OD1	19:S:146:LEU:N	2.32	0.63
1:A:243:GLU:OE2	1:A:243:GLU:N	2.31	0.63
22:W:340:HIS:O	22:W:340:HIS:CD2	2.52	0.63
1:A:1122:LEU:HD22	1:A:1124:ASP:OD1	1.98	0.63
18:R:187:ALA:HB2	18:R:244:LEU:HD21	1.81	0.62
18:R:284:GLU:OE2	18:R:287:LEU:N	2.32	0.62
7:G:44:LYS:HE3	7:G:44:LYS:HA	1.80	0.62
8:H:26:ILE:HD11	8:H:70:VAL:HG22	1.81	0.62
7:G:42:ASP:OD2	7:G:43:TYR:N	2.32	0.62
2:B:379:LYS:HE3	2:B:379:LYS:HA	1.82	0.62
25:Z:223:SER:OG	25:Z:317:CYS:SG	2.50	0.62
20:T:318:VAL:O	20:T:318:VAL:HG22	2.00	0.62
18:R:208:ARG:H	18:R:208:ARG:HD2	1.64	0.62
20:T:364:PHE:O	20:T:368:ALA:N	2.30	0.62
3:C:531:MET:O	3:C:533:ARG:NH2	2.33	0.62
2:B:280:GLN:N	2:B:280:GLN:OE1	2.33	0.61
2:B:634:ASP:OD1	2:B:635:VAL:N	2.31	0.61
15:O:138:ASP:O	15:O:138:ASP:OD2	2.18	0.61
7:G:81:ARG:O	7:G:81:ARG:HG2	1.99	0.61
1:A:120:GLU:N	1:A:120:GLU:OE1	2.34	0.61
2:B:311:GLU:OE2	2:B:312:LEU:N	2.33	0.61
1:A:1094:ASP:OD1	1:A:1095:ALA:N	2.33	0.61
1:A:1093:ASP:O	10:J:77:ALA:HB3	2.00	0.61
1:A:296:HIS:CE1	1:A:301:ALA:HB3	2.35	0.61
1:A:897:ILE:HD12	13:M:165:LEU:HD21	1.83	0.61
6:F:86:LYS:HE3	6:F:91:GLN:CA	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:165:ALA:HB3	6:F:234:ASP:OD2	2.00	0.60
19:S:135:MET:SD	19:S:135:MET:N	2.69	0.60
3:C:293:ILE:HD12	3:C:308:LEU:HD21	1.83	0.60
6:F:239:LEU:O	6:F:270:TYR:OH	2.18	0.60
3:C:438:ARG:NH1	6:F:293:PHE:CG	2.69	0.60
10:J:34:ILE:HD12	10:J:34:ILE:O	2.01	0.60
1:A:1143:GLU:OE1	1:A:1143:GLU:N	2.35	0.60
6:F:84:LYS:HD3	6:F:86:LYS:HD3	1.81	0.60
3:C:88:TYR:CZ	3:C:111:LEU:HD11	2.36	0.60
7:G:41:THR:O	7:G:44:LYS:NZ	2.24	0.60
20:T:338:LYS:NZ	23:X:28:DT:OP1	2.22	0.60
6:F:250:MET:CE	6:F:252:ILE:HG22	2.32	0.59
10:J:89:GLU:N	10:J:89:GLU:OE1	2.35	0.59
1:A:109:CYS:SG	1:A:163:ASN:ND2	2.73	0.59
6:F:134:LYS:HA	6:F:153:TYR:CE1	2.38	0.59
6:F:176:PHE:HA	6:F:179:VAL:HG12	1.83	0.59
13:M:103:LEU:HD12	13:M:104:ILE:N	2.17	0.59
6:F:231:SER:O	6:F:233:GLU:N	2.35	0.59
2:B:257:THR:OG1	4:D:146:GLU:OE2	2.20	0.59
6:F:84:LYS:HA	6:F:86:LYS:CD	2.32	0.58
3:C:121:VAL:O	3:C:125:VAL:HG12	2.02	0.58
1:A:1099:ARG:HG2	10:J:80:MET:HG2	1.84	0.58
4:D:138:ILE:HD12	4:D:138:ILE:H	1.68	0.58
1:A:1195:ASP:O	10:J:46:LEU:HB3	2.03	0.58
6:F:296:CYS:SG	28:F:401:SF4:S4	2.96	0.58
8:H:142:MET:SD	8:H:142:MET:N	2.77	0.58
18:R:204:ILE:HG22	19:S:392:TYR:OH	2.03	0.58
18:R:208:ARG:HD2	18:R:208:ARG:N	2.18	0.58
18:R:295:MET:SD	18:R:296:ILE:N	2.77	0.58
2:B:257:THR:OG1	4:D:147:THR:OG1	2.22	0.58
9:I:110:GLU:HA	9:I:113:ILE:HD12	1.86	0.58
19:S:405:ALA:HB3	20:T:364:PHE:HB3	1.86	0.58
21:U:17:ARG:O	21:U:21:THR:HG23	2.03	0.58
1:A:1239:HIS:CD2	10:J:56:ALA:HB3	2.39	0.58
20:T:365:ASP:O	20:T:369:HIS:CD2	2.57	0.58
1:A:1113:ILE:HG22	1:A:1137:ILE:HD11	1.85	0.58
10:J:86:SER:OG	10:J:87:ALA:N	2.36	0.58
2:B:75:LEU:HD11	2:B:117:ILE:HG12	1.86	0.57
6:F:82:ALA:HA	6:F:94:LEU:HD13	1.85	0.57
24:Y:-14:DG:H2'	24:Y:-13:DT:C6	2.39	0.57
1:A:485:THR:O	1:A:487:ARG:NH1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:243:ILE:HA	6:F:248:VAL:HG11	1.85	0.57
2:B:271:GLU:N	2:B:271:GLU:OE1	2.37	0.57
18:R:188:ARG:NH1	20:T:360:ARG:O	2.38	0.57
1:A:283:LEU:O	1:A:287:ILE:HG22	2.04	0.57
3:C:252:VAL:HG23	3:C:271:LEU:HD21	1.86	0.57
6:F:86:LYS:HE3	6:F:91:GLN:HG3	1.85	0.57
19:S:288:LEU:HD13	19:S:293:VAL:HB	1.85	0.57
1:A:1100:LEU:HD23	1:A:1104:ARG:NH2	2.20	0.57
13:M:31:ASP:OD2	13:M:32:GLU:N	2.38	0.57
22:W:149:TYR:HE1	25:Z:320:VAL:HG22	1.68	0.57
1:A:267:VAL:HB	1:A:277:ASP:HA	1.85	0.57
2:B:39:LEU:O	2:B:40:VAL:HG12	2.04	0.57
22:W:376:VAL:HG21	22:W:383:ASP:C	2.26	0.57
6:F:251:THR:HB	6:F:268:LYS:HA	1.87	0.56
17:Q:40:LEU:HD22	17:Q:45:CYS:HB3	1.86	0.56
19:S:112:GLN:O	19:S:116:VAL:HG13	2.04	0.56
20:T:342:LYS:HE3	20:T:342:LYS:HA	1.86	0.56
3:C:88:TYR:CG	3:C:111:LEU:HD21	2.40	0.56
6:F:84:LYS:CB	6:F:94:LEU:HD23	2.35	0.56
6:F:86:LYS:HE3	6:F:91:GLN:HA	1.87	0.56
15:O:66:GLU:N	15:O:66:GLU:OE1	2.39	0.56
6:F:167:TYR:HA	6:F:172:PHE:HA	1.87	0.56
6:F:220:ILE:HG22	6:F:226:SER:HB2	1.86	0.56
8:H:119:LYS:HD2	8:H:120:PHE:HB2	1.87	0.56
6:F:86:LYS:NZ	6:F:87:GLY:O	2.32	0.56
1:A:1167:VAL:O	1:A:1167:VAL:HG13	2.04	0.56
1:A:1221:GLU:HB2	10:J:74:HIS:CE1	2.41	0.56
1:A:1319:ALA:O	1:A:1324:THR:HG22	2.05	0.56
2:B:232:GLU:N	2:B:232:GLU:OE1	2.39	0.56
9:I:81:ALA:O	9:I:85:GLN:NE2	2.39	0.56
22:W:147:LYS:NZ	25:Z:318:GLU:O	2.26	0.56
18:R:258:MET:SD	18:R:258:MET:N	2.79	0.56
8:H:2:PHE:CD2	9:I:16:VAL:HG21	2.41	0.56
18:R:287:LEU:HD13	19:S:150:SER:HB2	1.87	0.56
19:S:231:PHE:CZ	19:S:247:LEU:HA	2.40	0.56
1:A:1101:VAL:HG22	1:A:1104:ARG:NH1	2.21	0.56
2:B:72:MET:O	2:B:72:MET:HG3	2.06	0.55
6:F:230:LEU:HD12	6:F:235:ILE:HB	1.87	0.55
6:F:250:MET:HE1	6:F:252:ILE:HG22	1.89	0.55
6:F:287:CYS:SG	28:F:401:SF4:S2	3.05	0.55
18:R:202:MET:N	18:R:211:ALA:O	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:ILE:HG22	2:B:318:LEU:HG	1.89	0.55
6:F:296:CYS:SG	28:F:401:SF4:S1	3.04	0.55
1:A:1108:THR:O	10:J:49:VAL:N	2.39	0.55
9:I:82:GLU:O	9:I:86:LEU:HG	2.07	0.55
24:Y:-29:DA:H2'	24:Y:-28:DA:C8	2.41	0.55
1:A:575:LYS:HE2	1:A:575:LYS:HA	1.88	0.55
1:A:1199:VAL:HG13	1:A:1200:VAL:N	2.21	0.55
3:C:85:MET:SD	3:C:85:MET:N	2.77	0.55
6:F:240:ASN:HA	6:F:243:ILE:HG12	1.87	0.55
7:G:89:LYS:HD3	7:G:89:LYS:N	2.22	0.55
17:Q:31:GLU:OE1	17:Q:31:GLU:N	2.38	0.55
20:T:312:PHE:O	20:T:351:ARG:NH2	2.38	0.55
6:F:201:ASN:O	6:F:203:MET:N	2.40	0.55
1:A:1195:ASP:HA	10:J:46:LEU:HB2	1.88	0.55
3:C:269:THR:O	3:C:273:MET:HE3	2.07	0.55
7:G:106:LEU:HD12	7:G:107:PRO:CD	2.28	0.55
1:A:267:VAL:O	19:S:50:LEU:HD23	2.07	0.54
13:M:17:ILE:HD11	13:M:103:LEU:HD21	1.89	0.54
18:R:202:MET:HG2	18:R:213:ILE:HD11	1.88	0.54
18:R:241:VAL:HA	18:R:244:LEU:HD12	1.89	0.54
22:W:199:ASP:CG	22:W:266:ILE:HD11	2.27	0.54
6:F:86:LYS:HE3	6:F:91:GLN:N	2.22	0.54
24:Y:-24:DA:H2'	24:Y:-23:DG:O4'	2.08	0.54
3:C:441:LYS:NZ	6:F:293:PHE:CE2	2.76	0.54
6:F:300:GLY:O	6:F:301:GLU:C	2.46	0.54
1:A:367:THR:HG22	1:A:368:VAL:N	2.23	0.54
1:A:978:GLU:OE2	1:A:982:LYS:NZ	2.41	0.54
1:A:1109:LEU:HD13	10:J:48:GLU:HA	1.90	0.54
7:G:63:GLU:O	7:G:67:THR:HG22	2.07	0.54
13:M:103:LEU:HD12	13:M:104:ILE:H	1.73	0.54
5:E:418:ARG:HA	5:E:421:MET:SD	2.48	0.53
6:F:239:LEU:O	6:F:243:ILE:HG23	2.09	0.53
8:H:116:GLN:O	8:H:116:GLN:NE2	2.39	0.53
13:M:163:TYR:HB2	13:M:165:LEU:CD1	2.38	0.53
18:R:263:ASP:OD1	18:R:264:VAL:N	2.41	0.53
6:F:252:ILE:HG23	6:F:254:ALA:N	2.16	0.53
10:J:74:HIS:HB3	10:J:75:PRO:HD2	1.90	0.53
3:C:88:TYR:CD2	3:C:111:LEU:HD21	2.43	0.53
10:J:69:CYS:SG	10:J:73:GLU:N	2.82	0.53
3:C:441:LYS:NZ	6:F:293:PHE:CZ	2.77	0.53
5:E:86:ALA:HB1	5:E:88:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:ILE:HG22	7:G:85:GLU:H	1.73	0.53
8:H:26:ILE:HD11	8:H:70:VAL:CG2	2.37	0.53
1:A:1065:LEU:HD23	1:A:1066:GLY:N	2.24	0.53
11:K:5:GLN:OE1	11:K:5:GLN:N	2.41	0.53
24:Y:-26:DA:H2'	24:Y:-25:DT:C6	2.43	0.53
6:F:200:GLN:O	6:F:205:GLN:N	2.41	0.53
6:F:206:ARG:HD2	6:F:207:ASN:N	2.24	0.53
19:S:167:LEU:HB3	19:S:172:LEU:HD21	1.90	0.53
1:A:1195:ASP:H	10:J:44:PRO:HB2	1.74	0.53
3:C:376:GLU:OE2	3:C:423:LEU:HD22	2.09	0.53
1:A:1136:ARG:O	1:A:1140:LEU:HD13	2.08	0.53
2:B:75:LEU:HD13	2:B:119:TYR:HB3	1.91	0.53
6:F:251:THR:O	6:F:251:THR:CG2	2.57	0.53
7:G:60:LEU:O	7:G:64:LEU:HD23	2.08	0.53
6:F:251:THR:H	6:F:268:LYS:HG2	1.74	0.52
1:A:40:ASN:OD1	19:S:60:GLY:N	2.41	0.52
11:K:241:LEU:HD23	11:K:241:LEU:H	1.74	0.52
2:B:135:ARG:H	2:B:412:THR:HG22	1.75	0.52
6:F:308:ILE:HG12	7:G:38:PHE:CE2	2.44	0.52
1:A:720:GLY:HA3	1:A:759:ILE:HD11	1.90	0.52
6:F:200:GLN:O	6:F:201:ASN:C	2.48	0.52
13:M:121:MET:H	13:M:121:MET:CE	2.22	0.52
2:B:722:THR:HG22	2:B:723:LYS:H	1.74	0.52
6:F:78:ASP:O	6:F:80:GLN:N	2.42	0.52
9:I:101:VAL:O	9:I:104:SER:OG	2.26	0.52
13:M:199:THR:HG23	13:M:201:GLY:H	1.74	0.52
21:U:97:ILE:N	21:U:134:ALA:O	2.38	0.52
24:Y:-31:DT:H2'	24:Y:-30:DT:C6	2.43	0.52
1:A:97:TYR:HB3	1:A:250:LEU:HD21	1.91	0.52
4:D:331:ILE:HD12	4:D:331:ILE:N	2.24	0.52
13:M:118:LEU:HD23	13:M:127:LEU:HD12	1.91	0.52
19:S:204:THR:O	19:S:208:VAL:HG22	2.10	0.52
24:Y:-29:DA:H2'	24:Y:-28:DA:H8	1.74	0.52
6:F:243:ILE:HA	6:F:248:VAL:CG1	2.39	0.52
13:M:18:MET:HE2	13:M:33:LEU:HA	1.90	0.52
19:S:231:PHE:CZ	19:S:250:PHE:HB3	2.45	0.52
1:A:1192:LEU:HD12	1:A:1192:LEU:O	2.10	0.52
24:Y:-25:DT:H2'	24:Y:-24:DA:C8	2.45	0.52
3:C:438:ARG:HD3	6:F:293:PHE:CZ	2.45	0.52
6:F:293:PHE:O	6:F:294:ASP:C	2.48	0.52
1:A:1094:ASP:OD1	10:J:75:PRO:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1122:LEU:HG	1:A:1123:PRO:HD2	1.91	0.51
2:B:458:GLN:N	2:B:458:GLN:OE1	2.43	0.51
25:Z:386:MET:SD	25:Z:387:LEU:N	2.83	0.51
6:F:249:GLU:O	6:F:268:LYS:HB3	2.10	0.51
18:R:172:VAL:HG12	18:R:219:MET:CE	2.40	0.51
18:R:180:LEU:HD22	18:R:200:VAL:HG23	1.91	0.51
2:B:812:ASP:OD2	16:P:15:MET:HE1	2.11	0.51
7:G:33:LYS:HA	7:G:33:LYS:HE2	1.93	0.51
10:J:39:THR:HG22	10:J:39:THR:O	2.10	0.51
19:S:270:LEU:O	19:S:273:LEU:HD12	2.09	0.51
24:Y:-18:DG:H1'	24:Y:-17:DA:C8	2.46	0.51
3:C:514:ILE:HG13	7:G:61:LYS:HE2	1.91	0.51
5:E:313:GLY:O	5:E:317:VAL:HG23	2.11	0.51
8:H:119:LYS:HD2	8:H:119:LYS:C	2.30	0.51
10:J:52:VAL:HG13	10:J:53:LEU:HG	1.92	0.51
7:G:89:LYS:HA	7:G:92:MET:SD	2.51	0.51
1:A:1089:LEU:HD22	1:A:1098:ALA:HA	1.91	0.51
1:A:1212:ILE:HD11	10:J:106:TRP:CD1	2.45	0.51
2:B:325:GLU:OE1	2:B:325:GLU:N	2.37	0.51
3:C:109:GLU:HA	3:C:109:GLU:OE2	2.11	0.51
6:F:118:LEU:O	6:F:123:ILE:HD11	2.11	0.51
21:U:133:ARG:NH1	25:Z:64:ARG:O	2.42	0.51
2:B:89:GLU:OE2	2:B:89:GLU:N	2.33	0.51
6:F:188:LEU:HD11	6:F:270:TYR:CB	2.40	0.51
3:C:267:VAL:HA	3:C:270:MET:SD	2.51	0.51
7:G:41:THR:OG1	7:G:44:LYS:NZ	2.40	0.51
2:B:751:ILE:HG22	2:B:752:GLU:HG2	1.92	0.51
18:R:191:GLU:OE2	20:T:322:PHE:N	2.44	0.51
20:T:371:LEU:O	20:T:375:LEU:HG	2.11	0.51
1:A:302:LYS:HZ2	1:A:304:GLN:H	1.59	0.50
3:C:139:MET:SD	3:C:140:ASP:N	2.84	0.50
18:R:210:THR:HB	23:X:28:DT:H5"	1.93	0.50
21:U:46:MET:SD	21:U:46:MET:N	2.84	0.50
21:U:63:TRP:CH2	21:U:107:VAL:HG21	2.46	0.50
22:W:306:GLN:NE2	22:W:340:HIS:O	2.36	0.50
24:Y:-23:DG:H2'	24:Y:-22:DG:C8	2.46	0.50
1:A:776:SER:HB2	1:A:777:PRO:HD3	1.94	0.50
2:B:722:THR:HG23	2:B:962:THR:HA	1.92	0.50
7:G:80:GLU:OE1	7:G:80:GLU:N	2.43	0.50
12:L:98:ARG:O	12:L:102:GLU:HG3	2.10	0.50
19:S:266:LEU:O	19:S:270:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:325:ILE:HD11	20:T:337:ILE:HG21	1.92	0.50
22:W:187:TRP:CE2	22:W:191:LEU:HD11	2.45	0.50
21:U:27:GLU:O	21:U:31:GLU:HG2	2.11	0.50
1:A:252:LEU:O	1:A:252:LEU:HD12	2.11	0.50
4:D:332:ARG:HG3	4:D:336:ARG:HH12	1.77	0.50
5:E:319:MET:SD	5:E:319:MET:N	2.84	0.50
3:C:487:ILE:O	3:C:489:GLU:N	2.45	0.50
6:F:75:ARG:HH12	6:F:78:ASP:HB2	1.76	0.50
9:I:53:ILE:O	9:I:59:ARG:NH1	2.45	0.50
22:W:340:HIS:O	22:W:340:HIS:CG	2.65	0.50
3:C:473:SER:HB2	3:C:474:MET:HE1	1.94	0.50
6:F:82:ALA:N	6:F:94:LEU:HD13	2.25	0.50
11:K:50:ARG:NH1	11:K:52:ASP:OD2	2.44	0.50
19:S:76:VAL:HG22	19:S:118:VAL:HG13	1.93	0.50
21:U:8:GLN:N	21:U:8:GLN:OE1	2.44	0.50
21:U:105:ASP:OD1	21:U:106:GLU:N	2.45	0.50
3:C:441:LYS:NZ	6:F:293:PHE:CD2	2.79	0.50
3:C:487:ILE:O	3:C:490:MET:HE1	2.12	0.50
10:J:82:LEU:HD21	10:J:94:PHE:HE1	1.76	0.49
1:A:1096:ASP:H	10:J:76:ARG:HA	1.77	0.49
3:C:293:ILE:CD1	3:C:308:LEU:HD21	2.42	0.49
6:F:190:SER:O	6:F:194:THR:HG23	2.13	0.49
6:F:217:TRP:CD1	6:F:230:LEU:HG	2.47	0.49
6:F:265:GLY:HA3	6:F:268:LYS:HD2	1.94	0.49
8:H:115:GLN:HG2	8:H:117:PRO:HD2	1.94	0.49
1:A:1223:TYR:HA	10:J:102:CYS:SG	2.52	0.49
3:C:368:LEU:HD21	6:F:244:TYR:HB3	1.93	0.49
5:E:321:VAL:HG12	5:E:423:TRP:CH2	2.47	0.49
6:F:84:LYS:HB3	6:F:94:LEU:HD23	1.94	0.49
21:U:14:LEU:HD22	21:U:36:MET:HE1	1.93	0.49
1:A:1096:ASP:HA	10:J:78:TYR:CD2	2.47	0.49
2:B:407:ARG:HG2	2:B:407:ARG:HH11	1.78	0.49
6:F:79:SER:O	6:F:90:ASN:ND2	2.45	0.49
6:F:251:THR:O	6:F:253:ILE:HD12	2.12	0.49
6:F:287:CYS:SG	28:F:401:SF4:S1	3.10	0.49
6:F:308:ILE:HG23	7:G:38:PHE:CE2	2.41	0.49
20:T:310:MET:O	20:T:310:MET:HE3	2.13	0.49
22:W:194:LYS:O	22:W:197:VAL:HG22	2.11	0.49
1:A:1305:ARG:HG3	1:A:1306:PHE:CD1	2.48	0.49
3:C:383:PHE:HB3	6:F:244:TYR:HE2	1.78	0.49
5:E:318:ALA:HB1	5:E:325:TRP:HB3	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:108:ARG:NH1	7:G:109:GLU:OE2	2.45	0.49
20:T:352:ILE:O	20:T:355:ALA:HB3	2.12	0.49
2:B:75:LEU:HD11	2:B:117:ILE:CG1	2.42	0.49
7:G:80:GLU:OE2	7:G:81:ARG:NH2	2.45	0.49
8:H:22:LEU:O	8:H:26:ILE:HG22	2.11	0.49
2:B:135:ARG:N	2:B:412:THR:HG22	2.27	0.49
2:B:228:ASN:OD1	2:B:229:THR:N	2.46	0.49
2:B:622:GLU:OE2	2:B:626:HIS:NE2	2.45	0.49
3:C:473:SER:O	3:C:474:MET:SD	2.71	0.49
1:A:101:VAL:HG22	1:A:250:LEU:HD22	1.95	0.49
1:A:1221:GLU:HB3	10:J:72:CYS:SG	2.53	0.49
2:B:375:ASP:C	2:B:375:ASP:OD2	2.51	0.49
19:S:273:LEU:HD13	19:S:293:VAL:HG11	1.95	0.49
1:A:1058:VAL:O	1:A:1058:VAL:HG22	2.12	0.49
2:B:267:PRO:HA	2:B:270:GLU:OE1	2.12	0.49
6:F:84:LYS:HE3	6:F:95:VAL:HG23	1.95	0.49
11:K:140:PHE:O	11:K:211:LEU:HD12	2.12	0.49
21:U:33:TRP:CH2	21:U:84:GLY:HA3	2.48	0.49
25:Z:309:TYR:N	25:Z:321:ILE:O	2.43	0.49
1:A:1379:PHE:CE2	9:I:84:LEU:HD13	2.48	0.48
5:E:348:VAL:HG13	5:E:348:VAL:O	2.13	0.48
10:J:3:LEU:N	10:J:3:LEU:HD12	2.28	0.48
13:M:111:THR:HG23	13:M:114:ALA:H	1.78	0.48
19:S:285:VAL:O	19:S:287:ARG:NH1	2.46	0.48
1:A:219:ASN:OD1	1:A:219:ASN:C	2.50	0.48
5:E:314:ILE:O	5:E:318:ALA:N	2.46	0.48
6:F:188:LEU:HD11	6:F:270:TYR:HB2	1.95	0.48
2:B:264:ALA:HB3	2:B:343:ILE:HD11	1.96	0.48
3:C:438:ARG:NH1	6:F:293:PHE:CD1	2.82	0.48
6:F:238:ILE:HA	6:F:241:THR:HG23	1.96	0.48
10:J:2:LEU:C	10:J:3:LEU:HD12	2.33	0.48
23:X:34:DC:O4'	23:X:34:DC:O2	2.31	0.48
1:A:1101:VAL:HG12	1:A:1105:ILE:HD12	1.96	0.48
2:B:601:LYS:HG3	2:B:601:LYS:O	2.12	0.48
3:C:105:LEU:HB3	3:C:125:VAL:HG23	1.95	0.48
9:I:92:VAL:HG13	9:I:93:THR:HG23	1.95	0.48
10:J:36:ARG:HA	10:J:36:ARG:NH1	2.29	0.48
1:A:1188:VAL:HG22	1:A:1191:PHE:HD2	1.78	0.48
6:F:243:ILE:CA	6:F:248:VAL:HG11	2.43	0.48
1:A:430:ARG:HD3	1:A:440:MET:HE2	1.95	0.48
1:A:1202:GLN:OE1	10:J:52:VAL:HG21	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:LEU:HD12	2:B:76:LYS:N	2.29	0.48
3:C:376:GLU:OE1	3:C:376:GLU:HA	2.13	0.48
6:F:239:LEU:HD22	6:F:266:HIS:ND1	2.28	0.48
9:I:59:ARG:NH1	9:I:59:ARG:HB2	2.28	0.48
1:A:137:LEU:HA	1:A:140:ARG:HG2	1.95	0.48
7:G:112:PRO:O	7:G:113:ARG:HG2	2.14	0.48
24:Y:-56:DC:C2	24:Y:-55:DC:C5	3.01	0.48
1:A:315:LEU:O	1:A:315:LEU:HD12	2.13	0.48
1:A:1082:THR:O	1:A:1082:THR:OG1	2.28	0.48
1:A:1240:GLY:HA3	10:J:56:ALA:HB2	1.96	0.48
3:C:395:LEU:HD21	3:C:424:TYR:CZ	2.48	0.48
3:C:507:ASN:HB3	7:G:58:LEU:HD11	1.96	0.48
4:D:132:MET:SD	4:D:132:MET:N	2.87	0.48
5:E:77:ILE:HG21	5:E:97:MET:SD	2.54	0.48
5:E:246:LEU:HD23	5:E:246:LEU:O	2.14	0.48
5:E:291:VAL:HG12	5:E:326:VAL:HG12	1.96	0.48
6:F:166:TRP:HH2	6:F:237:THR:HG1	1.53	0.48
3:C:93:TYR:HB2	7:G:57:MET:CE	2.44	0.47
6:F:217:TRP:HE1	6:F:231:SER:HA	1.79	0.47
21:U:70:TYR:HB3	21:U:74:ILE:HG23	1.96	0.47
24:Y:-27:DA:H2'	24:Y:-26:DA:C8	2.49	0.47
1:A:1140:LEU:HD11	10:J:91:MET:HE3	1.95	0.47
1:A:1198:LYS:HA	10:J:47:LYS:HA	1.96	0.47
3:C:266:ILE:O	3:C:270:MET:SD	2.72	0.47
3:C:487:ILE:O	3:C:490:MET:CE	2.62	0.47
6:F:83:GLY:O	6:F:86:LYS:HD2	2.14	0.47
15:O:137:VAL:O	15:O:138:ASP:HB3	2.15	0.47
18:R:286:GLU:OE1	18:R:286:GLU:HA	2.15	0.47
1:A:1096:ASP:HB3	10:J:76:ARG:HD2	1.95	0.47
3:C:308:LEU:O	3:C:312:LEU:HG	2.13	0.47
3:C:441:LYS:HE3	6:F:293:PHE:CZ	2.49	0.47
3:C:524:GLU:HA	3:C:527:ILE:HG22	1.97	0.47
1:A:1096:ASP:H	10:J:77:ALA:N	2.13	0.47
1:A:1100:LEU:CD1	10:J:80:MET:SD	3.02	0.47
1:A:1199:VAL:CG1	1:A:1200:VAL:N	2.77	0.47
6:F:39:GLN:HA	6:F:50:ARG:HH12	1.79	0.47
6:F:175:GLU:O	6:F:178:GLU:HG2	2.13	0.47
6:F:243:ILE:CB	6:F:248:VAL:HG11	2.42	0.47
19:S:235:GLN:HB2	19:S:294:VAL:HG21	1.96	0.47
20:T:335:ILE:HD12	20:T:336:GLU:N	2.29	0.47
1:A:66:ASP:OD1	1:A:66:ASP:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1116:GLU:O	2:B:1120:MET:HG3	2.15	0.47
6:F:93:LYS:HA	6:F:96:TYR:HB3	1.96	0.47
18:R:188:ARG:NH2	20:T:358:GLU:O	2.48	0.47
1:A:1104:ARG:CZ	10:J:56:ALA:HA	2.45	0.47
3:C:522:LEU:HD12	3:C:522:LEU:H	1.80	0.47
6:F:248:VAL:HG22	6:F:268:LYS:HB2	1.97	0.47
6:F:287:CYS:HA	6:F:290:CYS:HB2	1.96	0.47
10:J:86:SER:HB3	10:J:89:GLU:OE2	2.14	0.47
13:M:159:LEU:C	13:M:159:LEU:HD23	2.35	0.47
20:T:320:THR:HG23	20:T:356:PHE:CZ	2.50	0.47
22:W:149:TYR:CE1	25:Z:320:VAL:HG22	2.50	0.47
23:X:39:DC:H2"	23:X:40:DA:C8	2.50	0.47
1:A:1185:MET:SD	1:A:1185:MET:N	2.88	0.47
1:A:1201:VAL:HG22	1:A:1202:GLN:N	2.29	0.47
2:B:1106:ILE:HD11	2:B:1110:CYS:SG	2.55	0.47
8:H:88:LYS:O	8:H:100:SER:N	2.43	0.47
11:K:261:VAL:HG23	11:K:278:PRO:HA	1.97	0.47
13:M:168:ASN:C	13:M:168:ASN:OD1	2.53	0.47
18:R:267:PRO:HB3	19:S:358:LEU:HD21	1.97	0.47
19:S:133:LEU:HD21	19:S:138:ILE:HD11	1.97	0.47
2:B:258:GLU:O	2:B:261:VAL:HG12	2.15	0.47
6:F:82:ALA:HA	6:F:94:LEU:CD1	2.45	0.47
6:F:308:ILE:HG12	7:G:38:PHE:CD2	2.50	0.47
9:I:82:GLU:HA	9:I:85:GLN:OE1	2.15	0.47
22:W:193:ARG:O	22:W:197:VAL:HG13	2.14	0.47
1:A:1379:PHE:CZ	9:I:84:LEU:HD13	2.50	0.46
7:G:56:TYR:O	7:G:60:LEU:HG	2.16	0.46
10:J:102:CYS:HG	10:J:104:HIS:H	1.60	0.46
13:M:121:MET:H	13:M:121:MET:HE3	1.80	0.46
1:A:1044:PRO:HB3	1:A:1280:MET:SD	2.55	0.46
1:A:1100:LEU:HB2	10:J:78:TYR:HE1	1.79	0.46
2:B:88:GLU:OE2	2:B:88:GLU:HA	2.15	0.46
6:F:265:GLY:HA3	6:F:268:LYS:HG3	1.96	0.46
7:G:84:ILE:HG22	7:G:85:GLU:N	2.30	0.46
10:J:82:LEU:HD23	10:J:82:LEU:N	2.30	0.46
13:M:110:MET:SD	13:M:114:ALA:HB3	2.55	0.46
1:A:379:GLU:OE2	1:A:479:ARG:NH1	2.47	0.46
1:A:1122:LEU:HD23	1:A:1123:PRO:N	2.30	0.46
1:A:1197:PRO:HD2	10:J:45:LYS:HA	1.98	0.46
3:C:342:LEU:O	3:C:345:LEU:HD12	2.16	0.46
6:F:289:LEU:O	6:F:290:CYS:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:53:GLY:O	7:G:57:MET:SD	2.73	0.46
10:J:53:LEU:O	10:J:57:ALA:HB2	2.15	0.46
18:R:298:PRO:HD3	18:R:323:GLU:OE1	2.15	0.46
24:Y:-28:DA:H2'	24:Y:-27:DA:C8	2.51	0.46
1:A:1212:ILE:HG23	1:A:1214:ILE:HG23	1.97	0.46
3:C:404:MET:SD	3:C:404:MET:N	2.89	0.46
1:A:35:GLN:NE2	1:A:87:ASP:OD2	2.48	0.46
1:A:1134:LEU:N	1:A:1134:LEU:HD12	2.31	0.46
13:M:86:THR:O	13:M:90:TYR:CD1	2.68	0.46
1:A:258:PRO:HB2	1:A:262:ILE:HD11	1.98	0.46
1:A:1095:ALA:N	10:J:77:ALA:H	2.12	0.46
1:A:1225:LEU:HD13	10:J:96:LYS:HE3	1.97	0.46
5:E:344:VAL:HG12	5:E:345:PRO:O	2.15	0.46
19:S:228:ALA:O	19:S:232:LEU:HG	2.16	0.46
1:A:630:ASP:OD1	15:O:98:ARG:NH1	2.49	0.46
1:A:1124:ASP:OD1	1:A:1125:ASP:N	2.49	0.46
1:A:1303:ILE:O	1:A:1303:ILE:HG22	2.16	0.46
3:C:266:ILE:HG22	3:C:270:MET:HE1	1.97	0.46
3:C:428:ILE:HD12	3:C:428:ILE:H	1.80	0.46
5:E:343:GLY:O	5:E:345:PRO:HD2	2.16	0.46
1:A:1264:ARG:NH1	1:A:1292:ASP:OD1	2.49	0.46
3:C:24:ILE:HG21	3:C:53:ALA:HB1	1.97	0.46
3:C:514:ILE:HD13	3:C:514:ILE:N	2.31	0.46
6:F:243:ILE:HG13	6:F:244:TYR:HD1	1.80	0.46
1:A:590:LYS:HB3	1:A:591:PRO:HD3	1.98	0.46
1:A:927:ASN:O	1:A:931:VAL:HG12	2.16	0.46
1:A:1140:LEU:O	10:J:80:MET:CE	2.64	0.46
2:B:228:ASN:OD1	2:B:229:THR:HG23	2.16	0.46
5:E:314:ILE:HG21	5:E:325:TRP:CE2	2.51	0.46
6:F:240:ASN:O	6:F:243:ILE:HG12	2.15	0.46
1:A:860:ASP:C	1:A:860:ASP:OD1	2.53	0.46
1:A:1140:LEU:HB3	1:A:1142:LEU:CD1	2.46	0.46
1:A:1221:GLU:HB3	10:J:72:CYS:HB3	1.97	0.46
3:C:118:MET:SD	3:C:122:VAL:HG13	2.56	0.46
6:F:235:ILE:O	6:F:239:LEU:HG	2.16	0.46
6:F:266:HIS:CG	6:F:266:HIS:O	2.68	0.46
8:H:98:HIS:CD2	8:H:108:LEU:HD13	2.51	0.46
18:R:214:PHE:CE2	24:Y:-25:DT:H2"	2.51	0.46
10:J:14:VAL:HG22	10:J:23:PHE:CD1	2.51	0.45
1:A:112:CYS:HB3	1:A:159:CYS:SG	2.56	0.45
1:A:654:THR:HG22	1:A:654:THR:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:LEU:O	3:C:12:LEU:HD23	2.16	0.45
3:C:384:ALA:O	3:C:385:MET:HG3	2.16	0.45
5:E:366:VAL:HG13	5:E:366:VAL:O	2.16	0.45
7:G:42:ASP:OD2	7:G:42:ASP:C	2.54	0.45
9:I:93:THR:O	9:I:97:ILE:HD12	2.16	0.45
24:Y:-62:DT:H2'	24:Y:-61:DC:H6	1.81	0.45
19:S:250:PHE:CD1	19:S:250:PHE:C	2.90	0.45
19:S:288:LEU:HD12	19:S:288:LEU:C	2.36	0.45
22:W:147:LYS:HG3	25:Z:191:ILE:HD12	1.99	0.45
1:A:1122:LEU:HD23	1:A:1124:ASP:H	1.81	0.45
2:B:225:LEU:C	2:B:225:LEU:HD23	2.37	0.45
2:B:392:ILE:CG2	2:B:393:PRO:HD3	2.47	0.45
6:F:236:GLU:HG3	6:F:264:ASP:HB3	1.99	0.45
7:G:57:MET:C	7:G:61:LYS:HE3	2.37	0.45
9:I:63:PRO:O	9:I:66:VAL:HG22	2.17	0.45
13:M:99:ILE:HG22	13:M:100:THR:N	2.32	0.45
16:P:15:MET:C	16:P:16:ILE:HD13	2.36	0.45
20:T:318:VAL:HB	20:T:362:PHE:CE2	2.51	0.45
20:T:325:ILE:CD1	20:T:337:ILE:HG21	2.46	0.45
20:T:367:PHE:O	20:T:368:ALA:C	2.53	0.45
1:A:1344:SER:O	1:A:1348:ILE:HG23	2.16	0.45
2:B:554:LYS:HD2	2:B:554:LYS:O	2.16	0.45
2:B:722:THR:HG22	2:B:723:LYS:N	2.30	0.45
6:F:244:TYR:O	6:F:245:ASP:CB	2.64	0.45
19:S:388:GLU:OE1	19:S:388:GLU:N	2.48	0.45
19:S:398:GLU:HB2	20:T:361:PRO:HB2	1.98	0.45
22:W:356:MET:CE	22:W:378:TYR:HB3	2.47	0.45
22:W:373:ARG:NH1	24:Y:-60:DC:OP2	2.49	0.45
1:A:251:ILE:N	1:A:251:ILE:HD13	2.32	0.45
1:A:368:VAL:HG12	1:A:369:ILE:N	2.32	0.45
1:A:1197:PRO:CD	10:J:45:LYS:HA	2.47	0.45
1:A:1223:TYR:C	10:J:99:ASN:H	2.20	0.45
2:B:79:ASN:N	2:B:116:ASP:OD1	2.47	0.45
3:C:381:GLU:OE2	3:C:392:LYS:NZ	2.49	0.45
19:S:297:ILE:HA	19:S:300:LEU:CD1	2.46	0.45
23:X:34:DC:H4'	23:X:34:DC:OP1	2.17	0.45
1:A:1211:VAL:HG22	1:A:1212:ILE:N	2.24	0.45
1:A:1223:TYR:C	10:J:102:CYS:SG	2.95	0.45
1:A:1306:PHE:CD1	1:A:1306:PHE:N	2.84	0.45
2:B:189:ILE:HA	2:B:203:VAL:HG12	1.99	0.45
3:C:510:ASP:HA	3:C:513:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:243:ILE:N	6:F:270:TYR:OH	2.49	0.45
18:R:244:LEU:HD23	19:S:393:LEU:CD1	2.47	0.45
6:F:86:LYS:CE	6:F:91:GLN:HA	2.46	0.45
6:F:169:ASP:CG	6:F:169:ASP:O	2.55	0.45
6:F:174:SER:HA	6:F:177:VAL:HG22	1.98	0.45
10:J:25:CYS:SG	10:J:26:ASN:N	2.90	0.45
18:R:207:PRO:HG2	18:R:229:GLN:O	2.16	0.45
20:T:335:ILE:HD12	20:T:335:ILE:C	2.37	0.45
1:A:1195:ASP:H	10:J:45:LYS:N	2.15	0.45
3:C:398:MET:HB3	3:C:404:MET:CE	2.47	0.45
6:F:82:ALA:CA	6:F:94:LEU:HD13	2.46	0.45
6:F:267:MET:HE2	6:F:267:MET:C	2.37	0.45
11:K:116:HIS:O	11:K:116:HIS:ND1	2.50	0.45
19:S:231:PHE:O	19:S:235:GLN:NE2	2.48	0.45
20:T:336:GLU:O	20:T:340:LYS:HG2	2.17	0.45
1:A:1377:LEU:HD23	1:A:1377:LEU:H	1.82	0.45
19:S:231:PHE:O	19:S:235:GLN:HG2	2.16	0.45
23:X:22:DA:H2'	23:X:23:DC:C6	2.51	0.45
23:X:22:DA:H2'	23:X:23:DC:H6	1.82	0.45
1:A:171:LEU:C	1:A:171:LEU:HD23	2.37	0.44
3:C:88:TYR:CE1	3:C:111:LEU:HD11	2.52	0.44
6:F:86:LYS:HG3	6:F:87:GLY:N	2.32	0.44
10:J:22:ARG:HD3	10:J:31:VAL:HG11	1.98	0.44
22:W:238:ALA:O	22:W:242:ILE:HG12	2.16	0.44
1:A:1099:ARG:HG2	10:J:80:MET:CG	2.47	0.44
1:A:1100:LEU:CB	10:J:78:TYR:HE1	2.29	0.44
1:A:1199:VAL:CG1	1:A:1200:VAL:H	2.30	0.44
3:C:22:GLU:O	3:C:26:VAL:HG13	2.18	0.44
6:F:201:ASN:OD1	6:F:204:ILE:HG12	2.17	0.44
6:F:213:SER:HA	6:F:216:VAL:HB	2.00	0.44
6:F:267:MET:CE	6:F:268:LYS:N	2.81	0.44
8:H:83:GLU:O	8:H:152:VAL:HG22	2.17	0.44
9:I:59:ARG:HB2	9:I:59:ARG:CZ	2.48	0.44
9:I:73:LEU:HD21	9:I:86:LEU:HD12	1.98	0.44
20:T:317:MET:HG3	20:T:367:PHE:CZ	2.52	0.44
22:W:192:LEU:HD23	22:W:283:PHE:CE2	2.53	0.44
1:A:46:ASN:OD1	1:A:46:ASN:C	2.56	0.44
4:D:120:LYS:HA	4:D:123:TRP:CD1	2.52	0.44
6:F:116:SER:O	6:F:117:ASN:HB2	2.17	0.44
6:F:216:VAL:HG11	6:F:266:HIS:CD2	2.53	0.44
22:W:376:VAL:HG13	22:W:382:ARG:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLY:O	1:A:257:VAL:HG22	2.18	0.44
1:A:1067:VAL:CG1	1:A:1068:PRO:HD3	2.47	0.44
5:E:183:GLU:HG2	6:F:117:ASN:C	2.38	0.44
6:F:84:LYS:HG2	6:F:116:SER:O	2.17	0.44
6:F:256:LYS:HB2	6:F:257:GLU:OE1	2.16	0.44
25:Z:52:ARG:O	25:Z:56:ARG:N	2.40	0.44
1:A:1089:LEU:HD23	1:A:1101:VAL:HG21	1.98	0.44
1:A:1383:GLU:HG2	1:A:1384:PHE:CD2	2.52	0.44
3:C:509:LEU:HD21	6:F:314:LEU:HD21	2.00	0.44
11:K:194:HIS:O	11:K:195:ASP:HB3	2.17	0.44
13:M:94:MET:SD	13:M:99:ILE:HB	2.58	0.44
15:O:27:ARG:NE	15:O:42:ASP:OD1	2.49	0.44
18:R:191:GLU:OE2	20:T:321:ASP:HB3	2.17	0.44
22:W:176:PHE:HE2	25:Z:226:GLN:HE21	1.59	0.44
1:A:1120:VAL:HG23	4:D:123:TRP:CE3	2.52	0.44
3:C:438:ARG:NH1	6:F:293:PHE:CE1	2.85	0.44
6:F:191:LYS:HD3	6:F:211:ALA:HA	2.00	0.44
15:O:34:SER:OG	15:O:35:PHE:N	2.50	0.44
23:X:28:DT:H2'	23:X:29:DT:C6	2.52	0.44
23:X:49:DA:C2	24:Y:-47:DG:C2	3.06	0.44
1:A:1193:LYS:O	10:J:45:LYS:NZ	2.49	0.44
1:A:1199:VAL:H	10:J:46:LEU:HA	1.83	0.44
3:C:518:GLU:O	3:C:522:LEU:HD12	2.18	0.44
5:E:375:THR:HG23	5:E:377:LEU:CD1	2.41	0.44
7:G:57:MET:O	7:G:61:LYS:HE3	2.18	0.44
8:H:149:ARG:O	8:H:196:GLY:N	2.48	0.44
18:R:252:ASP:CG	18:R:252:ASP:O	2.55	0.44
22:W:192:LEU:O	22:W:196:VAL:HG23	2.17	0.44
24:Y:-32:DC:H2'	24:Y:-32:DC:O2	2.17	0.44
2:B:329:ARG:HH21	2:B:527:CYS:HA	1.83	0.44
5:E:6:ASP:N	5:E:6:ASP:OD1	2.51	0.44
6:F:84:LYS:HB2	6:F:94:LEU:HD23	1.99	0.44
6:F:232:MET:O	6:F:233:GLU:C	2.56	0.44
19:S:402:PHE:O	20:T:364:PHE:CE2	2.71	0.44
20:T:318:VAL:HG11	20:T:325:ILE:HG23	1.98	0.44
1:A:1113:ILE:O	1:A:1133:SER:N	2.50	0.44
3:C:58:VAL:O	3:C:115:LYS:NZ	2.51	0.44
6:F:184:CYS:HB3	6:F:266:HIS:CE1	2.53	0.44
6:F:262:SER:OG	6:F:265:GLY:HA2	2.17	0.44
13:M:33:LEU:O	13:M:33:LEU:HD23	2.17	0.44
13:M:99:ILE:CG2	13:M:100:THR:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:204:ILE:HG13	18:R:207:PRO:O	2.18	0.44
1:A:235:VAL:N	1:A:236:PRO:HD2	2.32	0.43
2:B:951:ALA:HB2	2:B:976:LEU:CD2	2.48	0.43
5:E:319:MET:SD	5:E:328:LYS:NZ	2.65	0.43
6:F:308:ILE:O	6:F:309:TYR:C	2.55	0.43
6:F:310:MET:O	6:F:311:THR:C	2.56	0.43
7:G:37:LEU:HG	7:G:38:PHE:CD1	2.52	0.43
18:R:219:MET:SD	18:R:219:MET:C	2.96	0.43
1:A:222:VAL:HG22	1:A:226:LEU:HD23	2.00	0.43
1:A:780:MET:SD	2:B:935:PRO:HG2	2.58	0.43
1:A:1185:MET:HG2	1:A:1187:TYR:H	1.83	0.43
2:B:334:TYR:O	2:B:337:VAL:HG12	2.18	0.43
3:C:514:ILE:HG13	7:G:61:LYS:HZ3	1.82	0.43
4:D:336:ARG:HH21	4:D:338:GLN:HG3	1.82	0.43
5:E:371:VAL:O	5:E:375:THR:HG22	2.18	0.43
6:F:253:ILE:O	6:F:253:ILE:HG22	2.18	0.43
9:I:62:SER:OG	9:I:64:GLU:OE2	2.35	0.43
19:S:44:PHE:HA	19:S:47:GLU:HB3	2.00	0.43
20:T:325:ILE:O	20:T:329:PHE:HB2	2.18	0.43
20:T:338:LYS:HE2	20:T:342:LYS:HD3	2.00	0.43
23:X:18:DT:H2"	23:X:19:DC:C6	2.53	0.43
2:B:93:VAL:HG22	2:B:94:THR:N	2.32	0.43
3:C:404:MET:HB2	3:C:425:THR:O	2.18	0.43
13:M:84:ILE:HD11	24:Y:16:DG:OP1	2.19	0.43
18:R:172:VAL:HG12	18:R:219:MET:HE3	1.99	0.43
1:A:99:ARG:C	1:A:99:ARG:HD3	2.38	0.43
1:A:596:THR:HG22	1:A:597:GLY:N	2.33	0.43
1:A:1067:VAL:HG12	1:A:1068:PRO:HD3	2.01	0.43
1:A:1313:GLU:OE1	1:A:1313:GLU:N	2.50	0.43
2:B:230:LEU:HD23	2:B:234:ILE:CD1	2.48	0.43
2:B:276:GLN:HA	2:B:278:PHE:HE2	1.84	0.43
2:B:287:ILE:HD13	2:B:287:ILE:HA	1.93	0.43
6:F:180:LEU:HD23	6:F:238:ILE:HD13	2.01	0.43
7:G:103:TRP:CZ3	7:G:106:LEU:HD23	2.53	0.43
10:J:1:MET:HG3	10:J:40:ASN:OD1	2.19	0.43
18:R:180:LEU:HB2	18:R:192:TYR:CZ	2.54	0.43
1:A:1099:ARG:CG	10:J:80:MET:HB2	2.48	0.43
1:A:1120:VAL:HG23	4:D:123:TRP:HE3	1.82	0.43
2:B:522:ASP:OD1	2:B:523:VAL:N	2.51	0.43
6:F:91:GLN:HB3	6:F:126:ILE:HG13	1.99	0.43
21:U:100:ALA:HB2	21:U:141:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:VAL:O	2:B:40:VAL:HG22	2.19	0.43
2:B:974:GLU:HA	2:B:977:VAL:HG12	2.00	0.43
4:D:138:ILE:HD12	4:D:138:ILE:N	2.31	0.43
20:T:367:PHE:O	20:T:371:LEU:HD22	2.19	0.43
1:A:811:ASP:OD1	1:A:811:ASP:N	2.50	0.43
3:C:439:CYS:SG	6:F:282:LEU:HD22	2.59	0.43
5:E:298:MET:SD	5:E:299:SER:N	2.91	0.43
6:F:267:MET:O	6:F:268:LYS:C	2.57	0.43
1:A:238:LEU:C	1:A:239:LEU:HD12	2.39	0.43
2:B:71:PRO:O	2:B:72:MET:HB3	2.19	0.43
2:B:551:ASP:O	2:B:551:ASP:OD2	2.36	0.43
6:F:266:HIS:HA	6:F:270:TYR:HE2	1.83	0.43
9:I:112:GLN:O	9:I:116:LEU:HG	2.19	0.43
12:L:44:LEU:HD12	12:L:80:ILE:HD11	2.00	0.43
19:S:205:MET:HA	19:S:208:VAL:HG22	2.01	0.43
24:Y:-33:DG:H2"	24:Y:-32:DC:O4'	2.17	0.43
24:Y:-30:DT:H2"	24:Y:-29:DA:H5'	2.01	0.43
1:A:415:HIS:O	1:A:417:GLY:N	2.48	0.43
1:A:934:CYS:O	1:A:1005:ARG:NH2	2.47	0.43
2:B:145:CYS:SG	2:B:146:VAL:N	2.92	0.43
2:B:312:LEU:HD12	2:B:316:THR:HB	2.01	0.43
3:C:60:HIS:CB	3:C:62:LEU:HD23	2.49	0.43
19:S:206:GLN:CD	19:S:301:LEU:HD22	2.38	0.43
21:U:136:HIS:HB2	21:U:138:THR:HG23	2.01	0.43
1:A:1225:LEU:HD13	10:J:96:LYS:CE	2.49	0.43
4:D:254:LEU:O	4:D:258:LEU:HG	2.18	0.43
5:E:321:VAL:O	5:E:321:VAL:HG23	2.19	0.43
5:E:381:ASP:OD1	5:E:381:ASP:N	2.52	0.43
6:F:235:ILE:HG23	6:F:236:GLU:N	2.34	0.43
18:R:279:GLN:HG2	18:R:280:PHE:CD2	2.54	0.43
1:A:1098:ALA:HB3	10:J:77:ALA:HA	2.01	0.42
3:C:78:GLN:O	3:C:82:VAL:HG23	2.19	0.42
5:E:314:ILE:HG21	5:E:325:TRP:CZ2	2.54	0.42
18:R:206:GLU:O	18:R:236:LYS:NZ	2.51	0.42
1:A:250:LEU:O	1:A:250:LEU:HD23	2.19	0.42
2:B:281:MET:HE2	2:B:282:GLN:N	2.34	0.42
5:E:321:VAL:HG12	5:E:423:TRP:HH2	1.83	0.42
6:F:77:LYS:O	6:F:81:ASN:HB2	2.19	0.42
6:F:243:ILE:HG13	6:F:244:TYR:CD1	2.54	0.42
9:I:7:ASN:C	9:I:7:ASN:OD1	2.57	0.42
10:J:6:PRO:HD2	10:J:30:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:36:ASP:O	12:L:36:ASP:OD2	2.37	0.42
16:P:21:GLU:HA	16:P:21:GLU:OE1	2.19	0.42
18:R:286:GLU:HG2	19:S:135:MET:SD	2.59	0.42
20:T:337:ILE:HA	20:T:340:LYS:HG2	2.01	0.42
22:W:192:LEU:HD23	22:W:283:PHE:HE2	1.84	0.42
1:A:84:GLY:C	1:A:257:VAL:HG22	2.39	0.42
1:A:219:ASN:H	1:A:222:VAL:CG1	2.33	0.42
1:A:1117:ILE:HG22	10:J:41:ARG:HD2	2.01	0.42
2:B:75:LEU:CD1	2:B:117:ILE:HG12	2.48	0.42
3:C:159:ARG:NH2	3:C:189:LEU:O	2.46	0.42
3:C:368:LEU:HD21	6:F:244:TYR:CB	2.49	0.42
6:F:301:GLU:O	6:F:303:SER:N	2.52	0.42
7:G:83:ASP:OD2	7:G:84:ILE:HG13	2.19	0.42
8:H:38:VAL:HG11	8:H:183:PRO:HG2	2.00	0.42
10:J:30:TYR:CD1	10:J:31:VAL:N	2.87	0.42
10:J:95:TYR:CD2	10:J:106:TRP:HB2	2.55	0.42
10:J:99:ASN:O	10:J:100:ALA:HB2	2.20	0.42
11:K:133:THR:HG23	11:K:135:ILE:HG22	2.00	0.42
18:R:188:ARG:HH21	19:S:391:GLN:HG2	1.84	0.42
19:S:152:THR:HG22	19:S:156:ILE:HD11	2.01	0.42
24:Y:-51:DA:H4'	24:Y:-50:DG:OP1	2.19	0.42
5:E:7:ASP:HB2	5:E:8:PRO:HD2	2.02	0.42
7:G:73:TYR:CD1	7:G:73:TYR:N	2.87	0.42
18:R:234:ALA:HA	18:R:237:TYR:CD2	2.54	0.42
19:S:226:ILE:HD13	19:S:226:ILE:N	2.34	0.42
22:W:145:PHE:N	22:W:145:PHE:CD1	2.88	0.42
1:A:1108:THR:OG1	10:J:49:VAL:HG13	2.20	0.42
1:A:1112:GLU:OE1	1:A:1112:GLU:N	2.46	0.42
3:C:398:MET:HB3	3:C:404:MET:HE1	2.01	0.42
5:E:350:CYS:O	5:E:354:ASP:OD1	2.36	0.42
6:F:245:ASP:OD1	6:F:247:LYS:HB2	2.20	0.42
22:W:199:ASP:OD2	22:W:266:ILE:HD11	2.19	0.42
1:A:401:ILE:CG2	1:A:402:ASN:N	2.82	0.42
1:A:596:THR:HG22	1:A:597:GLY:H	1.85	0.42
1:A:1139:LEU:HD21	10:J:81:GLN:CD	2.39	0.42
1:A:1143:GLU:HB2	10:J:53:LEU:HD13	2.02	0.42
2:B:680:SER:OG	2:B:681:PRO:HD3	2.20	0.42
6:F:228:VAL:HG12	6:F:229:GLU:H	1.84	0.42
6:F:278:PRO:HB2	6:F:279:PRO:HD2	2.01	0.42
8:H:115:GLN:HE21	8:H:117:PRO:HD2	1.85	0.42
12:L:38:HIS:O	12:L:38:HIS:ND1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:-16:DC:H2"	24:Y:-15:DA:H5'	2.01	0.42
25:Z:80:ASP:OD1	25:Z:81:ARG:N	2.53	0.42
3:C:82:VAL:HG12	3:C:82:VAL:O	2.20	0.42
5:E:320:LEU:HD21	5:E:325:TRP:CE2	2.55	0.42
6:F:239:LEU:HD13	6:F:266:HIS:HB2	2.01	0.42
10:J:48:GLU:O	10:J:48:GLU:HG3	2.20	0.42
13:M:18:MET:CE	13:M:33:LEU:HA	2.49	0.42
13:M:110:MET:SD	13:M:110:MET:C	2.98	0.42
16:P:27:GLU:N	16:P:27:GLU:OE1	2.53	0.42
18:R:289:PRO:HG2	23:X:33:DG:H1'	2.02	0.42
23:X:31:DA:H2'	23:X:32:DA:C8	2.55	0.42
1:A:25:PRO:HA	1:A:28:MET:HG2	2.01	0.42
3:C:510:ASP:O	3:C:514:ILE:HG12	2.20	0.42
16:P:32:ASP:OD2	16:P:32:ASP:C	2.58	0.42
18:R:201:ILE:HG13	18:R:212:LEU:HD13	2.01	0.42
22:W:168:LYS:NZ	25:Z:316:ASP:OD2	2.47	0.42
24:Y:-13:DT:H2"	24:Y:-12:DA:H5'	2.02	0.42
1:A:687:ALA:HB3	1:A:688:PRO:HD3	2.02	0.42
3:C:385:MET:HG2	6:F:241:THR:HG21	2.01	0.42
5:E:355:PHE:CZ	5:E:374:VAL:HG11	2.55	0.42
6:F:94:LEU:HD12	6:F:94:LEU:HA	1.78	0.42
6:F:308:ILE:HA	6:F:311:THR:HB	2.01	0.42
7:G:57:MET:HA	7:G:60:LEU:HG	2.01	0.42
21:U:83:TYR:CG	21:U:125:ILE:HG23	2.54	0.42
2:B:70:ASP:OD2	2:B:70:ASP:C	2.58	0.42
2:B:228:ASN:O	2:B:292:ARG:NH1	2.52	0.42
2:B:241:LYS:HA	2:B:245:VAL:O	2.20	0.42
3:C:90:ARG:NH1	3:C:518:GLU:OE1	2.53	0.42
3:C:531:MET:HE2	3:C:531:MET:HA	2.02	0.42
5:E:378:CYS:SG	5:E:379:ALA:N	2.93	0.42
6:F:237:THR:O	6:F:241:THR:HG23	2.19	0.42
6:F:243:ILE:CG2	6:F:270:TYR:OH	2.68	0.42
6:F:250:MET:HE1	6:F:252:ILE:H	1.85	0.42
22:W:308:ILE:HG13	22:W:320:ILE:HG23	2.02	0.42
1:A:575:LYS:O	1:A:575:LYS:HD3	2.19	0.41
1:A:995:THR:HG22	1:A:997:PRO:HD2	2.02	0.41
1:A:1196:LEU:CB	1:A:1197:PRO:HD3	2.45	0.41
1:A:1224:LYS:N	10:J:98:CYS:HA	2.35	0.41
2:B:119:TYR:CD2	2:B:402:VAL:HG12	2.54	0.41
2:B:224:TYR:HB3	2:B:233:ASP:HB2	2.02	0.41
2:B:877:ASP:OD2	2:B:877:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:379:GLN:OE1	3:C:379:GLN:N	2.48	0.41
3:C:490:MET:CE	3:C:490:MET:H	2.33	0.41
5:E:317:VAL:HA	5:E:328:LYS:HD3	2.02	0.41
6:F:249:GLU:H	6:F:269:LEU:HB2	1.85	0.41
6:F:313:TRP:HA	6:F:316:PHE:CE2	2.55	0.41
13:M:112:PRO:HA	13:M:115:LYS:HB2	2.02	0.41
23:X:33:DG:H3'	23:X:34:DC:H5"	2.02	0.41
1:A:173:LYS:HD2	1:A:173:LYS:HA	1.93	0.41
1:A:267:VAL:HG13	19:S:50:LEU:HA	2.00	0.41
1:A:435:GLY:O	1:A:437:ARG:HG2	2.20	0.41
1:A:1104:ARG:NH1	10:J:55:GLY:O	2.51	0.41
2:B:250:GLU:OE1	2:B:251:ILE:N	2.53	0.41
2:B:391:VAL:HG23	2:B:392:ILE:N	2.35	0.41
6:F:250:MET:HA	6:F:268:LYS:HE3	2.02	0.41
6:F:286:PRO:O	6:F:287:CYS:C	2.58	0.41
6:F:293:PHE:HB3	6:F:294:ASP:H	1.30	0.41
7:G:59:ALA:O	7:G:63:GLU:OE2	2.37	0.41
10:J:74:HIS:HB3	10:J:75:PRO:CD	2.50	0.41
1:A:137:LEU:HA	1:A:140:ARG:CG	2.51	0.41
1:A:267:VAL:HG13	19:S:49:ASN:O	2.20	0.41
1:A:296:HIS:ND1	1:A:306:ILE:HD11	2.35	0.41
1:A:437:ARG:HH21	1:A:439:LYS:HD3	1.86	0.41
1:A:1043:GLU:HB3	1:A:1044:PRO:HD3	2.02	0.41
2:B:1032:THR:O	2:B:1034:GLN:N	2.52	0.41
6:F:141:SER:O	6:F:145:SER:HA	2.21	0.41
6:F:181:ASN:O	6:F:242:LEU:HD11	2.20	0.41
6:F:228:VAL:HG12	6:F:229:GLU:N	2.35	0.41
8:H:131:TYR:HB3	8:H:135:GLU:HB3	2.02	0.41
9:I:59:ARG:O	9:I:60:HIS:CG	2.73	0.41
20:T:370:LEU:O	20:T:374:VAL:HG22	2.21	0.41
25:Z:161:SER:HA	25:Z:164:ILE:HG22	2.01	0.41
1:A:1105:ILE:HG22	1:A:1207:VAL:HG11	2.02	0.41
2:B:307:GLU:O	2:B:311:GLU:HG3	2.21	0.41
2:B:478:MET:C	2:B:479:LEU:HD12	2.40	0.41
2:B:1083:CYS:SG	2:B:1085:LEU:HD23	2.60	0.41
3:C:62:LEU:HD12	3:C:82:VAL:HG22	2.03	0.41
19:S:232:LEU:HD21	19:S:269:LEU:HD11	2.01	0.41
25:Z:63:LEU:HD21	25:Z:329:VAL:HG13	2.01	0.41
3:C:498:GLN:O	3:C:502:LEU:HG	2.21	0.41
4:D:369:ARG:HA	4:D:369:ARG:NE	2.36	0.41
5:E:244:GLU:O	5:E:244:GLU:OE1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:250:MET:HE2	6:F:252:ILE:HG22	2.02	0.41
11:K:23:ASN:O	11:K:303:ARG:NH2	2.50	0.41
17:Q:6:ARG:HG2	17:Q:13:ILE:HD13	2.03	0.41
21:U:46:MET:SD	25:Z:133:ARG:NH1	2.93	0.41
1:A:105:LEU:HD21	1:A:218:LEU:HD13	2.01	0.41
1:A:1132:LEU:HB2	1:A:1134:LEU:HD11	2.01	0.41
2:B:413:ASN:HA	2:B:416:VAL:HG22	2.03	0.41
5:E:295:ALA:O	5:E:298:MET:SD	2.79	0.41
8:H:116:GLN:HB3	8:H:117:PRO:HD3	2.02	0.41
13:M:66:ASP:OD1	13:M:67:ASP:N	2.53	0.41
13:M:187:ARG:HB2	13:M:187:ARG:CZ	2.50	0.41
22:W:357:LEU:HD12	22:W:375:ILE:HD13	2.02	0.41
1:A:1381:THR:O	1:A:1385:HIS:NE2	2.53	0.41
3:C:19:GLU:OE1	3:C:19:GLU:N	2.54	0.41
3:C:55:CYS:SG	3:C:56:VAL:N	2.93	0.41
3:C:364:ARG:O	3:C:368:LEU:HD23	2.20	0.41
5:E:320:LEU:HD23	5:E:325:TRP:CE3	2.55	0.41
6:F:185:PHE:O	6:F:189:GLN:HG2	2.20	0.41
19:S:260:TYR:N	19:S:261:PRO:HD2	2.36	0.41
24:Y:-10:DC:H2"	24:Y:-9:DC:C6	2.56	0.41
25:Z:388:HIS:HB3	25:Z:399:PHE:CZ	2.55	0.41
1:A:250:LEU:C	1:A:251:ILE:HD13	2.41	0.41
1:A:1111:GLY:HA2	10:J:86:SER:HA	2.03	0.41
2:B:407:ARG:HH22	19:S:81:ARG:HD3	1.84	0.41
4:D:143:GLU:OE1	4:D:143:GLU:N	2.53	0.41
5:E:297:LEU:HD21	5:E:314:ILE:HD11	2.03	0.41
6:F:217:TRP:NE1	6:F:230:LEU:HG	2.36	0.41
16:P:23:HIS:NE2	17:Q:64:PRO:HB3	2.36	0.41
22:W:317:TRP:CD1	25:Z:386:MET:CE	3.04	0.41
1:A:430:ARG:NH2	19:S:9:ASP:OD2	2.54	0.41
1:A:646:MET:CE	15:O:95:LYS:HE2	2.50	0.41
1:A:1140:LEU:O	10:J:80:MET:HE1	2.21	0.41
1:A:1198:LYS:H	10:J:45:LYS:HB2	1.86	0.41
1:A:1239:HIS:CG	10:J:56:ALA:HB3	2.55	0.41
2:B:741:VAL:HA	2:B:927:ILE:O	2.21	0.41
2:B:777:CYS:SG	2:B:778:THR:N	2.94	0.41
3:C:267:VAL:O	3:C:271:LEU:HG	2.21	0.41
5:E:400:PHE:CE2	5:E:402:LEU:HD23	2.56	0.41
6:F:26:CYS:HB3	6:F:76:ILE:HB	2.03	0.41
6:F:248:VAL:HG22	6:F:268:LYS:CB	2.51	0.41
6:F:249:GLU:N	6:F:269:LEU:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:26:ILE:HG23	8:H:27:ALA:N	2.35	0.41
9:I:62:SER:O	9:I:65:ILE:HG22	2.20	0.41
10:J:1:MET:SD	10:J:1:MET:C	2.99	0.41
10:J:95:TYR:HD2	10:J:106:TRP:HB2	1.86	0.41
11:K:228:VAL:HG11	11:K:231:ALA:HB2	2.03	0.41
12:L:94:GLU:HB2	12:L:95:PRO:HD3	2.03	0.41
15:O:128:ASP:OD1	15:O:129:ALA:N	2.53	0.41
19:S:44:PHE:N	19:S:44:PHE:CD1	2.88	0.41
19:S:381:ASP:OD1	19:S:381:ASP:N	2.54	0.41
20:T:309:ASP:OD1	20:T:309:ASP:C	2.59	0.41
1:A:319:LEU:HA	1:A:322:ASN:O	2.21	0.41
1:A:531:THR:HG22	1:A:536:GLU:O	2.20	0.41
1:A:817:SER:O	1:A:818:LEU:HD23	2.21	0.41
1:A:1105:ILE:HG13	10:J:55:GLY:H	1.84	0.41
3:C:139:MET:O	3:C:198:LYS:HA	2.20	0.41
3:C:531:MET:HG3	3:C:533:ARG:HG3	2.02	0.41
6:F:21:ARG:HE	6:F:25:LEU:HG	1.86	0.41
9:I:64:GLU:HA	9:I:67:ARG:HG2	2.03	0.41
11:K:252:GLU:HA	11:K:255:ARG:NH1	2.36	0.41
13:M:87:ILE:HA	13:M:90:TYR:HD1	1.86	0.41
25:Z:213:THR:HA	25:Z:293:MET:HE1	2.03	0.41
1:A:1089:LEU:HD12	10:J:98:CYS:SG	2.61	0.40
1:A:1109:LEU:HD23	10:J:84:THR:O	2.21	0.40
1:A:1152:SER:HB2	1:A:1202:GLN:HB3	2.03	0.40
1:A:1323:LYS:HA	23:X:-2:DC:OP1	2.21	0.40
3:C:91:TYR:O	3:C:94:THR:HG22	2.21	0.40
6:F:294:ASP:HB2	6:F:295:ASP:H	1.63	0.40
11:K:187:GLU:OE1	11:K:188:GLY:N	2.55	0.40
14:N:118:TRP:HB3	14:N:123:LEU:HD21	2.02	0.40
19:S:201:LEU:N	19:S:201:LEU:HD23	2.37	0.40
21:U:96:LYS:HD2	21:U:134:ALA:HA	2.03	0.40
23:X:28:DT:H2"	23:X:29:DT:O4'	2.22	0.40
1:A:1223:TYR:H	10:J:99:ASN:HB3	1.86	0.40
2:B:392:ILE:HG23	2:B:393:PRO:HD3	2.03	0.40
5:E:370:GLU:O	5:E:370:GLU:HG2	2.21	0.40
6:F:94:LEU:O	6:F:98:ILE:HG12	2.22	0.40
6:F:231:SER:O	6:F:232:MET:C	2.60	0.40
7:G:54:GLU:OE1	7:G:54:GLU:N	2.43	0.40
20:T:374:VAL:HG23	20:T:375:LEU:HD23	2.03	0.40
21:U:96:LYS:HB2	21:U:136:HIS:CD2	2.56	0.40
21:U:96:LYS:HB2	21:U:136:HIS:NE2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLU:HG2	1:A:199:THR:N	2.36	0.40
1:A:296:HIS:NE2	1:A:305:MET:SD	2.95	0.40
1:A:428:MET:O	1:A:428:MET:SD	2.79	0.40
1:A:822:GLU:HG2	1:A:825:SER:HB3	2.02	0.40
1:A:1210:ALA:HB3	10:J:105:ARG:HD3	2.02	0.40
5:E:246:LEU:HD23	5:E:246:LEU:C	2.41	0.40
7:G:64:LEU:O	7:G:68:MET:HG3	2.20	0.40
11:K:339:GLU:OE2	11:K:343:VAL:HG23	2.21	0.40
19:S:202:SER:O	19:S:205:MET:SD	2.79	0.40
24:Y:-16:DC:H2'	24:Y:-15:DA:O4'	2.21	0.40
1:A:353:ARG:HE	1:A:873:ARG:NH2	2.19	0.40
2:B:227:HIS:ND1	2:B:228:ASN:N	2.69	0.40
3:C:88:TYR:HB2	3:C:89:PRO:HD3	2.03	0.40
3:C:292:GLU:O	3:C:295:ARG:HG2	2.21	0.40
6:F:84:LYS:NZ	6:F:95:VAL:HG23	2.37	0.40
10:J:22:ARG:HA	10:J:33:ASN:HA	2.03	0.40
10:J:102:CYS:SG	10:J:104:HIS:N	2.86	0.40
18:R:165:LEU:HD21	18:R:318:ARG:HG3	2.03	0.40
18:R:233:ALA:HB1	18:R:237:TYR:OH	2.21	0.40
19:S:106:ILE:N	19:S:106:ILE:HD12	2.36	0.40
19:S:289:ASP:OD1	19:S:291:ARG:N	2.54	0.40
22:W:356:MET:SD	22:W:357:LEU:N	2.94	0.40
1:A:114:HIS:HB2	1:A:158:HIS:CE1	2.56	0.40
2:B:1060:ALA:O	2:B:1064:LEU:HD22	2.21	0.40
2:B:1092:CYS:O	2:B:1096:LYS:N	2.50	0.40
6:F:38:ILE:HG22	6:F:50:ARG:HH11	1.86	0.40
6:F:112:ILE:O	6:F:116:SER:N	2.52	0.40
8:H:84:ILE:O	8:H:85:LEU:HD13	2.22	0.40
16:P:50:LYS:N	16:P:50:LYS:HD2	2.36	0.40
18:R:188:ARG:HG2	19:S:394:ARG:HG3	2.03	0.40
19:S:129:HIS:O	19:S:130:ASN:HB3	2.21	0.40
19:S:132:PRO:HB2	19:S:172:LEU:HD13	2.04	0.40
23:X:28:DT:C6	23:X:29:DT:H72	2.56	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%)	1304 (95%)	72 (5%)	1 (0%)	48 77
2	B	1091/1133 (96%)	1052 (96%)	38 (4%)	1 (0%)	48 77
3	C	508/534 (95%)	491 (97%)	16 (3%)	1 (0%)	44 72
4	D	180/398 (45%)	170 (94%)	10 (6%)	0	100 100
5	E	396/666 (60%)	379 (96%)	17 (4%)	0	100 100
6	F	300/316 (95%)	240 (80%)	45 (15%)	15 (5%)	1 11
7	G	80/223 (36%)	70 (88%)	10 (12%)	0	100 100
8	H	185/204 (91%)	178 (96%)	7 (4%)	0	100 100
9	I	122/148 (82%)	118 (97%)	4 (3%)	0	100 100
10	J	105/108 (97%)	82 (78%)	23 (22%)	0	100 100
11	K	341/346 (99%)	334 (98%)	7 (2%)	0	100 100
12	L	105/133 (79%)	102 (97%)	3 (3%)	0	100 100
13	M	207/210 (99%)	198 (96%)	9 (4%)	0	100 100
14	N	76/127 (60%)	73 (96%)	3 (4%)	0	100 100
15	O	146/150 (97%)	140 (96%)	6 (4%)	0	100 100
16	P	44/58 (76%)	40 (91%)	4 (9%)	0	100 100
17	Q	64/67 (96%)	63 (98%)	1 (2%)	0	100 100
18	R	176/200 (88%)	172 (98%)	4 (2%)	0	100 100
19	S	357/419 (85%)	344 (96%)	13 (4%)	0	100 100
20	T	76/484 (16%)	71 (93%)	5 (7%)	0	100 100
21	U	139/368 (38%)	137 (99%)	2 (1%)	0	100 100
22	W	240/1519 (16%)	237 (99%)	3 (1%)	0	100 100
25	Z	383/411 (93%)	370 (97%)	13 (3%)	0	100 100
All	All	6698/9612 (70%)	6365 (95%)	315 (5%)	18 (0%)	38 67

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	86	LYS
6	F	160	SER
6	F	232	MET
6	F	245	ASP
6	F	263	VAL
6	F	268	LYS
6	F	302	ILE
2	B	40	VAL
6	F	295	ASP
6	F	82	ALA
6	F	273	VAL
6	F	301	GLU
6	F	293	PHE
6	F	299	GLY
3	C	488	GLU
6	F	286	PRO
6	F	294	ASP
1	A	1197	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1204/1212 (99%)	1183 (98%)	21 (2%)	56 74
2	B	959/988 (97%)	942 (98%)	17 (2%)	54 73
3	C	458/476 (96%)	444 (97%)	14 (3%)	35 61
4	D	167/347 (48%)	162 (97%)	5 (3%)	36 61
5	E	358/581 (62%)	346 (97%)	12 (3%)	32 58
6	F	268/280 (96%)	239 (89%)	29 (11%)	5 21
7	G	79/195 (40%)	72 (91%)	7 (9%)	8 28
8	H	168/181 (93%)	162 (96%)	6 (4%)	30 57
9	I	116/136 (85%)	114 (98%)	2 (2%)	56 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	J	93/94 (99%)	89 (96%)	4 (4%)	25 52
11	K	299/302 (99%)	298 (100%)	1 (0%)	91 94
12	L	96/119 (81%)	96 (100%)	0	100 100
13	M	191/192 (100%)	186 (97%)	5 (3%)	41 65
14	N	68/111 (61%)	68 (100%)	0	100 100
15	O	129/131 (98%)	129 (100%)	0	100 100
16	P	43/55 (78%)	42 (98%)	1 (2%)	45 68
17	Q	55/56 (98%)	55 (100%)	0	100 100
18	R	152/172 (88%)	143 (94%)	9 (6%)	16 43
19	S	324/365 (89%)	312 (96%)	12 (4%)	29 56
20	T	70/440 (16%)	67 (96%)	3 (4%)	25 52
21	U	124/334 (37%)	121 (98%)	3 (2%)	44 67
22	W	215/1250 (17%)	211 (98%)	4 (2%)	52 72
25	Z	340/356 (96%)	332 (98%)	8 (2%)	44 67
All	All	5976/8373 (71%)	5813 (97%)	163 (3%)	41 65

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	128	TYR
1	A	158	HIS
1	A	162	PHE
1	A	234	ASP
1	A	294	LYS
1	A	295	LYS
1	A	305	MET
1	A	312	PHE
1	A	428	MET
1	A	627	LYS
1	A	630	ASP
1	A	725	ASP
1	A	864	LYS
1	A	916	ASP
1	A	1127	PHE
1	A	1185	MET
1	A	1191	PHE

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Mol	Chain	Res	Type
1	A	1213	HIS
1	A	1236	MET
1	A	1313	GLU
2	B	81	TYR
2	B	91	PHE
2	B	281	MET
2	B	289	ASN
2	B	311	GLU
2	B	354	ARG
2	B	357	TYR
2	B	367	GLN
2	B	400	PHE
2	B	463	ARG
2	B	573	SER
2	B	660	GLU
2	B	812	ASP
2	B	877	ASP
2	B	1078	ASP
2	B	1086	LEU
2	B	1131	TYR
3	C	118	MET
3	C	139	MET
3	C	270	MET
3	C	345	LEU
3	C	356	GLU
3	C	362	CYS
3	C	393	ASP
3	C	429	LEU
3	C	434	MET
3	C	438	ARG
3	C	474	MET
3	C	490	MET
3	C	524	GLU
3	C	531	MET
4	D	123	TRP
4	D	132	MET
4	D	156	ARG
4	D	282	GLN
4	D	373	MET
5	E	60	MET
5	E	195	PHE
5	E	198	LYS

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Mol	Chain	Res	Type
5	E	244	GLU
5	E	294	PHE
5	E	296	ASN
5	E	298	MET
5	E	354	ASP
5	E	377	LEU
5	E	378	CYS
5	E	381	ASP
5	E	421	MET
6	F	42	MET
6	F	85	MET
6	F	150	TYR
6	F	166	TRP
6	F	169	ASP
6	F	172	PHE
6	F	185	PHE
6	F	187	PHE
6	F	196	ARG
6	F	247	LYS
6	F	250	MET
6	F	267	MET
6	F	271	ARG
6	F	273	VAL
6	F	274	ASN
6	F	276	ILE
6	F	277	ILE
6	F	280	THR
6	F	283	VAL
6	F	287	CYS
6	F	289	LEU
6	F	290	CYS
6	F	293	PHE
6	F	294	ASP
6	F	295	ASP
6	F	302	ILE
6	F	303	SER
6	F	308	ILE
6	F	315	GLU
7	G	42	ASP
7	G	68	MET
7	G	71	MET
7	G	81	ARG

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Mol	Chain	Res	Type
7	G	83	ASP
7	G	91	TYR
7	G	92	MET
8	H	19	GLU
8	H	119	LYS
8	H	135	GLU
8	H	141	TYR
8	H	142	MET
8	H	180	LYS
9	I	1	MET
9	I	40	GLN
10	J	22	ARG
10	J	40	ASN
10	J	94	PHE
10	J	95	TYR
11	K	64	ASP
13	M	54	ARG
13	M	94	MET
13	M	121	MET
13	M	129	GLN
13	M	181	ARG
16	P	52	LEU
18	R	192	TYR
18	R	208	ARG
18	R	214	PHE
18	R	252	ASP
18	R	253	PHE
18	R	258	MET
18	R	280	PHE
18	R	295	MET
18	R	325	PHE
19	S	44	PHE
19	S	51	ARG
19	S	62	ASN
19	S	135	MET
19	S	205	MET
19	S	213	GLU
19	S	231	PHE
19	S	260	TYR
19	S	273	LEU
19	S	282	TRP
19	S	296	HIS

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Mol	Chain	Res	Type
19	S	300	LEU
20	T	329	PHE
20	T	362	PHE
20	T	365	ASP
21	U	47	ARG
21	U	111	GLN
21	U	140	MET
22	W	149	TYR
22	W	153	LYS
22	W	214	TYR
22	W	378	TYR
25	Z	51	TRP
25	Z	61	LEU
25	Z	151	ARG
25	Z	204	MET
25	Z	216	ARG
25	Z	282	ASP
25	Z	359	MET
25	Z	386	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	124	GLN
8	H	98	HIS
10	J	101	GLN
20	T	369	HIS
22	W	340	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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.

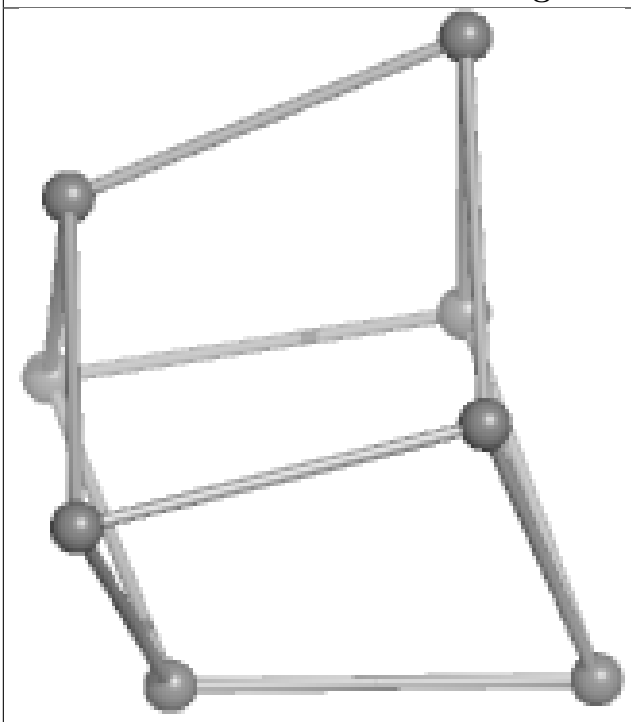
1 monomer is involved in 9 short contacts:

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

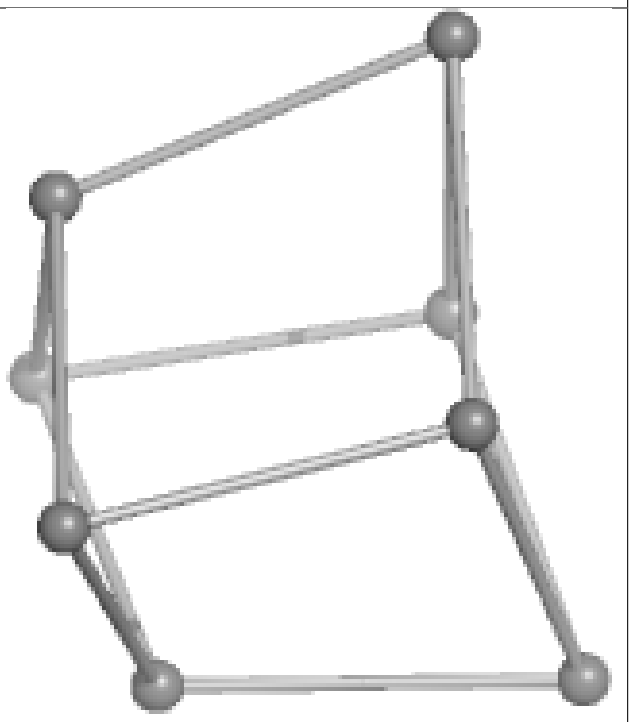
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

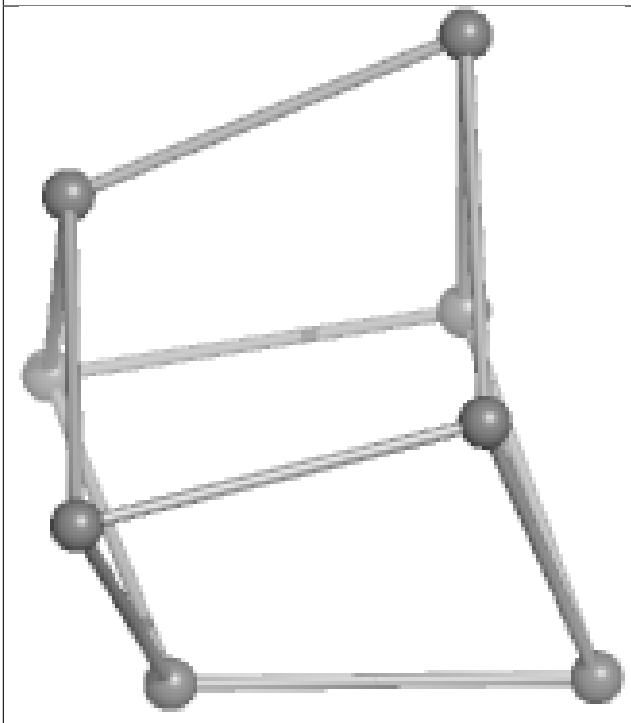
Ligand SF4 F 401



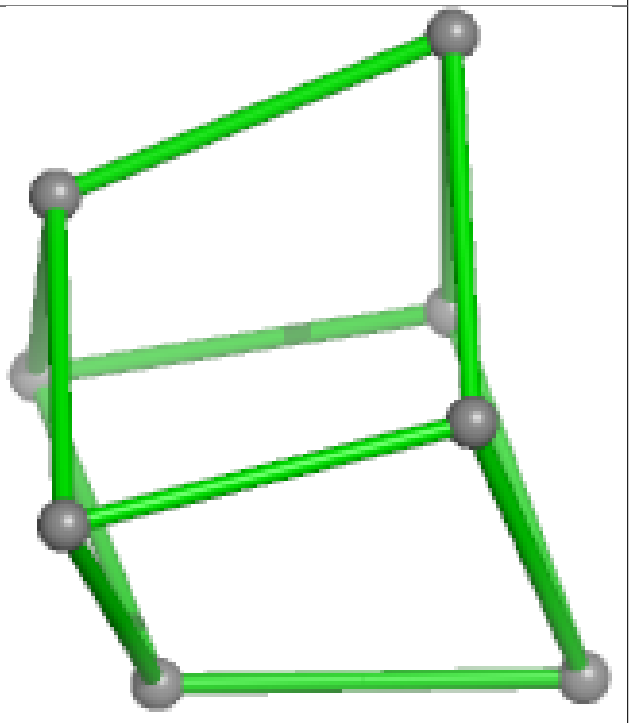
Bond lengths



Bond angles



Torsions



Rings

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.

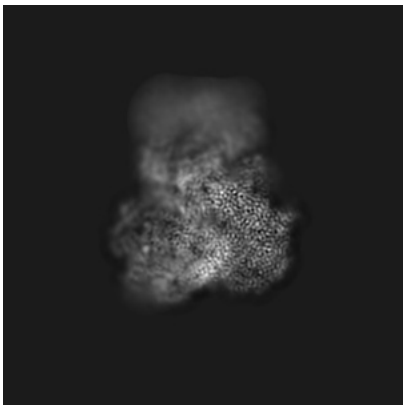
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50730. These allow visual inspection of the internal detail of the map and identification of artifacts.

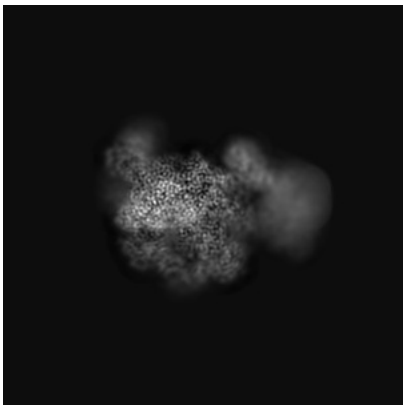
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

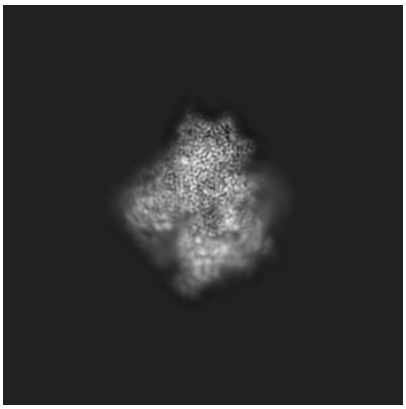
6.1.1 Primary map



X

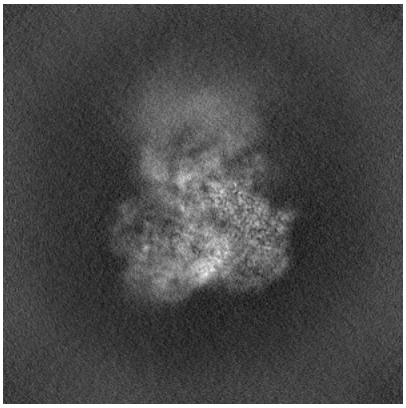


Y

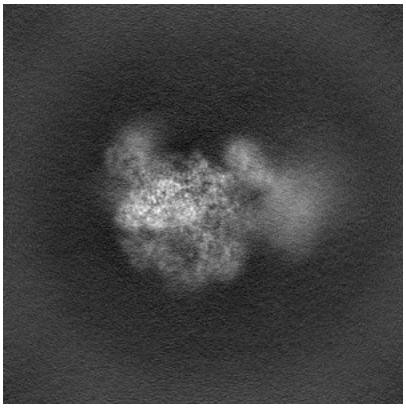


Z

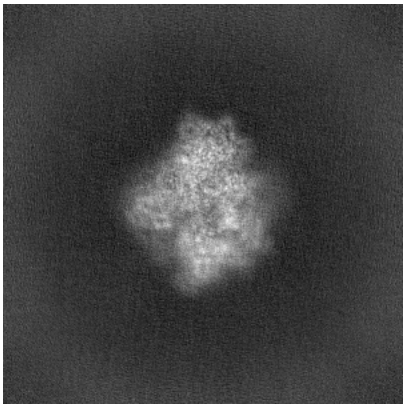
6.1.2 Raw map



X



Y

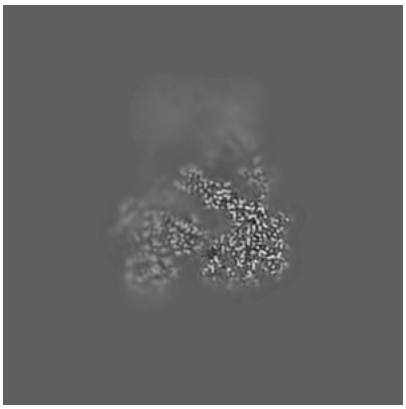


Z

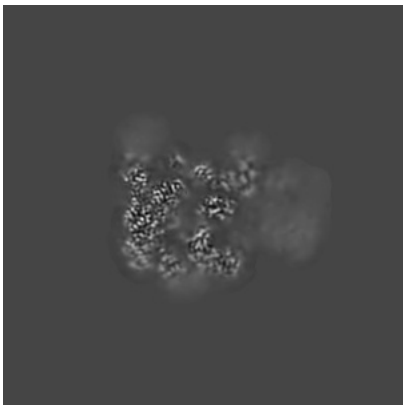
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

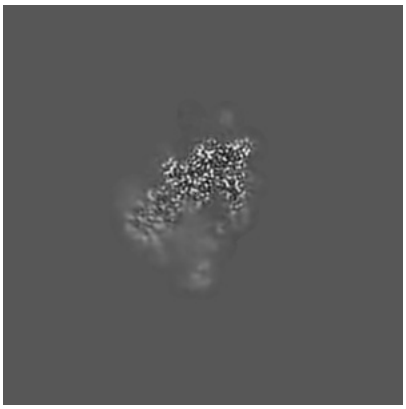
6.2.1 Primary map



X Index: 210

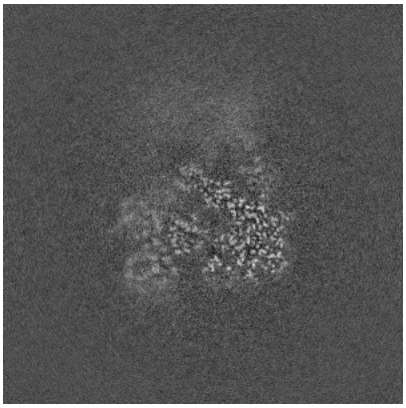


Y Index: 210

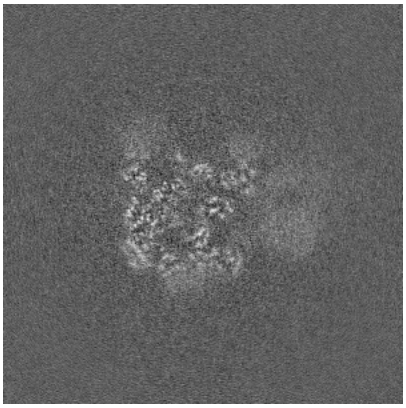


Z Index: 210

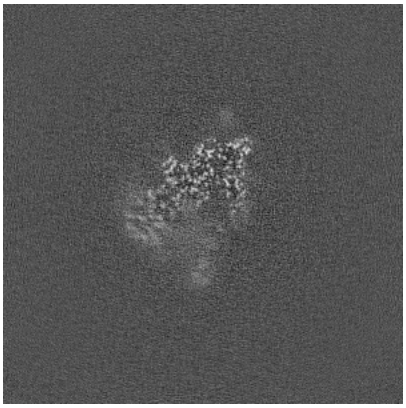
6.2.2 Raw map



X Index: 210



Y Index: 210

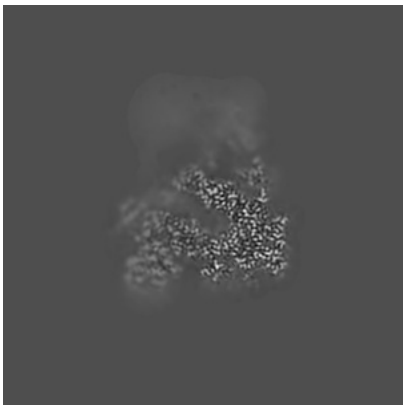


Z Index: 210

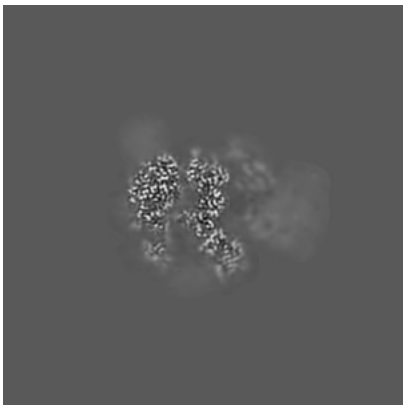
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

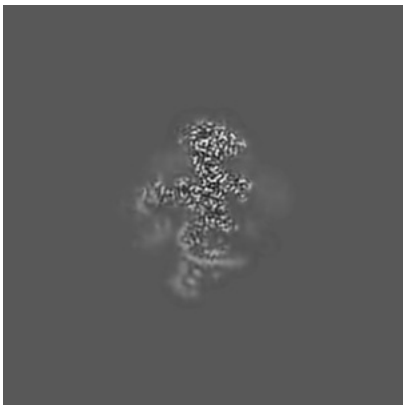
6.3.1 Primary map



X Index: 212

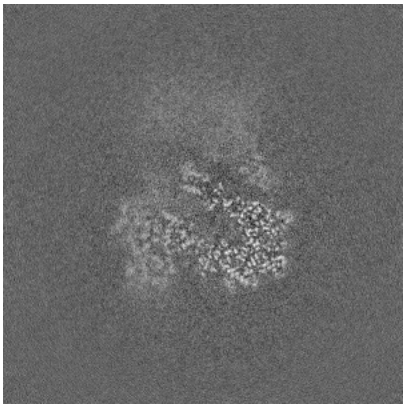


Y Index: 229

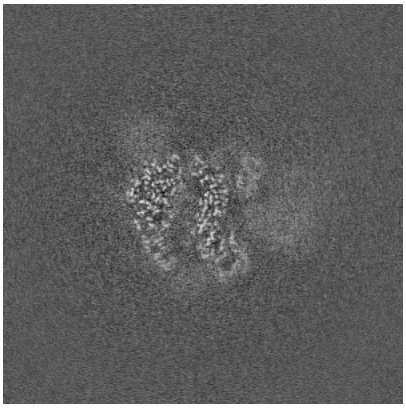


Z Index: 164

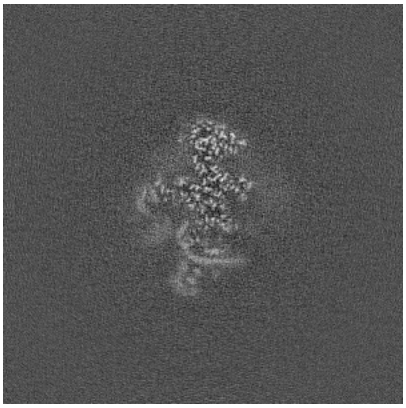
6.3.2 Raw map



X Index: 206



Y Index: 224

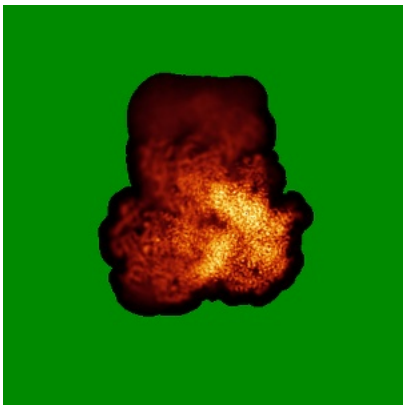


Z Index: 164

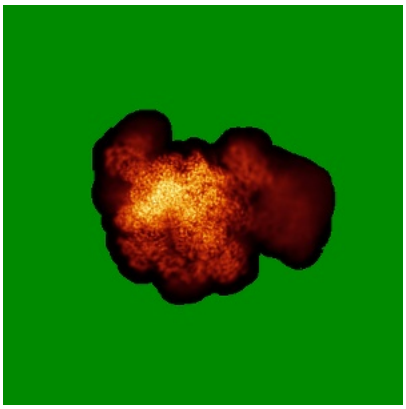
The images above show the largest variance slices of the map in three orthogonal directions.

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

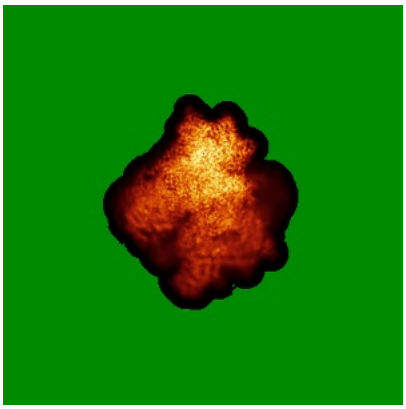
6.4.1 Primary map



X

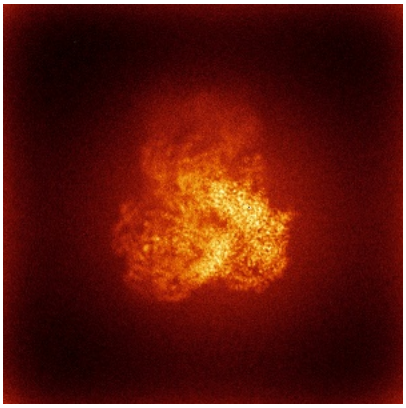


Y

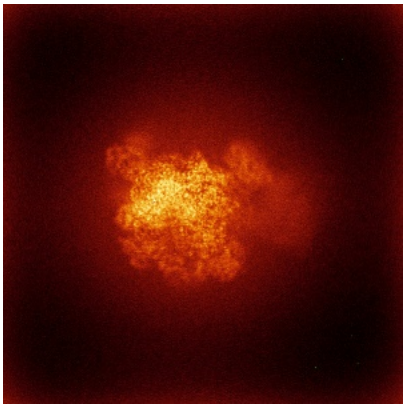


Z

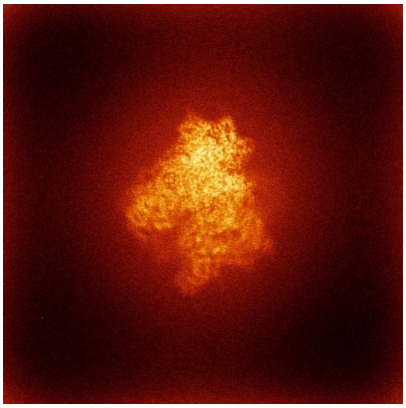
6.4.2 Raw map



X



Y

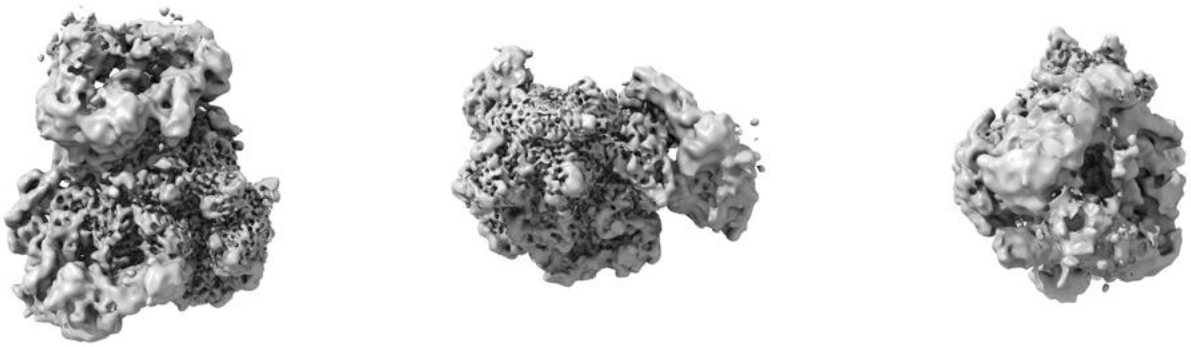


Z

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)

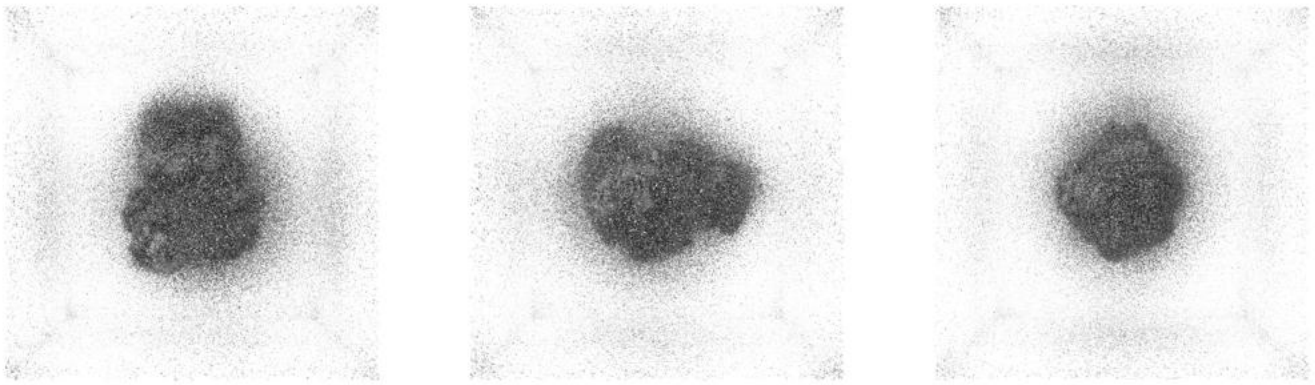
6.5.1 Primary map



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.

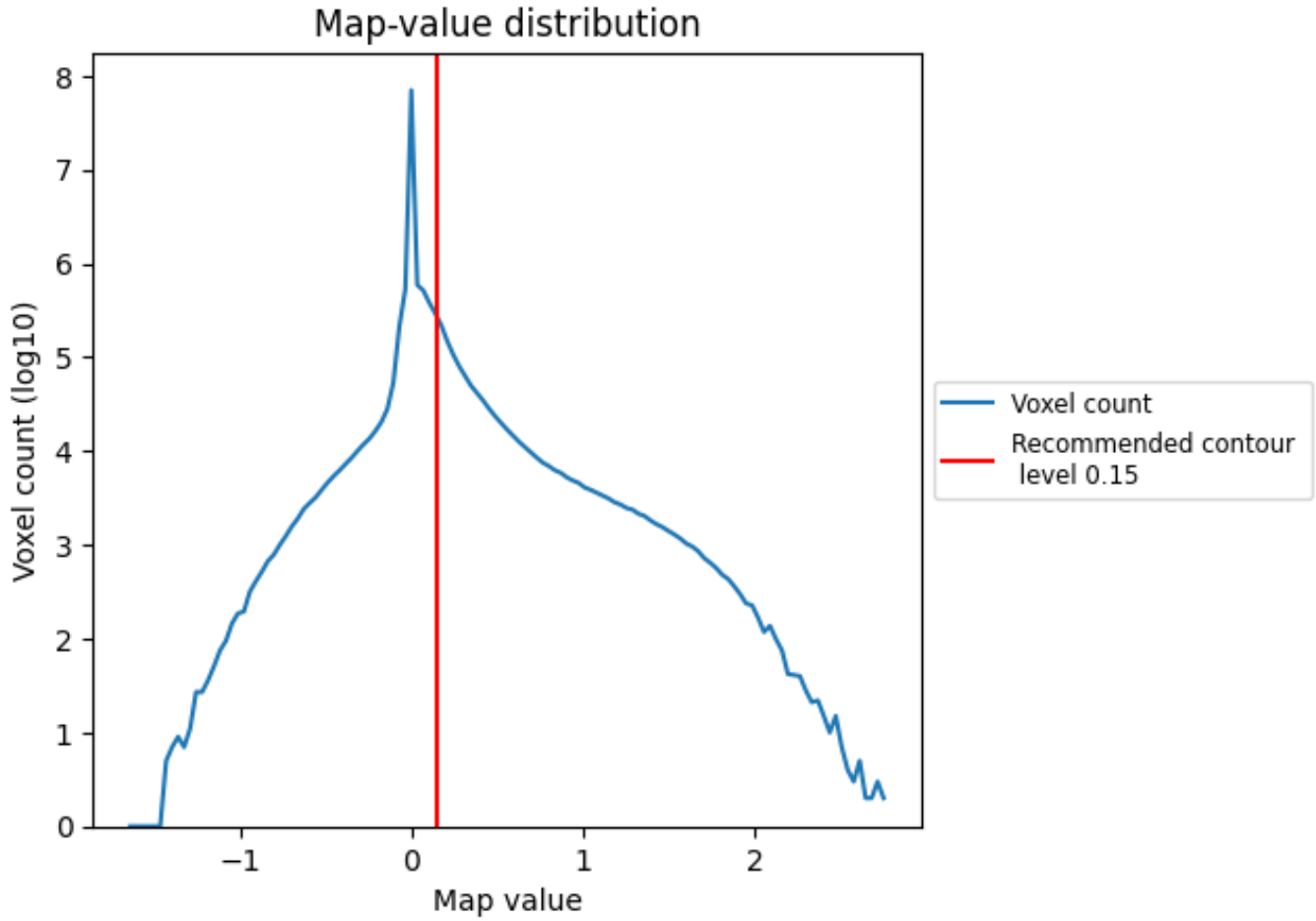
6.6 Mask visualisation (i)

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

7 Map analysis

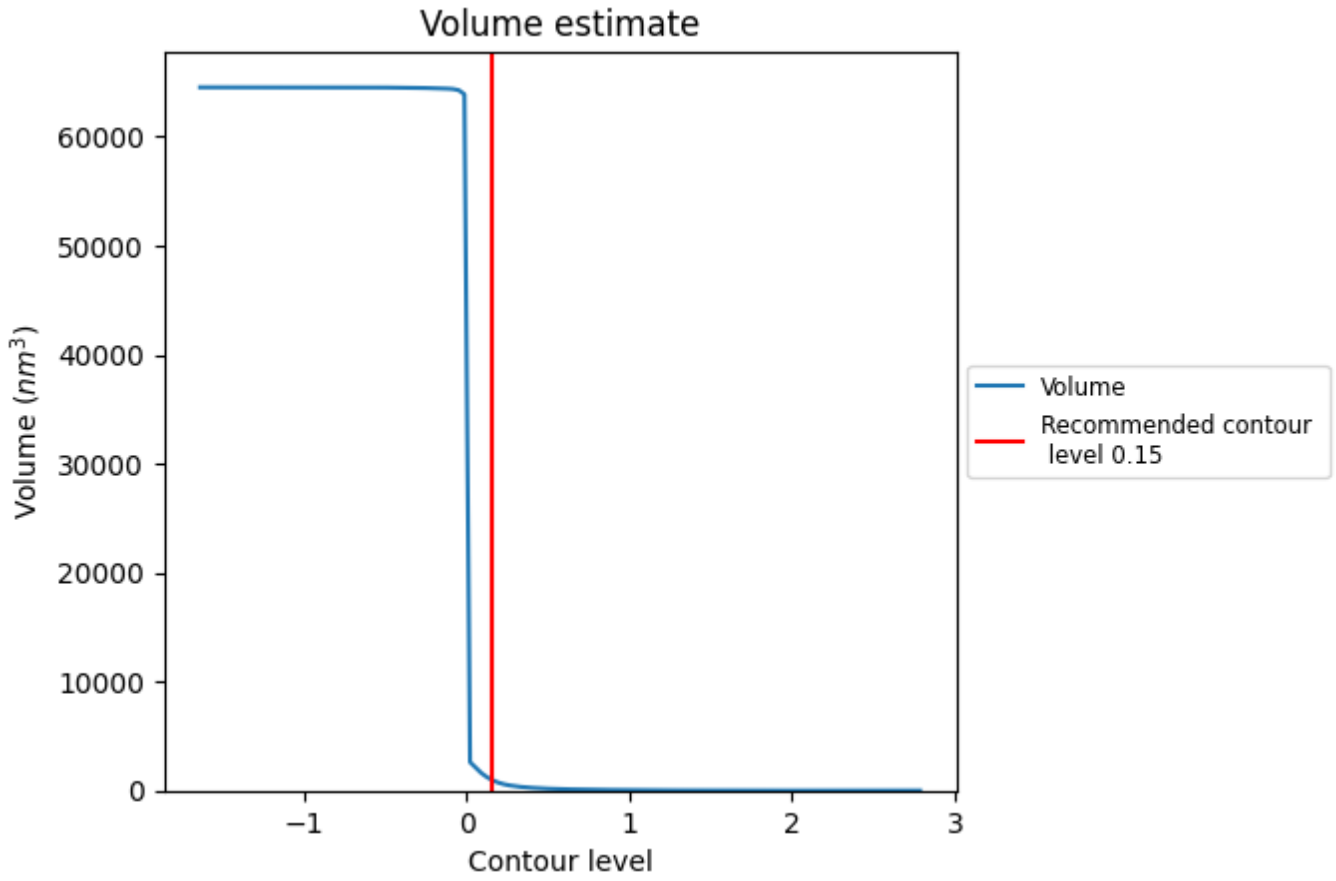
This section contains the results of statistical analysis of the map.

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.

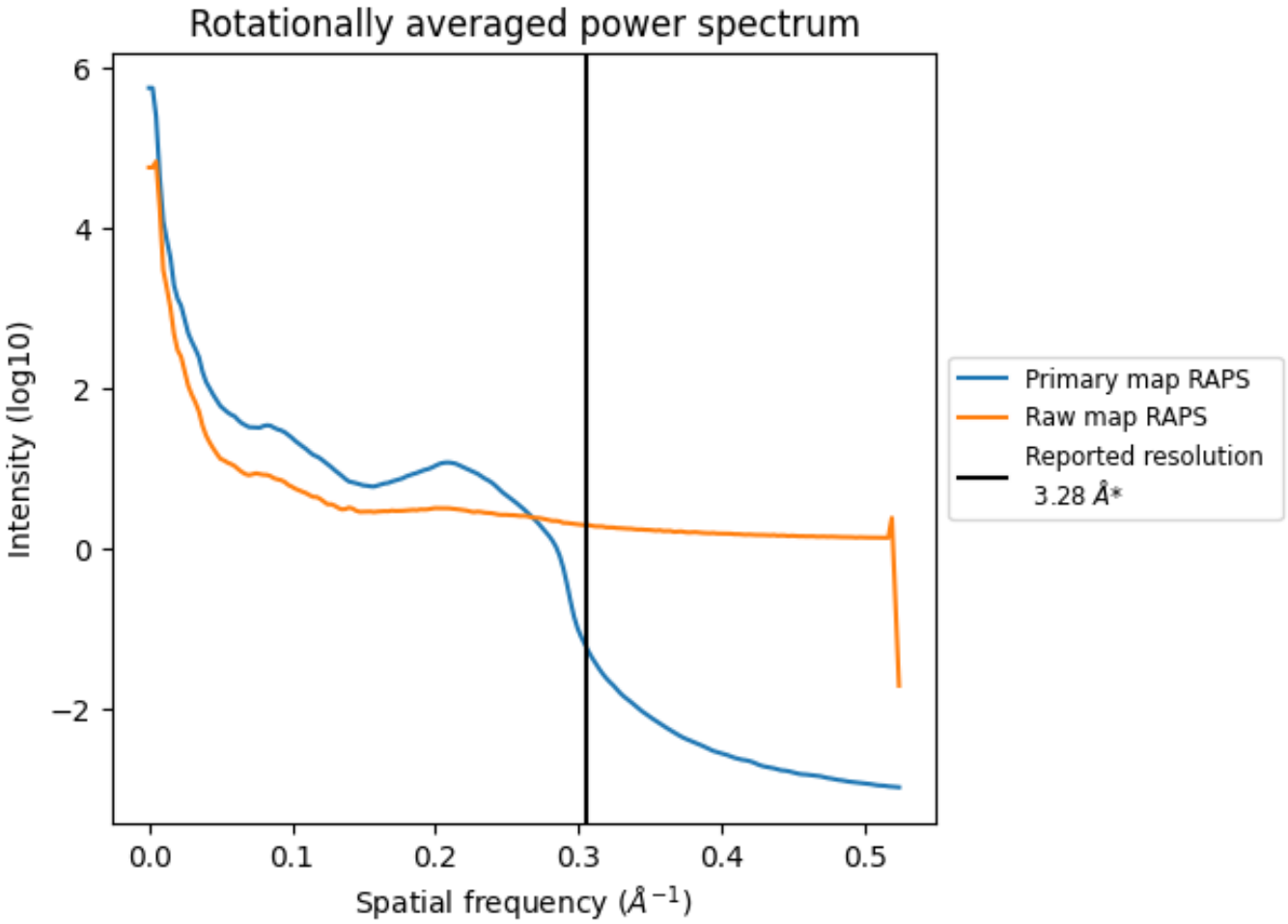
7.2 Volume estimate



The volume at the recommended contour level is 1022 nm^3; this corresponds to an approximate mass of 924 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)

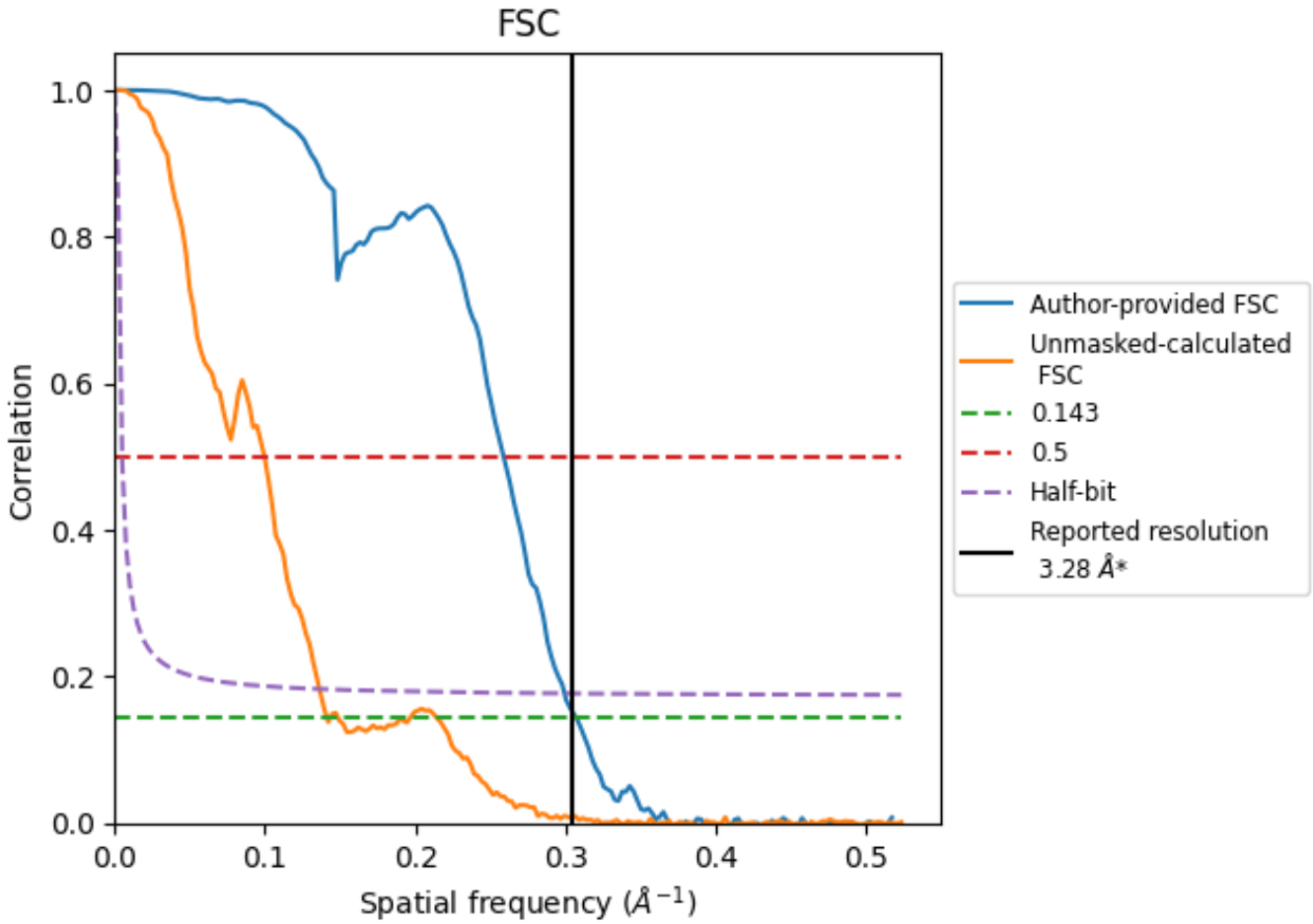


*Reported resolution corresponds to spatial frequency of 0.305 $Å^{-1}$

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 0.305 Å^{-1}

8.2 Resolution estimates (i)

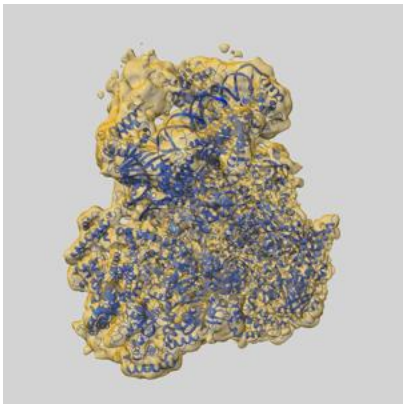
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.26	3.86	3.34
Unmasked-calculated*	7.08	10.03	7.34

*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 7.08 differs from the reported value 3.28 by more than 10 %

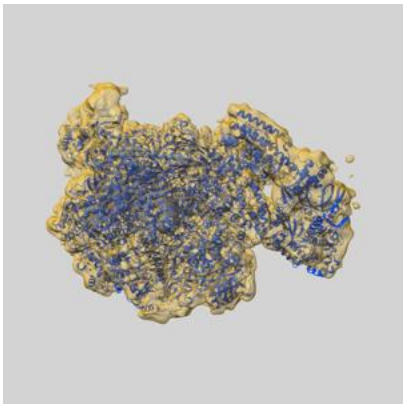
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50730 and PDB model 9FSO. Per-residue inclusion information can be found in section 3 on page 11.

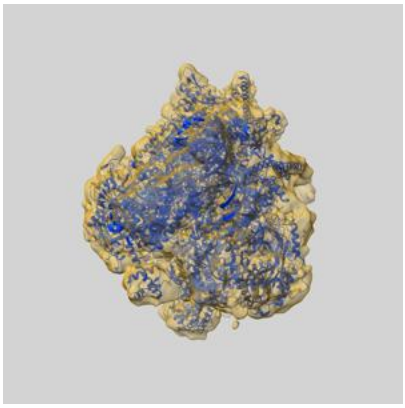
9.1 Map-model overlay



X



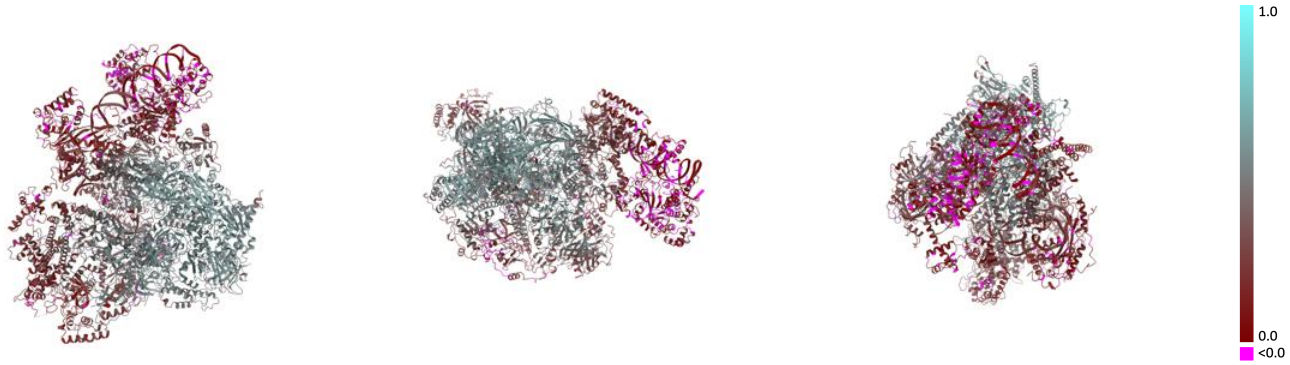
Y



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.

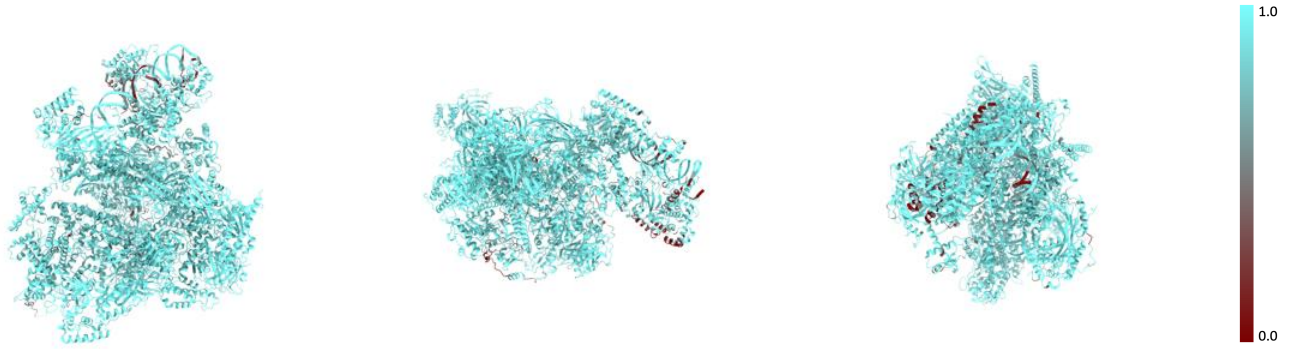
9.2 Q-score mapped to coordinate model (i)



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.

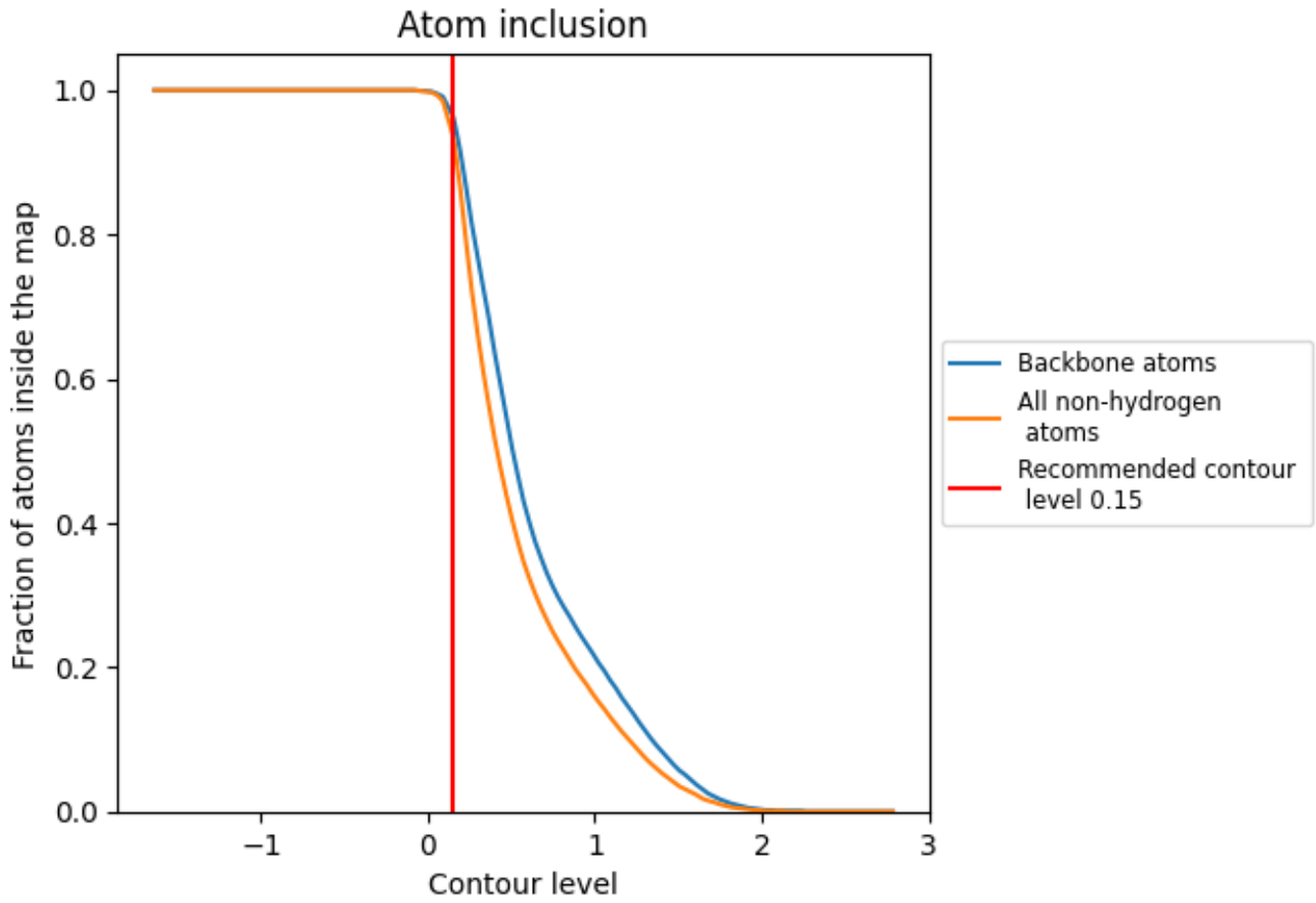
9.3 Atom inclusion mapped to coordinate model (i)



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, 96% of all backbone atoms, 94% 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	0.9370	0.3420
A	0.9550	0.4480
B	0.9770	0.5060
C	0.9290	0.2550
D	0.8660	0.2850
E	0.9220	0.3170
F	0.9320	0.1750
G	0.9680	0.2710
H	0.9850	0.3590
I	0.9760	0.2670
J	0.7480	0.1540
K	0.9910	0.5390
L	0.9960	0.5260
M	0.9890	0.3760
N	0.9800	0.5360
O	0.9900	0.5030
P	0.9870	0.5190
Q	0.9860	0.5630
R	0.9810	0.1830
S	0.9170	0.2840
T	0.9740	0.1390
U	0.8470	0.0480
W	0.8450	0.1080
X	0.8610	0.1840
Y	0.8860	0.1640
Z	0.8470	0.0820