Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 07:37 pm GMT

PDB ID	:	5OQM
EMDB ID	:	EMD-3850
Title	:	STRUCTURE OF YEAST TRANSCRIPTION PRE-INITIATION COMPLEX WITH TFIIH AND CORE MEDIATOR
Authors	:	Schilbach, S.; Hantsche, M.; Tegunov, D.; Dienemann, C.; Wigge, C.; Urlaub, H.; Cramer, P.
Deposited on	:	2017-08-13
Resolution	:	5.80 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 (i) 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 (i)) were used in the production of this report:

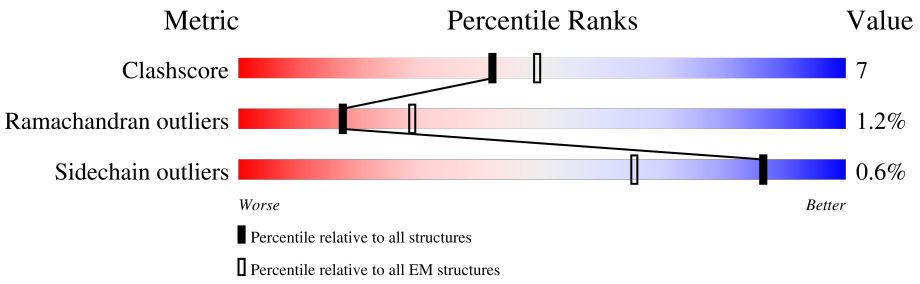
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 5.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1733	66% 14% 19%
2	B	1224	73% 21% 6%
3	C	318	68% 14% 18%
4	D	221	62% 9% 29%
5	E	215	87% 11% •
6	F	155	42% 12% 46%
7	G	171	70% 30%
8	H	146	• 71% 23% 7%

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Mol	Chain	Length	Quality of chain
9	I	122	71% 23% 5%
10	J	70	80% 13% 7%
11	K	120	77% 17% 7%
12	L	70	50% 14% 36%
13	M	345	63% 17% 19%
14	N	106	40% 32% 28%
15	O	240	60% 15% 25%
16	Q	747	15% 5% 80%
17	R	400	38% 10% 52%
18	T	106	5% 40% 28% 32%
19	U	286	24% 8% 68%
20	V	122	71% 11% 18%
21	W	541	40% 7% 52%
22	X	328	44% 5% 51%
23	0	778	75% 14% 10%
24	1	510	5% 88% 8%
25	2	553	68% 29%
26	3	321	39% 57%
27	4	333	84% 11%
28	5	72	6% 65% 26% 8%
29	6	461	67% 6% 27%
30	7	843	36% 12% 52%
31	Z	43	88% 12%
32	a	295	49% 49%
33	b	223	70% 29%

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Mol	Chain	Length	Quality of chain
34	c	115	85% 14%
35	d	687	63% 36%
36	e	307	76% 24%
37	f	210	95%
38	g	121	70% 30%
39	h	300	44% 56%
40	i	223	61% 39%
41	j	149	44% 56%
42	k	157	80% 19%
43	l	745	62% 37%
44	m	220	45% 53%
45	n	140	95%
46	o	151	66% 34%

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
49	SF4	0	901	-	-	X	-

2 Entry composition (i)

There are 49 unique types of molecules in this entry. The entry contains 79757 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1398	10997	6931	1927	2078	61	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1152	9178	5807	1608	1708	55	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	262	2061	1299	343	406	13	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	157	1253	779	220	252	2	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	213	1744	1107	308	318	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	83	670	428	114	125	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1340	861	222	249	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	136	1089	686	184	215	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	116	944	581	172	181	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	65	532	339	93	94	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	112	904	580	154	168	2	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	45	358	221	71	62	4	0	0

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	279	2175	1382	373	403	17	0	0

- Molecule 14 is a DNA chain called NONTEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	N	76	1533	747	288	422	76	0	0

- Molecule 15 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	180	1416	921	242	247	6	0	0

- Molecule 16 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	148	1144	733	195	212	4	0	0

- Molecule 17 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	190	1303	812	238	246	7	0	0

- Molecule 18 is a DNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	T	72	1440	706	254	408	72	0	0

- Molecule 19 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	U	92	757	474	130	150	3	0	0

- Molecule 20 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	100	782	492	130	156	4	0	0

- Molecule 21 is a protein called Transcription factor TFIIE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	258	1825	1147	321	351	6	0	0

- Molecule 22 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	X	160	1004	620	184	196	4	0	0

- Molecule 23 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	0	698	4844	3051	856	907	30	0	0

- Molecule 24 is a protein called General transcription and DNA repair factor IIH subunit TFB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	1	491	3060	1893	570	590	7	0	0

- Molecule 25 is a protein called General transcription and DNA repair factor IIH subunit TFB2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	2	395	2160	1317	413	430	0	0

- Molecule 26 is a protein called RNA polymerase II transcription factor B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	3	138	860	533	160	160	7	0	0

- Molecule 27 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	4	297	1475	877	297	297	4	0	0

- Molecule 28 is a protein called General transcription and DNA repair factor IIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	5	66	498	314	89	93	2	0	0

- Molecule 29 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	6	335	2197	1355	399	422	21	0	0

- Molecule 30 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	7	408	3148	2000	557	572	19	0	0

- Molecule 31 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	Z	43	215	129	43	43	0	0

- Molecule 32 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	a	149	741	443	149	149	0	0

- Molecule 33 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	b	158	839	511	161	167	0	0

- Molecule 34 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	c	99	809	506	137	163	3	0	0

- Molecule 35 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	d	442	3065	1942	539	577	7	0	0

- Molecule 36 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	e	232	1822	1161	297	355	9	0	0

- Molecule 37 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	f	203	1560	987	263	305	5	0	0

- Molecule 38 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	g	85	667	420	110	133	4	1	0

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	h	131	654	392	131	131	0	0

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	i	136	1096	704	190	197	5	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	14	SER	-	insertion	UNP Q08278
i	16	THR	PRO	conflict	UNP Q08278
i	17	SER	PRO	conflict	UNP Q08278
i	19	SER	PRO	conflict	UNP Q08278

- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	j	66	328	196	66	66	0	0

- Molecule 42 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	k	127	630	376	127	127	0	0

- Molecule 43 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	l	471	2344	1402	471	471	0	0

- Molecule 44 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	m	103	512	306	103	103	0	0

- Molecule 45 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	n	136	999	623	171	201	4	0	0

- Molecule 46 is a protein called Mediator of RNA polymerase II transcription subunit 31,Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	o	99	760	499	121	136	4	0	0

- Molecule 47 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
47	A	2	2	2	0

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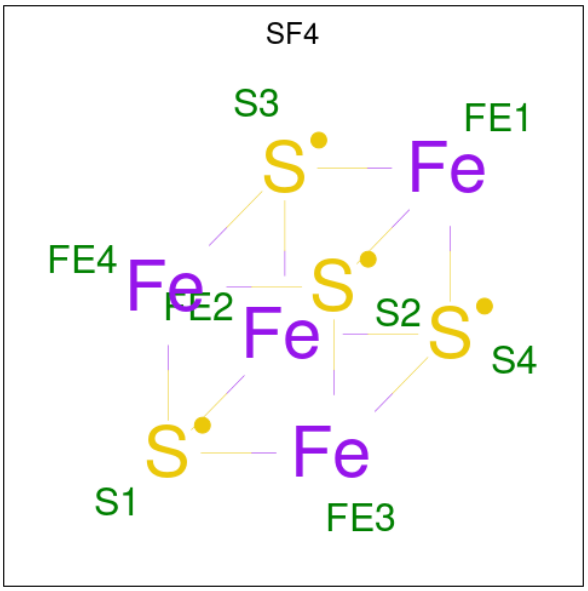
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
47	B	1	1	1	0
47	C	1	1	1	0
47	I	2	2	2	0
47	J	1	1	1	0
47	L	1	1	1	0
47	M	1	1	1	0
47	W	1	1	1	0
47	3	2	2	2	0
47	4	1	1	1	0
47	6	3	3	3	0

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 49 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



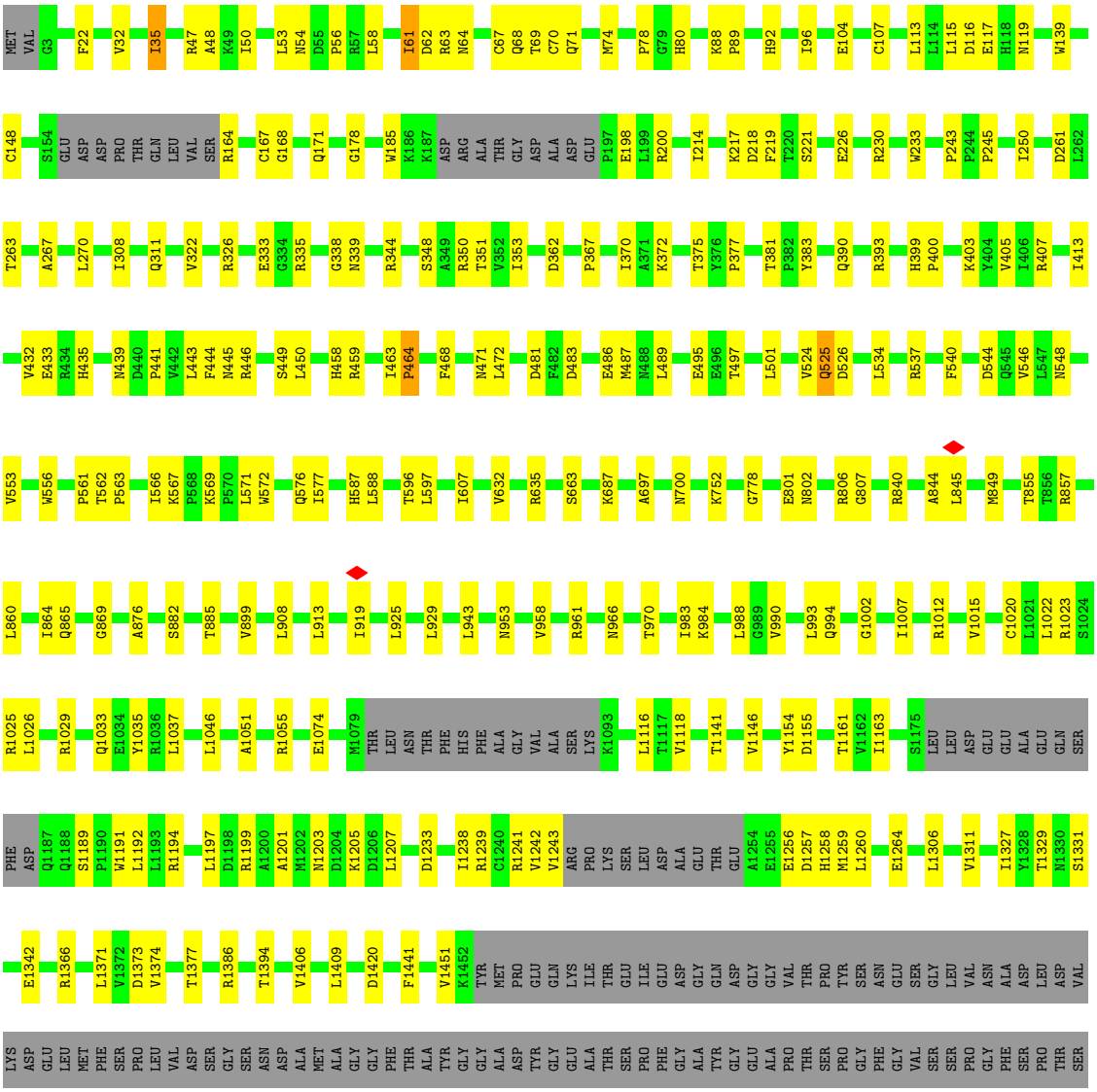
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
49	0	1	8	4	4	0

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.

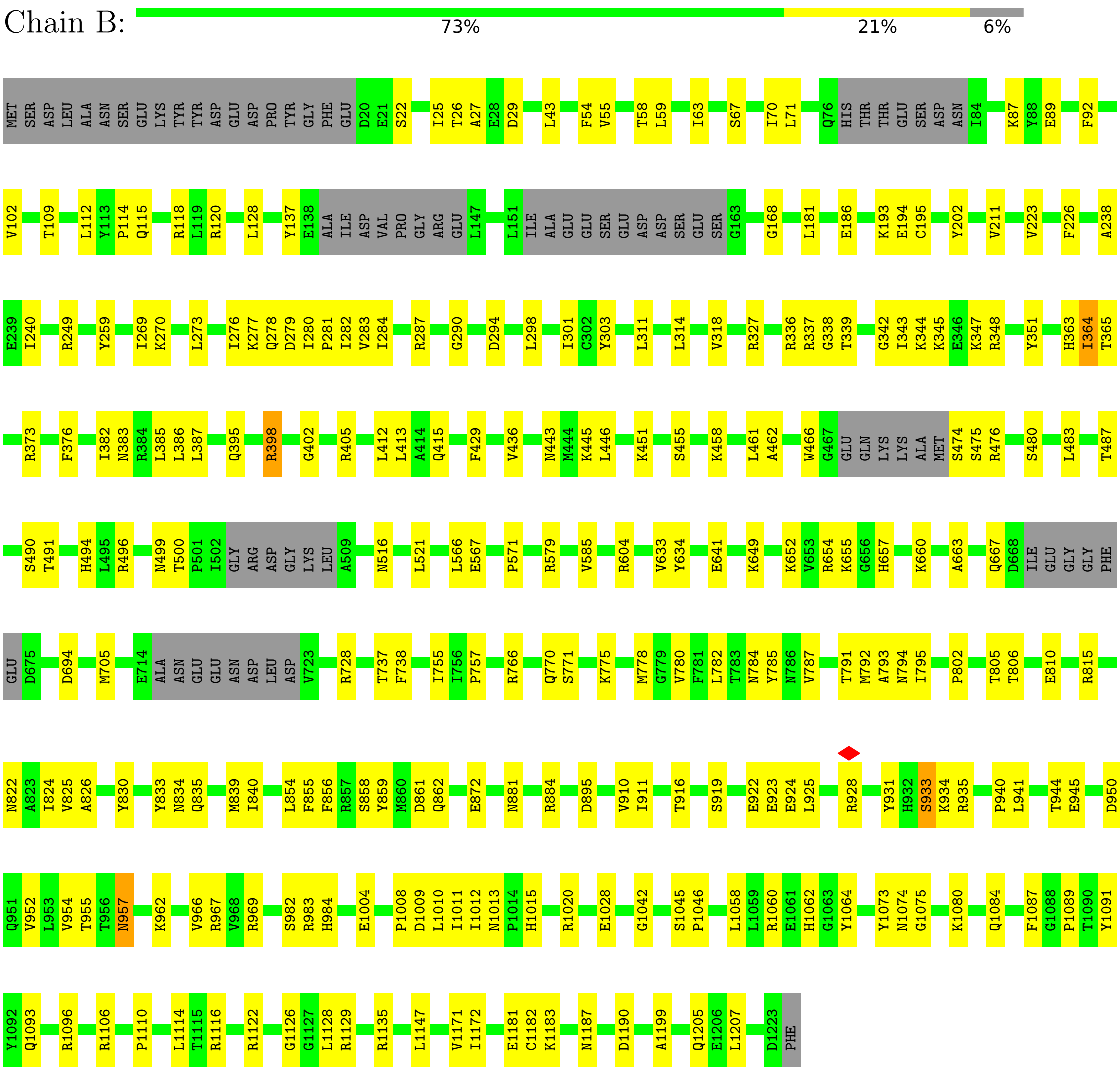
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A: 66% 14% 19%



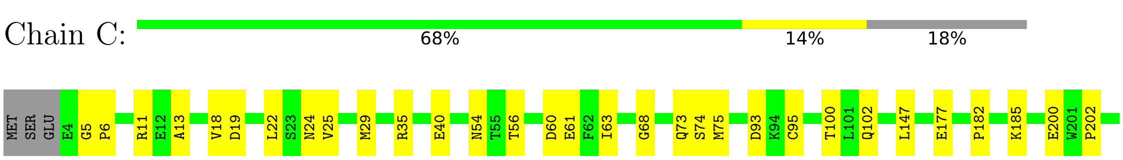
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

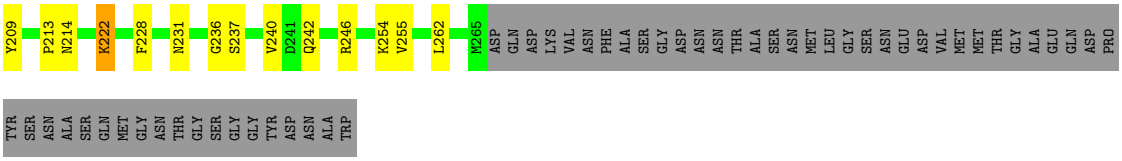
Chain B:



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

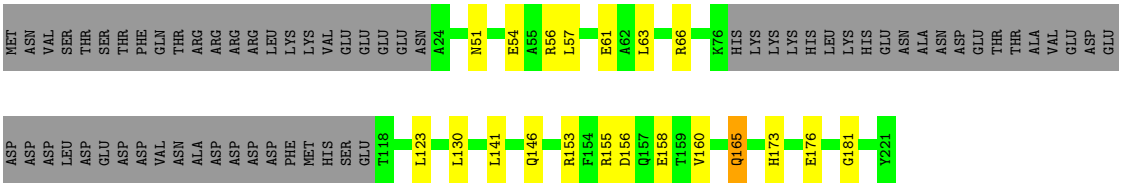
Chain C:





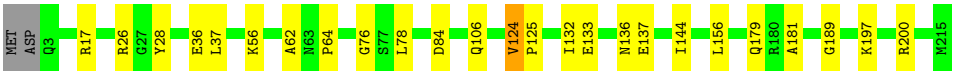
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:



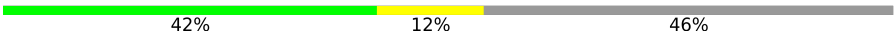
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

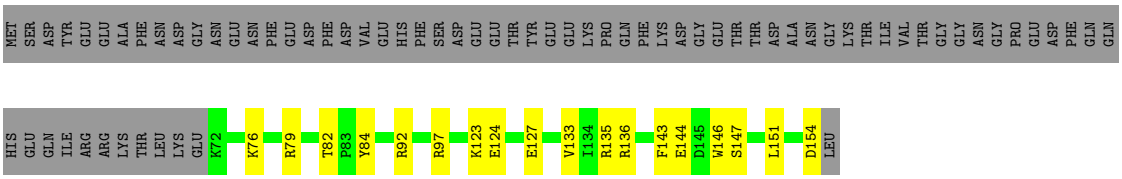
Chain E:



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

Chain F:



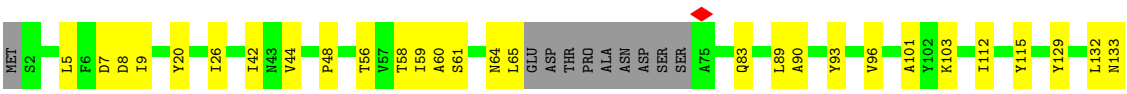


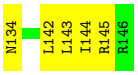
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:

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

Chain H:





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

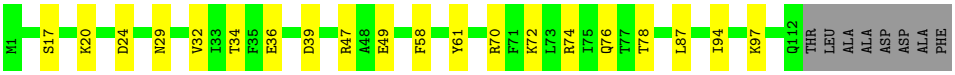
Chain I:

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

Chain J:

• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:

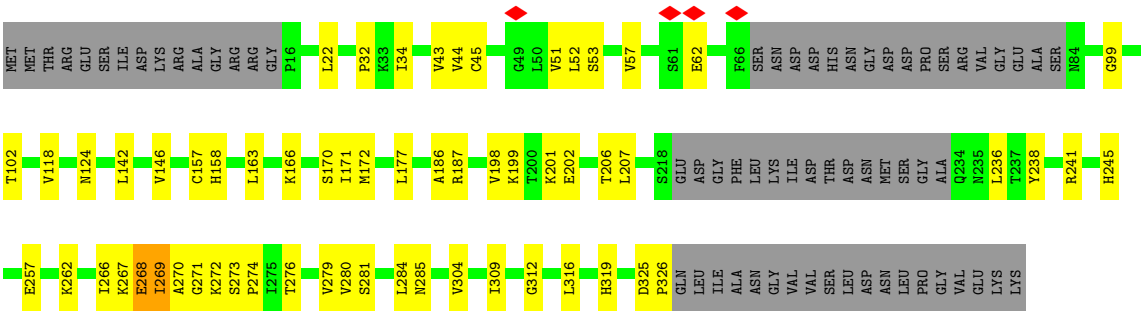


• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:

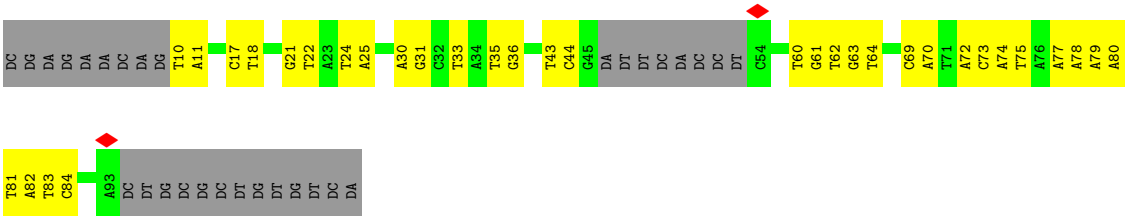
• Molecule 13: Transcription initiation factor IIB

Chain M:



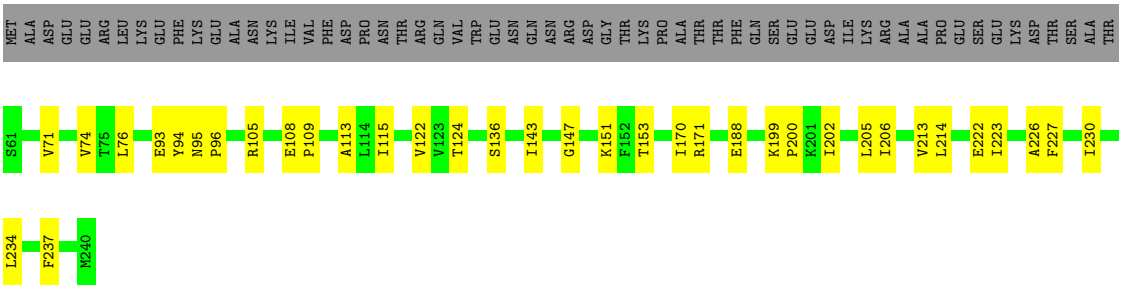
• Molecule 14: NONTEMPLATE DNA

Chain N:



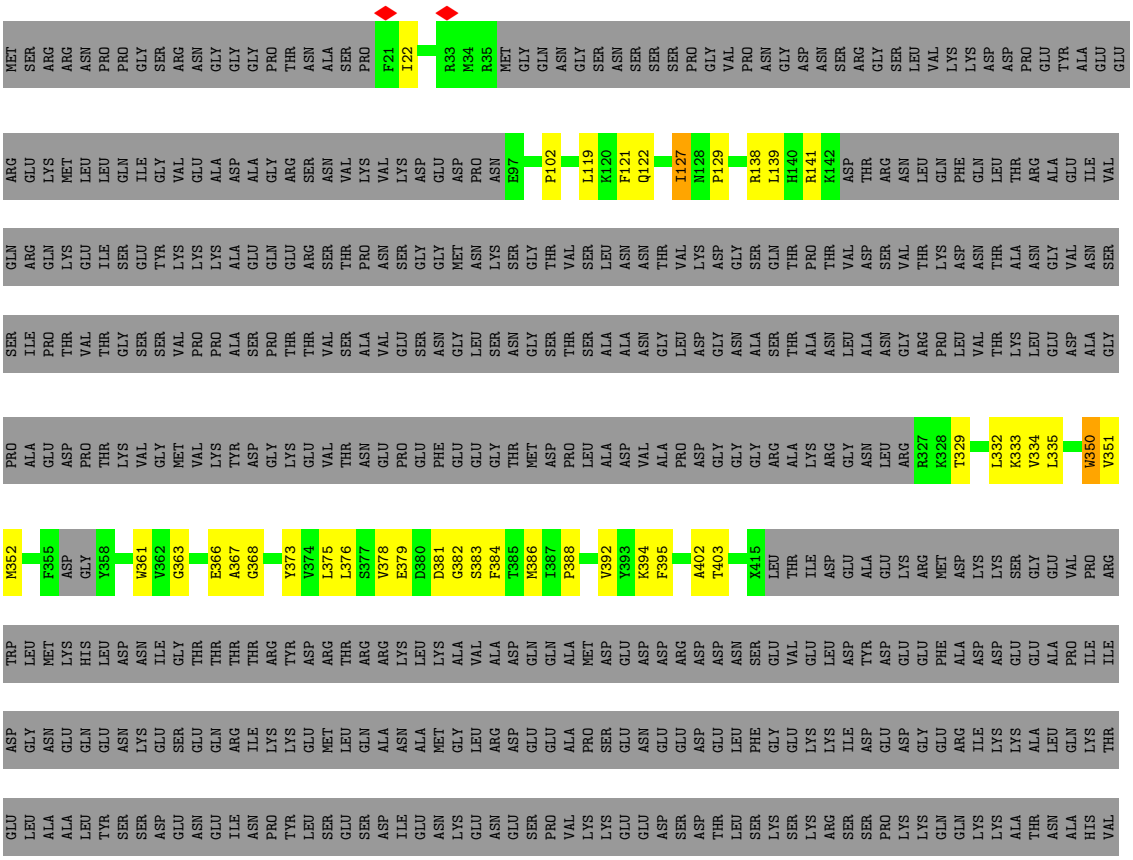
• Molecule 15: TATA-box-binding protein

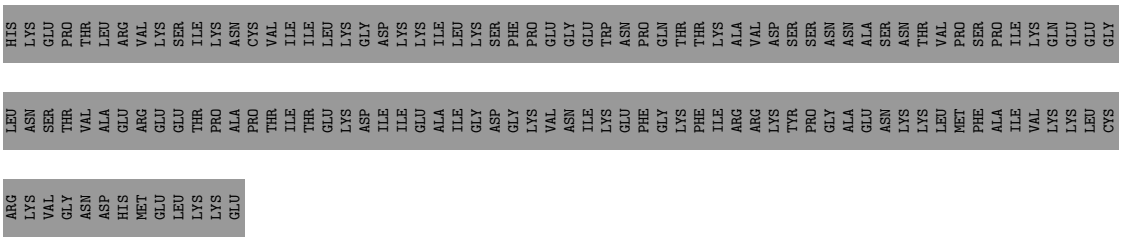
Chain O: 60% 15% 25%



• Molecule 16: Transcription initiation factor IIF subunit alpha

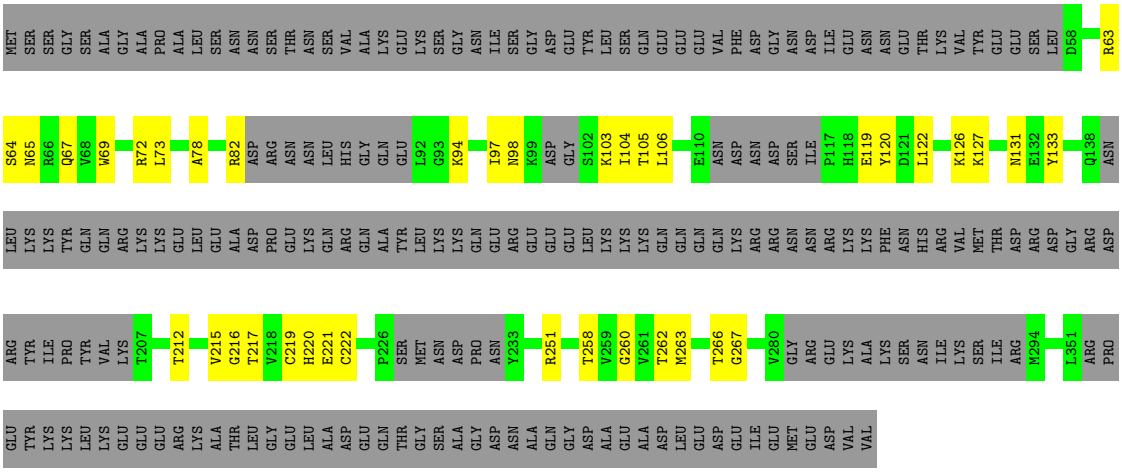
Chain Q: 15% 5% 80%





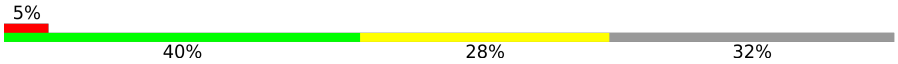
- Molecule 17: Transcription initiation factor IIF subunit beta

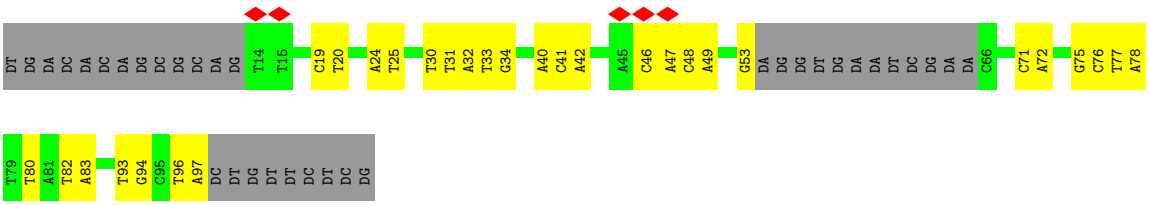
Chain R:



- Molecule 18: TEMPLATE DNA

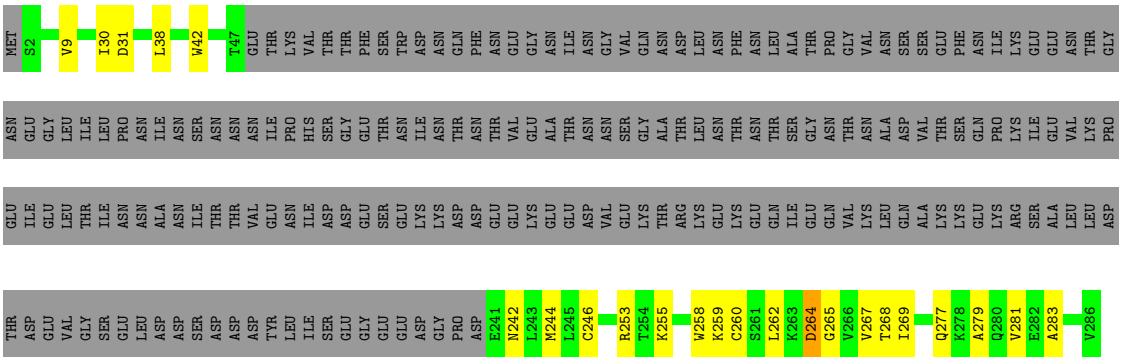
Chain T:





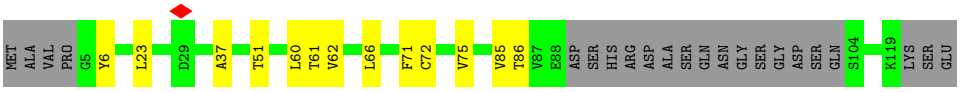
- Molecule 19: Transcription initiation factor IIA large subunit

Chain U:



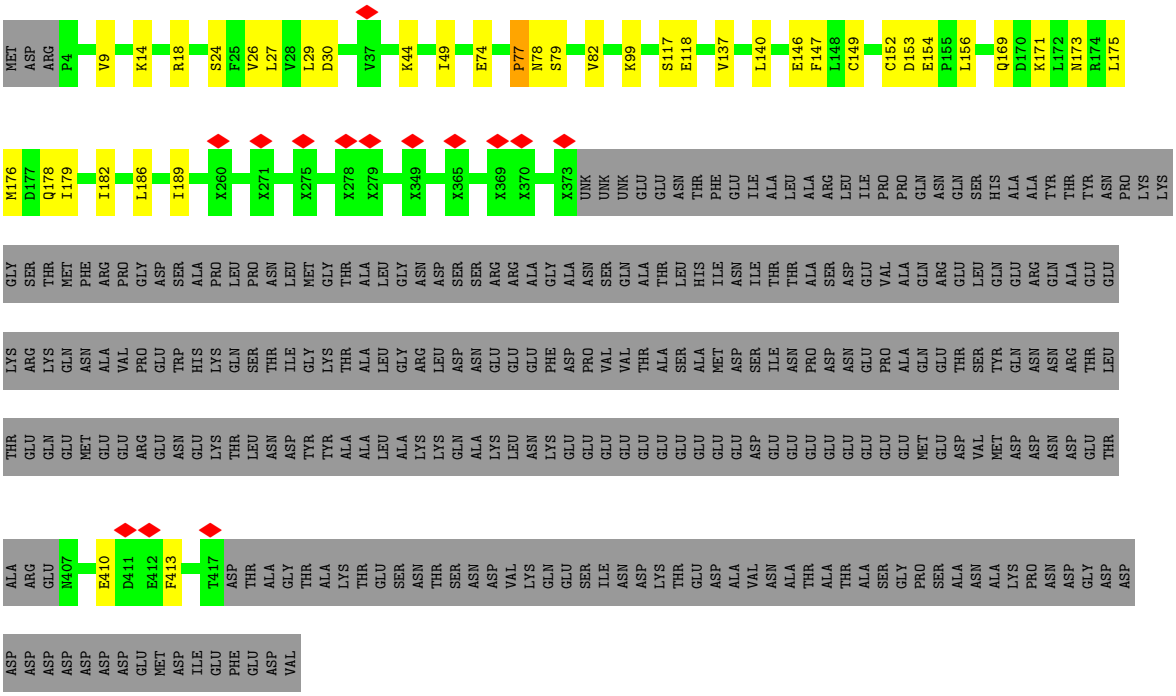
• Molecule 20: Transcription initiation factor IIA subunit 2

Chain V:



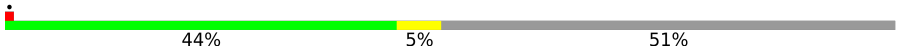
• Molecule 21: Transcription factor TFIIE subunit

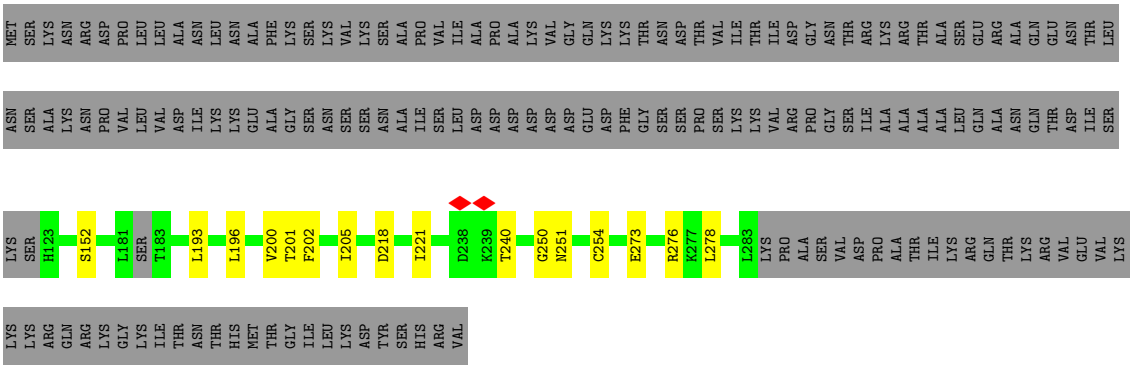
Chain W:



• Molecule 22: Transcription initiation factor IIE subunit beta

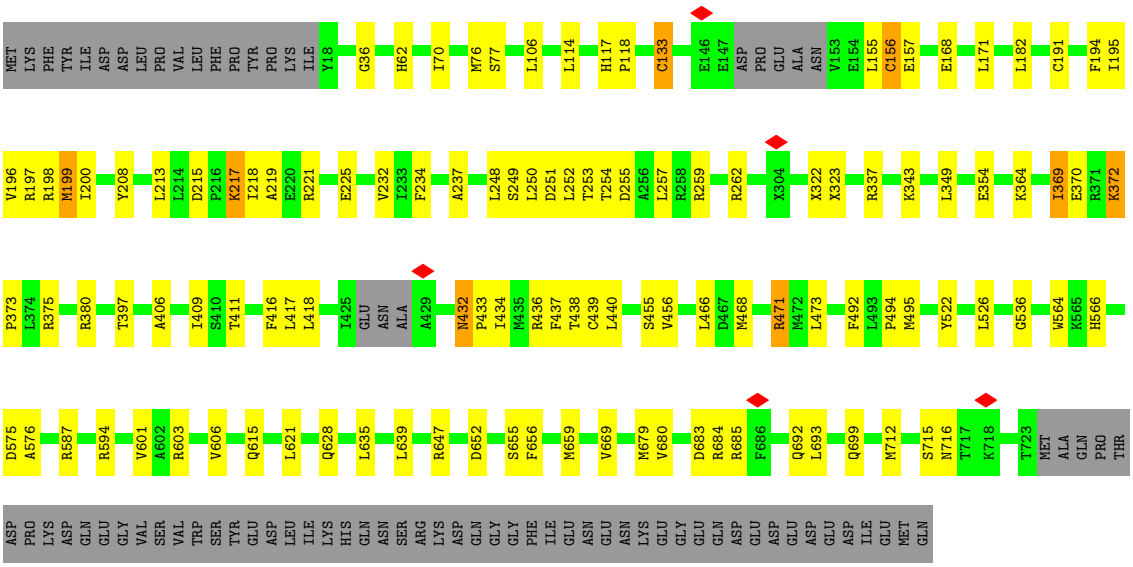
Chain X:





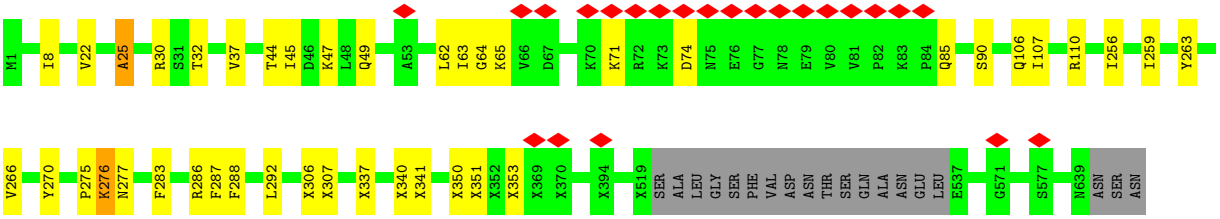
• Molecule 23: General transcription and DNA repair factor IIH helicase subunit XPD

Chain 0:



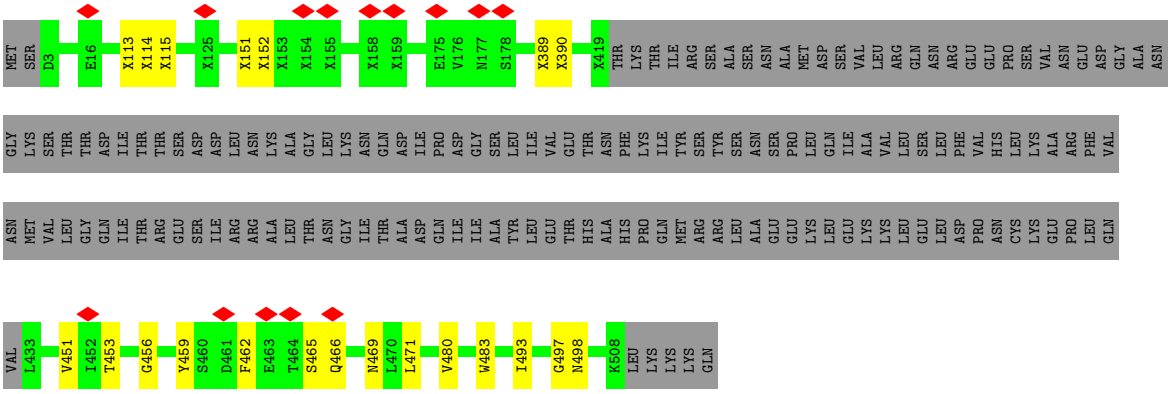
• Molecule 24: General transcription and DNA repair factor IIH subunit TFB1

Chain 1:



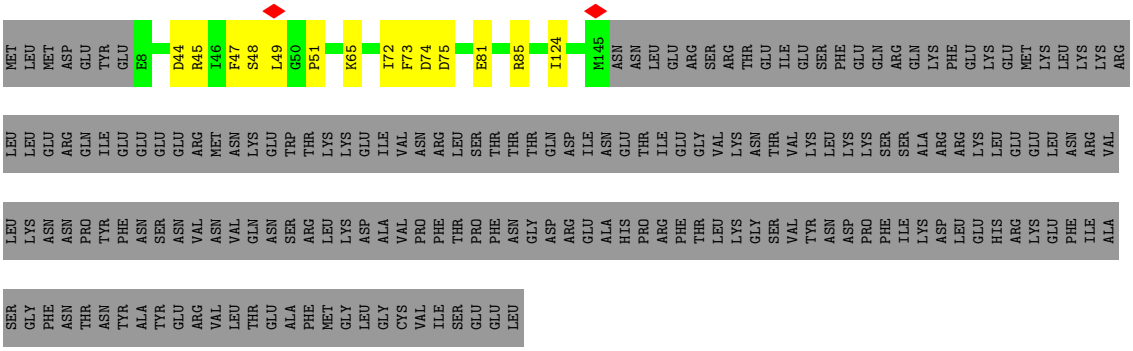
• Molecule 25: General transcription and DNA repair factor IIH subunit TFB2

Chain 2:



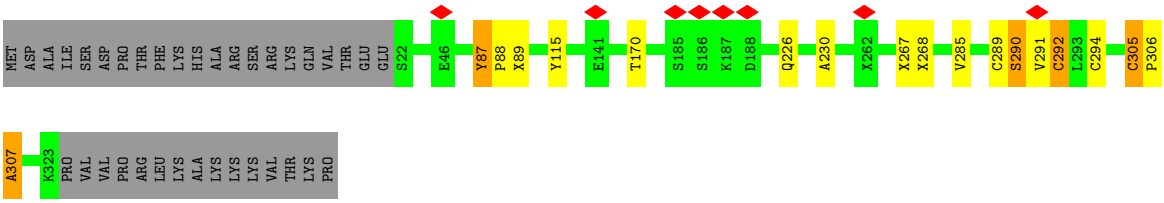
• Molecule 26: RNA polymerase II transcription factor B subunit 3

Chain 3:



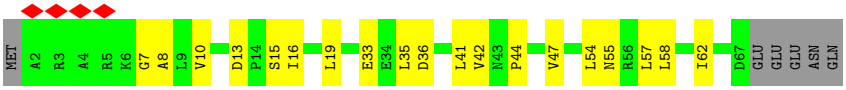
• Molecule 27: General transcription and DNA repair factor IIH subunit TFB4

Chain 4:



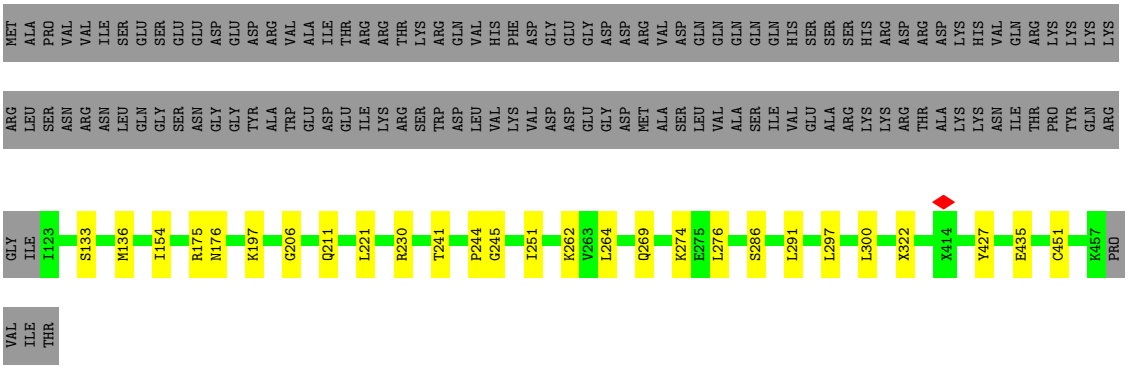
• Molecule 28: General transcription and DNA repair factor IIH subunit TFB5

Chain 5:



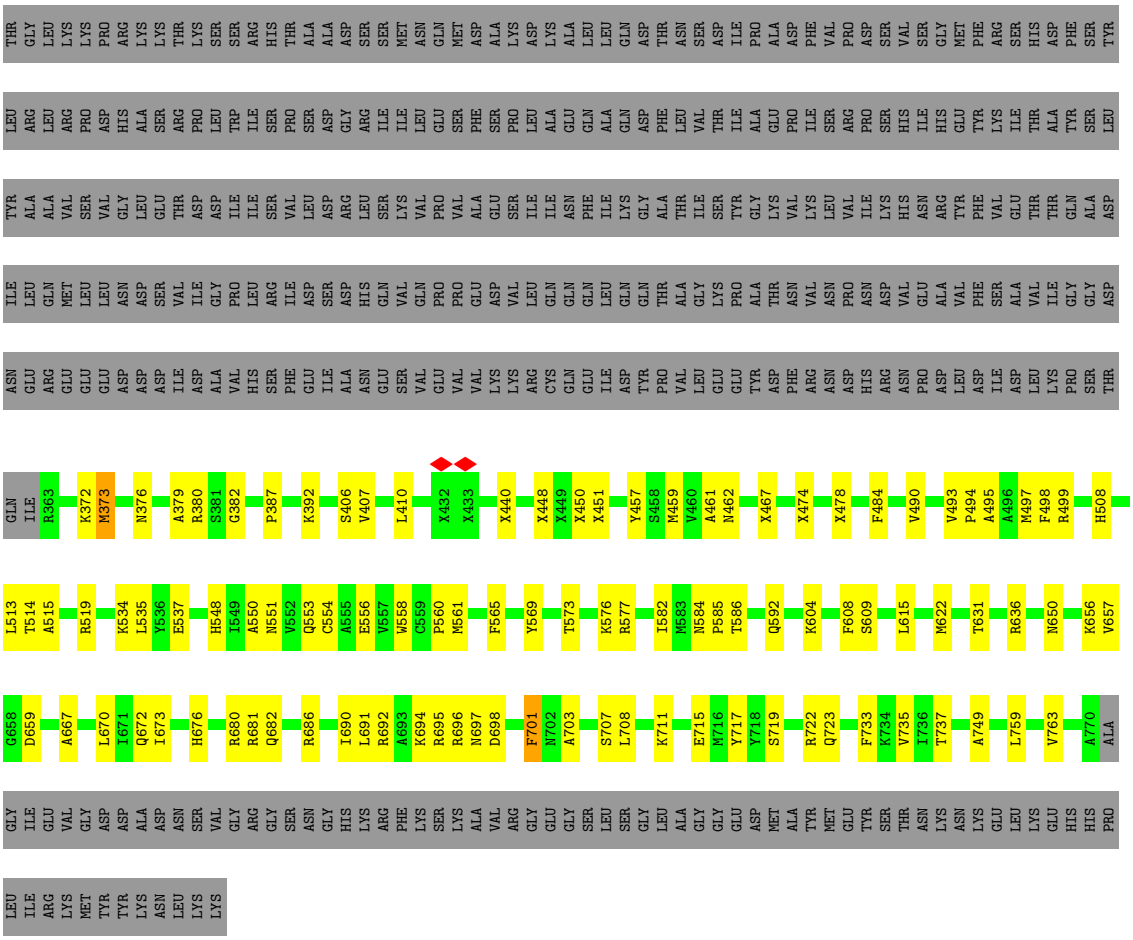
• Molecule 29: General transcription and DNA repair factor IIH subunit SSL1

Chain 6:



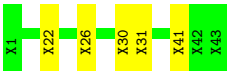
• Molecule 30: General transcription and DNA repair factor IIH helicase subunit XPB

Chain 7:



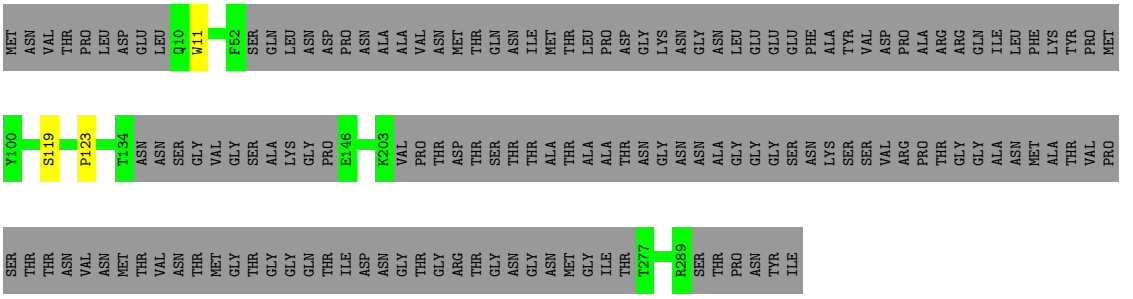
• Molecule 31: Unknown protein

Chain Z: 88% 12%



• Molecule 32: Mediator of RNA polymerase II transcription subunit 6

Chain a: 49% • 49%



• Molecule 33: Mediator of RNA polymerase II transcription subunit 8

Chain b: 70% 29%

MET SER GLN SER THR ALA SER LEU VAL PRO GLU GLY ASN GLN GLY SER LEU GLN GLU ASP VAL SER PHE ASP PHE ASN GLY VAL PRO GLY Q31 P60 F172 LYS ASN GLU GLU SER LEU SER GLU GLU HIS ALA SER LEU LEU VAL ARG ASP SER LYS PRO SER LYS P195 K210

PRO ILE ILE THR GLY SER THR SER THR SER SER SER ASN

- Molecule 34: Mediator of RNA polymerase II transcription subunit 11

Chain c: 85% 14%

MET GLN PRO P4 K38 P83 ILE ASN VAL ASN LYS LYS ALA LEU GLY Q93 P111 SER LYS SER LYS

- Molecule 35: Mediator of RNA polymerase II transcription subunit 17

Chain d: 63% 36%

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

GLU GLY ASP GLU LEU GLU ASN LYS THR LYS LYS ASP ASN ASP LYS ASN LEU LYS PHE LEU LYS ASN LYS ASP SER LEU VAL SER ASN PRO HIS GLU ILE TYR GLY SER MET PRO L99 R110 GLY PRO GLY PHE LYS PHE VAL ASP LEU ASN E121 L131 GLY SER ASP SER SER ASP

GLY HIS ASN SER GLU LYS LYS ASP THR ASP GLY ALA ASP GLU ASN VAL GLN ILE GLY GLU ASP PHE MET GLU VAL ASP TYR GLU ASP LYS ASP ASN PRO VAL ASP SER ARG ASN GLU THR ASP HIS LYS THR ASN GLU ASN GLY GLU THR ASP ASP ASN ILE GLU THR VAL MET THR GLN

GLU Q199 V262 S317 K324 ILE ARG ASP ARG THR SER GLY GLN K333 G340 TYR GLU ASP SER GLY SER THR TYR LYS HIS D351 I357 ARG ASN ASN ILE GLU SER GLN N365 P370 H371 SER SER SER VAL PHE LYS GLY THR ASP PHE VAL H383 R390 I397

R413 ASP SER GLU SER GLU GLU ALA GLU THR LYS D424 D484 SER ILE VAL ASN HIS GLU GLN ASP L493 G529 N532 L540 I541 P571 V580 GLU ARG GLU GLN PRO GLN GLU ASN LYS ASN ILE ASP ASP E594 K608 E654 Q684 LYS LYS VAL

- Molecule 36: Mediator of RNA polymerase II transcription subunit 18

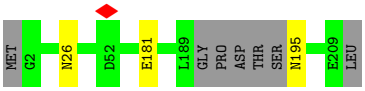
Chain e: 76% 24%

MET V2 F93 THR ASN ASP LYS ILE PRO LEU ASN TYR ALA MET THR ARG ASN ILE LEU HIS ASN THR VAL PRO GLN VAL THR ASN PHE ASN SER THR ASN GLU ASP GLN ASN ASN SER LYS HIS THR GLU ASP THR VAL ASN GLU SER ARG ASN SER ASP ASP ILE ILE ASP VAL ASP

MET ASP ALA SER PRO ALA PRO SER ASN E159 S260 ARG GLY THR D264 A301 HIS GLY ASN ILE LEU ILE

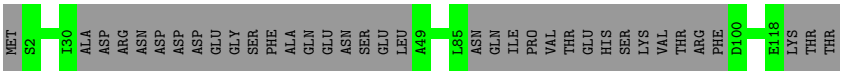
- Molecule 37: Mediator of RNA polymerase II transcription subunit 20

Chain f: 95%



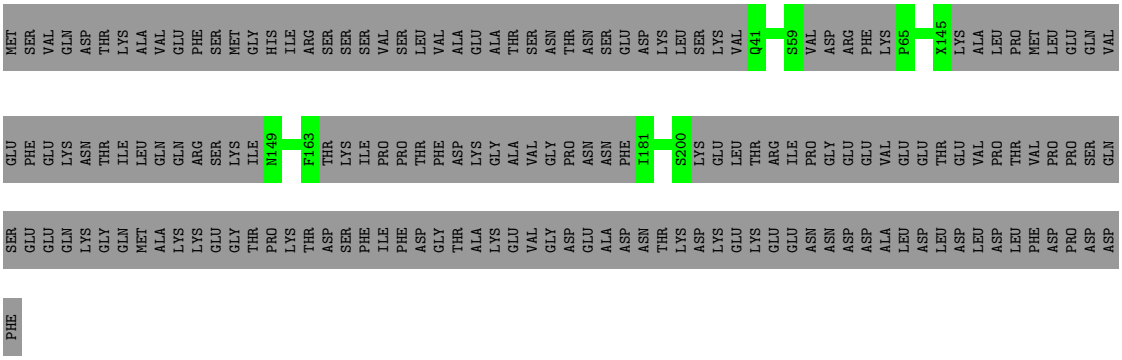
• Molecule 38: Mediator of RNA polymerase II transcription subunit 22

Chain g:



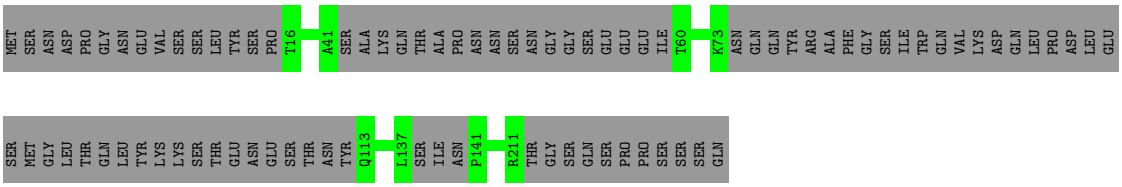
• Molecule 39: Mediator of RNA polymerase II transcription subunit 4

Chain h:



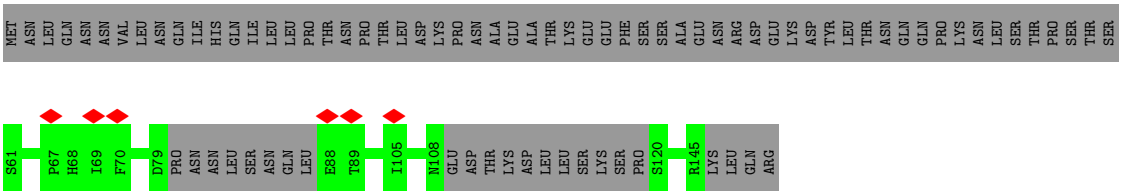
• Molecule 40: Mediator of RNA polymerase II transcription subunit 7

Chain i:



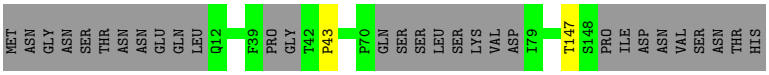
• Molecule 41: Mediator of RNA polymerase II transcription subunit 9

Chain j:



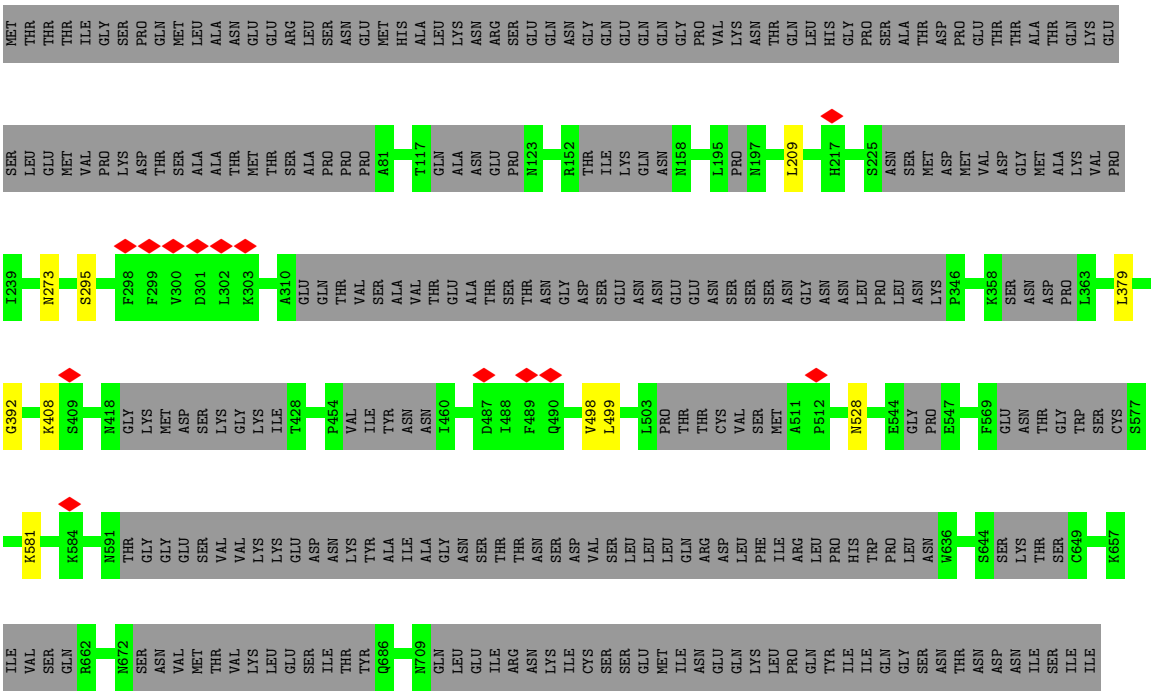
• Molecule 42: Mediator of RNA polymerase II transcription subunit 10

Chain k:



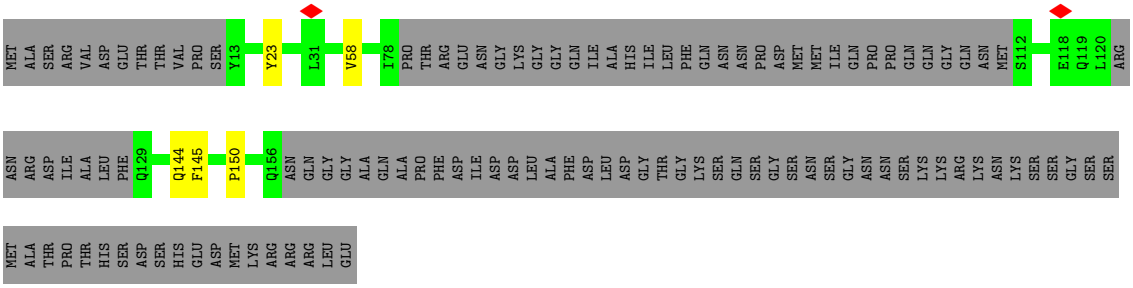
• Molecule 43: Mediator of RNA polymerase II transcription subunit 14

Chain l:



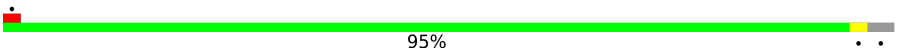
• Molecule 44: Mediator of RNA polymerase II transcription subunit 19

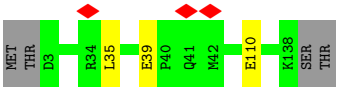
Chain m:



• Molecule 45: Mediator of RNA polymerase II transcription subunit 21

Chain n:

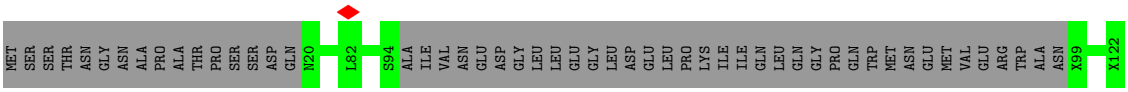




• Molecule 46: Mediator of RNA polymerase II transcription subunit 31,Mediator of RNA polymerase II transcription subunit 31

Chain o:

66%
34%


MET SER SER THR ASN GLY ASN ALA PRO ALA THR PRO SER SER ASP GLN N20 L82 S94 ALA ILE VAL ASN GLU ASP GLY LEU LEU GLU GLY LEU ASP GLU LEU PRO LYS ILE ILE GLN LEU GLN GLY PRO GLN TRP MET ASN GLU MET VAL GLU ARG TRP ALA ASN X99 X122

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16000	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 ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.700	Depositor
Minimum map value	-0.340	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	479.5, 479.5, 479.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	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	0.25	0/11192	0.40	0/15128
2	B	0.24	0/9357	0.40	0/12618
3	C	0.24	0/2099	0.40	0/2845
4	D	0.23	0/1262	0.37	0/1693
5	E	0.24	0/1780	0.38	0/2395
6	F	0.24	0/682	0.38	0/922
7	G	0.25	0/1368	0.42	0/1844
8	H	0.25	0/1107	0.42	0/1499
9	I	0.24	0/962	0.43	0/1295
10	J	0.28	0/541	0.41	0/727
11	K	0.24	0/922	0.38	0/1244
12	L	0.23	0/360	0.45	0/478
13	M	0.24	0/2204	0.40	0/2963
14	N	0.54	0/1724	0.93	0/2614
15	O	0.25	0/1443	0.43	0/1942
16	Q	0.25	0/1108	0.43	0/1495
17	R	0.24	0/1312	0.42	0/1777
18	T	0.53	0/1614	0.96	0/2442
19	U	0.22	0/766	0.38	0/1032
20	V	0.23	0/789	0.40	0/1066
21	W	0.24	0/1566	0.39	0/2117
22	X	0.24	0/1013	0.40	0/1385
23	0	0.26	0/4739	0.41	0/6431
24	1	0.25	0/2198	0.39	0/2983
25	2	0.24	0/1631	0.37	0/2243
26	3	0.24	0/870	0.42	0/1190
27	4	0.27	0/1282	0.52	0/1780
28	5	0.23	0/502	0.41	0/677
29	6	0.27	0/1996	0.42	0/2713
30	7	0.24	0/2980	0.38	0/4019
32	a	0.25	0/737	0.42	0/1023
33	b	0.23	0/841	0.36	0/1166

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	c	0.23	0/817	0.35	0/1096
35	d	0.25	0/3089	0.40	0/4188
36	e	0.24	0/1854	0.41	0/2509
37	f	0.24	0/1584	0.40	0/2145
38	g	0.22	0/665	0.35	0/894
39	h	0.29	0/570	0.35	0/791
40	i	0.32	0/1112	0.40	0/1494
41	j	0.36	0/325	0.41	0/449
42	k	0.24	0/627	0.42	0/870
43	l	0.23	0/2328	0.42	0/3227
44	m	0.23	0/509	0.42	0/706
45	n	0.25	0/1005	0.35	0/1357
46	o	0.24	0/661	0.35	0/902
All	All	0.27	0/78093	0.44	0/106374

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10997	0	11080	166	0
2	B	9178	0	9195	166	0
3	C	2061	0	2029	29	0
4	D	1253	0	1275	12	0
5	E	1744	0	1771	14	0
6	F	670	0	690	11	0
7	G	1340	0	1357	32	0
8	H	1089	0	1062	21	0
9	I	944	0	899	31	0
10	J	532	0	542	6	0
11	K	904	0	911	13	0
12	L	358	0	381	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	2175	0	2283	41	0
14	N	1533	0	860	32	0
15	O	1416	0	1493	22	0
16	Q	1144	0	1021	30	0
17	R	1303	0	1110	29	0
18	T	1440	0	820	28	0
19	U	757	0	747	13	0
20	V	782	0	790	10	0
21	W	1825	0	1546	27	0
22	X	1004	0	730	8	0
23	0	4844	0	4241	82	0
24	1	3060	0	2050	26	0
25	2	2160	0	1075	13	0
26	3	860	0	620	11	0
27	4	1475	0	624	9	0
28	5	498	0	506	12	0
29	6	2197	0	1738	15	0
30	7	3148	0	3001	67	0
31	Z	215	0	49	5	0
32	a	741	0	298	0	0
33	b	839	0	424	0	0
34	c	809	0	807	0	0
35	d	3065	0	2684	0	0
36	e	1822	0	1825	0	0
37	f	1560	0	1573	0	0
38	g	667	0	678	0	0
39	h	654	0	268	0	0
40	i	1096	0	1110	0	0
41	j	328	0	130	0	0
42	k	630	0	265	0	0
43	l	2344	0	979	0	0
44	m	512	0	212	0	0
45	n	999	0	925	0	0
46	o	760	0	656	0	0
47	3	2	0	0	0	0
47	4	1	0	0	0	0
47	6	3	0	0	0	0
47	A	2	0	0	0	0
47	B	1	0	0	0	0
47	C	1	0	0	0	0
47	I	2	0	0	0	0
47	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	L	1	0	0	0	0
47	M	1	0	0	0	0
47	W	1	0	0	0	0
48	A	1	0	0	0	0
49	0	8	0	0	3	0
All	All	79757	0	69330	892	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (892) 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)
9:I:54:GLU:O	9:I:89:GLN:N	1.93	1.02
19:U:242:ASN:HA	19:U:268:THR:O	1.62	0.99
31:Z:31:UNK:HA	31:Z:41:UNK:CB	1.93	0.97
1:A:70:CYS:SG	1:A:80:HIS:NE2	2.40	0.95
31:Z:30:UNK:O	31:Z:41:UNK:CB	2.18	0.91
17:R:98:ASN:HB3	17:R:103:LYS:O	1.71	0.91
9:I:54:GLU:HB3	9:I:88:SER:OG	1.72	0.90
16:Q:138:ARG:O	16:Q:352:MET:HA	1.72	0.89
17:R:106:LEU:O	17:R:119:GLU:HA	1.72	0.89
23:0:594:ARG:NH1	29:6:241:THR:O	2.08	0.85
2:B:70:ILE:HD11	16:Q:333:LYS:HB2	1.59	0.84
9:I:54:GLU:HA	9:I:90:GLN:H	1.43	0.84
18:T:30:DT:H2"	18:T:31:DT:H71	1.58	0.84
3:C:11:ARG:NH1	3:C:209:TYR:OH	2.12	0.82
9:I:54:GLU:CB	9:I:88:SER:OG	2.27	0.82
23:0:252:LEU:O	23:0:434:ILE:HA	1.78	0.82
21:W:14:LYS:O	21:W:18:ARG:HB2	1.79	0.81
25:2:151:UNK:O	25:2:152:UNK:CB	2.29	0.81
23:0:191:CYS:HG	49:0:901:SF4:FE4	0.96	0.80
18:T:19:DC:H2"	18:T:20:DT:H71	1.65	0.79
21:W:149:CYS:O	21:W:153:ASP:N	2.16	0.79
23:0:635:LEU:O	23:0:639:LEU:HB2	1.83	0.78
2:B:835:GLN:HA	2:B:1013:ASN:ND2	1.99	0.77
24:1:64:GLY:HA3	24:1:85:GLN:O	1.83	0.77
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.65	0.77
30:7:672:GLN:HE21	30:7:722:ARG:HH12	1.31	0.77
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.67	0.77
4:D:57:LEU:O	4:D:61:GLU:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:O	2:B:1205:GLN:NE2	2.18	0.76
2:B:839:MET:HG2	2:B:1012:ILE:HG22	1.66	0.76
18:T:77:DT:H2'	18:T:78:DA:H8	1.47	0.76
25:2:114:UNK:O	25:2:115:UNK:CB	2.35	0.75
24:1:350:UNK:O	24:1:351:UNK:CB	2.35	0.75
25:2:113:UNK:O	25:2:114:UNK:CB	2.34	0.74
16:Q:376:LEU:HD21	16:Q:386:MET:HE3	1.69	0.74
23:0:323:UNK:CB	23:0:380:ARG:NH2	2.51	0.74
11:K:20:LYS:HB2	11:K:34:THR:HB	1.67	0.74
3:C:75:MET:O	3:C:246:ARG:NH2	2.21	0.74
1:A:1055:ARG:NH1	6:F:154:ASP:O	2.20	0.73
8:H:56:THR:O	8:H:144:ILE:HA	1.86	0.73
1:A:441:PRO:HA	1:A:458:HIS:O	1.88	0.73
9:I:101:PHE:HB2	9:I:110:PHE:O	1.89	0.73
27:4:289:CYS:HB2	27:4:294:CYS:H	1.54	0.72
3:C:56:THR:HG22	3:C:147:LEU:HD21	1.70	0.72
12:L:32:ALA:HB2	12:L:55:ILE:HB	1.70	0.72
21:W:149:CYS:HB2	21:W:156:LEU:HD21	1.70	0.72
13:M:279:VAL:HG11	13:M:304:VAL:HG11	1.70	0.72
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.55	0.72
16:Q:127:ILE:HG22	16:Q:129:PRO:HD3	1.70	0.71
25:2:389:UNK:O	25:2:390:UNK:CB	2.39	0.71
23:0:526:LEU:HD22	23:0:621:LEU:HD21	1.73	0.71
7:G:10:ASN:HA	7:G:70:PHE:O	1.92	0.70
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.73	0.70
9:I:19:ASP:HB3	9:I:24:ARG:O	1.92	0.69
13:M:99:GLY:H	13:M:102:THR:HG21	1.58	0.69
1:A:524:VAL:HG12	1:A:525:GLN:HG2	1.75	0.69
16:Q:375:LEU:O	16:Q:386:MET:HA	1.91	0.69
18:T:82:DT:H2'	18:T:83:DA:C8	2.28	0.69
14:N:63:DG:H2"	14:N:64:DT:C5	2.28	0.69
30:7:672:GLN:HE21	30:7:722:ARG:NH1	1.91	0.69
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.72	0.69
24:1:256:ILE:HD13	24:1:259:ILE:HD11	1.75	0.69
7:G:101:VAL:HG21	7:G:145:VAL:HG21	1.73	0.69
30:7:558:TRP:HE1	30:7:735:VAL:HB	1.57	0.68
8:H:96:VAL:HA	8:H:142:LEU:O	1.93	0.68
13:M:34:ILE:HG22	13:M:45:CYS:HA	1.75	0.68
30:7:592:GLN:HE22	30:7:749:ALA:H	1.41	0.68
13:M:236:LEU:HD11	13:M:257:GLU:HG3	1.74	0.68
1:A:35:ILE:HG22	1:A:270:LEU:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HG22	1:A:62:ASP:H	1.59	0.68
3:C:18:VAL:HG21	3:C:240:VAL:HG21	1.76	0.67
1:A:1146:VAL:HG23	1:A:1197:LEU:HD22	1.77	0.67
30:7:376:ASN:HD21	30:7:380:ARG:HB3	1.58	0.67
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.75	0.67
1:A:807:GLY:HA3	2:B:728:ARG:HH21	1.60	0.67
26:3:51:PRO:HD3	26:3:65:LYS:HE3	1.77	0.67
2:B:825:VAL:HA	2:B:1010:LEU:O	1.93	0.67
23:0:712:MET:O	23:0:716:ASN:ND2	2.27	0.67
24:1:47:LYS:HB2	24:1:63:ILE:HD12	1.77	0.67
17:R:64:SER:HA	17:R:216:GLY:HA2	1.77	0.67
2:B:373:ARG:HG3	2:B:566:LEU:HD23	1.75	0.67
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.77	0.66
23:0:669:VAL:HG21	23:0:679:MET:HB2	1.77	0.66
1:A:1451:VAL:HG12	7:G:20:PRO:HB3	1.76	0.66
13:M:157:CYS:SG	13:M:158:HIS:N	2.68	0.66
16:Q:121:PHE:HB2	17:R:131:ASN:HB3	1.78	0.66
13:M:267:LYS:HE2	13:M:270:ALA:HB2	1.78	0.66
29:6:221:LEU:HD13	29:6:230:ARG:HB3	1.78	0.66
2:B:67:SER:HB2	2:B:92:PHE:H	1.61	0.65
2:B:770:GLN:NE2	2:B:982:SER:O	2.29	0.65
2:B:383:ASN:O	2:B:387:LEU:HB2	1.96	0.65
23:0:364:LYS:HZ2	23:0:369:ILE:H	1.45	0.65
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.70	0.65
2:B:1171:VAL:HA	2:B:1181:GLU:O	1.97	0.65
2:B:826:ALA:HB3	2:B:1011:ILE:HG12	1.79	0.65
2:B:822:ASN:O	10:J:48:ARG:NH1	2.30	0.64
15:O:170:ILE:HD13	15:O:234:LEU:HD22	1.78	0.64
1:A:178:GLY:HA2	1:A:311:GLN:HE22	1.63	0.64
3:C:11:ARG:NH2	3:C:19:ASP:OD2	2.30	0.64
23:0:248:LEU:HD13	23:0:416:PHE:HE1	1.63	0.64
1:A:69:THR:HG23	1:A:80:HIS:CD2	2.32	0.64
21:W:413:PHE:HB3	24:1:49:GLN:HB3	1.78	0.64
2:B:115:GLN:NE2	2:B:787:VAL:O	2.31	0.64
4:D:173:HIS:HB3	4:D:176:GLU:HG3	1.80	0.64
23:0:253:THR:O	23:0:255:ASP:N	2.26	0.64
1:A:1329:THR:HG22	1:A:1331:SER:H	1.62	0.64
3:C:13:ALA:HA	3:C:18:VAL:HG22	1.80	0.64
23:0:191:CYS:SG	49:0:901:SF4:FE4	1.90	0.63
24:1:8:ILE:HB	24:1:90:SER:HB2	1.77	0.63
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:114:LEU:HD23	7:G:162:SER:HB3	1.81	0.63
13:M:274:PRO:HD2	15:O:188:GLU:HG2	1.81	0.63
30:7:558:TRP:HB3	30:7:711:LYS:HE2	1.81	0.63
1:A:70:CYS:SG	1:A:80:HIS:CE1	2.91	0.63
23:0:248:LEU:HB2	23:0:439:CYS:HB3	1.79	0.63
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.81	0.62
23:0:603:ARG:NH1	23:0:628:GLN:HG3	2.13	0.62
1:A:860:LEU:HD11	1:A:1394:THR:HA	1.80	0.62
17:R:126:LYS:HB3	17:R:221:GLU:HB2	1.79	0.62
21:W:178:GLN:NE2	22:X:254:CYS:SG	2.73	0.62
1:A:68:GLN:O	1:A:71:GLN:NE2	2.33	0.62
23:0:251:ASP:OD1	23:0:436:ARG:NE	2.32	0.62
25:2:483:TRP:NE1	28:5:36:ASP:OD2	2.31	0.62
2:B:490:SER:O	2:B:494:HIS:HB2	2.00	0.62
2:B:944:THR:HG21	2:B:1122:ARG:HH12	1.63	0.62
30:7:560:PRO:HD2	30:7:586:THR:HG21	1.80	0.62
30:7:604:LYS:NZ	30:7:650:ASN:OD1	2.32	0.62
1:A:544:ASP:HB2	11:K:47:ARG:HH12	1.65	0.62
13:M:163:LEU:O	13:M:166:LYS:NZ	2.33	0.62
1:A:1189:SER:N	1:A:1242:VAL:O	2.31	0.62
2:B:25:ILE:HA	2:B:655:LYS:HE3	1.82	0.62
19:U:259:LYS:HA	19:U:281:VAL:O	2.00	0.62
23:0:217:LYS:HG3	23:0:218:ILE:HG12	1.81	0.62
13:M:118:VAL:HG22	13:M:124:ASN:HD21	1.65	0.61
1:A:1199:ARG:O	1:A:1203:ASN:ND2	2.33	0.61
7:G:96:GLN:NE2	21:W:146:GLU:OE2	2.33	0.61
1:A:562:THR:O	1:A:576:GLN:NE2	2.34	0.61
3:C:25:VAL:HG13	3:C:29:MET:HB3	1.83	0.61
23:0:257:LEU:HB3	23:0:343:LYS:NZ	2.16	0.61
23:0:495:MET:SD	23:0:684:ARG:NH2	2.73	0.61
27:4:289:CYS:HB3	27:4:292:CYS:SG	2.40	0.61
27:4:305:CYS:O	27:4:307:ALA:N	2.34	0.61
2:B:249:ARG:HG2	2:B:415:GLN:HE22	1.64	0.61
27:4:87:TYR:O	27:4:89:UNK:N	2.34	0.61
1:A:32:VAL:HG12	2:B:1183:LYS:HE2	1.81	0.61
16:Q:373:TYR:OH	17:R:72:ARG:NH2	2.34	0.61
30:7:565:PHE:O	30:7:569:TYR:HB2	2.01	0.61
30:7:673:ILE:HG12	30:7:708:LEU:HD12	1.82	0.61
30:7:656:LYS:NZ	30:7:686:ARG:HH21	1.98	0.61
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.23	0.60
25:2:456:GLY:HA3	25:2:493:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:4:285:VAL:HA	29:6:322:UNK:O	2.00	0.60
2:B:193:LYS:HB3	2:B:787:VAL:HG21	1.83	0.60
30:7:631:THR:HB	30:7:636:ARG:HE	1.66	0.60
1:A:481:ASP:O	1:A:483:ASP:OD1	2.20	0.60
1:A:185:TRP:HB2	1:A:198:GLU:O	2.02	0.60
14:N:30:DA:H2'	14:N:31:DG:C8	2.36	0.60
1:A:115:LEU:O	1:A:164:ARG:NH1	2.35	0.60
4:D:57:LEU:O	4:D:61:GLU:CB	2.50	0.60
30:7:672:GLN:HE22	30:7:686:ARG:HH22	1.48	0.60
1:A:1257:ASP:OD1	1:A:1258:HIS:N	2.35	0.60
8:H:129:TYR:O	8:H:133:ASN:ND2	2.35	0.60
30:7:493:VAL:O	30:7:495:ALA:N	2.35	0.60
1:A:537:ARG:HD2	8:H:20:TYR:CZ	2.37	0.59
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.83	0.59
3:C:22:LEU:O	3:C:228:PHE:HB2	2.02	0.59
23:0:322:UNK:CB	23:0:380:ARG:HH12	2.14	0.59
1:A:483:ASP:OD1	1:A:483:ASP:N	2.35	0.59
4:D:66:ARG:NH2	7:G:47:CYS:SG	2.75	0.59
18:T:77:DT:H2'	18:T:78:DA:C8	2.34	0.59
13:M:281:SER:O	13:M:285:ASN:ND2	2.31	0.59
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.84	0.59
13:M:22:LEU:HB3	13:M:52:LEU:HD23	1.83	0.59
14:N:82:DA:H4'	30:7:676:HIS:HE1	1.66	0.59
23:0:364:LYS:NZ	23:0:370:GLU:H	1.99	0.59
2:B:919:SER:HB2	2:B:922:GLU:HB2	1.84	0.59
7:G:4:ILE:HG12	7:G:77:VAL:HG22	1.84	0.59
31:Z:31:UNK:CA	31:Z:41:UNK:CB	2.77	0.59
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.36	0.59
2:B:298:LEU:HD23	2:B:311:LEU:HD22	1.84	0.59
3:C:54:ASN:HD21	3:C:63:ILE:HD12	1.68	0.59
8:H:101:ALA:HA	8:H:115:TYR:O	2.02	0.59
16:Q:139:LEU:HA	16:Q:351:VAL:O	2.02	0.59
30:7:680:ARG:HB3	30:7:722:ARG:HB2	1.84	0.59
2:B:969:ARG:NH2	3:C:60:ASP:OD2	2.36	0.59
11:K:49:GLU:OE2	11:K:97:LYS:NZ	2.35	0.58
18:T:30:DT:OP1	30:7:657:VAL:HA	2.03	0.58
23:0:354:GLU:HB2	23:0:418:LEU:HB2	1.84	0.58
2:B:1106:ARG:NH2	2:B:1110:PRO:O	2.34	0.58
3:C:73:GLN:HE21	3:C:74:SER:H	1.50	0.58
19:U:244:MET:HG3	19:U:267:VAL:HG22	1.85	0.58
1:A:1342:GLU:OE1	5:E:200:ARG:NH2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:31:DT:H2'	18:T:32:DA:C8	2.38	0.58
17:R:104:ILE:HD11	17:R:122:LEU:HD22	1.86	0.58
19:U:246:CYS:HB3	19:U:265:GLY:HA3	1.85	0.58
22:X:200:VAL:HG12	22:X:201:THR:HG23	1.85	0.58
23:0:257:LEU:HB3	23:0:343:LYS:HZ2	1.68	0.58
1:A:333:GLU:OE1	2:B:1129:ARG:NH2	2.37	0.58
1:A:390:GLN:OE1	1:A:393:ARG:NH2	2.37	0.58
7:G:84:GLY:CA	7:G:147:ILE:O	2.52	0.58
29:6:264:LEU:HD22	29:6:300:LEU:HD13	1.85	0.58
9:I:19:ASP:O	9:I:23:ASN:HA	2.04	0.58
16:Q:141:ARG:HA	16:Q:350:TRP:HA	1.85	0.58
17:R:104:ILE:HD11	17:R:122:LEU:HB3	1.86	0.58
29:6:291:LEU:HD22	29:6:297:LEU:HD13	1.86	0.58
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.86	0.58
1:A:250:ILE:HD13	13:M:62:GLU:HG3	1.85	0.57
1:A:348:SER:HA	1:A:489:LEU:O	2.04	0.57
2:B:858:SER:HA	2:B:966:VAL:O	2.04	0.57
9:I:82:GLU:HG2	9:I:104:LEU:HD12	1.85	0.57
11:K:29:ASN:ND2	11:K:78:THR:O	2.37	0.57
8:H:65:LEU:HD21	8:H:89:LEU:HD13	1.86	0.57
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.85	0.57
1:A:1146:VAL:HG12	1:A:1201:ALA:HB1	1.85	0.57
1:A:326:ARG:HG2	1:A:1406:VAL:HG11	1.86	0.57
2:B:881:ASN:O	2:B:933:SER:OG	2.23	0.57
7:G:8:SER:HA	7:G:72:VAL:O	2.05	0.57
30:7:474:UNK:O	30:7:478:UNK:CB	2.51	0.57
23:0:364:LYS:HZ2	23:0:369:ILE:N	2.03	0.57
1:A:687:LYS:NZ	1:A:801:GLU:OE1	2.38	0.57
23:0:337:ARG:NH2	26:3:74:ASP:OD2	2.38	0.57
27:4:267:UNK:O	27:4:268:UNK:CB	2.51	0.57
18:T:41:DC:H2"	18:T:42:DA:C8	2.39	0.57
3:C:5:GLY:O	3:C:24:ASN:ND2	2.36	0.57
7:G:84:GLY:HA2	7:G:147:ILE:O	2.05	0.57
13:M:284:LEU:HD22	13:M:316:LEU:HG	1.86	0.57
30:7:490:VAL:H	30:7:514:THR:HB	1.70	0.56
19:U:262:LEU:HB2	19:U:279:ALA:HB3	1.86	0.56
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.05	0.56
17:R:98:ASN:CB	17:R:103:LYS:O	2.50	0.56
24:1:283:PHE:O	24:1:287:PHE:HB3	2.06	0.56
1:A:544:ASP:O	1:A:548:ASN:ND2	2.38	0.56
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1009:ASP:OD2	10:J:48:ARG:NH2	2.38	0.56
9:I:55:THR:HG22	9:I:100:PHE:CD2	2.40	0.56
14:N:43:DT:H1'	14:N:44:DC:H5'	1.87	0.56
1:A:443:LEU:HG	1:A:501:LEU:HD21	1.87	0.56
7:G:138:THR:HG22	7:G:139:ILE:H	1.70	0.56
17:R:67:GLN:HB3	17:R:219:CYS:HB2	1.87	0.56
23:0:76:MET:HB2	24:1:341:UNK:HA	1.88	0.56
1:A:335:ARG:HH22	2:B:1114:LEU:HD11	1.69	0.56
7:G:84:GLY:N	7:G:147:ILE:O	2.39	0.56
23:0:468:MET:SD	23:0:468:MET:N	2.79	0.56
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.38	0.56
3:C:242:GLN:O	3:C:246:ARG:HB2	2.06	0.56
10:J:48:ARG:O	10:J:52:THR:OG1	2.15	0.56
11:K:36:GLU:OE1	11:K:70:ARG:NH1	2.39	0.56
29:6:175:ARG:NH1	29:6:176:ASN:OD1	2.38	0.56
1:A:261:ASP:HB3	1:A:322:VAL:HG13	1.88	0.56
2:B:794:ASN:HA	2:B:854:LEU:O	2.06	0.56
5:E:17:ARG:HH12	5:E:36:GLU:HA	1.71	0.56
16:Q:122:GLN:HB2	16:Q:394:LYS:HE3	1.87	0.56
24:1:288:PHE:O	24:1:292:LEU:CB	2.53	0.56
5:E:28:TYR:HA	5:E:64:PRO:HA	1.86	0.55
13:M:177:LEU:HD22	13:M:207:LEU:HD11	1.87	0.55
1:A:445:ASN:OD1	1:A:449:SER:OG	2.21	0.55
2:B:785:TYR:O	2:B:967:ARG:NH1	2.32	0.55
1:A:62:ASP:O	1:A:64:ASN:N	2.35	0.55
13:M:241:ARG:O	13:M:245:HIS:ND1	2.35	0.55
22:X:202:PHE:HE1	24:1:32:THR:O	1.89	0.55
29:6:154:ILE:HD13	29:6:197:LYS:NZ	2.22	0.55
30:7:698:ASP:HB2	30:7:701:PHE:HB2	1.89	0.55
2:B:71:LEU:HD21	2:B:436:VAL:HG11	1.88	0.55
2:B:118:ARG:NH2	2:B:202:TYR:OH	2.38	0.55
3:C:73:GLN:NE2	3:C:237:SER:O	2.38	0.55
13:M:34:ILE:HG21	13:M:52:LEU:HD22	1.87	0.55
1:A:908:LEU:HA	1:A:1029:ARG:HH22	1.72	0.55
8:H:112:ILE:HG23	8:H:132:LEU:HD12	1.89	0.55
9:I:54:GLU:HG2	9:I:90:GLN:HB3	1.89	0.55
19:U:30:ILE:HG23	19:U:31:ASP:H	1.71	0.55
1:A:185:TRP:HZ3	1:A:200:ARG:HB2	1.72	0.55
1:A:899:VAL:H	1:A:929:LEU:HD11	1.72	0.55
13:M:274:PRO:HD2	15:O:188:GLU:CG	2.36	0.55
23:0:114:LEU:HD21	23:0:196:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:HD11	1:A:1371:LEU:HD23	1.89	0.55
23:0:36:GLY:HA2	23:0:455:SER:H	1.72	0.55
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.72	0.55
12:L:30:ILE:HB	12:L:57:LEU:HB2	1.88	0.55
15:O:74:VAL:HG21	15:O:136:SER:HB3	1.88	0.55
23:0:575:ASP:OD1	23:0:576:ALA:N	2.40	0.55
24:1:64:GLY:CA	24:1:85:GLN:O	2.53	0.54
2:B:347:LYS:O	2:B:351:TYR:HB2	2.07	0.54
4:D:141:LEU:HD13	7:G:46:LEU:HB3	1.88	0.54
15:O:205:LEU:HB2	15:O:213:VAL:HB	1.90	0.54
14:N:60:DT:H2"	14:N:61:DG:C8	2.42	0.54
2:B:298:LEU:HG	2:B:314:LEU:HD13	1.89	0.54
2:B:211:VAL:O	2:B:480:SER:HA	2.07	0.54
13:M:202:GLU:OE2	13:M:206:THR:OG1	2.24	0.54
1:A:1386:ARG:CZ	18:T:53:DG:H5"	2.37	0.54
2:B:278:GLN:HB2	2:B:337:ARG:HD2	1.88	0.54
9:I:29:CYS:SG	9:I:31:THR:OG1	2.66	0.54
13:M:43:VAL:HG12	13:M:53:SER:HB3	1.90	0.54
30:7:515:ALA:HB1	30:7:692:ARG:NH1	2.23	0.54
2:B:303:TYR:HD1	2:B:571:PRO:HB3	1.73	0.54
7:G:160:ILE:HD11	21:W:137:VAL:HG21	1.90	0.54
23:0:587:ARG:HH11	23:0:615:GLN:HB2	1.73	0.54
1:A:1155:ASP:OD2	1:A:1241:ARG:NH2	2.39	0.54
3:C:6:PRO:HB3	3:C:25:VAL:HG23	1.90	0.54
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.90	0.54
1:A:115:LEU:HD22	1:A:119:ASN:HD22	1.73	0.54
2:B:429:PHE:CZ	16:Q:332:LEU:HB2	2.43	0.54
7:G:47:CYS:SG	7:G:48:VAL:N	2.81	0.54
30:7:691:LEU:HA	30:7:694:LYS:HZ1	1.72	0.54
1:A:588:LEU:HD13	1:A:632:VAL:HG21	1.89	0.53
1:A:1441:PHE:O	6:F:92:ARG:NH1	2.41	0.53
18:T:32:DA:H5"	30:7:440:UNK:CB	2.38	0.53
24:1:22:VAL:HG23	24:1:25:ALA:H	1.74	0.53
1:A:700:ASN:HB2	9:I:98:VAL:HG22	1.91	0.53
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.88	0.53
2:B:923:GLU:HB3	2:B:925:LEU:HG	1.91	0.53
2:B:1106:ARG:HH11	2:B:1126:GLY:HA2	1.74	0.53
2:B:833:TYR:HB2	2:B:840:ILE:HD11	1.90	0.53
5:E:76:GLY:N	5:E:106:GLN:OE1	2.39	0.53
21:W:14:LYS:NZ	21:W:30:ASP:OD1	2.41	0.53
24:1:266:VAL:HG22	24:1:287:PHE:HZ	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:276:THR:HA	13:M:279:VAL:HG12	1.91	0.53
1:A:48:ALA:HB3	1:A:56:PRO:HD3	1.90	0.53
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.90	0.53
10:J:2:ILE:HD13	10:J:57:ILE:HG21	1.90	0.53
2:B:1060:ARG:NH1	3:C:200:GLU:O	2.42	0.53
24:1:44:THR:HA	24:1:65:LYS:HE2	1.91	0.53
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.39	0.53
14:N:77:DA:H2"	14:N:78:DA:O5'	2.09	0.53
14:N:82:DA:H4'	30:7:676:HIS:CE1	2.44	0.53
24:1:283:PHE:O	24:1:287:PHE:CB	2.56	0.53
30:7:407:VAL:HG22	30:7:484:PHE:HB3	1.91	0.53
2:B:1042:GLY:HA2	16:Q:22:ILE:HA	1.90	0.53
17:R:105:THR:HA	17:R:120:TYR:O	2.09	0.53
17:R:127:LYS:HA	17:R:220:HIS:CE1	2.43	0.53
23:0:492:PHE:HE2	23:0:715:SER:HB3	1.73	0.53
16:Q:366:GLU:HB3	16:Q:392:VAL:HG13	1.90	0.53
23:0:322:UNK:C	23:0:380:ARG:HH12	2.21	0.53
26:3:81:GLU:O	26:3:85:ARG:CB	2.57	0.53
15:O:113:ALA:HA	15:O:122:VAL:O	2.09	0.52
20:V:71:PHE:HA	20:V:75:VAL:O	2.09	0.52
23:0:471:ARG:HA	23:0:471:ARG:HH11	1.74	0.52
23:0:601:VAL:HG12	23:0:603:ARG:H	1.74	0.52
23:0:603:ARG:HH12	23:0:628:GLN:HG3	1.73	0.52
2:B:862:GLN:OE1	2:B:957:ASN:ND2	2.42	0.52
23:0:221:ARG:HG2	23:0:225:GLU:OE2	2.09	0.52
29:6:269:GLN:HB3	29:6:274:LYS:NZ	2.23	0.52
2:B:128:LEU:HB2	2:B:168:GLY:O	2.09	0.52
9:I:56:ALA:O	9:I:89:GLN:HG3	2.08	0.52
30:7:490:VAL:HG23	30:7:514:THR:HB	1.92	0.52
1:A:226:GLU:HA	1:A:230:ARG:HE	1.74	0.52
2:B:458:LYS:O	2:B:462:ALA:HB2	2.09	0.52
4:D:51:ASN:HD22	4:D:181:GLY:HA3	1.74	0.52
13:M:199:LYS:O	13:M:201:LYS:N	2.42	0.52
16:Q:366:GLU:O	16:Q:368:GLY:N	2.43	0.52
2:B:342:GLY:O	2:B:344:LYS:N	2.41	0.52
2:B:1091:TYR:HE2	2:B:1093:GLN:HE21	1.58	0.52
5:E:62:ALA:HB3	5:E:78:LEU:HB3	1.90	0.52
30:7:585:PRO:HG3	30:7:759:LEU:HD23	1.91	0.52
1:A:88:LYS:HD3	1:A:89:PRO:HD2	1.92	0.52
1:A:1154:TYR:HE2	9:I:18:GLU:HB2	1.75	0.52
2:B:806:THR:HG23	2:B:1045:SER:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1060:ARG:HH12	3:C:202:PRO:HD3	1.75	0.52
28:5:16:ILE:HD13	28:5:19:LEU:HD12	1.92	0.52
30:7:448:UNK:C	30:7:450:UNK:H	2.23	0.52
2:B:757:PRO:HD3	2:B:983:ARG:HE	1.75	0.51
2:B:55:VAL:HA	2:B:59:LEU:HD13	1.90	0.51
2:B:791:THR:HG22	2:B:792:MET:HG3	1.91	0.51
3:C:100:THR:OG1	3:C:102:GLN:NE2	2.43	0.51
5:E:26:ARG:HH12	5:E:189:GLY:HA3	1.74	0.51
2:B:376:PHE:HD2	2:B:566:LEU:HG	1.75	0.51
2:B:826:ALA:O	2:B:1011:ILE:HA	2.10	0.51
3:C:35:ARG:NH2	11:K:39:ASP:OD2	2.41	0.51
27:4:290:SER:C	27:4:292:CYS:H	2.14	0.51
22:X:193:LEU:HA	22:X:196:LEU:HD12	1.91	0.51
23:0:77:SER:HB3	24:1:337:UNK:HA	1.92	0.51
23:0:208:TYR:HE2	23:0:213:LEU:HB2	1.75	0.51
2:B:345:LYS:HA	2:B:348:ARG:HG2	1.91	0.51
16:Q:334:VAL:HG12	16:Q:335:LEU:H	1.76	0.51
30:7:672:GLN:NE2	30:7:722:ARG:HH12	2.06	0.51
2:B:737:THR:OG1	9:I:66:PRO:O	2.27	0.51
24:1:106:GLN:HB3	24:1:286:ARG:NH1	2.26	0.51
30:7:690:ILE:O	30:7:694:LYS:NZ	2.41	0.51
2:B:771:SER:O	2:B:775:LYS:NZ	2.44	0.51
13:M:280:VAL:HG12	13:M:309:ILE:HA	1.92	0.51
2:B:43:LEU:O	2:B:496:ARG:NH1	2.41	0.51
23:0:194:PHE:HD1	23:0:197:ARG:HH21	1.59	0.51
23:0:250:LEU:HB3	23:0:437:PHE:CE2	2.46	0.51
30:7:576:LYS:HB2	30:7:576:LYS:NZ	2.26	0.51
1:A:534:LEU:HD11	1:A:577:ILE:HD11	1.93	0.51
1:A:840:ARG:O	1:A:844:ALA:HB2	2.11	0.51
2:B:22:SER:O	2:B:654:ARG:NH2	2.44	0.51
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.93	0.51
3:C:19:ASP:HB2	3:C:231:ASN:HD22	1.76	0.51
11:K:61:TYR:HA	11:K:72:LYS:O	2.11	0.51
15:O:115:ILE:HD13	15:O:143:ILE:HD11	1.92	0.51
28:5:54:LEU:HA	28:5:57:LEU:HG	1.93	0.51
2:B:102:VAL:O	2:B:109:THR:HA	2.12	0.51
15:O:206:ILE:HD13	15:O:234:LEU:HD21	1.93	0.51
23:0:106:LEU:HD11	23:0:196:VAL:HG22	1.93	0.51
30:7:373:MET:SD	30:7:373:MET:N	2.84	0.51
25:2:459:TYR:OH	25:2:498:ASN:OD1	2.21	0.50
9:I:55:THR:HG22	9:I:100:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:466:LEU:H	23:0:466:LEU:HD23	1.75	0.50
1:A:63:ARG:HA	1:A:74:MET:HG2	1.92	0.50
2:B:755:ILE:O	2:B:983:ARG:NE	2.45	0.50
3:C:222:LYS:H	3:C:222:LYS:HD3	1.76	0.50
30:7:656:LYS:HZ1	30:7:686:ARG:HH21	1.56	0.50
1:A:752:LYS:HG3	2:B:1015:HIS:HB3	1.92	0.50
8:H:142:LEU:HG	8:H:144:ILE:HD11	1.92	0.50
21:W:99:LYS:HG2	21:W:186:LEU:HD13	1.92	0.50
1:A:553:VAL:HB	1:A:556:TRP:HB2	1.92	0.50
2:B:641:GLU:HB2	2:B:652:LYS:HE2	1.93	0.50
9:I:54:GLU:HA	9:I:90:GLN:N	2.21	0.50
1:A:1020:CYS:SG	1:A:1023:ARG:NH2	2.85	0.50
2:B:413:LEU:HD21	2:B:461:LEU:HD11	1.93	0.50
20:V:62:VAL:HG22	20:V:85:VAL:HG22	1.92	0.50
1:A:864:ILE:HG22	1:A:865:GLN:HG3	1.93	0.50
1:A:1116:LEU:HD11	1:A:1311:VAL:HG23	1.94	0.50
9:I:86:PHE:O	9:I:100:PHE:HB2	2.12	0.50
15:O:202:ILE:HD11	15:O:222:GLU:HB3	1.94	0.50
16:Q:119:LEU:HD12	17:R:133:TYR:HB2	1.93	0.50
7:G:111:THR:HB	7:G:114:LEU:HD13	1.92	0.50
8:H:8:ASP:OD1	8:H:9:ILE:N	2.44	0.50
24:1:351:UNK:O	24:1:353:UNK:N	2.45	0.50
1:A:961:ARG:NH1	1:A:1035:TYR:OH	2.44	0.50
1:A:984:LYS:O	1:A:988:LEU:HB2	2.12	0.50
7:G:95:SER:OG	7:G:98:GLY:O	2.23	0.50
13:M:187:ARG:HH11	13:M:241:ARG:HH21	1.59	0.50
15:O:93:GLU:OE2	15:O:105:ARG:NH1	2.45	0.50
23:0:372:LYS:N	23:0:373:PRO:HD3	2.27	0.50
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.94	0.49
5:E:56:LYS:NZ	5:E:84:ASP:OD2	2.43	0.49
17:R:73:LEU:HD23	17:R:78:ALA:HA	1.92	0.49
29:6:133:SER:H	29:6:136:MET:HG2	1.76	0.49
30:7:548:HIS:HB2	30:7:697:ASN:HA	1.93	0.49
6:F:82:THR:HG22	6:F:84:TYR:H	1.76	0.49
16:Q:352:MET:HG3	16:Q:361:TRP:HB2	1.94	0.49
2:B:63:ILE:O	2:B:67:SER:HB3	2.13	0.49
2:B:766:ARG:HE	2:B:1020:ARG:HB3	1.77	0.49
17:R:263:MET:O	17:R:266:THR:OG1	2.28	0.49
21:W:24:SER:HA	21:W:27:LEU:HD22	1.94	0.49
1:A:1029:ARG:O	1:A:1033:GLN:HB3	2.12	0.49
1:A:1386:ARG:NH2	18:T:53:DG:H5”	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.94	0.49
14:N:33:DT:O2	18:T:75:DG:N2	2.46	0.49
23:0:432:ASN:O	23:0:434:ILE:HG13	2.12	0.49
2:B:402:GLY:O	2:B:405:ARG:NH1	2.41	0.49
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.93	0.49
30:7:551:ASN:O	30:7:703:ALA:HB3	2.12	0.49
1:A:1191:TRP:CZ3	9:I:43:VAL:HG21	2.48	0.49
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.12	0.49
2:B:87:LYS:HB2	2:B:137:TYR:HB2	1.93	0.49
3:C:185:LYS:HE2	3:C:213:PRO:HB3	1.93	0.49
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.93	0.49
1:A:1199:ARG:NH1	1:A:1233:ASP:O	2.45	0.49
16:Q:363:GLY:HA2	16:Q:395:PHE:HA	1.95	0.49
21:W:77:PRO:O	21:W:79:SER:N	2.46	0.49
24:1:276:LYS:H	24:1:276:LYS:HD3	1.77	0.49
29:6:154:ILE:HD13	29:6:197:LYS:HZ2	1.78	0.49
30:7:691:LEU:HA	30:7:694:LYS:NZ	2.27	0.49
1:A:869:GLY:HA3	1:A:1366:ARG:HD2	1.93	0.49
2:B:226:PHE:HD1	2:B:395:GLN:HE21	1.60	0.49
9:I:14:LEU:HA	9:I:28:GLU:O	2.13	0.49
19:U:283:ALA:HB1	20:V:66:LEU:HB2	1.94	0.49
24:1:306:UNK:O	24:1:307:UNK:CB	2.60	0.49
1:A:495:GLU:OE1	1:A:495:GLU:N	2.46	0.49
1:A:597:LEU:HD13	8:H:103:LYS:HD3	1.94	0.49
2:B:793:ALA:O	2:B:855:PHE:HA	2.13	0.49
22:X:273:GLU:HG2	22:X:276:ARG:HH11	1.77	0.49
26:3:45:ARG:O	26:3:49:LEU:HG	2.12	0.49
1:A:446:ARG:O	1:A:449:SER:OG	2.31	0.49
1:A:526:ASP:OD1	2:B:1015:HIS:ND1	2.45	0.49
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.95	0.49
14:N:24:DT:H2"	14:N:25:DA:N7	2.27	0.49
28:5:33:GLU:HB2	28:5:41:LEU:HB3	1.95	0.49
1:A:63:ARG:HH11	13:M:57:VAL:HG22	1.76	0.48
1:A:966:ASN:O	1:A:970:THR:OG1	2.25	0.48
6:F:133:VAL:HA	6:F:147:SER:HA	1.95	0.48
8:H:89:LEU:HG	8:H:90:ALA:H	1.78	0.48
9:I:19:ASP:CB	9:I:24:ARG:O	2.60	0.48
11:K:32:VAL:HG22	11:K:74:ARG:HG2	1.94	0.48
14:N:78:DA:H4'	14:N:79:DA:OP1	2.13	0.48
16:Q:381:ASP:OD1	16:Q:382:GLY:N	2.42	0.48
17:R:73:LEU:HD23	17:R:78:ALA:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:4:290:SER:N	27:4:292:CYS:SG	2.86	0.48
11:K:24:ASP:HB2	11:K:32:VAL:HG23	1.95	0.48
4:D:54:GLU:HB2	4:D:160:VAL:HG11	1.95	0.48
8:H:26:ILE:HG13	8:H:42:ILE:HD12	1.95	0.48
18:T:30:DT:H2"	18:T:31:DT:C7	2.38	0.48
30:7:553:GLN:HB2	30:7:703:ALA:O	2.13	0.48
1:A:69:THR:HG23	1:A:80:HIS:NE2	2.28	0.48
2:B:810:GLU:HB2	2:B:815:ARG:HH12	1.79	0.48
2:B:931:TYR:O	2:B:933:SER:N	2.43	0.48
15:O:95:ASN:N	15:O:95:ASN:OD1	2.47	0.48
31:Z:22:UNK:O	31:Z:26:UNK:CB	2.62	0.48
13:M:267:LYS:HG3	13:M:268:GLU:H	1.78	0.48
23:0:323:UNK:CB	23:0:380:ARG:HH22	2.26	0.48
13:M:118:VAL:HG22	13:M:124:ASN:ND2	2.28	0.48
23:0:234:PHE:HB3	23:0:237:ALA:HB2	1.95	0.48
23:0:322:UNK:CA	23:0:380:ARG:HH12	2.27	0.48
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.79	0.48
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.95	0.48
15:O:214:LEU:HD22	15:O:223:ILE:HG23	1.96	0.48
21:W:118:GLU:HB2	26:3:49:LEU:HD22	1.96	0.48
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.95	0.47
18:T:46:DC:H2"	18:T:47:DA:C8	2.49	0.47
21:W:176:MET:HA	21:W:179:ILE:HG22	1.95	0.47
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.96	0.47
2:B:445:LYS:NZ	17:R:267:GLY:O	2.36	0.47
1:A:139:TRP:HH2	14:N:60:DT:OP1	1.98	0.47
2:B:70:ILE:HG22	2:B:89:GLU:HG3	1.97	0.47
15:O:171:ARG:HB2	15:O:237:PHE:HB3	1.96	0.47
1:A:864:ILE:HG12	1:A:1374:VAL:HG22	1.97	0.47
2:B:458:LYS:O	2:B:462:ALA:CB	2.63	0.47
16:Q:102:PRO:HA	17:R:94:LYS:HA	1.97	0.47
17:R:69:TRP:CD1	17:R:219:CYS:HB3	2.49	0.47
23:0:156:CYS:SG	23:0:157:GLU:N	2.87	0.47
29:6:251:ILE:HG12	29:6:276:LEU:HD13	1.95	0.47
2:B:861:ASP:OD1	2:B:862:GLN:N	2.48	0.47
5:E:156:LEU:HD11	5:E:197:LYS:HB2	1.96	0.47
23:0:259:ARG:HG2	23:0:262:ARG:HH21	1.78	0.47
1:A:481:ASP:OD2	1:A:483:ASP:OD2	2.31	0.47
5:E:179:GLN:HG2	5:E:181:ALA:H	1.78	0.47
13:M:312:GLY:O	13:M:316:LEU:HB2	2.14	0.47
17:R:122:LEU:HD21	17:R:222:CYS:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:257:LEU:HD13	23:0:343:LYS:HG2	1.96	0.47
26:3:47:PHE:HB2	26:3:65:LYS:HG2	1.96	0.47
30:7:608:PHE:HE2	30:7:670:LEU:HB3	1.79	0.47
1:A:381:THR:HG23	1:A:383:TYR:H	1.78	0.47
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.96	0.47
2:B:398:ARG:H	2:B:398:ARG:HD2	1.80	0.47
20:V:60:LEU:HA	20:V:86:THR:O	2.15	0.47
21:W:74:GLU:CB	21:W:82:VAL:O	2.63	0.47
23:0:417:LEU:O	23:0:438:THR:HB	2.14	0.47
30:7:495:ALA:HB3	30:7:498:PHE:CD1	2.50	0.47
7:G:123:ALA:HA	7:G:128:PRO:HB3	1.97	0.47
9:I:54:GLU:CG	9:I:88:SER:OG	2.62	0.47
11:K:17:SER:H	11:K:20:LYS:HZ1	1.62	0.47
25:2:453:THR:HG22	28:5:10:VAL:HG22	1.95	0.47
28:5:55:ASN:HA	28:5:58:LEU:HG	1.96	0.47
1:A:58:LEU:HA	1:A:80:HIS:HB2	1.96	0.47
2:B:810:GLU:HG3	2:B:815:ARG:HH22	1.79	0.47
21:W:117:SER:O	26:3:49:LEU:HD13	2.14	0.47
30:7:410:LEU:HB3	30:7:457:TYR:CZ	2.50	0.47
9:I:88:SER:O	9:I:91:ARG:NH1	2.47	0.47
15:O:94:TYR:CZ	15:O:96:PRO:HG3	2.50	0.47
16:Q:402:ALA:O	16:Q:403:THR:HG23	2.15	0.47
1:A:990:VAL:HG12	1:A:994:GLN:HE21	1.80	0.46
2:B:336:ARG:HD2	2:B:348:ARG:NH1	2.30	0.46
4:D:123:LEU:HD21	4:D:146:GLN:HA	1.97	0.46
31:Z:30:UNK:C	31:Z:41:UNK:CB	2.93	0.46
1:A:471:ASN:OD1	1:A:472:LEU:N	2.48	0.46
1:A:882:SER:O	1:A:1025:ARG:NH2	2.43	0.46
6:F:76:LYS:HA	6:F:79:ARG:HE	1.79	0.46
30:7:406:SER:HA	30:7:451:UNK:CB	2.45	0.46
1:A:806:ARG:HD2	2:B:728:ARG:HA	1.97	0.46
2:B:194:GLU:HA	2:B:784:ASN:HD22	1.80	0.46
2:B:364:ILE:HG22	2:B:365:THR:HG22	1.96	0.46
7:G:44:TYR:OH	7:G:157:ILE:O	2.28	0.46
17:R:97:ILE:HA	17:R:104:ILE:HG22	1.97	0.46
28:5:8:ALA:HB3	28:5:42:VAL:O	2.15	0.46
30:7:534:LYS:HD2	30:7:537:GLU:OE2	2.15	0.46
2:B:363:HIS:CD2	2:B:364:ILE:HG13	2.49	0.46
30:7:565:PHE:HE2	30:7:763:VAL:HG21	1.81	0.46
30:7:659:ASP:HB3	30:7:686:ARG:HG3	1.96	0.46
1:A:308:ILE:HG23	1:A:311:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:63:ARG:C	17:R:65:ASN:H	2.18	0.46
18:T:48:DC:C2	18:T:49:DA:C8	3.04	0.46
20:V:72:CYS:O	20:V:75:VAL:HB	2.15	0.46
10:J:17:LYS:HB3	10:J:39:LEU:HD13	1.96	0.46
18:T:71:DC:H2"	18:T:72:DA:C8	2.50	0.46
22:X:218:ASP:HA	22:X:221:ILE:HD12	1.97	0.46
26:3:44:ASP:O	26:3:48:SER:OG	2.23	0.46
28:5:13:ASP:OD1	28:5:15:SER:OG	2.23	0.46
1:A:596:THR:HG22	1:A:597:LEU:H	1.80	0.46
1:A:1012:ARG:HH21	1:A:1015:VAL:HG11	1.81	0.46
2:B:933:SER:OG	2:B:934:LYS:N	2.49	0.46
2:B:1004:GLU:OE1	2:B:1064:TYR:OH	2.27	0.46
14:N:21:DG:H1'	14:N:22:DT:H5'	1.98	0.46
23:0:494:PRO:HB2	23:0:699:GLN:HE22	1.80	0.46
1:A:561:PRO:HB2	1:A:576:GLN:HE21	1.80	0.46
2:B:634:TYR:HA	2:B:694:ASP:HA	1.98	0.46
2:B:1172:ILE:HD11	2:B:1183:LYS:HD2	1.98	0.46
9:I:54:GLU:HB3	9:I:88:SER:CB	2.46	0.46
18:T:40:DA:H2"	18:T:41:DC:H5'	1.97	0.46
23:0:133:CYS:HA	49:0:901:SF4:S4	2.56	0.46
23:0:564:TRP:O	23:0:566:HIS:N	2.40	0.46
30:7:495:ALA:HB3	30:7:498:PHE:HD1	1.80	0.46
1:A:563:PRO:HG2	1:A:566:ILE:HG13	1.98	0.46
2:B:301:ILE:O	2:B:383:ASN:ND2	2.49	0.46
23:0:372:LYS:HD3	23:0:375:ARG:NH1	2.31	0.46
1:A:993:LEU:HD13	1:A:1046:LEU:HD22	1.98	0.46
19:U:38:LEU:O	19:U:42:TRP:HB2	2.15	0.46
21:W:18:ARG:CZ	22:X:250:GLY:H	2.28	0.46
30:7:719:SER:O	30:7:723:GLN:HG2	2.16	0.46
1:A:855:THR:HG21	1:A:857:ARG:HH21	1.81	0.45
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.81	0.45
2:B:824:ILE:HD13	2:B:1089:PRO:HB3	1.98	0.45
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.98	0.45
25:2:466:GLN:OE1	25:2:466:GLN:N	2.47	0.45
18:T:33:DT:OP1	30:7:467:UNK:CB	2.64	0.45
23:0:70:ILE:HB	23:0:232:VAL:HA	1.96	0.45
26:3:72:ILE:H	26:3:72:ILE:HG13	1.62	0.45
30:7:554:CYS:HB2	30:7:733:PHE:HA	1.97	0.45
1:A:53:LEU:HD21	1:A:267:ALA:HB2	1.99	0.45
2:B:314:LEU:O	2:B:318:VAL:HG23	2.16	0.45
7:G:21:ARG:HG3	7:G:25:TYR:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:HIS:HA	1:A:607:ILE:O	2.16	0.45
4:D:158:GLU:OE1	4:D:158:GLU:N	2.41	0.45
14:N:61:DG:C2	18:T:47:DA:C2	3.05	0.45
23:0:652:ASP:O	23:0:656:PHE:HB3	2.16	0.45
24:1:45:ILE:HD12	24:1:62:LEU:HB3	1.97	0.45
21:W:171:LYS:O	21:W:175:LEU:HB2	2.16	0.45
23:0:171:LEU:HD22	23:0:199:MET:HG2	1.99	0.45
29:6:427:TYR:O	29:6:435:GLU:HA	2.16	0.45
1:A:92:HIS:O	1:A:96:ILE:HG13	2.17	0.45
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.52	0.45
2:B:249:ARG:HG2	2:B:415:GLN:NE2	2.29	0.45
2:B:924:GLU:H	2:B:928:ARG:HD2	1.79	0.45
6:F:135:ARG:HA	6:F:144:GLU:O	2.16	0.45
9:I:83:ASN:HA	9:I:104:LEU:HG	1.99	0.45
24:1:107:ILE:HD12	24:1:110:ARG:HH11	1.81	0.45
30:7:573:THR:HA	30:7:577:ARG:HD2	1.97	0.45
1:A:463:ILE:HD12	1:A:464:PRO:O	2.17	0.45
2:B:290:GLY:HA2	2:B:327:ARG:HD2	1.98	0.45
2:B:737:THR:HB	9:I:66:PRO:CB	2.47	0.45
12:L:43:THR:HG22	12:L:43:THR:O	2.16	0.45
21:W:24:SER:HA	21:W:27:LEU:HB2	1.98	0.45
1:A:1146:VAL:HG11	1:A:1207:LEU:CD1	2.47	0.45
2:B:238:ALA:HB2	2:B:385:LEU:HD13	1.99	0.45
14:N:79:DA:H1'	14:N:80:DA:H5'	1.98	0.45
16:Q:379:GLU:OE2	16:Q:383:SER:OG	2.35	0.45
21:W:179:ILE:HD12	21:W:182:ILE:HD12	1.97	0.45
30:7:561:MET:SD	30:7:584:ASN:ND2	2.90	0.45
7:G:23:LYS:O	7:G:26:LEU:HB2	2.16	0.45
25:2:462:PHE:HE1	25:2:471:LEU:HD12	1.82	0.45
30:7:556:GLU:HG2	30:7:707:SER:HB3	1.98	0.45
1:A:350:ARG:HA	1:A:487:MET:O	2.17	0.45
1:A:439:ASN:HA	1:A:459:ARG:HG3	1.99	0.45
7:G:165:GLU:HG2	26:3:65:LYS:NZ	2.31	0.45
8:H:5:LEU:HD22	8:H:134:ASN:HB3	1.99	0.45
23:0:106:LEU:HD22	23:0:199:MET:HB3	1.99	0.45
23:0:215:ASP:H	23:0:219:ALA:HB2	1.81	0.45
16:Q:352:MET:CG	16:Q:361:TRP:HB2	2.47	0.44
17:R:133:TYR:CD1	17:R:217:THR:HG22	2.52	0.44
30:7:392:LYS:HD3	30:7:513:LEU:HB3	2.00	0.44
2:B:859:TYR:OH	2:B:945:GLU:OE1	2.35	0.44
15:O:76:LEU:HD13	15:O:143:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:202:ILE:HG13	15:O:226:ALA:HB2	1.98	0.44
15:O:227:PHE:HA	15:O:230:ILE:HG22	1.99	0.44
16:Q:376:LEU:CD2	16:Q:386:MET:HE3	2.44	0.44
20:V:61:THR:HB	20:V:86:THR:HB	1.98	0.44
21:W:169:GLN:NE2	21:W:173:ASN:OD1	2.45	0.44
23:0:196:VAL:O	23:0:200:ILE:HG12	2.17	0.44
24:1:263:TYR:HB2	24:1:266:VAL:HG23	1.98	0.44
1:A:104:GLU:OE1	1:A:139:TRP:NE1	2.47	0.44
1:A:367:PRO:HD2	1:A:370:ILE:HD12	1.98	0.44
2:B:663:ALA:O	2:B:667:GLN:HB2	2.17	0.44
29:6:176:ASN:HA	29:6:206:GLY:HA3	2.00	0.44
20:V:23:LEU:HD13	20:V:37:ALA:HB1	1.99	0.44
21:W:152:CYS:O	21:W:154:GLU:HG3	2.17	0.44
1:A:481:ASP:C	1:A:483:ASP:OD1	2.56	0.44
2:B:499:ASN:OD1	2:B:500:THR:N	2.50	0.44
28:5:62:ILE:HA	30:7:717:TYR:CZ	2.53	0.44
2:B:281:PRO:HD2	2:B:284:ILE:HD12	2.00	0.44
2:B:412:LEU:HB3	2:B:466:TRP:CE2	2.53	0.44
13:M:44:VAL:HG22	13:M:51:VAL:HA	2.00	0.44
13:M:166:LYS:HB3	13:M:170:SER:HB3	2.00	0.44
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.00	0.44
13:M:262:LYS:O	13:M:266:ILE:HG13	2.17	0.44
18:T:75:DG:H1'	18:T:76:DC:H5'	1.98	0.44
23:0:168:GLU:HA	23:0:199:MET:HE2	2.00	0.44
29:6:262:LYS:HE2	29:6:264:LEU:HD21	1.99	0.44
1:A:1051:ALA:O	1:A:1055:ARG:HG2	2.18	0.44
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.00	0.44
6:F:123:LYS:NZ	6:F:127:GLU:OE2	2.51	0.44
14:N:72:DA:H5'	14:N:72:DA:C8	2.53	0.44
19:U:260:CYS:HB2	19:U:281:VAL:HB	1.99	0.44
1:A:362:ASP:OD2	1:A:459:ARG:NH1	2.51	0.43
1:A:882:SER:OG	1:A:953:ASN:ND2	2.51	0.43
4:D:63:LEU:HD13	4:D:130:LEU:HD13	1.99	0.43
7:G:102:GLN:HE22	7:G:107:LYS:HE2	1.83	0.43
14:N:73:DC:H2"	14:N:74:DA:C8	2.52	0.43
23:0:197:ARG:HG3	23:0:221:ARG:NH1	2.33	0.43
1:A:116:ASP:OD1	1:A:117:GLU:N	2.43	0.43
1:A:339:ASN:HB3	2:B:1199:ALA:HB1	2.00	0.43
1:A:351:THR:O	1:A:486:GLU:HA	2.18	0.43
1:A:1035:TYR:HB3	1:A:1037:LEU:HG	2.01	0.43
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:954:VAL:HG11	2:B:962:LYS:HE3	1.98	0.43
9:I:54:GLU:CA	9:I:88:SER:OG	2.66	0.43
14:N:69:DC:H2"	14:N:70:DA:C8	2.53	0.43
14:N:83:DT:H2"	14:N:84:DC:C5	2.54	0.43
21:W:99:LYS:HE3	22:X:278:LEU:HD13	2.00	0.43
30:7:459:MET:O	30:7:462:ASN:ND2	2.51	0.43
1:A:405:VAL:HG13	1:A:432:VAL:HG22	2.01	0.43
1:A:407:ARG:HH11	1:A:413:ILE:HD11	1.83	0.43
13:M:198:VAL:HG12	13:M:198:VAL:O	2.18	0.43
13:M:267:LYS:CG	13:M:268:GLU:H	2.31	0.43
14:N:60:DT:H2"	14:N:61:DG:H8	1.81	0.43
19:U:9:VAL:HG13	20:V:51:THR:HG21	1.99	0.43
30:7:608:PHE:CG	30:7:686:ARG:NH1	2.87	0.43
1:A:925:LEU:HD22	1:A:983:ILE:HB	2.01	0.43
2:B:223:VAL:HG22	2:B:240:ILE:HD12	1.99	0.43
13:M:325:ASP:HB3	13:M:326:PRO:HD3	2.00	0.43
14:N:77:DA:H4'	14:N:78:DA:OP1	2.18	0.43
19:U:267:VAL:HG12	19:U:269:ILE:HG13	2.01	0.43
23:0:232:VAL:HB	23:0:456:VAL:HG13	1.99	0.43
23:0:432:ASN:O	23:0:434:ILE:N	2.52	0.43
30:7:495:ALA:O	30:7:499:ARG:HG2	2.18	0.43
1:A:377:PRO:HB3	1:A:433:GLU:HG2	2.00	0.43
1:A:1146:VAL:HG11	1:A:1207:LEU:HD12	2.00	0.43
13:M:171:ILE:H	13:M:171:ILE:HG13	1.66	0.43
14:N:74:DA:H1'	14:N:75:DT:H5"	2.00	0.43
23:0:217:LYS:NZ	23:0:218:ILE:HD11	2.34	0.43
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.99	0.43
2:B:376:PHE:HE2	2:B:567:GLU:HA	1.84	0.43
7:G:97:HIS:O	7:G:112:LYS:N	2.51	0.43
17:R:258:THR:O	17:R:260:GLY:N	2.42	0.43
30:7:382:GLY:HA3	30:7:535:LEU:HG	2.00	0.43
1:A:167:CYS:SG	1:A:168:GLY:N	2.92	0.43
1:A:546:VAL:HG21	1:A:572:TRP:HB2	1.99	0.43
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.53	0.43
7:G:143:ILE:HG13	7:G:170:ALA:HA	2.01	0.43
8:H:5:LEU:HD11	8:H:61:SER:HB3	2.00	0.43
13:M:187:ARG:NH1	13:M:241:ARG:HH21	2.17	0.43
23:0:416:PHE:CE2	23:0:437:PHE:HB2	2.54	0.43
1:A:113:LEU:HD11	1:A:218:ASP:HA	2.01	0.43
2:B:276:ILE:HA	2:B:338:GLY:HA3	1.99	0.43
2:B:1058:LEU:O	2:B:1062:HIS:ND1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1074:ASN:OD1	2:B:1075:GLY:N	2.52	0.43
8:H:64:ASN:OD1	8:H:65:LEU:N	2.52	0.43
19:U:253:ARG:HD2	19:U:258:TRP:CZ2	2.54	0.43
30:7:515:ALA:HB1	30:7:692:ARG:HH12	1.83	0.43
5:E:144:ILE:H	5:E:144:ILE:HG13	1.71	0.43
17:R:262:THR:O	17:R:266:THR:HG23	2.19	0.43
18:T:80:DT:H6	18:T:80:DT:H2'	1.70	0.43
24:1:266:VAL:O	24:1:270:TYR:HB2	2.19	0.43
25:2:480:VAL:HG11	25:2:497:GLY:HA3	2.00	0.43
26:3:44:ASP:O	26:3:48:SER:CB	2.67	0.43
30:7:387:PRO:HB3	30:7:692:ARG:HD3	2.01	0.43
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.00	0.43
1:A:697:ALA:HB1	9:I:97:MET:HE3	2.01	0.43
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.84	0.43
16:Q:388:PRO:HB2	17:R:82:ARG:NH1	2.34	0.43
1:A:849:MET:SD	1:A:849:MET:N	2.92	0.42
1:A:1386:ARG:NH1	18:T:53:DG:H5"	2.34	0.42
12:L:38:LEU:HD23	12:L:40:LEU:HD23	2.01	0.42
15:O:199:LYS:HA	15:O:200:PRO:HA	1.85	0.42
1:A:372:LYS:HA	1:A:435:HIS:HD2	1.84	0.42
14:N:17:DC:H1'	14:N:18:DT:H5'	2.01	0.42
17:R:105:THR:OG1	17:R:106:LEU:N	2.52	0.42
1:A:1260:LEU:O	1:A:1264:GLU:HG3	2.19	0.42
3:C:262:LEU:HD22	11:K:87:LEU:HD23	2.01	0.42
14:N:33:DT:C2	18:T:75:DG:N2	2.87	0.42
15:O:94:TYR:O	20:V:71:PHE:HD2	2.02	0.42
28:5:44:PRO:HA	28:5:47:VAL:HG23	2.01	0.42
1:A:148:CYS:O	1:A:168:GLY:HA2	2.19	0.42
1:A:362:ASP:O	1:A:458:HIS:ND1	2.51	0.42
1:A:375:THR:HB	1:A:403:LYS:HD3	2.00	0.42
1:A:443:LEU:HD21	1:A:501:LEU:HD11	2.00	0.42
9:I:103:CYS:SG	9:I:105:SER:OG	2.71	0.42
13:M:268:GLU:C	13:M:270:ALA:H	2.23	0.42
15:O:108:GLU:HA	15:O:109:PRO:HA	1.87	0.42
18:T:24:DA:H2'	18:T:25:DT:H71	2.02	0.42
1:A:913:LEU:HD11	1:A:919:ILE:HG13	2.02	0.42
2:B:186:GLU:OE2	10:J:62:ARG:NH1	2.52	0.42
2:B:474:SER:O	2:B:476:ARG:N	2.52	0.42
2:B:487:THR:HG23	2:B:490:SER:H	1.85	0.42
13:M:142:LEU:HD23	13:M:146:VAL:HG11	2.01	0.42
18:T:93:DT:H2"	18:T:94:DG:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:VAL:O	2:B:287:ARG:HG2	2.19	0.42
7:G:98:GLY:HA3	7:G:110:VAL:O	2.20	0.42
14:N:43:DT:H2"	14:N:44:DC:H5'	2.01	0.42
18:T:33:DT:H2"	18:T:34:DG:C8	2.55	0.42
30:7:372:LYS:HB3	30:7:380:ARG:HH12	1.85	0.42
30:7:379:ALA:H	30:7:508:HIS:CE1	2.37	0.42
1:A:74:MET:O	2:B:1116:ARG:NH2	2.48	0.42
2:B:884:ARG:HG3	2:B:935:ARG:HE	1.84	0.42
2:B:950:ASP:HB2	2:B:969:ARG:HG2	2.02	0.42
14:N:80:DA:OP2	30:7:495:ALA:HB2	2.20	0.42
23:0:114:LEU:HA	23:0:182:LEU:HD21	2.01	0.42
24:1:30:ARG:HA	24:1:37:VAL:HG12	2.02	0.42
2:B:279:ASP:OD1	2:B:279:ASP:N	2.50	0.42
2:B:451:LYS:O	2:B:455:SER:HB2	2.20	0.42
14:N:43:DT:C1'	14:N:44:DC:H5'	2.50	0.42
21:W:9:VAL:HG22	21:W:189:ILE:HD13	2.01	0.42
21:W:77:PRO:C	21:W:79:SER:H	2.23	0.42
28:5:7:GLY:HA3	28:5:41:LEU:HD11	2.01	0.42
6:F:97:ARG:NE	6:F:124:GLU:OE1	2.39	0.42
8:H:7:ASP:OD1	8:H:58:THR:OG1	2.37	0.42
14:N:10:DT:H2"	14:N:11:DA:N7	2.35	0.42
15:O:151:LYS:HG2	15:O:153:THR:HG23	2.02	0.42
23:0:372:LYS:N	23:0:373:PRO:CD	2.83	0.42
1:A:54:ASN:OD1	1:A:54:ASN:N	2.52	0.41
3:C:19:ASP:HA	3:C:231:ASN:HA	2.01	0.41
6:F:146:TRP:HB3	6:F:151:LEU:HD21	2.02	0.41
14:N:61:DG:H2"	14:N:62:DT:C6	2.55	0.41
23:0:635:LEU:O	23:0:639:LEU:CB	2.62	0.41
23:0:692:GLN:HG3	23:0:693:LEU:HG	2.01	0.41
27:4:226:GLN:O	27:4:230:ALA:CB	2.68	0.41
29:6:211:GLN:HE22	29:6:245:GLY:C	2.23	0.41
1:A:1022:LEU:O	1:A:1026:LEU:HB2	2.20	0.41
7:G:83:LYS:HG2	7:G:149:GLY:HA2	2.01	0.41
30:7:497:MET:HG3	30:7:498:PHE:N	2.35	0.41
6:F:136:ARG:O	6:F:143:PHE:HA	2.21	0.41
21:W:26:VAL:HA	21:W:29:LEU:HB3	2.01	0.41
23:0:621:LEU:HA	23:0:680:VAL:HG23	2.02	0.41
1:A:53:LEU:HD23	1:A:263:THR:HG22	2.03	0.41
1:A:230:ARG:HB2	1:A:233:TRP:CG	2.55	0.41
1:A:1191:TRP:CZ3	1:A:1257:ASP:HB3	2.55	0.41
3:C:68:GLY:HA3	12:L:69:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:80:DA:H1'	14:N:81:DT:H5'	2.02	0.41
16:Q:376:LEU:HB2	17:R:69:TRP:HB2	2.01	0.41
1:A:348:SER:HB2	2:B:1128:LEU:HD12	2.01	0.41
2:B:54:PHE:O	2:B:58:THR:HB	2.21	0.41
2:B:793:ALA:HB3	2:B:856:PHE:HB2	2.02	0.41
13:M:269:ILE:HG23	13:M:272:LYS:HE3	2.03	0.41
14:N:35:DT:H2"	14:N:36:DG:C8	2.56	0.41
21:W:44:LYS:NZ	21:W:49:ILE:O	2.50	0.41
30:7:410:LEU:HB3	30:7:457:TYR:CE1	2.56	0.41
1:A:663:SER:OG	2:B:1084:GLN:O	2.25	0.41
2:B:70:ILE:HG21	16:Q:335:LEU:HD21	2.01	0.41
2:B:70:ILE:HG12	16:Q:335:LEU:HD21	2.03	0.41
2:B:778:MET:HA	2:B:1096:ARG:HH12	1.86	0.41
2:B:895:ASP:OD2	12:L:42:ARG:NH2	2.54	0.41
7:G:122:ASN:HB3	7:G:129:SER:O	2.21	0.41
16:Q:139:LEU:HD23	17:R:212:THR:HG21	2.03	0.41
23:0:198:ARG:HA	23:0:198:ARG:HH11	1.86	0.41
30:7:582:ILE:HG23	30:7:673:ILE:HG22	2.03	0.41
30:7:609:SER:HB2	30:7:615:LEU:HD13	2.02	0.41
2:B:1171:VAL:HG22	2:B:1182:CYS:HB2	2.03	0.41
5:E:136:ASN:OD1	5:E:137:GLU:N	2.54	0.41
11:K:58:PHE:HB3	11:K:76:GLN:HB3	2.01	0.41
13:M:171:ILE:HD12	13:M:172:MET:HG3	2.03	0.41
13:M:268:GLU:OE1	13:M:319:HIS:NE2	2.38	0.41
16:Q:378:VAL:HG22	16:Q:384:PHE:CD1	2.56	0.41
18:T:96:DT:H6	18:T:96:DT:H2'	1.73	0.41
23:0:492:PHE:CE2	23:0:715:SER:HB3	2.53	0.41
30:7:519:ARG:HE	30:7:682:GLN:HE22	1.67	0.41
1:A:481:ASP:N	1:A:481:ASP:OD1	2.52	0.41
1:A:481:ASP:CG	1:A:483:ASP:OD1	2.59	0.41
2:B:910:VAL:HA	2:B:940:PRO:HA	2.01	0.41
2:B:1183:LYS:HE3	2:B:1183:LYS:HB3	1.83	0.41
6:F:76:LYS:HB3	6:F:79:ARG:HH21	1.85	0.41
1:A:1194:ARG:HA	1:A:1238:ILE:O	2.20	0.41
2:B:259:TYR:HE1	2:B:270:LYS:HB2	1.85	0.41
4:D:165:GLN:HE21	4:D:165:GLN:HB3	1.68	0.41
5:E:124:VAL:H	5:E:125:PRO:HD2	1.85	0.41
7:G:93:SER:OG	7:G:100:GLU:OE1	2.39	0.41
9:I:55:THR:CG2	9:I:100:PHE:CE2	3.03	0.41
13:M:186:ALA:HB1	13:M:238:TYR:CZ	2.56	0.41
15:O:71:VAL:HG13	15:O:124:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:264:ASP:OD1	19:U:277:GLN:NE2	2.54	0.41
20:V:61:THR:O	20:V:85:VAL:HA	2.21	0.41
23:0:259:ARG:HH22	23:0:397:THR:HB	1.85	0.41
23:0:655:SER:O	23:0:659:MET:HB2	2.20	0.41
25:2:483:TRP:CZ2	28:5:35:LEU:HB3	2.55	0.41
1:A:1420:ASP:OD1	1:A:1420:ASP:N	2.54	0.41
2:B:1135:ARG:HG3	2:B:1147:LEU:HD11	2.03	0.41
21:W:140:LEU:HD22	21:W:147:PHE:HE1	1.85	0.41
23:0:155:LEU:O	23:0:156:CYS:HB2	2.21	0.41
25:2:465:SER:O	25:2:469:ASN:ND2	2.32	0.41
1:A:635:ARG:NH2	1:A:876:ALA:O	2.54	0.40
2:B:26:THR:OG1	2:B:27:ALA:N	2.54	0.40
2:B:102:VAL:HG23	2:B:112:LEU:HB2	2.03	0.40
2:B:657:HIS:HA	2:B:660:LYS:HZ3	1.86	0.40
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.54	0.40
7:G:45:ILE:HA	7:G:78:VAL:HG12	2.02	0.40
7:G:126:ASN:HA	7:G:127:PRO:HA	1.96	0.40
23:0:257:LEU:O	23:0:343:LYS:NZ	2.53	0.40
24:1:340:UNK:O	24:1:341:UNK:CB	2.69	0.40
1:A:497:THR:O	1:A:501:LEU:HB2	2.20	0.40
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.36	0.40
2:B:443:ASN:HD22	2:B:446:LEU:HG	1.86	0.40
2:B:649:LYS:HZ1	2:B:738:PHE:HD2	1.70	0.40
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.56	0.40
8:H:56:THR:HB	8:H:145:ARG:HG2	2.03	0.40
8:H:93:TYR:CG	8:H:143:LEU:HB3	2.56	0.40
14:N:73:DC:H2"	14:N:74:DA:N7	2.36	0.40
23:0:195:ILE:O	23:0:199:MET:HB2	2.21	0.40
1:A:214:ILE:HG22	1:A:219:PHE:HD2	1.87	0.40
1:A:217:LYS:O	1:A:221:SER:OG	2.33	0.40
1:A:802:ASN:HA	1:A:806:ARG:HH21	1.87	0.40
1:A:885:THR:HB	1:A:943:LEU:HD12	2.03	0.40
2:B:26:THR:HG23	2:B:29:ASP:H	1.86	0.40
2:B:780:VAL:HG22	2:B:795:ILE:HG23	2.04	0.40
3:C:255:VAL:HG21	11:K:94:ILE:HG21	2.04	0.40
4:D:56:ARG:HH22	4:D:155:ARG:HE	1.68	0.40
18:T:96:DT:H2"	18:T:97:DA:C8	2.56	0.40
23:0:406:ALA:HA	23:0:409:ILE:HG12	2.02	0.40
1:A:139:TRP:CH2	14:N:60:DT:OP1	2.75	0.40
8:H:90:ALA:HB1	8:H:96:VAL:HG21	2.03	0.40
9:I:54:GLU:HG2	9:I:88:SER:OG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LEU:HD12	1:A:1074:GLU:HG2	2.03	0.40
23:0:117:HIS:N	23:0:118:PRO:HD2	2.36	0.40
23:0:364:LYS:HZ3	23:0:370:GLU:H	1.66	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	1386/1733 (80%)	1298 (94%)	77 (6%)	11 (1%)	19	60
2	B	1136/1224 (93%)	1064 (94%)	62 (6%)	10 (1%)	17	56
3	C	260/318 (82%)	236 (91%)	20 (8%)	4 (2%)	10	45
4	D	153/221 (69%)	145 (95%)	7 (5%)	1 (1%)	22	62
5	E	211/215 (98%)	202 (96%)	8 (4%)	1 (0%)	29	69
6	F	81/155 (52%)	79 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	155 (92%)	13 (8%)	1 (1%)	25	66
8	H	132/146 (90%)	117 (89%)	12 (9%)	3 (2%)	6	33
9	I	114/122 (93%)	99 (87%)	15 (13%)	0	100	100
10	J	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	4	26
11	K	110/120 (92%)	109 (99%)	1 (1%)	0	100	100
12	L	43/70 (61%)	37 (86%)	6 (14%)	0	100	100
13	M	273/345 (79%)	252 (92%)	16 (6%)	5 (2%)	8	40
15	O	178/240 (74%)	164 (92%)	13 (7%)	1 (1%)	25	66
16	Q	129/747 (17%)	111 (86%)	15 (12%)	3 (2%)	6	33
17	R	176/400 (44%)	160 (91%)	15 (8%)	1 (1%)	25	66
19	U	88/286 (31%)	82 (93%)	4 (4%)	2 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	V	96/122 (79%)	92 (96%)	3 (3%)	1 (1%)	15	54
21	W	198/541 (37%)	189 (96%)	6 (3%)	3 (2%)	10	45
22	X	156/328 (48%)	129 (83%)	23 (15%)	4 (3%)	5	31
23	0	659/778 (85%)	590 (90%)	54 (8%)	15 (2%)	6	33
24	1	309/510 (61%)	297 (96%)	8 (3%)	4 (1%)	12	48
25	2	284/553 (51%)	266 (94%)	17 (6%)	1 (0%)	34	72
26	3	136/321 (42%)	114 (84%)	19 (14%)	3 (2%)	6	35
27	4	257/333 (77%)	231 (90%)	17 (7%)	9 (4%)	3	25
28	5	64/72 (89%)	59 (92%)	5 (8%)	0	100	100
29	6	289/461 (63%)	260 (90%)	26 (9%)	3 (1%)	15	54
30	7	361/843 (43%)	333 (92%)	23 (6%)	5 (1%)	11	46
32	a	141/295 (48%)	132 (94%)	6 (4%)	3 (2%)	7	36
33	b	154/223 (69%)	147 (96%)	6 (4%)	1 (1%)	25	66
34	c	95/115 (83%)	90 (95%)	5 (5%)	0	100	100
35	d	422/687 (61%)	387 (92%)	30 (7%)	5 (1%)	13	49
36	e	226/307 (74%)	212 (94%)	14 (6%)	0	100	100
37	f	199/210 (95%)	182 (92%)	16 (8%)	1 (0%)	29	69
38	g	79/121 (65%)	79 (100%)	0	0	100	100
39	h	107/300 (36%)	106 (99%)	1 (1%)	0	100	100
40	i	128/223 (57%)	122 (95%)	6 (5%)	0	100	100
41	j	60/149 (40%)	56 (93%)	4 (7%)	0	100	100
42	k	121/157 (77%)	111 (92%)	8 (7%)	2 (2%)	9	42
43	l	439/745 (59%)	402 (92%)	27 (6%)	10 (2%)	6	33
44	m	97/220 (44%)	82 (84%)	10 (10%)	5 (5%)	2	19
45	n	134/140 (96%)	126 (94%)	6 (4%)	2 (2%)	10	45
46	o	73/151 (48%)	69 (94%)	4 (6%)	0	100	100
All	All	9986/15488 (64%)	9231 (92%)	633 (6%)	122 (1%)	17	49

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Q	127	ILE
21	W	77	PRO

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Mol	Chain	Res	Type
23	0	156	CYS
23	0	254	THR
27	4	88	PRO
27	4	290	SER
43	l	499	LEU
44	m	58	VAL
2	B	830	TYR
2	B	933	SER
7	G	63	PRO
13	M	269	ILE
21	W	78	ASN
22	X	251	ASN
23	0	349	LEU
24	1	275	PRO
26	3	124	ILE
30	7	461	ALA
35	d	370	PRO
35	d	571	PRO
43	l	273	ASN
45	n	35	LEU
2	B	277	LYS
2	B	475	SER
3	C	214	ASN
8	H	60	ALA
13	M	268	GLU
19	U	255	LYS
22	X	152	SER
23	0	62	HIS
23	0	217	LYS
23	0	471	ARG
24	1	25	ALA
24	1	74	ASP
27	4	87	TYR
27	4	170	THR
27	4	291	VAL
27	4	307	ALA
29	6	244	PRO
30	7	494	PRO
30	7	550	ALA
30	7	696	ARG
32	a	119	SER
33	b	60	PRO

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Mol	Chain	Res	Type
43	l	295	SER
44	m	23	TYR
44	m	150	PRO
1	A	47	ARG
1	A	67	CYS
1	A	567	LYS
1	A	958	VAL
2	B	364	ILE
2	B	957	ASN
3	C	93	ASP
4	D	156	ASP
8	H	83	GLN
10	J	9	SER
19	U	264	ASP
20	V	6	TYR
23	0	432	ASN
23	0	683	ASP
24	1	277	ASN
25	2	451	VAL
27	4	115	TYR
27	4	305	CYS
27	4	306	PRO
29	6	451	CYS
30	7	667	ALA
32	a	11	TRP
32	a	123	PRO
42	k	147	THR
43	l	581	LYS
1	A	35	ILE
1	A	50	ILE
1	A	525	GLN
1	A	569	LYS
2	B	339	THR
2	B	705	MET
3	C	236	GLY
5	E	124	VAL
10	J	3	VAL
13	M	271	GLY
22	X	240	THR
23	0	249	SER
23	0	433	PRO
23	0	473	LEU

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Mol	Chain	Res	Type
23	0	606	VAL
26	3	75	ASP
29	6	286	SER
35	d	541	ILE
37	f	181	GLU
43	l	209	LEU
43	l	379	LEU
43	l	392	GLY
43	l	408	LYS
44	m	144	GLN
44	m	145	PHE
1	A	464	PRO
2	B	1046	PRO
13	M	273	SER
16	Q	329	THR
16	Q	367	ALA
21	W	410	GLU
26	3	73	PHE
35	d	317	SER
45	n	39	GLU
15	O	147	GLY
22	X	205	ILE
23	0	536	GLY
42	k	43	PRO
43	l	498	VAL
2	B	343	ILE
8	H	59	ILE
23	0	372	LYS
1	A	61	ILE
3	C	182	PRO
17	R	215	VAL
1	A	1327	ILE
13	M	32	PRO
23	0	369	ILE
35	d	397	ILE
43	l	528	ASN

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	1221/1520 (80%)	1218 (100%)	3 (0%)	93	96
2	B	1000/1061 (94%)	997 (100%)	3 (0%)	92	94
3	C	230/274 (84%)	228 (99%)	2 (1%)	78	87
4	D	139/200 (70%)	137 (99%)	2 (1%)	67	80
5	E	195/197 (99%)	194 (100%)	1 (0%)	88	93
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	119/128 (93%)	119 (100%)	0	100	100
9	I	110/116 (95%)	108 (98%)	2 (2%)	59	77
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	97/102 (95%)	97 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	245/299 (82%)	245 (100%)	0	100	100
15	O	152/205 (74%)	152 (100%)	0	100	100
16	Q	109/641 (17%)	108 (99%)	1 (1%)	78	87
17	R	107/363 (30%)	106 (99%)	1 (1%)	78	87
19	U	84/260 (32%)	84 (100%)	0	100	100
20	V	90/108 (83%)	90 (100%)	0	100	100
21	W	161/429 (38%)	161 (100%)	0	100	100
22	X	62/295 (21%)	62 (100%)	0	100	100
23	0	413/677 (61%)	406 (98%)	7 (2%)	60	78
24	1	179/306 (58%)	177 (99%)	2 (1%)	73	84
25	2	53/407 (13%)	53 (100%)	0	100	100
26	3	53/303 (18%)	53 (100%)	0	100	100
27	4	4/260 (2%)	3 (75%)	1 (25%)	0	3
28	5	53/66 (80%)	53 (100%)	0	100	100
29	6	173/378 (46%)	173 (100%)	0	100	100
30	7	315/695 (45%)	308 (98%)	7 (2%)	52	71
33	b	15/207 (7%)	15 (100%)	0	100	100
34	c	93/108 (86%)	92 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	d	256/642 (40%)	253 (99%)	3 (1%)	71	83
36	e	210/280 (75%)	210 (100%)	0	100	100
37	f	172/178 (97%)	170 (99%)	2 (1%)	71	83
38	g	75/113 (66%)	75 (100%)	0	100	100
40	i	118/209 (56%)	118 (100%)	0	100	100
45	n	96/132 (73%)	95 (99%)	1 (1%)	76	86
46	o	73/117 (62%)	73 (100%)	0	100	100
All	All	6797/11687 (58%)	6758 (99%)	39 (1%)	86	92

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	444	PHE
1	A	1259	MET
2	B	398	ARG
2	B	579	ARG
2	B	604	ARG
3	C	95	CYS
3	C	222	LYS
4	D	153	ARG
4	D	165	GLN
5	E	37	LEU
9	I	42	LEU
9	I	43	VAL
16	Q	350	TRP
17	R	251	ARG
23	0	133	CYS
23	0	199	MET
23	0	411	THR
23	0	440	LEU
23	0	522	TYR
23	0	647	ARG
23	0	685	ARG
24	1	71	LYS
24	1	276	LYS
27	4	292	CYS
30	7	373	MET
30	7	622	MET
30	7	681	ARG

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Mol	Chain	Res	Type
30	7	695	ARG
30	7	701	PHE
30	7	715	GLU
30	7	737	THR
34	c	38	LYS
35	d	390	ARG
35	d	540	LEU
35	d	608	LYS
37	f	26	ASN
37	f	195	ASN
45	n	110	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	64	ASN
1	A	68	GLN
1	A	256	GLN
1	A	311	GLN
1	A	313	GLN
1	A	339	ASN
1	A	363	GLN
1	A	517	ASN
1	A	525	GLN
1	A	589	GLN
1	A	611	GLN
1	A	640	GLN
1	A	698	GLN
1	A	745	GLN
1	A	760	GLN
1	A	881	GLN
1	A	953	ASN
1	A	965	GLN
1	A	968	GLN
1	A	994	GLN
1	A	1040	GLN
1	A	1130	GLN
1	A	1140	HIS
2	B	60	GLN
2	B	115	GLN
2	B	395	GLN

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Mol	Chain	Res	Type
2	B	415	GLN
2	B	433	GLN
2	B	573	GLN
2	B	657	HIS
2	B	667	GLN
2	B	763	GLN
2	B	1093	GLN
2	B	1161	HIS
2	B	1193	GLN
2	B	1195	HIS
3	C	73	GLN
3	C	102	GLN
3	C	224	GLN
3	C	231	ASN
3	C	242	GLN
3	C	264	GLN
4	D	157	GLN
4	D	165	GLN
4	D	179	GLN
7	G	96	GLN
7	G	102	GLN
8	H	83	GLN
9	I	60	GLN
10	J	53	HIS
11	K	112	GLN
13	M	90	ASN
13	M	114	GLN
13	M	193	GLN
13	M	235	ASN
15	O	91	ASN
15	O	158	GLN
16	Q	117	HIS
19	U	33	GLN
19	U	280	GLN
20	V	55	ASN
20	V	84	GLN
21	W	107	GLN
21	W	178	GLN
22	X	216	GLN
22	X	223	GLN
22	X	267	GLN
22	X	279	GLN

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Mol	Chain	Res	Type
23	0	239	ASN
23	0	651	ASN
23	0	716	ASN
24	1	38	HIS
24	1	49	GLN
24	1	92	ASN
24	1	258	ASN
28	5	11	GLN
28	5	22	GLN
29	6	211	GLN
29	6	212	ASN
29	6	269	GLN
29	6	281	ASN
29	6	302	ASN
30	7	491	HIS
30	7	508	HIS
30	7	584	ASN
30	7	592	GLN
30	7	648	GLN
30	7	672	GLN
30	7	676	HIS
30	7	682	GLN
34	c	25	GLN
34	c	51	HIS
35	d	642	ASN
35	d	646	HIS
35	d	684	GLN
36	e	3	GLN
36	e	167	GLN
36	e	205	ASN
36	e	214	GLN
37	f	26	ASN
37	f	68	GLN
37	f	75	ASN
37	f	195	ASN
38	g	60	ASN
40	i	159	HIS
45	n	98	GLN
46	o	20	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 17 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	$\#\|Z\| > 2$
49	SF4	0	901	23	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
49	SF4	0	901	23	-	-	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	0	901	SF4	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	1	3
21	W	2
25	2	1
27	4	1
39	h	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	394:UNK	C	465:UNK	N	84.00
1	W	289:UNK	C	349:UNK	N	45.11
1	1	121:ARG	C	168:UNK	N	38.20
1	2	281:ASP	C	380:UNK	N	36.23
1	W	194:ILE	C	259:UNK	N	35.82
1	4	97:UNK	C	103:UNK	N	15.93
1	1	353:UNK	C	369:UNK	N	14.71
1	h	125:LEU	C	130:UNK	N	5.44

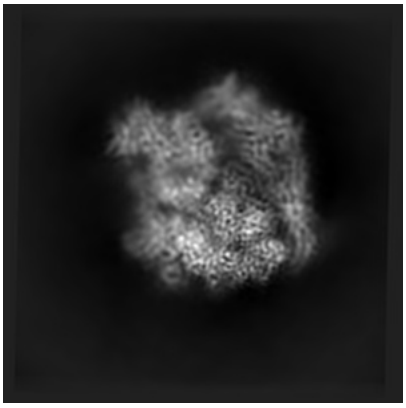
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3850. These allow visual inspection of the internal detail of the map and identification of artifacts.

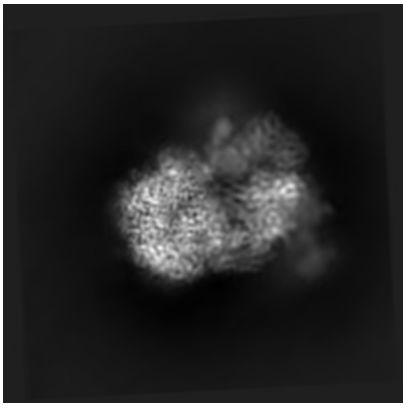
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

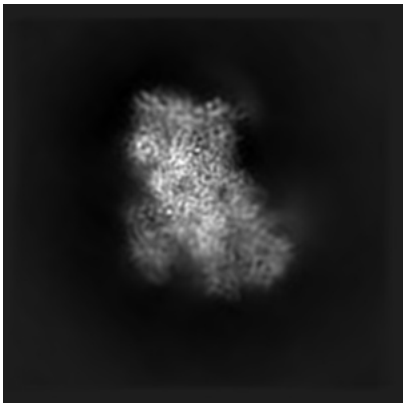
6.1.1 Primary map



X



Y

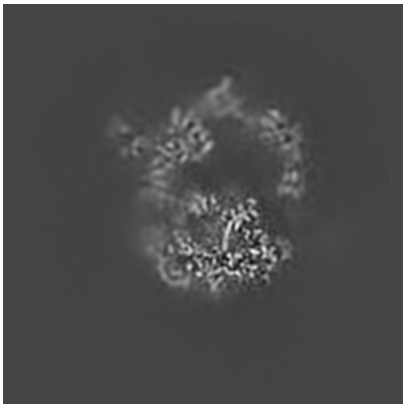


Z

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

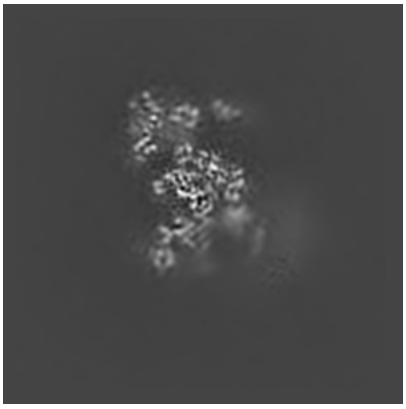
6.2 Central slices (i)

6.2.1 Primary map



X Index: 175

Y Index: 175

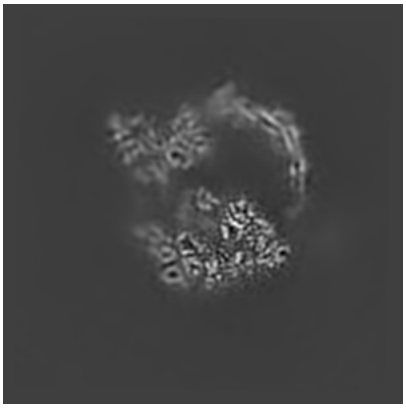


Z Index: 175

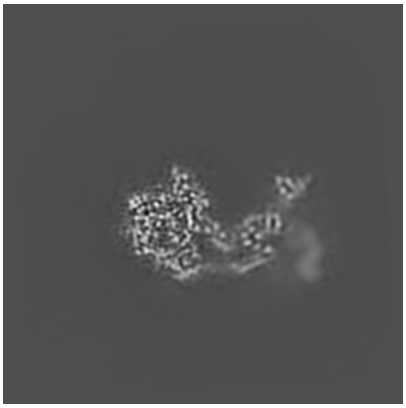
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 182



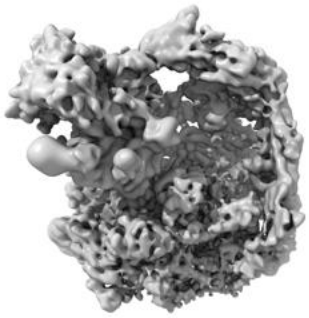
Y Index: 217

Z Index: 130

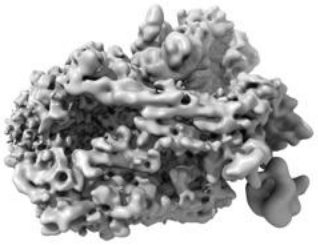
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

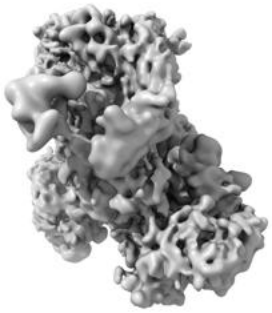
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

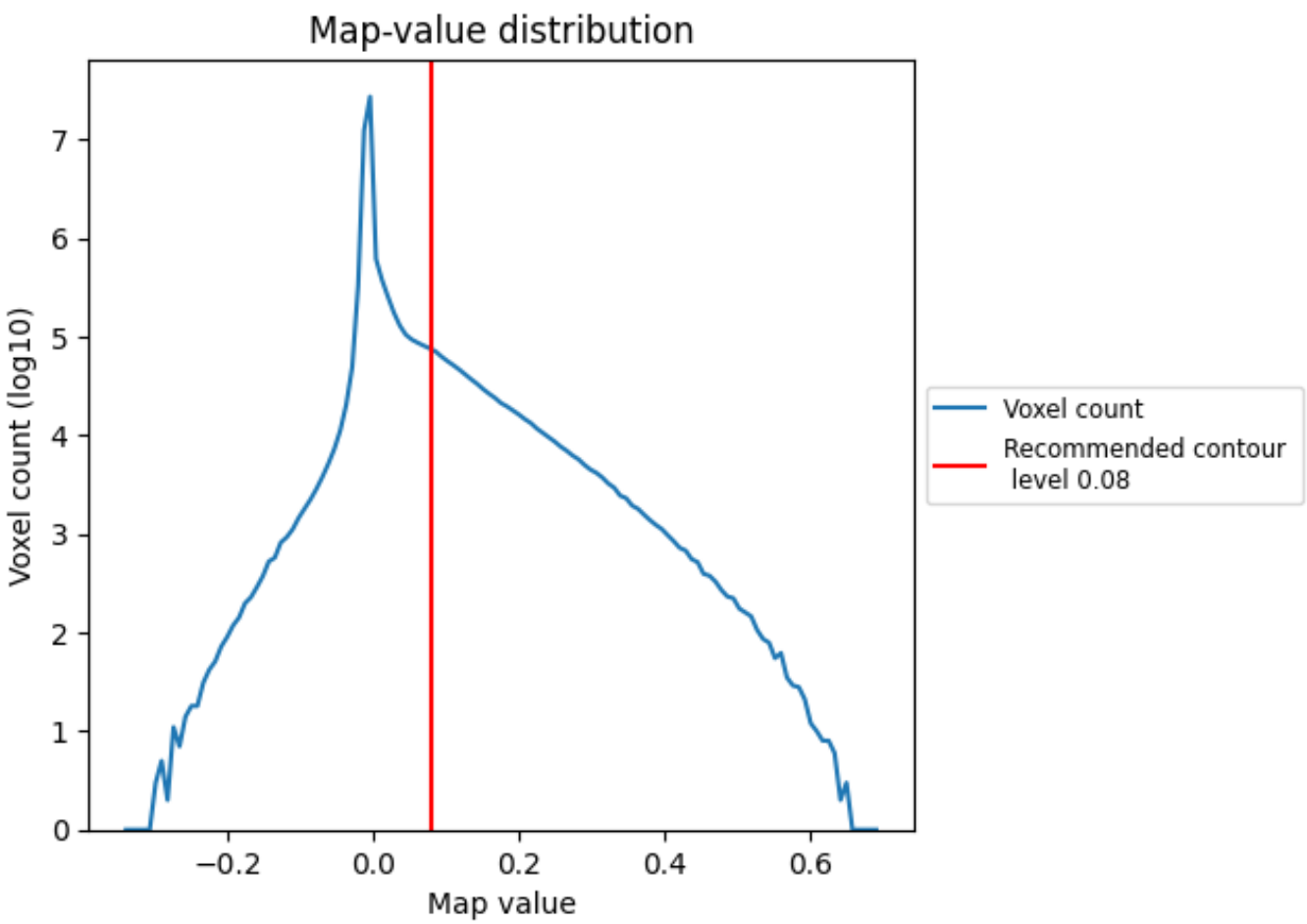
6.5 Mask visualisation (i)

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

7 Map analysis (i)

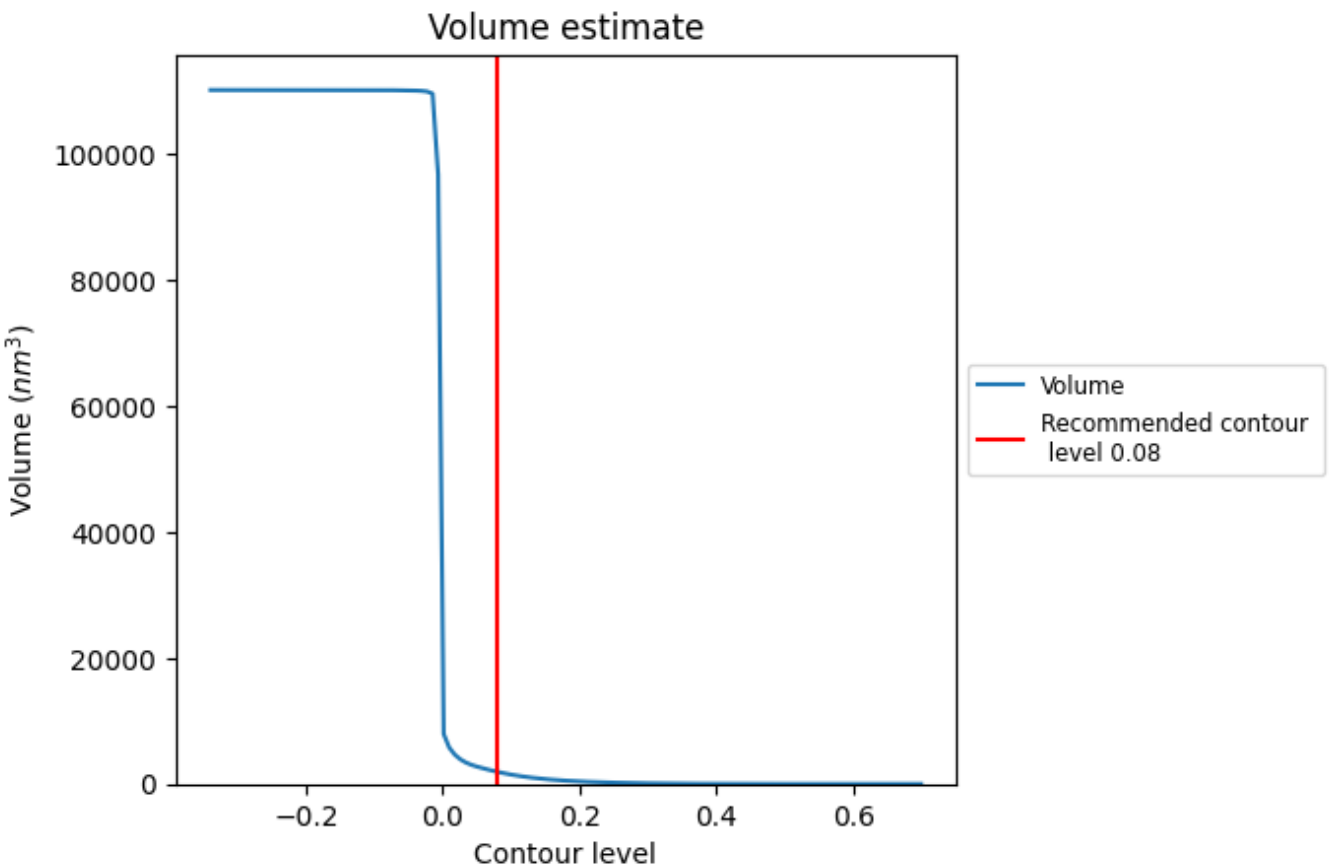
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

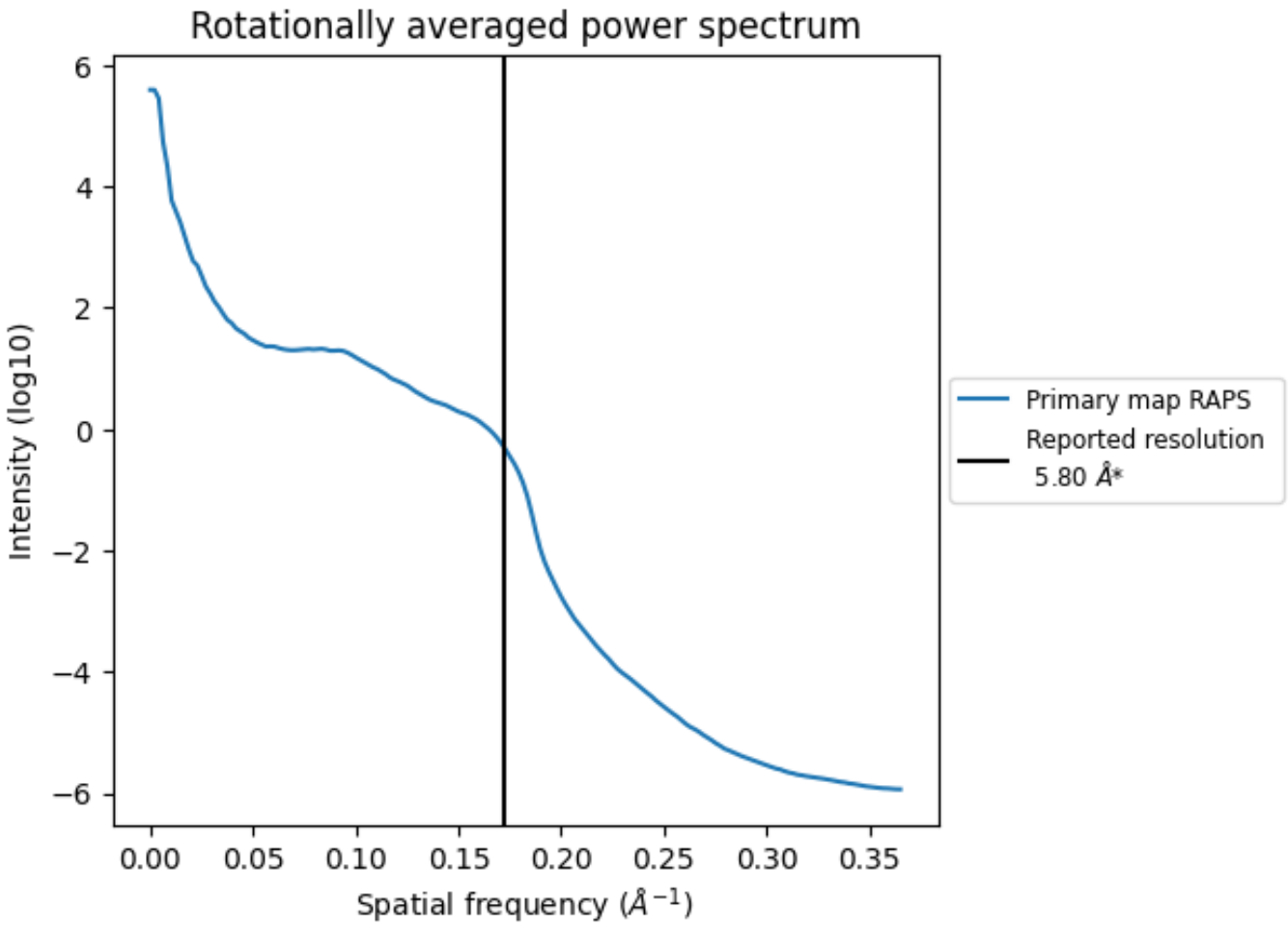
7.2 Volume estimate (i)



The volume at the recommended contour level is 1922 nm^3; this corresponds to an approximate mass of 1736 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 0.172 Å^{-1}

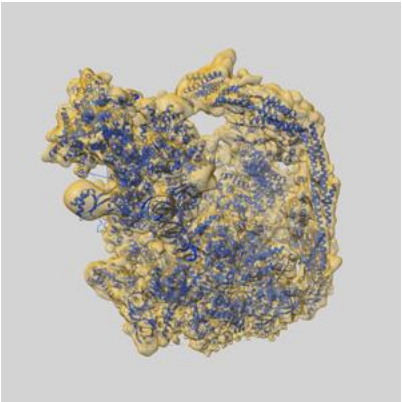
8 Fourier-Shell correlation (i)

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

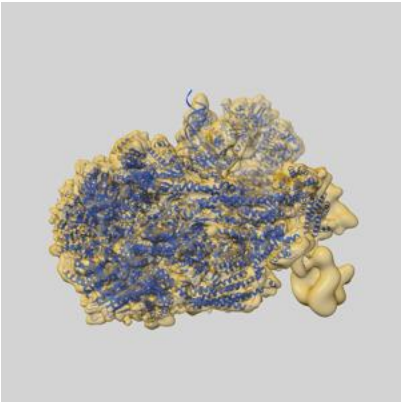
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3850 and PDB model 5OQM. Per-residue inclusion information can be found in section 3 on page 14.

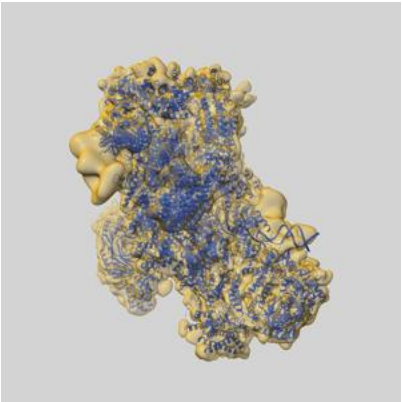
9.1 Map-model overlay (i)



X



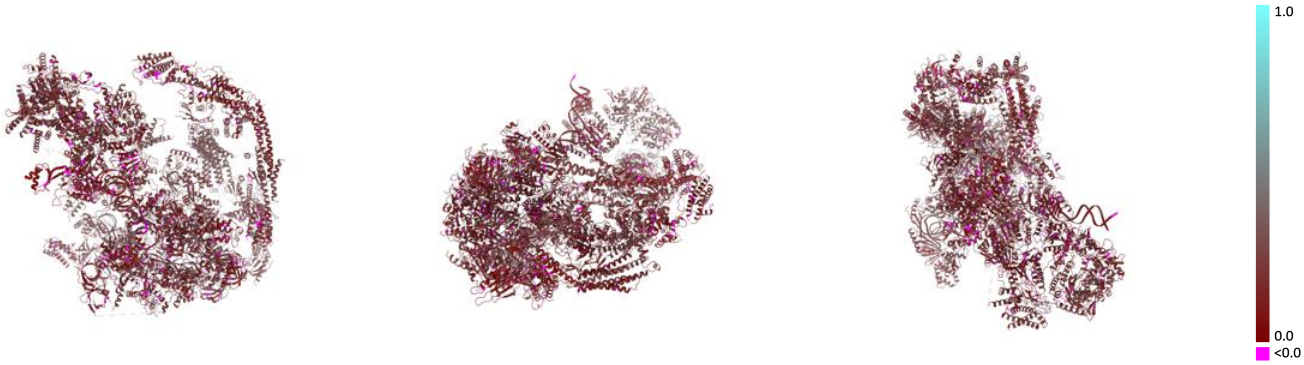
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

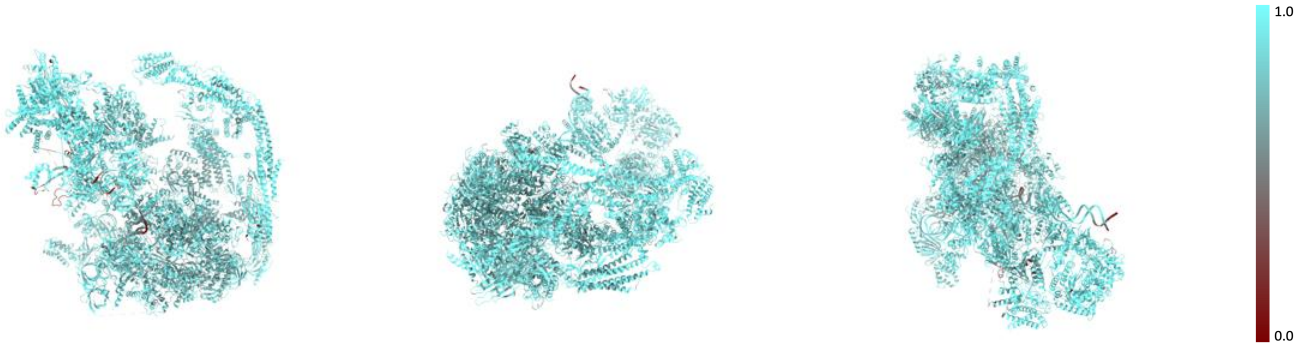
9.2 Q-score mapped to coordinate model (i)



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.

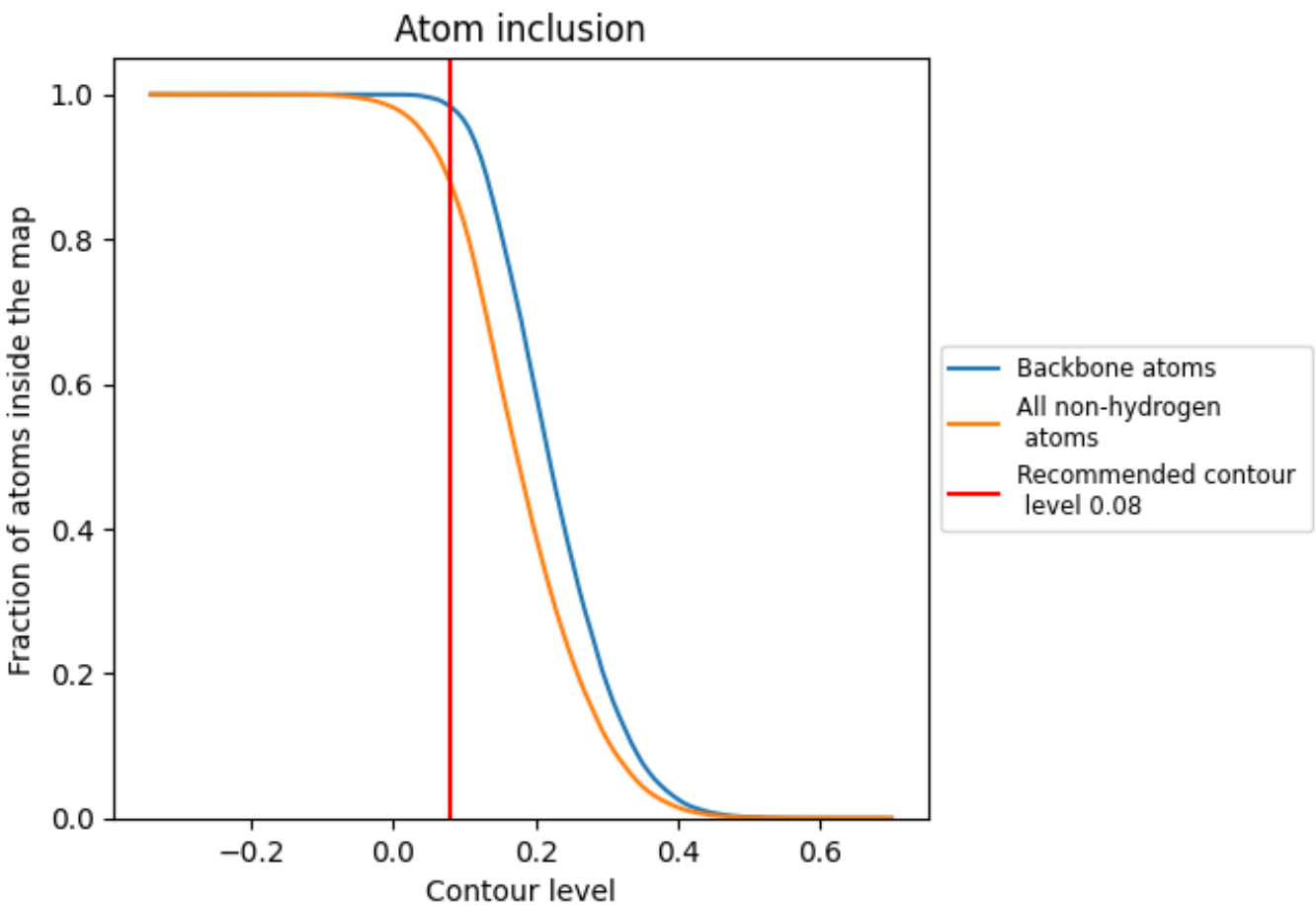
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8792	0.1830
0	0.9059	0.1670
1	0.8853	0.1810
2	0.9457	0.1890
3	0.9333	0.1940
4	0.9607	0.2140
5	0.9024	0.1230
6	0.9051	0.1750
7	0.9542	0.1340
A	0.8398	0.1930
B	0.8369	0.1900
C	0.8564	0.2160
D	0.8313	0.1700
E	0.8836	0.1950
F	0.8666	0.2250
G	0.8631	0.1950
H	0.8445	0.1890
I	0.8925	0.1850
J	0.8472	0.2000
K	0.8328	0.1960
L	0.8613	0.2160
M	0.8048	0.1650
N	0.9028	0.1940
O	0.8984	0.1520
Q	0.8664	0.1600
R	0.9191	0.2040
T	0.8424	0.1780
U	0.8907	0.1450
V	0.8970	0.1560
W	0.8471	0.1630
X	0.9158	0.1890
Z	0.9814	0.2250
a	0.9865	0.2400
b	0.9571	0.2420
c	0.8419	0.1340

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Chain	Atom inclusion	Q-score
d	0.8819	0.1750
e	0.8391	0.1810
f	0.8397	0.1880
g	0.8194	0.1460
h	0.9801	0.2510
i	0.9088	0.1670
j	0.8902	0.2320
k	0.9968	0.2120
l	0.9578	0.2150
m	0.9727	0.1220
n	0.8818	0.1530
o	0.8745	0.1490