Full wwPDB EM Validation Report ⓘ

Aug 7, 2024 – 02:55 pm BST

PDB ID	:	8PJ4
EMDB ID	:	EMD-17699
Title	:	Structure of human 48S translation initiation complex after eIF5 release (48S-4)
Authors	:	Petrychenko, V.; Yi, S.-H.; Liedtke, D.; Peng, B.Z.; Rodnina, M.V.; Fischer, N.
Deposited on	:	2023-06-22
Resolution	:	3.20 Å(reported)

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

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

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

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

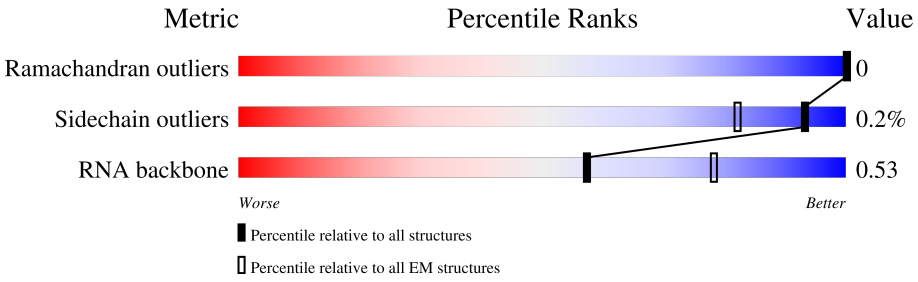
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	0	1220	51% 49%
2	1	814	60% 72% 28%
3	2	325	94% 94% 6%
4	3	218	70% 98%
5	4	357	32% 72% 28%
6	5	564	61% 92% 8%
7	6	374	48% 96%
8	7	255	7% 7% 14% 78%

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Mol	Chain	Length	Quality of chain
9	8	352	44% 90% 10%
10	9	25	96%
11	A	1869	69% 23% 6%
12	B	158	89% 10%
13	C	263	97%
14	D	194	91% 9%
15	E	143	98%
16	F	133	44% 56%
17	G	194	90% 9%
18	H	84	96%
19	I	151	99%
20	J	130	98%
21	K	83	98%
22	L	293	74% 25%
23	M	135	96%
24	N	295	70% 30%
25	O	264	80% 20%
26	P	151	87% 12%
27	Q	115	85% 14%
28	R	208	95% 5%
29	S	249	92% 8%
30	T	133	93% 6%
31	V	204	93% 7%
32	Y	146	96%
33	Z	243	93% 7%

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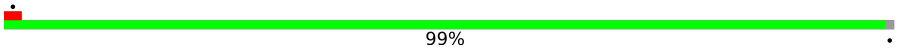
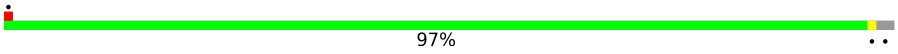
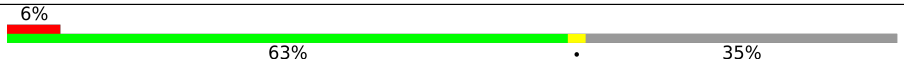
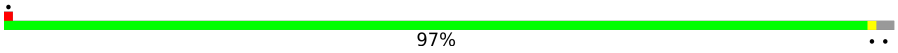
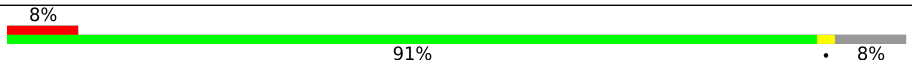
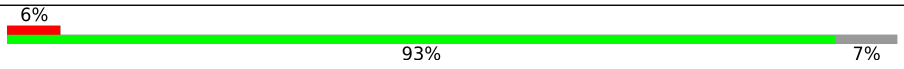
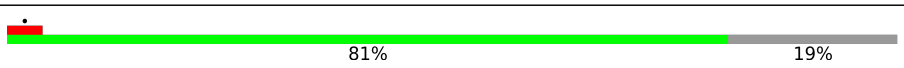
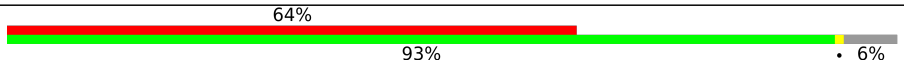
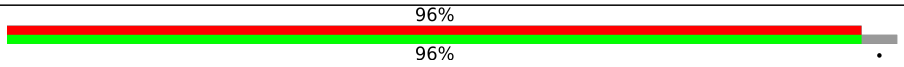
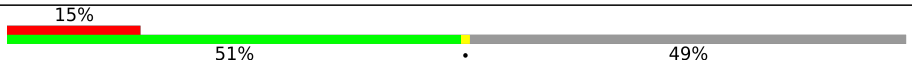
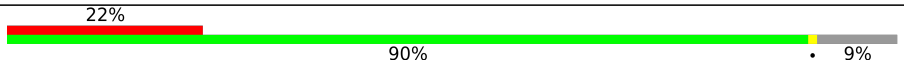
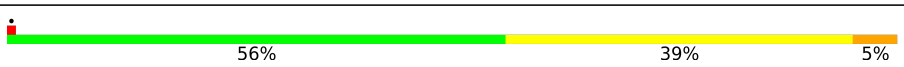
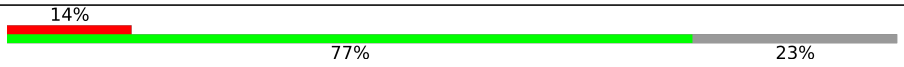
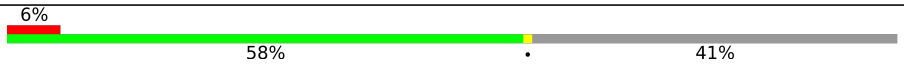
Mol	Chain	Length	Quality of chain
34	a	165	
35	b	145	
36	c	317	
37	d	145	
38	e	125	
39	f	152	
40	h	119	
41	i	56	
42	k	156	
43	m	132	
44	n	69	
45	o	320	
46	q	144	
47	r	315	
48	t	472	
49	u	1382	
50	v	445	
51	w	75	
52	x	548	
53	y	913	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 121694 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 Eukaryotic translation initiation factor 5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	621	Total	C	N	O	S	0	0
			4920	3135	850	913	22		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	588	Total	C	N	O	S	0	0
			3258	1986	633	634	5		

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	2	304	Total	C	N	O	0	0
			1493	885	304	304		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	213	Total	C	N	O	0	0
			1057	631	213	213		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	257	Total	C	N	O	0	0
			1272	757	257	258		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	520	Total	C	N	O	S	0	0
			4347	2814	721	793	19		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	362	Total	C	N	O	S	0	0
			2196	1348	414	427	7		

- Molecule 8 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	57	Total	C	N	O	P	0	0
			1218	547	231	383	57		

- Molecule 9 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	317	Total	C	N	O	0	0
			1574	937	318	319		

- Molecule 10 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 11 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1754	Total	C	N	O	P	0	0
			37429	16718	6714	12244	1753		

- Molecule 12 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	142	Total	C	N	O	S	0	0
			1166	743	218	199	6		

- Molecule 13 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	256	Total	C	N	O	S	0	0
			2035	1302	378	347	8		

- Molecule 14 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	177	Total	C	N	O	S	0	0
			1477	941	295	239	2		

- Molecule 15 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 16 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	58	Total	C	N	O	S	0	0
			452	279	98	74	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	125	PRO	LYS	conflict	UNP P62861

- Molecule 17 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	177	Total	C	N	O	S	0	0
			1430	917	260	252	1		

- Molecule 18 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 19 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 20 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 21 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 22 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 23 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 24 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 25 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 26 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	133	Total	C	N	O	S	0	0
			997	610	196	185	6		

- Molecule 27 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 28 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	R	198	Total	C	N	O	S	0	0
			1627	1021	322	279	5		

- Molecule 29 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 31 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 32 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 33 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 34 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	99	Total	C	N	O	S	0	0
			834	544	149	135	6		

- Molecule 35 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	131	Total	C	N	O	S	0	0
			1072	682	201	182	7		

- Molecule 36 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 37 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	142	Total	C	N	O	S	0	0
			1105	692	213	197	3		

- Molecule 38 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	81	Total	C	N	O	S	0	0
			649	420	119	109	1		

- Molecule 39 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	149	Total	C	N	O	S	0	0
			1227	770	249	207	1		

- Molecule 40 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 41 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	50	Total	C	N	O	S	0	0
			419	262	85	67	5		

- Molecule 42 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	68	Total	C	N	O	S	0	0
			554	349	103	95	7		

- Molecule 43 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 44 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	o	77	Total	C	N	O	0	0
			616	389	111	116		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	117	Total	C	N	O	S	1	0
			951	590	183	174	4		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	296	Total	C	N	O	S	0	0
			2138	1342	384	404	8		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	t	455	Total	C	N	O	S	0	0
			3439	2179	599	643	18		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	706	Total	C	N	O	S	1	0
			5383	3379	982	999	23		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	405	Total	C	N	O	S	0	0
			2740	1720	498	510	12		

- Molecule 51 is a RNA chain called Initiator Met-tRNA-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

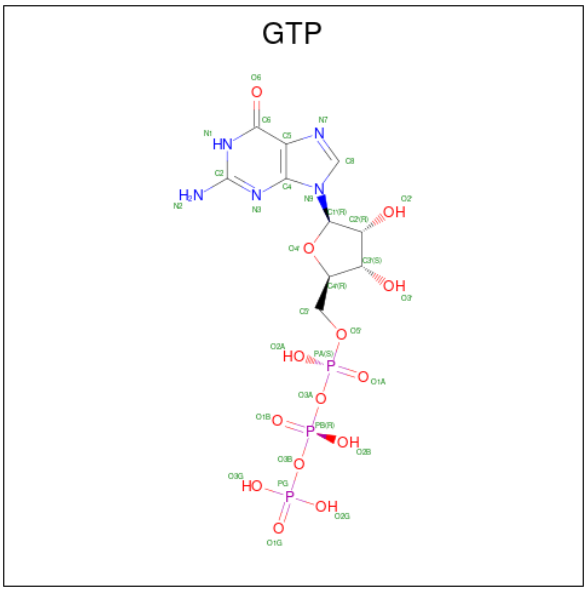
- Molecule 52 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	423	Total	C	N	O	S	0	0
			2842	1752	523	557	10		

- Molecule 53 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	543	Total	C	N	O	S	0	0
			4361	2743	776	809	33		

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
54	0	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 55 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
55	0	1	Total	Na	0
			1	1	

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	0	1	Total	Mg	0
			1	1	
56	A	87	Total	Mg	0
			87	87	
56	f	1	Total	Mg	0
			1	1	

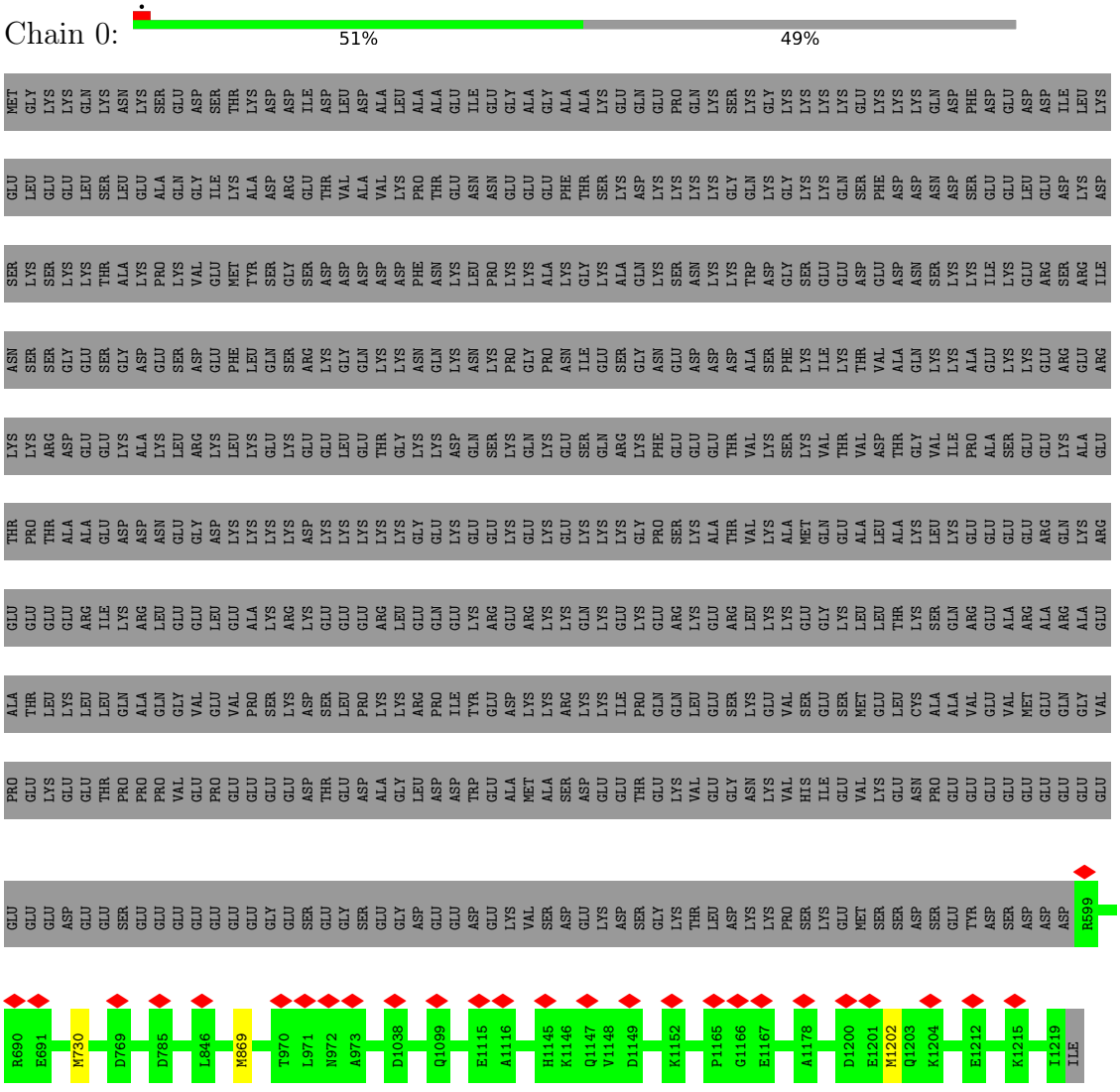
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	Q	1	Total	Zn	0
			1	1	
57	k	1	Total	Zn	0
			1	1	

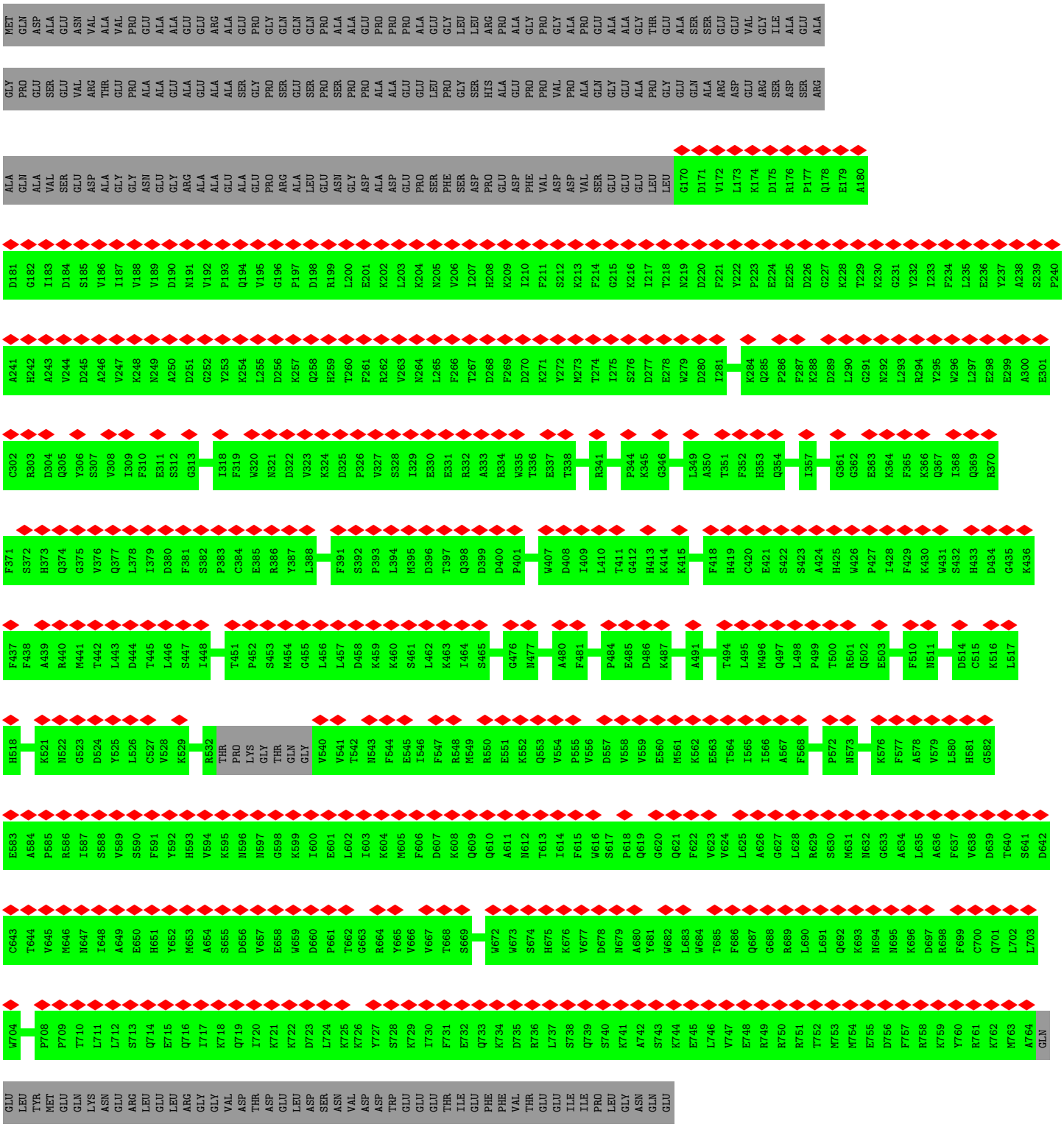
3 Residue-property plots (i)

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

• Molecule 1: Eukaryotic translation initiation factor 5B

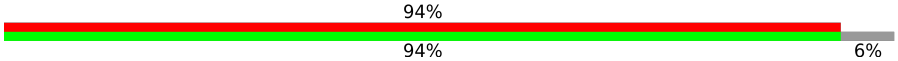


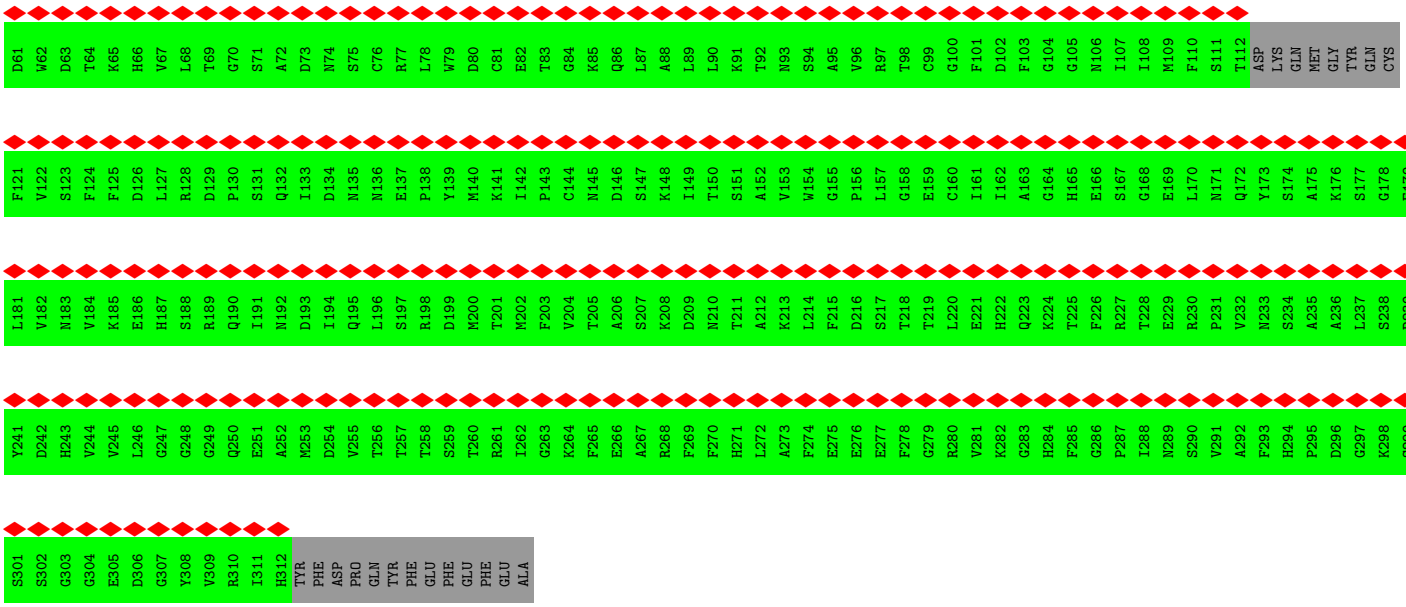
• Molecule 2: Eukaryotic translation initiation factor 3 subunit B



• Molecule 3: Eukaryotic translation initiation factor 3 subunit I

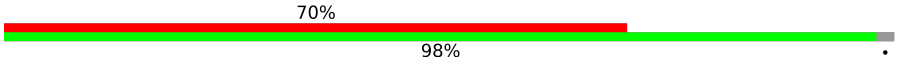
Chain 2:





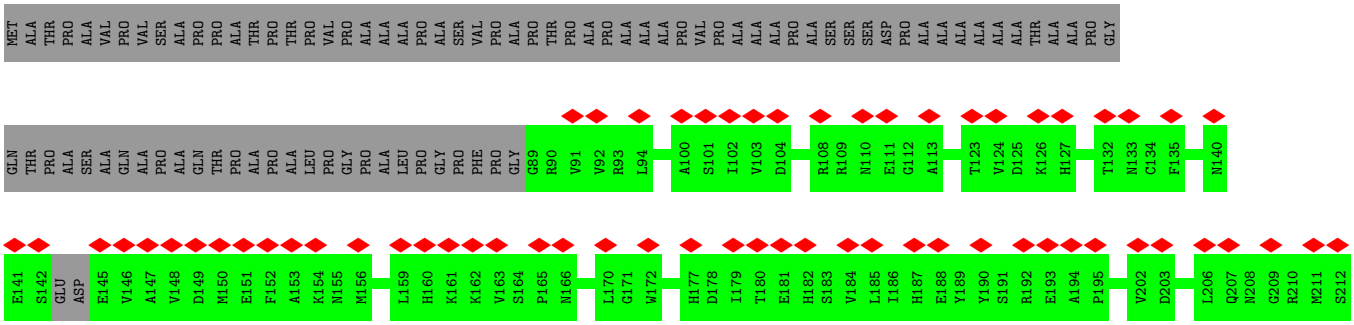
• Molecule 4: Eukaryotic translation initiation factor 3 subunit K

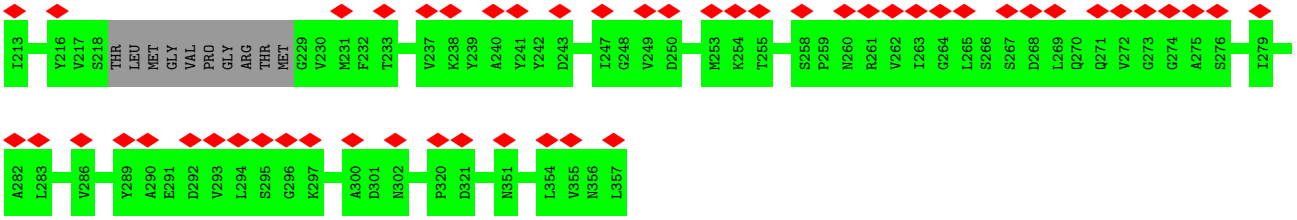
Chain 3:



• Molecule 5: Eukaryotic translation initiation factor 3 subunit F

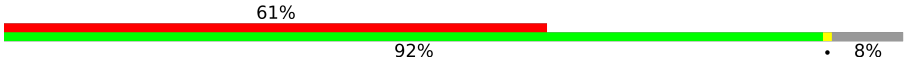
Chain 4:

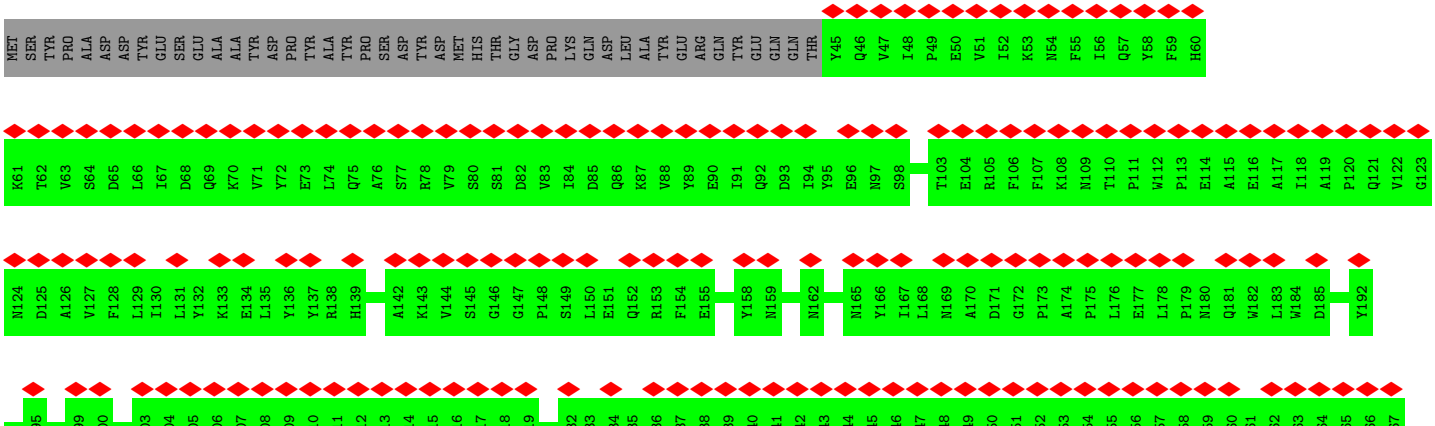




• Molecule 6: Eukaryotic translation initiation factor 3 subunit L

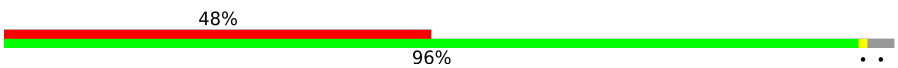
Chain 5:

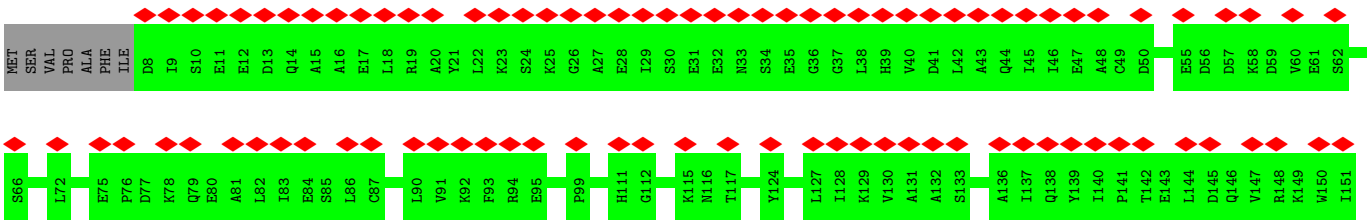


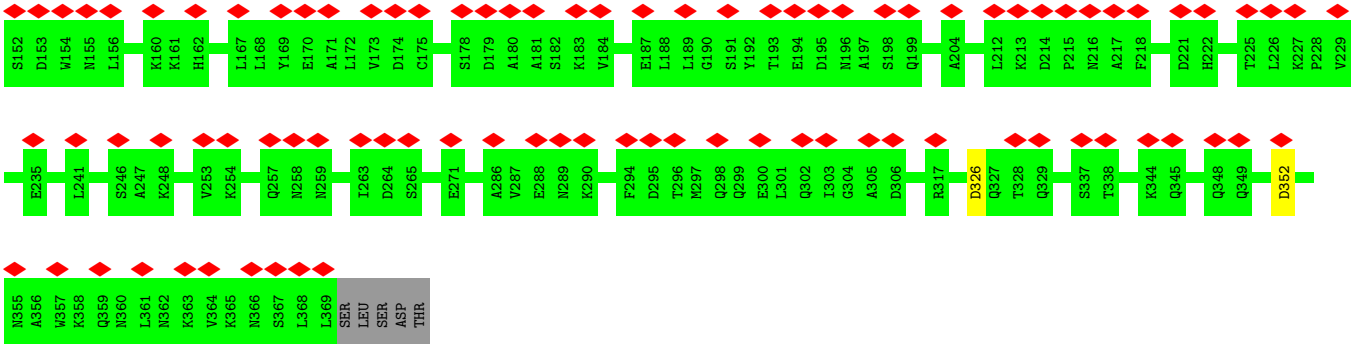


• Molecule 7: Eukaryotic translation initiation factor 3 subunit M

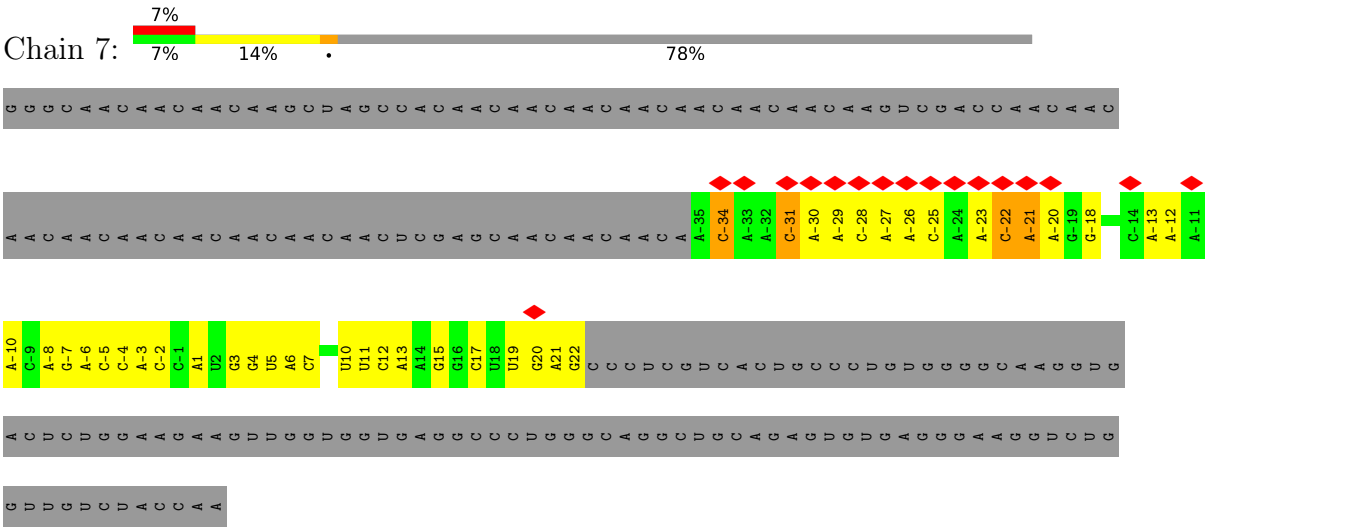
Chain 6:



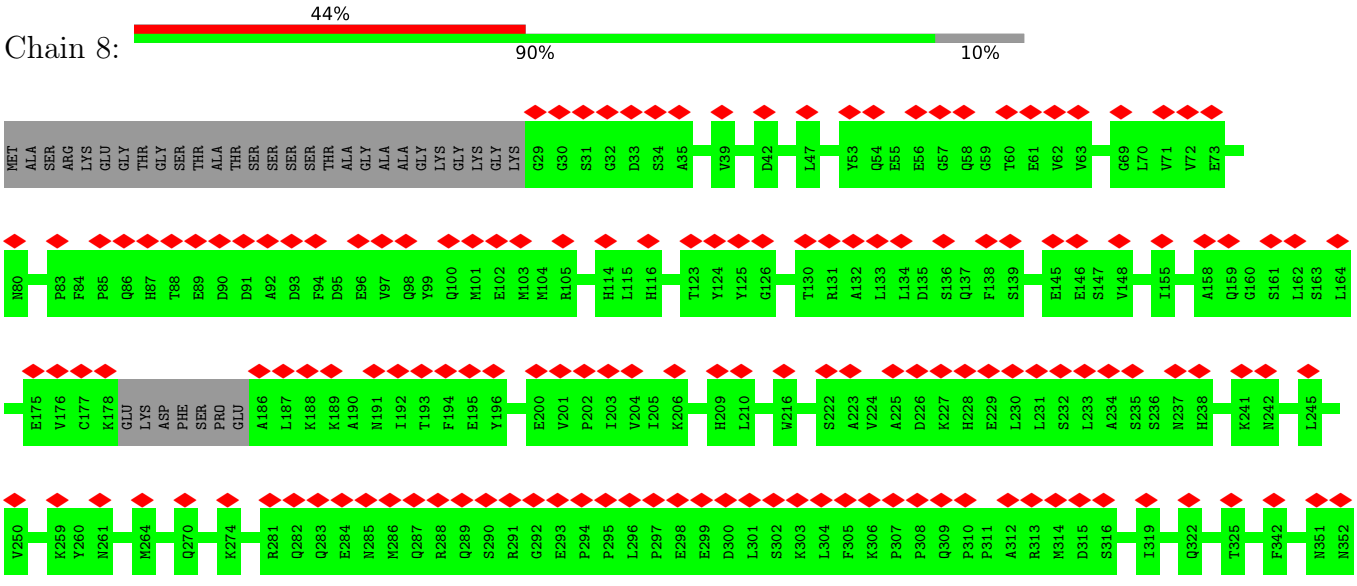




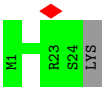
• Molecule 8: mRNA



• Molecule 9: Eukaryotic translation initiation factor 3 subunit H

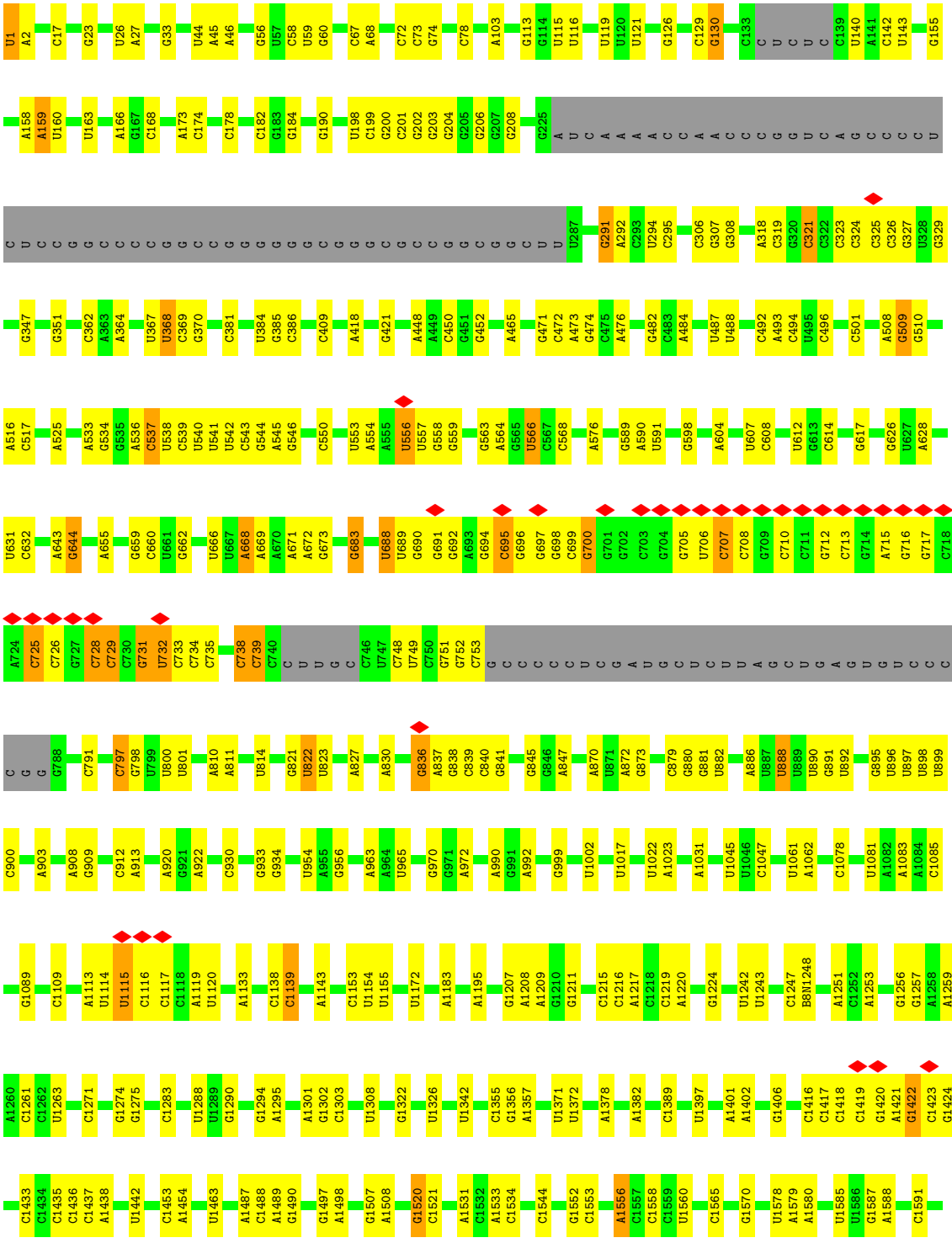


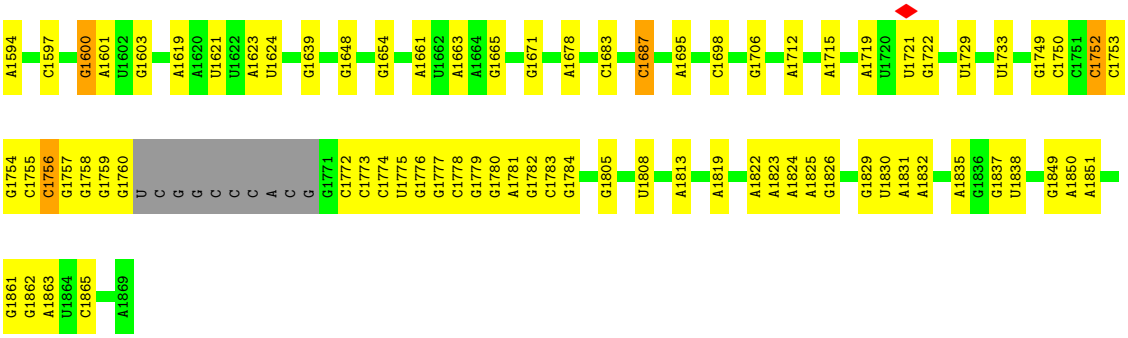
• Molecule 10: 60S ribosomal protein L41



• Molecule 11: 18S rRNA

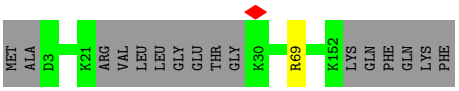
Chain A:





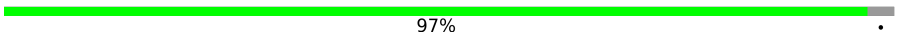
• Molecule 12: 40S ribosomal protein S11

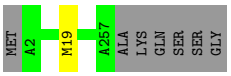
Chain B:



• Molecule 13: 40S ribosomal protein S4, X isoform

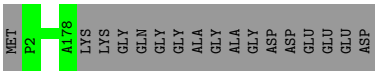
Chain C:





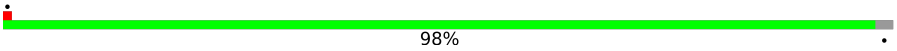
• Molecule 14: 40S ribosomal protein S9

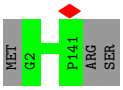
Chain D:



• Molecule 15: 40S ribosomal protein S23

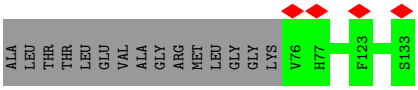
Chain E:





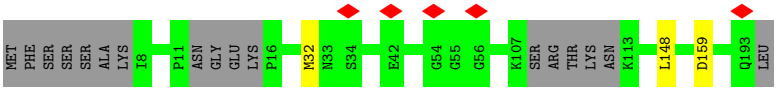
• Molecule 16: Small ribosomal subunit protein eS30

Chain F:



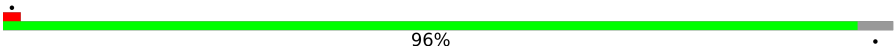
• Molecule 17: 40S ribosomal protein S7

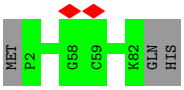
Chain G:



• Molecule 18: 40S ribosomal protein S27

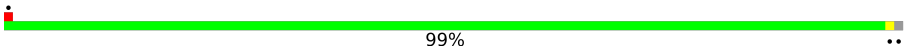
Chain H:

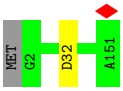




• Molecule 19: 40S ribosomal protein S13

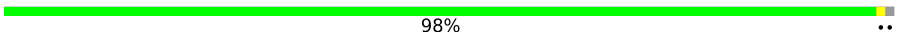
Chain I:





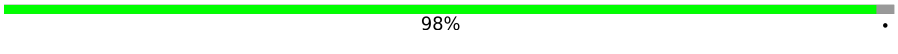
• Molecule 20: 40S ribosomal protein S15a

Chain J:



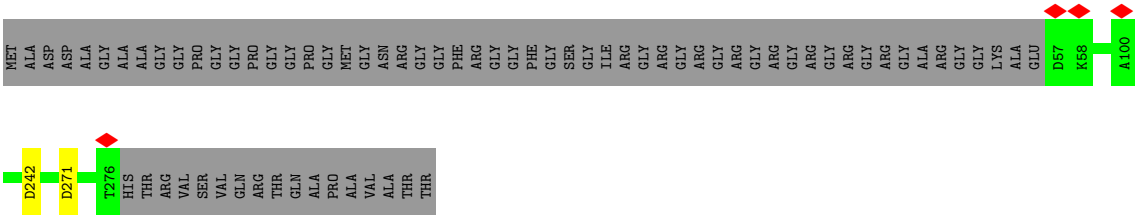
• Molecule 21: 40S ribosomal protein S21

Chain K:



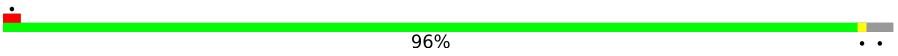
• Molecule 22: 40S ribosomal protein S2

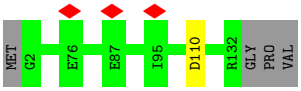
Chain L:



• Molecule 23: 40S ribosomal protein S17

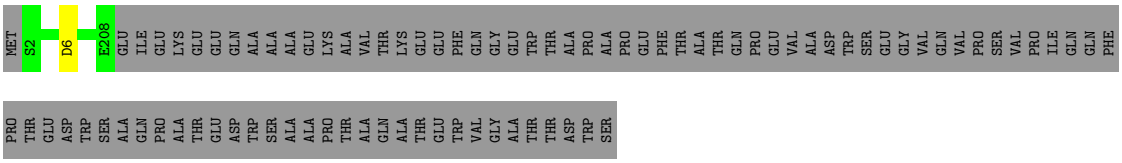
Chain M:





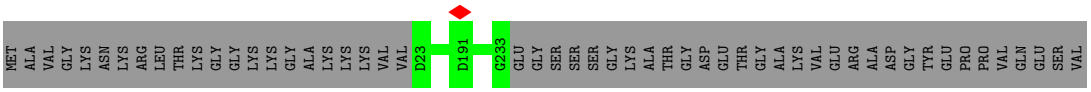
• Molecule 24: 40S ribosomal protein SA

Chain N:



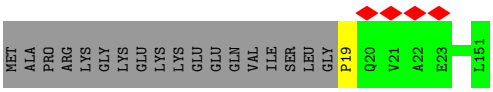
• Molecule 25: 40S ribosomal protein S3a

Chain O:



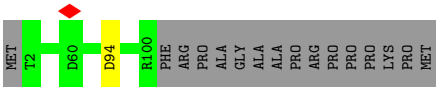
• Molecule 26: 40S ribosomal protein S14

Chain P:



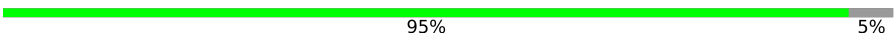
• Molecule 27: 40S ribosomal protein S26

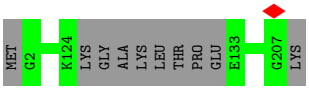
Chain Q:



• Molecule 28: 40S ribosomal protein S8

Chain R:



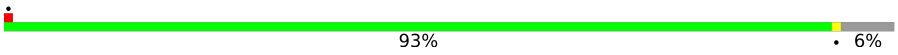


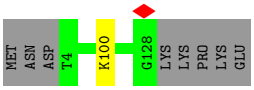
• Molecule 29: 40S ribosomal protein S6

Chain S:

• Molecule 30: 40S ribosomal protein S24

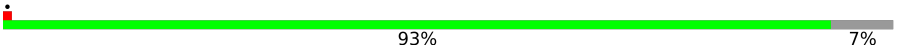
Chain T:

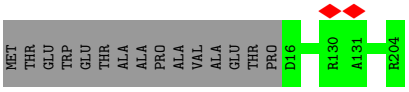




• Molecule 31: 40S ribosomal protein S5

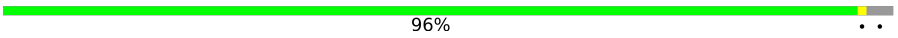
Chain V:

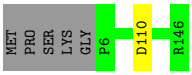




• Molecule 32: 40S ribosomal protein S16

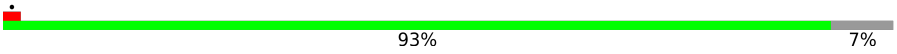
Chain Y:

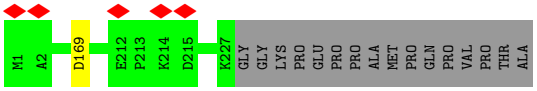




• Molecule 33: 40S ribosomal protein S3

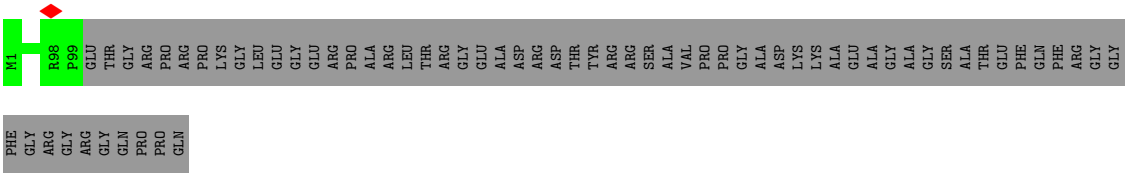
Chain Z:





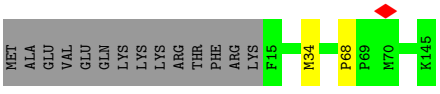
• Molecule 34: 40S ribosomal protein S10

Chain a:



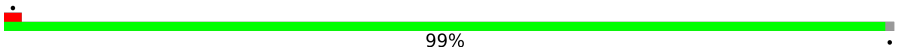
• Molecule 35: 40S ribosomal protein S15

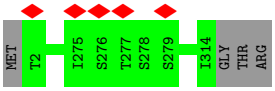
Chain b:



• Molecule 36: Receptor of activated protein C kinase 1

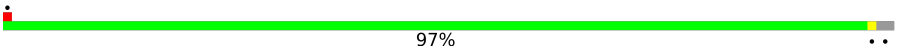
Chain c:

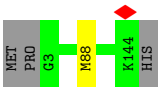




• Molecule 37: 40S ribosomal protein S19

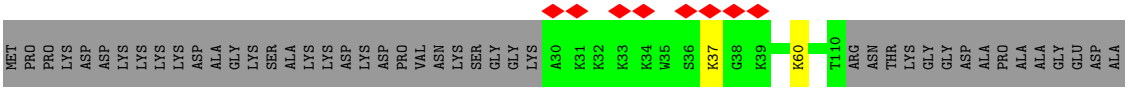
Chain d:





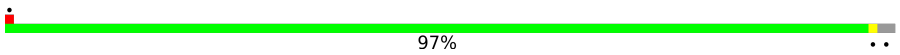
• Molecule 38: 40S ribosomal protein S25

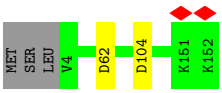
Chain e:



• Molecule 39: 40S ribosomal protein S18

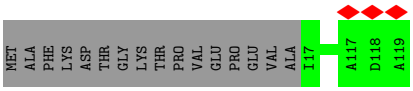
Chain f:





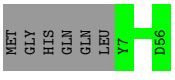
• Molecule 40: 40S ribosomal protein S20

Chain h:



• Molecule 41: 40S ribosomal protein S29

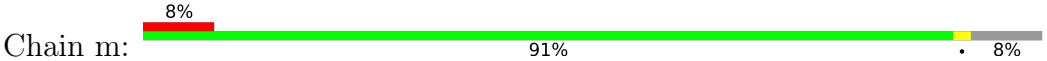
Chain i:

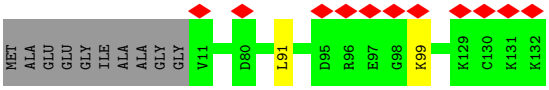


• Molecule 42: Ubiquitin

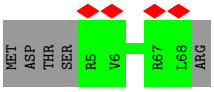
Chain k:

• Molecule 43: 40S ribosomal protein S12

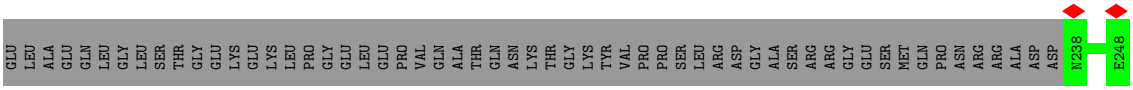


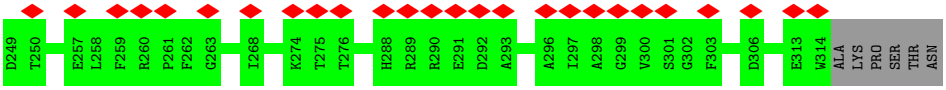


• Molecule 44: 40S ribosomal protein S28

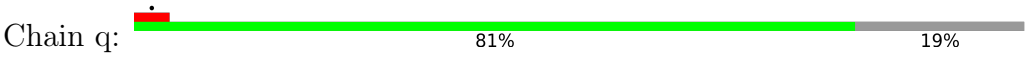


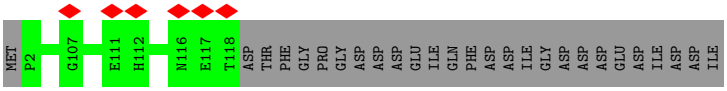
• Molecule 45: Eukaryotic translation initiation factor 3 subunit G



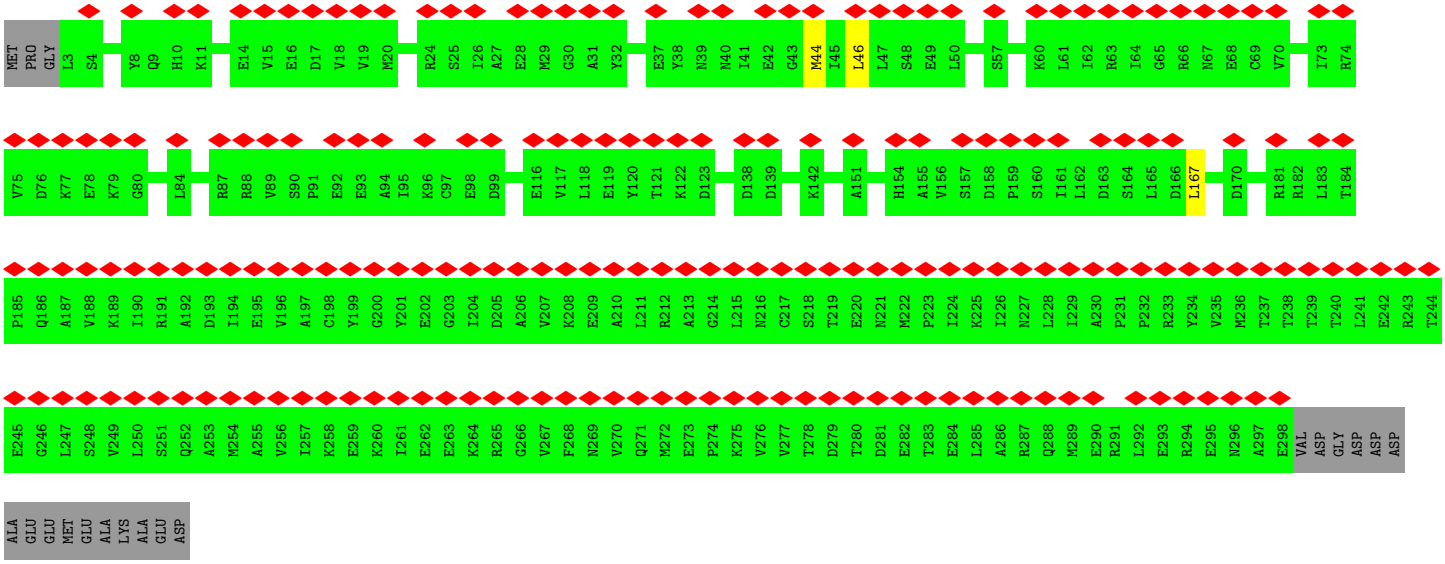


• Molecule 46: Eukaryotic translation initiation factor 1A, X-chromosomal



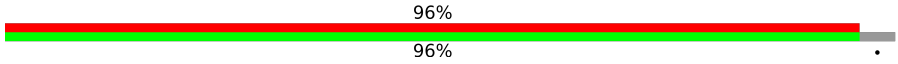


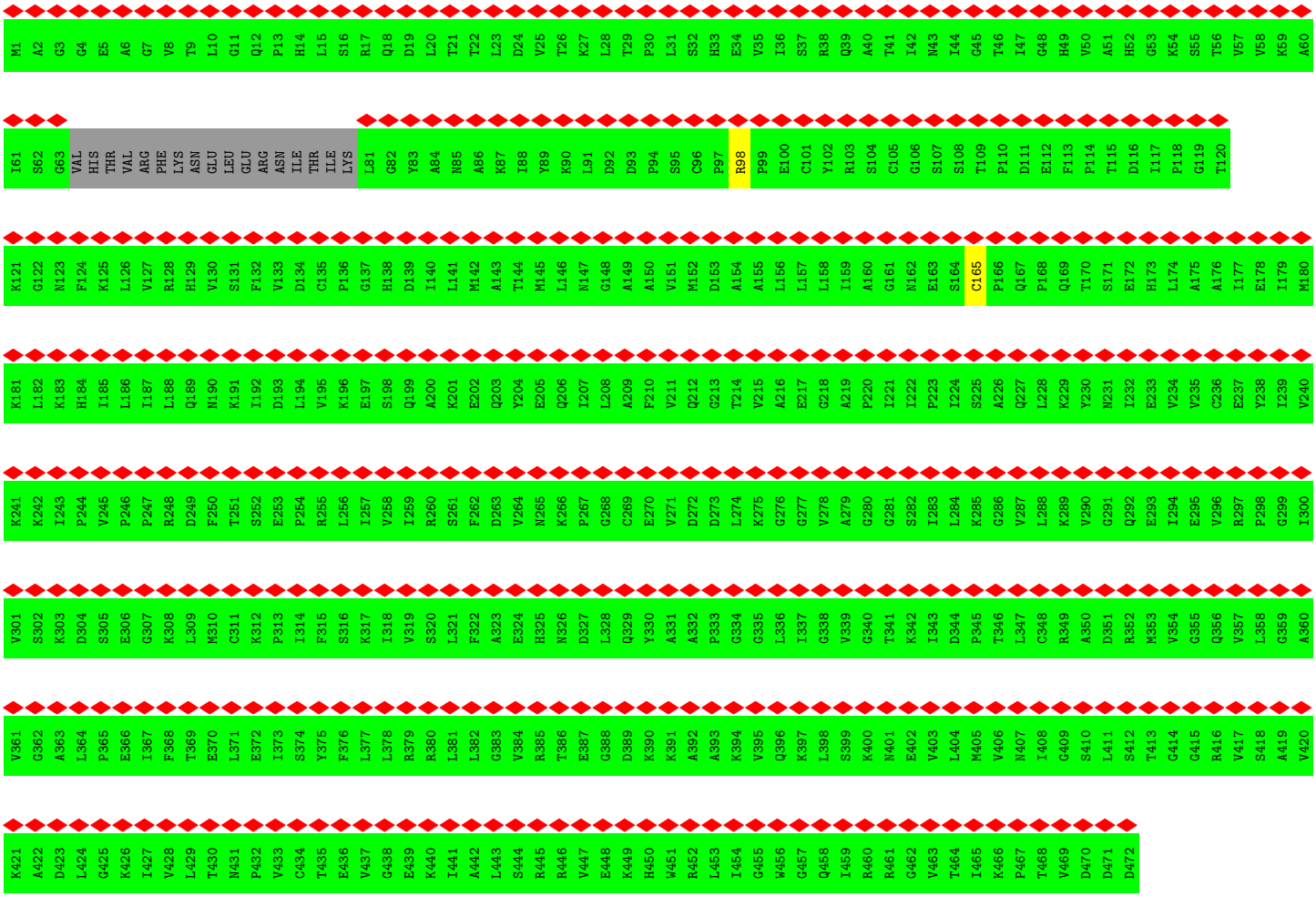
• Molecule 47: Eukaryotic translation initiation factor 2 subunit 1



• Molecule 48: Eukaryotic translation initiation factor 2 subunit 3

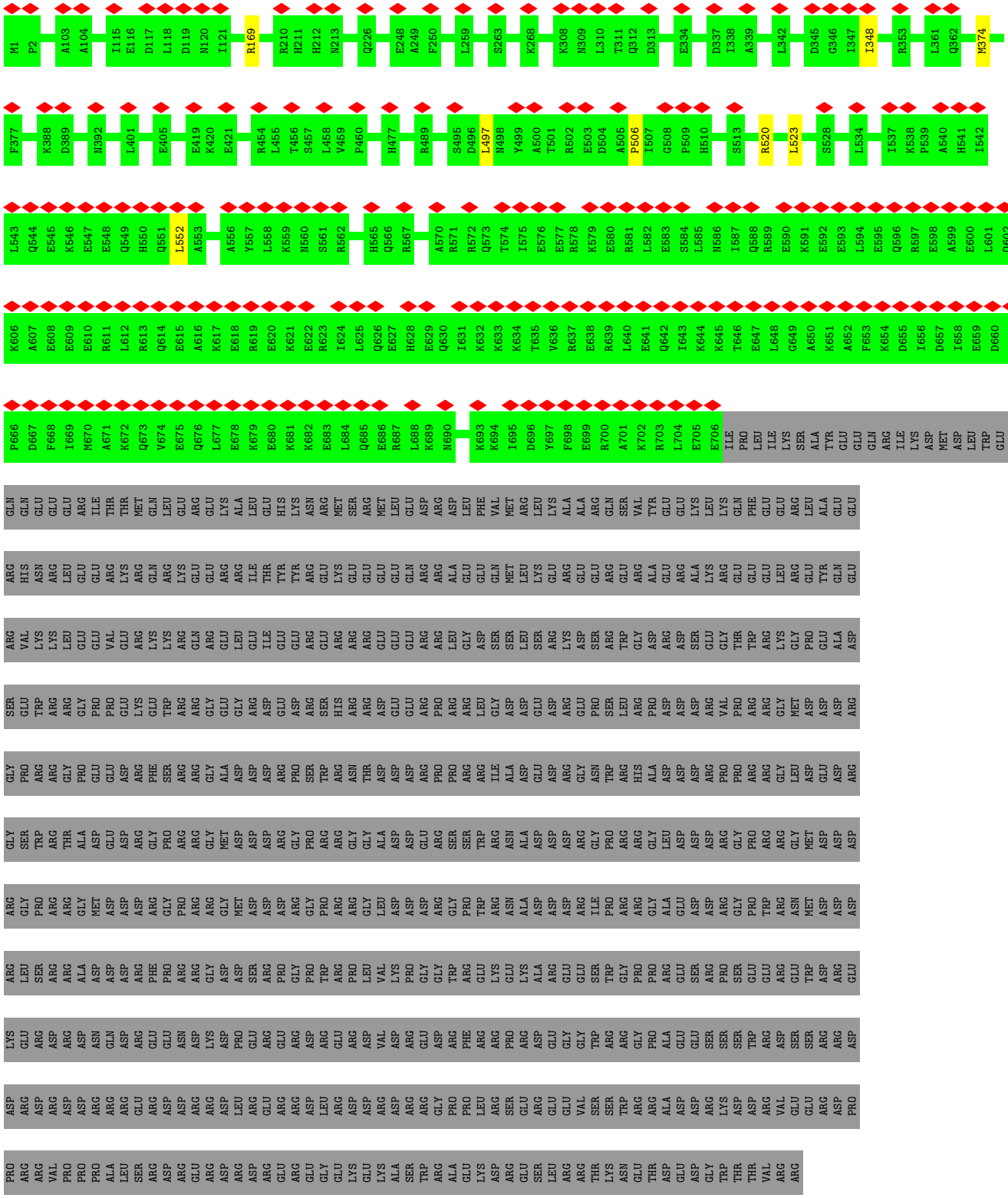
Chain t:



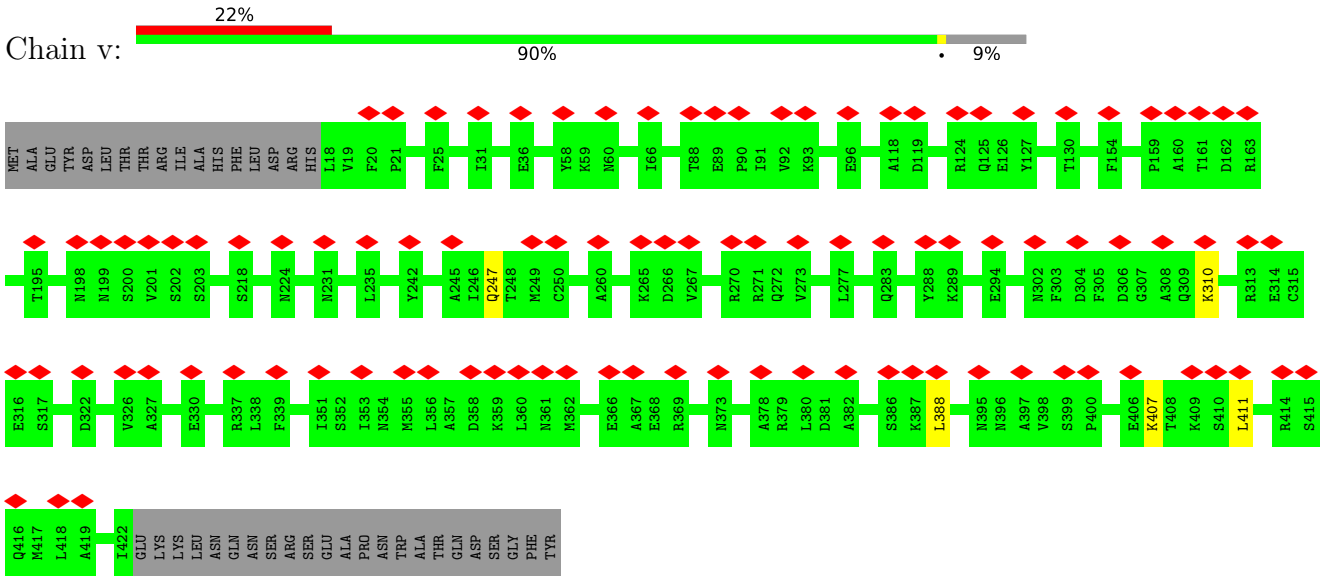


• Molecule 49: Eukaryotic translation initiation factor 3 subunit A

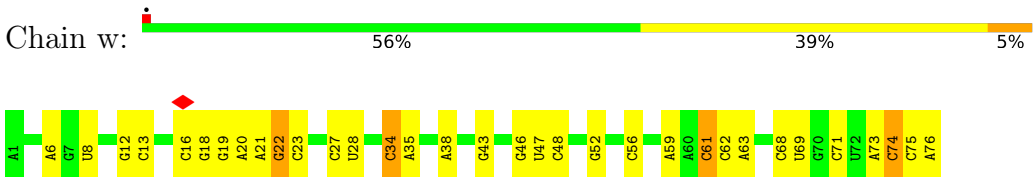
Chain u:



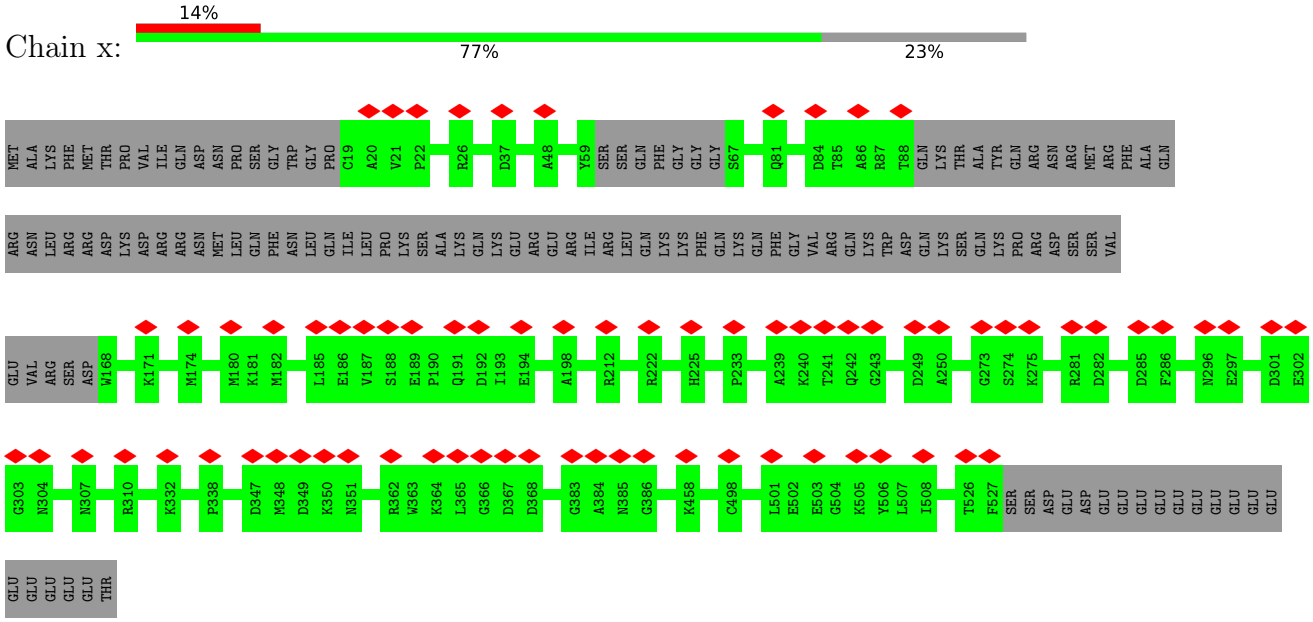
• Molecule 50: Eukaryotic translation initiation factor 3 subunit E



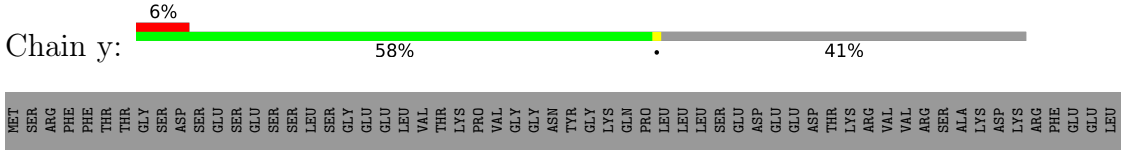
• Molecule 51: Initiator Met-tRNA-i

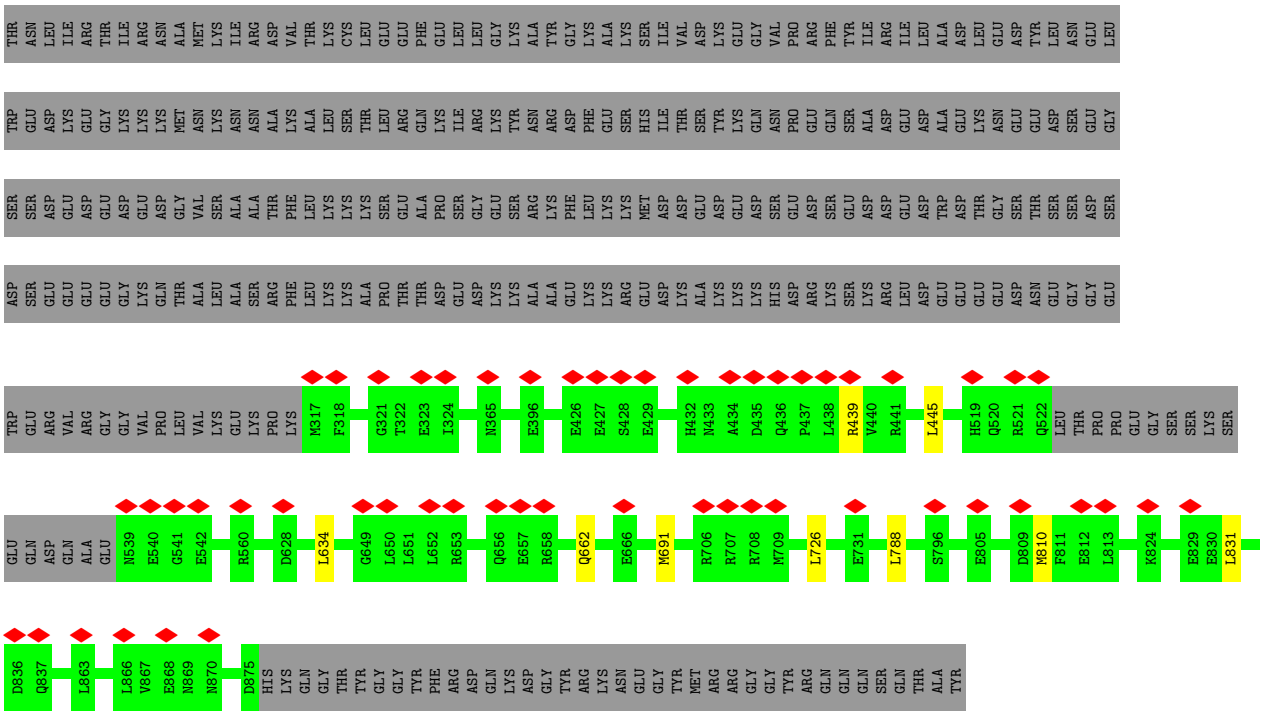


• Molecule 52: Eukaryotic translation initiation factor 3 subunit D



• Molecule 53: Eukaryotic translation initiation factor 3 subunit C




THR ASN LEU ILE ARG THR ILE ARG ASN ALA MET LYS ILE ARG ASP VAL THR LYS CYS LEU GLU GLU PHE GLU LEU LEU GLY LYS ALA TYR GLY LYS ALA LYS SER ILE VAL ASP LYS GLU GLY VAL PRO ARG PHE TYR ILE ARG ILE LEU ALA ASP LEU GLU ASP TYR LEU ASN GLU LEU
TRP GLU ASP LYS GLU GLY LYS LYS LYS MET ASN LYS ASN ASN ALA LYS ALA LEU SER THR LEU ARG GLN LYS ILE ARG LYS TYR ASN ARG ASP PHE GLU SER HIS ILE THR SER TYR LYS GLN ASN PRO GLU GLN SER ALA ASP GLU ASP ALA GLU LYS ASN GLU GLU ASP SER GLU GLY
SER SER ASP GLU ASP GLU ASP GLU ASP GLY VAL SER ALA ALA THR PHE LEU LYS LYS LYS SER GLU ALA PRO SER GLY GLU SER ARG LYS PHE LEU LYS LYS SER GLU ASP ASP GLU ASP GLU ASP SER GLU ASP SER GLU ASP ASP ASP GLU ASP TRP ASP THR GLY SER THR SER SER ASP SER
ASP SER GLU GLU GLU GLU GLY LYS GLN THR ALA LEU ALA SER ARG PHE LEU LYS LYS ALA PRO THR THR ASP GLU ASP LYS LYS ALA ALA GLU LYS LYS LYS ARG GLU ASP LYS ALA LYS LYS LYS HIS ASP ARG LYS SER LYS ARG LEU ASP GLU GLU GLU GLU ASP ASN GLU GLY GLY GLU
TRP GLU ARG VAL ARG GLY GLY VAL PRO LEU VAL LYS GLU LYS PRO LYS M317 F318 G321 T322 E323 I324 N365 E396 E426 E427 S428 E429 H432 N433 A434 D435 Q436 P437 L438 R439 V440 R441 L445 H519 Q520 R521 Q522 LEU THR PRO PRO GLU GLY SER SER LYS SER
GLU GLN ASP GLN ALA GLU N539 E540 G541 E542 R560 D628 L634 G649 L650 L651 L652 R653 Q656 E657 R658 Q662 E666 M691 R706 R707 R708 M709 L726 E731 L788 S796 E805 D809 M810 F811 E812 L813 K824 E829 E830 L831
D836 Q837 L863 L866 V867 E868 N869 N870 D875 HIS LYS GLN GLY THR TYR GLY GLY TYR PHE ARG ASP GLN LYS ASP GLY TYR ARG LYS ASN GLU GLY TYR MET ARG ARG GLY GLY TYR ARG GLN GLN GLN SER GLN THR ALA TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46318	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	22.337	Depositor
Minimum map value	-6.543	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	417.74402, 417.74402, 417.74402	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96700007, 0.96700007, 0.96700007	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: OMC, A2M, PSU, UR3, JMH, ZN, NA, 5MU, B8N, MG, GTP, 6MZ, 5MC, OMG, OMU, MA6

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	0	0.31	0/5002	0.62	2/6743 (0.0%)
2	1	0.28	0/3279	0.59	0/4534
3	2	0.26	0/1491	0.49	0/2068
4	3	0.24	0/1055	0.37	0/1469
5	4	0.25	0/1269	0.41	0/1762
6	5	0.28	0/4458	0.59	3/6027 (0.0%)
7	6	0.29	0/2212	0.58	2/3034 (0.1%)
8	7	0.44	4/1365 (0.3%)	0.91	3/2124 (0.1%)
9	8	0.25	0/1572	0.43	0/2187
10	9	0.32	0/231	0.82	0/294
11	A	0.40	0/41130	1.00	147/64100 (0.2%)
12	B	0.30	0/1186	0.57	0/1585
13	C	0.30	0/2077	0.64	1/2796 (0.0%)
14	D	0.30	0/1502	0.65	0/2008
15	E	0.31	0/1105	0.62	0/1476
16	F	0.30	0/459	0.65	0/607
17	G	0.31	0/1451	0.71	3/1942 (0.2%)
18	H	0.31	0/644	0.61	0/864
19	I	0.29	0/1232	0.61	1/1656 (0.1%)
20	J	0.31	0/1051	0.65	1/1406 (0.1%)
21	K	0.31	0/623	0.66	0/833
22	L	0.33	0/1743	0.65	2/2354 (0.1%)
23	M	0.35	0/1078	0.72	1/1447 (0.1%)
24	N	0.32	0/1670	0.66	1/2271 (0.0%)
25	O	0.30	0/1742	0.62	0/2330
26	P	0.36	0/1010	0.76	1/1353 (0.1%)
27	Q	0.31	0/805	0.68	1/1079 (0.1%)
28	R	0.28	0/1654	0.58	0/2203
29	S	0.28	0/1885	0.62	1/2510 (0.0%)
30	T	0.36	0/1032	0.67	0/1371
31	V	0.30	0/1516	0.63	0/2037
32	Y	0.31	0/1142	0.67	1/1528 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Z	0.31	0/1793	0.61	1/2414 (0.0%)
34	a	0.31	0/859	0.61	0/1159
35	b	0.33	0/1094	0.71	2/1464 (0.1%)
36	c	0.29	0/2493	0.60	0/3394
37	d	0.29	0/1123	0.62	1/1504 (0.1%)
38	e	0.41	0/657	0.62	0/878
39	f	0.30	0/1245	0.70	2/1665 (0.1%)
40	h	0.32	0/827	0.72	0/1110
41	i	0.33	0/429	0.63	0/568
42	k	0.43	0/566	0.81	1/753 (0.1%)
43	m	0.33	0/960	0.70	1/1286 (0.1%)
44	n	0.30	0/508	0.73	0/680
45	o	0.29	0/628	0.66	0/846
46	q	0.30	0/965	0.64	0/1282
47	r	0.31	0/2167	0.63	3/2943 (0.1%)
48	t	0.29	0/3494	0.64	1/4726 (0.0%)
49	u	0.31	0/5475	0.68	6/7432 (0.1%)
50	v	0.31	0/2778	0.67	3/3797 (0.1%)
51	w	0.42	0/1795	1.18	11/2798 (0.4%)
52	x	0.27	0/2885	0.58	0/3940
53	y	0.32	0/4436	0.70	7/5989 (0.1%)
All	All	0.34	4/126848 (0.0%)	0.80	210/180626 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	7	-34	C	C1'-N1	5.96	1.57	1.48
8	7	-25	C	C1'-N1	5.67	1.57	1.48
8	7	-31	C	C1'-N1	5.44	1.56	1.48
8	7	-22	C	C1'-N1	5.34	1.56	1.48

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	501	C	C2-N1-C1'	12.16	132.17	118.80
11	A	501	C	N1-C2-O2	11.96	126.07	118.90
11	A	882	U	N1-C2-O2	10.08	129.85	122.80
11	A	537	C	N3-C2-O2	-9.94	114.94	121.90
11	A	1453	C	N1-C2-O2	9.93	124.86	118.90
11	A	888	U	C2-N1-C1'	9.66	129.29	117.70
11	A	1115	U	C2-N1-C1'	9.43	129.01	117.70
11	A	1115	U	N1-C2-O2	9.33	129.33	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1453	C	C2-N1-C1'	9.31	129.04	118.80
51	w	74	C	N1-C2-O2	8.94	124.26	118.90
11	A	501	C	N3-C2-O2	-8.91	115.66	121.90
11	A	1115	U	N3-C2-O2	-8.88	115.98	122.20
11	A	501	C	C6-N1-C1'	-8.86	110.17	120.80
11	A	537	C	N1-C2-O2	8.69	124.12	118.90
51	w	74	C	N3-C2-O2	-8.65	115.85	121.90
11	A	1752	C	N1-C2-O2	8.62	124.07	118.90
11	A	882	U	N3-C2-O2	-8.61	116.18	122.20
11	A	556	U	C2-N1-C1'	8.57	127.99	117.70
51	w	74	C	C6-N1-C2	-8.49	116.90	120.30
11	A	882	U	C2-N1-C1'	8.48	127.88	117.70
11	A	888	U	N1-C2-O2	8.15	128.50	122.80
11	A	1752	C	C2-N1-C1'	8.09	127.69	118.80
11	A	888	U	N3-C2-O2	-8.01	116.59	122.20
35	b	68	PRO	CA-N-CD	-7.89	100.45	111.50
6	5	388	LEU	CA-CB-CG	7.76	133.14	115.30
19	I	32	ASP	CB-CG-OD1	7.75	125.27	118.30
11	A	706	U	C2-N1-C1'	7.72	126.97	117.70
11	A	556	U	N1-C2-O2	7.68	128.18	122.80
49	u	523	LEU	CA-CB-CG	7.61	132.81	115.30
53	y	726	LEU	CA-CB-CG	7.60	132.79	115.30
11	A	537	C	C6-N1-C2	-7.56	117.28	120.30
11	A	1520	G	C4-N9-C1'	7.56	136.32	126.50
11	A	1597	C	N3-C2-O2	-7.53	116.63	121.90
11	A	556	U	N3-C2-O2	-7.52	116.93	122.20
11	A	1453	C	N3-C2-O2	-7.52	116.64	121.90
39	f	104	ASP	CB-CG-OD1	7.49	125.04	118.30
22	L	242	ASP	CB-CG-OD1	7.46	125.02	118.30
11	A	729	C	C5-C6-N1	7.46	124.73	121.00
11	A	1139	C	C2-N1-C1'	7.43	126.97	118.80
11	A	706	U	N1-C2-O2	7.41	127.99	122.80
11	A	731	G	P-O3'-C3'	7.25	128.40	119.70
11	A	1022	U	C2-N1-C1'	7.22	126.37	117.70
7	6	352	ASP	CB-CG-OD1	7.15	124.73	118.30
51	w	22	G	P-O3'-C3'	7.11	128.24	119.70
8	7	-31	C	P-O3'-C3'	7.11	128.23	119.70
11	A	537	C	C2-N1-C1'	7.07	126.58	118.80
11	A	1597	C	N1-C2-O2	7.06	123.13	118.90
32	Y	110	ASP	CB-CG-OD1	7.04	124.64	118.30
17	G	159	ASP	CB-CG-OD1	7.01	124.61	118.30
33	Z	169	ASP	CB-CG-OD1	6.97	124.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	321	C	C2-N1-C1'	6.95	126.44	118.80
11	A	1752	C	N3-C2-O2	-6.92	117.06	121.90
11	A	965	U	N1-C2-O2	6.90	127.63	122.80
11	A	510	G	C8-N9-C4	-6.76	103.70	106.40
11	A	739	C	O5'-P-OP1	-6.73	99.64	105.70
11	A	1520	G	C8-N9-C1'	-6.72	118.26	127.00
11	A	706	U	N3-C2-O2	-6.72	117.49	122.20
11	A	707	C	C6-N1-C2	-6.70	117.62	120.30
17	G	32	MET	CA-CB-CG	6.70	124.68	113.30
11	A	1422	G	N3-C4-N9	6.63	129.98	126.00
11	A	501	C	C6-N1-C2	-6.61	117.65	120.30
27	Q	94	ASP	CB-CG-OD1	6.60	124.24	118.30
11	A	710	C	C5-C6-N1	6.60	124.30	121.00
11	A	501	C	C5-C6-N1	6.57	124.29	121.00
26	P	19	PRO	CA-N-CD	-6.57	102.30	111.50
11	A	836	G	C4-N9-C1'	6.50	134.96	126.50
11	A	1687	C	C6-N1-C2	-6.50	117.70	120.30
24	N	6	ASP	CB-CG-OD1	6.49	124.14	118.30
11	A	706	U	C5-C6-N1	6.49	125.94	122.70
11	A	1453	C	C6-N1-C1'	-6.47	113.04	120.80
11	A	1520	G	N3-C4-N9	6.47	129.88	126.00
39	f	62	ASP	CB-CG-OD1	6.46	124.12	118.30
8	7	-21	A	P-O3'-C3'	6.46	127.45	119.70
11	A	1422	G	C4-N9-C1'	6.46	134.89	126.50
11	A	723	C	N1-C2-O2	6.45	122.77	118.90
11	A	1139	C	N1-C2-O2	6.43	122.75	118.90
11	A	836	G	N3-C4-C5	-6.42	125.39	128.60
11	A	1261	C	N1-C2-O2	6.42	122.75	118.90
11	A	965	U	N3-C2-O2	-6.36	117.75	122.20
11	A	836	G	N3-C4-N9	6.32	129.79	126.00
11	A	168	C	N1-C2-O2	6.28	122.67	118.90
51	w	61	C	C2-N1-C1'	6.27	125.70	118.80
51	w	56	C	C5-C6-N1	6.27	124.13	121.00
37	d	88	MET	CA-CB-CG	6.22	123.88	113.30
51	w	34	C	C2-N1-C1'	6.15	125.57	118.80
23	M	110	ASP	CB-CG-OD1	6.09	123.78	118.30
11	A	1422	G	N3-C4-C5	-6.09	125.56	128.60
7	6	326	ASP	CB-CG-OD1	6.08	123.77	118.30
11	A	965	U	C2-N1-C1'	6.08	125.00	117.70
53	y	634	LEU	CA-CB-CG	6.07	129.25	115.30
11	A	710	C	C6-N1-C2	-6.05	117.88	120.30
11	A	888	U	C6-N1-C1'	-6.05	112.73	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1202	MET	CA-CB-CG	6.03	123.55	113.30
11	A	1453	C	C6-N1-C2	-6.02	117.89	120.30
11	A	1115	U	C6-N1-C1'	-6.02	112.78	121.20
6	5	277	LEU	CA-CB-CG	6.00	129.11	115.30
47	r	167	LEU	CA-CB-CG	6.00	129.10	115.30
47	r	44	MET	CA-CB-CG	5.99	123.49	113.30
11	A	708	C	C2-N1-C1'	5.99	125.39	118.80
11	A	707	C	C5-C6-N1	5.96	123.98	121.00
11	A	644	OMG	O3'-P-O5'	5.96	115.32	104.00
11	A	729	C	C6-N1-C2	-5.95	117.92	120.30
11	A	1756	C	N1-C2-O2	5.94	122.47	118.90
50	v	411	LEU	CA-CB-CG	5.90	128.87	115.30
8	7	-2	C	N1-C2-O2	5.88	122.43	118.90
11	A	1	U	OP1-P-O3'	5.86	118.09	105.20
51	w	56	C	C2-N1-C1'	5.86	125.24	118.80
11	A	1139	C	N3-C2-O2	-5.85	117.80	121.90
11	A	1687	C	C5-C6-N1	5.84	123.92	121.00
11	A	178	C	N1-C2-O2	5.83	122.40	118.90
11	A	201	C	N1-C2-O2	5.83	122.40	118.90
11	A	1453	C	C5-C6-N1	5.83	123.92	121.00
11	A	719	G	N7-C8-N9	5.81	116.00	113.10
11	A	1752	C	C6-N1-C1'	-5.80	113.83	120.80
20	J	38	LEU	CA-CB-CG	5.80	128.64	115.30
51	w	27	C	N1-C2-O2	5.79	122.38	118.90
11	A	735	C	C5-C6-N1	5.72	123.86	121.00
11	A	879	C	C2-N1-C1'	5.72	125.09	118.80
11	A	659	G	C4-N9-C1'	5.71	133.93	126.50
11	A	797	C	P-O3'-C3'	5.70	126.55	119.70
11	A	700	G	N3-C4-N9	5.70	129.42	126.00
11	A	708	C	C5-C6-N1	5.70	123.85	121.00
11	A	1271	C	N1-C2-O2	5.70	122.32	118.90
11	A	291	G	P-O3'-C3'	5.70	126.53	119.70
11	A	728	C	C6-N1-C2	-5.69	118.02	120.30
11	A	882	U	C6-N1-C1'	-5.66	113.28	121.20
13	C	19	MET	CG-SD-CE	-5.64	91.17	100.20
1	0	869	MET	CA-CB-CG	5.64	122.89	113.30
11	A	728	C	C5-C6-N1	5.64	123.82	121.00
11	A	1578	U	N3-C2-O2	-5.60	118.28	122.20
11	A	888	U	C5-C6-N1	5.59	125.50	122.70
11	A	1422	G	C8-N9-C1'	-5.58	119.74	127.00
53	y	831	LEU	CA-CB-CG	5.57	128.12	115.30
11	A	632	C	C2-N1-C1'	5.57	124.92	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1139	C	C6-N1-C2	-5.56	118.08	120.30
11	A	719	G	C8-N9-C4	-5.55	104.18	106.40
11	A	1600	G	P-O3'-C3'	5.55	126.36	119.70
11	A	1172	U	C2-N1-C1'	5.55	124.36	117.70
11	A	368	U	P-O3'-C3'	5.54	126.35	119.70
11	A	700	G	C6-C5-N7	-5.52	127.09	130.40
49	u	552	LEU	CA-CB-CG	5.51	127.98	115.30
11	A	1565	C	C2-N1-C1'	5.50	124.85	118.80
17	G	148	LEU	CA-CB-CG	5.47	127.89	115.30
11	A	130	G	C4-N9-C1'	5.46	133.60	126.50
11	A	1022	U	C6-N1-C1'	-5.46	113.56	121.20
11	A	1591	C	N1-C2-O2	5.45	122.17	118.90
11	A	882	U	C5-C6-N1	5.44	125.42	122.70
11	A	836	G	C8-N9-C1'	-5.42	119.95	127.00
11	A	732	U	O5'-P-OP1	-5.42	100.82	105.70
11	A	1116	C	N1-C2-O2	5.42	122.15	118.90
51	w	56	C	N1-C2-O2	5.40	122.14	118.90
11	A	688	U	P-O3'-C3'	5.38	126.16	119.70
53	y	810	MET	CA-CB-CG	5.35	122.39	113.30
11	A	725	C	C6-N1-C2	-5.34	118.16	120.30
11	A	556	U	C6-N1-C1'	-5.34	113.73	121.20
11	A	1556	A	C2-N3-C4	5.33	113.27	110.60
11	A	1520	G	N3-C4-C5	-5.33	125.94	128.60
11	A	321	C	N1-C2-O2	5.32	122.09	118.90
11	A	1261	C	N3-C2-O2	-5.32	118.17	121.90
11	A	509	OMG	O3'-P-O5'	5.32	114.11	104.00
11	A	666	U	C2-N1-C1'	5.32	124.08	117.70
11	A	1115	U	C5-C6-N1	5.29	125.35	122.70
50	v	388	LEU	CA-CB-CG	5.28	127.45	115.30
49	u	497	LEU	CA-CB-CG	5.28	127.44	115.30
11	A	1078	C	C6-N1-C2	-5.27	118.19	120.30
11	A	1172	U	N1-C2-O2	5.27	126.49	122.80
6	5	327	ARG	CA-CB-CG	5.27	124.98	113.40
42	k	132	MET	CA-CB-CG	5.26	122.25	113.30
11	A	1389	C	C2-N1-C1'	5.26	124.58	118.80
11	A	695	C	N3-C2-O2	-5.25	118.23	121.90
35	b	34	MET	CA-CB-CG	5.23	122.19	113.30
11	A	739	C	C6-N1-C2	-5.23	118.21	120.30
11	A	1600	G	OP1-P-O3'	5.23	116.70	105.20
11	A	1261	C	C2-N1-C1'	5.22	124.54	118.80
11	A	494	C	N1-C2-O2	5.21	122.03	118.90
47	r	46	LEU	CA-CB-CG	5.21	127.29	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	723	C	N3-C2-O2	-5.20	118.26	121.90
11	A	1078	C	C2-N1-C1'	5.20	124.52	118.80
11	A	130	G	N3-C4-N9	5.19	129.11	126.00
49	u	348	ILE	CG1-CB-CG2	-5.19	99.98	111.40
22	L	271	ASP	CB-CG-OD1	5.18	122.96	118.30
11	A	706	U	C6-N1-C2	-5.17	117.90	121.00
11	A	1078	C	N1-C2-O2	5.16	122.00	118.90
50	v	247	GLN	CA-CB-CG	5.16	124.76	113.40
11	A	738	C	N3-C2-O2	-5.16	118.29	121.90
48	t	165	CYS	CA-CB-SG	5.15	123.27	114.00
11	A	1687	C	C2-N1-C1'	5.14	124.46	118.80
11	A	566	U	C2-N1-C1'	5.14	123.86	117.70
11	A	1578	U	N1-C2-O2	5.13	126.39	122.80
11	A	1078	C	N3-C2-O2	-5.12	118.32	121.90
11	A	1139	C	O4'-C1'-N1	5.11	112.29	108.20
43	m	91	LEU	CA-CB-CG	5.10	127.03	115.30
11	A	731	G	OP1-P-O3'	5.10	116.41	105.20
11	A	1416	C	N1-C2-O2	5.10	121.96	118.90
11	A	725	C	C5-C6-N1	5.09	123.55	121.00
53	y	445	LEU	CB-CG-CD1	-5.09	102.35	111.00
49	u	506	PRO	CA-N-CD	-5.09	104.38	111.50
11	A	537	C	O4'-C1'-N1	5.08	112.27	108.20
11	A	888	U	C6-N1-C2	-5.07	117.96	121.00
51	w	61	C	N1-C2-O2	5.07	121.94	118.90
11	A	556	U	C5-C6-N1	5.06	125.23	122.70
11	A	130	G	N3-C4-C5	-5.06	126.07	128.60
29	S	122	PRO	CA-N-CD	-5.05	104.43	111.50
11	A	321	C	C6-N1-C2	-5.05	118.28	120.30
53	y	691	MET	CA-CB-CG	5.04	121.87	113.30
53	y	788	LEU	CA-CB-CG	5.04	126.89	115.30
11	A	1600	G	N3-C4-N9	5.03	129.02	126.00
49	u	374	MET	CA-CB-CG	5.03	121.85	113.30
11	A	723	C	C2-N1-C1'	5.02	124.33	118.80
11	A	1683	C	N1-C2-O2	5.01	121.91	118.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	0	619/1220 (51%)	587 (95%)	32 (5%)	0	100	100
2	1	584/814 (72%)	539 (92%)	45 (8%)	0	100	100
3	2	300/325 (92%)	291 (97%)	9 (3%)	0	100	100
4	3	209/218 (96%)	202 (97%)	7 (3%)	0	100	100
5	4	251/357 (70%)	238 (95%)	13 (5%)	0	100	100
6	5	518/564 (92%)	501 (97%)	17 (3%)	0	100	100
7	6	360/374 (96%)	338 (94%)	22 (6%)	0	100	100
9	8	313/352 (89%)	290 (93%)	23 (7%)	0	100	100
10	9	22/25 (88%)	22 (100%)	0	0	100	100
12	B	138/158 (87%)	135 (98%)	3 (2%)	0	100	100
13	C	254/263 (97%)	248 (98%)	6 (2%)	0	100	100
14	D	175/194 (90%)	168 (96%)	7 (4%)	0	100	100
15	E	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
16	F	56/133 (42%)	47 (84%)	9 (16%)	0	100	100
17	G	171/194 (88%)	164 (96%)	7 (4%)	0	100	100
18	H	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
19	I	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
20	J	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
21	K	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
22	L	218/293 (74%)	210 (96%)	8 (4%)	0	100	100
23	M	129/135 (96%)	123 (95%)	6 (5%)	0	100	100
24	N	205/295 (70%)	197 (96%)	8 (4%)	0	100	100
25	O	209/264 (79%)	203 (97%)	6 (3%)	0	100	100
26	P	131/151 (87%)	123 (94%)	8 (6%)	0	100	100
27	Q	97/115 (84%)	96 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	R	194/208 (93%)	190 (98%)	4 (2%)	0	100	100
29	S	228/249 (92%)	221 (97%)	7 (3%)	0	100	100
30	T	123/133 (92%)	123 (100%)	0	0	100	100
31	V	187/204 (92%)	178 (95%)	9 (5%)	0	100	100
32	Y	139/146 (95%)	132 (95%)	7 (5%)	0	100	100
33	Z	225/243 (93%)	222 (99%)	3 (1%)	0	100	100
34	a	97/165 (59%)	94 (97%)	3 (3%)	0	100	100
35	b	129/145 (89%)	122 (95%)	7 (5%)	0	100	100
36	c	311/317 (98%)	295 (95%)	16 (5%)	0	100	100
37	d	140/145 (97%)	134 (96%)	6 (4%)	0	100	100
38	e	79/125 (63%)	73 (92%)	6 (8%)	0	100	100
39	f	147/152 (97%)	138 (94%)	9 (6%)	0	100	100
40	h	101/119 (85%)	92 (91%)	9 (9%)	0	100	100
41	i	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
42	k	66/156 (42%)	61 (92%)	5 (8%)	0	100	100
43	m	120/132 (91%)	114 (95%)	6 (5%)	0	100	100
44	n	62/69 (90%)	57 (92%)	5 (8%)	0	100	100
45	o	75/320 (23%)	72 (96%)	3 (4%)	0	100	100
46	q	116/144 (81%)	111 (96%)	5 (4%)	0	100	100
47	r	294/315 (93%)	275 (94%)	19 (6%)	0	100	100
48	t	451/472 (96%)	439 (97%)	12 (3%)	0	100	100
49	u	705/1382 (51%)	656 (93%)	49 (7%)	0	100	100
50	v	403/445 (91%)	369 (92%)	34 (8%)	0	100	100
52	x	417/548 (76%)	394 (94%)	23 (6%)	0	100	100
53	y	539/913 (59%)	514 (95%)	25 (5%)	0	100	100
All	All	10926/14338 (76%)	10398 (95%)	528 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	0	546/1081 (50%)	545 (100%)	1 (0%)	93 98
2	1	97/702 (14%)	97 (100%)	0	100 100
6	5	477/515 (93%)	477 (100%)	0	100 100
7	6	112/335 (33%)	112 (100%)	0	100 100
9	8	1/310 (0%)	1 (100%)	0	100 100
10	9	23/24 (96%)	23 (100%)	0	100 100
12	B	129/142 (91%)	128 (99%)	1 (1%)	81 93
13	C	220/225 (98%)	220 (100%)	0	100 100
14	D	158/168 (94%)	158 (100%)	0	100 100
15	E	112/115 (97%)	112 (100%)	0	100 100
16	F	46/104 (44%)	46 (100%)	0	100 100
17	G	159/174 (91%)	159 (100%)	0	100 100
18	H	73/76 (96%)	73 (100%)	0	100 100
19	I	130/131 (99%)	130 (100%)	0	100 100
20	J	112/113 (99%)	112 (100%)	0	100 100
21	K	65/67 (97%)	65 (100%)	0	100 100
22	L	186/225 (83%)	186 (100%)	0	100 100
23	M	119/122 (98%)	119 (100%)	0	100 100
24	N	173/243 (71%)	173 (100%)	0	100 100
25	O	192/231 (83%)	192 (100%)	0	100 100
26	P	104/119 (87%)	104 (100%)	0	100 100
27	Q	86/98 (88%)	86 (100%)	0	100 100
28	R	172/180 (96%)	172 (100%)	0	100 100
29	S	200/218 (92%)	199 (100%)	1 (0%)	88 95
30	T	107/115 (93%)	106 (99%)	1 (1%)	78 91
31	V	159/170 (94%)	159 (100%)	0	100 100
32	Y	117/121 (97%)	117 (100%)	0	100 100
33	Z	190/202 (94%)	190 (100%)	0	100 100
34	a	90/136 (66%)	90 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	b	117/130 (90%)	117 (100%)	0	100 100
36	c	272/275 (99%)	272 (100%)	0	100 100
37	d	112/115 (97%)	112 (100%)	0	100 100
38	e	71/103 (69%)	69 (97%)	2 (3%)	43 74
39	f	129/132 (98%)	129 (100%)	0	100 100
40	h	94/107 (88%)	94 (100%)	0	100 100
41	i	44/49 (90%)	44 (100%)	0	100 100
42	k	61/140 (44%)	59 (97%)	2 (3%)	38 71
43	m	104/108 (96%)	103 (99%)	1 (1%)	76 90
44	n	57/62 (92%)	57 (100%)	0	100 100
45	o	64/277 (23%)	64 (100%)	0	100 100
46	q	100/123 (81%)	100 (100%)	0	100 100
47	r	190/280 (68%)	190 (100%)	0	100 100
48	t	380/397 (96%)	379 (100%)	1 (0%)	92 96
49	u	528/1259 (42%)	526 (100%)	2 (0%)	91 95
50	v	206/406 (51%)	204 (99%)	2 (1%)	76 90
52	x	207/494 (42%)	207 (100%)	0	100 100
53	y	472/811 (58%)	470 (100%)	2 (0%)	91 95
All	All	7563/11730 (64%)	7547 (100%)	16 (0%)	93 98

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	730	MET
12	B	69	ARG
29	S	98	ARG
30	T	100	LYS
38	e	37	LYS
38	e	60	LYS
42	k	85	TYR
42	k	138	ARG
43	m	99	LYS
48	t	98	ARG
49	u	169	ARG
49	u	520	ARG
50	v	310	LYS

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Mol	Chain	Res	Type
50	v	407	LYS
53	y	439	ARG
53	y	662	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	639	HIS
1	0	1103	ASN
2	1	502	GLN
17	G	163	GLN
24	N	113	GLN
32	Y	24	HIS
32	Y	114	GLN
46	q	37	GLN
48	t	39	GLN
49	u	110	GLN
50	v	377	ASN
53	y	701	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1741/1869 (93%)	407 (23%)	13 (0%)
51	w	74/75 (98%)	31 (41%)	0
8	7	56/255 (21%)	37 (66%)	3 (5%)
All	All	1871/2199 (85%)	475 (25%)	16 (0%)

All (475) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-34	C
8	7	-31	C
8	7	-30	A
8	7	-29	A
8	7	-28	C
8	7	-27	A
8	7	-26	A
8	7	-23	A
8	7	-22	C

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Mol	Chain	Res	Type
8	7	-21	A
8	7	-20	A
8	7	-18	G
8	7	-13	A
8	7	-12	A
8	7	-10	A
8	7	-8	A
8	7	-7	G
8	7	-6	A
8	7	-5	C
8	7	-4	C
8	7	-3	A
8	7	1	A
8	7	3	G
8	7	4	G
8	7	5	U
8	7	6	A
8	7	7	C
8	7	10	U
8	7	11	U
8	7	12	C
8	7	13	A
8	7	15	G
8	7	17	C
8	7	19	U
8	7	20	G
8	7	21	A
8	7	22	G
11	A	2	A
11	A	17	C
11	A	23	G
11	A	26	U
11	A	33	G
11	A	44	U
11	A	45	A
11	A	46	A
11	A	56	G
11	A	58	C
11	A	59	U
11	A	60	G
11	A	67	C
11	A	68	A

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Mol	Chain	Res	Type
11	A	72	C
11	A	73	C
11	A	74	G
11	A	78	C
11	A	103	A
11	A	113	G
11	A	115	U
11	A	126	G
11	A	129	C
11	A	130	G
11	A	140	U
11	A	142	C
11	A	143	U
11	A	155	G
11	A	158	A
11	A	159	A2M
11	A	160	U
11	A	163	U
11	A	173	A
11	A	182	C
11	A	184	G
11	A	190	G
11	A	198	U
11	A	199	C
11	A	200	G
11	A	202	G
11	A	203	G
11	A	204	G
11	A	206	G
11	A	208	G
11	A	291	G
11	A	292	A
11	A	294	U
11	A	295	C
11	A	306	C
11	A	307	G
11	A	308	G
11	A	318	A
11	A	319	C
11	A	321	C
11	A	323	C
11	A	324	C

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Mol	Chain	Res	Type
11	A	325	C
11	A	326	C
11	A	327	G
11	A	329	G
11	A	347	G
11	A	351	G
11	A	362	C
11	A	364	A
11	A	368	U
11	A	369	C
11	A	370	G
11	A	381	C
11	A	384	U
11	A	385	G
11	A	386	C
11	A	409	C
11	A	418	A
11	A	421	G
11	A	448	A
11	A	450	C
11	A	452	G
11	A	465	A
11	A	471	G
11	A	472	C
11	A	473	A
11	A	474	G
11	A	476	A
11	A	482	G
11	A	487	U
11	A	488	U
11	A	492	C
11	A	493	A
11	A	496	C
11	A	508	A
11	A	509	OMG
11	A	516	A
11	A	517	OMC
11	A	525	A
11	A	533	A
11	A	534	G
11	A	536	A
11	A	537	C

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Mol	Chain	Res	Type
11	A	538	U
11	A	539	C
11	A	540	U
11	A	541	U
11	A	542	U
11	A	543	C
11	A	544	G
11	A	545	A
11	A	546	G
11	A	550	C
11	A	553	U
11	A	554	A
11	A	556	U
11	A	557	U
11	A	558	G
11	A	559	G
11	A	563	G
11	A	564	A
11	A	566	U
11	A	568	C
11	A	576	A
11	A	589	G
11	A	590	A
11	A	591	U
11	A	598	G
11	A	604	A
11	A	607	U
11	A	608	C
11	A	614	C
11	A	617	G
11	A	626	G
11	A	628	A
11	A	631	U
11	A	643	A
11	A	644	OMG
11	A	655	A
11	A	660	C
11	A	662	G
11	A	668	A2M
11	A	669	A
11	A	671	A
11	A	672	A

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Mol	Chain	Res	Type
11	A	673	G
11	A	683	OMG
11	A	688	U
11	A	689	U
11	A	690	G
11	A	691	G
11	A	692	G
11	A	695	C
11	A	696	G
11	A	697	G
11	A	698	G
11	A	699	C
11	A	700	G
11	A	705	G
11	A	707	C
11	A	712	G
11	A	713	C
11	A	715	A
11	A	717	G
11	A	719	G
11	A	720	A
11	A	721	G
11	A	723	C
11	A	725	C
11	A	726	C
11	A	728	C
11	A	729	C
11	A	731	G
11	A	732	U
11	A	733	C
11	A	734	C
11	A	738	C
11	A	739	C
11	A	748	C
11	A	749	U
11	A	751	G
11	A	752	G
11	A	753	C
11	A	791	C
11	A	798	G
11	A	800	U
11	A	801	U

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Mol	Chain	Res	Type
11	A	810	A
11	A	811	A
11	A	821	G
11	A	822	PSU
11	A	827	A
11	A	830	A
11	A	836	G
11	A	837	A
11	A	838	G
11	A	839	C
11	A	840	C
11	A	841	G
11	A	845	G
11	A	847	A
11	A	870	A
11	A	872	A
11	A	873	G
11	A	880	G
11	A	881	G
11	A	886	A
11	A	888	U
11	A	890	U
11	A	891	G
11	A	892	U
11	A	895	G
11	A	896	U
11	A	897	U
11	A	898	U
11	A	899	U
11	A	900	C
11	A	903	A
11	A	908	A
11	A	909	G
11	A	913	A
11	A	920	A
11	A	922	A
11	A	930	C
11	A	933	G
11	A	934	G
11	A	954	U
11	A	956	G
11	A	963	A

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Mol	Chain	Res	Type
11	A	970	G
11	A	972	A
11	A	990	A
11	A	992	A
11	A	999	G
11	A	1002	U
11	A	1017	U
11	A	1023	A
11	A	1045	U
11	A	1047	C
11	A	1061	U
11	A	1062	A
11	A	1083	A
11	A	1085	C
11	A	1089	G
11	A	1109	C
11	A	1113	A
11	A	1114	U
11	A	1115	U
11	A	1117	C
11	A	1119	A
11	A	1120	U
11	A	1133	A
11	A	1138	C
11	A	1139	C
11	A	1143	A
11	A	1153	C
11	A	1154	U
11	A	1155	U
11	A	1183	A
11	A	1195	A
11	A	1207	G
11	A	1208	A
11	A	1209	A
11	A	1211	G
11	A	1215	C
11	A	1216	C
11	A	1217	A
11	A	1220	A
11	A	1224	G
11	A	1242	U
11	A	1247	C

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Mol	Chain	Res	Type
11	A	1251	A
11	A	1253	A
11	A	1256	G
11	A	1257	G
11	A	1259	A
11	A	1263	U
11	A	1274	G
11	A	1275	G
11	A	1283	C
11	A	1288	U
11	A	1290	G
11	A	1294	G
11	A	1295	A
11	A	1301	A
11	A	1302	G
11	A	1303	C
11	A	1308	U
11	A	1322	G
11	A	1326	U
11	A	1342	U
11	A	1355	C
11	A	1356	G
11	A	1357	A
11	A	1371	U
11	A	1372	U
11	A	1378	A
11	A	1382	A
11	A	1397	U
11	A	1401	A
11	A	1402	A
11	A	1406	G
11	A	1417	C
11	A	1418	C
11	A	1419	C
11	A	1420	G
11	A	1421	A
11	A	1422	G
11	A	1423	C
11	A	1424	G
11	A	1433	C
11	A	1435	C
11	A	1436	C

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Mol	Chain	Res	Type
11	A	1437	C
11	A	1438	A
11	A	1442	U
11	A	1454	A
11	A	1463	U
11	A	1487	A
11	A	1488	C
11	A	1489	A
11	A	1490	G
11	A	1497	G
11	A	1498	A
11	A	1507	G
11	A	1508	A
11	A	1520	G
11	A	1521	C
11	A	1531	A
11	A	1533	A
11	A	1534	C
11	A	1544	C
11	A	1552	G
11	A	1553	C
11	A	1556	A
11	A	1558	C
11	A	1560	U
11	A	1570	G
11	A	1579	A
11	A	1580	A
11	A	1585	U
11	A	1587	G
11	A	1588	A
11	A	1594	A
11	A	1600	G
11	A	1601	A
11	A	1603	G
11	A	1619	A
11	A	1621	U
11	A	1623	A
11	A	1624	U
11	A	1639	G
11	A	1648	G
11	A	1654	G
11	A	1661	A

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Mol	Chain	Res	Type
11	A	1663	A
11	A	1665	G
11	A	1671	G
11	A	1687	C
11	A	1695	A
11	A	1698	C
11	A	1706	G
11	A	1712	A
11	A	1715	A
11	A	1719	A
11	A	1721	U
11	A	1722	G
11	A	1729	U
11	A	1733	U
11	A	1749	G
11	A	1750	C
11	A	1752	C
11	A	1753	C
11	A	1754	G
11	A	1755	C
11	A	1756	C
11	A	1757	G
11	A	1758	G
11	A	1759	G
11	A	1760	G
11	A	1772	C
11	A	1773	C
11	A	1774	C
11	A	1775	U
11	A	1776	G
11	A	1777	G
11	A	1778	C
11	A	1779	G
11	A	1780	G
11	A	1781	A
11	A	1782	G
11	A	1783	C
11	A	1784	G
11	A	1805	G
11	A	1808	U
11	A	1813	A
11	A	1819	A

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Mol	Chain	Res	Type
11	A	1822	A
11	A	1823	A
11	A	1824	A
11	A	1825	A
11	A	1826	G
11	A	1829	G
11	A	1831	A
11	A	1835	A
11	A	1837	G
11	A	1838	U
11	A	1849	G
11	A	1861	G
11	A	1862	G
11	A	1863	A
11	A	1865	C
51	w	6	A
51	w	8	U
51	w	12	G
51	w	13	C
51	w	16	C
51	w	18	G
51	w	19	G
51	w	20	A
51	w	21	A
51	w	22	G
51	w	23	C
51	w	28	U
51	w	34	C
51	w	35	A
51	w	38	A
51	w	43	G
51	w	46	G
51	w	47	U
51	w	48	C
51	w	52	G
51	w	59	A
51	w	61	C
51	w	62	C
51	w	63	A
51	w	68	C
51	w	69	U
51	w	71	C

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Mol	Chain	Res	Type
51	w	73	A
51	w	74	C
51	w	75	C
51	w	76	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	-31	C
8	7	-21	A
8	7	-5	C
11	A	1	U
11	A	291	G
11	A	367	U
11	A	368	U
11	A	541	U
11	A	644	OMG
11	A	688	U
11	A	694	G
11	A	716	G
11	A	731	G
11	A	797	C
11	A	912	C
11	A	1600	G

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

29 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
11	A2M	A	166	11	18,25,26	4.28	8 (44%)	18,36,39	3.74	4 (22%)
11	A2M	A	668	56,11	18,25,26	4.20	8 (44%)	18,36,39	3.79	6 (33%)
11	A2M	A	1031	11	18,25,26	4.33	8 (44%)	18,36,39	3.75	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	5MU	A	814	11	19,22,23	0.47	0	28,32,35	1.15	2 (7%)
11	MA6	A	1851	11	18,26,27	1.35	3 (16%)	19,38,41	3.22	2 (10%)
11	OMG	A	509	56,11	18,26,27	2.65	9 (50%)	19,38,41	2.55	9 (47%)
11	PSU	A	822	11	18,21,22	1.07	1 (5%)	22,30,33	1.78	5 (22%)
11	PSU	A	119	11	18,21,22	1.00	1 (5%)	22,30,33	1.61	4 (18%)
11	A2M	A	27	56,11	18,25,26	4.28	9 (50%)	18,36,39	3.78	5 (27%)
11	OMC	A	174	56,11	19,22,23	0.56	0	26,31,34	0.78	1 (3%)
11	6MZ	A	1832	56,11	18,25,26	1.77	2 (11%)	16,36,39	2.49	5 (31%)
11	PSU	A	1081	11	18,21,22	1.03	1 (5%)	22,30,33	1.75	4 (18%)
11	PSU	A	1243	11	18,21,22	1.05	1 (5%)	22,30,33	1.79	4 (18%)
11	OMG	A	683	11	18,26,27	1.09	1 (5%)	19,38,41	1.09	2 (10%)
11	UR3	A	1830	11	19,22,23	2.79	8 (42%)	26,32,35	1.51	4 (15%)
11	OMC	A	1703	11	19,22,23	0.57	0	26,31,34	0.66	0
11	OMU	A	116	11	19,22,23	3.02	6 (31%)	26,31,34	1.64	5 (19%)
11	A2M	A	159	11	18,25,26	4.34	8 (44%)	18,36,39	3.85	5 (27%)
11	5MC	A	1374	11	18,22,23	0.56	0	26,32,35	0.53	0
11	B8N	A	1248	11	24,29,30	3.05	6 (25%)	29,42,45	1.83	6 (20%)
11	PSU	A	612	11	18,21,22	0.98	1 (5%)	22,30,33	1.78	5 (22%)
11	PSU	A	823	11	18,21,22	1.08	1 (5%)	22,30,33	1.75	4 (18%)
11	MA6	A	1850	11	18,26,27	1.31	2 (11%)	19,38,41	3.13	2 (10%)
11	OMC	A	517	11	19,22,23	0.55	0	26,31,34	0.65	0
11	JMH	A	1219	56,11	18,22,23	2.93	5 (27%)	21,32,35	1.73	5 (23%)
11	A2M	A	1678	11	18,25,26	4.34	8 (44%)	18,36,39	3.86	5 (27%)
11	OMU	A	121	11	19,22,23	3.00	6 (31%)	26,31,34	1.71	5 (19%)
11	A2M	A	484	11	18,25,26	4.21	9 (50%)	18,36,39	3.87	5 (27%)
11	OMG	A	644	11	18,26,27	2.44	7 (38%)	19,38,41	2.66	10 (52%)

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
11	A2M	A	166	11	-	1/5/27/28	0/3/3/3
11	A2M	A	668	56,11	-	2/5/27/28	0/3/3/3
11	A2M	A	1031	11	-	1/5/27/28	0/3/3/3
11	5MU	A	814	11	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MA6	A	1851	11	-	4/7/29/30	0/3/3/3
11	OMG	A	509	56,11	-	3/5/27/28	0/3/3/3
11	PSU	A	822	11	-	2/7/25/26	0/2/2/2
11	PSU	A	119	11	-	0/7/25/26	0/2/2/2
11	A2M	A	27	56,11	-	1/5/27/28	0/3/3/3
11	OMC	A	174	56,11	-	0/9/27/28	0/2/2/2
11	6MZ	A	1832	56,11	-	2/5/27/28	0/3/3/3
11	PSU	A	1081	11	-	1/7/25/26	0/2/2/2
11	PSU	A	1243	11	-	0/7/25/26	0/2/2/2
11	OMG	A	683	11	-	3/5/27/28	0/3/3/3
11	UR3	A	1830	11	-	2/7/25/26	0/2/2/2
11	OMC	A	1703	11	-	0/9/27/28	0/2/2/2
11	OMU	A	116	11	-	1/9/27/28	0/2/2/2
11	A2M	A	159	11	-	3/5/27/28	0/3/3/3
11	5MC	A	1374	11	-	0/7/25/26	0/2/2/2
11	B8N	A	1248	11	-	5/16/34/35	0/2/2/2
11	PSU	A	612	11	-	0/7/25/26	0/2/2/2
11	PSU	A	823	11	-	0/7/25/26	0/2/2/2
11	MA6	A	1850	11	-	3/7/29/30	0/3/3/3
11	OMC	A	517	11	-	2/9/27/28	0/2/2/2
11	JMH	A	1219	56,11	-	1/7/25/26	0/2/2/2
11	A2M	A	1678	11	-	1/5/27/28	0/3/3/3
11	OMU	A	121	11	-	0/9/27/28	0/2/2/2
11	A2M	A	484	11	-	1/5/27/28	0/3/3/3
11	OMG	A	644	11	-	4/5/27/28	0/3/3/3

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1031	A2M	C3'-C2'	-12.89	1.24	1.52
11	A	1678	A2M	C3'-C2'	-12.79	1.24	1.52
11	A	27	A2M	C3'-C2'	-12.77	1.24	1.52
11	A	159	A2M	C3'-C2'	-12.73	1.24	1.52
11	A	166	A2M	C3'-C2'	-12.70	1.24	1.52
11	A	484	A2M	C3'-C2'	-12.32	1.25	1.52
11	A	668	A2M	C3'-C2'	-12.29	1.25	1.52
11	A	1219	JMH	C2-N1	8.35	1.50	1.38
11	A	1248	B8N	C4-N3	-8.13	1.25	1.40
11	A	159	A2M	O4'-C1'	7.99	1.52	1.41
11	A	1031	A2M	O4'-C1'	7.62	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1678	A2M	O4'-C1'	7.48	1.51	1.41
11	A	1248	B8N	C6-N1	7.46	1.55	1.36
11	A	166	A2M	O4'-C1'	7.46	1.51	1.41
11	A	27	A2M	O4'-C1'	7.45	1.51	1.41
11	A	484	A2M	O4'-C1'	7.40	1.51	1.41
11	A	1830	UR3	C2-N1	7.38	1.49	1.38
11	A	116	OMU	C2-N1	7.12	1.49	1.38
11	A	116	OMU	C2-N3	7.11	1.50	1.38
11	A	121	OMU	C2-N3	7.02	1.50	1.38
11	A	121	OMU	C2-N1	6.94	1.49	1.38
11	A	668	A2M	O4'-C4'	-6.90	1.29	1.45
11	A	668	A2M	O4'-C1'	6.90	1.50	1.41
11	A	1678	A2M	O4'-C4'	-6.72	1.30	1.45
11	A	166	A2M	O4'-C4'	-6.47	1.30	1.45
11	A	1031	A2M	O4'-C4'	-6.41	1.30	1.45
11	A	159	A2M	O4'-C4'	-6.40	1.30	1.45
11	A	484	A2M	O4'-C4'	-6.33	1.30	1.45
11	A	27	A2M	O4'-C4'	-6.30	1.30	1.45
11	A	116	OMU	C6-C5	6.12	1.49	1.35
11	A	121	OMU	C6-C5	6.12	1.49	1.35
11	A	1830	UR3	C6-C5	6.09	1.49	1.35
11	A	1219	JMH	C6-C5	6.01	1.49	1.35
11	A	1832	6MZ	C6-N6	5.82	1.44	1.35
11	A	1248	B8N	C6-C5	5.49	1.42	1.34
11	A	1678	A2M	C3'-C4'	5.27	1.66	1.53
11	A	509	OMG	C4-N3	5.23	1.50	1.37
11	A	1219	JMH	C2-N3	5.23	1.49	1.39
11	A	159	A2M	C3'-C4'	5.16	1.66	1.53
11	A	509	OMG	C2-N3	5.14	1.45	1.33
11	A	1031	A2M	C3'-C4'	5.11	1.66	1.53
11	A	1830	UR3	C2-N3	5.08	1.48	1.39
11	A	484	A2M	C3'-C4'	5.07	1.66	1.53
11	A	1248	B8N	C2-N1	5.06	1.54	1.39
11	A	509	OMG	C2-N2	5.03	1.46	1.34
11	A	668	A2M	C3'-C4'	5.01	1.65	1.53
11	A	27	A2M	C3'-C4'	4.97	1.65	1.53
11	A	166	A2M	C3'-C4'	4.87	1.65	1.53
11	A	644	OMG	C2-N2	4.81	1.45	1.34
11	A	644	OMG	C4-N3	4.76	1.48	1.37
11	A	644	OMG	C2-N3	4.52	1.44	1.33
11	A	116	OMU	C4-N3	4.17	1.46	1.38
11	A	121	OMU	C4-N3	4.10	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1248	B8N	C1'-C5	3.71	1.58	1.50
11	A	484	A2M	O2'-C2'	3.49	1.51	1.42
11	A	27	A2M	O2'-C2'	3.49	1.51	1.42
11	A	1031	A2M	O2'-C2'	3.48	1.51	1.42
11	A	159	A2M	O2'-C2'	3.45	1.51	1.42
11	A	1248	B8N	O2-C2	-3.43	1.16	1.22
11	A	1243	PSU	C6-C5	3.42	1.39	1.35
11	A	668	A2M	O2'-C2'	3.38	1.51	1.42
11	A	166	A2M	O2'-C2'	3.37	1.51	1.42
11	A	1678	A2M	O2'-C2'	3.37	1.51	1.42
11	A	822	PSU	C6-C5	3.36	1.39	1.35
11	A	823	PSU	C6-C5	3.33	1.39	1.35
11	A	644	OMG	C6-N1	3.31	1.42	1.37
11	A	119	PSU	C6-C5	3.30	1.39	1.35
11	A	509	OMG	C6-N1	3.29	1.42	1.37
11	A	1081	PSU	C6-C5	3.24	1.39	1.35
11	A	159	A2M	C6-N6	3.15	1.45	1.34
11	A	1678	A2M	C6-N6	3.14	1.45	1.34
11	A	484	A2M	C6-N6	3.13	1.45	1.34
11	A	166	A2M	C6-N6	3.12	1.45	1.34
11	A	668	A2M	C6-N6	3.12	1.45	1.34
11	A	27	A2M	C6-N6	3.12	1.45	1.34
11	A	1851	MA6	C2-N3	3.11	1.37	1.32
11	A	1031	A2M	C6-N6	3.09	1.45	1.34
11	A	612	PSU	C6-C5	3.02	1.38	1.35
11	A	1830	UR3	C6-N1	3.01	1.45	1.38
11	A	1850	MA6	C2-N3	3.01	1.36	1.32
11	A	683	OMG	C6-N1	-2.95	1.33	1.37
11	A	1850	MA6	C5-C4	-2.86	1.33	1.40
11	A	1851	MA6	C5-C4	-2.86	1.33	1.40
11	A	166	A2M	C5-C4	-2.82	1.33	1.40
11	A	1678	A2M	C5-C4	-2.81	1.33	1.40
11	A	27	A2M	C5-C4	-2.81	1.33	1.40
11	A	1031	A2M	C5-C4	-2.80	1.33	1.40
11	A	1219	JMH	C6-N1	2.80	1.44	1.38
11	A	668	A2M	C5-C4	-2.75	1.33	1.40
11	A	509	OMG	C5-C6	2.75	1.53	1.47
11	A	644	OMG	C5-C6	2.73	1.52	1.47
11	A	159	A2M	C5-C4	-2.72	1.33	1.40
11	A	484	A2M	C5-C4	-2.69	1.33	1.40
11	A	509	OMG	O6-C6	-2.67	1.17	1.23
11	A	121	OMU	C6-N1	2.61	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	116	OMU	C6-N1	2.58	1.44	1.38
11	A	1219	JMH	C5-C4	2.52	1.48	1.42
11	A	644	OMG	O6-C6	-2.47	1.18	1.23
11	A	644	OMG	C5-C4	-2.43	1.36	1.43
11	A	509	OMG	C5-C4	-2.38	1.37	1.43
11	A	509	OMG	C2-N1	2.32	1.43	1.37
11	A	1830	UR3	O2-C2	-2.28	1.18	1.22
11	A	1830	UR3	O4-C4	-2.28	1.18	1.23
11	A	121	OMU	C5-C4	2.21	1.48	1.43
11	A	1832	6MZ	C5-C4	-2.21	1.35	1.40
11	A	1830	UR3	C5-C4	2.18	1.49	1.43
11	A	484	A2M	C2-N3	2.16	1.35	1.32
11	A	116	OMU	C5-C4	2.15	1.48	1.43
11	A	159	A2M	C2-N3	2.14	1.35	1.32
11	A	484	A2M	O3'-C3'	2.11	1.47	1.43
11	A	1678	A2M	O3'-C3'	2.11	1.47	1.43
11	A	166	A2M	O3'-C3'	2.10	1.47	1.43
11	A	27	A2M	C2-N3	2.10	1.35	1.32
11	A	1830	UR3	C4-N3	2.10	1.45	1.40
11	A	668	A2M	O3'-C3'	2.08	1.47	1.43
11	A	509	OMG	O2'-C2'	-2.06	1.37	1.42
11	A	1851	MA6	C4-N3	2.05	1.38	1.35
11	A	27	A2M	O3'-C3'	2.01	1.47	1.43
11	A	1031	A2M	C2-N3	2.00	1.35	1.32

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1851	MA6	N1-C6-N6	-12.58	103.82	117.06
11	A	1850	MA6	N1-C6-N6	-12.38	104.02	117.06
11	A	159	A2M	C1'-N9-C4	10.52	145.12	126.64
11	A	484	A2M	C1'-N9-C4	10.42	144.95	126.64
11	A	1678	A2M	C1'-N9-C4	10.40	144.92	126.64
11	A	27	A2M	C1'-N9-C4	10.06	144.31	126.64
11	A	1031	A2M	C1'-N9-C4	9.72	143.71	126.64
11	A	668	A2M	C1'-N9-C4	9.60	143.51	126.64
11	A	166	A2M	C1'-N9-C4	9.53	143.38	126.64
11	A	668	A2M	C5-C6-N6	9.11	134.20	120.35
11	A	1678	A2M	C5-C6-N6	8.96	133.97	120.35
11	A	166	A2M	C5-C6-N6	8.96	133.97	120.35
11	A	1031	A2M	C5-C6-N6	8.94	133.94	120.35
11	A	159	A2M	C5-C6-N6	8.82	133.75	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	484	A2M	C5-C6-N6	8.80	133.72	120.35
11	A	27	A2M	C5-C6-N6	8.67	133.53	120.35
11	A	644	OMG	O2'-C2'-C1'	6.23	121.44	109.09
11	A	668	A2M	N6-C6-N1	-6.09	105.93	118.57
11	A	1031	A2M	N6-C6-N1	-6.00	106.13	118.57
11	A	1678	A2M	N6-C6-N1	-5.95	106.23	118.57
11	A	159	A2M	N6-C6-N1	-5.94	106.24	118.57
11	A	166	A2M	N6-C6-N1	-5.94	106.24	118.57
11	A	484	A2M	N6-C6-N1	-5.94	106.25	118.57
11	A	1832	6MZ	N3-C2-N1	-5.92	119.42	128.68
11	A	27	A2M	N6-C6-N1	-5.92	106.29	118.57
11	A	166	A2M	N3-C2-N1	-5.87	119.50	128.68
11	A	27	A2M	N3-C2-N1	-5.75	119.69	128.68
11	A	1678	A2M	N3-C2-N1	-5.73	119.73	128.68
11	A	1851	MA6	N3-C2-N1	-5.65	119.84	128.68
11	A	484	A2M	N3-C2-N1	-5.60	119.92	128.68
11	A	1031	A2M	N3-C2-N1	-5.59	119.94	128.68
11	A	1832	6MZ	C2-N1-C6	5.43	121.24	116.59
11	A	509	OMG	O2'-C2'-C1'	5.41	119.82	109.09
11	A	668	A2M	N3-C2-N1	-5.40	120.23	128.68
11	A	159	A2M	N3-C2-N1	-5.37	120.29	128.68
11	A	121	OMU	C4-N3-C2	-5.24	119.67	126.58
11	A	644	OMG	O3'-C3'-C4'	5.18	126.03	111.05
11	A	1850	MA6	N3-C2-N1	-5.17	120.60	128.68
11	A	116	OMU	C4-N3-C2	-4.93	120.08	126.58
11	A	1248	B8N	C5-C4-N3	4.86	125.17	116.17
11	A	1832	6MZ	C9-N6-C6	4.78	126.99	122.87
11	A	1243	PSU	N1-C2-N3	4.70	120.45	115.13
11	A	509	OMG	O3'-C3'-C4'	4.63	124.44	111.05
11	A	1081	PSU	C4-N3-C2	-4.55	119.78	126.34
11	A	822	PSU	C4-N3-C2	-4.50	119.85	126.34
11	A	823	PSU	C4-N3-C2	-4.50	119.85	126.34
11	A	822	PSU	N1-C2-N3	4.50	120.23	115.13
11	A	1830	UR3	C4-N3-C2	-4.49	120.33	124.56
11	A	1243	PSU	C4-N3-C2	-4.49	119.87	126.34
11	A	612	PSU	N1-C2-N3	4.49	120.22	115.13
11	A	1081	PSU	N1-C2-N3	4.48	120.20	115.13
11	A	612	PSU	C4-N3-C2	-4.47	119.90	126.34
11	A	823	PSU	N1-C2-N3	4.42	120.14	115.13
11	A	1248	B8N	C4-N3-C2	-4.37	119.93	125.46
11	A	119	PSU	N1-C2-N3	4.18	119.86	115.13
11	A	119	PSU	C4-N3-C2	-4.12	120.40	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	1219	JMH	C1'-N1-C2	4.01	123.77	116.99
11	A	1248	B8N	C31-N3-C4	3.95	123.13	117.31
11	A	509	OMG	C5-C6-N1	3.92	120.87	113.95
11	A	121	OMU	N3-C2-N1	3.74	119.85	114.89
11	A	1219	JMH	C6-N1-C2	-3.69	118.49	121.79
11	A	509	OMG	O3'-C3'-C2'	3.62	121.45	111.17
11	A	644	OMG	O3'-C3'-C2'	3.60	121.39	111.17
11	A	1830	UR3	C1'-N1-C2	3.57	123.02	116.99
11	A	116	OMU	N3-C2-N1	3.56	119.61	114.89
11	A	1219	JMH	O2-C2-N3	-3.48	116.44	121.34
11	A	509	OMG	C2-N1-C6	-3.41	118.81	125.10
11	A	121	OMU	C5-C4-N3	3.38	119.90	114.84
11	A	644	OMG	C5-C6-N1	3.35	119.86	113.95
11	A	1248	B8N	N3-C2-N1	3.34	121.47	116.76
11	A	116	OMU	C5-C4-N3	3.27	119.73	114.84
11	A	509	OMG	C5'-C4'-C3'	3.14	126.93	115.18
11	A	644	OMG	C2-N1-C6	-2.90	119.76	125.10
11	A	1830	UR3	C6-N1-C2	-2.88	119.21	121.79
11	A	612	PSU	O2-C2-N1	-2.87	119.63	122.79
11	A	121	OMU	O4-C4-C5	-2.86	120.12	125.16
11	A	116	OMU	O4-C4-C5	-2.86	120.13	125.16
11	A	814	5MU	C1'-N1-C2	2.81	122.65	117.57
11	A	814	5MU	O2-C2-N1	2.72	126.40	122.79
11	A	1243	PSU	O2-C2-N1	-2.65	119.87	122.79
11	A	823	PSU	O2-C2-N1	-2.64	119.89	122.79
11	A	509	OMG	O6-C6-C5	-2.60	119.29	124.37
11	A	822	PSU	O2-C2-N1	-2.53	120.00	122.79
11	A	644	OMG	N2-C2-N1	2.52	122.07	116.71
11	A	1219	JMH	O3'-C3'-C2'	2.46	119.79	111.82
11	A	119	PSU	O2-C2-N1	-2.42	120.13	122.79
11	A	683	OMG	C5-C6-N1	2.41	118.21	113.95
11	A	823	PSU	C6-N1-C2	-2.41	120.22	122.68
11	A	644	OMG	N1-C2-N3	-2.39	118.85	123.32
11	A	1243	PSU	C6-N1-C2	-2.36	120.27	122.68
11	A	119	PSU	C6-N1-C2	-2.31	120.32	122.68
11	A	1081	PSU	O2-C2-N1	-2.31	120.25	122.79
11	A	822	PSU	O4'-C1'-C2'	2.28	108.36	105.14
11	A	668	A2M	C3'-C2'-C1'	2.28	107.17	102.89
11	A	822	PSU	C6-N1-C2	-2.27	120.37	122.68
11	A	1248	B8N	O4'-C1'-C2'	2.24	108.30	105.14
11	A	174	OMC	C1'-N1-C2	2.24	123.42	118.42
11	A	683	OMG	C8-N7-C5	2.22	107.22	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	612	PSU	O4'-C1'-C2'	2.22	108.27	105.14
11	A	1832	6MZ	C4-C5-N7	-2.21	107.09	109.40
11	A	1830	UR3	O2-C2-N3	-2.20	118.23	121.34
11	A	121	OMU	O2-C2-N1	-2.20	119.86	122.79
11	A	612	PSU	C6-N1-C2	-2.18	120.45	122.68
11	A	644	OMG	O6-C6-C5	-2.17	120.13	124.37
11	A	668	A2M	C2'-C3'-C4'	2.16	106.69	101.99
11	A	1832	6MZ	C1'-N9-C4	-2.16	122.85	126.64
11	A	27	A2M	O4'-C1'-C2'	-2.15	102.86	106.59
11	A	644	OMG	O5'-C5'-C4'	2.13	116.25	108.99
11	A	159	A2M	C2'-C3'-C4'	2.13	106.61	101.99
11	A	484	A2M	C3'-C2'-C1'	2.12	106.87	102.89
11	A	1219	JMH	O3'-C3'-C4'	2.11	117.16	111.05
11	A	509	OMG	C8-N7-C5	2.11	107.01	102.99
11	A	1248	B8N	O2-C2-N3	-2.07	119.12	121.99
11	A	1081	PSU	C6-N1-C2	-2.07	120.57	122.68
11	A	509	OMG	N1-C2-N3	-2.04	119.51	123.32
11	A	644	OMG	C5'-C4'-C3'	2.04	122.82	115.18
11	A	1678	A2M	O2'-C2'-C1'	-2.02	105.09	109.09
11	A	116	OMU	O2-C2-N1	-2.00	120.12	122.79

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	27	A2M	C1'-C2'-O2'-CM'
11	A	116	OMU	C1'-C2'-O2'-CM2
11	A	159	A2M	C3'-C4'-C5'-O5'
11	A	159	A2M	C1'-C2'-O2'-CM'
11	A	166	A2M	C1'-C2'-O2'-CM'
11	A	484	A2M	C1'-C2'-O2'-CM'
11	A	509	OMG	C1'-C2'-O2'-CM2
11	A	644	OMG	C3'-C4'-C5'-O5'
11	A	644	OMG	C1'-C2'-O2'-CM2
11	A	668	A2M	O4'-C4'-C5'-O5'
11	A	822	PSU	C3'-C4'-C5'-O5'
11	A	1031	A2M	C1'-C2'-O2'-CM'
11	A	1678	A2M	C1'-C2'-O2'-CM'
11	A	1830	UR3	O4'-C1'-N1-C2
11	A	1832	6MZ	N1-C6-N6-C9
11	A	1850	MA6	C5-C6-N6-C10
11	A	1851	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
11	A	683	OMG	O4'-C4'-C5'-O5'
11	A	683	OMG	C3'-C4'-C5'-O5'
11	A	683	OMG	C1'-C2'-O2'-CM2
11	A	1248	B8N	O4'-C4'-C5'-O5'
11	A	1248	B8N	C3'-C4'-C5'-O5'
11	A	159	A2M	O4'-C4'-C5'-O5'
11	A	668	A2M	C3'-C4'-C5'-O5'
11	A	822	PSU	O4'-C4'-C5'-O5'
11	A	1851	MA6	C3'-C4'-C5'-O5'
11	A	1830	UR3	O4'-C1'-N1-C6
11	A	517	OMC	C3'-C4'-C5'-O5'
11	A	517	OMC	O4'-C4'-C5'-O5'
11	A	644	OMG	O4'-C4'-C5'-O5'
11	A	644	OMG	C4'-C5'-O5'-P
11	A	1850	MA6	C5-C6-N6-C9
11	A	1851	MA6	C5-C6-N6-C10
11	A	1850	MA6	N1-C6-N6-C10
11	A	509	OMG	C3'-C4'-C5'-O5'
11	A	1248	B8N	C31-C32-C33-C34
11	A	1248	B8N	N34-C33-C34-O36
11	A	1081	PSU	C4'-C5'-O5'-P
11	A	1851	MA6	C4'-C5'-O5'-P
11	A	1248	B8N	N34-C33-C34-O35
11	A	1832	6MZ	C5-C6-N6-C9
11	A	509	OMG	O4'-C4'-C5'-O5'
11	A	1219	JMH	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 93 ligands modelled in this entry, 92 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	$\#\|Z\| > 2$
54	GTP	0	2001	55,56	26,34,34	1.12	2 (7%)	32,54,54	1.75	6 (18%)

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
54	GTP	0	2001	55,56	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	0	2001	GTP	C5-C6	-3.91	1.39	1.47
54	0	2001	GTP	C2-N3	2.10	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	0	2001	GTP	PA-O3A-PB	-5.30	114.63	132.83
54	0	2001	GTP	C5-C6-N1	3.29	119.75	113.95
54	0	2001	GTP	C8-N7-C5	3.19	109.06	102.99
54	0	2001	GTP	C2-N1-C6	-2.93	119.71	125.10
54	0	2001	GTP	C3'-C2'-C1'	2.82	105.23	100.98
54	0	2001	GTP	PB-O3B-PG	-2.53	124.15	132.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

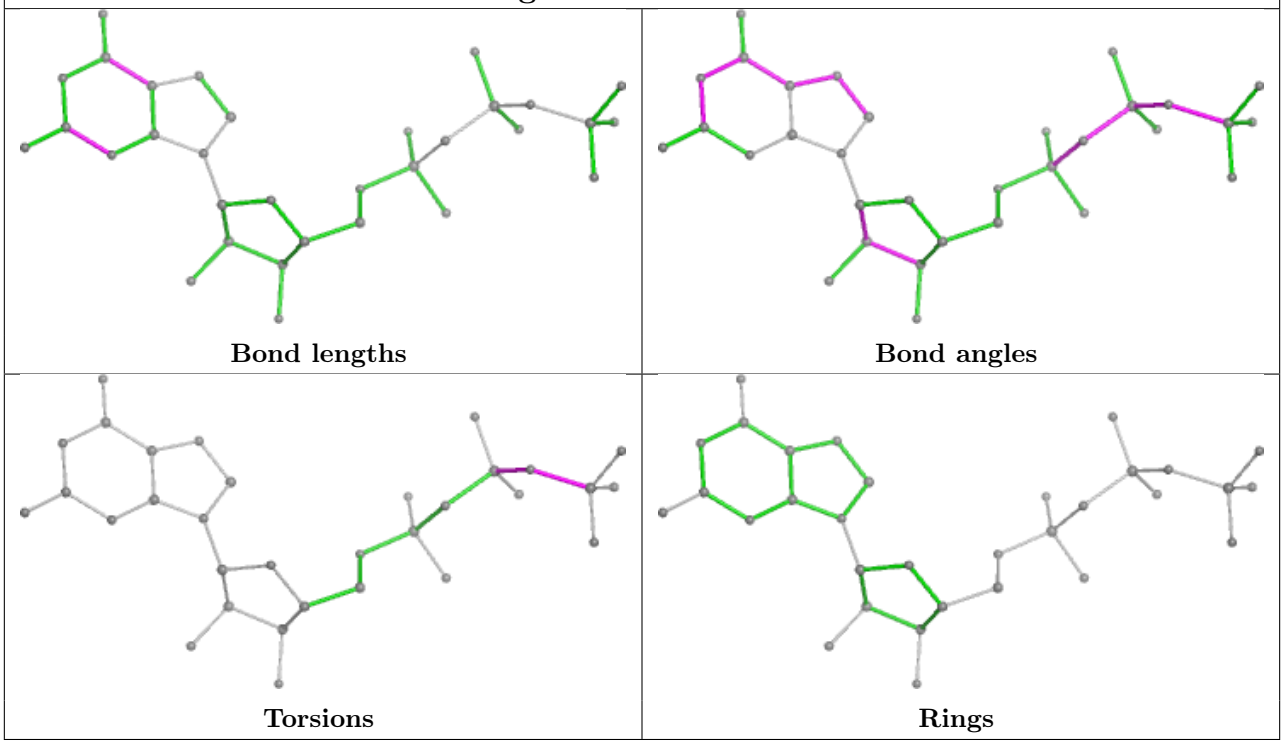
Mol	Chain	Res	Type	Atoms
54	0	2001	GTP	PB-O3B-PG-O2G
54	0	2001	GTP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP 0 2001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

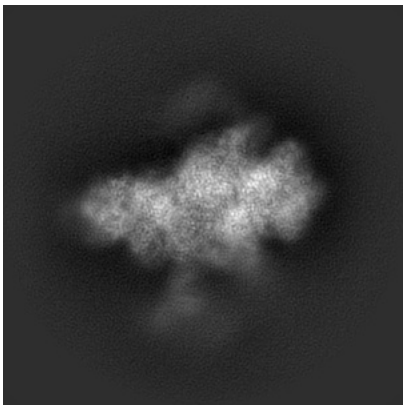
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17699. These allow visual inspection of the internal detail of the map and identification of artifacts.

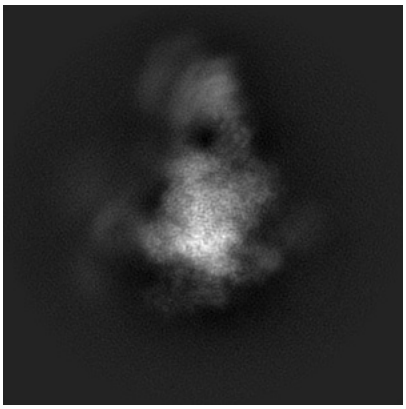
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

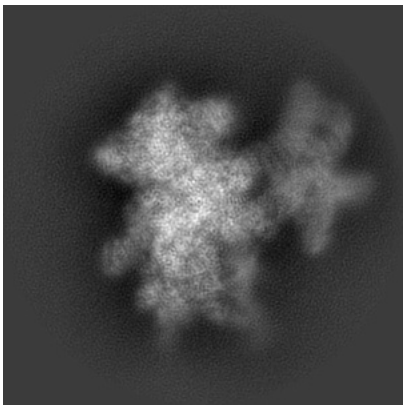
6.1.1 Primary map



X

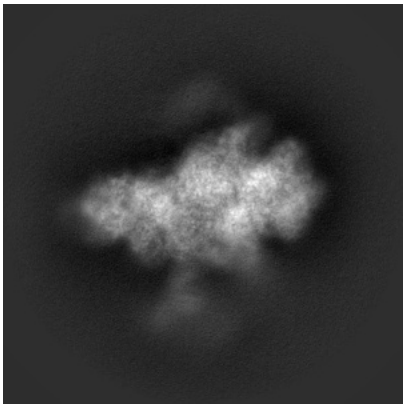


Y

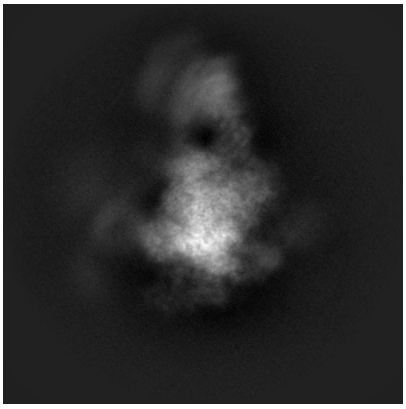


Z

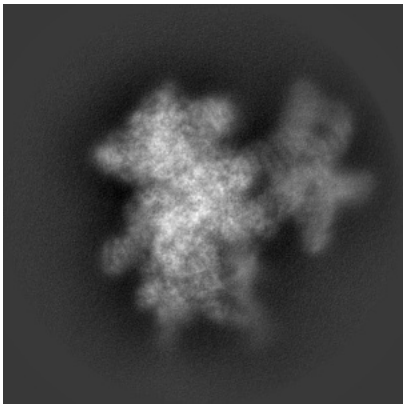
6.1.2 Raw map



X



Y

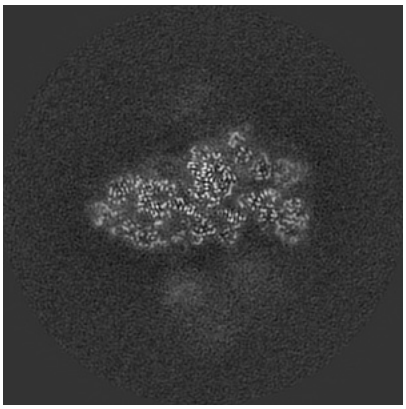


Z

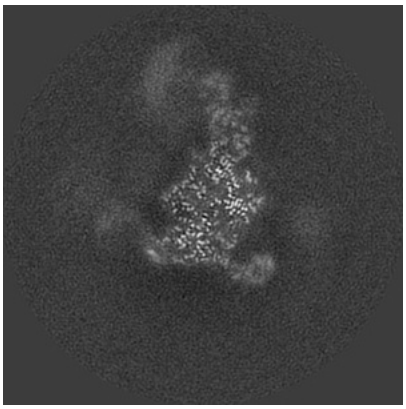
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

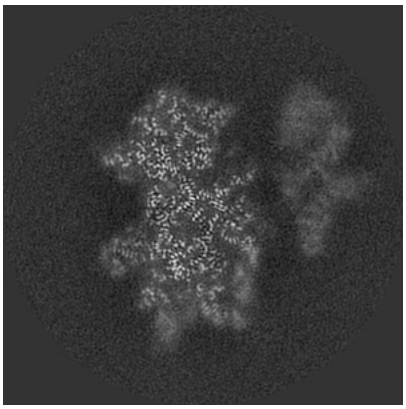
6.2.1 Primary map



X Index: 216

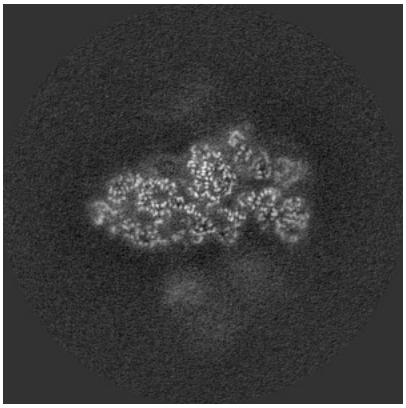


Y Index: 216

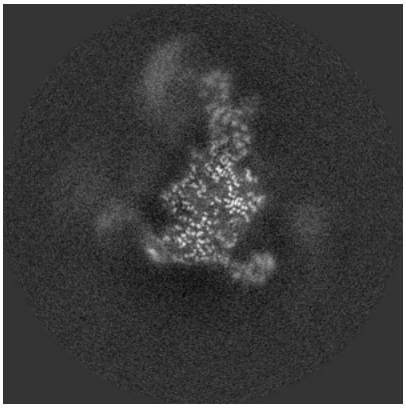


Z Index: 216

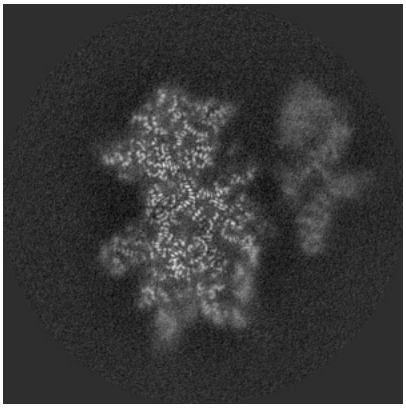
6.2.2 Raw map



X Index: 180



Y Index: 180

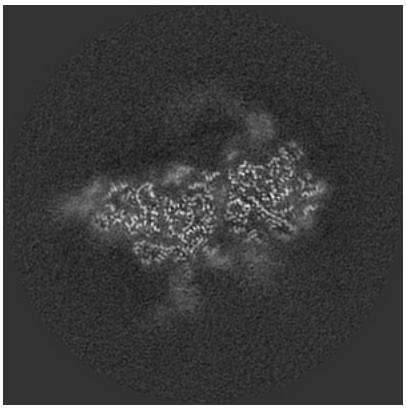


Z Index: 180

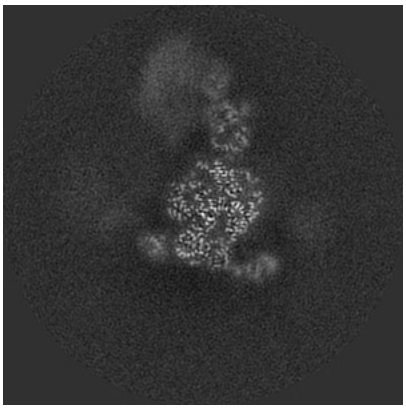
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

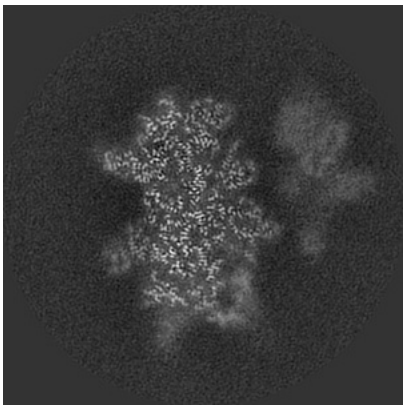
6.3.1 Primary map



X Index: 176

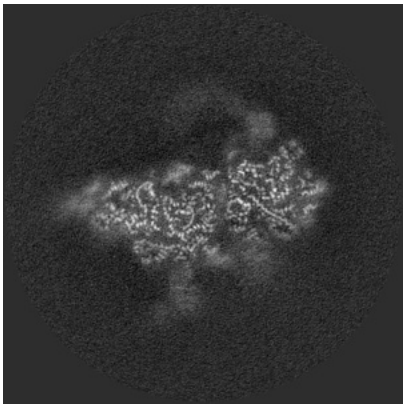


Y Index: 222

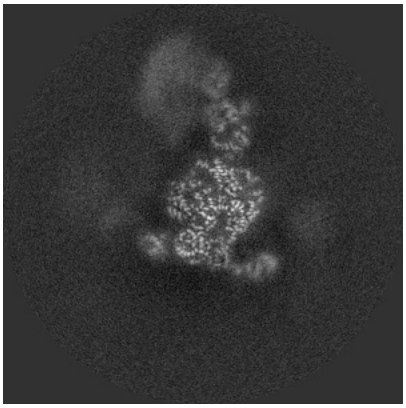


Z Index: 209

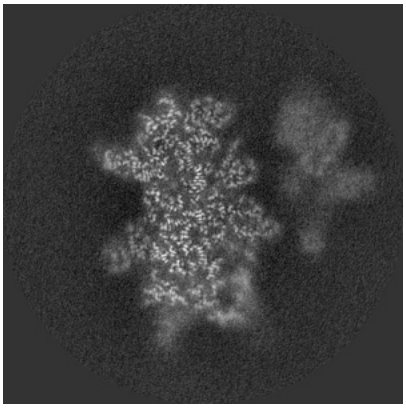
6.3.2 Raw map



X Index: 147



Y Index: 185

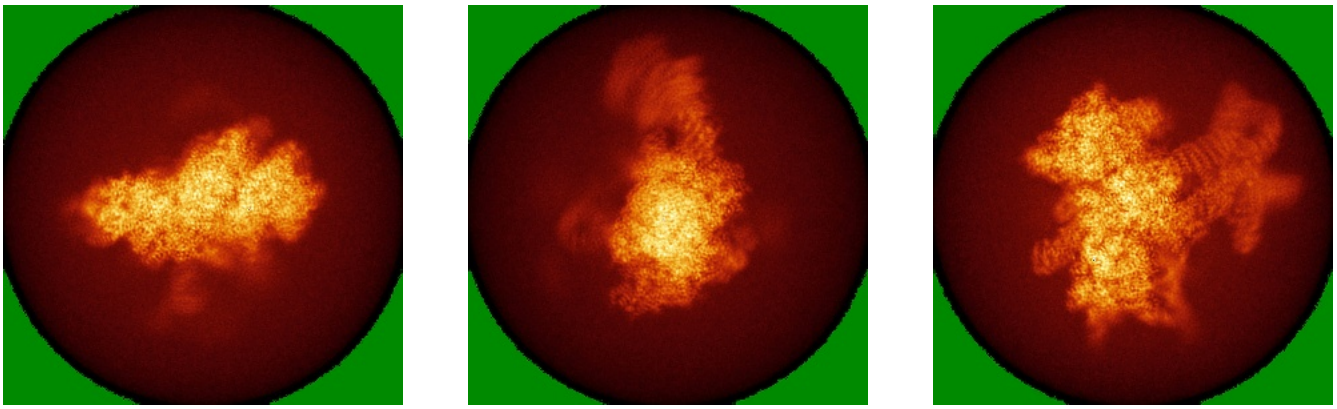


Z Index: 174

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

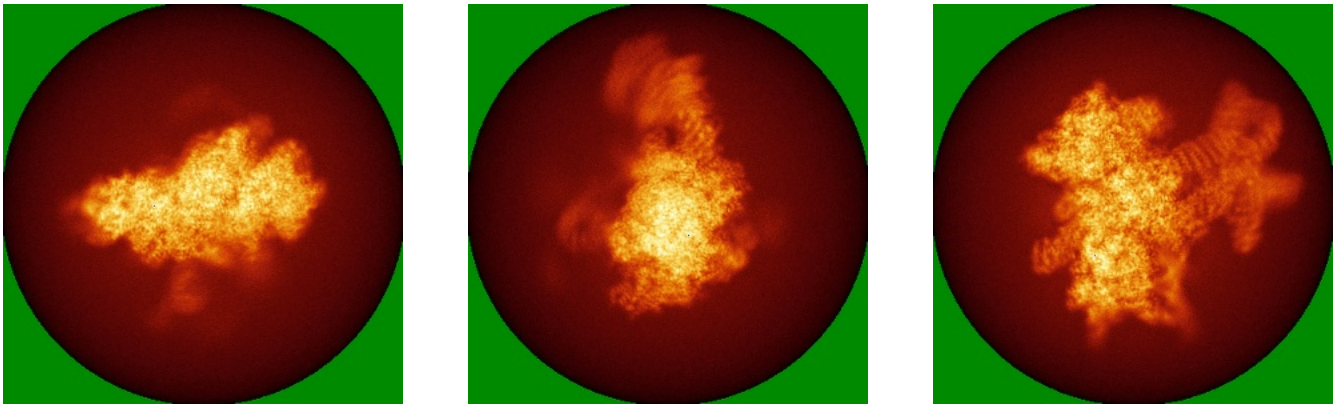
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

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

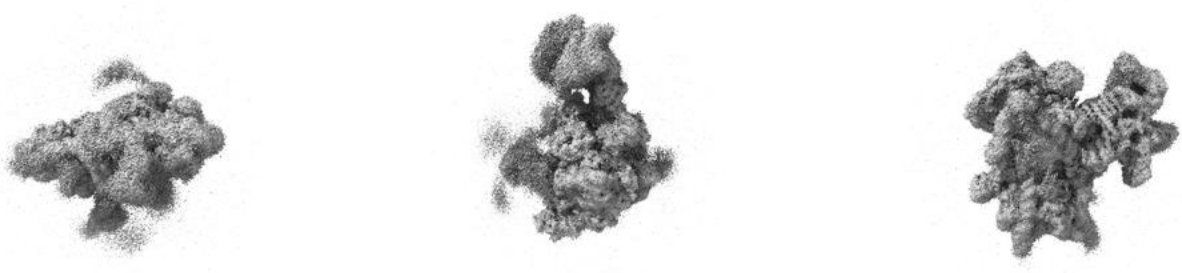
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

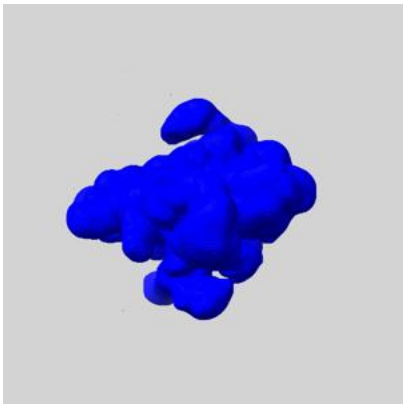
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

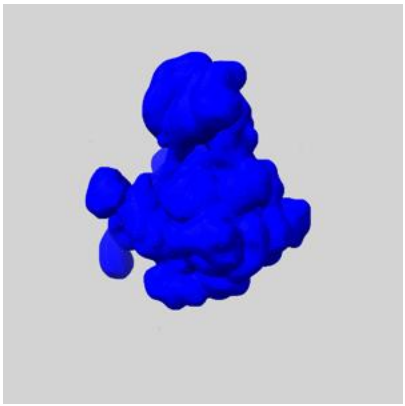
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

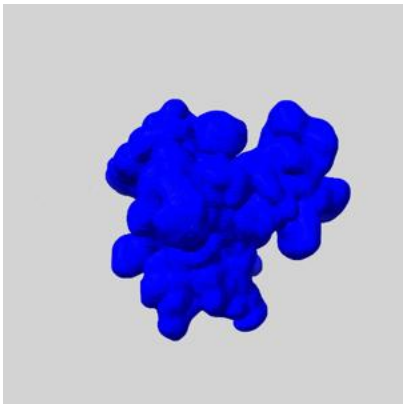
6.6.1 emd_17699_msk_1.map (i)



X



Y

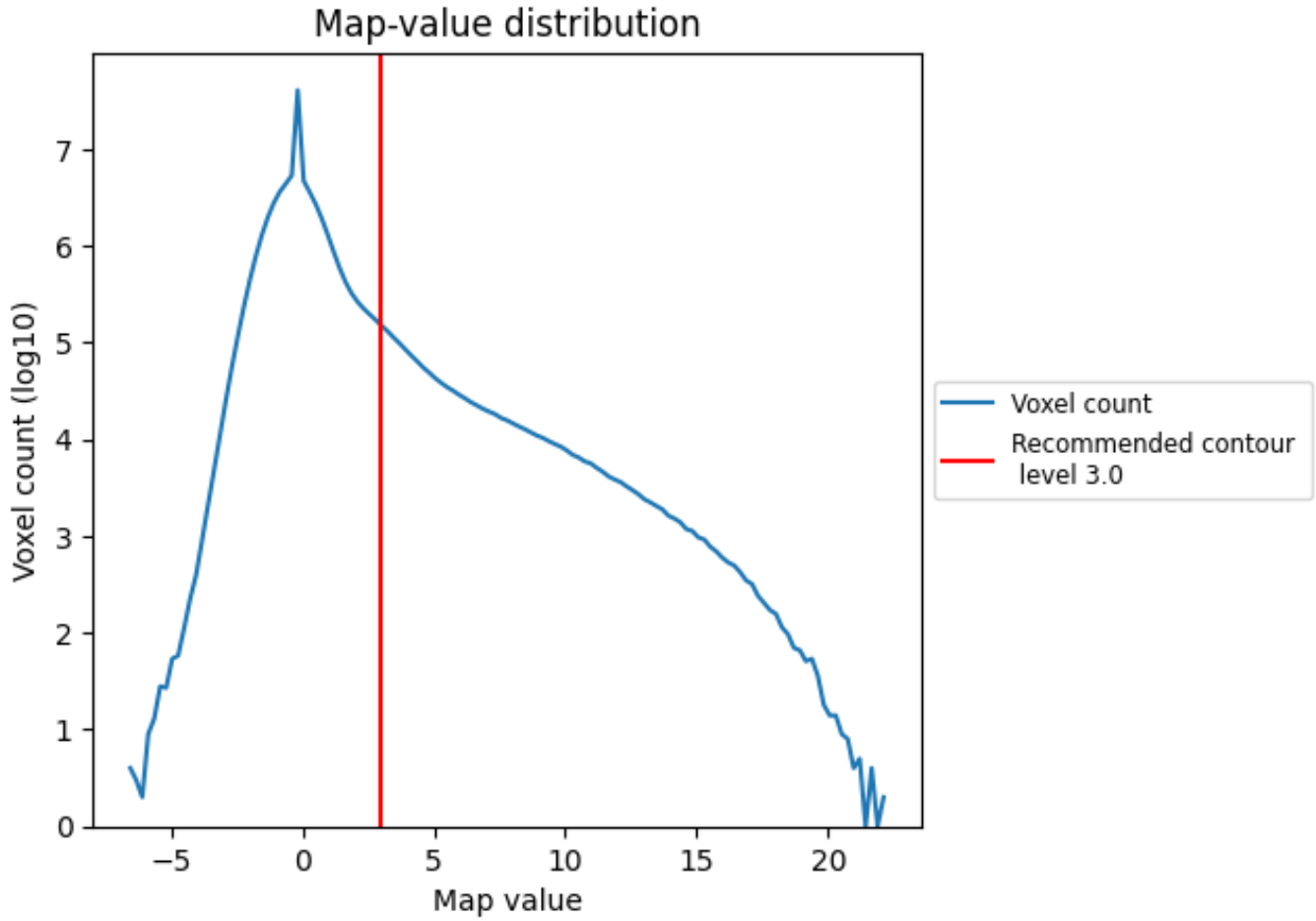


Z

7 Map analysis

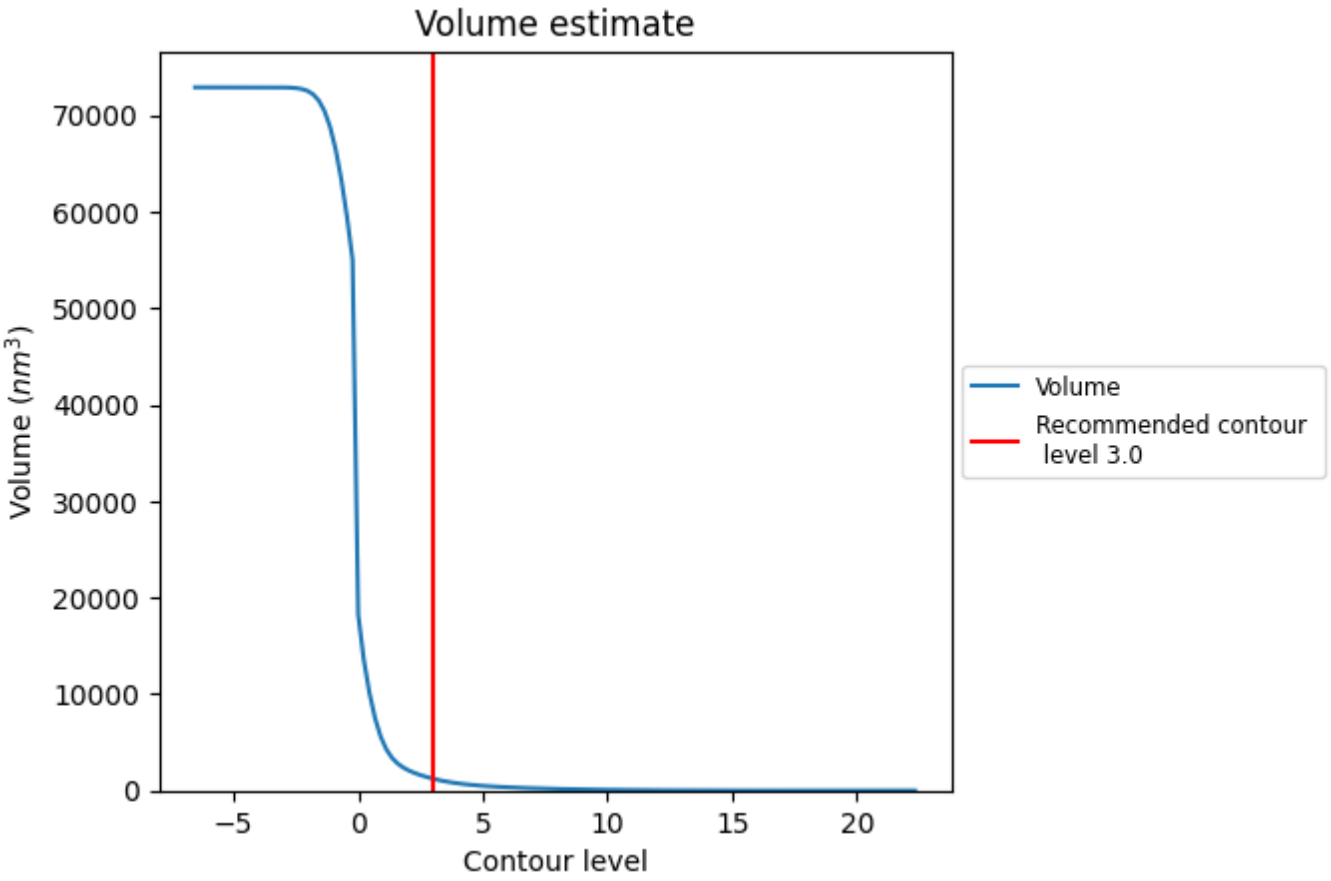
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

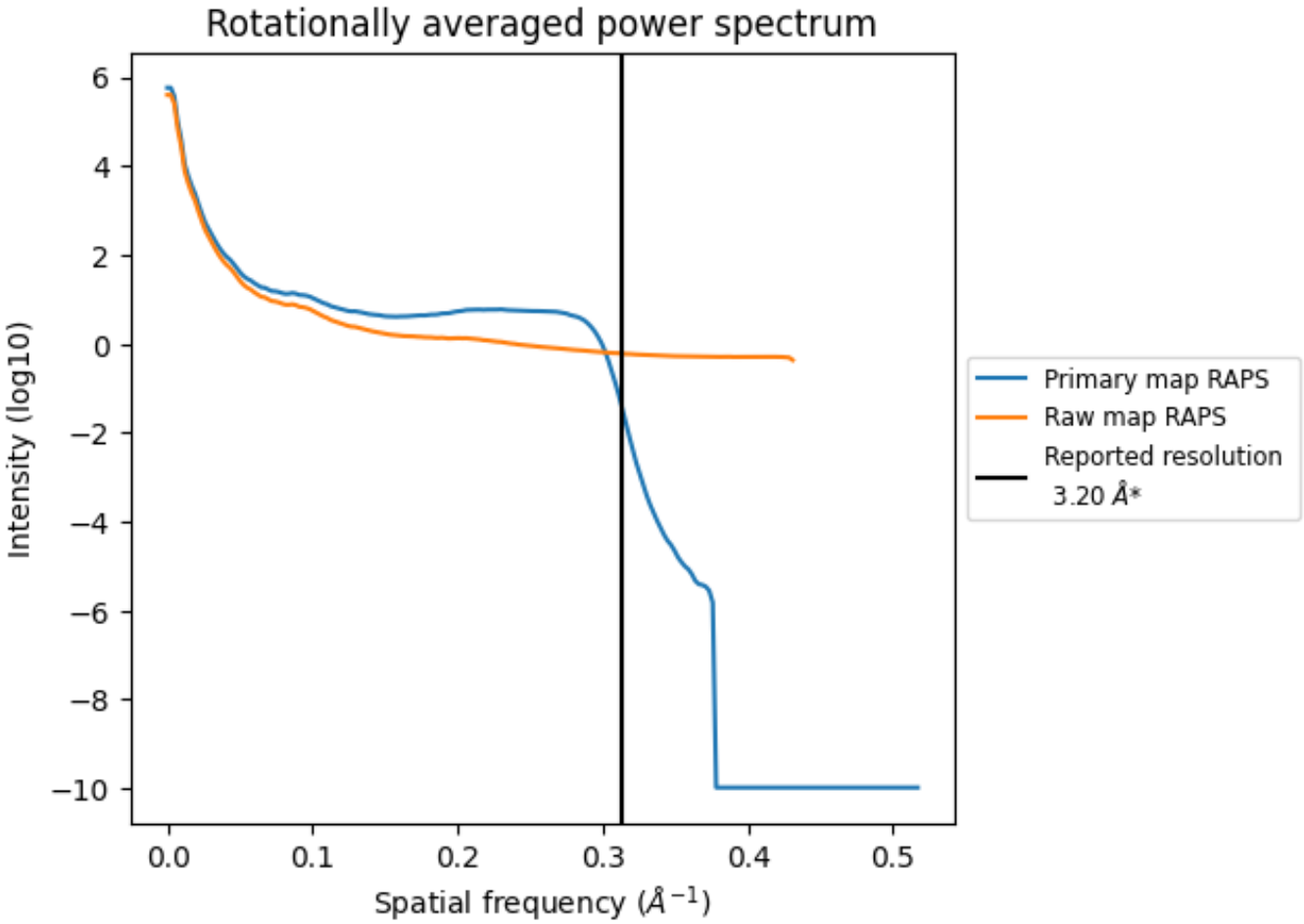
7.2 Volume estimate



The volume at the recommended contour level is 1228 nm^3; this corresponds to an approximate mass of 1109 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)

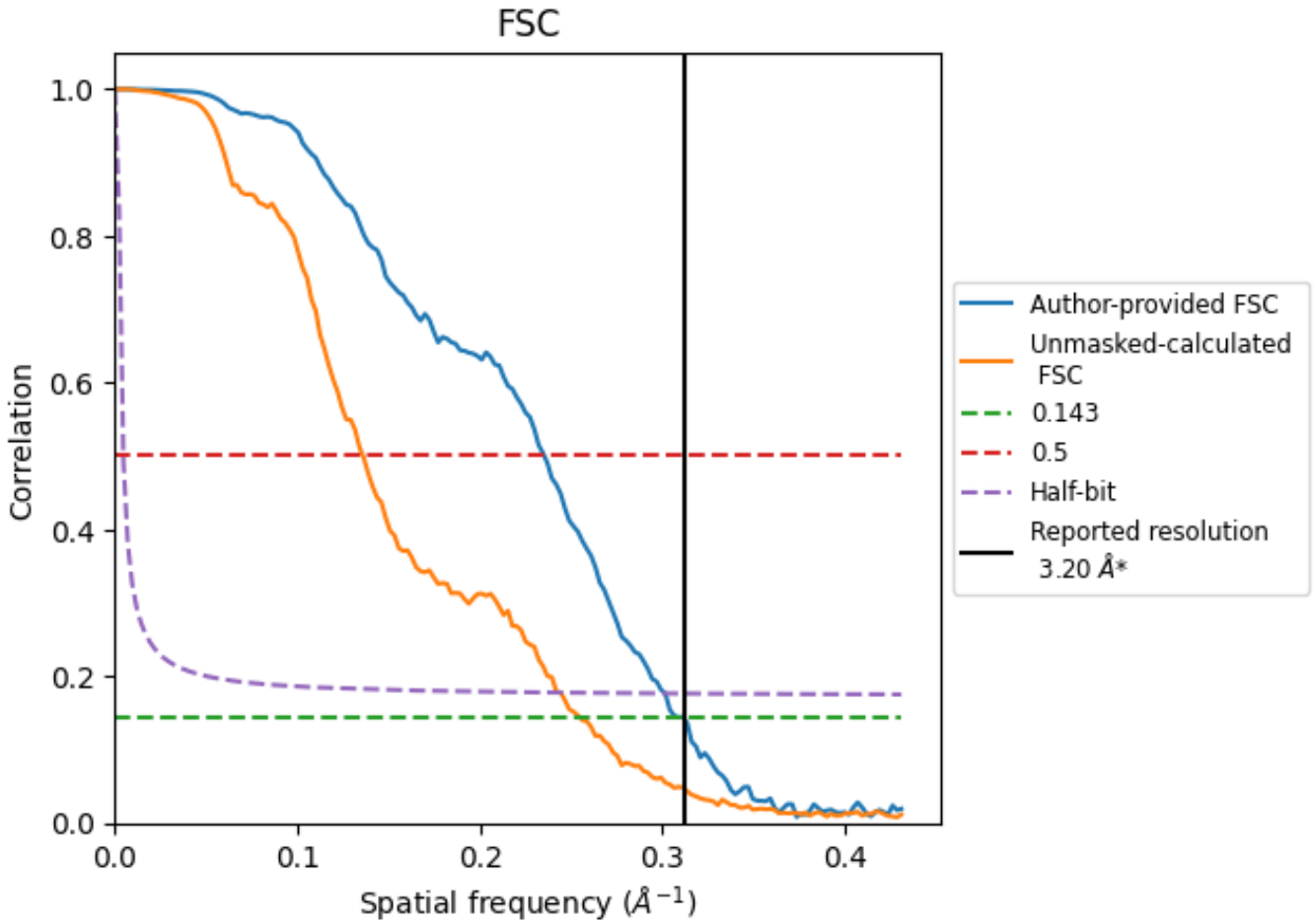


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

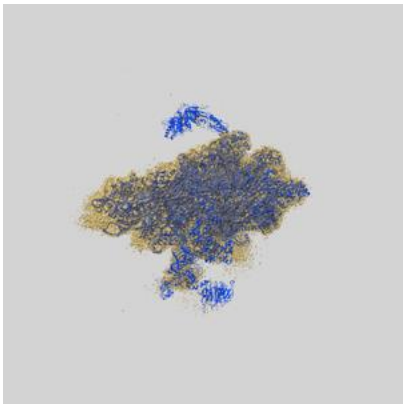
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	4.25	3.32
Unmasked-calculated*	3.92	7.35	4.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 3.2 by more than 10 %

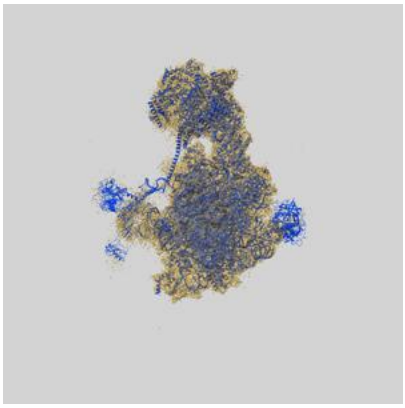
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17699 and PDB model 8PJ4. Per-residue inclusion information can be found in section 3 on page 14.

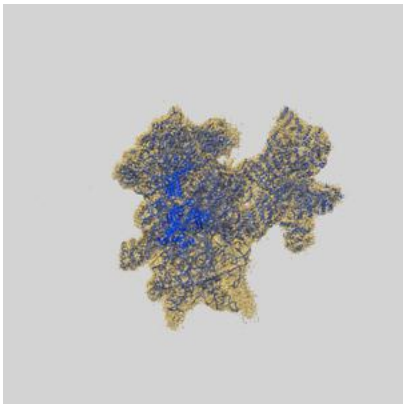
9.1 Map-model overlay



X



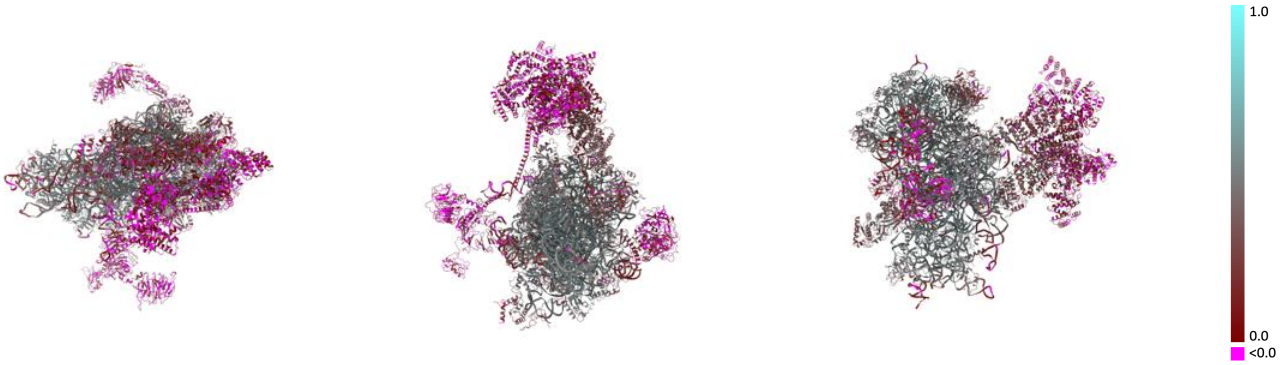
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 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.

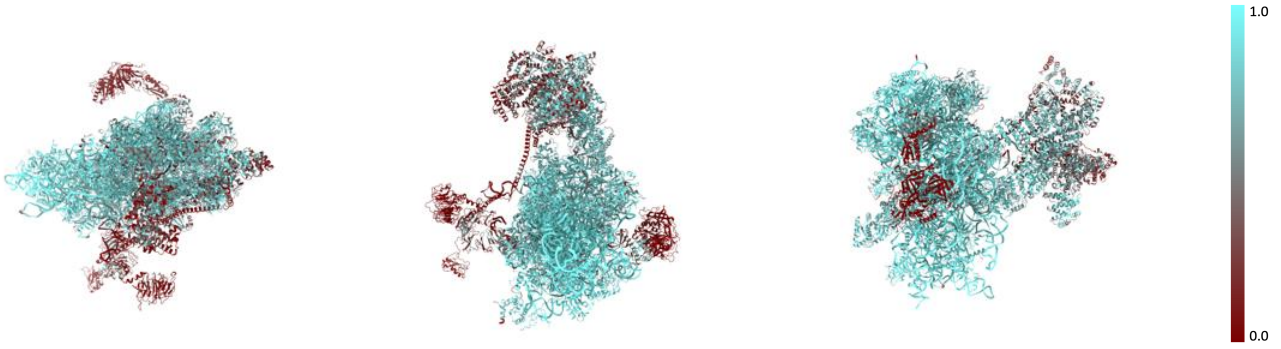
9.2 Q-score mapped to coordinate model (i)



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.

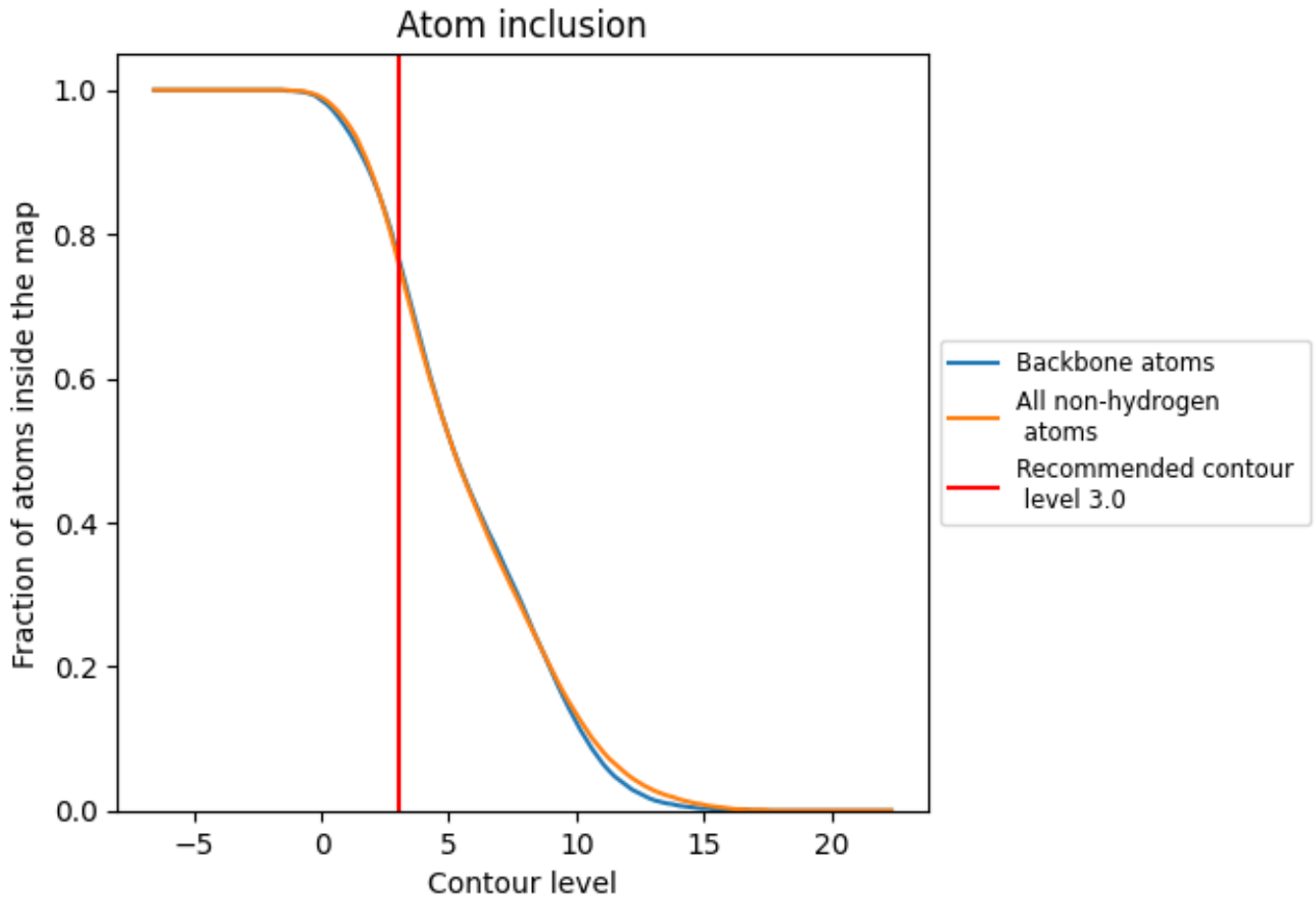
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.0).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7640	0.3610
0	0.7650	0.3440
1	0.2110	0.0910
2	0.0010	0.0010
3	0.3310	0.0280
4	0.5490	0.0800
5	0.3200	0.0380
6	0.4880	0.0730
7	0.6010	0.2300
8	0.5060	0.1010
9	0.8760	0.4570
A	0.9590	0.4670
B	0.9120	0.5040
C	0.9280	0.5060
D	0.8950	0.4980
E	0.9010	0.5150
F	0.8240	0.4430
G	0.8150	0.4210
H	0.8600	0.4650
I	0.8920	0.4920
J	0.9090	0.5130
K	0.8510	0.4850
L	0.8710	0.4990
M	0.8260	0.4620
N	0.8870	0.4920
O	0.8780	0.4770
P	0.8780	0.4810
Q	0.9260	0.5000
R	0.9320	0.4780
S	0.9140	0.4380
T	0.9100	0.4710
V	0.8800	0.4870
Y	0.9430	0.5120
Z	0.8300	0.4710
a	0.9010	0.4730

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	0.9010	0.4820
c	0.8820	0.4550
d	0.9380	0.5060
e	0.8020	0.4720
f	0.8900	0.4670
h	0.8670	0.4520
i	0.9530	0.5260
k	0.8430	0.3240
m	0.7320	0.2900
n	0.7880	0.4440
o	0.5260	0.2060
q	0.7930	0.4620
r	0.3250	0.1750
t	0.0050	0.0630
u	0.6040	0.2230
v	0.6110	0.1290
w	0.9170	0.2640
x	0.6870	0.2840
y	0.7280	0.2830