Full wwPDB EM Validation Report (i)

Apr 16, 2024 – 10:51 am BST

PDB ID	:	8PPL
EMDB ID	:	EMD-17805
Title	:	MERS-CoV Nsp1 bound to the human 43S pre-initiation complex
Authors	:	Schubert, K.; Karousis, E.D.; Ban, I.; Lapointe, C.P.; Leibundgut, M.; Baeumlin, E.; Kummerant, E.; Scaiola, A.; Schoenhut, T.; Ziegelmueller, J.; Puglisi, J.D.; Muehlemann, O.; Ban, N.
Deposited on	:	2023-07-07
Resolution	:	2.65 Å(reported)
Based on initial models	:	6ZOL, 6ZOK

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

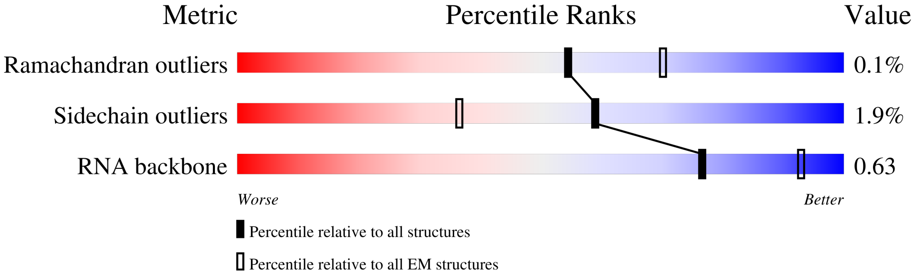
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

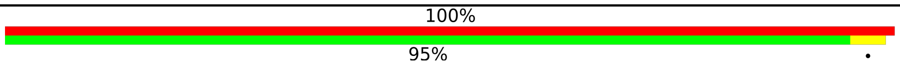
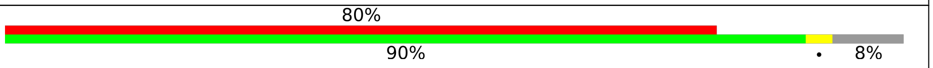
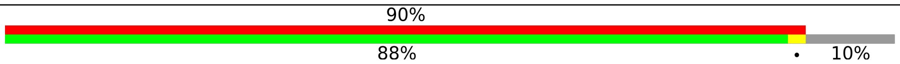
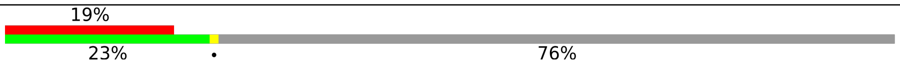
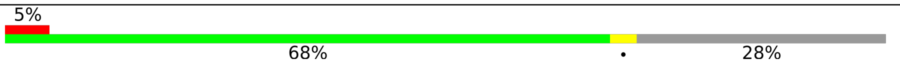
The reported resolution of this entry is 2.65 Å.

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	I3	218	
2	I4	357	
3	I5	564	
4	I6	374	
5	I8	352	
6	Io	320	
7	Ip	113	
8	Iq	144	

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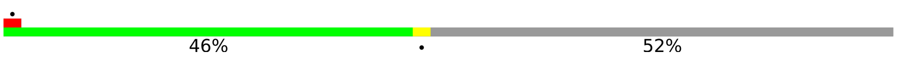
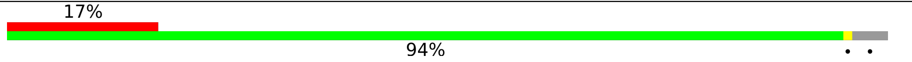
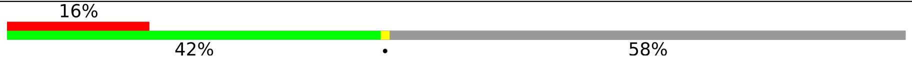
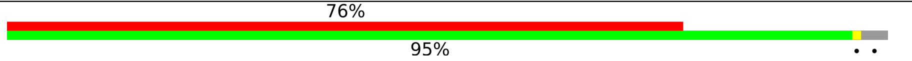
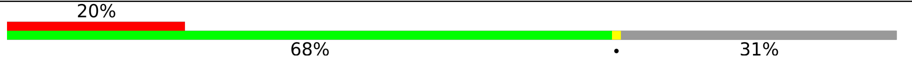
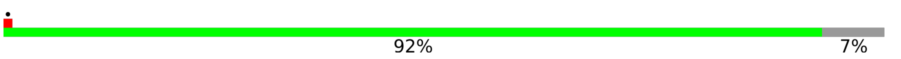
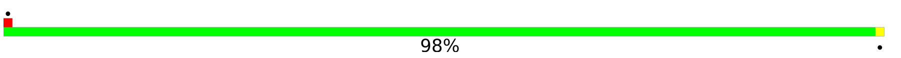
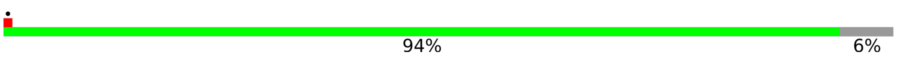
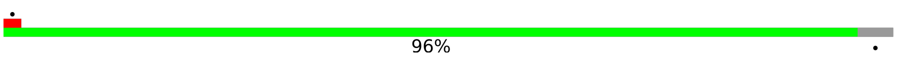
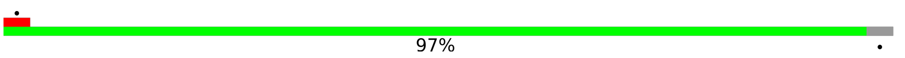
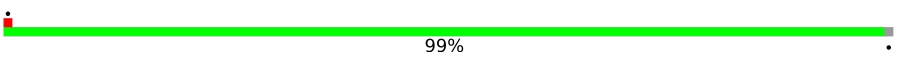
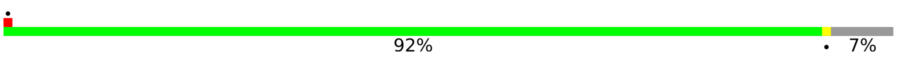
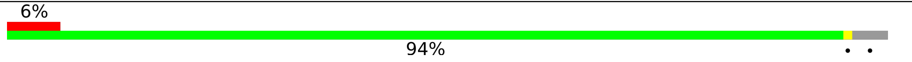
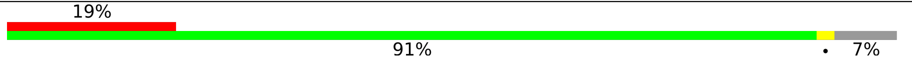
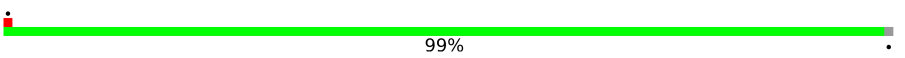
Mol	Chain	Length	Quality of chain
9	Ir	315	
10	Is	333	
11	It	472	
12	Iu	1382	
13	Iv	445	
14	Iw	75	
15	Ix	548	
16	Iy	913	
17	A2	1869	
18	AA	295	
19	AB	264	
20	AC	293	
21	AD	243	
22	AE	263	
23	AF	204	
24	AG	249	
25	AH	194	
26	AI	208	
27	AJ	194	
28	AK	165	
29	AL	158	
30	AM	132	
31	AN	151	
32	AO	151	
33	AP	145	

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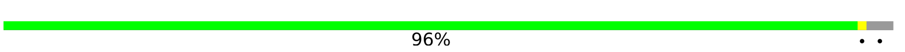
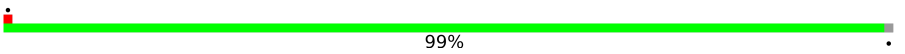
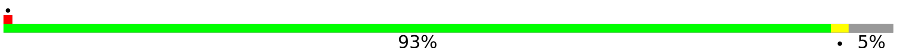
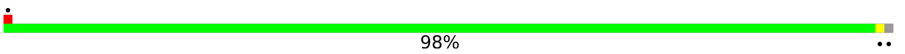
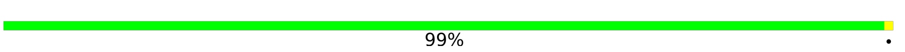
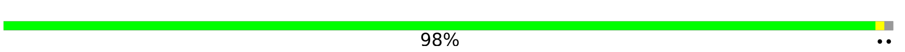
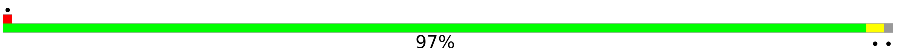
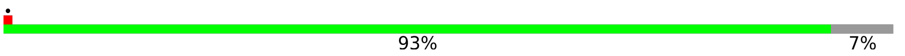
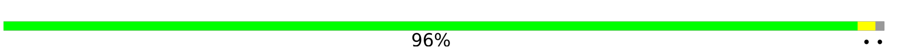
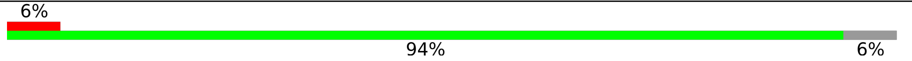
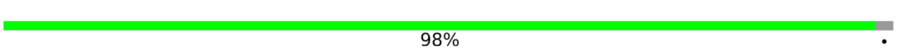
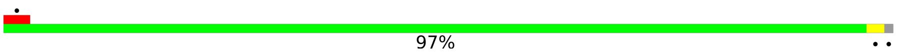
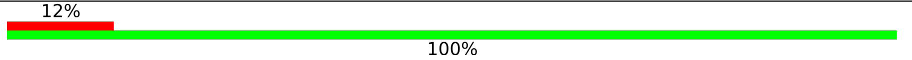
Mol	Chain	Length	Quality of chain
34	AQ	146	
35	AR	135	
36	AS	152	
37	AT	145	
38	AU	119	
39	AV	83	
40	AW	130	
41	AX	143	
42	AY	133	
43	AZ	125	
44	Aa	115	
45	Ab	84	
46	Ac	69	
47	Ad	56	
48	Ae	133	
49	Af	156	
50	Ag	317	
51	Ah	25	
52	Aj	216	

2 Entry composition ⓘ

There are 58 unique types of molecules in this entry. The entry contains 118236 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 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	I3	217	1750	1116	288	334	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I4	268	2087	1315	355	405	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I5	372	3111	2011	520	563	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I6	345	2751	1753	464	517	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I8	318	2594	1641	444	494	15	0	0

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

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

- Molecule 7 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Ip	105	797	501	145	149	2	0	0

- Molecule 8 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Iq	103	835	525	148	158	4	0	0

- Molecule 9 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Ir	293	2368	1486	415	454	13	0	0

- Molecule 10 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Is	159	1288	813	238	228	9	0	0

- Molecule 11 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	It	451	3445	2191	605	632	17	0	0

- Molecule 12 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Iu	587	4830	3048	869	891	22	0	0

- Molecule 13 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Iv	430	3553	2272	602	658	21	0	0

- Molecule 14 is a RNA chain called Met-tRNAi(Met).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Iw	75	Total	C	N	O	P	0	0
			1624	728	299	522	75		

- Molecule 15 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ix	455	Total	C	N	O	S	0	0
			3680	2311	640	707	22		

- Molecule 16 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Iy	633	Total	C	N	O	S	0	0
			4949	3102	886	928	33		

- Molecule 17 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A2	1780	Total	C	N	O	P	0	0
			38049	17008	6822	12439	1780		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AA	216	Total	C	N	O	S	0	0
			1708	1085	299	316	8		

- Molecule 19 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AB	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 20 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AC	218	Total	C	N	O	S	1	0
			1698	1099	292	297	10		

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AD	225	Total 1752	C 1117	N 315	O 313	S 7	0	0

- Molecule 22 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AE	262	Total 2076	C 1324	N 386	O 358	S 8	0	0

- Molecule 23 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AF	192	Total 1517	C 948	N 287	O 275	S 7	0	0

- Molecule 24 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AG	240	Total 1945	C 1212	N 393	O 333	S 7	0	0

- Molecule 25 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AH	188	Total 1515	C 966	N 279	O 269	S 1	0	0

- Molecule 26 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AI	205	Total 1682	C 1056	N 331	O 290	S 5	0	0

- Molecule 27 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AJ	180	Total 1499	C 955	N 300	O 242	S 2	0	0

- Molecule 28 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AK	97	Total 816	C 533	N 144	O 133	S 6	0	0

- Molecule 29 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AL	151	Total 1229	C 782	N 230	O 211	S 6	0	0

- Molecule 30 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AM	123	Total 953	C 598	N 169	O 177	S 9	0	0

- Molecule 31 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AN	149	Total 1202	C 770	N 228	O 203	S 1	0	0

- Molecule 32 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AO	135	Total 1010	C 618	N 198	O 188	S 6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	138	IAS	ASP	modified residue	UNP P62263

- Molecule 33 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AP	131	Total 1075	C 682	N 204	O 182	S 7	0	0

- Molecule 34 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	AQ	142	1128	717	213	195	3	0	0

- Molecule 35 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	AR	134	1082	680	201	197	4	0	0

- Molecule 36 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	AS	145	1200	753	242	204	1	0	0

- Molecule 37 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	AT	144	1123	704	217	199	3	0	0

- Molecule 38 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	AU	101	803	504	153	142	4	0	0

- Molecule 39 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	AV	83	639	395	117	122	5	0	0

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

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

- Molecule 41 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	AX	141	1112	703	222	184	3	2	0

- Molecule 42 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	AY	124	1014	641	198	170	5	0	0

- Molecule 43 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	AZ	72	574	368	104	101	1	0	0

- Molecule 44 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Aa	101	814	507	170	132	5	0	0

- Molecule 45 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Ab	83	650	408	121	114	7	0	0

- Molecule 46 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Ac	65	512	311	103	96	2	0	0

- Molecule 47 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Ad	55	458	286	94	73	5	0	0

- Molecule 48 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Ae	59	467	290	102	74	1	0	0

- Molecule 49 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Af	74	610	385	117	101	7	0	0

- Molecule 50 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	Ag	314	2440	1537	425	466	12	0	0

- Molecule 51 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Ah	25	239	145	64	27	3	0	0

- Molecule 52 is a protein called Host translation inhibitor nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	Aj	29	227	145	36	44	2	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aj	-22	MET	-	initiating methionine	UNP K9N7C7
Aj	-21	ALA	-	expression tag	UNP K9N7C7
Aj	-20	ASP	-	expression tag	UNP K9N7C7
Aj	-19	TYR	-	expression tag	UNP K9N7C7
Aj	-18	LYS	-	expression tag	UNP K9N7C7
Aj	-17	ASP	-	expression tag	UNP K9N7C7
Aj	-16	HIS	-	expression tag	UNP K9N7C7
Aj	-15	ASP	-	expression tag	UNP K9N7C7
Aj	-14	GLY	-	expression tag	UNP K9N7C7
Aj	-13	ASP	-	expression tag	UNP K9N7C7
Aj	-12	TYR	-	expression tag	UNP K9N7C7
Aj	-11	LYS	-	expression tag	UNP K9N7C7

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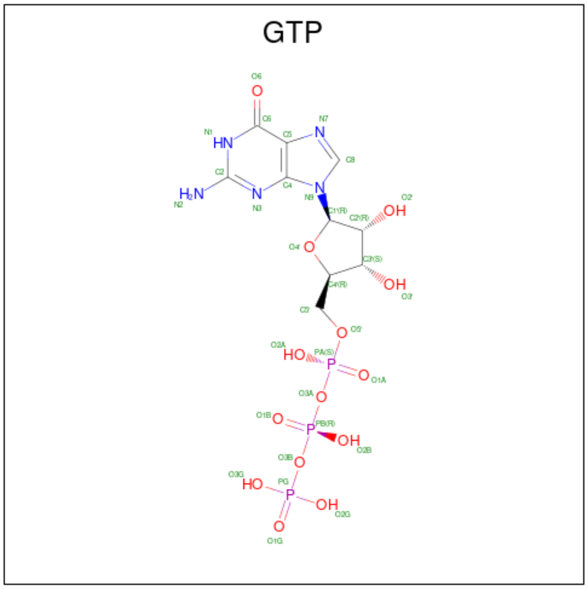
Chain	Residue	Modelled	Actual	Comment	Reference
Aj	-10	ASP	-	expression tag	UNP K9N7C7
Aj	-9	HIS	-	expression tag	UNP K9N7C7
Aj	-8	ASP	-	expression tag	UNP K9N7C7
Aj	-7	ILE	-	expression tag	UNP K9N7C7
Aj	-6	ASP	-	expression tag	UNP K9N7C7
Aj	-5	TYR	-	expression tag	UNP K9N7C7
Aj	-4	LYS	-	expression tag	UNP K9N7C7
Aj	-3	ASP	-	expression tag	UNP K9N7C7
Aj	-2	ASP	-	expression tag	UNP K9N7C7
Aj	-1	ASP	-	expression tag	UNP K9N7C7
Aj	0	ASP	-	expression tag	UNP K9N7C7
Aj	1	LYS	-	expression tag	UNP K9N7C7

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
53	Is	1	Total Zn 1 1	0
53	Aa	1	Total Zn 1 1	0
53	Ad	1	Total Zn 1 1	0
53	Af	1	Total Zn 1 1	0

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

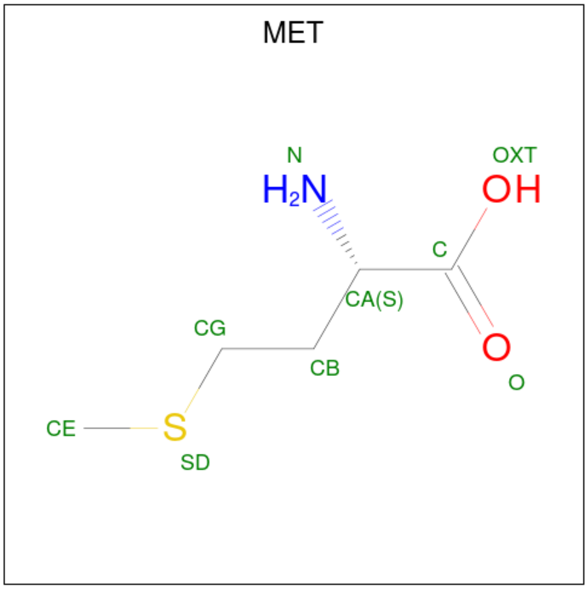


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	It	1	32	10	5	14	3	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
55	It	1	1	1	0
55	A2	110	110	110	0
55	AG	1	1	1	0
55	AS	2	2	2	0
55	AT	1	1	1	0
55	AX	1	1	1	0

- Molecule 56 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
56	Iw	1	8	5	1	1	1	0

- Molecule 57 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	AltConf
57	Iw	2	Total X 2 2	0
57	A2	122	Total X 122 122	0
57	AJ	1	Total X 1 1	0
57	AN	1	Total X 1 1	0
57	AO	2	Total X 2 2	0
57	Ad	1	Total X 1 1	0

- Molecule 58 is water.

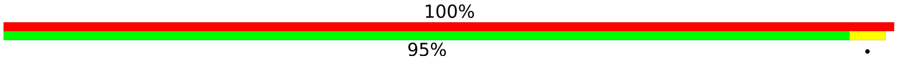
Mol	Chain	Residues	Atoms	AltConf
58	It	2	Total O 2 2	0

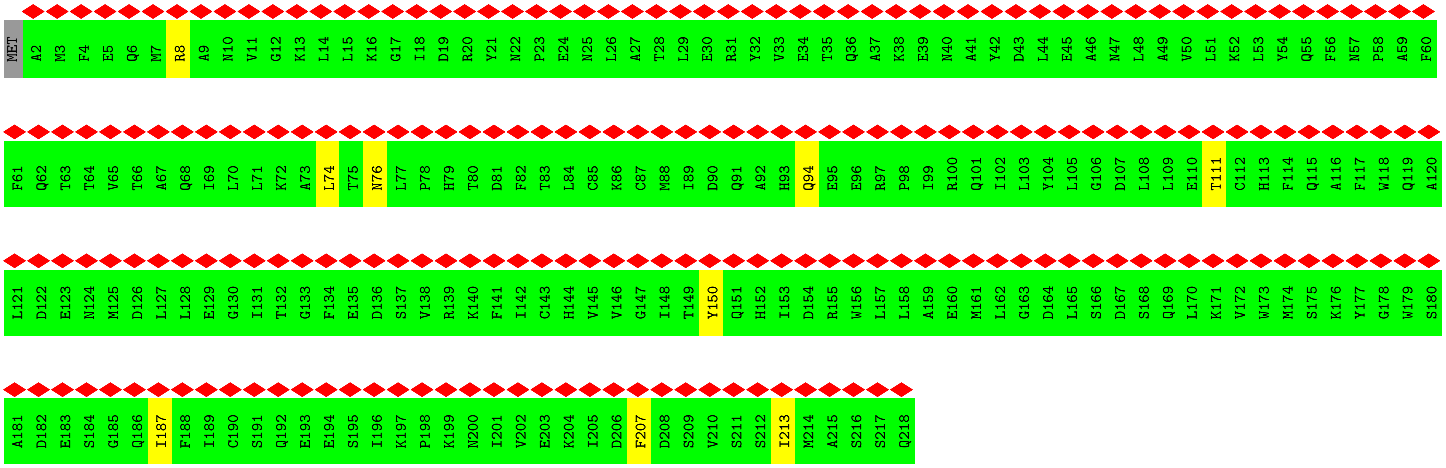
3 Residue-property plots ⓘ

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 3 subunit K

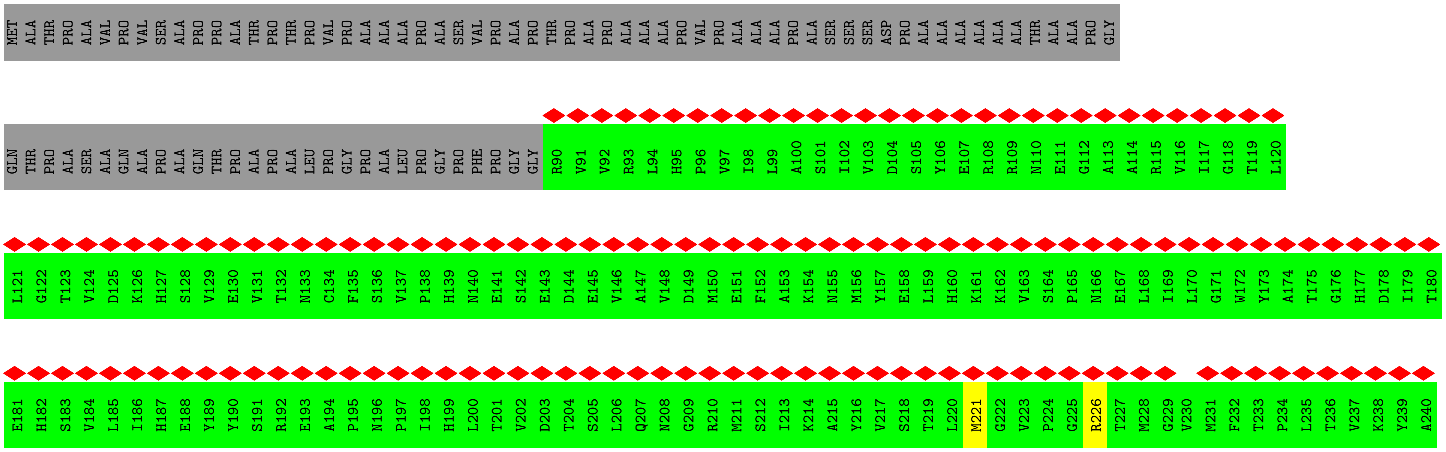
Chain I3:

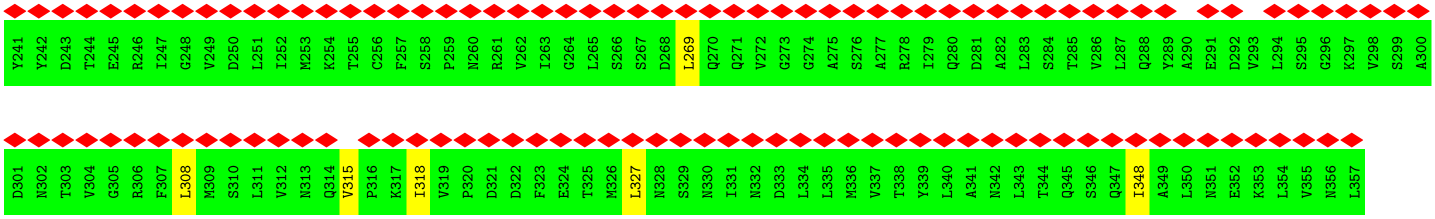




- Molecule 2: Eukaryotic translation initiation factor 3 subunit F

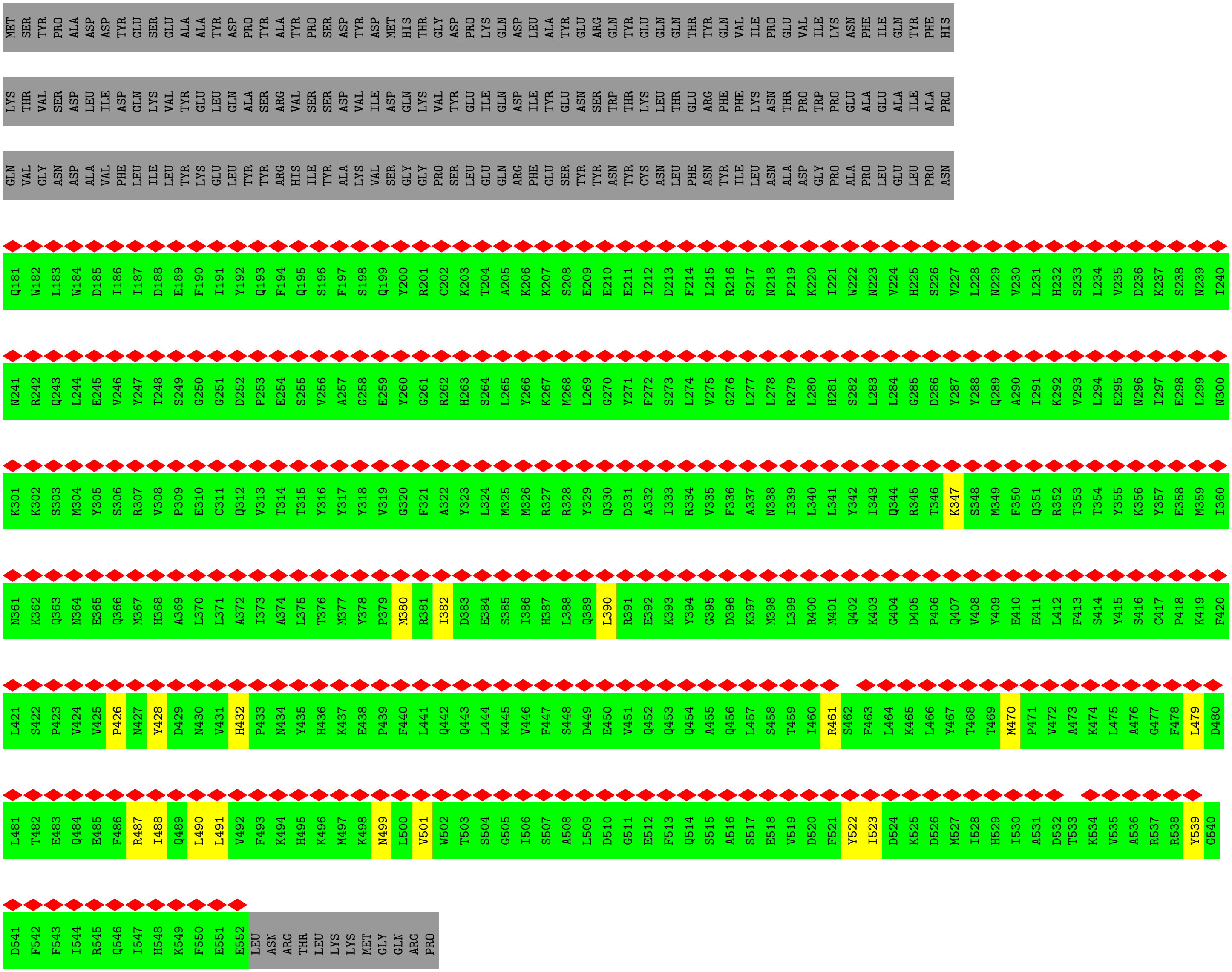
Chain I4:





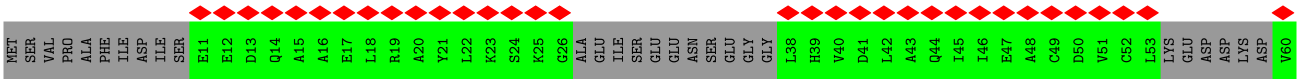
- Molecule 3: Eukaryotic translation initiation factor 3 subunit L

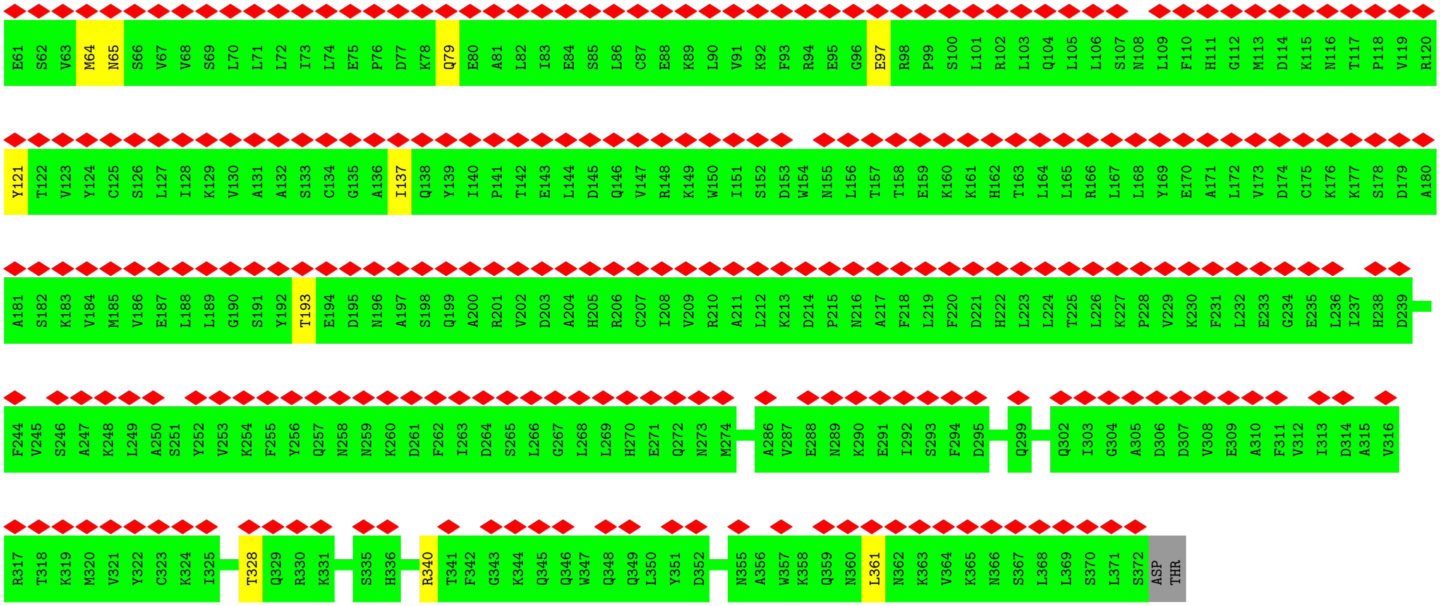
Chain I5:



- Molecule 4: Eukaryotic translation initiation factor 3 subunit M

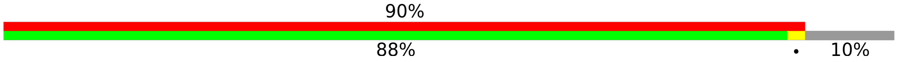
Chain I6:

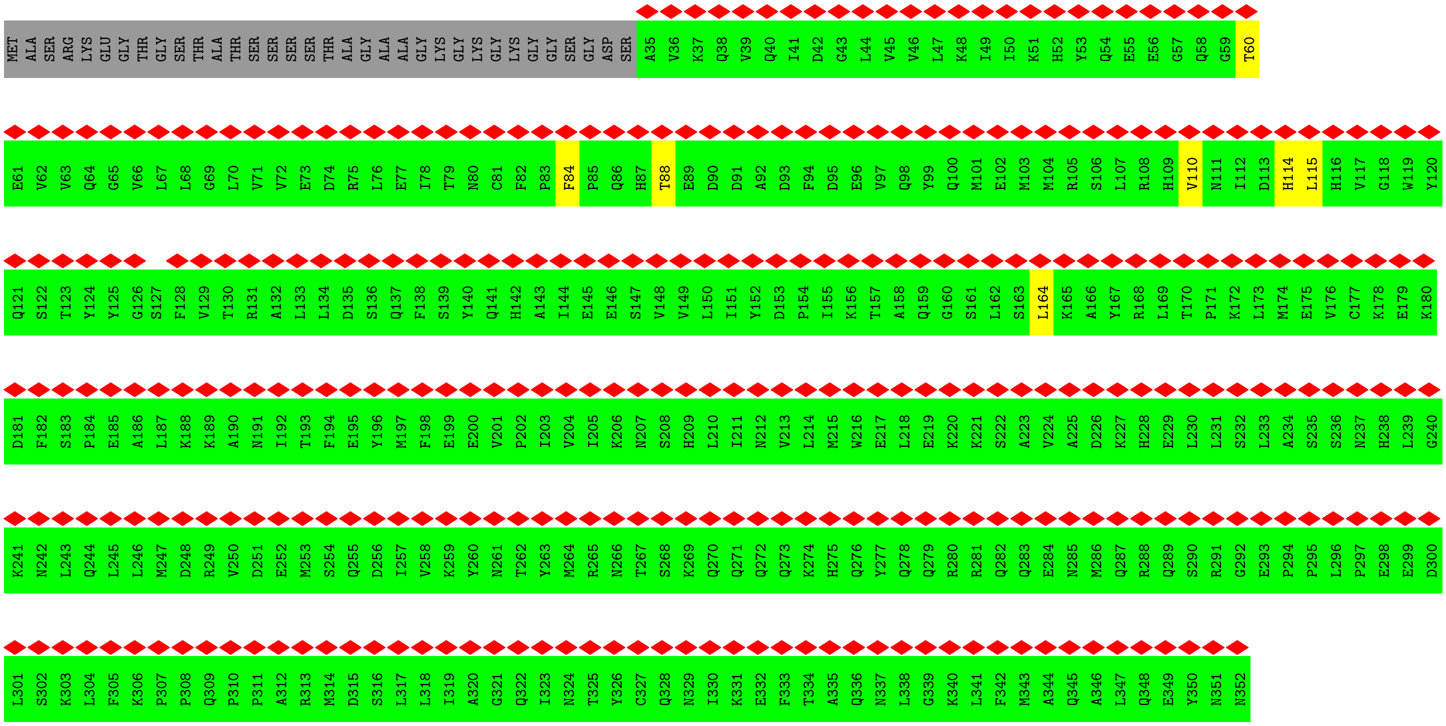




- Molecule 5: Eukaryotic translation initiation factor 3 subunit H

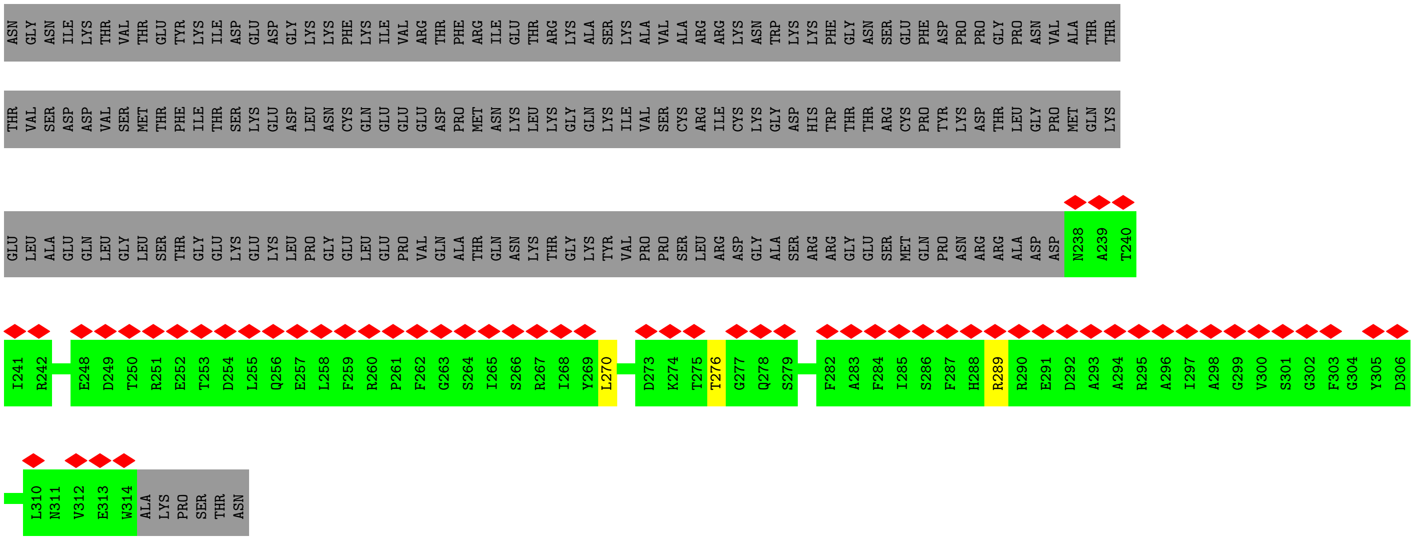
Chain I8:





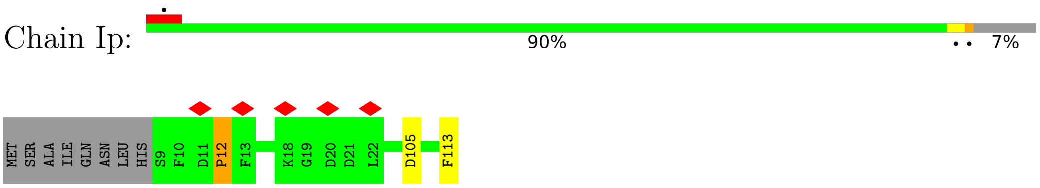
- Molecule 6: Eukaryotic translation initiation factor 3 subunit G

Chain Io:



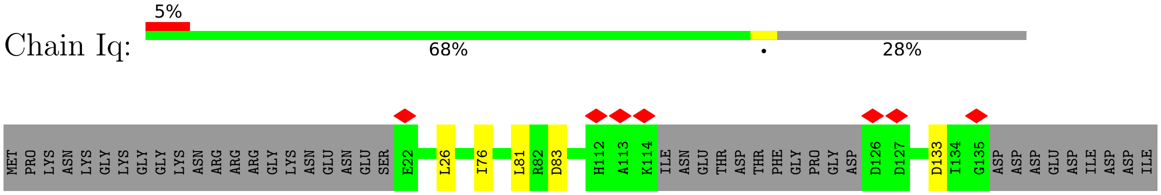
- Molecule 7: Eukaryotic translation initiation factor 1

Chain Ip:



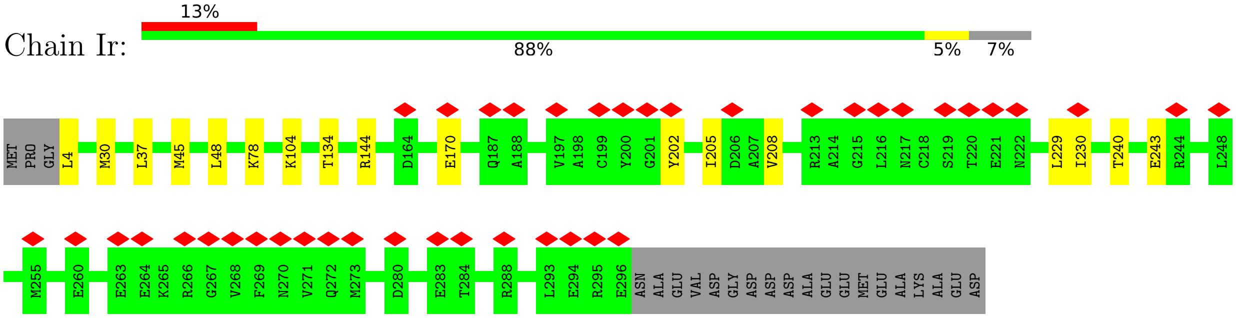
- Molecule 8: Eukaryotic translation initiation factor 1A, X-chromosomal

Chain Iq:



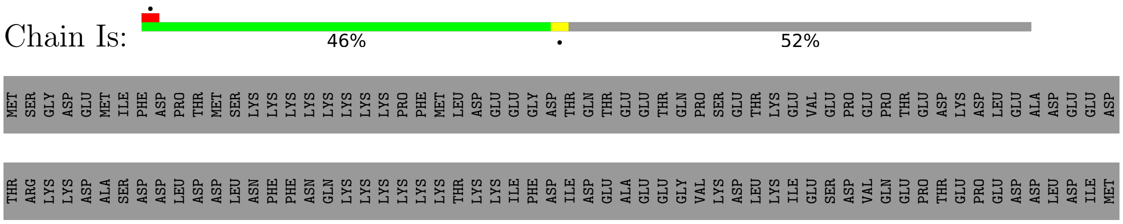
- Molecule 9: Eukaryotic translation initiation factor 2 subunit 1

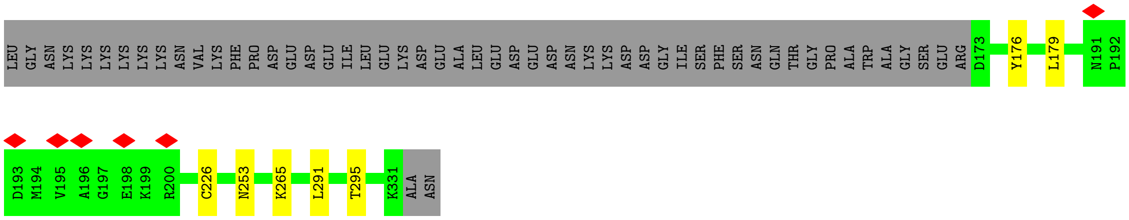
Chain Ir:



- Molecule 10: Eukaryotic translation initiation factor 2 subunit 2

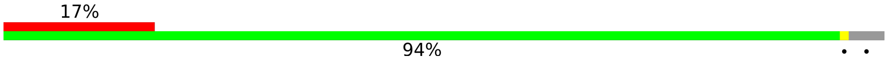
Chain Is:

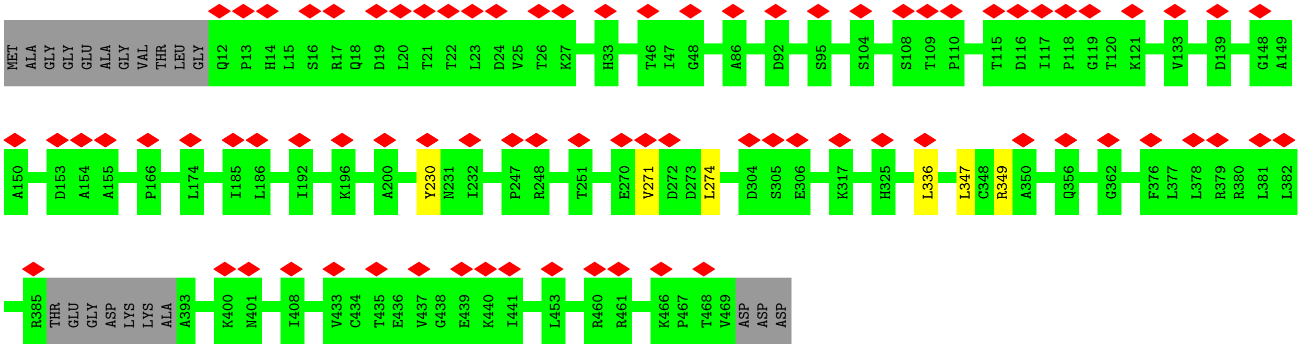




- Molecule 11: Eukaryotic translation initiation factor 2 subunit 3

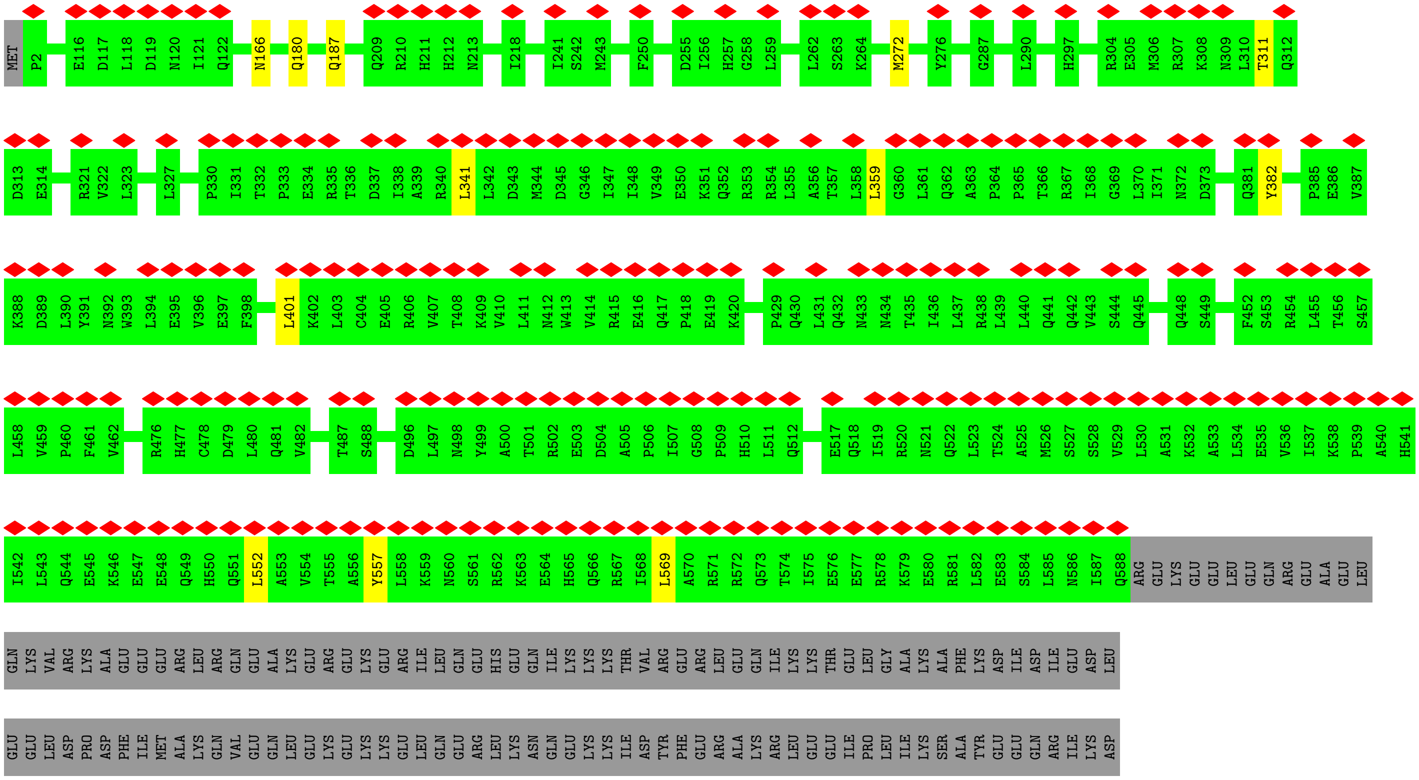
Chain It:

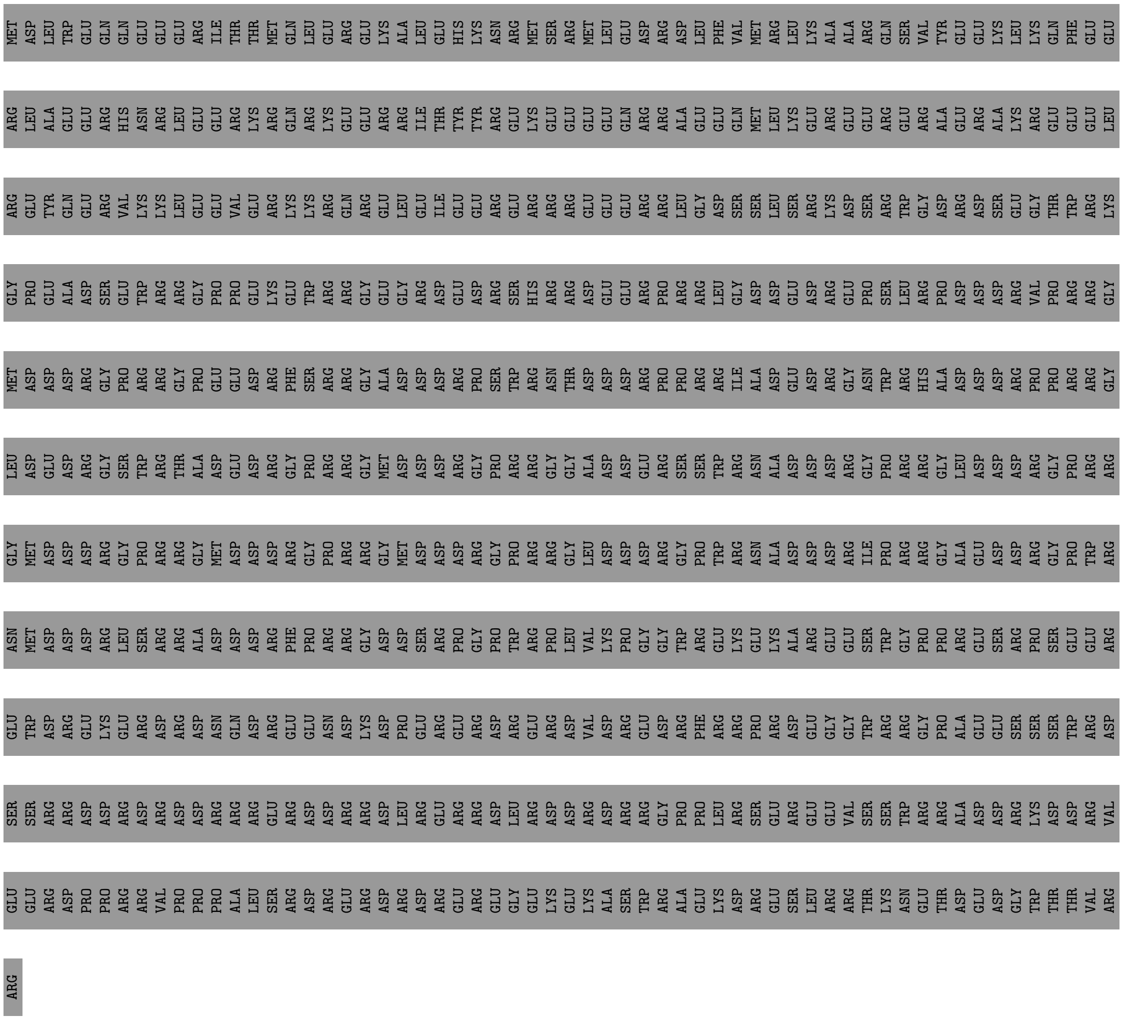




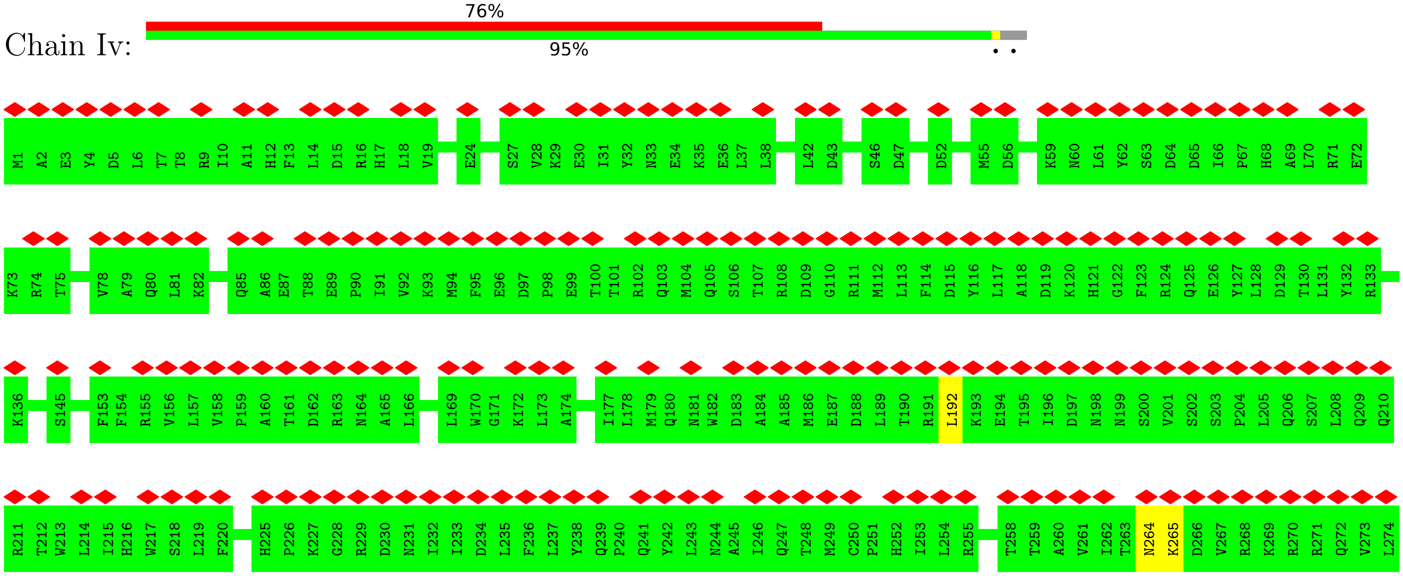
- Molecule 12: Eukaryotic translation initiation factor 3 subunit A

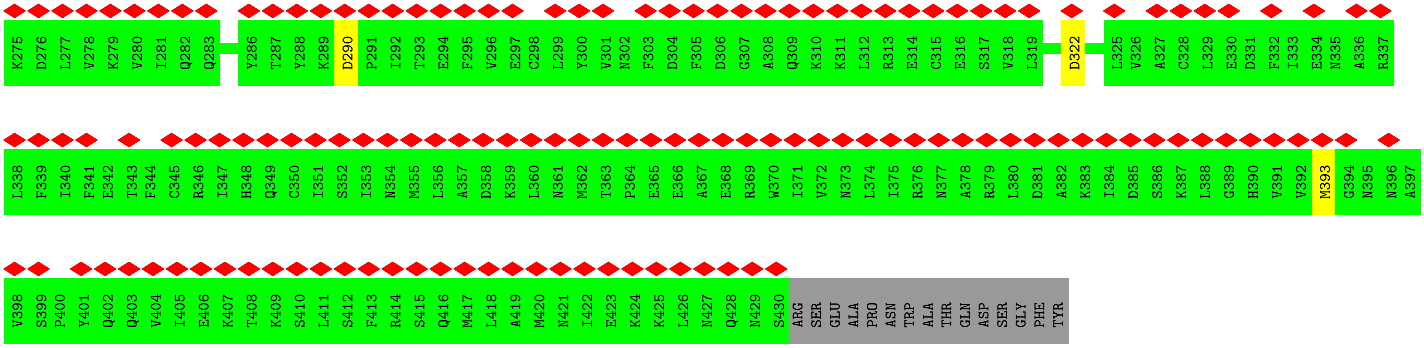
Chain Iu:





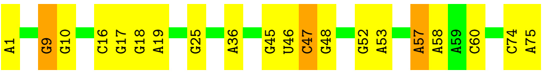
- Molecule 13: Eukaryotic translation initiation factor 3 subunit E





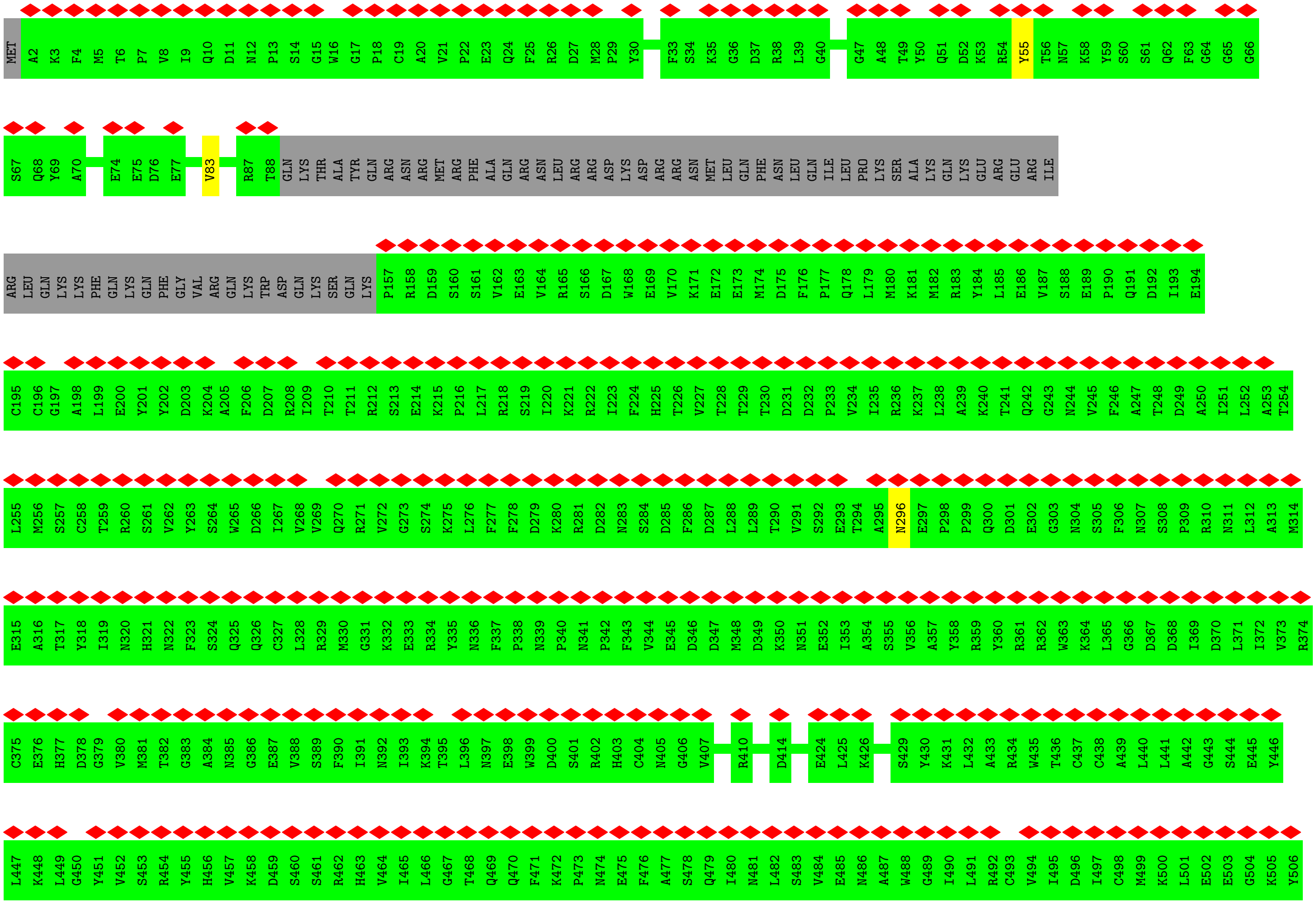
- Molecule 14: Met-tRNAi(Met)

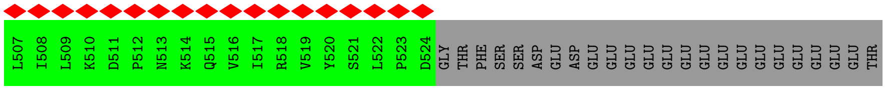
Chain Iw:



- Molecule 15: Eukaryotic translation initiation factor 3 subunit D

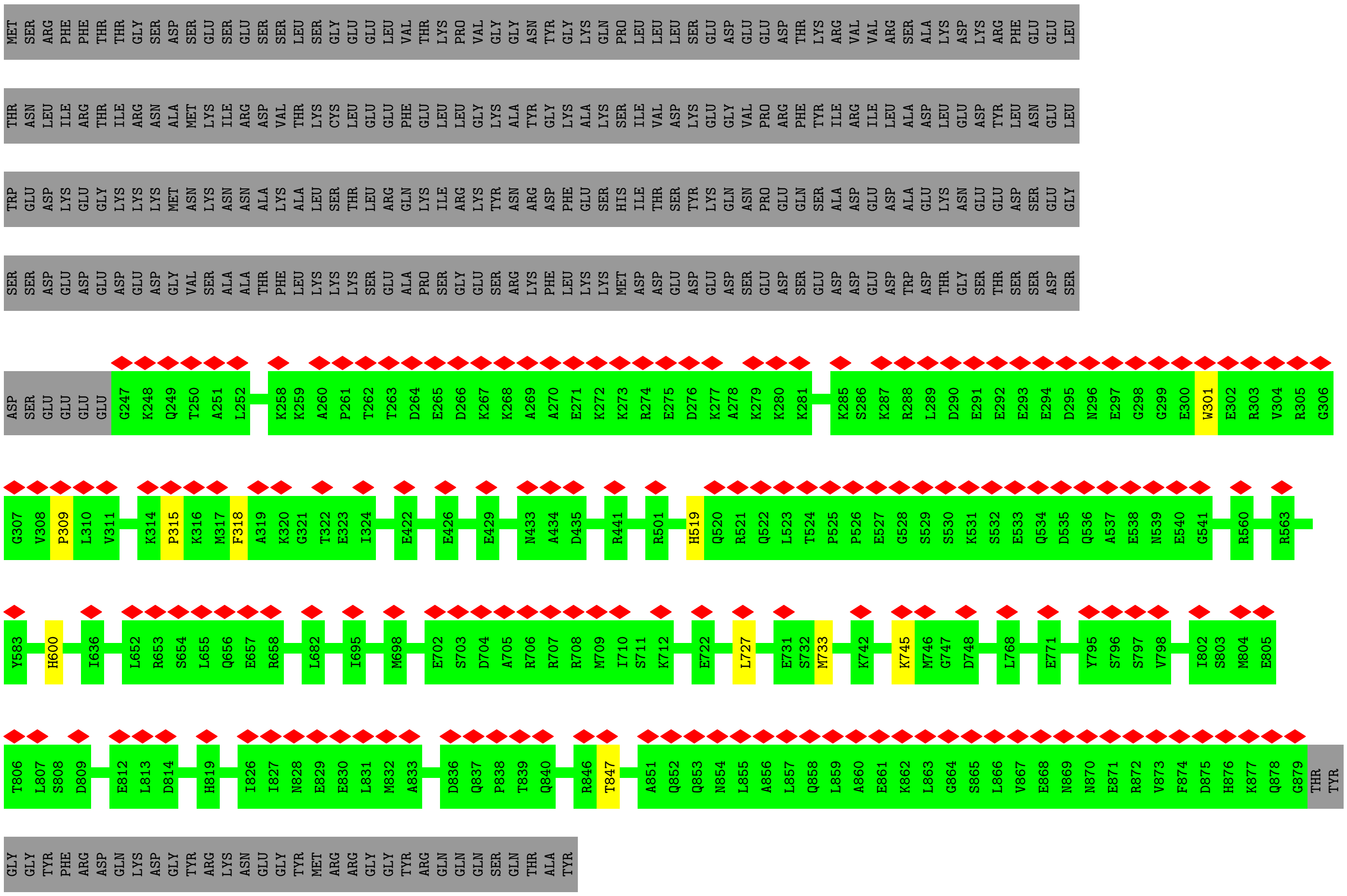
Chain Ix:





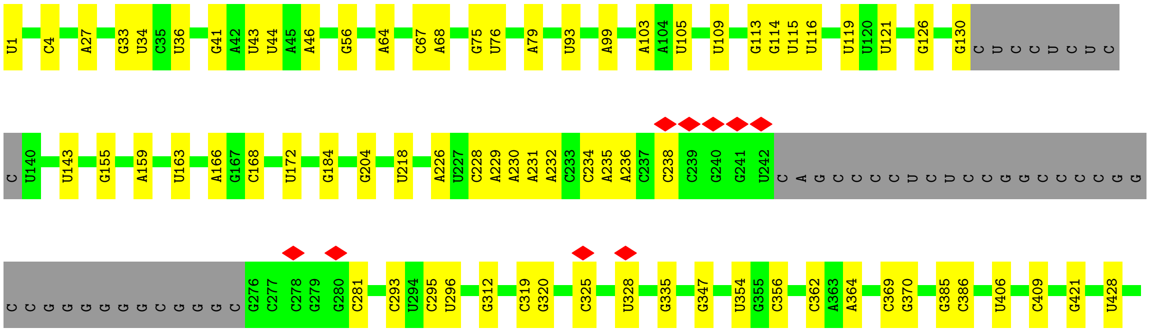
- Molecule 16: Eukaryotic translation initiation factor 3 subunit C

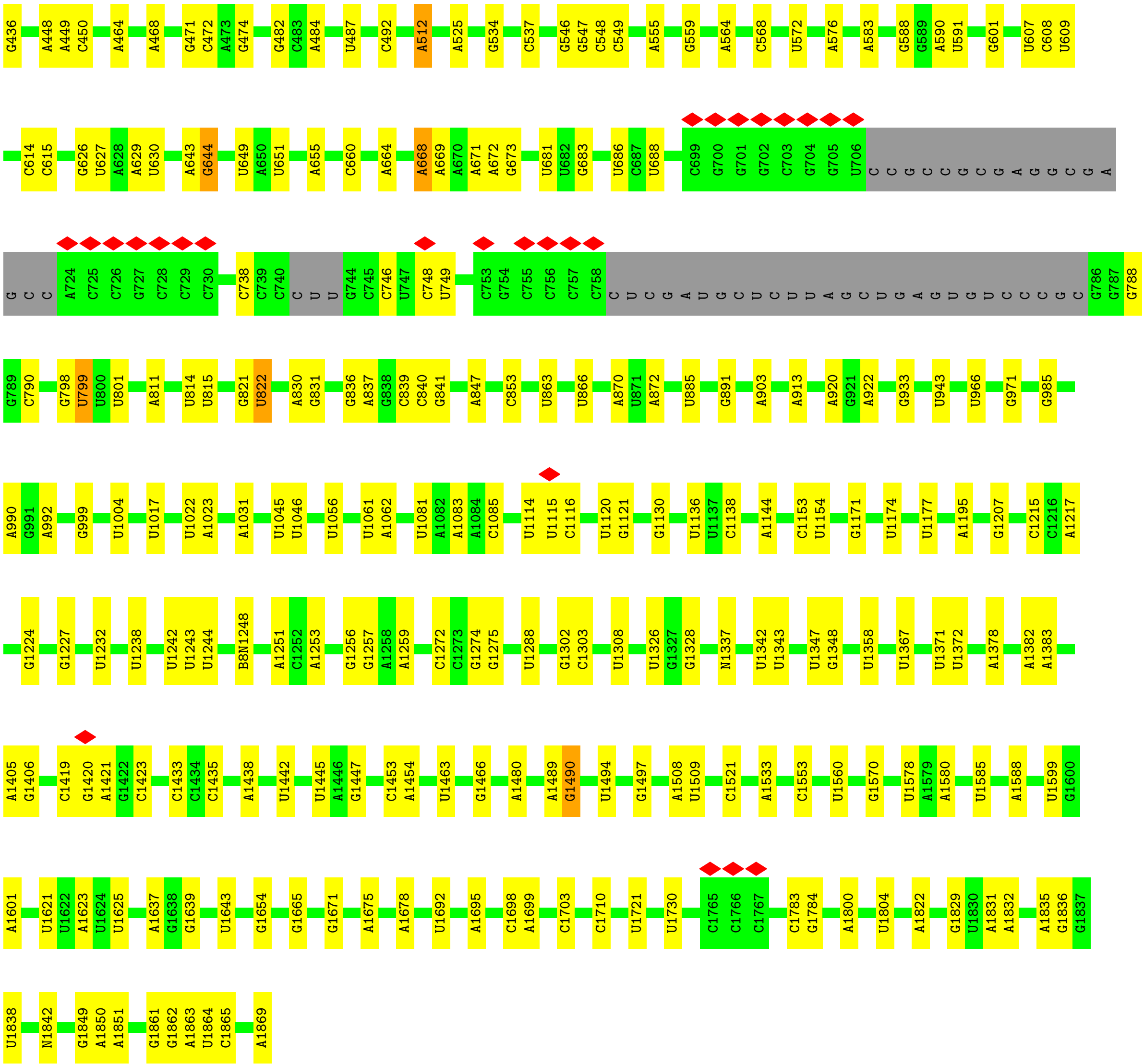
Chain Iy:



- Molecule 17: 18S rRNA

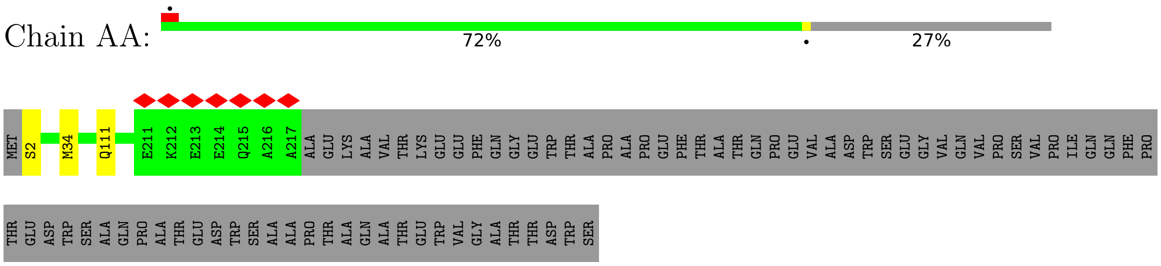
Chain A2:





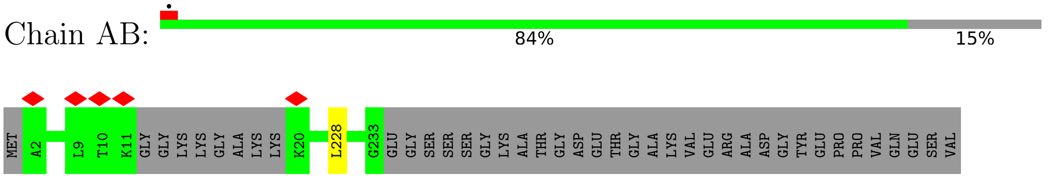
- Molecule 18: 40S ribosomal protein SA

Chain AA:



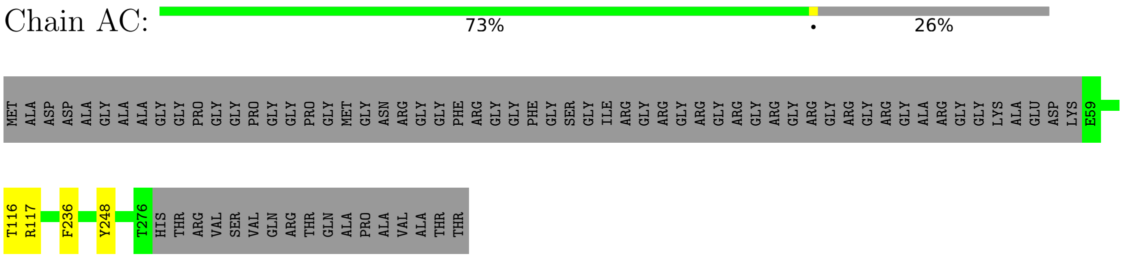
- Molecule 19: 40S ribosomal protein S3a

Chain AB:



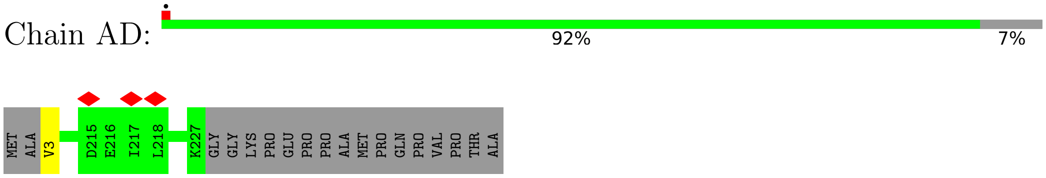
- Molecule 20: 40S ribosomal protein S2

Chain AC:



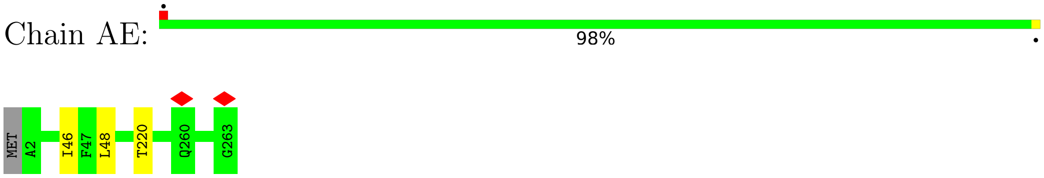
- Molecule 21: 40S ribosomal protein S3

Chain AD:



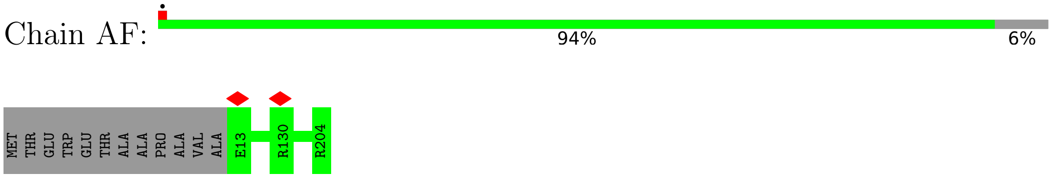
- Molecule 22: 40S ribosomal protein S4, X isoform

Chain AE:



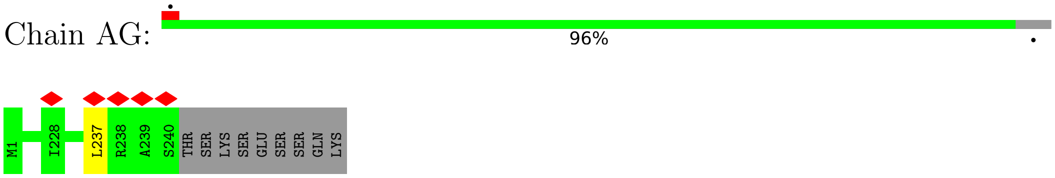
- Molecule 23: 40S ribosomal protein S5

Chain AF:



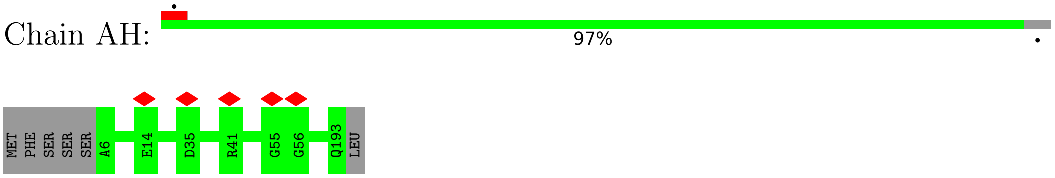
- Molecule 24: 40S ribosomal protein S6

Chain AG:



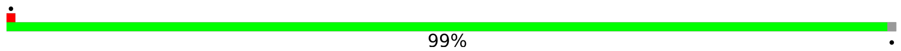
- Molecule 25: 40S ribosomal protein S7

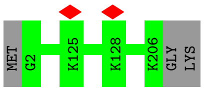
Chain AH:



- Molecule 26: 40S ribosomal protein S8

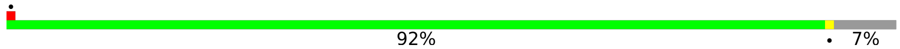
Chain AI:





- Molecule 27: 40S ribosomal protein S9

Chain AJ:

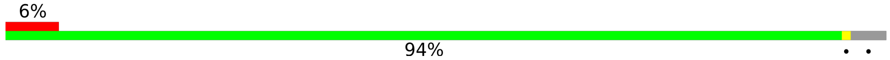


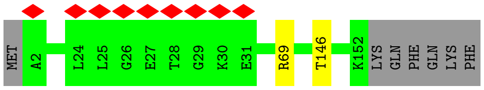
- Molecule 28: 40S ribosomal protein S10

Chain AK:

- Molecule 29: 40S ribosomal protein S11

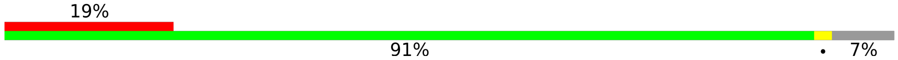
Chain AL:

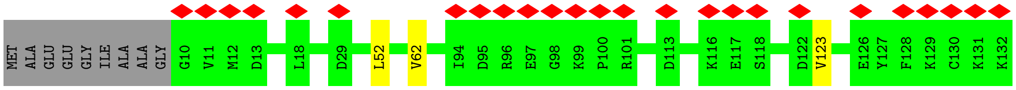




- Molecule 30: 40S ribosomal protein S12

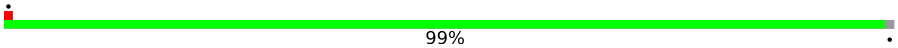
Chain AM:

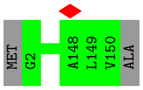




- Molecule 31: 40S ribosomal protein S13

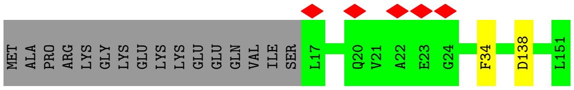
Chain AN:





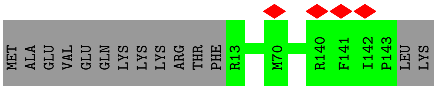
- Molecule 32: 40S ribosomal protein S14

Chain AO:



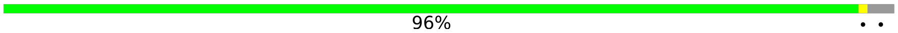
- Molecule 33: 40S ribosomal protein S15

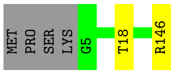
Chain AP:



- Molecule 34: 40S ribosomal protein S16

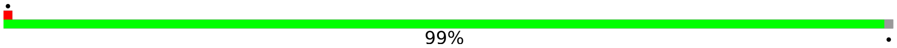
Chain AQ:

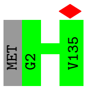




- Molecule 35: 40S ribosomal protein S17

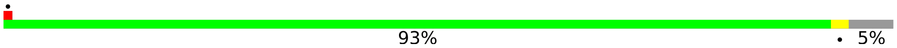
Chain AR:

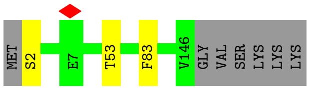




- Molecule 36: Small ribosomal subunit protein uS13

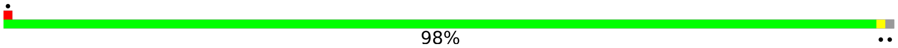
Chain AS:

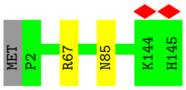




- Molecule 37: Small ribosomal subunit protein eS19

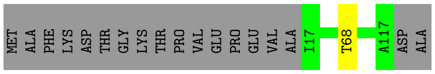
Chain AT:





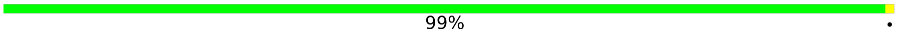
- Molecule 38: 40S ribosomal protein S20

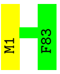
Chain AU:



- Molecule 39: 40S ribosomal protein S21

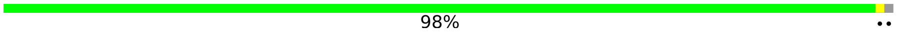
Chain AV:

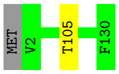




- Molecule 40: 40S ribosomal protein S15a

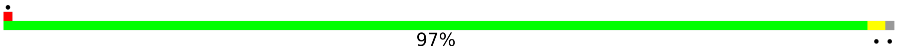
Chain AW:

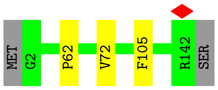




- Molecule 41: 40S ribosomal protein S23

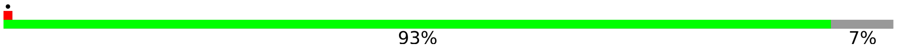
Chain AX:

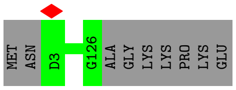




- Molecule 42: 40S ribosomal protein S24

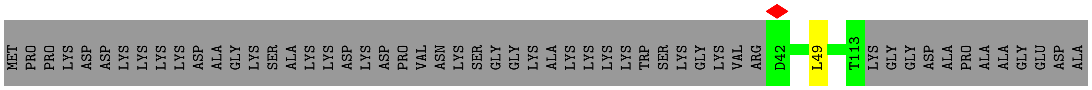
Chain AY:





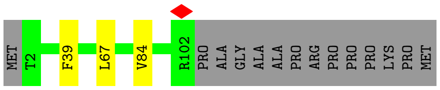
- Molecule 43: 40S ribosomal protein S25

Chain AZ:



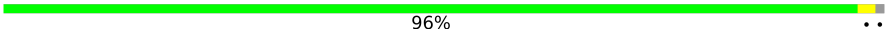
- Molecule 44: 40S ribosomal protein S26

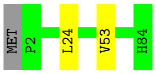
Chain Aa:



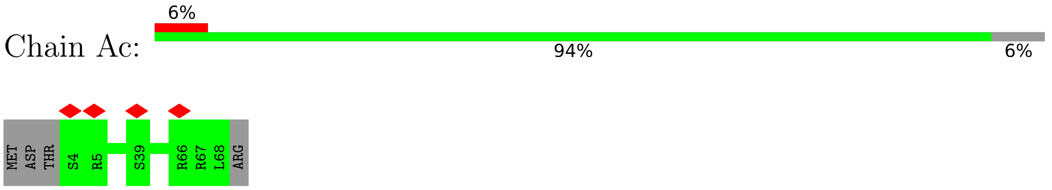
- Molecule 45: 40S ribosomal protein S27

Chain Ab:

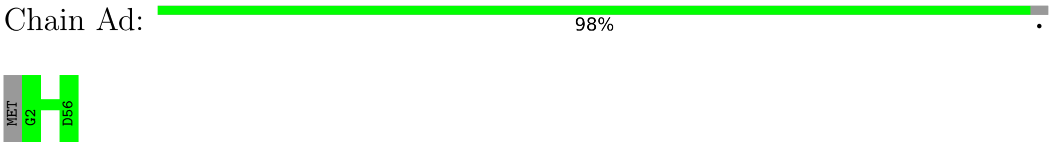




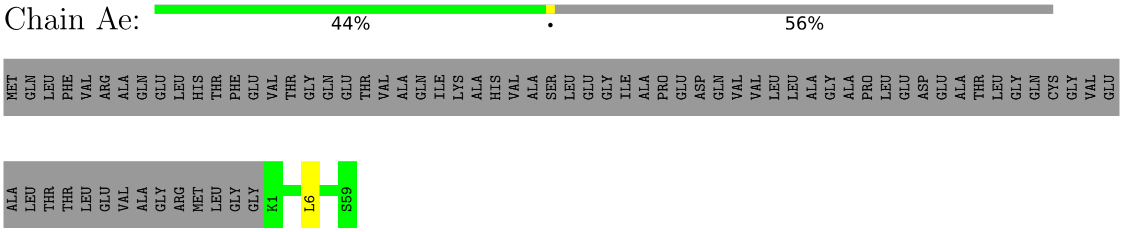
- Molecule 46: 40S ribosomal protein S28



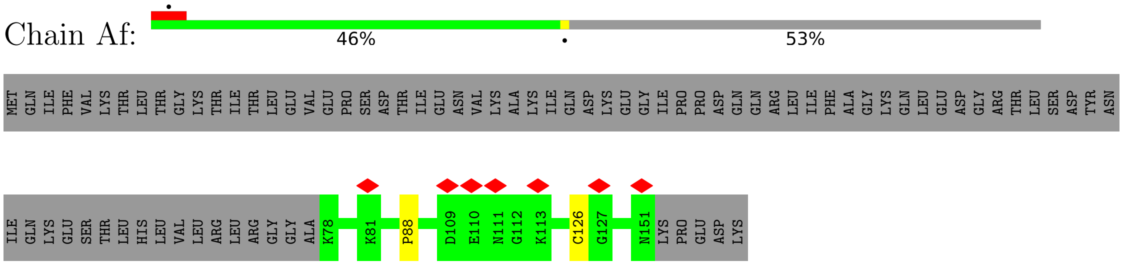
- Molecule 47: 40S ribosomal protein S29



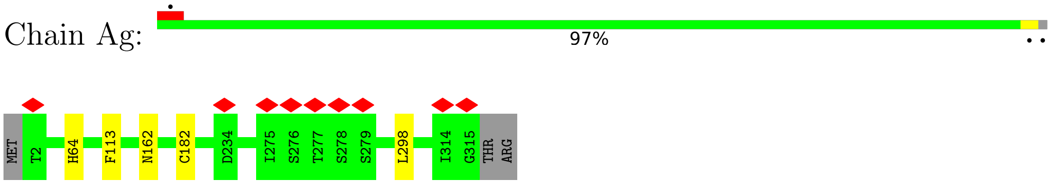
- Molecule 48: Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein



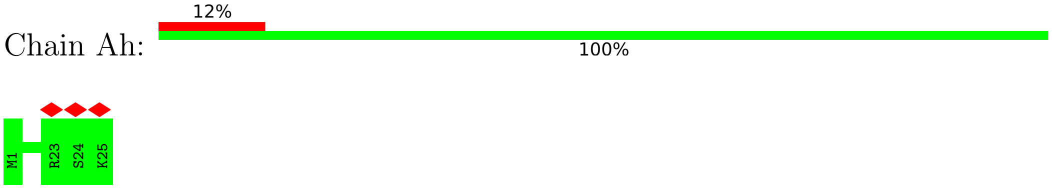
- Molecule 49: Ubiquitin-40S ribosomal protein S27a



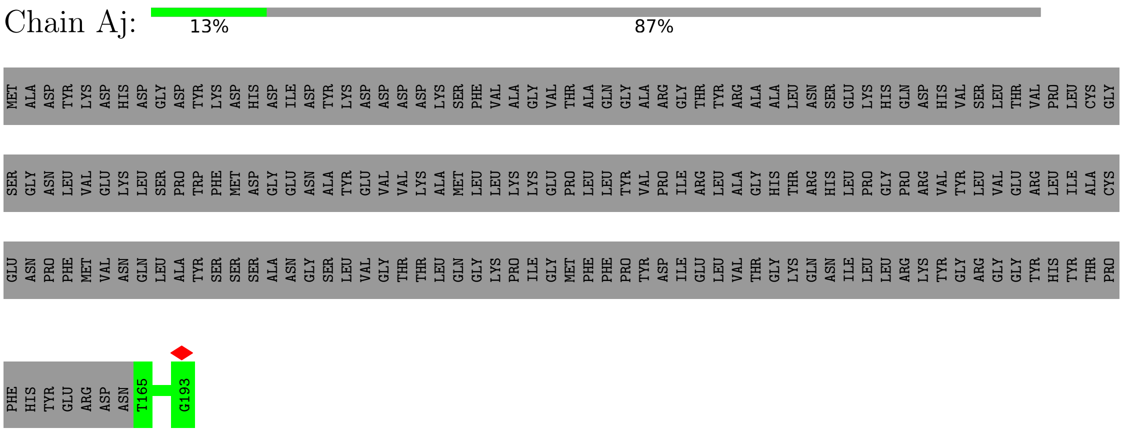
- Molecule 50: Receptor of activated protein C kinase 1



- Molecule 51: 60S ribosomal protein L41



- Molecule 52: Host translation inhibitor nsp1


Chain Aj:
13%
87%
MET ALA ASP TYR LYS ASP HIS ASP GLY ASP TYR LYS ASP HIS ASP ILE ASP TYR LYS ASP ASP ASP ASP LYS SER PHE VAL ALA GLY VAL THR ALA GLN GLY ALA ARG GLY THR TYR ARG ALA ALA LEU ASN SER GLU LYS HIS GLN ASP HIS VAL SER LEU THR VAL PRO LEU CYS GLY
SER GLY ASN LEU VAL GLU LYS LEU SER PRO TRP PHE MET ASP GLY GLU ASN ALA TYR GLU VAL VAL LYS ALA MET LEU LEU LYS LYS GLU PRO LEU LEU TYR VAL PRO ILE ARG LEU ALA GLY HIS THR ARG HIS LEU PRO GLY PRO ARG VAL TYR LEU VAL GLU ARG LEU ILE ALA CYS
GLU ASN PRO PHE MET VAL ASN GLN LEU ALA TYR SER SER SER ALA ASN GLY SER LEU VAL GLY THR THR LEU GLN GLY LYS PRO ILE GLY MET PHE PHE PRO TYR ASP ILE GLU LEU VAL THR GLY LYS GLN ASN ILE LEU LEU ARG LYS TYR GLY ARG GLY GLY TYR HIS TYR THR PRO
PHE HIS TYR GLU ARG ASP ASN T165 G193

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	218516	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 $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.673	Depositor
Minimum map value	-0.615	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	596.4, 596.4, 596.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	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: GTP, OMU, G7M, A2M, PSU, 1MG, NMM, 1MA, 5MC, 6MZ, OMG, B8N, MA6, IAS, SAC, AME, MG, UNX, H2U, OMC, ZN, HY3, 4AC, T6A, 2MG

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	I3	0.23	0/1785	0.43	0/2414
2	I4	0.24	0/2123	0.44	0/2885
3	I5	0.24	0/3187	0.44	0/4299
4	I6	0.23	0/2793	0.41	0/3770
5	I8	0.23	0/2645	0.41	0/3570
6	Io	0.25	0/628	0.52	0/846
7	Ip	0.25	0/808	0.52	1/1085 (0.1%)
8	Iq	0.24	0/845	0.48	0/1128
9	Ir	0.24	0/2400	0.50	0/3234
10	Is	0.25	0/1309	0.48	0/1757
11	It	0.24	0/3502	0.46	0/4739
12	Iu	0.23	0/4919	0.43	0/6647
13	Iv	0.23	0/3626	0.42	0/4902
14	Iw	0.37	1/1601 (0.1%)	0.70	0/2492
15	Ix	0.24	0/3763	0.46	0/5089
16	Iy	0.25	0/5032	0.45	2/6800 (0.0%)
17	A2	0.28	1/40497 (0.0%)	0.70	15/63121 (0.0%)
18	AA	0.26	0/1736	0.47	0/2359
19	AB	0.25	0/1841	0.47	0/2459
20	AC	0.26	0/1737	0.47	0/2346
21	AD	0.25	0/1780	0.49	0/2397
22	AE	0.26	0/2118	0.51	0/2849
23	AF	0.24	0/1539	0.49	0/2071
24	AG	0.24	0/1968	0.53	0/2619
25	AH	0.25	0/1538	0.47	0/2060
26	AI	0.25	0/1711	0.52	0/2282
27	AJ	0.25	0/1524	0.52	0/2035
28	AK	0.24	0/840	0.44	0/1133
29	AL	0.27	0/1250	0.52	0/1673
30	AM	0.23	0/963	0.42	0/1291
31	AN	0.25	0/1226	0.48	0/1649

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	AO	0.26	0/1014	0.54	0/1358
33	AP	0.25	0/1097	0.49	0/1467
34	AQ	0.26	0/1146	0.51	0/1534
35	AR	0.25	0/1097	0.48	0/1474
36	AS	0.24	0/1209	0.54	0/1620
37	AT	0.24	0/1130	0.46	0/1513
38	AU	0.24	0/813	0.52	0/1092
39	AV	0.26	0/635	0.49	0/850
40	AW	0.26	0/1051	0.50	0/1406
41	AX	0.25	0/1127	0.50	0/1501
42	AY	0.25	0/1031	0.50	0/1370
43	AZ	0.24	0/580	0.47	0/780
44	Aa	0.26	0/828	0.54	0/1109
45	Ab	0.25	0/664	0.46	0/891
46	Ac	0.24	0/514	0.58	0/688
47	Ad	0.26	0/469	0.52	0/623
48	Ae	0.26	0/473	0.53	0/623
49	Af	0.32	0/622	0.50	0/822
50	Ag	0.24	0/2497	0.48	0/3399
51	Ah	0.22	0/240	0.67	0/305
52	Aj	0.25	0/232	0.36	0/311
All	All	0.26	2/121703 (0.0%)	0.57	18/172737 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A2	1	U	OP3-P	-10.66	1.48	1.61
14	Iw	1	A	OP3-P	-10.60	1.48	1.61

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	356	C	C2-N1-C1’	8.03	127.63	118.80
17	A2	1453	C	C2-N1-C1’	8.02	127.63	118.80
17	A2	356	C	N1-C2-O2	7.84	123.60	118.90
17	A2	1453	C	N1-C2-O2	7.41	123.34	118.90
7	Ip	12	PRO	N-CA-CB	6.66	111.29	103.30
17	A2	356	C	N3-C2-O2	-6.23	117.54	121.90
17	A2	630	U	C2-N1-C1’	6.08	125.00	117.70
16	Iy	315	PRO	N-CA-CB	5.77	110.22	103.30
17	A2	1453	C	N3-C2-O2	-5.77	117.86	121.90
17	A2	356	C	C6-N1-C1’	-5.74	113.92	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	293	C	C2-N1-C1'	5.69	125.06	118.80
17	A2	293	C	N1-C2-O2	5.67	122.31	118.90
17	A2	1453	C	C6-N1-C1'	-5.55	114.14	120.80
16	Iy	309	PRO	N-CA-CB	5.47	109.87	103.30
17	A2	630	U	N1-C2-O2	5.46	126.62	122.80
17	A2	853	C	C2-N1-C1'	5.26	124.58	118.80
17	A2	1453	C	C6-N1-C2	-5.21	118.22	120.30
17	A2	1022	U	C2-N1-C1'	5.05	123.75	117.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	I3	215/218 (99%)	205 (95%)	10 (5%)	0	100	100
2	I4	266/357 (74%)	261 (98%)	5 (2%)	0	100	100
3	I5	370/564 (66%)	340 (92%)	30 (8%)	0	100	100
4	I6	339/374 (91%)	326 (96%)	12 (4%)	1 (0%)	41	56
5	I8	316/352 (90%)	308 (98%)	8 (2%)	0	100	100
6	Io	75/320 (23%)	71 (95%)	4 (5%)	0	100	100
7	Ip	103/113 (91%)	99 (96%)	3 (3%)	1 (1%)	15	23
8	Iq	99/144 (69%)	97 (98%)	2 (2%)	0	100	100
9	Ir	291/315 (92%)	278 (96%)	12 (4%)	1 (0%)	41	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	Is	157/333 (47%)	151 (96%)	6 (4%)	0	100	100
11	It	447/472 (95%)	443 (99%)	4 (1%)	0	100	100
12	Iu	585/1382 (42%)	570 (97%)	15 (3%)	0	100	100
13	Iv	428/445 (96%)	424 (99%)	2 (0%)	2 (0%)	29	43
15	Ix	451/548 (82%)	443 (98%)	8 (2%)	0	100	100
16	Iy	631/913 (69%)	617 (98%)	13 (2%)	1 (0%)	47	64
18	AA	214/295 (72%)	210 (98%)	4 (2%)	0	100	100
19	AB	220/264 (83%)	216 (98%)	4 (2%)	0	100	100
20	AC	217/293 (74%)	215 (99%)	2 (1%)	0	100	100
21	AD	223/243 (92%)	223 (100%)	0	0	100	100
22	AE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
23	AF	190/204 (93%)	182 (96%)	8 (4%)	0	100	100
24	AG	238/249 (96%)	238 (100%)	0	0	100	100
25	AH	186/194 (96%)	183 (98%)	3 (2%)	0	100	100
26	AI	203/208 (98%)	200 (98%)	3 (2%)	0	100	100
27	AJ	178/194 (92%)	176 (99%)	2 (1%)	0	100	100
28	AK	95/165 (58%)	93 (98%)	2 (2%)	0	100	100
29	AL	149/158 (94%)	148 (99%)	1 (1%)	0	100	100
30	AM	121/132 (92%)	114 (94%)	7 (6%)	0	100	100
31	AN	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
32	AO	131/151 (87%)	130 (99%)	1 (1%)	0	100	100
33	AP	129/145 (89%)	128 (99%)	1 (1%)	0	100	100
34	AQ	140/146 (96%)	138 (99%)	2 (1%)	0	100	100
35	AR	132/135 (98%)	132 (100%)	0	0	100	100
36	AS	143/152 (94%)	139 (97%)	4 (3%)	0	100	100
37	AT	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
38	AU	99/119 (83%)	97 (98%)	2 (2%)	0	100	100
39	AV	81/83 (98%)	81 (100%)	0	0	100	100
40	AW	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
41	AX	140/143 (98%)	138 (99%)	2 (1%)	0	100	100
42	AY	122/133 (92%)	122 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	AZ	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
44	Aa	99/115 (86%)	99 (100%)	0	0	100	100
45	Ab	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
46	Ac	63/69 (91%)	63 (100%)	0	0	100	100
47	Ad	53/56 (95%)	53 (100%)	0	0	100	100
48	Ae	57/133 (43%)	56 (98%)	1 (2%)	0	100	100
49	Af	72/156 (46%)	66 (92%)	5 (7%)	1 (1%)	11	16
50	Ag	312/317 (98%)	298 (96%)	14 (4%)	0	100	100
51	Ah	23/25 (92%)	23 (100%)	0	0	100	100
52	Aj	27/216 (12%)	27 (100%)	0	0	100	100
All	All	9656/12641 (76%)	9431 (98%)	218 (2%)	7 (0%)	54	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	Ip	12	PRO
9	Ir	202	TYR
13	Iv	265	LYS
13	Iv	264	ASN
16	Iy	301	TRP
4	I6	97	GLU
49	Af	88	PRO

5.3.2 Protein sidechains ⓘ

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	I3	192/193 (100%)	183 (95%)	9 (5%)	26	40
2	I4	237/289 (82%)	229 (97%)	8 (3%)	37	53
3	I5	342/515 (66%)	323 (94%)	19 (6%)	21	33
4	I6	308/335 (92%)	299 (97%)	9 (3%)	42	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I8	290/310 (94%)	283 (98%)	7 (2%)	49	67
6	Io	64/277 (23%)	61 (95%)	3 (5%)	26	40
7	Ip	77/96 (80%)	75 (97%)	2 (3%)	46	64
8	Iq	88/123 (72%)	83 (94%)	5 (6%)	20	31
9	Ir	264/280 (94%)	248 (94%)	16 (6%)	18	29
10	Is	144/304 (47%)	137 (95%)	7 (5%)	25	38
11	It	384/397 (97%)	378 (98%)	6 (2%)	62	78
12	Iu	540/1259 (43%)	528 (98%)	12 (2%)	52	70
13	Iv	394/406 (97%)	390 (99%)	4 (1%)	76	86
15	Ix	406/494 (82%)	403 (99%)	3 (1%)	84	91
16	Iy	516/811 (64%)	509 (99%)	7 (1%)	67	81
18	AA	179/242 (74%)	177 (99%)	2 (1%)	73	85
19	AB	203/231 (88%)	202 (100%)	1 (0%)	88	94
20	AC	185/225 (82%)	181 (98%)	4 (2%)	52	70
21	AD	189/202 (94%)	188 (100%)	1 (0%)	88	94
22	AE	224/225 (100%)	221 (99%)	3 (1%)	69	82
23	AF	162/170 (95%)	162 (100%)	0	100	100
24	AG	209/218 (96%)	208 (100%)	1 (0%)	88	94
25	AH	168/174 (97%)	168 (100%)	0	100	100
26	AI	178/180 (99%)	178 (100%)	0	100	100
27	AJ	160/168 (95%)	158 (99%)	2 (1%)	69	82
28	AK	88/136 (65%)	87 (99%)	1 (1%)	73	85
29	AL	135/142 (95%)	133 (98%)	2 (2%)	65	80
30	AM	104/108 (96%)	101 (97%)	3 (3%)	42	60
31	AN	130/131 (99%)	130 (100%)	0	100	100
32	AO	104/118 (88%)	103 (99%)	1 (1%)	76	86
33	AP	117/130 (90%)	117 (100%)	0	100	100
34	AQ	117/121 (97%)	115 (98%)	2 (2%)	60	77
35	AR	121/122 (99%)	121 (100%)	0	100	100
36	AS	125/131 (95%)	123 (98%)	2 (2%)	62	78
37	AT	113/114 (99%)	112 (99%)	1 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	AU	93/107 (87%)	92 (99%)	1 (1%)	73	85
39	AV	66/66 (100%)	66 (100%)	0	100	100
40	AW	112/113 (99%)	111 (99%)	1 (1%)	78	87
41	AX	114/114 (100%)	112 (98%)	2 (2%)	59	75
42	AY	108/115 (94%)	108 (100%)	0	100	100
43	AZ	64/103 (62%)	63 (98%)	1 (2%)	62	78
44	Aa	88/98 (90%)	85 (97%)	3 (3%)	37	53
45	Ab	75/76 (99%)	73 (97%)	2 (3%)	44	63
46	Ac	58/62 (94%)	58 (100%)	0	100	100
47	Ad	48/49 (98%)	48 (100%)	0	100	100
48	Ae	48/104 (46%)	47 (98%)	1 (2%)	53	72
49	Af	67/140 (48%)	66 (98%)	1 (2%)	65	80
50	Ag	272/275 (99%)	267 (98%)	5 (2%)	59	75
51	Ah	24/24 (100%)	24 (100%)	0	100	100
52	Aj	24/182 (13%)	24 (100%)	0	100	100
All	All	8518/11005 (77%)	8358 (98%)	160 (2%)	59	74

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I3	8	ARG
1	I3	74	LEU
1	I3	76	ASN
1	I3	94	GLN
1	I3	111	THR
1	I3	150	TYR
1	I3	187	ILE
1	I3	207	PHE
1	I3	213	ILE
2	I4	221	MET
2	I4	226	ARG
2	I4	269	LEU
2	I4	308	LEU
2	I4	315	VAL
2	I4	318	ILE
2	I4	327	LEU
2	I4	348	ILE

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Mol	Chain	Res	Type
3	I5	347	LYS
3	I5	380	MET
3	I5	382	ILE
3	I5	390	LEU
3	I5	426	PRO
3	I5	428	TYR
3	I5	432	HIS
3	I5	461	ARG
3	I5	470	MET
3	I5	479	LEU
3	I5	487	ARG
3	I5	488	ILE
3	I5	490	LEU
3	I5	491	LEU
3	I5	499	ASN
3	I5	501	VAL
3	I5	522	TYR
3	I5	523	ILE
3	I5	539	TYR
4	I6	64	MET
4	I6	65	ASN
4	I6	79	GLN
4	I6	121	TYR
4	I6	137	ILE
4	I6	193	THR
4	I6	328	THR
4	I6	340	ARG
4	I6	361	LEU
5	I8	60	THR
5	I8	84	PHE
5	I8	88	THR
5	I8	110	VAL
5	I8	114	HIS
5	I8	115	LEU
5	I8	164	LEU
6	Io	270	LEU
6	Io	276	THR
6	Io	289	ARG
7	Ip	105	ASP
7	Ip	113	PHE
8	Iq	26	LEU
8	Iq	76	ILE

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Mol	Chain	Res	Type
8	Iq	81	LEU
8	Iq	83	ASP
8	Iq	133	ASP
9	Ir	4	LEU
9	Ir	30	MET
9	Ir	37	LEU
9	Ir	45	MET
9	Ir	48	LEU
9	Ir	78	LYS
9	Ir	104	LYS
9	Ir	134	THR
9	Ir	144	ARG
9	Ir	170	GLU
9	Ir	205	ILE
9	Ir	208	VAL
9	Ir	229	LEU
9	Ir	230	ILE
9	Ir	240	THR
9	Ir	243	GLU
10	Is	176	TYR
10	Is	179	LEU
10	Is	226	CYS
10	Is	253	ASN
10	Is	265	LYS
10	Is	291	LEU
10	Is	295	THR
11	It	230	TYR
11	It	271	VAL
11	It	274	LEU
11	It	336	LEU
11	It	347	LEU
11	It	349	ARG
12	Iu	166	ASN
12	Iu	180	GLN
12	Iu	187	GLN
12	Iu	272	MET
12	Iu	311	THR
12	Iu	341	LEU
12	Iu	359	LEU
12	Iu	382	TYR
12	Iu	401	LEU
12	Iu	552	LEU

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Mol	Chain	Res	Type
12	Iu	557	TYR
12	Iu	569	LEU
13	Iv	192	LEU
13	Iv	290	ASP
13	Iv	322	ASP
13	Iv	393	MET
15	Ix	55	TYR
15	Ix	83	VAL
15	Ix	296	ASN
16	Iy	318	PHE
16	Iy	519	HIS
16	Iy	600	HIS
16	Iy	727	LEU
16	Iy	733	MET
16	Iy	745	LYS
16	Iy	847	THR
18	AA	34	MET
18	AA	111	GLN
19	AB	228	LEU
20	AC	116	THR
20	AC	117	ARG
20	AC	236	PHE
20	AC	248	TYR
21	AD	3	VAL
22	AE	46	ILE
22	AE	48	LEU
22	AE	220	THR
24	AG	237	LEU
27	AJ	29	LEU
27	AJ	106	LEU
28	AK	72	THR
29	AL	69	ARG
29	AL	146	THR
30	AM	52	LEU
30	AM	62	VAL
30	AM	123	VAL
32	AO	34	PHE
34	AQ	18	THR
34	AQ	146	ARG
36	AS	53	THR
36	AS	83	PHE
37	AT	85	ASN

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Mol	Chain	Res	Type
38	AU	68	THR
40	AW	105	THR
41	AX	72	VAL
41	AX	105	PHE
43	AZ	49	LEU
44	Aa	39	PHE
44	Aa	67	LEU
44	Aa	84	VAL
45	Ab	24	LEU
45	Ab	53	VAL
48	Ae	6	LEU
49	Af	126	CYS
50	Ag	64	HIS
50	Ag	113	PHE
50	Ag	162	ASN
50	Ag	182	CYS
50	Ag	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	I3	6	GLN
1	I3	47	ASN
1	I3	62	GLN
1	I3	68	GLN
1	I3	91	GLN
1	I3	119	GLN
1	I3	218	GLN
2	I4	139	HIS
2	I4	270	GLN
2	I4	302	ASN
3	I5	195	GLN
3	I5	199	GLN
3	I5	229	ASN
3	I5	243	GLN
3	I5	344	GLN
3	I5	364	ASN
3	I5	366	GLN
4	I6	79	GLN
4	I6	205	HIS
4	I6	339	HIS
4	I6	359	GLN

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Mol	Chain	Res	Type
5	I8	159	GLN
5	I8	207	ASN
5	I8	209	HIS
5	I8	238	HIS
5	I8	242	ASN
7	Ip	36	GLN
7	Ip	84	GLN
8	Iq	33	GLN
8	Iq	72	ASN
8	Iq	96	ASN
9	Ir	187	GLN
9	Ir	228	ASN
10	Is	232	GLN
10	Is	266	GLN
10	Is	292	GLN
12	Iu	25	GLN
12	Iu	47	HIS
12	Iu	73	GLN
12	Iu	122	GLN
12	Iu	180	GLN
12	Iu	301	HIS
12	Iu	312	GLN
12	Iu	441	GLN
12	Iu	477	HIS
12	Iu	522	GLN
13	Iv	49	ASN
13	Iv	216	HIS
13	Iv	361	ASN
15	Ix	31	GLN
15	Ix	57	ASN
15	Ix	62	GLN
15	Ix	311	ASN
15	Ix	336	ASN
15	Ix	339	ASN
15	Ix	403	HIS
15	Ix	456	HIS
15	Ix	486	ASN
16	Iy	364	ASN
16	Iy	415	ASN
16	Iy	534	GLN
16	Iy	595	GLN
16	Iy	597	ASN

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Mol	Chain	Res	Type
16	Iy	630	HIS
16	Iy	648	GLN
16	Iy	713	GLN
16	Iy	753	HIS
16	Iy	845	HIS
16	Iy	858	GLN
21	AD	4	GLN
22	AE	17	HIS
22	AE	50	ASN
22	AE	67	GLN
22	AE	161	GLN
22	AE	188	ASN
23	AF	83	ASN
25	AH	114	GLN
26	AI	165	GLN
28	AK	39	ASN
29	AL	112	HIS
30	AM	19	GLN
36	AS	105	ASN
37	AT	126	GLN
39	AV	2	GLN
39	AV	49	GLN
40	AW	56	HIS
40	AW	90	GLN
45	Ab	49	HIS
47	Ad	3	HIS
50	Ag	20	GLN
50	Ag	26	GLN
50	Ag	159	ASN
50	Ag	178	ASN
50	Ag	226	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	Iw	74/75 (98%)	14 (18%)	0
17	A2	1768/1869 (94%)	230 (13%)	0
All	All	1842/1944 (94%)	244 (13%)	0

All (244) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	Iw	9	1MG
14	Iw	16	C
14	Iw	17	G
14	Iw	18	G
14	Iw	19	A
14	Iw	47	5MC
14	Iw	48	G
14	Iw	52	G
14	Iw	53	A
14	Iw	57	1MA
14	Iw	58	A
14	Iw	60	C
14	Iw	74	C
14	Iw	75	A
17	A2	4	C
17	A2	33	G
17	A2	41	G
17	A2	43	U
17	A2	44	U
17	A2	46	A
17	A2	56	G
17	A2	64	A
17	A2	67	C
17	A2	68	A
17	A2	75	G
17	A2	76	U
17	A2	79	A
17	A2	103	A
17	A2	113	G
17	A2	114	G
17	A2	115	U
17	A2	126	G
17	A2	130	G
17	A2	143	U
17	A2	155	G
17	A2	163	U
17	A2	168	C
17	A2	184	G
17	A2	204	G
17	A2	226	A
17	A2	228	C
17	A2	229	A
17	A2	230	A

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Mol	Chain	Res	Type
17	A2	231	A
17	A2	232	A
17	A2	234	C
17	A2	235	A
17	A2	236	A
17	A2	238	C
17	A2	281	C
17	A2	295	C
17	A2	312	G
17	A2	319	C
17	A2	320	G
17	A2	325	C
17	A2	328	U
17	A2	335	G
17	A2	347	G
17	A2	362	C
17	A2	364	A
17	A2	369	C
17	A2	370	G
17	A2	385	G
17	A2	386	C
17	A2	409	C
17	A2	421	G
17	A2	448	A
17	A2	449	A
17	A2	450	C
17	A2	464	A
17	A2	471	G
17	A2	472	C
17	A2	474	G
17	A2	482	G
17	A2	487	U
17	A2	492	C
17	A2	512	A2M
17	A2	525	A
17	A2	534	G
17	A2	537	C
17	A2	546	G
17	A2	547	G
17	A2	548	C
17	A2	549	C
17	A2	555	A

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Mol	Chain	Res	Type
17	A2	559	G
17	A2	564	A
17	A2	568	C
17	A2	583	A
17	A2	588	G
17	A2	591	U
17	A2	607	U
17	A2	608	C
17	A2	614	C
17	A2	615	C
17	A2	626	G
17	A2	629	A
17	A2	643	A
17	A2	644	OMG
17	A2	655	A
17	A2	660	C
17	A2	664	A
17	A2	668	A2M
17	A2	669	A
17	A2	671	A
17	A2	672	A
17	A2	673	G
17	A2	688	U
17	A2	738	C
17	A2	746	C
17	A2	748	C
17	A2	749	U
17	A2	788	G
17	A2	790	C
17	A2	798	G
17	A2	799	OMU
17	A2	811	A
17	A2	821	G
17	A2	822	PSU
17	A2	830	A
17	A2	831	G
17	A2	836	G
17	A2	837	A
17	A2	839	C
17	A2	840	C
17	A2	841	G
17	A2	847	A

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Mol	Chain	Res	Type
17	A2	870	A
17	A2	872	A
17	A2	885	U
17	A2	891	G
17	A2	903	A
17	A2	913	A
17	A2	920	A
17	A2	922	A
17	A2	933	G
17	A2	943	U
17	A2	971	G
17	A2	985	G
17	A2	990	A
17	A2	992	A
17	A2	999	G
17	A2	1017	U
17	A2	1023	A
17	A2	1061	U
17	A2	1062	A
17	A2	1083	A
17	A2	1085	C
17	A2	1114	U
17	A2	1115	U
17	A2	1116	C
17	A2	1120	U
17	A2	1121	G
17	A2	1130	G
17	A2	1138	C
17	A2	1144	A
17	A2	1153	C
17	A2	1154	U
17	A2	1171	G
17	A2	1195	A
17	A2	1207	G
17	A2	1215	C
17	A2	1217	A
17	A2	1224	G
17	A2	1227	G
17	A2	1242	U
17	A2	1243	U
17	A2	1251	A
17	A2	1253	A

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Mol	Chain	Res	Type
17	A2	1256	G
17	A2	1257	G
17	A2	1259	A
17	A2	1274	G
17	A2	1275	G
17	A2	1302	G
17	A2	1303	C
17	A2	1308	U
17	A2	1342	U
17	A2	1343	U
17	A2	1348	G
17	A2	1358	U
17	A2	1371	U
17	A2	1372	U
17	A2	1378	A
17	A2	1382	A
17	A2	1405	A
17	A2	1406	G
17	A2	1419	C
17	A2	1420	G
17	A2	1421	A
17	A2	1423	C
17	A2	1433	C
17	A2	1435	C
17	A2	1438	A
17	A2	1454	A
17	A2	1463	U
17	A2	1466	G
17	A2	1480	A
17	A2	1489	A
17	A2	1490	OMG
17	A2	1494	U
17	A2	1497	G
17	A2	1508	A
17	A2	1509	U
17	A2	1521	C
17	A2	1533	A
17	A2	1553	C
17	A2	1560	U
17	A2	1570	G
17	A2	1578	U
17	A2	1580	A

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Mol	Chain	Res	Type
17	A2	1585	U
17	A2	1588	A
17	A2	1599	U
17	A2	1601	A
17	A2	1621	U
17	A2	1623	A
17	A2	1637	A
17	A2	1654	G
17	A2	1665	G
17	A2	1671	G
17	A2	1675	A
17	A2	1695	A
17	A2	1698	C
17	A2	1699	A
17	A2	1710	C
17	A2	1721	U
17	A2	1730	U
17	A2	1783	C
17	A2	1784	G
17	A2	1800	A
17	A2	1822	A
17	A2	1829	G
17	A2	1831	A
17	A2	1835	A
17	A2	1836	G
17	A2	1838	U
17	A2	1849	G
17	A2	1861	G
17	A2	1862	G
17	A2	1863	A
17	A2	1864	U
17	A2	1865	C
17	A2	1869	A

There are no RNA pucker outliers to report.

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

100 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	$\#\|Z\|>2$
17	PSU	A2	609	17	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
17	OMU	A2	116	17	19,22,23	1.19	3 (15%)	26,31,34	1.69	4 (15%)
17	OMG	A2	644	17	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
17	PSU	A2	1445	17	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
32	IAS	AO	138	32	6,7,8	0.96	0	6,8,10	1.33	1 (16%)
14	2MG	Iw	10	14	18,26,27	0.89	1 (5%)	16,38,41	1.13	2 (12%)
17	PSU	A2	36	17	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
17	OMG	A2	601	17	18,26,27	0.95	1 (5%)	19,38,41	1.07	2 (10%)
17	PSU	A2	572	17	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
17	OMC	A2	1703	17	19,22,23	0.81	0	26,31,34	0.83	1 (3%)
14	1MA	Iw	57	14	16,25,26	1.62	2 (12%)	18,37,40	1.24	3 (16%)
17	A2M	A2	166	17	18,25,26	1.03	1 (5%)	18,36,39	1.23	2 (11%)
17	OMC	A2	797	17	19,22,23	0.81	0	26,31,34	0.84	0
14	H2U	Iw	46	14	18,21,22	1.00	2 (11%)	21,30,33	1.72	1 (4%)
17	OMU	A2	1442	55,17	19,22,23	1.22	3 (15%)	26,31,34	1.71	4 (15%)
17	PSU	A2	1046	17	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
17	OMU	A2	1326	55,17	19,22,23	1.19	3 (15%)	26,31,34	1.72	5 (19%)
17	PSU	A2	1692	17	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
17	PSU	A2	801	17	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)
17	OMU	A2	354	17	19,22,23	1.25	3 (15%)	26,31,34	1.75	4 (15%)
17	PSU	A2	1045	17	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
17	OMC	A2	517	17	19,22,23	0.81	0	26,31,34	0.83	0
17	PSU	A2	822	17	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
17	PSU	A2	109	17	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
17	PSU	A2	1347	17	18,21,22	1.34	2 (11%)	22,30,33	1.95	4 (18%)
17	PSU	A2	34	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
17	PSU	A2	1244	17	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
17	A2M	A2	1031	17	18,25,26	0.99	1 (5%)	18,36,39	1.23	2 (11%)
17	OMG	A2	1447	17	18,26,27	0.95	1 (5%)	19,38,41	1.08	2 (10%)
17	PSU	A2	686	17	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
17	PSU	A2	866	17	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
17	OMG	A2	1490	55,17	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)
17	OMG	A2	436	17	18,26,27	0.94	1 (5%)	19,38,41	1.13	2 (10%)
17	OMU	A2	1804	17	19,22,23	1.21	2 (10%)	26,31,34	1.71	4 (15%)
17	OMC	A2	1391	17	19,22,23	0.82	0	26,31,34	0.82	0
17	4AC	A2	1337	17	21,24,25	1.09	2 (9%)	29,34,37	1.00	2 (6%)
17	6MZ	A2	1832	55,17	18,25,26	0.89	1 (5%)	16,36,39	1.75	4 (25%)
17	B8N	A2	1248	17	24,29,30	1.28	3 (12%)	29,42,45	1.28	3 (10%)
17	4AC	A2	1842	17	21,24,25	1.10	2 (9%)	29,34,37	1.17	2 (6%)
17	A2M	A2	1678	17	18,25,26	0.98	1 (5%)	18,36,39	1.24	2 (11%)
17	PSU	A2	814	17	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
17	PSU	A2	1136	17	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
41	HY3	AX	62	41	6,8,9	2.17	1 (16%)	5,10,12	1.13	1 (20%)
17	PSU	A2	218	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
17	PSU	A2	1056	17	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
17	PSU	A2	1625	17	18,21,22	1.39	2 (11%)	22,30,33	1.88	3 (13%)
17	OMU	A2	172	17	19,22,23	1.19	2 (10%)	26,31,34	1.73	5 (19%)
17	PSU	A2	105	17	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
17	OMU	A2	121	17	19,22,23	1.22	3 (15%)	26,31,34	1.73	5 (19%)
17	A2M	A2	576	17	18,25,26	1.01	1 (5%)	18,36,39	1.24	2 (11%)
17	PSU	A2	93	17	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
17	PSU	A2	651	17	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
17	OMU	A2	627	17	19,22,23	1.18	2 (10%)	26,31,34	1.72	5 (19%)
17	A2M	A2	668	55,17	18,25,26	0.93	1 (5%)	18,36,39	1.28	2 (11%)
14	5MC	Iw	47	14	18,22,23	0.61	0	26,32,35	0.82	1 (3%)
17	PSU	A2	863	17	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
17	PSU	A2	1177	17	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
17	PSU	A2	296	17	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
17	A2M	A2	159	17	18,25,26	0.99	1 (5%)	18,36,39	1.22	2 (11%)
17	PSU	A2	1004	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
17	PSU	A2	1367	17	18,21,22	1.35	2 (11%)	22,30,33	1.92	4 (18%)
17	OMU	A2	1288	17	19,22,23	1.21	3 (15%)	26,31,34	1.70	4 (15%)
37	NMM	AT	67	37	9,11,12	1.63	1 (11%)	6,12,14	3.45	2 (33%)
17	PSU	A2	649	17	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
17	PSU	A2	119	17	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
17	OMG	A2	683	17	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	A2M	A2	590	17	18,25,26	1.01	1 (5%)	18,36,39	1.20	2 (11%)
17	PSU	A2	1232	17	18,21,22	1.37	2 (11%)	22,30,33	1.93	4 (18%)
17	OMU	A2	799	17	19,22,23	1.21	3 (15%)	26,31,34	1.68	4 (15%)
14	G7M	Iw	45	14	20,26,27	2.96	7 (35%)	17,39,42	1.04	1 (5%)
17	PSU	A2	1174	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
17	PSU	A2	406	17	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
14	1MG	Iw	9	14	18,26,27	0.79	0	19,39,42	1.10	2 (10%)
14	T6A	Iw	36	14	27,34,35	0.97	2 (7%)	29,49,52	1.64	5 (17%)
17	OMU	A2	428	17	19,22,23	1.20	3 (15%)	26,31,34	1.72	5 (19%)
17	PSU	A2	681	17	18,21,22	1.37	3 (16%)	22,30,33	1.90	3 (13%)
17	A2M	A2	468	17	18,25,26	1.02	1 (5%)	18,36,39	1.29	2 (11%)
17	MA6	A2	1850	17	18,26,27	1.10	2 (11%)	19,38,41	1.95	3 (15%)
18	SAC	AA	2	18	7,8,9	0.52	0	8,9,11	0.86	1 (12%)
17	PSU	A2	966	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
17	MA6	A2	1851	17	18,26,27	1.10	2 (11%)	19,38,41	1.93	3 (15%)
17	A2M	A2	1383	17	18,25,26	1.01	1 (5%)	18,36,39	1.29	2 (11%)
17	A2M	A2	512	17	18,25,26	0.98	1 (5%)	18,36,39	1.20	2 (11%)
17	A2M	A2	484	17	18,25,26	1.03	1 (5%)	18,36,39	1.22	2 (11%)
17	OMC	A2	174	55,17	19,22,23	0.82	0	26,31,34	0.79	0
17	A2M	A2	99	55,17	18,25,26	1.06	1 (5%)	18,36,39	1.23	2 (11%)
17	OMG	A2	1328	17	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
17	PSU	A2	1081	17	18,21,22	1.39	3 (16%)	22,30,33	1.86	3 (13%)
17	G7M	A2	1639	14,17	20,26,27	2.93	7 (35%)	17,39,42	0.97	1 (5%)
17	PSU	A2	815	17	18,21,22	1.36	3 (16%)	22,30,33	1.92	3 (13%)
17	OMC	A2	1272	17	19,22,23	0.83	0	26,31,34	0.90	1 (3%)
17	PSU	A2	1643	55,17	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
36	SAC	AS	2	36	7,8,9	0.53	0	8,9,11	0.91	1 (12%)
17	PSU	A2	1238	17	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
14	2MG	Iw	25	14	18,26,27	0.88	1 (5%)	16,38,41	1.17	2 (12%)
17	A2M	A2	27	55,17	18,25,26	0.99	1 (5%)	18,36,39	1.21	2 (11%)
39	AME	AV	1	39	9,10,11	0.47	0	9,11,13	0.87	1 (11%)
17	OMC	A2	462	17	19,22,23	0.82	0	26,31,34	0.82	0

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
17	PSU	A2	609	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	116	17	-	1/9/27/28	0/2/2/2
17	OMG	A2	644	17	-	4/5/27/28	0/3/3/3
17	PSU	A2	1445	17	-	0/7/25/26	0/2/2/2
32	IAS	AO	138	32	-	2/7/7/8	-
14	2MG	Iw	10	14	-	0/5/27/28	0/3/3/3
17	PSU	A2	36	17	-	0/7/25/26	0/2/2/2
17	OMG	A2	601	17	-	0/5/27/28	0/3/3/3
17	PSU	A2	572	17	-	0/7/25/26	0/2/2/2
17	OMC	A2	1703	17	-	1/9/27/28	0/2/2/2
14	1MA	Iw	57	14	-	0/3/25/26	0/3/3/3
17	A2M	A2	166	17	-	0/5/27/28	0/3/3/3
17	OMC	A2	797	17	-	1/9/27/28	0/2/2/2
14	H2U	Iw	46	14	-	1/7/38/39	0/2/2/2
17	OMU	A2	1442	55,17	-	1/9/27/28	0/2/2/2
17	PSU	A2	1046	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	1326	55,17	-	0/9/27/28	0/2/2/2
17	PSU	A2	1692	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	801	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	354	17	-	1/9/27/28	0/2/2/2
17	PSU	A2	1045	17	-	0/7/25/26	0/2/2/2
17	OMC	A2	517	17	-	0/9/27/28	0/2/2/2
17	PSU	A2	822	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	109	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1347	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	34	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1244	17	-	0/7/25/26	0/2/2/2
17	A2M	A2	1031	17	-	1/5/27/28	0/3/3/3
17	OMG	A2	1447	17	-	2/5/27/28	0/3/3/3
17	PSU	A2	686	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	866	17	-	0/7/25/26	0/2/2/2
17	OMG	A2	1490	55,17	-	0/5/27/28	0/3/3/3
17	OMG	A2	436	17	-	1/5/27/28	0/3/3/3
17	OMU	A2	1804	17	-	0/9/27/28	0/2/2/2
17	OMC	A2	1391	17	-	0/9/27/28	0/2/2/2
17	4AC	A2	1337	17	-	2/11/29/30	0/2/2/2
17	6MZ	A2	1832	55,17	-	0/5/27/28	0/3/3/3
17	B8N	A2	1248	17	-	4/16/34/35	0/2/2/2
17	4AC	A2	1842	17	-	4/11/29/30	0/2/2/2
17	A2M	A2	1678	17	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PSU	A2	814	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1136	17	-	0/7/25/26	0/2/2/2
41	HY3	AX	62	41	-	0/1/12/14	0/1/1/1
17	PSU	A2	218	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1056	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1625	17	-	2/7/25/26	0/2/2/2
17	OMU	A2	172	17	-	0/9/27/28	0/2/2/2
17	PSU	A2	105	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	121	17	-	0/9/27/28	0/2/2/2
17	A2M	A2	576	17	-	2/5/27/28	0/3/3/3
17	PSU	A2	93	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	651	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	627	17	-	1/9/27/28	0/2/2/2
17	A2M	A2	668	55,17	-	2/5/27/28	0/3/3/3
14	5MC	Iw	47	14	-	3/7/25/26	0/2/2/2
17	PSU	A2	863	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1177	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	296	17	-	0/7/25/26	0/2/2/2
17	A2M	A2	159	17	-	1/5/27/28	0/3/3/3
17	PSU	A2	1004	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	1367	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	1288	17	-	1/9/27/28	0/2/2/2
37	NMM	AT	67	37	-	1/9/11/13	-
17	PSU	A2	649	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	119	17	-	0/7/25/26	0/2/2/2
17	OMG	A2	683	17	-	3/5/27/28	0/3/3/3
17	A2M	A2	590	17	-	0/5/27/28	0/3/3/3
17	PSU	A2	1232	17	-	0/7/25/26	0/2/2/2
17	OMU	A2	799	17	-	3/9/27/28	0/2/2/2
14	G7M	Iw	45	14	-	0/3/25/26	0/3/3/3
17	PSU	A2	1174	17	-	0/7/25/26	0/2/2/2
17	PSU	A2	406	17	-	0/7/25/26	0/2/2/2
14	1MG	Iw	9	14	-	2/3/25/26	0/3/3/3
14	T6A	Iw	36	14	-	4/19/41/42	0/3/3/3
17	OMU	A2	428	17	-	4/9/27/28	0/2/2/2
17	PSU	A2	681	17	-	0/7/25/26	0/2/2/2
17	A2M	A2	468	17	-	1/5/27/28	0/3/3/3
17	MA6	A2	1850	17	-	0/7/29/30	0/3/3/3
18	SAC	AA	2	18	-	2/7/8/10	-
17	PSU	A2	966	17	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MA6	A2	1851	17	-	2/7/29/30	0/3/3/3
17	A2M	A2	1383	17	-	0/5/27/28	0/3/3/3
17	A2M	A2	512	17	-	3/5/27/28	0/3/3/3
17	A2M	A2	484	17	-	0/5/27/28	0/3/3/3
17	OMC	A2	174	55,17	-	0/9/27/28	0/2/2/2
17	A2M	A2	99	55,17	-	2/5/27/28	0/3/3/3
17	OMG	A2	1328	17	-	1/5/27/28	0/3/3/3
17	PSU	A2	1081	17	-	0/7/25/26	0/2/2/2
17	G7M	A2	1639	14,17	-	0/3/25/26	0/3/3/3
17	PSU	A2	815	17	-	0/7/25/26	0/2/2/2
17	OMC	A2	1272	17	-	0/9/27/28	0/2/2/2
17	PSU	A2	1643	55,17	-	0/7/25/26	0/2/2/2
36	SAC	AS	2	36	-	0/7/8/10	-
17	PSU	A2	1238	17	-	0/7/25/26	0/2/2/2
14	2MG	Iw	25	14	-	0/5/27/28	0/3/3/3
17	A2M	A2	27	55,17	-	0/5/27/28	0/3/3/3
39	AME	AV	1	39	-	2/9/10/12	-
17	OMC	A2	462	17	-	0/9/27/28	0/2/2/2

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Iw	45	G7M	C5-C4	7.34	1.53	1.39
17	A2	1639	G7M	O6-C6	7.23	1.38	1.23
17	A2	1639	G7M	C5-C4	7.22	1.53	1.39
14	Iw	45	G7M	O6-C6	7.19	1.37	1.23
14	Iw	57	1MA	C2-N3	5.05	1.35	1.29
41	AX	62	HY3	C3-CA	-4.98	1.50	1.55
14	Iw	45	G7M	C2-N2	4.47	1.44	1.34
37	AT	67	NMM	CZ-NH2	4.42	1.45	1.34
17	A2	1639	G7M	C2-N2	4.42	1.44	1.34
14	Iw	45	G7M	C2-N1	3.82	1.47	1.37
17	A2	1639	G7M	C2-N1	3.80	1.47	1.37
14	Iw	45	G7M	C2-N3	3.38	1.41	1.33
17	A2	1639	G7M	C8-N9	3.38	1.39	1.33
14	Iw	57	1MA	C6-N6	3.33	1.36	1.27
17	A2	1850	MA6	C5-N7	3.32	1.51	1.39
17	A2	1851	MA6	C5-N7	3.30	1.51	1.39
14	Iw	45	G7M	C8-N9	3.25	1.39	1.33
14	Iw	45	G7M	C6-N1	3.24	1.42	1.37
17	A2	1639	G7M	C6-N1	3.19	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A2	296	PSU	C6-C5	3.16	1.39	1.35
17	A2	1248	B8N	C4-N3	-3.15	1.34	1.40
17	A2	1639	G7M	C2-N3	3.14	1.40	1.33
17	A2	866	PSU	C6-C5	3.12	1.39	1.35
17	A2	1625	PSU	C6-C5	3.07	1.38	1.35
17	A2	93	PSU	C6-C5	3.06	1.38	1.35
17	A2	609	PSU	C6-C5	3.05	1.38	1.35
17	A2	218	PSU	C6-C5	3.04	1.38	1.35
17	A2	966	PSU	C6-C5	3.02	1.38	1.35
17	A2	105	PSU	C6-C5	3.02	1.38	1.35
17	A2	1238	PSU	C6-C5	3.02	1.38	1.35
17	A2	1174	PSU	C6-C5	3.01	1.38	1.35
17	A2	1232	PSU	C6-C5	3.01	1.38	1.35
17	A2	1445	PSU	C6-C5	3.00	1.38	1.35
17	A2	1842	4AC	C4-N4	-2.99	1.35	1.39
17	A2	1244	PSU	C6-C5	2.99	1.38	1.35
17	A2	814	PSU	C6-C5	2.99	1.38	1.35
17	A2	815	PSU	C6-C5	2.98	1.38	1.35
17	A2	1004	PSU	C6-C5	2.97	1.38	1.35
17	A2	34	PSU	C6-C5	2.97	1.38	1.35
17	A2	1177	PSU	C6-C5	2.97	1.38	1.35
17	A2	1337	4AC	C4-N4	-2.96	1.35	1.39
17	A2	119	PSU	C6-C5	2.96	1.38	1.35
17	A2	109	PSU	C6-C5	2.96	1.38	1.35
17	A2	649	PSU	C6-C5	2.95	1.38	1.35
17	A2	1643	PSU	C6-C5	2.95	1.38	1.35
17	A2	1692	PSU	C6-C5	2.95	1.38	1.35
17	A2	651	PSU	C6-C5	2.95	1.38	1.35
17	A2	1081	PSU	C6-C5	2.95	1.38	1.35
17	A2	1046	PSU	C6-C5	2.95	1.38	1.35
17	A2	863	PSU	C6-C5	2.94	1.38	1.35
17	A2	686	PSU	C6-C5	2.93	1.38	1.35
17	A2	1136	PSU	C6-C5	2.93	1.38	1.35
17	A2	406	PSU	C6-C5	2.93	1.38	1.35
17	A2	801	PSU	C6-C5	2.92	1.38	1.35
17	A2	1367	PSU	C6-C5	2.92	1.38	1.35
17	A2	572	PSU	C6-C5	2.92	1.38	1.35
17	A2	36	PSU	C6-C5	2.91	1.38	1.35
17	A2	1056	PSU	C6-C5	2.91	1.38	1.35
17	A2	822	PSU	C6-C5	2.89	1.38	1.35
17	A2	1045	PSU	C6-C5	2.88	1.38	1.35
17	A2	681	PSU	C6-C5	2.86	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A2	109	PSU	C4-N3	-2.85	1.33	1.38
17	A2	1347	PSU	C4-N3	-2.85	1.33	1.38
17	A2	1248	B8N	C6-C5	2.85	1.39	1.34
17	A2	651	PSU	C4-N3	-2.85	1.33	1.38
17	A2	686	PSU	C4-N3	-2.84	1.33	1.38
17	A2	801	PSU	C4-N3	-2.84	1.33	1.38
17	A2	1347	PSU	C6-C5	2.83	1.38	1.35
17	A2	681	PSU	C4-N3	-2.82	1.33	1.38
17	A2	1367	PSU	C4-N3	-2.82	1.33	1.38
17	A2	1232	PSU	C4-N3	-2.81	1.33	1.38
17	A2	1081	PSU	C4-N3	-2.81	1.33	1.38
17	A2	1136	PSU	C4-N3	-2.81	1.33	1.38
17	A2	1692	PSU	C4-N3	-2.80	1.33	1.38
17	A2	1625	PSU	C4-N3	-2.79	1.33	1.38
17	A2	609	PSU	C4-N3	-2.79	1.33	1.38
17	A2	406	PSU	C4-N3	-2.78	1.33	1.38
17	A2	863	PSU	C4-N3	-2.78	1.33	1.38
17	A2	34	PSU	C4-N3	-2.78	1.33	1.38
17	A2	649	PSU	C4-N3	-2.78	1.33	1.38
17	A2	1045	PSU	C4-N3	-2.77	1.33	1.38
17	A2	1174	PSU	C4-N3	-2.77	1.33	1.38
17	A2	572	PSU	C4-N3	-2.77	1.33	1.38
17	A2	1004	PSU	C4-N3	-2.77	1.33	1.38
17	A2	93	PSU	C4-N3	-2.77	1.33	1.38
17	A2	1177	PSU	C4-N3	-2.76	1.33	1.38
17	A2	814	PSU	C4-N3	-2.76	1.33	1.38
17	A2	105	PSU	C4-N3	-2.76	1.33	1.38
17	A2	815	PSU	C4-N3	-2.76	1.33	1.38
17	A2	119	PSU	C4-N3	-2.76	1.33	1.38
17	A2	1643	PSU	C4-N3	-2.76	1.33	1.38
17	A2	296	PSU	C4-N3	-2.75	1.33	1.38
17	A2	36	PSU	C4-N3	-2.75	1.33	1.38
17	A2	1445	PSU	C4-N3	-2.75	1.33	1.38
17	A2	1046	PSU	C4-N3	-2.75	1.33	1.38
17	A2	866	PSU	C4-N3	-2.74	1.33	1.38
17	A2	966	PSU	C4-N3	-2.73	1.33	1.38
17	A2	1244	PSU	C4-N3	-2.73	1.33	1.38
17	A2	1238	PSU	C4-N3	-2.73	1.33	1.38
17	A2	218	PSU	C4-N3	-2.72	1.33	1.38
17	A2	1056	PSU	C4-N3	-2.69	1.33	1.38
17	A2	822	PSU	C4-N3	-2.67	1.33	1.38
17	A2	601	OMG	C6-N1	-2.66	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A2	354	OMU	C4-N3	-2.65	1.33	1.38
17	A2	1490	OMG	C6-N1	-2.61	1.34	1.37
17	A2	644	OMG	C6-N1	-2.61	1.34	1.37
17	A2	121	OMU	C4-N3	-2.60	1.33	1.38
17	A2	1447	OMG	C6-N1	-2.59	1.34	1.37
17	A2	683	OMG	C6-N1	-2.58	1.34	1.37
17	A2	1442	OMU	C4-N3	-2.58	1.33	1.38
17	A2	436	OMG	C6-N1	-2.57	1.34	1.37
17	A2	1248	B8N	C2-N3	-2.56	1.34	1.38
17	A2	428	OMU	C4-N3	-2.54	1.34	1.38
17	A2	1804	OMU	C4-N3	-2.54	1.34	1.38
17	A2	172	OMU	C4-N3	-2.53	1.34	1.38
14	Iw	10	2MG	C6-N1	-2.52	1.34	1.37
14	Iw	46	H2U	C2-N3	-2.52	1.33	1.38
17	A2	484	A2M	C5-C4	2.51	1.47	1.40
17	A2	116	OMU	C4-N3	-2.50	1.34	1.38
17	A2	1328	OMG	C6-N1	-2.50	1.34	1.37
17	A2	1326	OMU	C4-N3	-2.50	1.34	1.38
17	A2	627	OMU	C4-N3	-2.49	1.34	1.38
17	A2	1288	OMU	C4-N3	-2.49	1.34	1.38
17	A2	799	OMU	C4-N3	-2.49	1.34	1.38
17	A2	590	A2M	C5-C4	2.46	1.47	1.40
14	Iw	25	2MG	C6-N1	-2.44	1.34	1.37
17	A2	99	A2M	C5-C4	2.44	1.47	1.40
17	A2	468	A2M	C5-C4	2.39	1.47	1.40
17	A2	159	A2M	C5-C4	2.39	1.47	1.40
14	Iw	36	T6A	C5-C4	2.39	1.47	1.40
17	A2	576	A2M	C5-C4	2.39	1.47	1.40
17	A2	166	A2M	C5-C4	2.36	1.47	1.40
17	A2	1832	6MZ	C5-C4	2.34	1.47	1.40
17	A2	354	OMU	C2-N3	-2.33	1.33	1.38
17	A2	27	A2M	C5-C4	2.33	1.47	1.40
17	A2	1383	A2M	C5-C4	2.32	1.47	1.40
17	A2	512	A2M	C5-C4	2.31	1.47	1.40
17	A2	1678	A2M	C5-C4	2.31	1.47	1.40
17	A2	121	OMU	C2-N3	-2.31	1.33	1.38
17	A2	1031	A2M	C5-C4	2.29	1.47	1.40
17	A2	1442	OMU	C2-N3	-2.29	1.33	1.38
17	A2	668	A2M	C5-C4	2.27	1.46	1.40
17	A2	1326	OMU	C2-N3	-2.26	1.33	1.38
17	A2	1850	MA6	C4-N3	-2.26	1.32	1.35
17	A2	172	OMU	C2-N3	-2.25	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A2	428	OMU	C2-N3	-2.25	1.34	1.38
14	Iw	46	H2U	C4-N3	-2.24	1.33	1.37
17	A2	1842	4AC	C7-N4	-2.24	1.33	1.37
17	A2	1851	MA6	C4-N3	-2.24	1.32	1.35
17	A2	116	OMU	C2-N3	-2.19	1.34	1.38
17	A2	1804	OMU	C2-N3	-2.16	1.34	1.38
17	A2	627	OMU	C2-N3	-2.15	1.34	1.38
17	A2	1288	OMU	C2-N3	-2.12	1.34	1.38
17	A2	1337	4AC	C7-N4	-2.11	1.33	1.37
17	A2	1081	PSU	C2-N3	-2.10	1.33	1.37
17	A2	354	OMU	C5-C4	-2.10	1.39	1.43
17	A2	116	OMU	C5-C4	-2.09	1.39	1.43
17	A2	799	OMU	C2-N3	-2.09	1.34	1.38
17	A2	121	OMU	C5-C4	-2.07	1.39	1.43
17	A2	1442	OMU	C5-C4	-2.05	1.39	1.43
17	A2	428	OMU	C5-C4	-2.04	1.39	1.43
17	A2	1288	OMU	C2-N1	2.03	1.41	1.38
17	A2	799	OMU	C5-C4	-2.03	1.39	1.43
17	A2	815	PSU	C2-N3	-2.01	1.34	1.37
14	Iw	36	T6A	C10-N6	-2.01	1.33	1.37
17	A2	681	PSU	C2-N3	-2.01	1.34	1.37
17	A2	1326	OMU	C5-C4	-2.00	1.39	1.43

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	AT	67	NMM	NE-CZ-NH2	-7.19	112.89	119.48
14	Iw	46	H2U	C4-N3-C2	-6.91	120.06	125.79
17	A2	1347	PSU	N1-C2-N3	6.18	122.13	115.13
17	A2	1232	PSU	N1-C2-N3	6.14	122.09	115.13
17	A2	651	PSU	N1-C2-N3	6.14	122.09	115.13
17	A2	814	PSU	N1-C2-N3	6.12	122.06	115.13
17	A2	406	PSU	N1-C2-N3	6.09	122.03	115.13
17	A2	686	PSU	N1-C2-N3	6.08	122.02	115.13
17	A2	866	PSU	N1-C2-N3	6.07	122.01	115.13
17	A2	1643	PSU	N1-C2-N3	6.07	122.01	115.13
17	A2	1238	PSU	N1-C2-N3	6.07	122.00	115.13
17	A2	1445	PSU	N1-C2-N3	6.07	122.00	115.13
17	A2	815	PSU	N1-C2-N3	6.06	122.00	115.13
17	A2	1367	PSU	N1-C2-N3	6.06	122.00	115.13
17	A2	609	PSU	N1-C2-N3	6.05	121.99	115.13
17	A2	296	PSU	N1-C2-N3	6.05	121.99	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A2	34	PSU	N1-C2-N3	6.05	121.98	115.13
17	A2	105	PSU	N1-C2-N3	6.05	121.98	115.13
17	A2	681	PSU	N1-C2-N3	6.04	121.98	115.13
17	A2	1625	PSU	N1-C2-N3	6.04	121.97	115.13
17	A2	801	PSU	N1-C2-N3	6.04	121.97	115.13
17	A2	109	PSU	N1-C2-N3	6.03	121.97	115.13
17	A2	822	PSU	N1-C2-N3	6.03	121.96	115.13
17	A2	966	PSU	N1-C2-N3	6.03	121.96	115.13
17	A2	1004	PSU	N1-C2-N3	6.02	121.95	115.13
17	A2	1046	PSU	N1-C2-N3	6.01	121.94	115.13
17	A2	218	PSU	N1-C2-N3	6.01	121.94	115.13
17	A2	1136	PSU	N1-C2-N3	6.01	121.94	115.13
17	A2	1692	PSU	N1-C2-N3	6.01	121.94	115.13
17	A2	1045	PSU	N1-C2-N3	6.01	121.94	115.13
17	A2	649	PSU	N1-C2-N3	5.99	121.92	115.13
17	A2	93	PSU	N1-C2-N3	5.99	121.92	115.13
17	A2	36	PSU	N1-C2-N3	5.99	121.92	115.13
17	A2	1056	PSU	N1-C2-N3	5.99	121.92	115.13
17	A2	1174	PSU	N1-C2-N3	5.99	121.91	115.13
14	Iw	36	T6A	C2-N1-C6	5.98	121.72	116.59
17	A2	1244	PSU	N1-C2-N3	5.97	121.89	115.13
17	A2	119	PSU	N1-C2-N3	5.96	121.89	115.13
17	A2	1177	PSU	N1-C2-N3	5.96	121.88	115.13
17	A2	863	PSU	N1-C2-N3	5.96	121.88	115.13
17	A2	572	PSU	N1-C2-N3	5.93	121.85	115.13
17	A2	1081	PSU	N1-C2-N3	5.83	121.74	115.13
17	A2	1851	MA6	C4-C5-N7	-5.72	103.43	109.40
17	A2	1850	MA6	C4-C5-N7	-5.64	103.52	109.40
17	A2	1832	6MZ	C2-N1-C6	5.42	121.24	116.59
17	A2	172	OMU	C4-N3-C2	-4.60	120.51	126.58
17	A2	1326	OMU	C4-N3-C2	-4.58	120.54	126.58
17	A2	428	OMU	C4-N3-C2	-4.57	120.55	126.58
17	A2	354	OMU	C4-N3-C2	-4.57	120.56	126.58
17	A2	121	OMU	C4-N3-C2	-4.53	120.60	126.58
17	A2	1442	OMU	C4-N3-C2	-4.48	120.67	126.58
17	A2	1804	OMU	C4-N3-C2	-4.48	120.67	126.58
17	A2	627	OMU	C4-N3-C2	-4.47	120.68	126.58
17	A2	1288	OMU	C4-N3-C2	-4.43	120.74	126.58
17	A2	799	OMU	C4-N3-C2	-4.42	120.75	126.58
17	A2	116	OMU	C4-N3-C2	-4.36	120.82	126.58
17	A2	1850	MA6	N3-C2-N1	-4.32	121.92	128.68
17	A2	121	OMU	N3-C2-N1	4.24	120.52	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A2	354	OMU	N3-C2-N1	4.20	120.46	114.89
17	A2	1850	MA6	C1'-N9-C4	-4.14	119.36	126.64
17	A2	1442	OMU	N3-C2-N1	4.14	120.39	114.89
17	A2	1804	OMU	N3-C2-N1	4.14	120.38	114.89
17	A2	1851	MA6	C1'-N9-C4	-4.12	119.41	126.64
37	AT	67	NMM	NE-CZ-NH1	4.10	127.95	120.26
17	A2	801	PSU	C4-N3-C2	-4.10	120.43	126.34
17	A2	172	OMU	N3-C2-N1	4.09	120.33	114.89
17	A2	1326	OMU	N3-C2-N1	4.09	120.32	114.89
17	A2	1851	MA6	N3-C2-N1	-4.09	122.29	128.68
17	A2	1288	OMU	N3-C2-N1	4.08	120.31	114.89
17	A2	428	OMU	N3-C2-N1	4.08	120.30	114.89
17	A2	1347	PSU	C4-N3-C2	-4.07	120.48	126.34
17	A2	686	PSU	C4-N3-C2	-4.07	120.48	126.34
17	A2	116	OMU	N3-C2-N1	4.06	120.27	114.89
17	A2	799	OMU	N3-C2-N1	4.05	120.26	114.89
17	A2	1232	PSU	C4-N3-C2	-4.04	120.52	126.34
17	A2	1842	4AC	N4-C4-N3	4.04	120.63	113.85
17	A2	815	PSU	C4-N3-C2	-4.04	120.52	126.34
17	A2	814	PSU	C4-N3-C2	-4.03	120.54	126.34
17	A2	1445	PSU	C4-N3-C2	-4.03	120.54	126.34
17	A2	1367	PSU	C4-N3-C2	-4.01	120.56	126.34
17	A2	105	PSU	C4-N3-C2	-4.00	120.58	126.34
17	A2	1056	PSU	C4-N3-C2	-3.99	120.59	126.34
17	A2	109	PSU	C4-N3-C2	-3.98	120.60	126.34
17	A2	1177	PSU	C4-N3-C2	-3.98	120.60	126.34
17	A2	651	PSU	C4-N3-C2	-3.98	120.61	126.34
17	A2	296	PSU	C4-N3-C2	-3.98	120.61	126.34
17	A2	406	PSU	C4-N3-C2	-3.98	120.61	126.34
17	A2	1136	PSU	C4-N3-C2	-3.97	120.62	126.34
17	A2	1045	PSU	C4-N3-C2	-3.97	120.62	126.34
17	A2	866	PSU	C4-N3-C2	-3.97	120.62	126.34
17	A2	1643	PSU	C4-N3-C2	-3.97	120.62	126.34
17	A2	627	OMU	N3-C2-N1	3.97	120.16	114.89
17	A2	93	PSU	C4-N3-C2	-3.96	120.63	126.34
17	A2	572	PSU	C4-N3-C2	-3.96	120.63	126.34
17	A2	966	PSU	C4-N3-C2	-3.96	120.64	126.34
17	A2	218	PSU	C4-N3-C2	-3.96	120.64	126.34
17	A2	681	PSU	C4-N3-C2	-3.96	120.64	126.34
17	A2	649	PSU	C4-N3-C2	-3.95	120.64	126.34
17	A2	1692	PSU	C4-N3-C2	-3.95	120.64	126.34
17	A2	34	PSU	C4-N3-C2	-3.95	120.65	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	1004	PSU	C4-N3-C2	-3.95	120.65	126.34
17	A2	36	PSU	C4-N3-C2	-3.94	120.66	126.34
17	A2	1174	PSU	C4-N3-C2	-3.94	120.67	126.34
17	A2	609	PSU	C4-N3-C2	-3.92	120.69	126.34
17	A2	1238	PSU	C4-N3-C2	-3.91	120.71	126.34
17	A2	119	PSU	C4-N3-C2	-3.91	120.71	126.34
17	A2	863	PSU	C4-N3-C2	-3.89	120.74	126.34
17	A2	1046	PSU	C4-N3-C2	-3.88	120.75	126.34
17	A2	1244	PSU	C4-N3-C2	-3.88	120.75	126.34
17	A2	822	PSU	C4-N3-C2	-3.86	120.78	126.34
17	A2	1625	PSU	C4-N3-C2	-3.84	120.81	126.34
17	A2	1081	PSU	C4-N3-C2	-3.74	120.95	126.34
17	A2	428	OMU	C5-C4-N3	3.66	120.32	114.84
17	A2	172	OMU	C5-C4-N3	3.65	120.31	114.84
17	A2	354	OMU	C5-C4-N3	3.64	120.29	114.84
17	A2	1326	OMU	C5-C4-N3	3.64	120.28	114.84
17	A2	822	PSU	O2-C2-N1	-3.63	118.79	122.79
17	A2	627	OMU	C5-C4-N3	3.63	120.27	114.84
17	A2	1056	PSU	O2-C2-N1	-3.61	118.81	122.79
17	A2	1804	OMU	C5-C4-N3	3.56	120.17	114.84
17	A2	1643	PSU	O2-C2-N1	-3.56	118.88	122.79
17	A2	121	OMU	C5-C4-N3	3.55	120.16	114.84
17	A2	1442	OMU	C5-C4-N3	3.55	120.16	114.84
17	A2	1288	OMU	C5-C4-N3	3.55	120.15	114.84
17	A2	116	OMU	C5-C4-N3	3.55	120.15	114.84
17	A2	799	OMU	C5-C4-N3	3.54	120.14	114.84
17	A2	296	PSU	O2-C2-N1	-3.51	118.93	122.79
17	A2	814	PSU	O2-C2-N1	-3.50	118.93	122.79
17	A2	1347	PSU	O2-C2-N1	-3.50	118.93	122.79
17	A2	1445	PSU	O2-C2-N1	-3.50	118.94	122.79
17	A2	609	PSU	O2-C2-N1	-3.49	118.95	122.79
17	A2	105	PSU	O2-C2-N1	-3.46	118.98	122.79
17	A2	1238	PSU	O2-C2-N1	-3.46	118.98	122.79
17	A2	863	PSU	O2-C2-N1	-3.46	118.98	122.79
17	A2	1004	PSU	O2-C2-N1	-3.45	118.99	122.79
17	A2	1046	PSU	O2-C2-N1	-3.45	118.99	122.79
17	A2	1692	PSU	O2-C2-N1	-3.45	118.99	122.79
17	A2	1174	PSU	O2-C2-N1	-3.44	119.00	122.79
17	A2	93	PSU	O2-C2-N1	-3.44	119.00	122.79
17	A2	1367	PSU	O2-C2-N1	-3.44	119.00	122.79
17	A2	866	PSU	O2-C2-N1	-3.42	119.02	122.79
17	A2	686	PSU	O2-C2-N1	-3.42	119.02	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A2	218	PSU	O2-C2-N1	-3.42	119.02	122.79
17	A2	649	PSU	O2-C2-N1	-3.41	119.03	122.79
17	A2	1248	B8N	C4-N3-C2	-3.41	121.15	125.46
17	A2	406	PSU	O2-C2-N1	-3.40	119.05	122.79
17	A2	1045	PSU	O2-C2-N1	-3.40	119.05	122.79
17	A2	1232	PSU	O2-C2-N1	-3.39	119.06	122.79
17	A2	36	PSU	O2-C2-N1	-3.38	119.07	122.79
17	A2	681	PSU	O2-C2-N1	-3.37	119.08	122.79
17	A2	34	PSU	O2-C2-N1	-3.36	119.09	122.79
17	A2	651	PSU	O2-C2-N1	-3.36	119.09	122.79
17	A2	1244	PSU	O2-C2-N1	-3.36	119.09	122.79
17	A2	109	PSU	O2-C2-N1	-3.35	119.10	122.79
17	A2	1625	PSU	O2-C2-N1	-3.35	119.11	122.79
17	A2	801	PSU	O2-C2-N1	-3.34	119.11	122.79
17	A2	966	PSU	O2-C2-N1	-3.34	119.12	122.79
17	A2	119	PSU	O2-C2-N1	-3.33	119.12	122.79
17	A2	815	PSU	O2-C2-N1	-3.32	119.14	122.79
17	A2	572	PSU	O2-C2-N1	-3.28	119.18	122.79
14	Iw	36	T6A	N6-C10-N11	3.27	118.33	113.76
17	A2	1177	PSU	O2-C2-N1	-3.27	119.19	122.79
17	A2	1136	PSU	O2-C2-N1	-3.25	119.21	122.79
17	A2	1678	A2M	N3-C2-N1	-3.25	123.61	128.68
17	A2	166	A2M	N3-C2-N1	-3.24	123.61	128.68
17	A2	1031	A2M	N3-C2-N1	-3.24	123.62	128.68
17	A2	590	A2M	N3-C2-N1	-3.24	123.62	128.68
17	A2	1081	PSU	O2-C2-N1	-3.21	119.26	122.79
17	A2	159	A2M	N3-C2-N1	-3.19	123.69	128.68
17	A2	468	A2M	N3-C2-N1	-3.19	123.69	128.68
17	A2	1383	A2M	N3-C2-N1	-3.18	123.71	128.68
17	A2	27	A2M	N3-C2-N1	-3.18	123.71	128.68
17	A2	512	A2M	N3-C2-N1	-3.16	123.74	128.68
17	A2	668	A2M	N3-C2-N1	-3.15	123.75	128.68
14	Iw	36	T6A	N3-C2-N1	-3.15	123.76	128.68
17	A2	576	A2M	N3-C2-N1	-3.14	123.76	128.68
17	A2	428	OMU	O4-C4-C5	-3.13	119.65	125.16
17	A2	627	OMU	O4-C4-C5	-3.10	119.71	125.16
17	A2	1248	B8N	N3-C2-N1	3.09	121.12	116.76
17	A2	1326	OMU	O4-C4-C5	-3.02	119.84	125.16
17	A2	116	OMU	O4-C4-C5	-3.02	119.85	125.16
17	A2	172	OMU	O4-C4-C5	-2.99	119.89	125.16
17	A2	99	A2M	N3-C2-N1	-2.99	124.01	128.68
17	A2	1442	OMU	O4-C4-C5	-2.98	119.93	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A2	121	OMU	O4-C4-C5	-2.97	119.94	125.16
17	A2	354	OMU	O4-C4-C5	-2.96	119.95	125.16
17	A2	1639	G7M	C2-N1-C6	-2.96	119.65	125.10
17	A2	1804	OMU	O4-C4-C5	-2.96	119.96	125.16
17	A2	799	OMU	O4-C4-C5	-2.96	119.96	125.16
17	A2	1288	OMU	O4-C4-C5	-2.96	119.96	125.16
14	Iw	45	G7M	C2-N1-C6	-2.93	119.70	125.10
17	A2	1832	6MZ	N3-C2-N1	-2.92	124.11	128.68
17	A2	1337	4AC	N4-C4-N3	2.92	118.75	113.85
17	A2	484	A2M	N3-C2-N1	-2.89	124.17	128.68
17	A2	99	A2M	C4-C5-N7	-2.85	106.43	109.40
17	A2	159	A2M	C4-C5-N7	-2.71	106.58	109.40
17	A2	27	A2M	C4-C5-N7	-2.71	106.58	109.40
17	A2	484	A2M	C4-C5-N7	-2.69	106.60	109.40
17	A2	166	A2M	C4-C5-N7	-2.68	106.60	109.40
17	A2	468	A2M	C4-C5-N7	-2.67	106.61	109.40
17	A2	1031	A2M	C4-C5-N7	-2.66	106.62	109.40
17	A2	512	A2M	C4-C5-N7	-2.65	106.63	109.40
17	A2	576	A2M	C4-C5-N7	-2.65	106.64	109.40
17	A2	1383	A2M	C4-C5-N7	-2.63	106.66	109.40
17	A2	1678	A2M	C4-C5-N7	-2.62	106.67	109.40
14	Iw	57	1MA	C3'-C2'-C1'	2.57	104.85	100.98
17	A2	668	A2M	C4-C5-N7	-2.57	106.72	109.40
32	AO	138	IAS	OD1-CG-CB	-2.56	117.96	125.43
14	Iw	36	T6A	C4-C5-N7	-2.55	106.74	109.40
39	AV	1	AME	O-C-CA	-2.52	118.18	124.78
17	A2	1337	4AC	C6-C5-C4	2.51	120.04	116.96
17	A2	1842	4AC	C6-C5-C4	2.46	119.97	116.96
14	Iw	9	1MG	C5-C6-N1	2.46	117.59	113.90
17	A2	590	A2M	C4-C5-N7	-2.45	106.84	109.40
14	Iw	25	2MG	C8-N7-C5	2.44	107.63	102.99
36	AS	2	SAC	O-C-CA	-2.43	118.41	124.78
14	Iw	9	1MG	C8-N7-C5	2.42	107.59	102.99
17	A2	436	OMG	C5-C6-N1	2.37	118.14	113.95
17	A2	644	OMG	C5-C6-N1	2.36	118.12	113.95
17	A2	436	OMG	C8-N7-C5	2.35	107.47	102.99
17	A2	601	OMG	C5-C6-N1	2.35	118.09	113.95
18	AA	2	SAC	O-C-CA	-2.34	118.64	124.78
17	A2	683	OMG	C5-C6-N1	2.33	118.06	113.95
17	A2	1447	OMG	C8-N7-C5	2.33	107.42	102.99
14	Iw	25	2MG	C5-C6-N1	2.33	118.06	113.95
17	A2	683	OMG	C8-N7-C5	2.32	107.41	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A2	1328	OMG	C8-N7-C5	2.32	107.41	102.99
14	Iw	10	2MG	C5-C6-N1	2.32	118.05	113.95
17	A2	1328	OMG	C5-C6-N1	2.32	118.04	113.95
14	Iw	10	2MG	C8-N7-C5	2.31	107.39	102.99
17	A2	1490	OMG	C8-N7-C5	2.29	107.36	102.99
17	A2	601	OMG	C8-N7-C5	2.29	107.36	102.99
17	A2	644	OMG	C8-N7-C5	2.29	107.36	102.99
17	A2	1447	OMG	C5-C6-N1	2.29	118.00	113.95
17	A2	1490	OMG	C5-C6-N1	2.29	118.00	113.95
14	Iw	57	1MA	C8-N7-C5	2.28	107.34	102.99
17	A2	1272	OMC	O2-C2-N3	-2.25	118.68	122.33
17	A2	172	OMU	O2-C2-N1	-2.24	119.81	122.79
17	A2	627	OMU	O2-C2-N1	-2.22	119.83	122.79
41	AX	62	HY3	O-C-CA	-2.20	118.70	124.83
14	Iw	36	T6A	N6-C6-N1	2.19	121.65	118.72
17	A2	1326	OMU	O2-C2-N1	-2.18	119.89	122.79
14	Iw	57	1MA	C5-C6-N1	2.18	117.15	113.90
14	Iw	47	5MC	C1'-N1-C6	-2.18	117.50	121.12
17	A2	428	OMU	O2-C2-N1	-2.17	119.90	122.79
17	A2	121	OMU	O2-C2-N1	-2.14	119.94	122.79
17	A2	1832	6MZ	C9-N6-C6	-2.14	121.03	122.87
17	A2	1248	B8N	C5-C4-N3	2.12	120.09	116.17
17	A2	801	PSU	C5-C6-N1	-2.12	118.94	122.11
17	A2	822	PSU	O4'-C1'-C2'	2.11	108.11	105.14
17	A2	1703	OMC	O2-C2-N3	-2.07	118.96	122.33
17	A2	1832	6MZ	C4-C5-N7	-2.05	107.26	109.40
17	A2	1347	PSU	C5-C6-N1	-2.04	119.04	122.11
17	A2	1445	PSU	C5-C6-N1	-2.04	119.05	122.11
17	A2	1367	PSU	C5-C6-N1	-2.02	119.08	122.11
17	A2	1232	PSU	C5-C6-N1	-2.01	119.09	122.11

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	AT	67	NMM	O-C-CA-CB
14	Iw	9	1MG	O4'-C4'-C5'-O5'
14	Iw	36	T6A	O10-C10-N6-C6
14	Iw	36	T6A	N11-C10-N6-C6
14	Iw	36	T6A	N6-C10-N11-C12
17	A2	512	A2M	O4'-C4'-C5'-O5'
17	A2	627	OMU	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
17	A2	644	OMG	O4'-C4'-C5'-O5'
17	A2	644	OMG	C3'-C4'-C5'-O5'
17	A2	799	OMU	C3'-C4'-C5'-O5'
17	A2	1248	B8N	N34-C33-C34-O35
17	A2	1337	4AC	O7-C7-N4-C4
17	A2	1337	4AC	CM7-C7-N4-C4
17	A2	1447	OMG	C3'-C4'-C5'-O5'
17	A2	1842	4AC	N3-C4-N4-C7
17	A2	1842	4AC	C5-C4-N4-C7
14	Iw	36	T6A	O10-C10-N11-C12
17	A2	428	OMU	C2'-C1'-N1-C6
17	A2	512	A2M	C3'-C4'-C5'-O5'
17	A2	668	A2M	O4'-C4'-C5'-O5'
17	A2	668	A2M	C3'-C4'-C5'-O5'
17	A2	1625	PSU	C3'-C4'-C5'-O5'
39	AV	1	AME	CT2-CT1-N-CA
39	AV	1	AME	OT-CT1-N-CA
14	Iw	9	1MG	C3'-C4'-C5'-O5'
17	A2	99	A2M	O4'-C4'-C5'-O5'
17	A2	1625	PSU	O4'-C4'-C5'-O5'
17	A2	1248	B8N	N34-C33-C34-O36
17	A2	428	OMU	C2'-C1'-N1-C2
17	A2	799	OMU	C4'-C5'-O5'-P
14	Iw	47	5MC	C3'-C4'-C5'-O5'
17	A2	576	A2M	C3'-C4'-C5'-O5'
17	A2	799	OMU	O4'-C4'-C5'-O5'
14	Iw	47	5MC	O4'-C4'-C5'-O5'
17	A2	1447	OMG	O4'-C4'-C5'-O5'
17	A2	576	A2M	O4'-C4'-C5'-O5'
17	A2	683	OMG	O4'-C4'-C5'-O5'
17	A2	1842	4AC	O7-C7-N4-C4
17	A2	1248	B8N	C32-C33-C34-O36
17	A2	428	OMU	O4'-C1'-N1-C6
17	A2	644	OMG	C4'-C5'-O5'-P
18	AA	2	SAC	C-CA-N-C1A
18	AA	2	SAC	CB-CA-N-C1A
17	A2	1248	B8N	C32-C33-C34-O35
17	A2	428	OMU	O4'-C1'-N1-C2
17	A2	354	OMU	C3'-C2'-O2'-CM2
17	A2	436	OMG	C3'-C2'-O2'-CM2
17	A2	797	OMC	C3'-C2'-O2'-CM2
17	A2	1288	OMU	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
17	A2	1328	OMG	C3'-C2'-O2'-CM2
17	A2	1442	OMU	C3'-C2'-O2'-CM2
14	Iw	47	5MC	C4'-C5'-O5'-P
17	A2	683	OMG	C3'-C2'-O2'-CM2
17	A2	1031	A2M	C3'-C2'-O2'-CM'
17	A2	1851	MA6	C4'-C5'-O5'-P
17	A2	116	OMU	C3'-C2'-O2'-CM2
17	A2	644	OMG	C3'-C2'-O2'-CM2
32	AO	138	IAS	O-C-CA-N
17	A2	1851	MA6	C3'-C4'-C5'-O5'
17	A2	1842	4AC	CM7-C7-N4-C4
17	A2	99	A2M	C3'-C4'-C5'-O5'
17	A2	683	OMG	C3'-C4'-C5'-O5'
17	A2	468	A2M	O4'-C4'-C5'-O5'
14	Iw	46	H2U	O4'-C1'-N1-C6
17	A2	1703	OMC	O4'-C4'-C5'-O5'
32	AO	138	IAS	CA-CB-CG-OD1
17	A2	512	A2M	C3'-C2'-O2'-CM'
17	A2	159	A2M	O4'-C4'-C5'-O5'

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 251 ligands modelled in this entry, 120 are monoatomic and 129 are unknown - leaving 2 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	$\#\|Z\|>2$
56	MET	Iw	101	14	6,7,8	0.48	0	2,7,9	0.24	0
54	GTP	It	1000	55	26,34,34	0.95	2 (7%)	32,54,54	0.89	2 (6%)

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
56	MET	Iw	101	14	-	0/5/6/8	-
54	GTP	It	1000	55	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	It	1000	GTP	C5-C6	-2.60	1.42	1.47
54	It	1000	GTP	C8-N7	-2.05	1.31	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	It	1000	GTP	O4'-C1'-C2'	-2.79	102.85	106.93
54	It	1000	GTP	O6-C6-C5	2.00	128.28	124.37

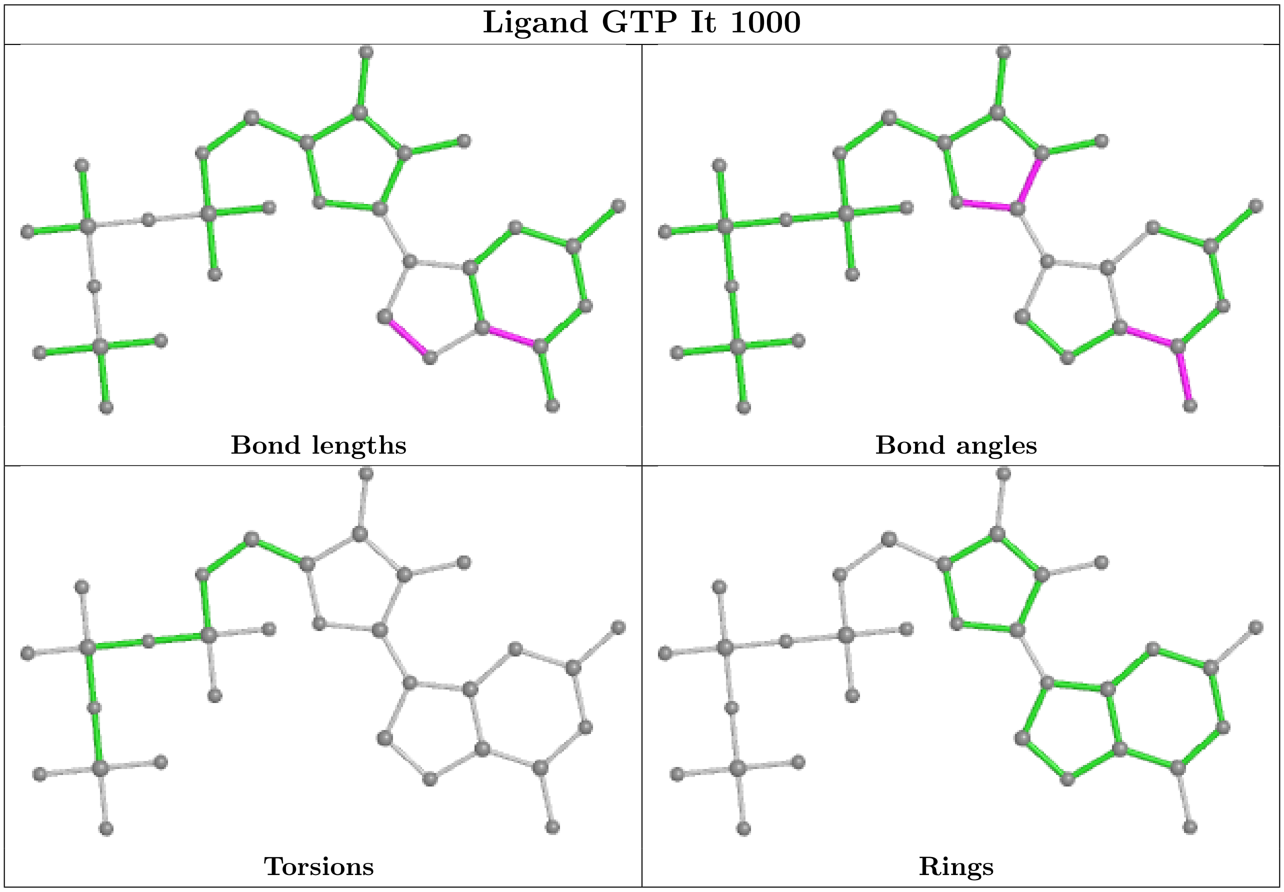
There are no chirality outliers.

There are no torsion outliers.

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 It 1000

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

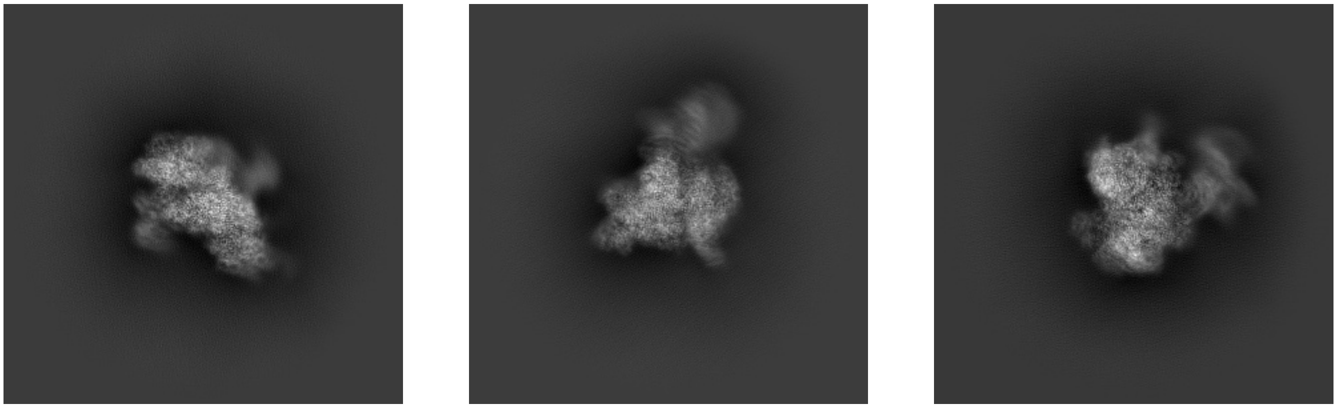
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17805. 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.

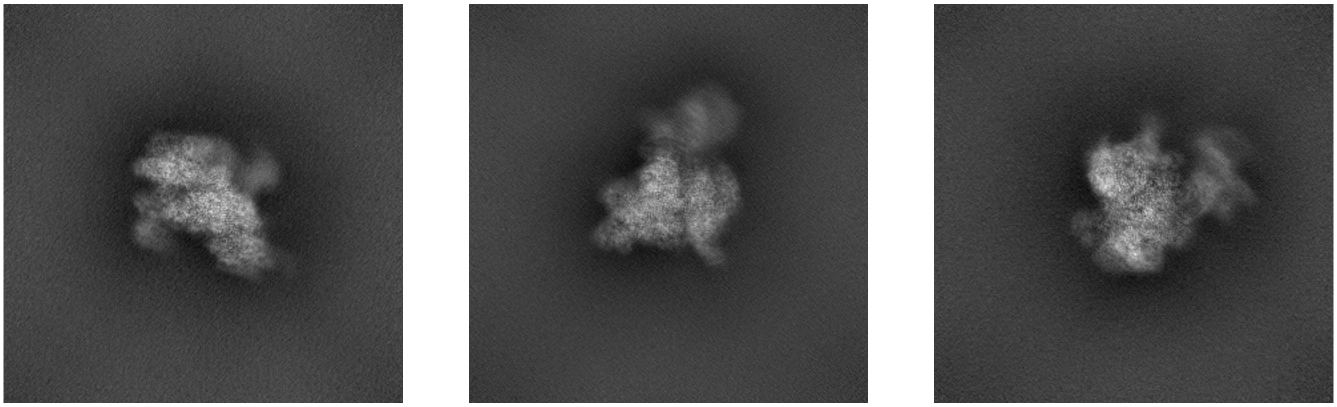
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map

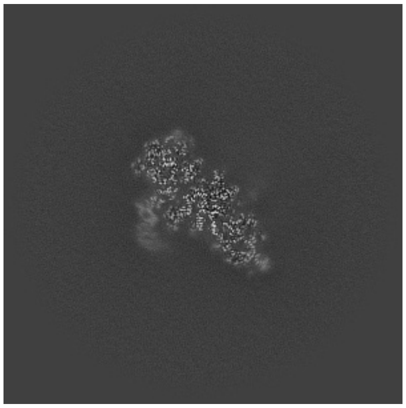


X Y Z

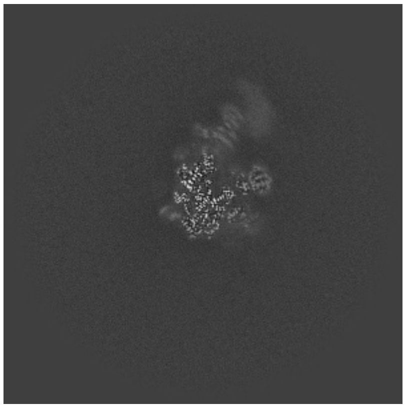
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

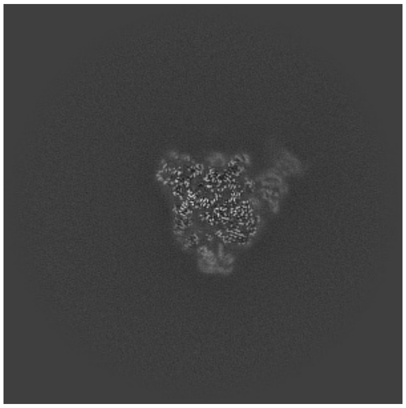
6.2.1 Primary map



X Index: 280

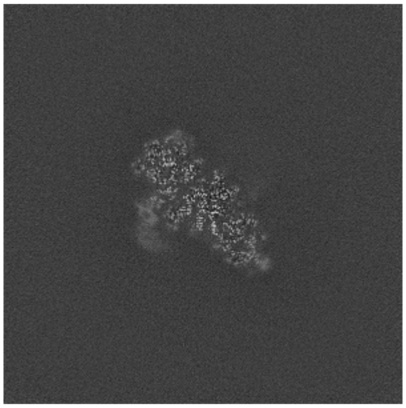


Y Index: 280

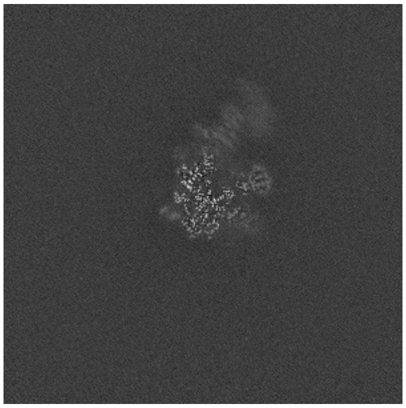


Z Index: 280

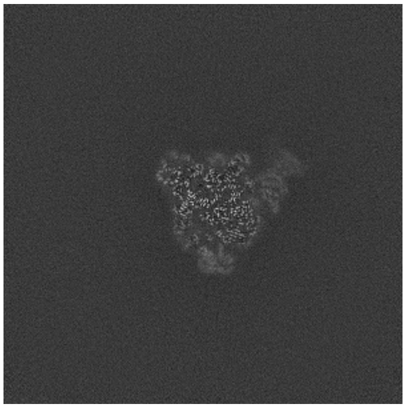
6.2.2 Raw map



X Index: 280



Y Index: 280

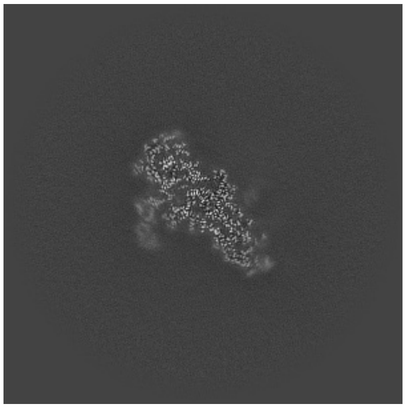


Z Index: 280

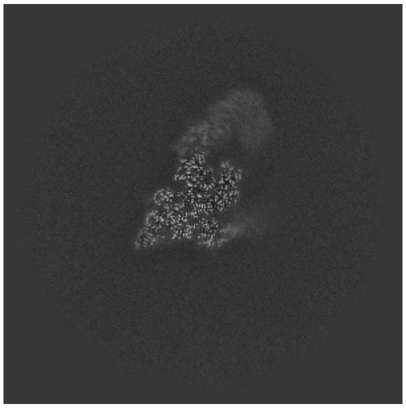
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

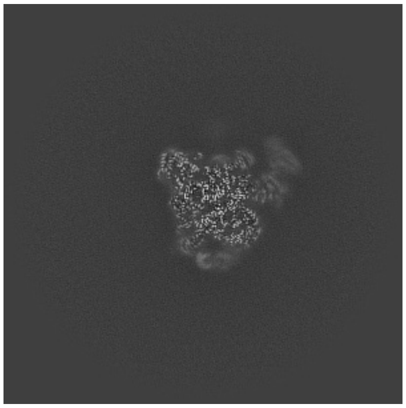
6.3.1 Primary map



X Index: 284

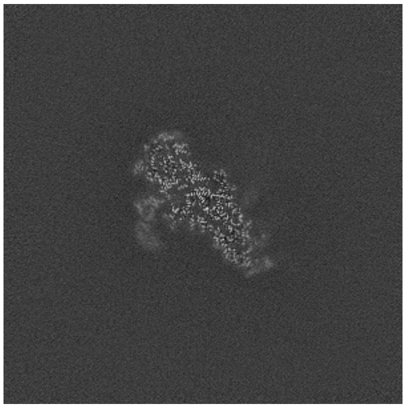


Y Index: 308

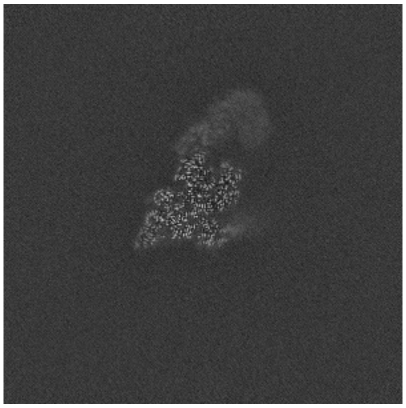


Z Index: 268

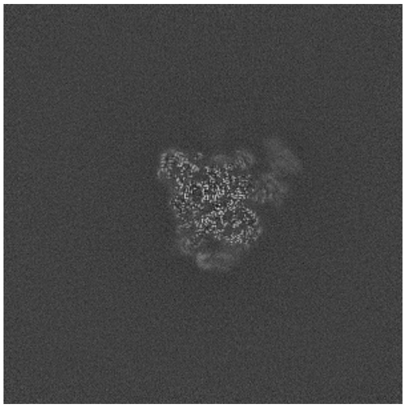
6.3.2 Raw map



X Index: 285



Y Index: 308

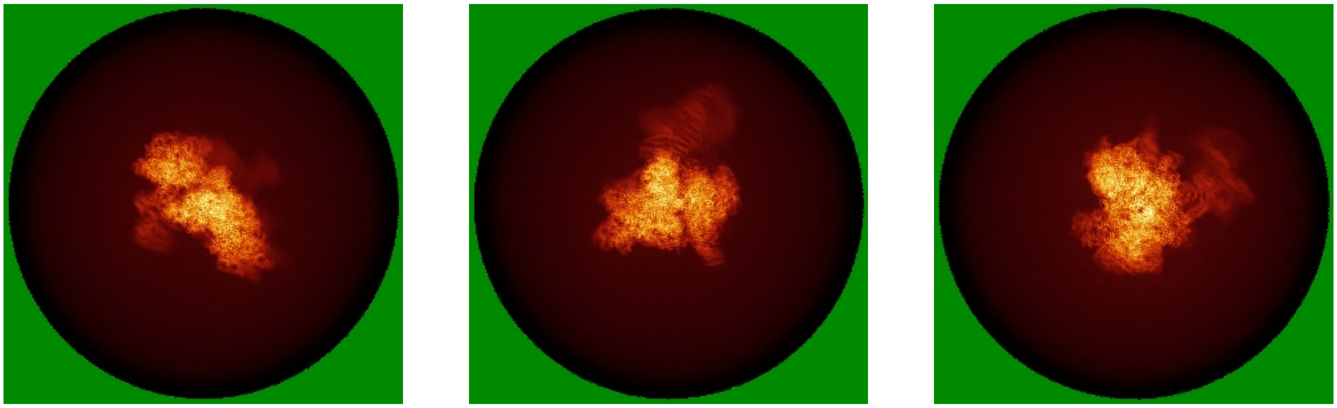


Z Index: 268

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

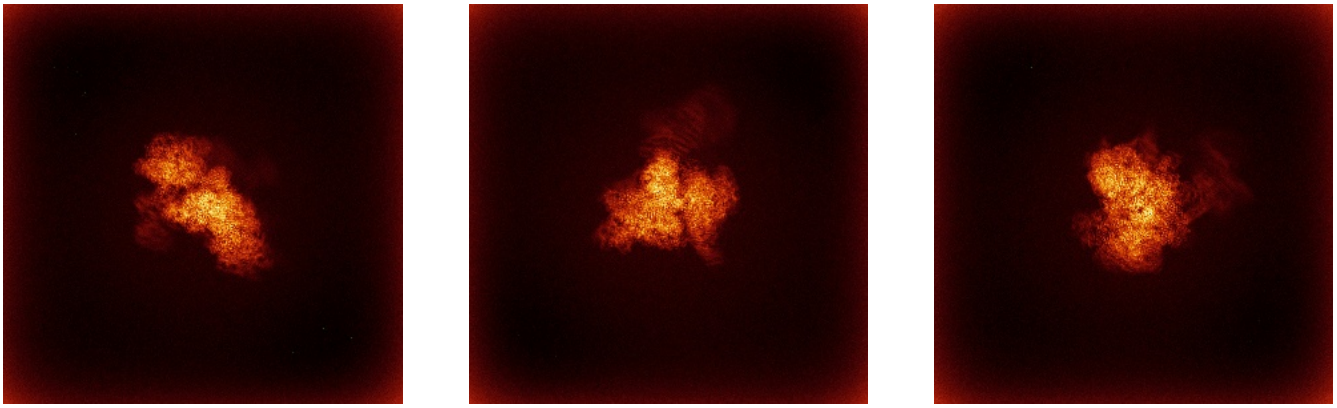
6.4 Orthogonal standard-deviation projections (False-color)

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 ⓘ

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

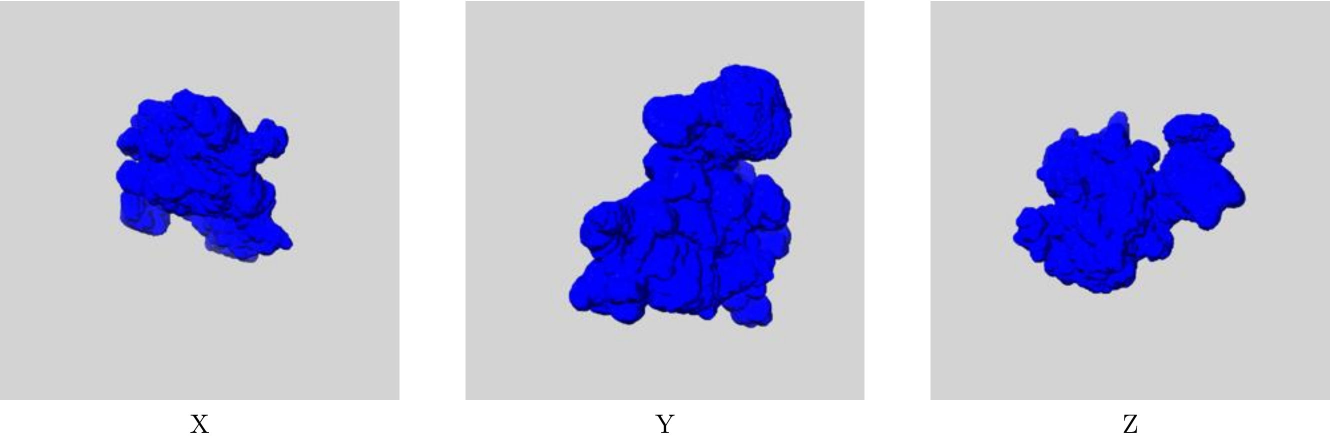
6.6 Mask visualisation ⓘ

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

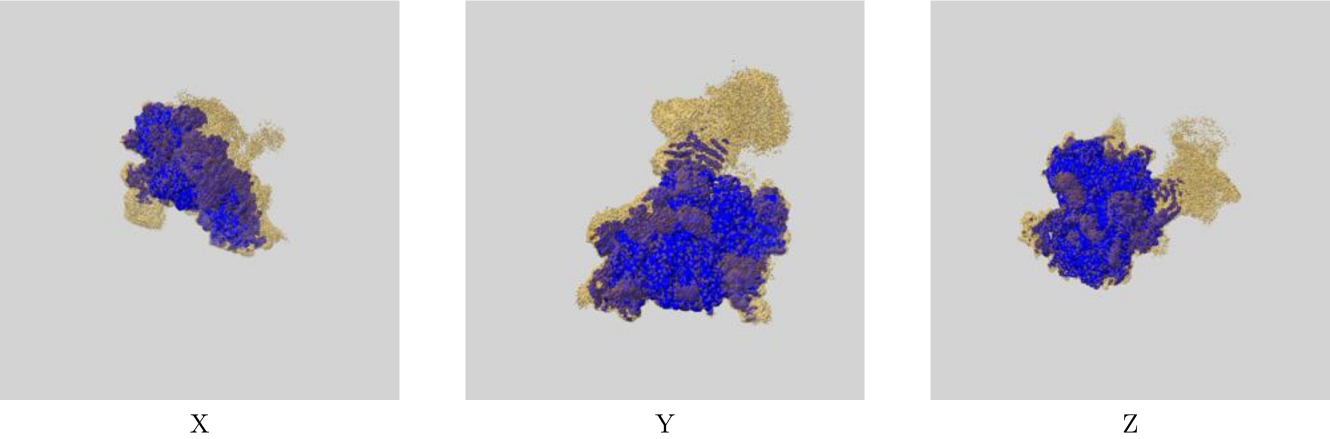
A mask typically either:

- 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_17805_msk_1.map ⓘ



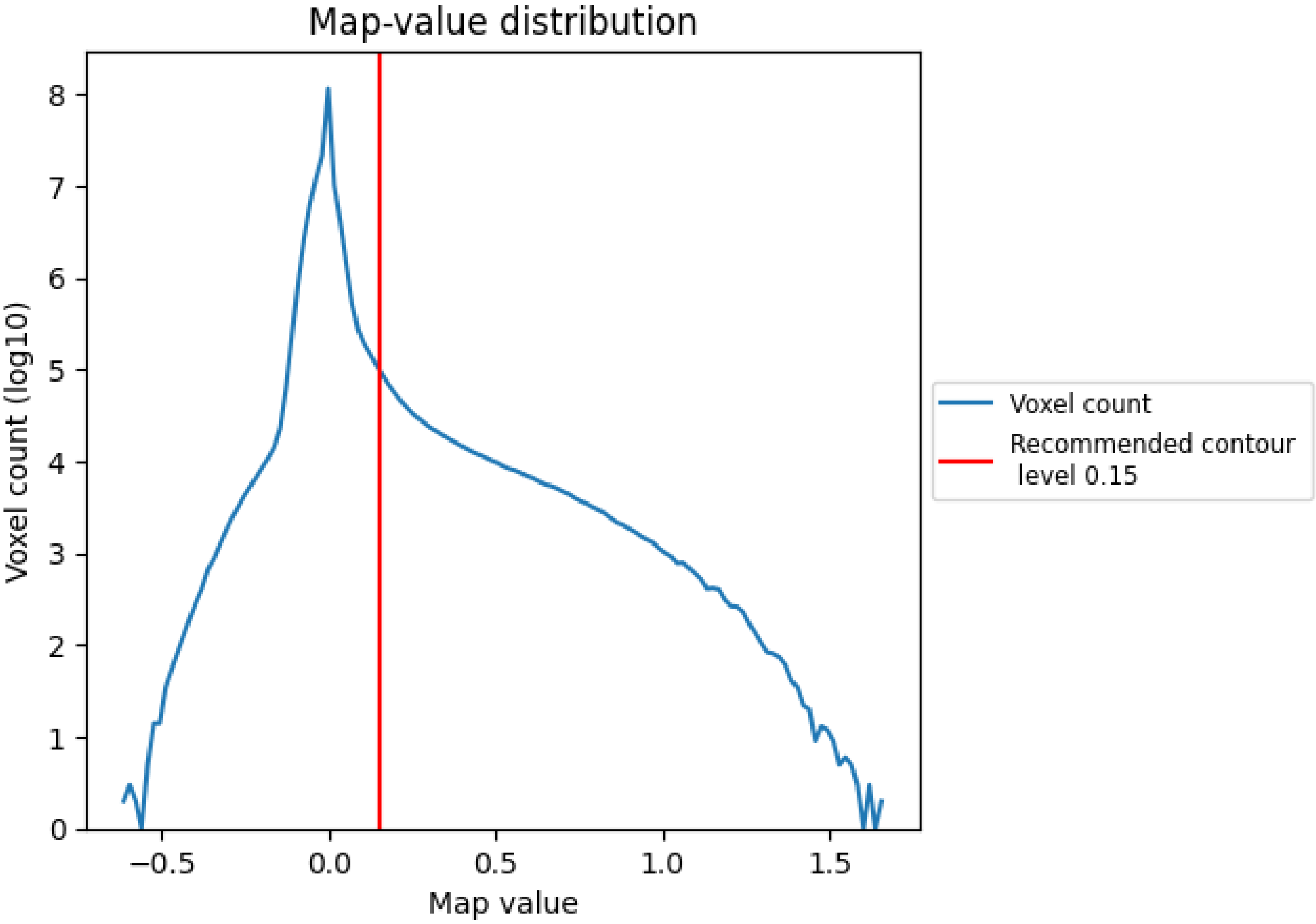
6.6.2 emd_17805_msk_2.map ⓘ



7 Map analysis (i)

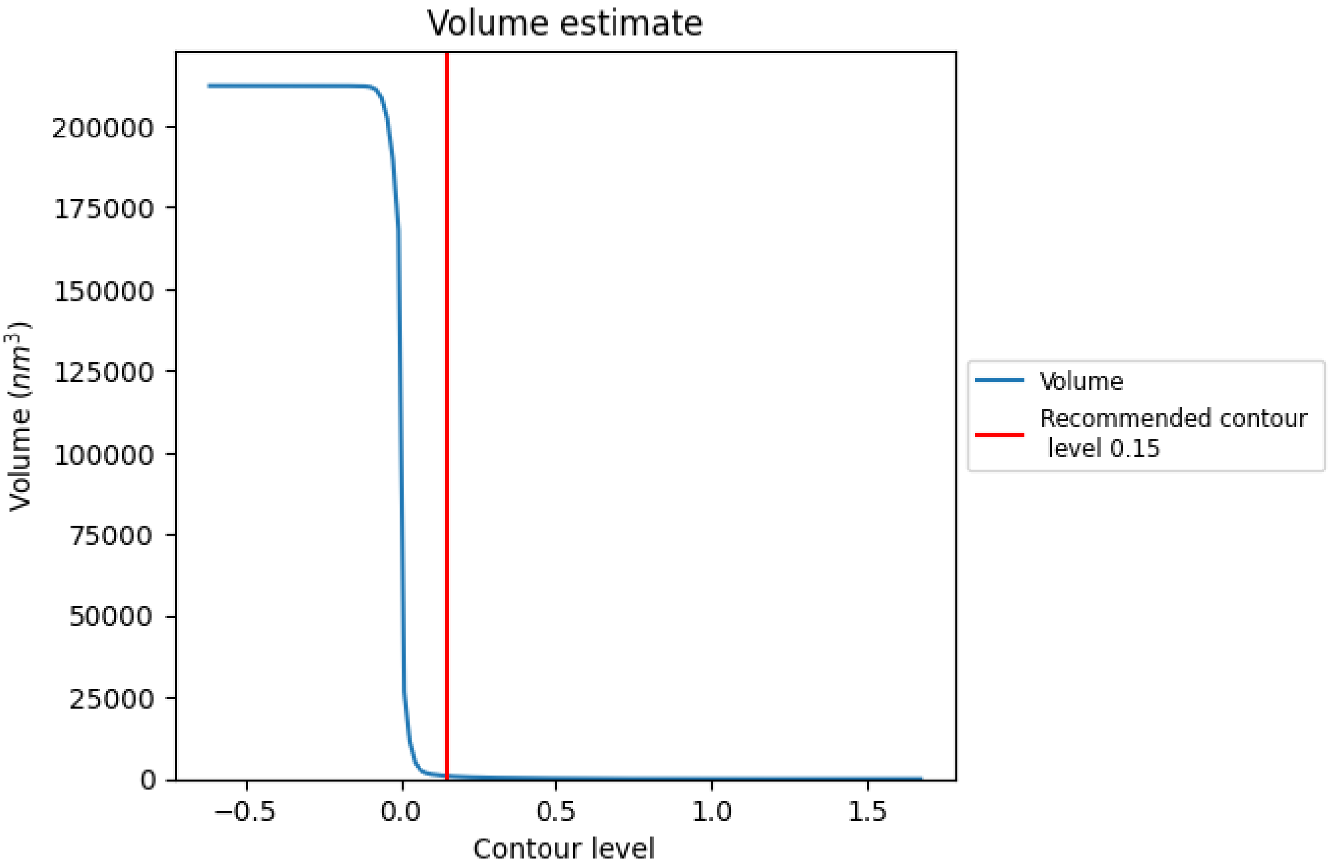
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

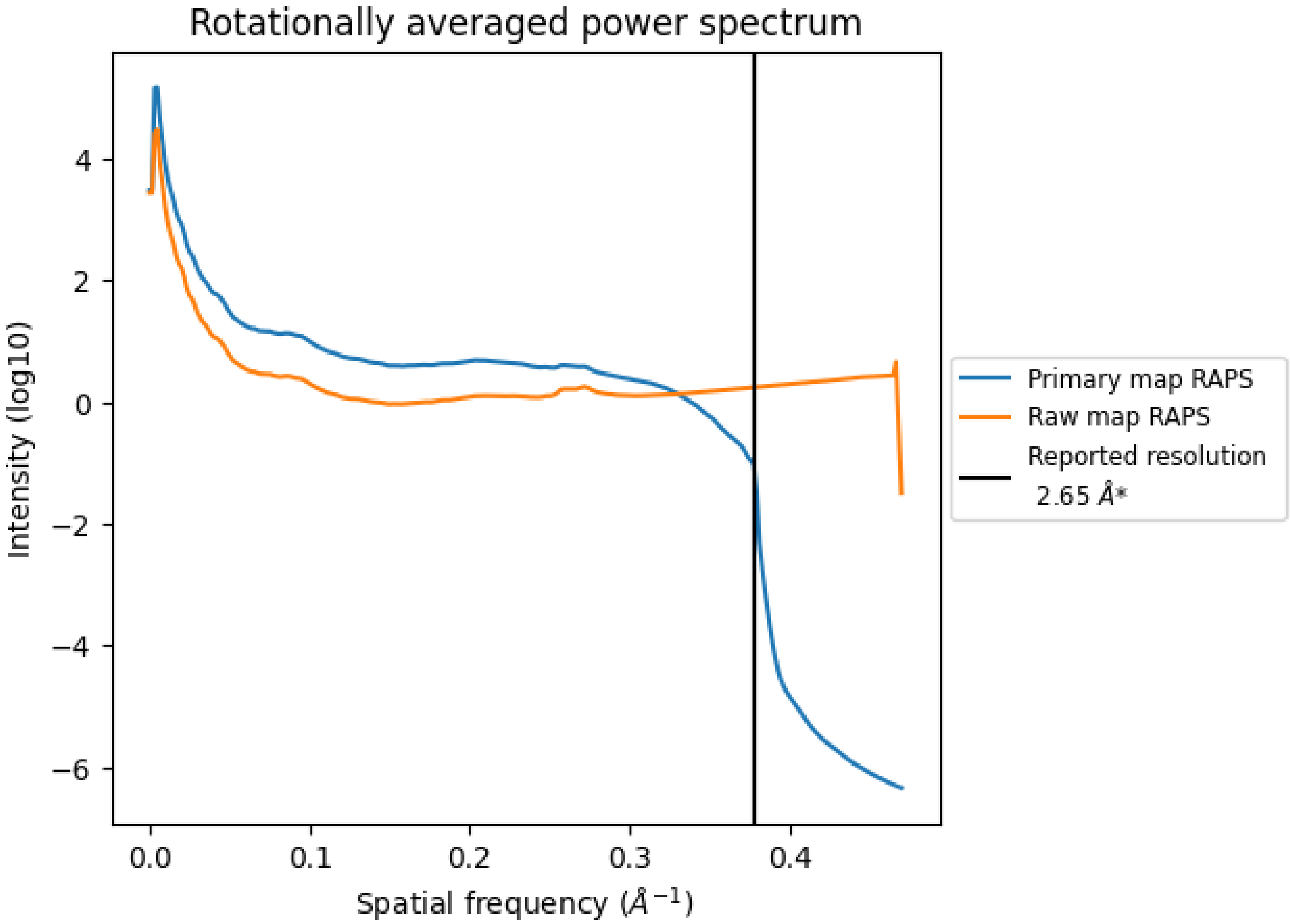
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 907 nm^3; this corresponds to an approximate mass of 819 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 ⓘ

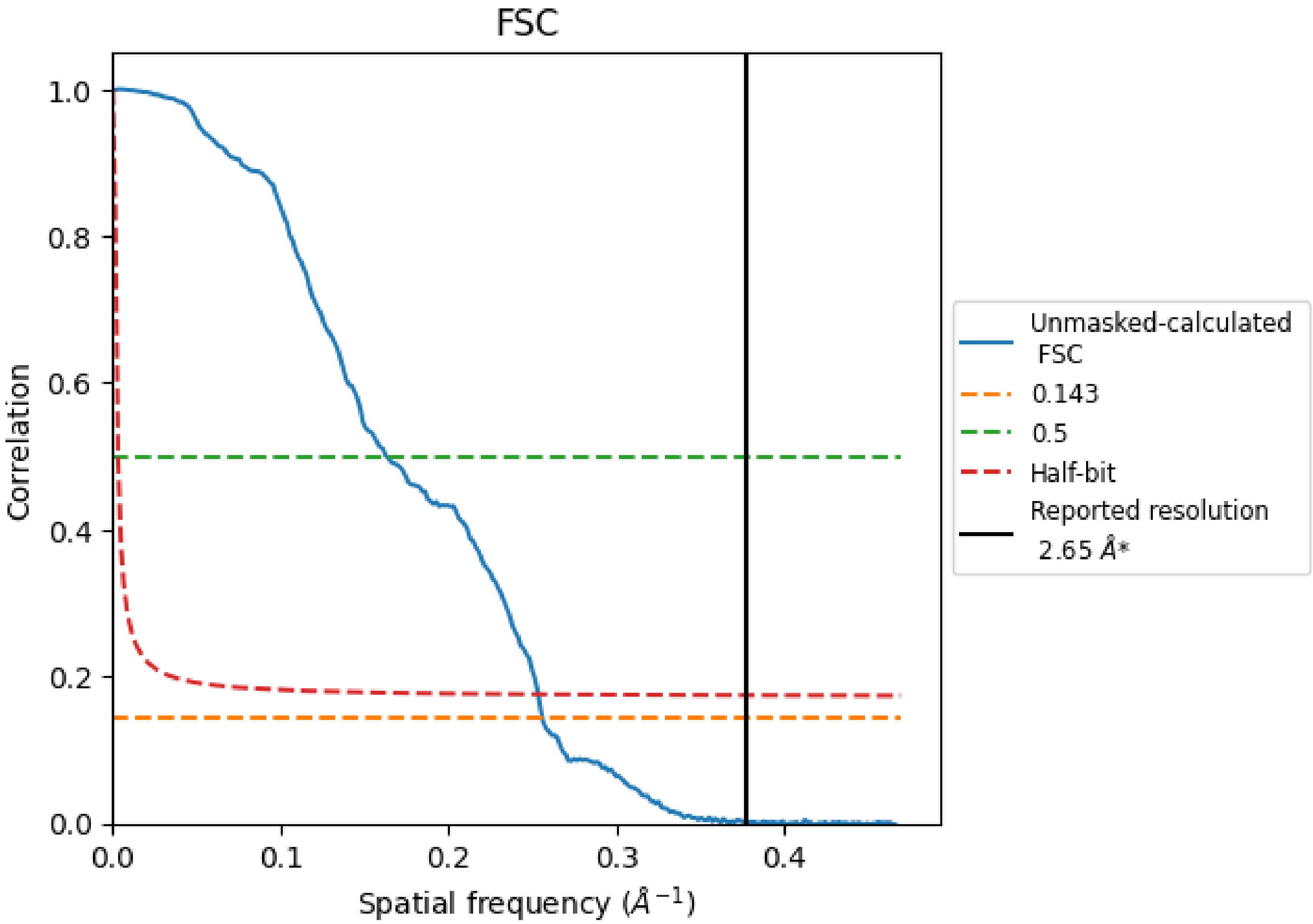


*Reported resolution corresponds to spatial frequency of 0.377 Å^{-1}

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 0.377 Å^{-1}

8.2 Resolution estimates

Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	6.12	3.95

*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 3.91 differs from the reported value 2.65 by more than 10 %

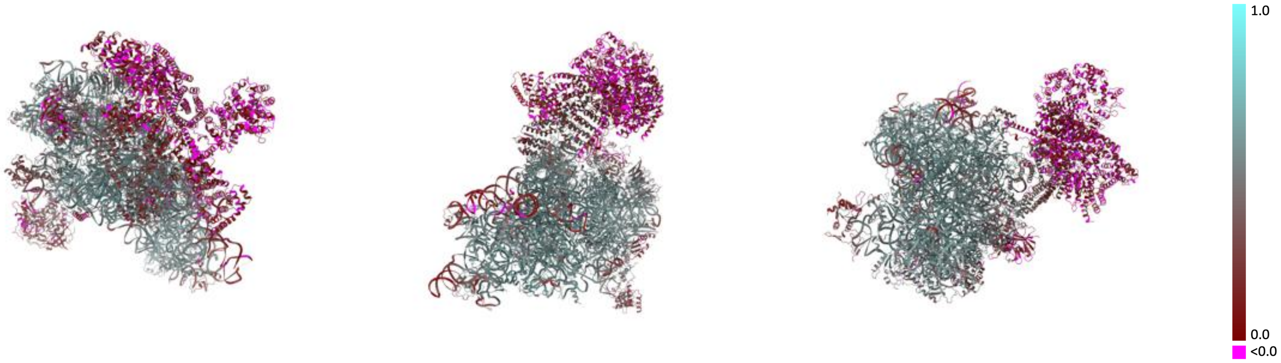
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-17805 and PDB model 8PPL. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay ⓘ

This section was not generated.

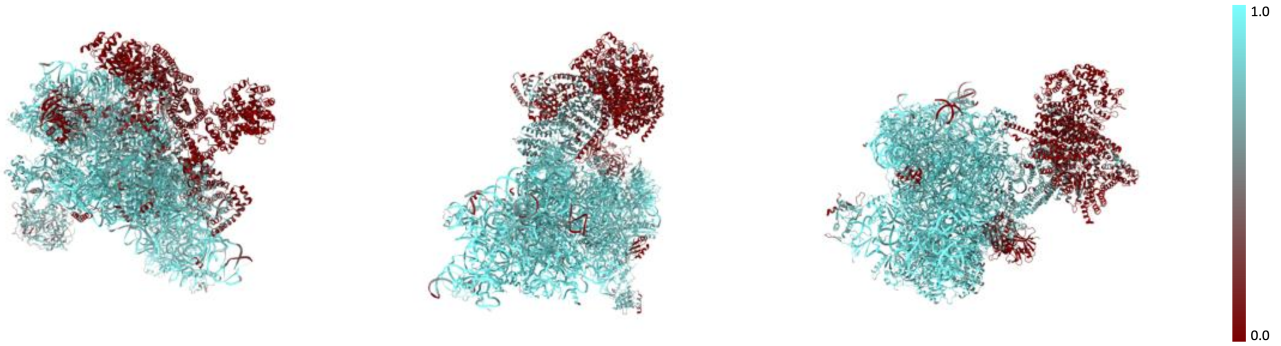
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

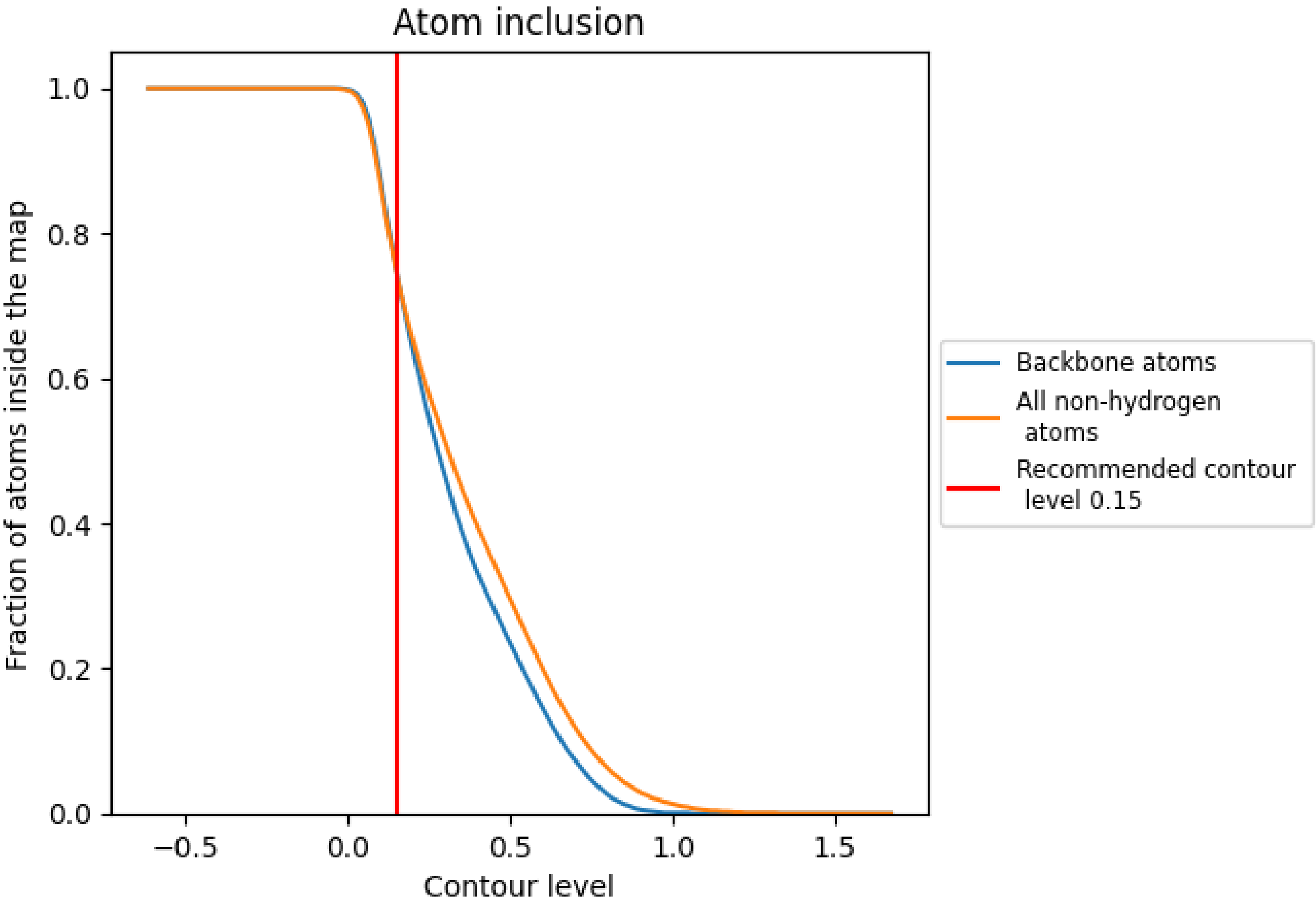
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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

9.4 Atom inclusion ⓘ



At the recommended contour level, 74% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7430	0.4270
A2	0.9630	0.5460
AA	0.9230	0.5740
AB	0.9150	0.5600
AC	0.9640	0.6080
AD	0.9120	0.5440
AE	0.9600	0.5900
AF	0.9290	0.5620
AG	0.8860	0.4830
AH	0.8370	0.4640
AI	0.9140	0.5340
AJ	0.9470	0.5870
AK	0.9110	0.5070
AL	0.9080	0.5640
AM	0.6040	0.2490
AN	0.9470	0.5800
AO	0.9260	0.5730
AP	0.8760	0.5200
AQ	0.9620	0.5850
AR	0.9020	0.5520
AS	0.9170	0.5350
AT	0.9310	0.5730
AU	0.8890	0.5310
AV	0.9380	0.5870
AW	0.9770	0.6210
AX	0.9600	0.6050
AY	0.9480	0.5710
AZ	0.8720	0.5110
Aa	0.9460	0.5900
Ab	0.9170	0.5590
Ac	0.8310	0.5210
Ad	0.9550	0.5900
Ae	0.9110	0.5580
Af	0.7220	0.3300
Ag	0.8790	0.4820

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Chain	Atom inclusion	Q-score
Ah	■ 0.8300	■ 0.5380
Aj	■ 0.9070	■ 0.5640
I3	■ 0.0100	■ 0.0450
I4	■ 0.0660	■ 0.0650
I5	■ 0.0280	■ 0.0790
I6	■ 0.1460	■ 0.1010
I8	■ 0.0440	■ 0.0650
Io	■ 0.1820	■ 0.2490
Ip	■ 0.8560	■ 0.5060
Iq	■ 0.8010	■ 0.5260
Ir	■ 0.6910	■ 0.2930
Is	■ 0.8090	■ 0.4270
It	■ 0.6150	■ 0.1920
Iu	■ 0.5100	■ 0.2280
Iv	■ 0.2250	■ 0.1000
Iw	■ 0.9840	■ 0.4350
Ix	■ 0.1410	■ 0.2120
Iy	■ 0.5820	■ 0.2770