



wwPDB EM Validation Summary Report ⓘ

Jun 21, 2026 – 12:54 pm BST

PDB ID : 6SKF / pdb_00006skf
EMDB ID : EMD-10223
Title : Cryo-EM Structure of T. kodakarensis 70S ribosome
Authors : Matzov, D.; Sas-Chen, A.; Thomas, J.M.; Santangelo, T.; Meier, J.L.; Schwartz, S.; Shalev-Benami, M.
Deposited on : 2019-08-15
Resolution : 2.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

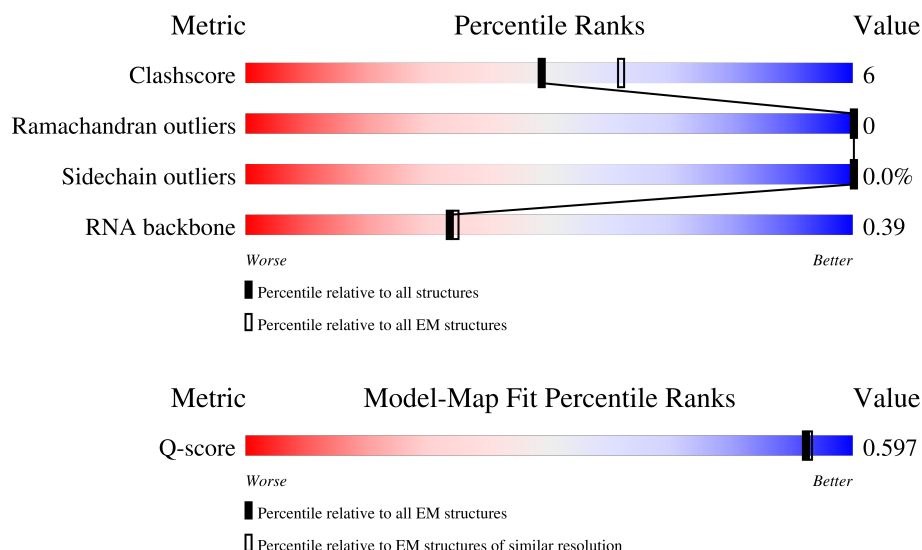
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.95 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13114 (2.45 - 3.45)

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 $\leq 5\%$. 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	Aa	1498	
2	Ab	201	
3	Ac	209	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	Ad	200	
5	Ae	180	
6	Af	243	
7	Ag	235	
8	Ah	125	
9	Ai	215	
10	Aj	130	
11	Ak	130	
12	Al	135	
13	Am	102	
14	An	140	
15	Ao	147	
16	Ap	149	
17	Aq	151	
18	Ar	56	
19	As	114	
20	At	67	
21	Au	133	
22	Av	150	
23	Aw	98	
24	Ax	65	
25	Ay	70	
26	Az	62	
27	BA	3037	
28	BB	126	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	BC	239	
30	BD	346	
31	BE	255	
32	BF	183	
33	BG	184	
34	BH	123	
34	BI	123	
35	BJ	182	
36	BK	142	
37	BL	141	
38	BM	83	
38	BN	83	
39	BO	148	
40	BP	194	
41	BQ	201	
42	BR	121	
43	BS	150	
44	BT	77	
45	BU	98	
46	BV	156	
47	BW	86	
48	BX	121	
49	BY	67	
50	BZ	66	
51	Ba	155	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	Bb	102	
53	Bc	90	
54	Bd	125	
55	Be	90	
56	Bg	86	
57	Bh	63	
58	Bi	51	
59	Bj	51	
60	Bk	37	
61	Bl	94	

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 161920 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	1463	Total	C	N	O	P	0	0
			31591	14101	5837	10190	1463		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	196	Total	C	N	O	S	0	0
			1580	1021	272	284	3		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ac	195	Total	C	N	O	S	0	0
			1524	973	277	271	3		

- Molecule 4 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ad	190	Total	C	N	O	S	0	0
			1550	997	277	273	3		

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ae	174	Total	C	N	O	S	0	0
			1454	912	287	253	2		

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Af	241	Total	C	N	O	S	0	0
			1945	1256	348	336	5		

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ag	223	Total	C	N	O	S	0	0
			1753	1107	327	312	7		

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ah	123	Total	C	N	O	S	0	0
			952	599	179	172	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ai	214	Total	C	N	O	S	0	0
			1715	1087	317	303	8		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Aj	129	Total	C	N	O	S	0	0
			1020	662	176	180	2		

- Molecule 11 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Ak	125	Total	C	N	O		0	0
			982	615	198	169			

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Al	133	Total	C	N	O	S	0	0
			1054	656	205	188	5		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Am	100	Total	C	N	O	S	0	0
			803	498	154	148	3		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	An	127	Total	C	N	O	S	0	0
			950	586	190	171	3		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ao	143	Total	C	N	O	S	0	0
			1122	712	216	192	2		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ap	135	Total	C	N	O	S	0	0
			1090	691	214	181	4		

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Aq	149	Total	C	N	O	S	0	0
			1217	776	233	206	2		

- Molecule 18 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Ar	54	Total	C	N	O	S	0	0
			447	284	92	65	6		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	As	108	Total	C	N	O	S	0	0
			879	560	164	152	3		

- Molecule 20 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	At	64	Total	C	N	O	S	0	0
			538	338	103	95	2		

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Au	116	Total	C	N	O	S	0	0
			952	608	175	163	6		

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Av	149	Total	C	N	O		0	0
			1216	788	215	213			

- Molecule 23 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Aw	95	Total	C	N	O	S	0	0
			777	497	131	146	3		

- Molecule 24 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ax	61	Total	C	N	O	S	0	0
			461	294	83	79	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ax	64	GLU	LEU	conflict	UNP Q5JE50

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ay	64	Total	C	N	O		0	0
			499	307	99	93			

- Molecule 26 is a protein called Predicted zinc-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Az	55	Total	C	N	O	S	0	0
			426	269	74	75	8		

- Molecule 27 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	BA	2929	Total	C	N	O	P	S	0	0
			63265	28239	11728	20367	2929	2		

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	BB	125	Total	C	N	O	P		0	0
			2678	1191	492	870	125			

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	BC	237	Total	C	N	O	S		0	0
			1820	1150	356	311	3			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	BD	344	Total	C	N	O	S		0	0
			2746	1765	505	469	7			

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	BE	255	Total	C	N	O	S		0	0
			2026	1286	389	347	4			

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	BF	169	Total	C	N	O	S		0	0
			1312	821	252	232	7			

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	BG	183	Total	C	N	O	S		0	0
			1463	942	253	266	2			

- Molecule 34 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BH	121	Total	C	N	O	S	0	0
			928	591	154	180	3		
34	BI	121	Total	C	N	O	S	0	0
			928	591	154	180	3		

- Molecule 35 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BJ	168	Total	C	N	O	S	0	0
			1378	877	258	236	7		

- Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	142	Total	C	N	O	S	0	0
			1146	731	213	198	4		

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	140	Total	C	N	O	S	0	0
			1055	658	214	180	3		

- Molecule 38 is a protein called 50S ribosomal protein L14e.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BM	81	Total	C	N	O	S	0	0
			610	382	119	108	1		
38	BN	81	Total	C	N	O	S	0	0
			610	382	119	108	1		

- Molecule 39 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BO	148	Total	C	N	O	S	0	0
			1165	742	222	198	3		

- Molecule 40 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BP	193	Total	C	N	O	S	0	0
			1582	1010	316	250	6		

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BQ	164	Total	C	N	O	S	0	0
			1314	841	243	228	2		

- Molecule 42 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BR	120	Total	C	N	O	S	0	0
			959	601	187	169	2		

- Molecule 43 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BS	146	Total	C	N	O	S	0	0
			1200	753	246	194	7		

- Molecule 44 is a protein called 50S ribosomal protein L18Ae.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	BT	74	Total	C	N	O	0	0
			624	399	113	112		

- Molecule 45 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BU	96	Total	C	N	O	S	0	0
			784	502	158	123	1		

- Molecule 46 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BV	154	Total	C	N	O	S	0	0
			1234	777	242	211	4		

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BW	85	Total	C	N	O	S	0	0
			683	438	119	123	3		

- Molecule 48 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BX	120	Total	C	N	O	S	0	0
			991	628	188	170	5		

- Molecule 49 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BY	62	Total	C	N	O	S	0	0
			524	334	99	85	6		

- Molecule 50 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BZ	60	Total	C	N	O	S	0	0
			506	314	98	90	4		

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ba	154	Total	C	N	O	S	0	0
			1242	788	235	214	5		

- Molecule 52 is a protein called 50S ribosomal protein L30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bb	96	Total	C	N	O	S	0	0
			730	473	123	133	1		

- Molecule 53 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Bc	89	Total	C	N	O	0	0
			721	463	140	118		

- Molecule 54 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bd	124	Total	C	N	O	S	0	0
			1022	650	208	162	2		

- Molecule 55 is a protein called 50S ribosomal protein L34e.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Be	89	Total	C	N	O	S	0	0
			728	454	155	110	9		

- Molecule 56 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Bg	84	Total	C	N	O	S	0	0
			630	392	132	101	5		

- Molecule 57 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Bh	62	Total	C	N	O	S	0	0
			512	314	118	75	5		

- Molecule 58 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Bi	50	Total	C	N	O	S	0	0
			432	276	97	59			

- Molecule 59 is a protein called 50S ribosomal protein L40e.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Bj	47	Total	C	N	O	S	0	0
			373	233	79	56	5		

- Molecule 60 is a protein called LSU ribosomal protein L41E.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Bk	36	Total	C	N	O	S	0	0
			345	218	86	39	2		

- Molecule 61 is a protein called 50S ribosomal protein L44e.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bl	93	Total	C	N	O	S	0	0
			778	494	160	119	5		

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	Ag	1	Total 1	Zn 1	0
62	Ar	1	Total 1	Zn 1	0
62	As	1	Total 1	Zn 1	0
62	Ax	1	Total 1	Zn 1	0
62	Az	2	Total 2	Zn 2	0
62	BY	1	Total 1	Zn 1	0
62	Be	1	Total 1	Zn 1	0
62	Bg	1	Total 1	Zn 1	0
62	Bh	1	Total 1	Zn 1	0
62	Bj	1	Total 1	Zn 1	0
62	Bl	1	Total 1	Zn 1	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		AltConf
63	Aa	714	Total 714	O 714	0
63	Ab	8	Total 8	O 8	0
63	Ac	10	Total 10	O 10	0
63	Ad	4	Total 4	O 4	0
63	Ae	13	Total 13	O 13	0
63	Af	14	Total 14	O 14	0
63	Ag	14	Total 14	O 14	0
63	Ah	2	Total 2	O 2	0
63	Ai	13	Total 13	O 13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
63	Aj	12	Total 12	O 12	0
63	Ak	8	Total 8	O 8	0
63	Al	7	Total 7	O 7	0
63	Am	2	Total 2	O 2	0
63	An	8	Total 8	O 8	0
63	Ao	10	Total 10	O 10	0
63	Ap	11	Total 11	O 11	0
63	Aq	10	Total 10	O 10	0
63	Ar	2	Total 2	O 2	0
63	As	6	Total 6	O 6	0
63	At	1	Total 1	O 1	0
63	Au	4	Total 4	O 4	0
63	Av	13	Total 13	O 13	0
63	Aw	1	Total 1	O 1	0
63	Ax	3	Total 3	O 3	0
63	Ay	4	Total 4	O 4	0
63	Az	4	Total 4	O 4	0
63	BA	1226	Total 1226	O 1226	0
63	BB	19	Total 19	O 19	0
63	BC	19	Total 19	O 19	0
63	BD	24	Total 24	O 24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
63	BE	11	Total 11	O 11	0
63	BG	6	Total 6	O 6	0
63	BJ	11	Total 11	O 11	0
63	BK	11	Total 11	O 11	0
63	BL	4	Total 4	O 4	0
63	BM	2	Total 2	O 2	0
63	BN	4	Total 4	O 4	0
63	BO	10	Total 10	O 10	0
63	BP	18	Total 18	O 18	0
63	BQ	7	Total 7	O 7	0
63	BR	8	Total 8	O 8	0
63	BS	7	Total 7	O 7	0
63	BT	3	Total 3	O 3	0
63	BU	7	Total 7	O 7	0
63	BV	7	Total 7	O 7	0
63	BW	4	Total 4	O 4	0
63	BX	6	Total 6	O 6	0
63	BY	3	Total 3	O 3	0
63	BZ	1	Total 1	O 1	0
63	Ba	10	Total 10	O 10	0
63	Bb	1	Total 1	O 1	0

Continued on next page...

Continued from previous page...

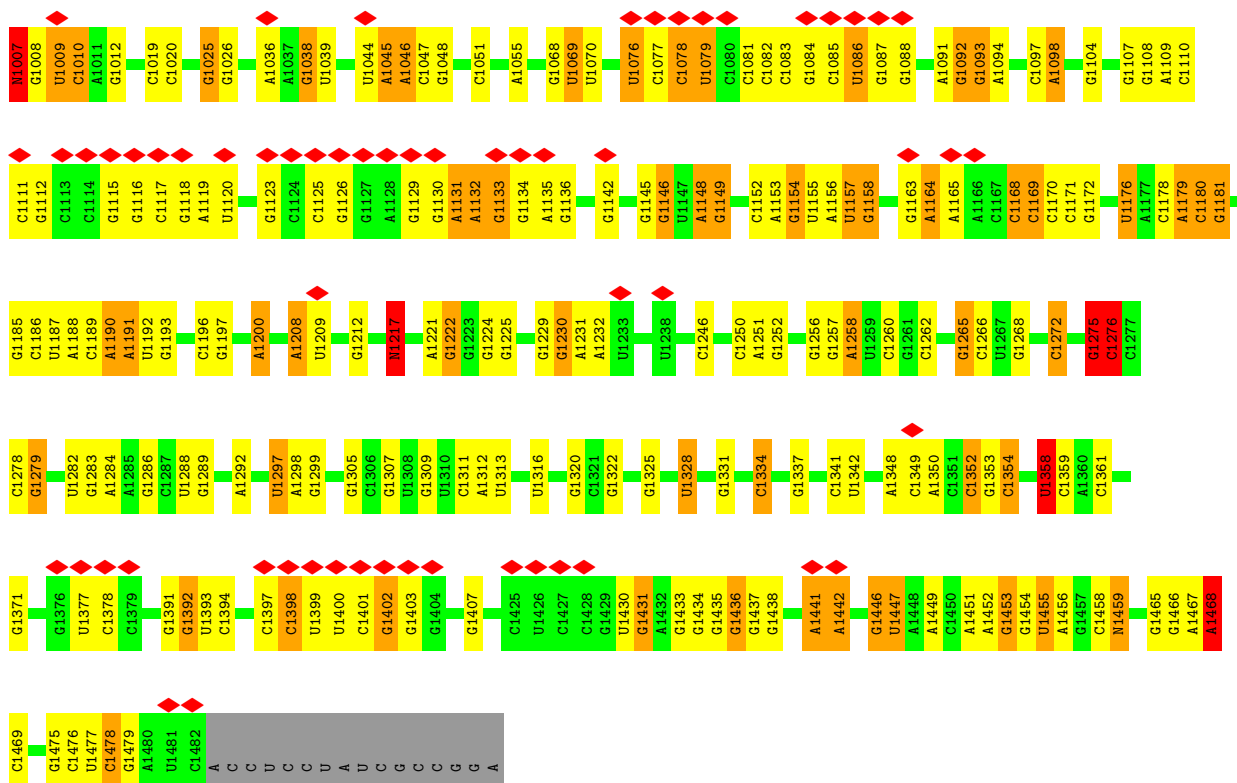
Mol	Chain	Residues	Atoms		AltConf
63	Bc	3	Total 3	O 3	0
63	Bd	5	Total 5	O 5	0
63	Be	3	Total 3	O 3	0
63	Bg	3	Total 3	O 3	0
63	Bh	11	Total 11	O 11	0
63	Bi	2	Total 2	O 2	0
63	Bj	2	Total 2	O 2	0
63	Bk	3	Total 3	O 3	0
63	Bl	8	Total 8	O 8	0

3 Residue-property plots [i](#)

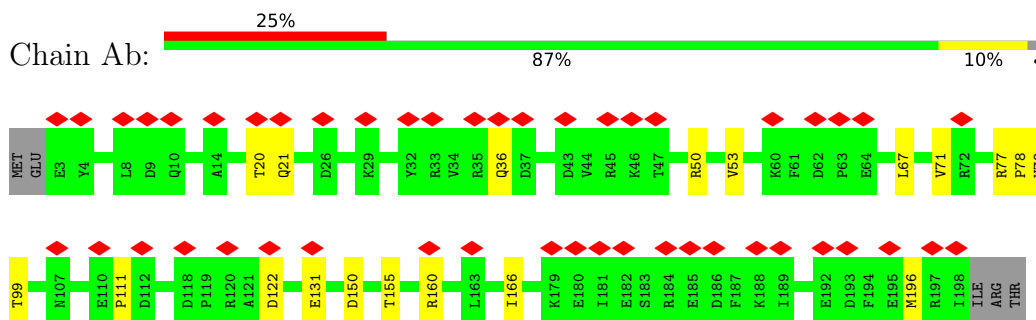
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

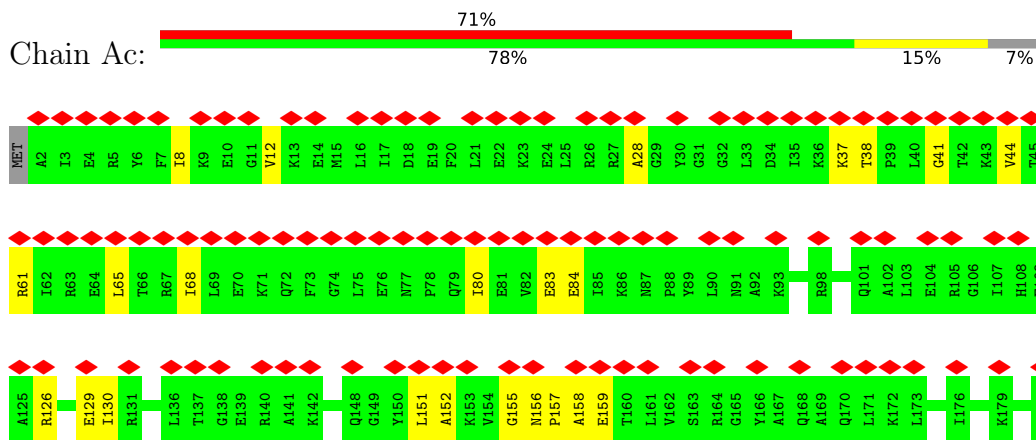




• Molecule 2: 30S ribosomal protein S2



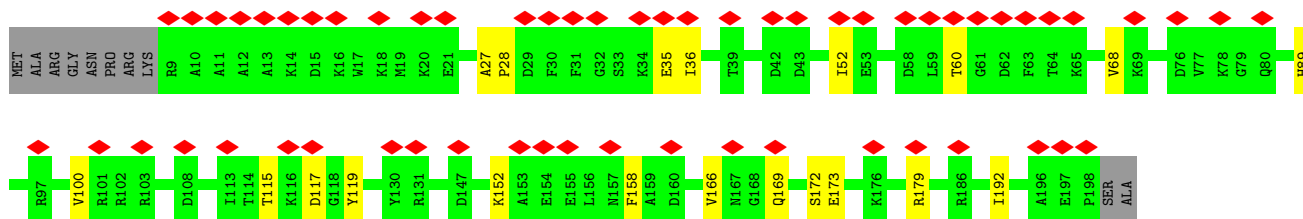
• Molecule 3: 30S ribosomal protein S3



GLU
ILE
VAL
GLY
GLU
GLU
GLU
VAL
SER
ASN
GLU
ALA
GLN

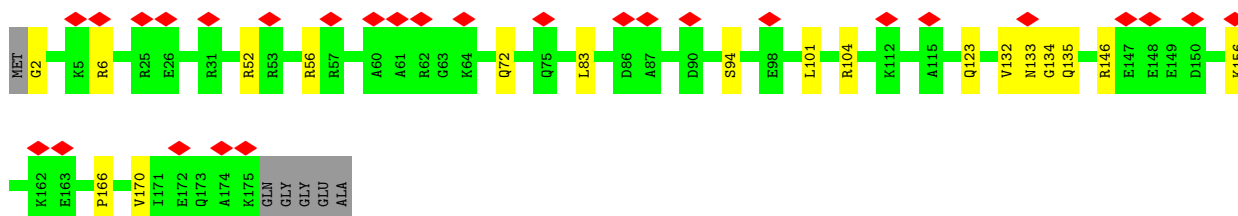
• Molecule 4: 30S ribosomal protein S3Ae

Chain Ad: 29% 85% 10% 5%



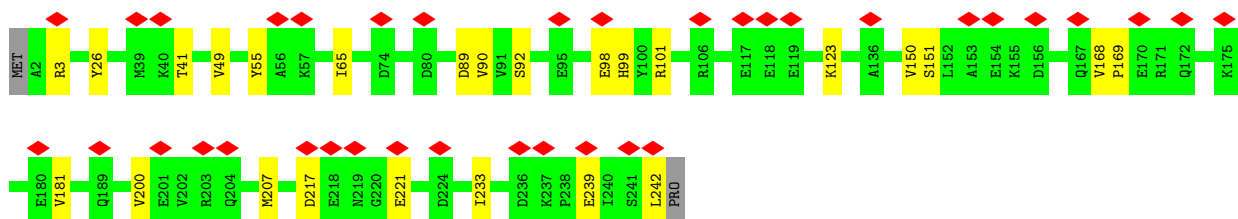
• Molecule 5: 30S ribosomal protein S4

Chain Ae: 16% 87% 10%



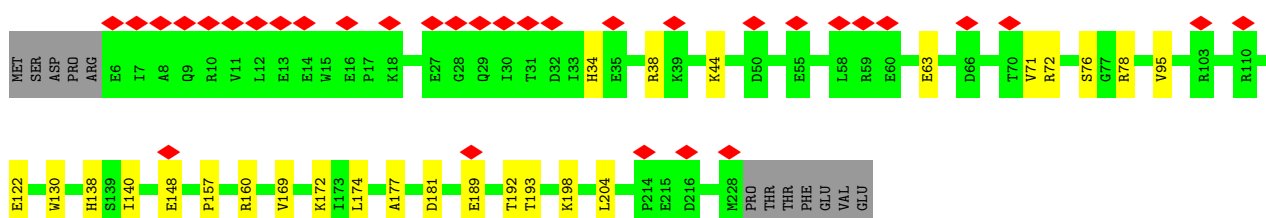
• Molecule 6: 30S ribosomal protein S4e

Chain Af: 15% 89% 10%

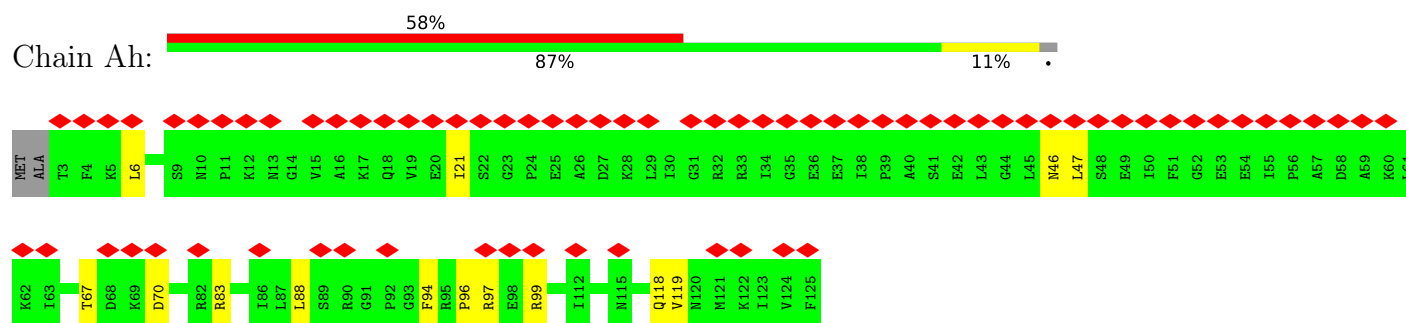


• Molecule 7: 30S ribosomal protein S5

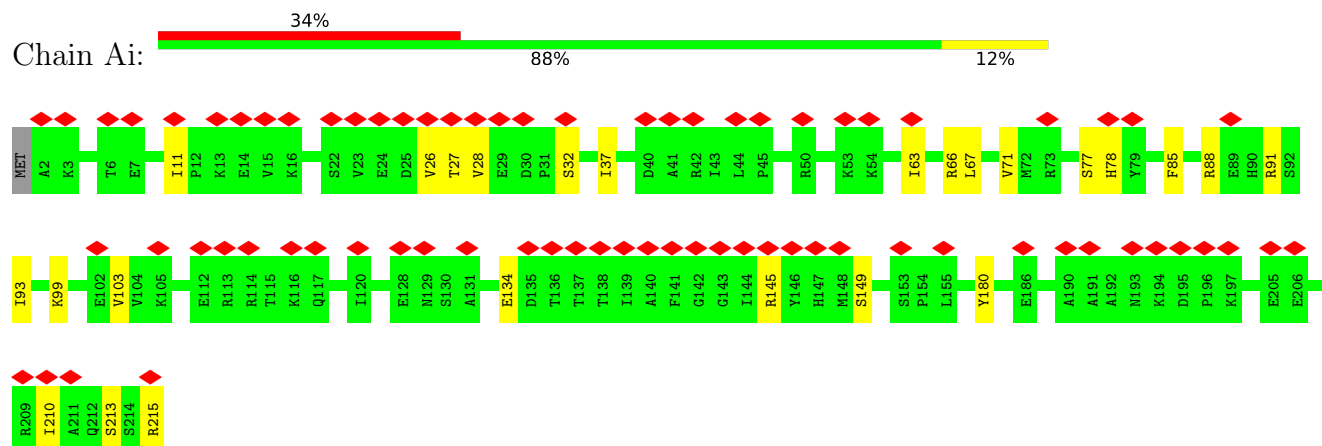
Chain Ag: 14% 84% 11% 5%



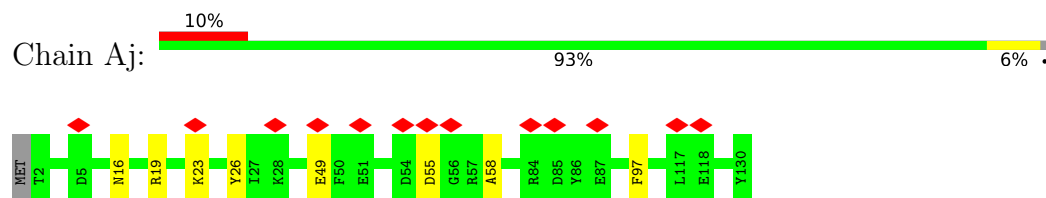
• Molecule 8: 30S ribosomal protein S6e



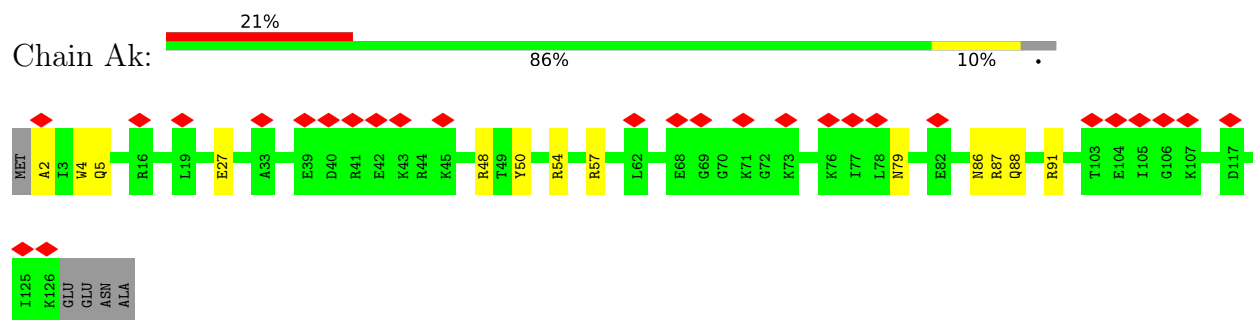
• Molecule 9: 30S ribosomal protein S7



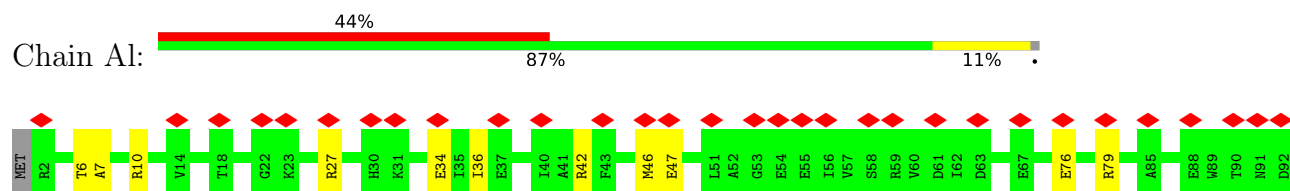
• Molecule 10: 30S ribosomal protein S8

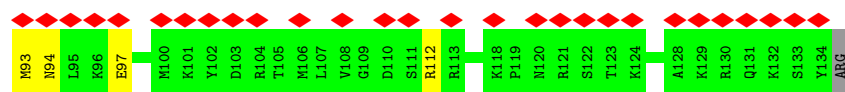


• Molecule 11: 30S ribosomal protein S8e

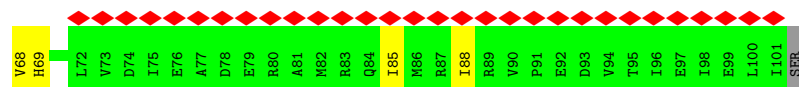
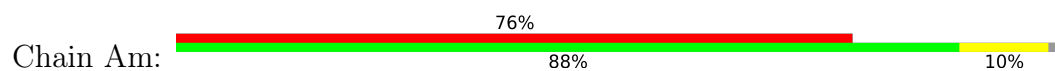


• Molecule 12: 30S ribosomal protein S9

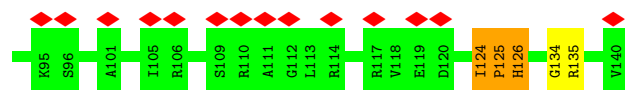
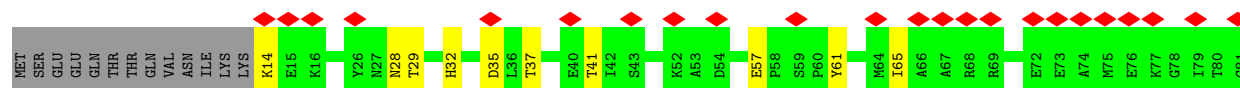
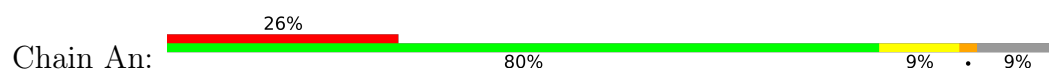




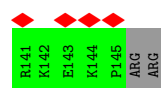
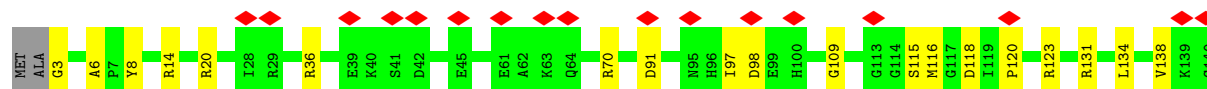
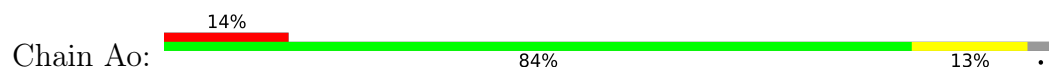
- Molecule 13: 30S ribosomal protein S10



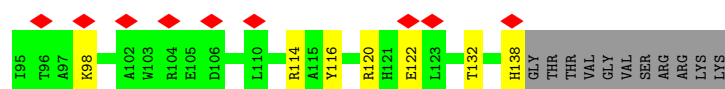
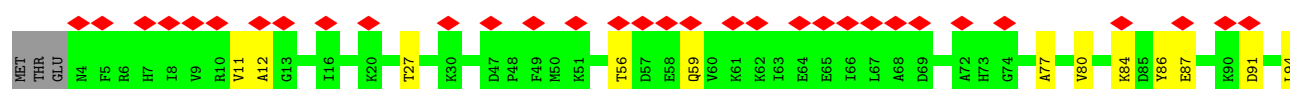
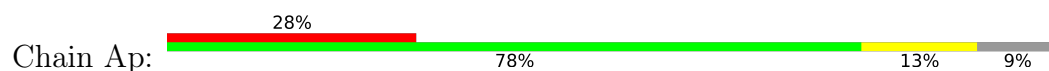
- Molecule 14: 30S ribosomal protein S11



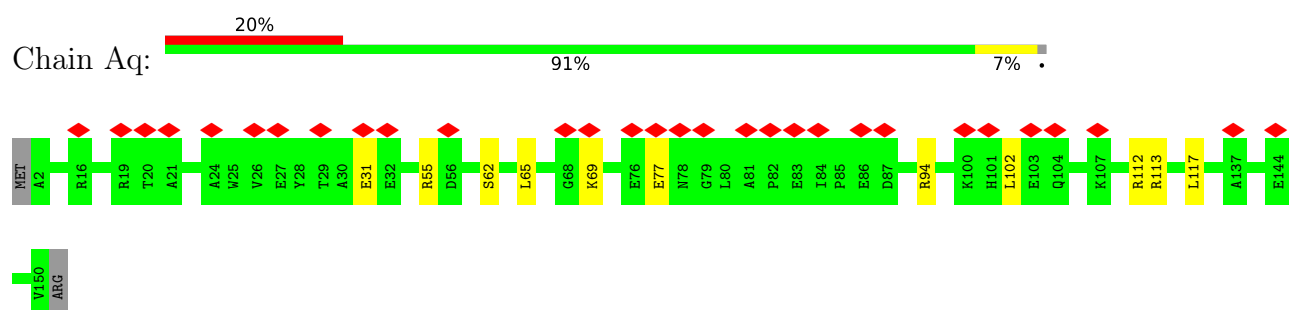
- Molecule 15: 30S ribosomal protein S12



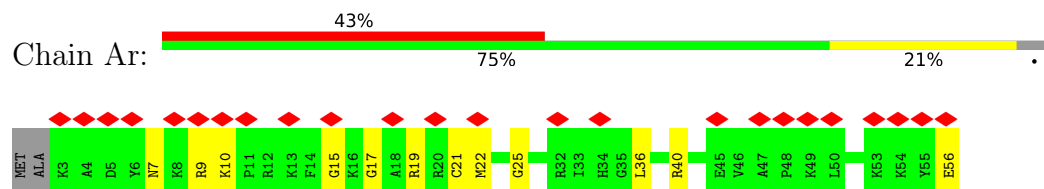
- Molecule 16: 30S ribosomal protein S13



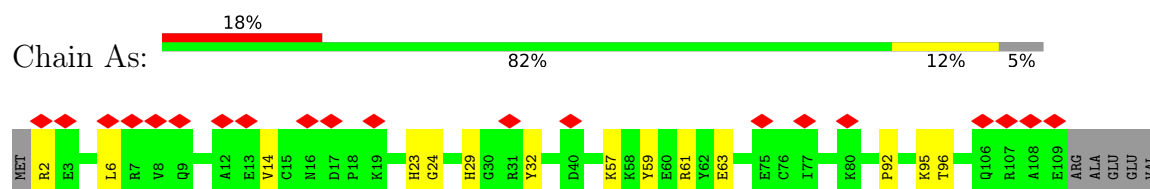
- Molecule 17: 30S ribosomal protein S15



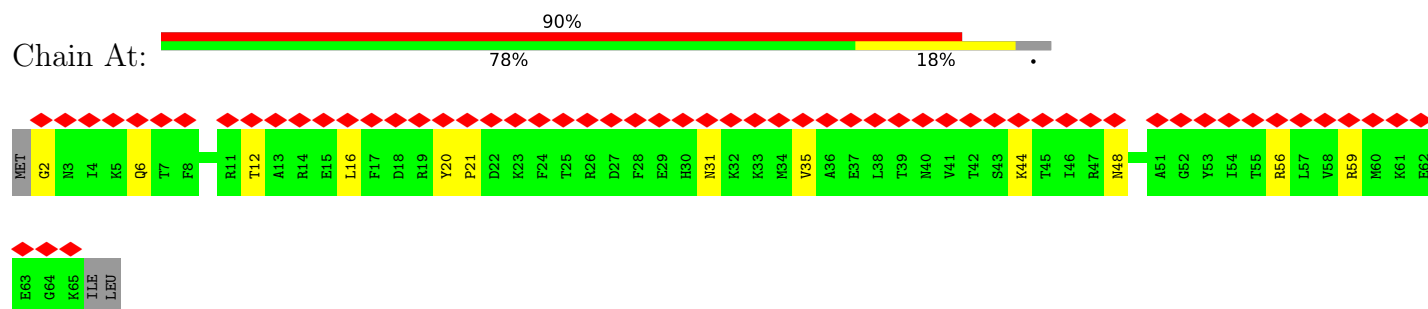
- Molecule 18: 30S ribosomal protein S14 type Z



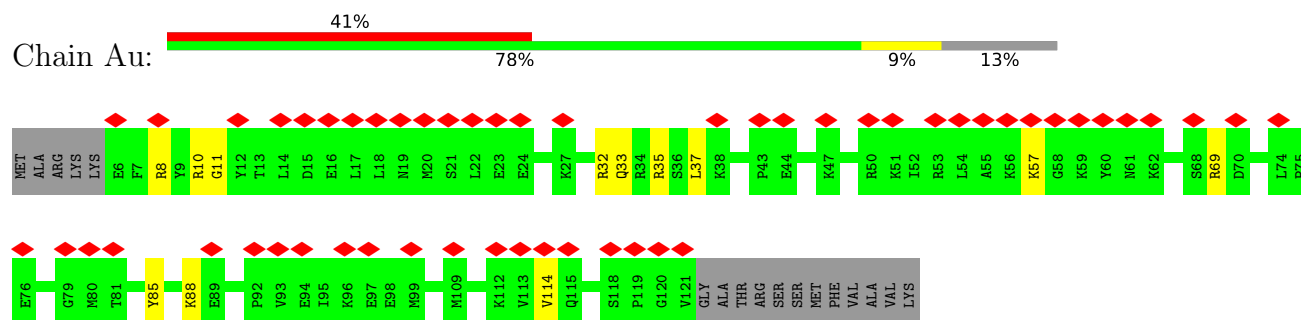
- Molecule 19: 30S ribosomal protein S17



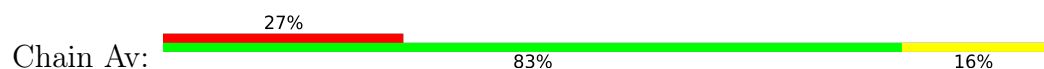
- Molecule 20: 30S ribosomal protein S17e

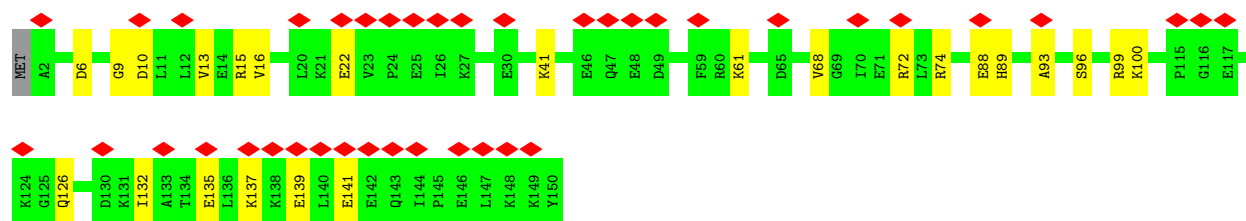


- Molecule 21: 30S ribosomal protein S19

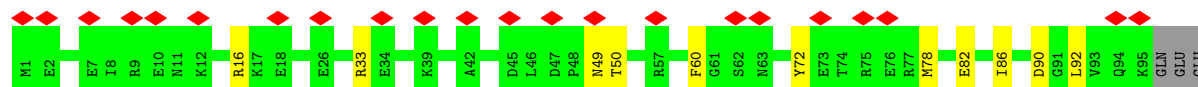
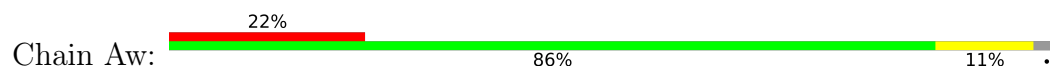


- Molecule 22: 30S ribosomal protein S19e

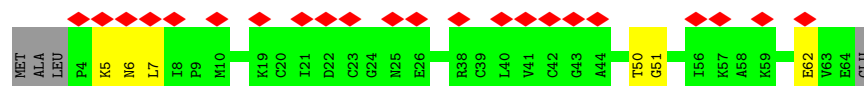
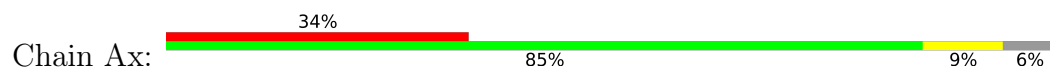




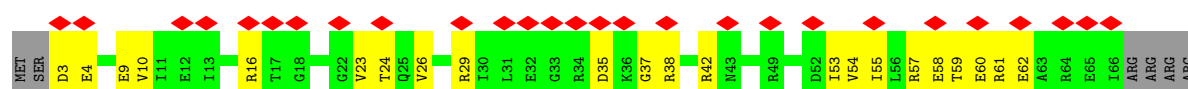
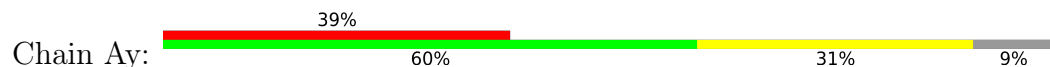
- Molecule 23: 30S ribosomal protein S24e



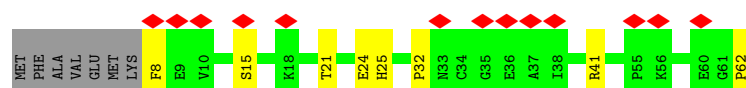
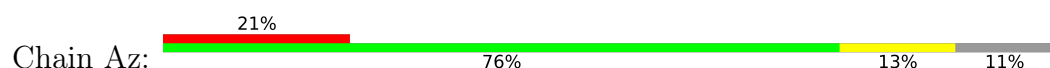
- Molecule 24: 30S ribosomal protein S27e



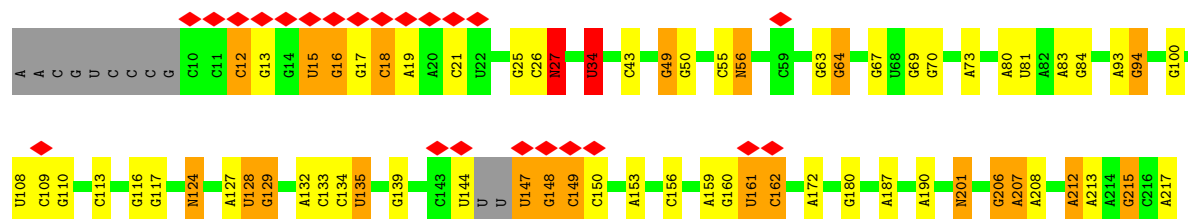
- Molecule 25: 30S ribosomal protein S28e

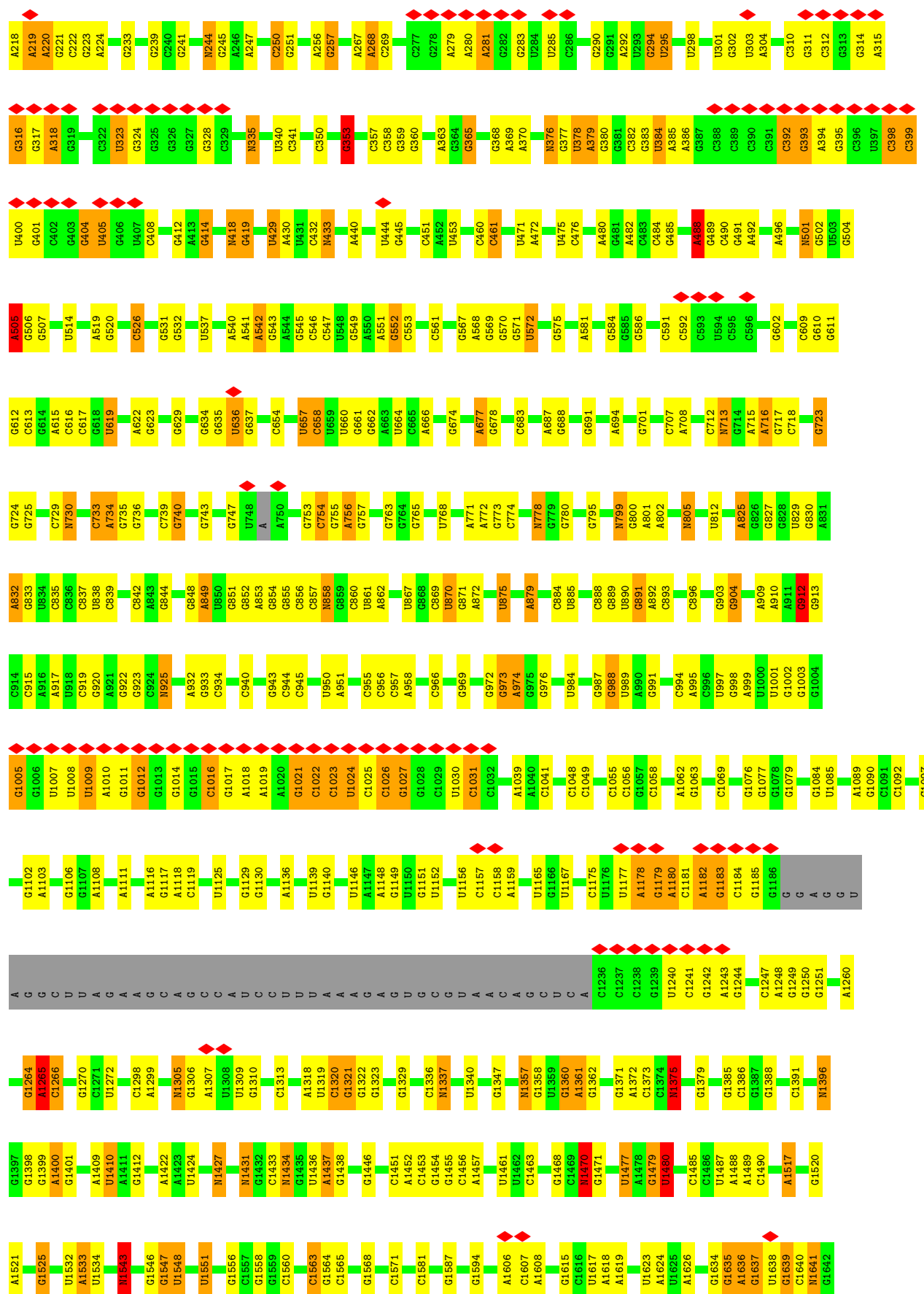


- Molecule 26: Predicted zinc-ribbon RNA-binding protein involved in translation

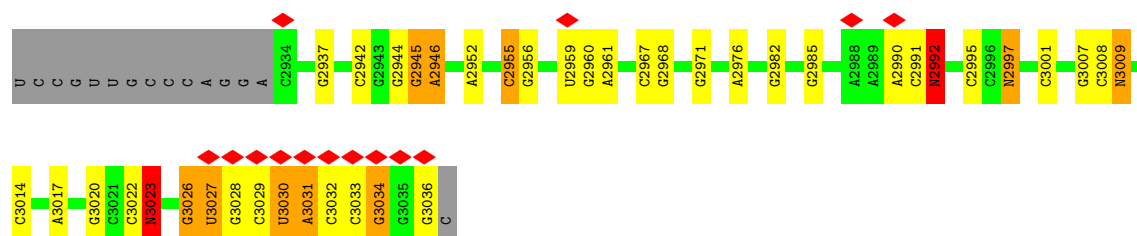


- Molecule 27: 23S rRNA

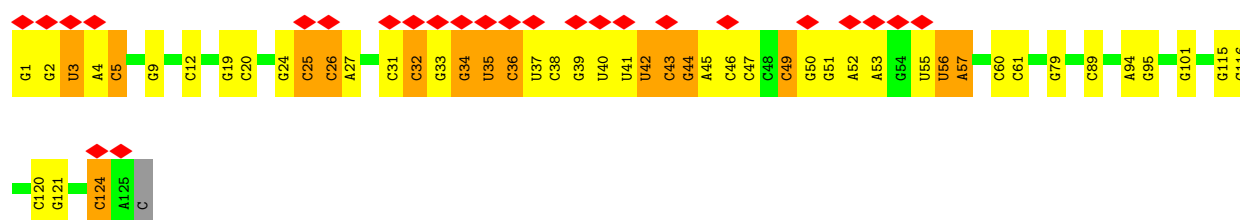




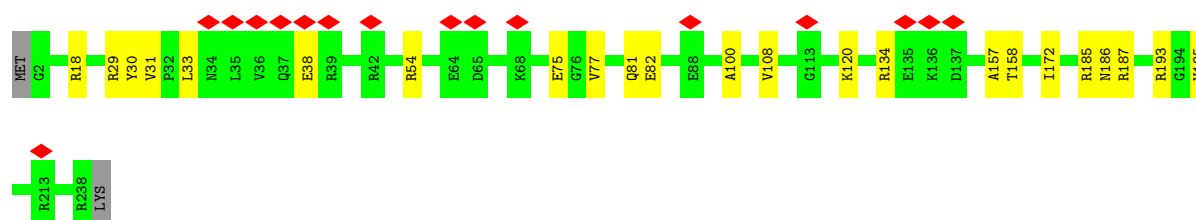




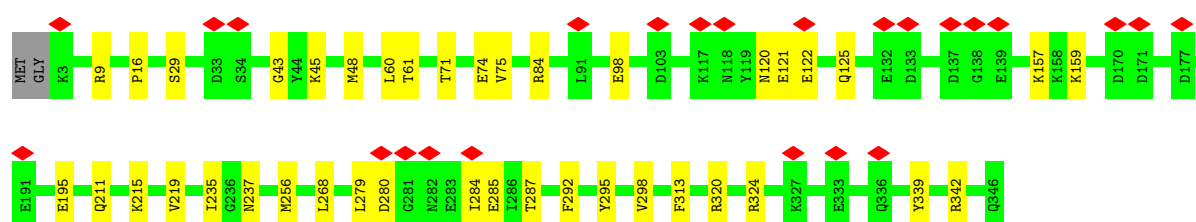
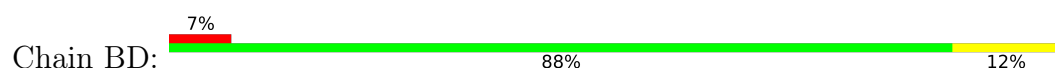
• Molecule 28: 5S rRNA



• Molecule 29: 50S ribosomal protein L2

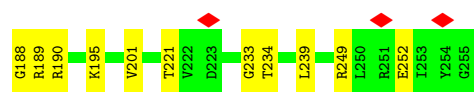


• Molecule 30: 50S ribosomal protein L3

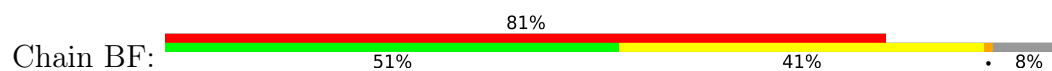


• Molecule 31: 50S ribosomal protein L4

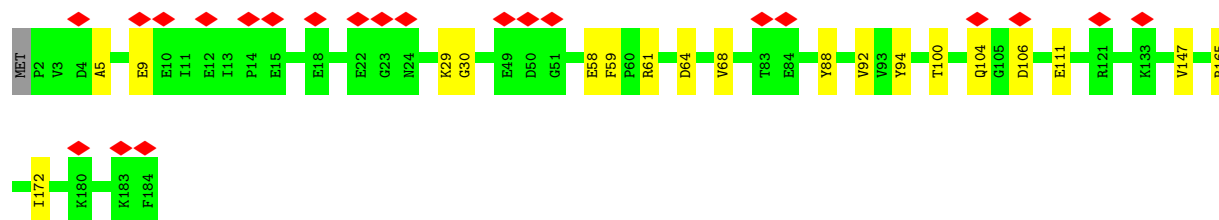
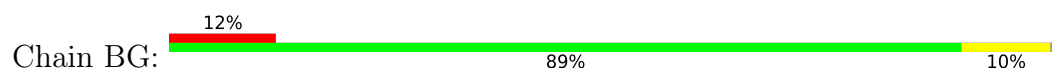




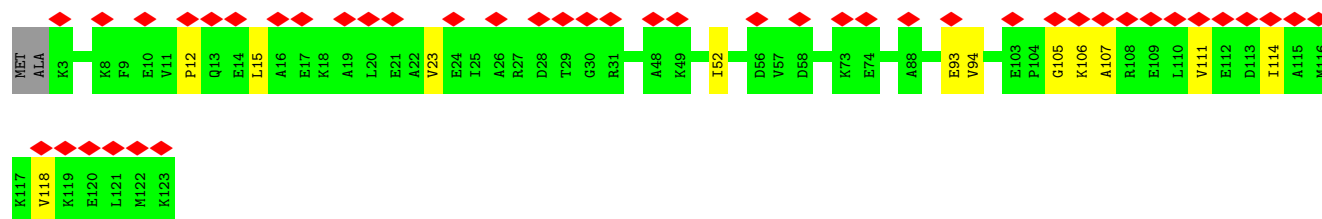
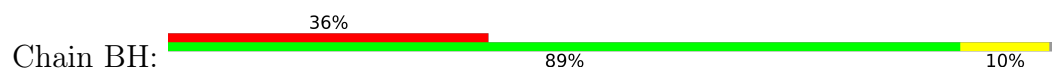
- Molecule 32: 50S ribosomal protein L5



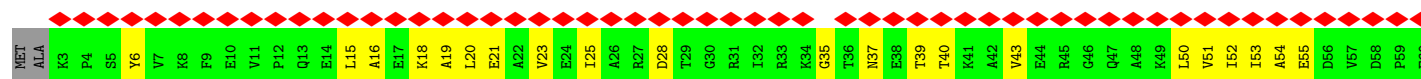
- Molecule 33: 50S ribosomal protein L6



- Molecule 34: 50S ribosomal protein L7Ae

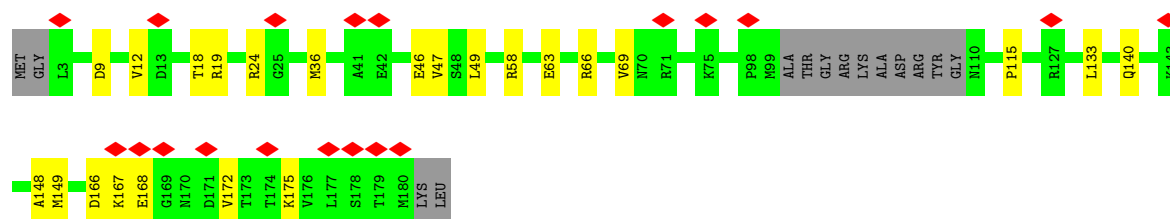
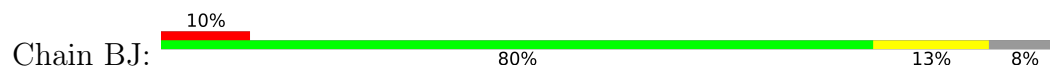


- Molecule 34: 50S ribosomal protein L7Ae

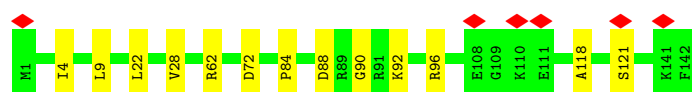




- Molecule 35: 50S ribosomal protein L10e



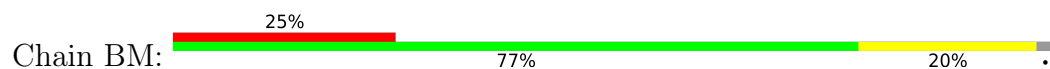
- Molecule 36: 50S ribosomal protein L13



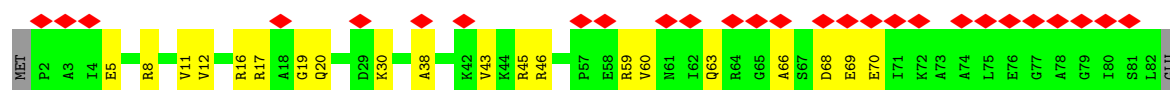
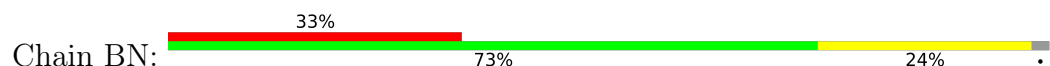
- Molecule 37: 50S ribosomal protein L14



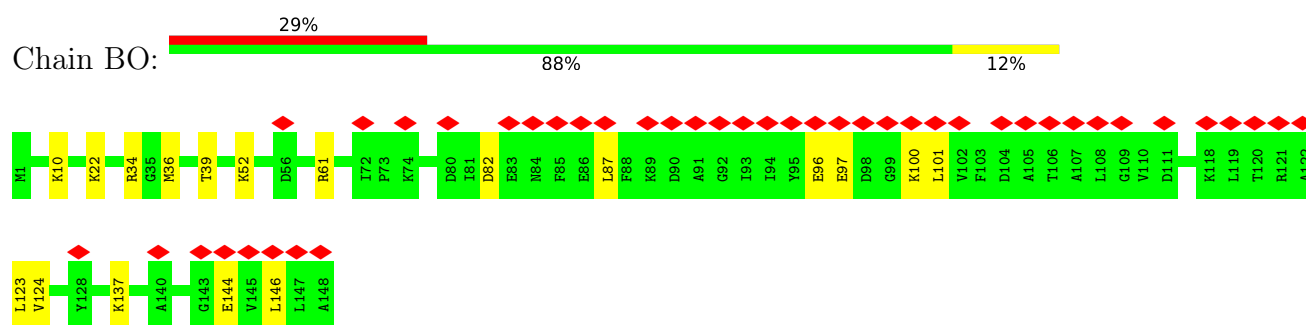
- Molecule 38: 50S ribosomal protein L14e



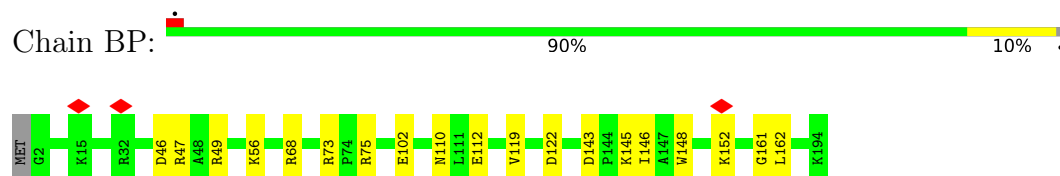
- Molecule 38: 50S ribosomal protein L14e



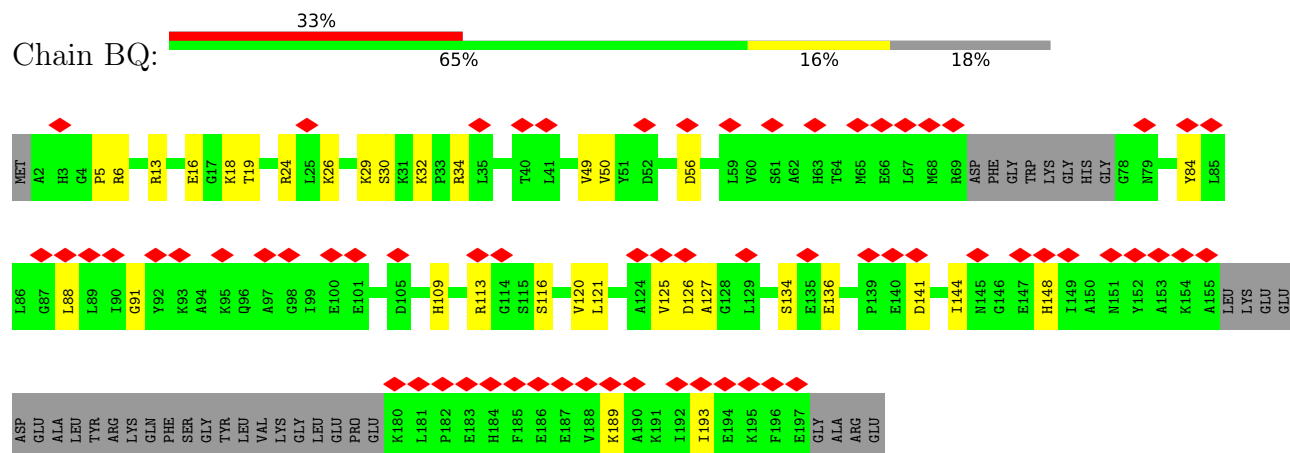
- Molecule 39: 50S ribosomal protein L15



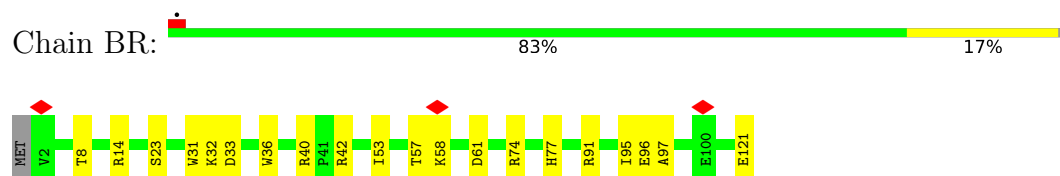
- Molecule 40: 50S ribosomal protein L15e



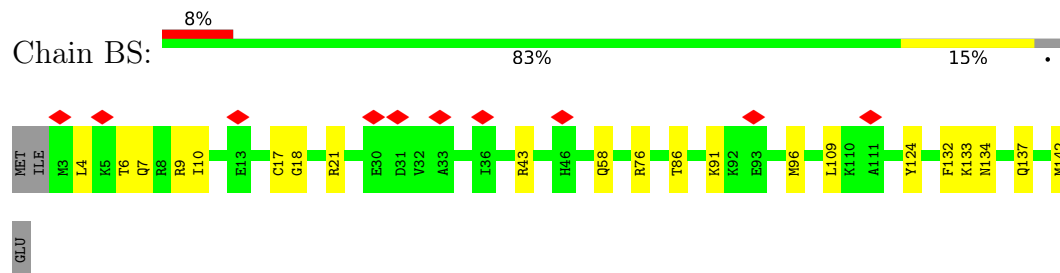
- Molecule 41: 50S ribosomal protein L18



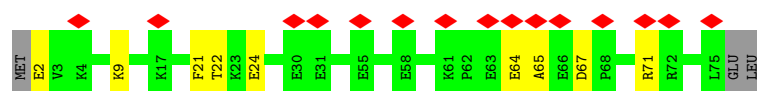
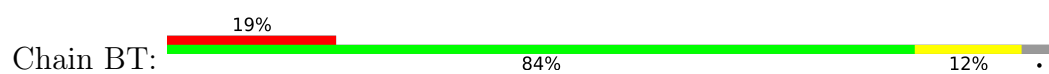
- Molecule 42: 50S ribosomal protein L18e



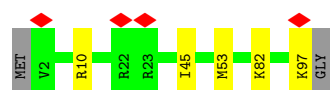
- Molecule 43: 50S ribosomal protein L19e



- Molecule 44: 50S ribosomal protein L18Ae



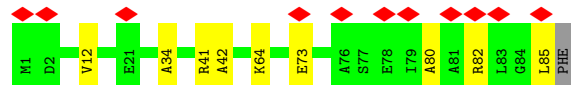
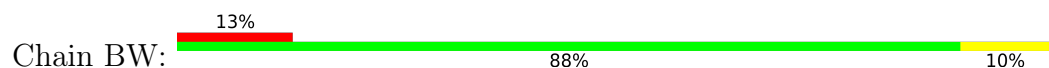
- Molecule 45: 50S ribosomal protein L21e



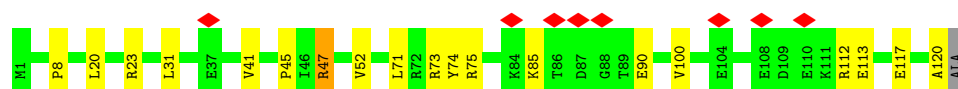
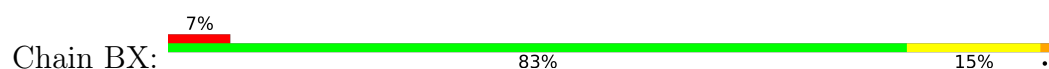
- Molecule 46: 50S ribosomal protein L22



- Molecule 47: 50S ribosomal protein L23



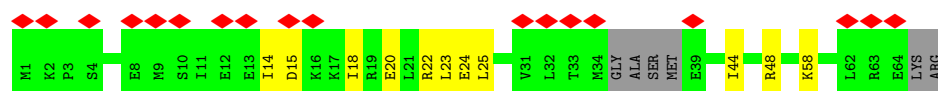
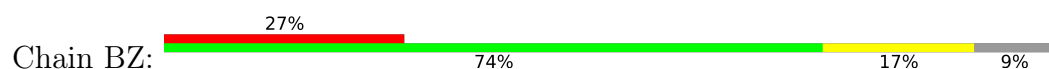
- Molecule 48: 50S ribosomal protein L24



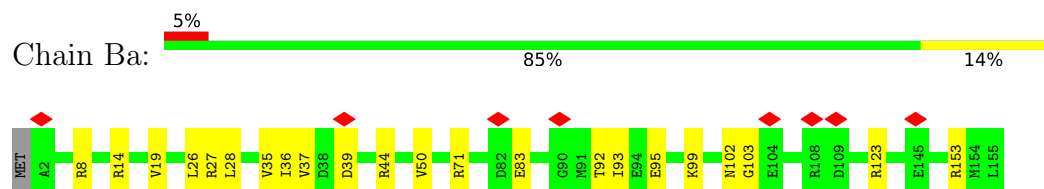
- Molecule 49: 50S ribosomal protein L24e



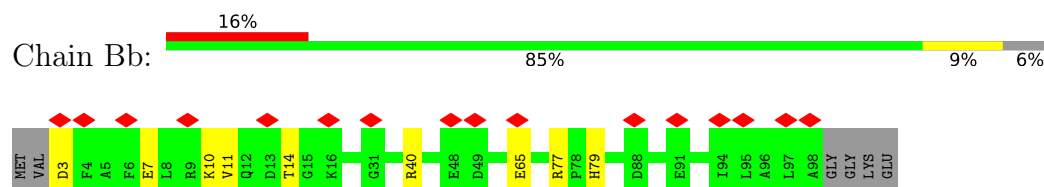
- Molecule 50: 50S ribosomal protein L29



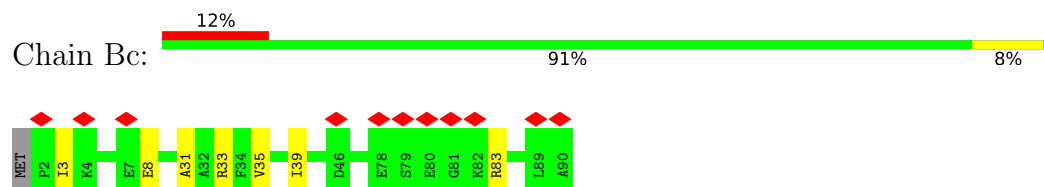
- Molecule 51: 50S ribosomal protein L30



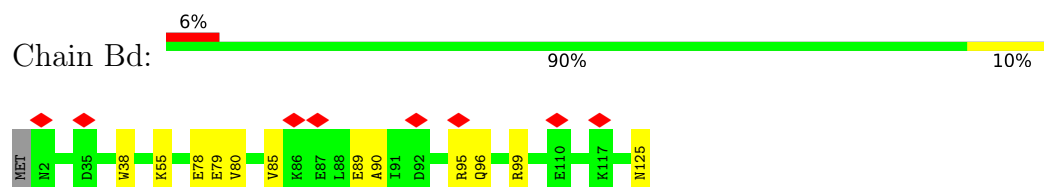
- Molecule 52: 50S ribosomal protein L30e



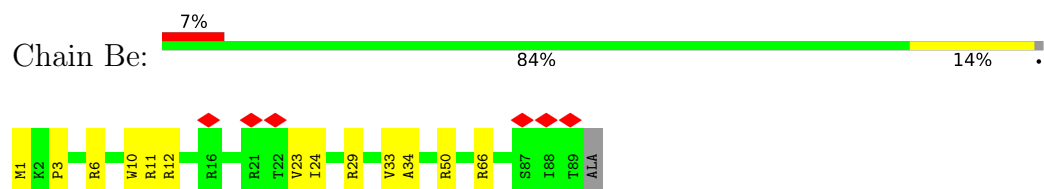
- Molecule 53: 50S ribosomal protein L31e



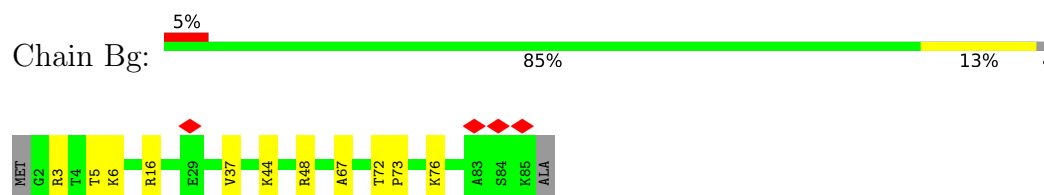
- Molecule 54: 50S ribosomal protein L32e



- Molecule 55: 50S ribosomal protein L34e



- Molecule 56: 50S ribosomal protein L37Ae

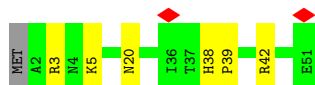
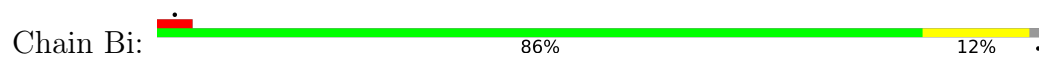


- Molecule 57: 50S ribosomal protein L37e

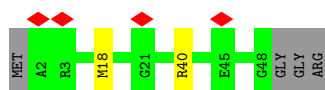
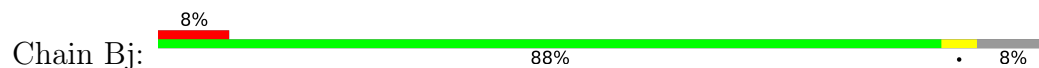




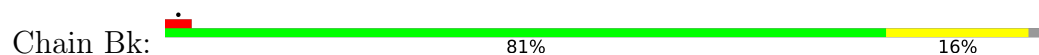
- Molecule 58: 50S ribosomal protein L39e



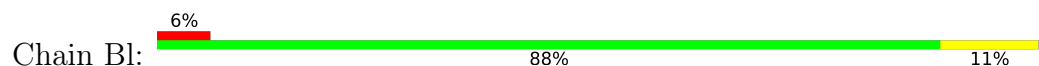
- Molecule 59: 50S ribosomal protein L40e



- Molecule 60: LSU ribosomal protein L41E



- Molecule 61: 50S ribosomal protein L44e



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53737	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 ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	29000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.441	Depositor
Minimum map value	-0.245	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, 5MC, OMU, ZN, A2M, 4SU, LV2, 6MZ, B8T, 5MU, 4AC, MA6, OMC, LHH, OMG

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	Aa	0.53	0/33361	0.48	2/52003 (0.0%)
2	Ab	0.30	0/1611	0.38	0/2179
3	Ac	0.25	0/1546	0.43	0/2075
4	Ad	0.29	0/1578	0.44	0/2119
5	Ae	0.34	0/1477	0.43	0/1980
6	Af	0.34	0/1991	0.38	0/2688
7	Ag	0.20	0/1779	0.39	0/2396
8	Ah	0.32	0/968	0.44	0/1300
9	Ai	0.29	0/1748	0.39	0/2347
10	Aj	0.35	0/1039	0.37	0/1397
11	Ak	0.34	0/991	0.38	0/1322
12	Al	0.28	0/1068	0.43	0/1430
13	Am	0.23	0/810	0.38	0/1087
14	An	0.69	2/968 (0.2%)	0.80	3/1304 (0.2%)
15	Ao	0.39	0/1139	0.44	0/1518
16	Ap	0.34	0/1113	0.48	0/1500
17	Aq	0.32	0/1241	0.39	0/1667
18	Ar	0.41	0/457	0.61	0/602
19	As	0.19	0/899	0.38	0/1214
20	At	0.21	0/545	0.42	0/725
21	Au	0.27	0/970	0.38	0/1295
22	Av	0.30	0/1249	0.40	0/1687
23	Aw	0.31	0/790	0.38	0/1063
24	Ax	0.16	0/469	0.40	0/633
25	Ay	0.30	0/501	0.47	0/672
26	Az	0.17	0/440	0.32	0/599
27	BA	0.69	2/66981 (0.0%)	0.56	2/104453 (0.0%)
28	BB	0.46	0/2993	0.47	0/4668
29	BC	0.62	0/1860	0.61	0/2511
30	BD	0.58	0/2815	0.56	0/3795
31	BE	0.57	0/2066	0.57	0/2785
32	BF	0.58	0/1329	0.80	2/1778 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BG	0.47	0/1490	0.52	0/2006
34	BH	0.38	0/941	0.44	0/1272
34	BI	0.26	0/941	0.47	0/1272
35	BJ	0.52	0/1407	0.58	0/1891
36	BK	0.59	0/1165	0.58	0/1558
37	BL	0.53	0/1067	0.53	0/1435
38	BM	0.47	0/614	0.53	0/824
38	BN	0.43	0/614	0.57	0/824
39	BO	0.52	0/1187	0.59	0/1583
40	BP	0.63	0/1621	0.58	0/2163
41	BQ	0.39	0/1342	0.47	0/1804
42	BR	0.53	0/971	0.50	0/1301
43	BS	0.55	0/1216	0.53	0/1607
44	BT	0.47	0/636	0.47	0/852
45	BU	0.54	0/806	0.53	0/1080
46	BV	0.78	2/1259 (0.2%)	0.80	3/1688 (0.2%)
47	BW	0.48	0/690	0.51	0/925
48	BX	0.50	0/1007	0.52	0/1344
49	BY	0.57	0/538	0.54	0/716
50	BZ	0.44	0/506	0.49	0/668
51	Ba	0.57	0/1259	0.55	0/1680
52	Bb	0.41	0/742	0.45	0/1001
53	Bc	0.53	0/736	0.49	0/990
54	Bd	0.60	0/1044	0.52	0/1394
55	Be	0.54	0/746	0.56	0/997
56	Bg	0.52	0/640	0.54	0/855
57	Bh	0.70	0/524	0.61	0/692
58	Bi	0.63	0/441	0.56	0/588
59	Bj	0.51	0/381	0.57	0/505
60	Bk	0.82	0/351	1.19	0/454
61	Bl	0.51	0/796	0.53	0/1056
All	All	0.58	6/166470 (0.0%)	0.53	12/245817 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
14	An	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	BV	75	PRO	N-CA	18.15	1.70	1.47
14	An	125	PRO	N-CA	18.07	1.70	1.47
27	BA	2581	4SU	O3'-P	5.22	1.61	1.56
27	BA	1969	OMU	O3'-P	5.04	1.61	1.56
14	An	124	ILE	C-N	5.02	1.45	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	An	124	ILE	CA-C-N	15.64	139.39	119.84
14	An	124	ILE	C-N-CA	15.64	139.39	119.84
46	BV	74	LYS	CA-C-N	14.71	138.23	119.84
46	BV	74	LYS	C-N-CA	14.71	138.23	119.84
14	An	125	PRO	CA-N-CD	-8.38	100.27	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	An	126	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	31591	0	15963	308	0
2	Ab	1580	0	1634	16	0
3	Ac	1524	0	1599	22	0
4	Ad	1550	0	1618	14	0
5	Ae	1454	0	1521	15	0
6	Af	1945	0	2028	22	0
7	Ag	1753	0	1822	20	0
8	Ah	952	0	997	12	0
9	Ai	1715	0	1779	18	0
10	Aj	1020	0	1066	6	0
11	Ak	982	0	1071	14	0
12	Al	1054	0	1105	12	0
13	Am	803	0	854	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	An	950	0	971	13	0
15	Ao	1122	0	1212	17	0
16	Ap	1090	0	1121	17	0
17	Aq	1217	0	1302	7	0
18	Ar	447	0	468	15	0
19	As	879	0	905	16	0
20	At	538	0	560	9	0
21	Au	952	0	1000	12	0
22	Av	1216	0	1236	18	0
23	Aw	777	0	797	7	0
24	Ax	461	0	492	6	0
25	Ay	499	0	528	17	0
26	Az	426	0	402	11	0
27	BA	63265	0	32020	545	0
28	BB	2678	0	1361	62	0
29	BC	1820	0	1902	18	0
30	BD	2746	0	2840	27	0
31	BE	2026	0	2128	24	0
32	BF	1312	0	1321	103	0
33	BG	1463	0	1520	16	0
34	BH	928	0	970	7	0
34	BI	928	0	970	28	0
35	BJ	1378	0	1409	20	0
36	BK	1146	0	1213	8	0
37	BL	1055	0	1134	4	0
38	BM	610	0	660	13	0
38	BN	610	0	660	18	0
39	BO	1165	0	1225	21	0
40	BP	1582	0	1677	16	0
41	BQ	1314	0	1359	26	0
42	BR	959	0	1018	20	0
43	BS	1200	0	1298	16	0
44	BT	624	0	647	8	0
45	BU	784	0	821	5	0
46	BV	1234	0	1274	16	0
47	BW	683	0	743	8	0
48	BX	991	0	1053	15	0
49	BY	524	0	512	2	0
50	BZ	506	0	559	7	0
51	Ba	1242	0	1332	15	0
52	Bb	730	0	768	5	0
53	Bc	721	0	776	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	Bd	1022	0	1106	9	0
55	Be	728	0	785	9	0
56	Bg	630	0	675	8	0
57	Bh	512	0	527	6	0
58	Bi	432	0	488	4	0
59	Bj	373	0	390	2	0
60	Bk	345	0	407	12	0
61	Bl	778	0	831	9	0
62	Ag	1	0	0	0	0
62	Ar	1	0	0	0	0
62	As	1	0	0	0	0
62	Ax	1	0	0	0	0
62	Az	2	0	0	0	0
62	BY	1	0	0	0	0
62	Be	1	0	0	0	0
62	Bg	1	0	0	0	0
62	Bh	1	0	0	0	0
62	Bj	1	0	0	0	0
62	Bl	1	0	0	0	0
63	Aa	714	0	0	43	0
63	Ab	8	0	0	0	0
63	Ac	10	0	0	0	0
63	Ad	4	0	0	2	0
63	Ae	13	0	0	0	0
63	Af	14	0	0	2	0
63	Ag	14	0	0	3	0
63	Ah	2	0	0	0	0
63	Ai	13	0	0	0	0
63	Aj	12	0	0	1	0
63	Ak	8	0	0	1	0
63	Al	7	0	0	1	0
63	Am	2	0	0	2	0
63	An	8	0	0	1	0
63	Ao	10	0	0	2	0
63	Ap	11	0	0	5	0
63	Aq	10	0	0	0	0
63	Ar	2	0	0	0	0
63	As	6	0	0	0	0
63	At	1	0	0	0	0
63	Au	4	0	0	0	0
63	Av	13	0	0	0	0
63	Aw	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	Ax	3	0	0	1	0
63	Ay	4	0	0	1	0
63	Az	4	0	0	2	0
63	BA	1226	0	0	91	0
63	BB	19	0	0	1	0
63	BC	19	0	0	0	0
63	BD	24	0	0	1	0
63	BE	11	0	0	2	0
63	BG	6	0	0	1	0
63	BJ	11	0	0	1	0
63	BK	11	0	0	4	0
63	BL	4	0	0	0	0
63	BM	2	0	0	1	0
63	BN	4	0	0	3	0
63	BO	10	0	0	7	0
63	BP	18	0	0	2	0
63	BQ	7	0	0	1	0
63	BR	8	0	0	2	0
63	BS	7	0	0	0	0
63	BT	3	0	0	2	0
63	BU	7	0	0	1	0
63	BV	7	0	0	0	0
63	BW	4	0	0	0	0
63	BX	6	0	0	2	0
63	BY	3	0	0	1	0
63	BZ	1	0	0	0	0
63	Ba	10	0	0	2	0
63	Bb	1	0	0	0	0
63	Bc	3	0	0	0	0
63	Bd	5	0	0	1	0
63	Be	3	0	0	0	0
63	Bg	3	0	0	1	0
63	Bh	11	0	0	1	0
63	Bi	2	0	0	0	0
63	Bj	2	0	0	0	0
63	Bk	3	0	0	1	0
63	Bl	8	0	0	3	0
All	All	161920	0	114430	1576	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1576 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BV:75:PRO:N	46:BV:75:PRO:CA	1.70	1.42
14:An:125:PRO:N	14:An:125:PRO:CA	1.70	1.30
32:BF:18:ARG:HG3	32:BF:142:ARG:NH1	1.48	1.25
27:BA:1759:A:OP1	63:BA:3101:HOH:O	1.54	1.21
28:BB:42:U:O2	32:BF:54:ILE:CB	1.88	1.21

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Ab	194/201 (96%)	181 (93%)	13 (7%)	0	100	100
3	Ac	193/209 (92%)	181 (94%)	12 (6%)	0	100	100
4	Ad	188/200 (94%)	172 (92%)	16 (8%)	0	100	100
5	Ae	172/180 (96%)	162 (94%)	10 (6%)	0	100	100
6	Af	239/243 (98%)	222 (93%)	17 (7%)	0	100	100
7	Ag	221/235 (94%)	207 (94%)	14 (6%)	0	100	100
8	Ah	121/125 (97%)	109 (90%)	12 (10%)	0	100	100
9	Ai	212/215 (99%)	200 (94%)	12 (6%)	0	100	100
10	Aj	127/130 (98%)	115 (91%)	12 (9%)	0	100	100
11	Ak	123/130 (95%)	114 (93%)	9 (7%)	0	100	100
12	Al	131/135 (97%)	123 (94%)	8 (6%)	0	100	100
13	Am	98/102 (96%)	90 (92%)	8 (8%)	0	100	100
14	An	125/140 (89%)	120 (96%)	5 (4%)	0	100	100
15	Ao	141/147 (96%)	137 (97%)	4 (3%)	0	100	100
16	Ap	133/149 (89%)	114 (86%)	19 (14%)	0	100	100
17	Aq	147/151 (97%)	141 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	Ar	52/56 (93%)	47 (90%)	5 (10%)	0	100	100
19	As	106/114 (93%)	100 (94%)	6 (6%)	0	100	100
20	At	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
21	Au	114/133 (86%)	108 (95%)	6 (5%)	0	100	100
22	Av	147/150 (98%)	134 (91%)	13 (9%)	0	100	100
23	Aw	93/98 (95%)	89 (96%)	4 (4%)	0	100	100
24	Ax	59/65 (91%)	57 (97%)	2 (3%)	0	100	100
25	Ay	62/70 (89%)	55 (89%)	7 (11%)	0	100	100
26	Az	53/62 (86%)	47 (89%)	6 (11%)	0	100	100
29	BC	235/239 (98%)	209 (89%)	26 (11%)	0	100	100
30	BD	342/346 (99%)	311 (91%)	31 (9%)	0	100	100
31	BE	253/255 (99%)	232 (92%)	21 (8%)	0	100	100
32	BF	165/183 (90%)	136 (82%)	29 (18%)	0	100	100
33	BG	181/184 (98%)	168 (93%)	13 (7%)	0	100	100
34	BH	119/123 (97%)	111 (93%)	8 (7%)	0	100	100
34	BI	119/123 (97%)	106 (89%)	13 (11%)	0	100	100
35	BJ	164/182 (90%)	149 (91%)	15 (9%)	0	100	100
36	BK	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
37	BL	138/141 (98%)	128 (93%)	10 (7%)	0	100	100
38	BM	79/83 (95%)	72 (91%)	7 (9%)	0	100	100
38	BN	79/83 (95%)	69 (87%)	10 (13%)	0	100	100
39	BO	146/148 (99%)	129 (88%)	17 (12%)	0	100	100
40	BP	191/194 (98%)	178 (93%)	13 (7%)	0	100	100
41	BQ	158/201 (79%)	144 (91%)	14 (9%)	0	100	100
42	BR	118/121 (98%)	106 (90%)	12 (10%)	0	100	100
43	BS	144/150 (96%)	128 (89%)	16 (11%)	0	100	100
44	BT	72/77 (94%)	68 (94%)	4 (6%)	0	100	100
45	BU	94/98 (96%)	88 (94%)	6 (6%)	0	100	100
46	BV	152/156 (97%)	143 (94%)	9 (6%)	0	100	100
47	BW	83/86 (96%)	71 (86%)	12 (14%)	0	100	100
48	BX	118/121 (98%)	111 (94%)	7 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	BY	60/67 (90%)	59 (98%)	1 (2%)	0	100	100
50	BZ	56/66 (85%)	54 (96%)	2 (4%)	0	100	100
51	Ba	152/155 (98%)	142 (93%)	10 (7%)	0	100	100
52	Bb	94/102 (92%)	86 (92%)	8 (8%)	0	100	100
53	Bc	87/90 (97%)	84 (97%)	3 (3%)	0	100	100
54	Bd	122/125 (98%)	113 (93%)	9 (7%)	0	100	100
55	Be	87/90 (97%)	77 (88%)	10 (12%)	0	100	100
56	Bg	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
57	Bh	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
58	Bi	48/51 (94%)	43 (90%)	5 (10%)	0	100	100
59	Bj	45/51 (88%)	39 (87%)	6 (13%)	0	100	100
60	Bk	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
61	Bl	91/94 (97%)	88 (97%)	3 (3%)	0	100	100
All	All	7621/8020 (95%)	7028 (92%)	593 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	Ab	170/175 (97%)	170 (100%)	0	100	100
3	Ac	154/168 (92%)	154 (100%)	0	100	100
4	Ad	162/169 (96%)	162 (100%)	0	100	100
5	Ae	153/156 (98%)	153 (100%)	0	100	100
6	Af	210/212 (99%)	210 (100%)	0	100	100
7	Ag	185/197 (94%)	185 (100%)	0	100	100
8	Ah	104/105 (99%)	104 (100%)	0	100	100
9	Ai	183/184 (100%)	183 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	Aj	106/107 (99%)	106 (100%)	0	100	100
11	Ak	101/105 (96%)	101 (100%)	0	100	100
12	Al	110/112 (98%)	110 (100%)	0	100	100
13	Am	89/91 (98%)	89 (100%)	0	100	100
14	An	94/108 (87%)	94 (100%)	0	100	100
15	Ao	117/120 (98%)	117 (100%)	0	100	100
16	Ap	111/123 (90%)	111 (100%)	0	100	100
17	Aq	129/131 (98%)	129 (100%)	0	100	100
18	Ar	45/46 (98%)	45 (100%)	0	100	100
19	As	96/101 (95%)	96 (100%)	0	100	100
20	At	58/61 (95%)	58 (100%)	0	100	100
21	Au	104/117 (89%)	104 (100%)	0	100	100
22	Av	125/126 (99%)	125 (100%)	0	100	100
23	Aw	85/88 (97%)	85 (100%)	0	100	100
24	Ax	53/56 (95%)	53 (100%)	0	100	100
25	Ay	53/59 (90%)	53 (100%)	0	100	100
26	Az	49/55 (89%)	49 (100%)	0	100	100
29	BC	185/187 (99%)	185 (100%)	0	100	100
30	BD	288/289 (100%)	288 (100%)	0	100	100
31	BE	212/212 (100%)	212 (100%)	0	100	100
32	BF	130/155 (84%)	130 (100%)	0	100	100
33	BG	158/159 (99%)	158 (100%)	0	100	100
34	BH	99/100 (99%)	99 (100%)	0	100	100
34	BI	99/100 (99%)	99 (100%)	0	100	100
35	BJ	144/153 (94%)	144 (100%)	0	100	100
36	BK	120/120 (100%)	120 (100%)	0	100	100
37	BL	104/105 (99%)	104 (100%)	0	100	100
38	BM	63/65 (97%)	63 (100%)	0	100	100
38	BN	63/65 (97%)	63 (100%)	0	100	100
39	BO	116/116 (100%)	116 (100%)	0	100	100
40	BP	161/162 (99%)	161 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	BQ	138/167 (83%)	138 (100%)	0	100	100
42	BR	101/102 (99%)	101 (100%)	0	100	100
43	BS	120/124 (97%)	120 (100%)	0	100	100
44	BT	69/72 (96%)	69 (100%)	0	100	100
45	BU	84/85 (99%)	84 (100%)	0	100	100
46	BV	129/131 (98%)	129 (100%)	0	100	100
47	BW	75/76 (99%)	75 (100%)	0	100	100
48	BX	109/109 (100%)	108 (99%)	1 (1%)	70	83
49	BY	54/58 (93%)	54 (100%)	0	100	100
50	BZ	57/61 (93%)	57 (100%)	0	100	100
51	Ba	132/133 (99%)	132 (100%)	0	100	100
52	Bb	76/80 (95%)	76 (100%)	0	100	100
53	Bc	75/76 (99%)	75 (100%)	0	100	100
54	Bd	106/107 (99%)	106 (100%)	0	100	100
55	Be	80/80 (100%)	80 (100%)	0	100	100
56	Bg	62/63 (98%)	62 (100%)	0	100	100
57	Bh	50/51 (98%)	50 (100%)	0	100	100
58	Bi	45/46 (98%)	45 (100%)	0	100	100
59	Bj	36/38 (95%)	36 (100%)	0	100	100
60	Bk	34/35 (97%)	34 (100%)	0	100	100
61	Bl	83/84 (99%)	83 (100%)	0	100	100
All	All	6503/6738 (96%)	6502 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BX	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
42	BR	54	ASN
53	Bc	55	ASN
42	BR	77	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	Ba	77	ASN
13	Am	25	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Aa	1457/1498 (97%)	283 (19%)	0
27	BA	2924/3037 (96%)	680 (23%)	46 (1%)
28	BB	124/126 (98%)	26 (20%)	2 (1%)
All	All	4505/4661 (96%)	989 (21%)	48 (1%)

5 of 989 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Aa	4	C
1	Aa	17	C
1	Aa	33	U
1	Aa	42	G
1	Aa	45	U

5 of 48 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	1928	C
27	BA	2268	G
27	BA	2053	U
27	BA	2173	G
27	BA	2482	A

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

229 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
27	4AC	BA	805	27	21,24,25	2.86	10 (47%)	29,34,37	1.40	7 (24%)
1	OMG	Aa	382	1	23,26,27	2.17	7 (30%)	33,38,41	1.71	7 (21%)
27	A2M	BA	879	27	22,25,26	3.46	10 (45%)	31,36,39	2.49	11 (35%)
1	LHH	Aa	1020	1	22,25,26	2.56	5 (22%)	29,35,38	1.85	8 (27%)
27	4AC	BA	1337	27	21,24,25	3.01	10 (47%)	29,34,37	1.18	3 (10%)
1	OMG	Aa	1107	1	23,26,27	2.25	9 (39%)	33,38,41	1.73	9 (27%)
1	5MC	Aa	1352	1	18,22,23	3.42	7 (38%)	26,32,35	1.15	3 (11%)
27	5MU	BA	298	27	19,22,23	4.46	7 (36%)	28,32,35	3.72	10 (35%)
27	OMG	BA	2152	27	23,26,27	2.10	6 (26%)	33,38,41	1.79	7 (21%)
27	OMG	BA	2527	27	23,26,27	2.12	6 (26%)	33,38,41	1.59	7 (21%)
27	4AC	BA	2997	27	21,24,25	3.17	9 (42%)	29,34,37	1.22	3 (10%)
27	OMG	BA	2550	27	23,26,27	2.15	6 (26%)	33,38,41	1.99	8 (24%)
1	5MC	Aa	457	1	18,22,23	4.90	15 (83%)	26,32,35	1.12	1 (3%)
1	4AC	Aa	136	1	21,24,25	3.33	9 (42%)	29,34,37	1.72	5 (17%)
27	OMG	BA	2324	27	23,26,27	2.17	7 (30%)	33,38,41	1.72	7 (21%)
27	OMG	BA	1799	27	23,26,27	2.24	9 (39%)	33,38,41	1.62	7 (21%)
1	OMG	Aa	659	1	23,26,27	2.18	8 (34%)	33,38,41	1.66	7 (21%)
1	OMG	Aa	876	1	23,26,27	2.26	8 (34%)	33,38,41	1.72	7 (21%)
1	5MU	Aa	917	1	19,22,23	1.39	4 (21%)	28,32,35	2.22	6 (21%)
27	A2M	BA	872	27	22,25,26	3.51	13 (59%)	31,36,39	2.56	10 (32%)
27	OMU	BA	2389	27	19,22,23	1.29	3 (15%)	26,31,34	1.84	6 (23%)
27	5MU	BA	2688	27	19,22,23	4.44	7 (36%)	28,32,35	3.70	11 (39%)
1	OMC	Aa	1354	1	19,22,23	2.75	7 (36%)	26,31,34	1.03	2 (7%)
27	4AC	BA	713	27	21,24,25	3.04	9 (42%)	29,34,37	1.17	2 (6%)
27	5MU	BA	2384	27	19,22,23	4.63	7 (36%)	28,32,35	3.73	12 (42%)
27	OMU	BA	1551	27	19,22,23	2.93	7 (36%)	26,31,34	1.77	5 (19%)
27	OMU	BA	657	27	19,22,23	2.56	6 (31%)	26,31,34	1.65	6 (23%)
1	OMC	Aa	1361	27,1	19,22,23	2.56	7 (36%)	26,31,34	0.82	0
1	OMU	Aa	479	1	19,22,23	2.97	8 (42%)	26,31,34	1.69	5 (19%)
27	4AC	BA	124	27	21,24,25	2.91	10 (47%)	29,34,37	1.21	3 (10%)
27	OMG	BA	552	27	23,26,27	2.16	8 (34%)	33,38,41	2.39	10 (30%)
27	4AC	BA	1434	27	21,24,25	2.91	10 (47%)	29,34,37	1.70	6 (20%)
27	4SU	BA	2553	27	18,21,22	3.87	8 (44%)	26,30,33	1.94	5 (19%)
27	5MC	BA	2863	27	18,22,23	3.13	7 (38%)	26,32,35	1.23	4 (15%)
27	A2M	BA	488	27	22,25,26	3.46	10 (45%)	31,36,39	2.44	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LV2	Aa	918	1	20,23,24	0.94	0	26,33,36	0.81	0
1	OMU	Aa	52	1	19,22,23	2.82	7 (36%)	26,31,34	1.62	4 (15%)
27	OMU	BA	2542	27	19,22,23	2.70	7 (36%)	26,31,34	1.75	5 (19%)
27	4AC	BA	1955	27	21,24,25	2.89	10 (47%)	29,34,37	1.16	4 (13%)
27	4AC	BA	1375	27	21,24,25	3.10	10 (47%)	29,34,37	1.32	4 (13%)
27	4AC	BA	1431	27	21,24,25	3.15	10 (47%)	29,34,37	1.41	6 (20%)
1	4AC	Aa	605	1	21,24,25	3.30	9 (42%)	29,34,37	1.91	7 (24%)
27	A2M	BA	1517	27	22,25,26	3.46	11 (50%)	31,36,39	2.42	9 (29%)
1	4AC	Aa	525	1	21,24,25	3.00	10 (47%)	29,34,37	1.88	6 (20%)
1	5MC	Aa	854	1	18,22,23	2.93	7 (38%)	26,32,35	1.46	5 (19%)
1	OMC	Aa	752	1	19,22,23	2.69	7 (36%)	26,31,34	0.98	1 (3%)
1	OMG	Aa	771	1	23,26,27	2.24	7 (30%)	33,38,41	1.71	7 (21%)
1	OMG	Aa	498	1	23,26,27	2.21	7 (30%)	33,38,41	1.68	7 (21%)
27	4AC	BA	433	27	21,24,25	3.00	9 (42%)	29,34,37	1.23	3 (10%)
27	4AC	BA	1470	27	21,24,25	3.05	9 (42%)	29,34,37	1.55	6 (20%)
27	4AC	BA	2590	27	21,24,25	3.04	10 (47%)	29,34,37	1.20	5 (17%)
27	4AC	BA	2797	27	21,24,25	2.96	10 (47%)	29,34,37	1.17	3 (10%)
1	4AC	Aa	458	1	21,24,25	1.02	1 (4%)	29,34,37	1.19	3 (10%)
27	4AC	BA	730	27	21,24,25	3.16	10 (47%)	29,34,37	1.37	5 (17%)
27	B8T	BA	357	27	19,22,23	0.79	0	26,31,34	0.85	1 (3%)
27	OMG	BA	2568	27	23,26,27	1.24	3 (13%)	33,38,41	2.09	8 (24%)
27	4AC	BA	2780	27	21,24,25	3.13	9 (42%)	29,34,37	1.67	7 (24%)
1	OMG	Aa	1025	1	23,26,27	2.18	7 (30%)	33,38,41	1.60	6 (18%)
27	4AC	BA	418	27	21,24,25	3.20	10 (47%)	29,34,37	1.17	4 (13%)
27	OMG	BA	2019	27	23,26,27	2.31	7 (30%)	33,38,41	2.02	9 (27%)
27	5MC	BA	2035	27	18,22,23	4.78	15 (83%)	26,32,35	1.19	2 (7%)
27	4AC	BA	2992	27	21,24,25	3.32	10 (47%)	29,34,37	1.39	5 (17%)
27	OMG	BA	2353	27	23,26,27	2.10	6 (26%)	33,38,41	1.63	9 (27%)
27	OMU	BA	619	27	19,22,23	2.81	7 (36%)	26,31,34	1.79	6 (23%)
27	OMG	BA	2016	27	23,26,27	2.22	7 (30%)	33,38,41	1.91	7 (21%)
1	LHH	Aa	229	1	22,25,26	2.50	5 (22%)	29,35,38	1.70	6 (20%)
27	OMU	BA	1776	27	19,22,23	2.71	7 (36%)	26,31,34	1.79	6 (23%)
27	4AC	BA	201	27	21,24,25	2.89	10 (47%)	29,34,37	1.65	6 (20%)
27	5MU	BA	1905	27	19,22,23	4.46	7 (36%)	28,32,35	3.81	11 (39%)
1	4AC	Aa	1217	1	21,24,25	3.44	9 (42%)	29,34,37	1.59	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	BA	925	27	21,24,25	1.06	1 (4%)	29,34,37	1.55	6 (20%)
27	LHH	BA	2457	27	22,25,26	2.52	5 (22%)	29,35,38	2.16	7 (24%)
27	5MC	BA	2055	27	18,22,23	3.24	7 (38%)	26,32,35	1.11	1 (3%)
1	OMG	Aa	446	1	23,26,27	2.20	7 (30%)	33,38,41	1.70	7 (21%)
1	OMC	Aa	190	1	19,22,23	2.74	7 (36%)	26,31,34	0.89	0
27	OMG	BA	2379	27	23,26,27	2.25	6 (26%)	33,38,41	1.68	6 (18%)
27	OMG	BA	1106	27	23,26,27	2.15	6 (26%)	33,38,41	1.60	7 (21%)
27	OMG	BA	912	27	23,26,27	2.23	7 (30%)	33,38,41	2.02	8 (24%)
27	4AC	BA	2121	27	21,24,25	2.90	10 (47%)	29,34,37	1.33	4 (13%)
1	4AC	Aa	298	1	21,24,25	3.17	9 (42%)	29,34,37	1.61	5 (17%)
27	A2M	BA	849	27	22,25,26	3.44	10 (45%)	31,36,39	2.72	13 (41%)
27	OMC	BA	869	27	19,22,23	2.60	7 (36%)	26,31,34	1.06	2 (7%)
27	OMC	BA	1750	27	19,22,23	2.54	7 (36%)	26,31,34	1.22	5 (19%)
27	OMC	BA	718	27	19,22,23	2.65	7 (36%)	26,31,34	1.30	4 (15%)
1	OMU	Aa	8	1	19,22,23	2.73	7 (36%)	26,31,34	1.85	8 (30%)
27	LHH	BA	617	27	22,25,26	2.53	5 (22%)	29,35,38	1.66	6 (20%)
27	4AC	BA	799	27	21,24,25	2.98	10 (47%)	29,34,37	1.33	3 (10%)
27	OMG	BA	1398	27	23,26,27	2.18	6 (26%)	33,38,41	1.58	7 (21%)
27	OMG	BA	2168	27	23,26,27	2.12	8 (34%)	33,38,41	1.81	11 (33%)
27	OMG	BA	1558	27	23,26,27	2.09	8 (34%)	33,38,41	1.70	8 (24%)
1	B8T	Aa	1051	1	19,22,23	0.80	0	26,31,34	0.89	1 (3%)
27	OMG	BA	64	27	23,26,27	2.10	6 (26%)	33,38,41	1.49	6 (18%)
27	5MU	BA	1548	27	19,22,23	4.67	7 (36%)	28,32,35	3.64	10 (35%)
27	OMG	BA	353	27	23,26,27	2.44	7 (30%)	33,38,41	2.05	8 (24%)
27	A2M	BA	2702	27	22,25,26	3.48	11 (50%)	31,36,39	2.34	10 (32%)
1	OMG	Aa	636	1	23,26,27	2.28	6 (26%)	33,38,41	1.81	8 (24%)
1	OMC	Aa	535	1	19,22,23	2.71	7 (36%)	26,31,34	0.93	0
27	OMC	BA	250	27	19,22,23	2.66	7 (36%)	26,31,34	1.42	5 (19%)
27	5MC	BA	1965	27	18,22,23	2.86	7 (38%)	26,32,35	1.15	2 (7%)
1	OMG	Aa	1026	1	23,26,27	2.22	7 (30%)	33,38,41	1.77	8 (24%)
27	OMG	BA	800	27	23,26,27	2.06	7 (30%)	33,38,41	1.44	4 (12%)
27	OMG	BA	365	27	23,26,27	2.09	7 (30%)	33,38,41	1.58	7 (21%)
1	4AC	Aa	682	1	21,24,25	3.23	9 (42%)	29,34,37	1.47	5 (17%)
1	B8T	Aa	1262	1	19,22,23	0.78	0	26,31,34	0.93	1 (3%)
27	OMC	BA	754	27	19,22,23	2.71	7 (36%)	26,31,34	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	OMG	BA	63	27	23,26,27	2.25	6 (26%)	33,38,41	1.81	7 (21%)
27	5MU	BA	537	27	19,22,23	4.44	7 (36%)	28,32,35	3.88	10 (35%)
27	A2M	BA	1265	27	22,25,26	3.40	9 (40%)	31,36,39	2.64	12 (38%)
1	6MZ	Aa	1449	1	22,25,26	1.33	4 (18%)	30,36,39	2.15	7 (23%)
27	5MU	BA	1085	27	19,22,23	4.18	7 (36%)	28,32,35	4.37	11 (39%)
27	OMC	BA	561	27	19,22,23	2.59	7 (36%)	26,31,34	0.94	1 (3%)
27	5MU	BA	875	27	19,22,23	4.58	7 (36%)	28,32,35	3.71	11 (39%)
27	4AC	BA	56	27	21,24,25	3.10	9 (42%)	29,34,37	1.35	5 (17%)
27	OMG	BA	2745	27	23,26,27	2.19	7 (30%)	33,38,41	1.82	6 (18%)
27	4AC	BA	1357	27	21,24,25	3.02	10 (47%)	29,34,37	1.38	6 (20%)
27	OMC	BA	2018	27	19,22,23	2.36	7 (36%)	26,31,34	1.07	3 (11%)
27	OMC	BA	2047	27	19,22,23	2.56	7 (36%)	26,31,34	1.06	1 (3%)
27	5MC	BA	2605	27	18,22,23	3.26	7 (38%)	26,32,35	0.90	1 (3%)
27	LHH	BA	2955	27	22,25,26	2.39	5 (22%)	29,35,38	2.00	6 (20%)
1	OMG	Aa	320	1	23,26,27	2.25	7 (30%)	33,38,41	1.77	8 (24%)
1	OMC	Aa	825	1	19,22,23	2.62	7 (36%)	26,31,34	0.86	0
27	OMG	BA	2728	27	23,26,27	2.21	7 (30%)	33,38,41	1.92	6 (18%)
1	OMG	Aa	246	1	23,26,27	2.14	7 (30%)	33,38,41	1.61	7 (21%)
27	OMU	BA	768	27	19,22,23	2.74	7 (36%)	26,31,34	1.74	4 (15%)
1	OMG	Aa	138	1	23,26,27	2.25	7 (30%)	33,38,41	1.69	7 (21%)
27	A2M	BA	1400	27	22,25,26	3.56	12 (54%)	31,36,39	2.31	8 (25%)
27	5MC	BA	2070	27	18,22,23	0.95	2 (11%)	26,32,35	1.20	3 (11%)
27	4AC	BA	1810	27	21,24,25	3.05	10 (47%)	29,34,37	1.44	5 (17%)
27	4AC	BA	335	27	21,24,25	3.13	9 (42%)	29,34,37	1.14	3 (10%)
27	OMU	BA	453	27	19,22,23	2.72	7 (36%)	26,31,34	1.82	5 (19%)
27	4AC	BA	501	27	21,24,25	3.05	9 (42%)	29,34,37	1.32	3 (10%)
1	4AC	Aa	818	1	21,24,25	3.11	10 (47%)	29,34,37	1.57	5 (17%)
27	4AC	BA	376	27	21,24,25	3.01	9 (42%)	29,34,37	1.32	5 (17%)
27	4AC	BA	778	27	21,24,25	3.14	10 (47%)	29,34,37	1.04	2 (6%)
27	4AC	BA	1543	27	21,24,25	3.12	9 (42%)	29,34,37	1.21	4 (13%)
1	5MC	Aa	1004	1	18,22,23	3.24	7 (38%)	26,32,35	1.14	2 (7%)
1	OMG	Aa	1265	1	23,26,27	2.22	8 (34%)	33,38,41	1.72	7 (21%)
27	OMG	BA	215	27	23,26,27	2.27	7 (30%)	33,38,41	1.94	7 (21%)
27	OMG	BA	723	27	23,26,27	2.19	9 (39%)	33,38,41	1.99	9 (27%)
1	OMG	Aa	994	1	23,26,27	2.33	8 (34%)	33,38,41	1.90	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	BA	244	27	21,24,25	2.99	10 (47%)	29,34,37	1.21	4 (13%)
1	OMG	Aa	532	1	23,26,27	2.16	7 (30%)	33,38,41	1.60	6 (18%)
27	4AC	BA	2838	27	21,24,25	3.16	9 (42%)	29,34,37	1.30	4 (13%)
1	OMG	Aa	450	1	23,26,27	2.15	7 (30%)	33,38,41	1.69	8 (24%)
27	OMU	BA	2610	27	19,22,23	3.04	8 (42%)	26,31,34	1.83	4 (15%)
27	A2M	BA	212	27	22,25,26	1.41	5 (22%)	31,36,39	2.16	10 (32%)
1	4AC	Aa	41	1	21,24,25	3.26	9 (42%)	29,34,37	1.68	5 (17%)
1	4AC	Aa	373	1	21,24,25	3.15	9 (42%)	29,34,37	1.45	6 (20%)
1	OMU	Aa	240	1	19,22,23	2.88	7 (36%)	26,31,34	1.76	4 (15%)
27	OMU	BA	34	27	19,22,23	2.62	7 (36%)	26,31,34	1.63	4 (15%)
1	5MC	Aa	1478	1	18,22,23	3.03	7 (38%)	26,32,35	1.48	6 (23%)
27	OMU	BA	1969	27	19,22,23	2.75	7 (36%)	26,31,34	1.73	5 (19%)
27	A2M	BA	505	27	22,25,26	3.54	10 (45%)	31,36,39	2.67	15 (48%)
1	MA6	Aa	1468	1	23,26,27	1.58	5 (21%)	34,38,41	3.24	11 (32%)
27	OMG	BA	1892	27	23,26,27	2.14	7 (30%)	33,38,41	1.73	8 (24%)
27	OMG	BA	1953	27	23,26,27	2.27	7 (30%)	33,38,41	1.78	7 (21%)
27	OMC	BA	2124	27	19,22,23	2.58	7 (36%)	26,31,34	1.08	3 (11%)
27	5MC	BA	944	27	18,22,23	2.92	7 (38%)	26,32,35	1.31	3 (11%)
1	OMG	Aa	852	1	23,26,27	2.22	7 (30%)	33,38,41	1.55	6 (18%)
27	4AC	BA	1427	27	21,24,25	2.99	9 (42%)	29,34,37	1.27	4 (13%)
27	4AC	BA	3009	27	21,24,25	3.09	10 (47%)	29,34,37	1.22	3 (10%)
27	OMU	BA	1319	27	19,22,23	2.75	7 (36%)	26,31,34	1.70	5 (19%)
27	OMU	BA	1340	27	19,22,23	2.65	7 (36%)	26,31,34	1.71	5 (19%)
1	A2M	Aa	352	1	22,25,26	1.43	4 (18%)	31,36,39	2.08	8 (25%)
1	OMG	Aa	892	1	23,26,27	2.16	7 (30%)	33,38,41	1.64	7 (21%)
1	4AC	Aa	697	1	21,24,25	3.24	9 (42%)	29,34,37	1.64	6 (20%)
27	A2M	BA	756	27	22,25,26	3.46	10 (45%)	31,36,39	2.45	11 (35%)
27	OMG	BA	2657	27	23,26,27	2.18	7 (30%)	33,38,41	1.73	7 (21%)
27	4AC	BA	2159	27	21,24,25	2.98	10 (47%)	29,34,37	1.32	5 (17%)
27	OMG	BA	290	27	23,26,27	2.18	8 (34%)	33,38,41	1.90	7 (21%)
1	4AC	Aa	358	1	21,24,25	3.25	9 (42%)	29,34,37	1.60	5 (17%)
1	5MC	Aa	942	1	18,22,23	3.37	7 (38%)	26,32,35	1.04	2 (7%)
1	5MC	Aa	1276	1	18,22,23	4.83	16 (88%)	26,32,35	1.16	2 (7%)
27	5MC	BA	2075	27	18,22,23	2.86	7 (38%)	26,32,35	1.02	1 (3%)
27	OMG	BA	2528	27	23,26,27	2.38	6 (26%)	33,38,41	2.01	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	OMC	BA	2595	27	19,22,23	2.57	7 (36%)	26,31,34	1.27	3 (11%)
27	4AC	BA	1305	27	21,24,25	3.31	10 (47%)	29,34,37	1.55	6 (20%)
27	A2M	BA	932	27	22,25,26	3.51	10 (45%)	31,36,39	2.48	11 (35%)
27	5MU	BA	572	27	19,22,23	4.45	7 (36%)	28,32,35	3.73	12 (42%)
27	OMG	BA	763	27	23,26,27	2.13	9 (39%)	33,38,41	1.83	9 (27%)
27	LHH	BA	526	27	22,25,26	2.41	5 (22%)	29,35,38	1.77	7 (24%)
27	OMG	BA	833	27	23,26,27	2.24	8 (34%)	33,38,41	1.92	7 (21%)
27	4AC	BA	1934	27	21,24,25	2.98	9 (42%)	29,34,37	1.31	4 (13%)
27	OMG	BA	2672	27	23,26,27	2.20	7 (30%)	33,38,41	1.87	7 (21%)
1	5MC	Aa	464	1	18,22,23	3.34	7 (38%)	26,32,35	1.22	2 (7%)
27	OMG	BA	575	27	23,26,27	2.10	8 (34%)	33,38,41	1.65	7 (21%)
1	4AC	Aa	569	1	21,24,25	3.15	9 (42%)	29,34,37	1.40	5 (17%)
27	4AC	BA	2832	27	21,24,25	3.03	10 (47%)	29,34,37	1.29	4 (13%)
1	4AC	Aa	827	1	21,24,25	3.18	9 (42%)	29,34,37	1.24	4 (13%)
1	MA6	Aa	1467	1	23,26,27	1.77	6 (26%)	34,38,41	3.01	11 (32%)
27	OMG	BA	1525	27	23,26,27	2.21	7 (30%)	33,38,41	1.84	8 (24%)
27	OMC	BA	2571	27	19,22,23	2.66	7 (36%)	26,31,34	1.28	4 (15%)
27	OMU	BA	2656	27	19,22,23	2.65	7 (36%)	26,31,34	1.67	4 (15%)
1	4AC	Aa	730	1	21,24,25	3.06	10 (47%)	29,34,37	1.68	5 (17%)
1	OMG	Aa	1434	1	23,26,27	2.15	7 (30%)	33,38,41	1.75	7 (21%)
1	OMG	Aa	381	1	23,26,27	2.22	7 (30%)	33,38,41	1.69	7 (21%)
1	OMC	Aa	296	1	19,22,23	2.62	7 (36%)	26,31,34	0.96	1 (3%)
1	5MC	Aa	1476	1	18,22,23	4.81	15 (83%)	26,32,35	1.20	2 (7%)
27	OMG	BA	1940	27	23,26,27	2.13	7 (30%)	33,38,41	1.53	7 (21%)
1	4AC	Aa	5	1	21,24,25	3.13	10 (47%)	29,34,37	1.64	5 (17%)
27	5MC	BA	1696	27	18,22,23	3.02	7 (38%)	26,32,35	1.07	2 (7%)
27	OMC	BA	2630	27	19,22,23	2.48	7 (36%)	26,31,34	1.10	2 (7%)
1	5MC	Aa	672	1	18,22,23	3.12	7 (38%)	26,32,35	1.20	2 (7%)
27	OMU	BA	1480	27	19,22,23	2.72	7 (36%)	26,31,34	1.59	4 (15%)
1	4AC	Aa	1459	1	21,24,25	2.56	7 (33%)	29,34,37	1.66	8 (27%)
1	4AC	Aa	1007	1	21,24,25	1.07	1 (4%)	29,34,37	1.16	4 (13%)
27	4AC	BA	3023	27	21,24,25	3.17	9 (42%)	29,34,37	1.33	7 (24%)
27	A2M	BA	825	27	22,25,26	3.51	12 (54%)	31,36,39	2.39	8 (25%)
27	4AC	BA	1396	27	21,24,25	3.07	10 (47%)	29,34,37	1.45	6 (20%)
27	OMG	BA	419	27	23,26,27	2.24	7 (30%)	33,38,41	3.02	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	BA	1899	27	21,24,25	2.96	10 (47%)	29,34,37	1.26	4 (13%)
1	OMU	Aa	304	1	19,22,23	2.87	7 (36%)	26,31,34	1.71	4 (15%)
1	2MG	Aa	670	1	23,26,27	2.69	8 (34%)	32,38,41	2.05	8 (25%)
1	OMG	Aa	1275	1	23,26,27	1.26	3 (13%)	33,38,41	1.94	6 (18%)
27	4AC	BA	27	27	21,24,25	3.17	10 (47%)	29,34,37	1.35	5 (17%)
27	4AC	BA	858	27	21,24,25	2.97	10 (47%)	29,34,37	1.65	2 (6%)
1	OMG	Aa	913	1	23,26,27	2.32	8 (34%)	33,38,41	2.21	11 (33%)
27	4SU	BA	2581	27	18,21,22	4.00	8 (44%)	26,30,33	2.26	5 (19%)
27	4AC	BA	1641	27	21,24,25	3.13	9 (42%)	29,34,37	1.25	5 (17%)
1	OMU	Aa	1358	1	19,22,23	2.52	7 (36%)	26,31,34	2.31	8 (30%)
27	OMC	BA	1820	27	19,22,23	2.58	7 (36%)	26,31,34	1.29	5 (19%)
1	4AC	Aa	501	1	21,24,25	3.24	9 (42%)	29,34,37	1.51	5 (17%)
1	4AC	Aa	847	1	21,24,25	3.09	10 (47%)	29,34,37	1.19	3 (10%)
27	OMC	BA	1790	27	19,22,23	2.51	7 (36%)	26,31,34	1.12	1 (3%)
27	OMG	BA	2521	27	23,26,27	2.20	6 (26%)	33,38,41	1.90	8 (24%)
27	OMC	BA	2545	27	19,22,23	2.58	7 (36%)	26,31,34	1.29	2 (7%)
27	OMG	BA	2010	27	23,26,27	2.14	7 (30%)	33,38,41	1.65	7 (21%)
1	B8T	Aa	1141	1	19,22,23	0.81	0	26,31,34	0.76	0
27	OMG	BA	674	27	23,26,27	1.94	7 (30%)	33,38,41	2.11	13 (39%)

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
27	4AC	BA	805	27	-	0/11/29/30	0/2/2/2
1	OMG	Aa	382	1	-	2/9/27/28	0/3/3/3
27	A2M	BA	879	27	-	0/9/27/28	0/3/3/3
1	LHH	Aa	1020	1	-	4/13/31/32	0/2/2/2
27	4AC	BA	1337	27	-	2/11/29/30	0/2/2/2
1	OMG	Aa	1107	1	-	3/9/27/28	0/3/3/3
1	5MC	Aa	1352	1	-	2/7/25/26	0/2/2/2
27	5MU	BA	298	27	-	0/7/25/26	0/2/2/2
27	OMG	BA	2152	27	-	2/9/27/28	0/3/3/3
27	OMG	BA	2527	27	-	2/9/27/28	0/3/3/3
27	4AC	BA	2997	27	-	0/11/29/30	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	OMG	BA	2550	27	-	2/9/27/28	0/3/3/3
1	5MC	Aa	457	1	-	2/7/25/26	0/2/2/2
1	4AC	Aa	136	1	-	2/11/29/30	0/2/2/2
27	OMG	BA	2324	27	-	0/9/27/28	0/3/3/3
27	OMG	BA	1799	27	-	3/9/27/28	0/3/3/3
1	OMG	Aa	659	1	-	0/9/27/28	0/3/3/3
1	OMG	Aa	876	1	-	2/9/27/28	0/3/3/3
1	5MU	Aa	917	1	-	2/7/25/26	0/2/2/2
27	A2M	BA	872	27	-	0/9/27/28	0/3/3/3
27	OMU	BA	2389	27	-	2/9/27/28	0/2/2/2
27	5MU	BA	2688	27	-	0/7/25/26	0/2/2/2
1	OMC	Aa	1354	1	-	2/9/27/28	0/2/2/2
27	4AC	BA	713	27	-	0/11/29/30	0/2/2/2
27	5MU	BA	2384	27	-	0/7/25/26	0/2/2/2
27	OMU	BA	1551	27	-	3/9/27/28	0/2/2/2
27	OMU	BA	657	27	-	1/9/27/28	0/2/2/2
1	OMC	Aa	1361	27,1	-	0/9/27/28	0/2/2/2
1	OMU	Aa	479	1	-	1/9/27/28	0/2/2/2
27	4AC	BA	124	27	-	0/11/29/30	0/2/2/2
27	OMG	BA	552	27	-	0/9/27/28	0/3/3/3
27	4AC	BA	1434	27	-	2/11/29/30	0/2/2/2
27	4SU	BA	2553	27	-	0/7/25/26	0/2/2/2
27	5MC	BA	2863	27	-	0/7/25/26	0/2/2/2
27	A2M	BA	488	27	-	3/9/27/28	0/3/3/3
1	LV2	Aa	918	1	-	0/9/29/30	0/2/2/2
1	OMU	Aa	52	1	-	2/9/27/28	0/2/2/2
27	OMU	BA	2542	27	-	0/9/27/28	0/2/2/2
27	4AC	BA	1955	27	-	2/11/29/30	0/2/2/2
27	4AC	BA	1375	27	-	2/11/29/30	0/2/2/2
27	4AC	BA	1431	27	-	0/11/29/30	0/2/2/2
1	4AC	Aa	605	1	-	1/11/29/30	0/2/2/2
27	A2M	BA	1517	27	-	1/9/27/28	0/3/3/3
1	4AC	Aa	525	1	-	5/11/29/30	0/2/2/2
1	5MC	Aa	854	1	-	1/7/25/26	0/2/2/2
1	OMC	Aa	752	1	-	0/9/27/28	0/2/2/2
1	OMG	Aa	771	1	-	0/9/27/28	0/3/3/3
1	OMG	Aa	498	1	-	0/9/27/28	0/3/3/3
27	4AC	BA	433	27	-	0/11/29/30	0/2/2/2
27	4AC	BA	1470	27	-	0/11/29/30	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	BA	2590	27	-	0/11/29/30	0/2/2/2
27	4AC	BA	2797	27	-	0/11/29/30	0/2/2/2
1	4AC	Aa	458	1	-	6/11/29/30	0/2/2/2
27	4AC	BA	730	27	-	0/11/29/30	0/2/2/2
27	B8T	BA	357	27	-	0/7/27/28	0/2/2/2
27	OMG	BA	2568	27	-	3/9/27/28	0/3/3/3
27	4AC	BA	2780	27	-	0/11/29/30	0/2/2/2
1	OMG	Aa	1025	1	-	1/9/27/28	0/3/3/3
27	4AC	BA	418	27	-	0/11/29/30	0/2/2/2
27	OMG	BA	2019	27	-	2/9/27/28	0/3/3/3
27	5MC	BA	2035	27	-	0/7/25/26	0/2/2/2
27	4AC	BA	2992	27	-	3/11/29/30	0/2/2/2
27	OMG	BA	2353	27	-	2/9/27/28	0/3/3/3
27	OMU	BA	619	27	-	1/9/27/28	0/2/2/2
27	OMG	BA	2016	27	-	0/9/27/28	0/3/3/3
1	LHH	Aa	229	1	-	3/13/31/32	0/2/2/2
27	OMU	BA	1776	27	-	0/9/27/28	0/2/2/2
27	4AC	BA	201	27	-	2/11/29/30	0/2/2/2
27	5MU	BA	1905	27	-	0/7/25/26	0/2/2/2
1	4AC	Aa	1217	1	-	4/11/29/30	0/2/2/2
27	4AC	BA	925	27	-	2/11/29/30	0/2/2/2
27	LHH	BA	2457	27	-	4/13/31/32	0/2/2/2
27	5MC	BA	2055	27	-	2/7/25/26	0/2/2/2
1	OMG	Aa	446	1	-	2/9/27/28	0/3/3/3
1	OMC	Aa	190	1	-	2/9/27/28	0/2/2/2
27	OMG	BA	2379	27	-	3/9/27/28	0/3/3/3
27	OMG	BA	1106	27	-	0/9/27/28	0/3/3/3
27	OMG	BA	912	27	-	0/9/27/28	0/3/3/3
27	4AC	BA	2121	27	-	0/11/29/30	0/2/2/2
1	4AC	Aa	298	1	-	0/11/29/30	0/2/2/2
27	A2M	BA	849	27	-	2/9/27/28	0/3/3/3
27	OMC	BA	869	27	-	2/9/27/28	0/2/2/2
27	OMC	BA	1750	27	-	0/9/27/28	0/2/2/2
27	OMC	BA	718	27	-	0/9/27/28	0/2/2/2
1	OMU	Aa	8	1	-	3/9/27/28	0/2/2/2
27	LHH	BA	617	27	-	5/13/31/32	0/2/2/2
27	4AC	BA	799	27	-	0/11/29/30	0/2/2/2
27	OMG	BA	1398	27	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	OMG	BA	2168	27	-	0/9/27/28	0/3/3/3
27	OMG	BA	1558	27	-	0/9/27/28	0/3/3/3
1	B8T	Aa	1051	1	-	0/7/27/28	0/2/2/2
27	OMG	BA	64	27	-	2/9/27/28	0/3/3/3
27	5MU	BA	1548	27	-	2/7/25/26	0/2/2/2
27	OMG	BA	353	27	-	2/9/27/28	0/3/3/3
27	A2M	BA	2702	27	-	1/9/27/28	0/3/3/3
1	OMG	Aa	636	1	-	2/9/27/28	0/3/3/3
1	OMC	Aa	535	1	-	0/9/27/28	0/2/2/2
27	OMC	BA	250	27	-	0/9/27/28	0/2/2/2
27	5MC	BA	1965	27	-	0/7/25/26	0/2/2/2
1	OMG	Aa	1026	1	-	1/9/27/28	0/3/3/3
27	OMG	BA	800	27	-	0/9/27/28	0/3/3/3
27	OMG	BA	365	27	-	1/9/27/28	0/3/3/3
1	4AC	Aa	682	1	-	0/11/29/30	0/2/2/2
1	B8T	Aa	1262	1	-	0/7/27/28	0/2/2/2
27	OMC	BA	754	27	-	2/9/27/28	0/2/2/2
27	OMG	BA	63	27	-	0/9/27/28	0/3/3/3
27	5MU	BA	537	27	-	0/7/25/26	0/2/2/2
27	A2M	BA	1265	27	-	2/9/27/28	0/3/3/3
1	6MZ	Aa	1449	1	-	0/9/27/28	0/3/3/3
27	5MU	BA	1085	27	-	0/7/25/26	0/2/2/2
27	OMC	BA	561	27	-	0/9/27/28	0/2/2/2
27	5MU	BA	875	27	-	2/7/25/26	0/2/2/2
27	4AC	BA	56	27	-	0/11/29/30	0/2/2/2
27	OMG	BA	2745	27	-	0/9/27/28	0/3/3/3
27	4AC	BA	1357	27	-	0/11/29/30	0/2/2/2
27	OMC	BA	2018	27	-	2/9/27/28	0/2/2/2
27	OMC	BA	2047	27	-	0/9/27/28	0/2/2/2
27	5MC	BA	2605	27	-	0/7/25/26	0/2/2/2
27	LHH	BA	2955	27	-	3/13/31/32	0/2/2/2
1	OMG	Aa	320	1	-	0/9/27/28	0/3/3/3
1	OMC	Aa	825	1	-	0/9/27/28	0/2/2/2
27	OMG	BA	2728	27	-	0/9/27/28	0/3/3/3
1	OMG	Aa	246	1	-	0/9/27/28	0/3/3/3
27	OMU	BA	768	27	-	0/9/27/28	0/2/2/2
1	OMG	Aa	138	1	-	0/9/27/28	0/3/3/3
27	A2M	BA	1400	27	-	1/9/27/28	0/3/3/3
27	5MC	BA	2070	27	-	0/7/25/26	0/2/2/2
27	4AC	BA	1810	27	-	2/11/29/30	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	BA	335	27	-	0/11/29/30	0/2/2/2
27	OMU	BA	453	27	-	2/9/27/28	0/2/2/2
27	4AC	BA	501	27	-	0/11/29/30	0/2/2/2
1	4AC	Aa	818	1	-	2/11/29/30	0/2/2/2
27	4AC	BA	376	27	-	0/11/29/30	0/2/2/2
27	4AC	BA	778	27	-	0/11/29/30	0/2/2/2
27	4AC	BA	1543	27	-	3/11/29/30	0/2/2/2
1	5MC	Aa	1004	1	-	2/7/25/26	0/2/2/2
1	OMG	Aa	1265	1	-	0/9/27/28	0/3/3/3
27	OMG	BA	215	27	-	2/9/27/28	0/3/3/3
27	OMG	BA	723	27	-	1/9/27/28	0/3/3/3
1	OMG	Aa	994	1	-	1/9/27/28	0/3/3/3
27	4AC	BA	244	27	-	1/11/29/30	0/2/2/2
1	OMG	Aa	532	1	-	2/9/27/28	0/3/3/3
27	4AC	BA	2838	27	-	2/11/29/30	0/2/2/2
1	OMG	Aa	450	1	-	0/9/27/28	0/3/3/3
27	OMU	BA	2610	27	-	3/9/27/28	0/2/2/2
27	A2M	BA	212	27	-	1/9/27/28	0/3/3/3
1	4AC	Aa	41	1	-	2/11/29/30	0/2/2/2
1	4AC	Aa	373	1	-	0/11/29/30	0/2/2/2
1	OMU	Aa	240	1	-	0/9/27/28	0/2/2/2
27	OMU	BA	34	27	-	1/9/27/28	0/2/2/2
1	5MC	Aa	1478	1	-	3/7/25/26	0/2/2/2
27	OMU	BA	1969	27	-	0/9/27/28	0/2/2/2
27	A2M	BA	505	27	-	2/9/27/28	0/3/3/3
1	MA6	Aa	1468	1	-	2/11/29/30	0/3/3/3
27	OMG	BA	1892	27	-	1/9/27/28	0/3/3/3
27	OMG	BA	1953	27	-	2/9/27/28	0/3/3/3
27	OMC	BA	2124	27	-	0/9/27/28	0/2/2/2
27	5MC	BA	944	27	-	0/7/25/26	0/2/2/2
1	OMG	Aa	852	1	-	0/9/27/28	0/3/3/3
27	4AC	BA	1427	27	-	0/11/29/30	0/2/2/2
27	4AC	BA	3009	27	-	2/11/29/30	0/2/2/2
27	OMU	BA	1319	27	-	0/9/27/28	0/2/2/2
27	OMU	BA	1340	27	-	0/9/27/28	0/2/2/2
1	A2M	Aa	352	1	-	1/9/27/28	0/3/3/3
1	OMG	Aa	892	1	-	3/9/27/28	0/3/3/3
1	4AC	Aa	697	1	-	4/11/29/30	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	A2M	BA	756	27	-	0/9/27/28	0/3/3/3
27	OMG	BA	2657	27	-	0/9/27/28	0/3/3/3
27	4AC	BA	2159	27	-	0/11/29/30	0/2/2/2
27	OMG	BA	290	27	-	0/9/27/28	0/3/3/3
1	4AC	Aa	358	1	-	2/11/29/30	0/2/2/2
1	5MC	Aa	942	1	-	0/7/25/26	0/2/2/2
1	5MC	Aa	1276	1	-	2/7/25/26	0/2/2/2
27	5MC	BA	2075	27	-	0/7/25/26	0/2/2/2
27	OMG	BA	2528	27	-	0/9/27/28	0/3/3/3
27	OMC	BA	2595	27	-	2/9/27/28	0/2/2/2
27	4AC	BA	1305	27	-	2/11/29/30	0/2/2/2
27	A2M	BA	932	27	-	0/9/27/28	0/3/3/3
27	5MU	BA	572	27	-	0/7/25/26	0/2/2/2
27	OMG	BA	763	27	-	0/9/27/28	0/3/3/3
27	LHH	BA	526	27	-	1/13/31/32	0/2/2/2
27	OMG	BA	833	27	-	0/9/27/28	0/3/3/3
27	4AC	BA	1934	27	-	0/11/29/30	0/2/2/2
27	OMG	BA	2672	27	-	0/9/27/28	0/3/3/3
1	5MC	Aa	464	1	-	0/7/25/26	0/2/2/2
27	OMG	BA	575	27	-	2/9/27/28	0/3/3/3
1	4AC	Aa	569	1	-	0/11/29/30	0/2/2/2
27	4AC	BA	2832	27	-	1/11/29/30	0/2/2/2
1	4AC	Aa	827	1	-	0/11/29/30	0/2/2/2
1	MA6	Aa	1467	1	-	0/11/29/30	0/3/3/3
27	OMG	BA	1525	27	-	2/9/27/28	0/3/3/3
27	OMC	BA	2571	27	-	2/9/27/28	0/2/2/2
27	OMU	BA	2656	27	-	0/9/27/28	0/2/2/2
1	4AC	Aa	730	1	-	2/11/29/30	0/2/2/2
1	OMG	Aa	1434	1	-	1/9/27/28	0/3/3/3
1	OMG	Aa	381	1	-	0/9/27/28	0/3/3/3
1	OMC	Aa	296	1	-	0/9/27/28	0/2/2/2
1	5MC	Aa	1476	1	-	0/7/25/26	0/2/2/2
27	OMG	BA	1940	27	-	2/9/27/28	0/3/3/3
1	4AC	Aa	5	1	-	4/11/29/30	0/2/2/2
27	5MC	BA	1696	27	-	0/7/25/26	0/2/2/2
27	OMC	BA	2630	27	-	0/9/27/28	0/2/2/2
1	5MC	Aa	672	1	-	0/7/25/26	0/2/2/2
27	OMU	BA	1480	27	-	2/9/27/28	0/2/2/2
1	4AC	Aa	1459	1	-	0/11/29/30	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	Aa	1007	1	-	2/11/29/30	0/2/2/2
27	4AC	BA	3023	27	-	2/11/29/30	0/2/2/2
27	A2M	BA	825	27	-	0/9/27/28	0/3/3/3
27	4AC	BA	1396	27	-	2/11/29/30	0/2/2/2
27	OMG	BA	419	27	-	2/9/27/28	0/3/3/3
27	4AC	BA	1899	27	-	0/11/29/30	0/2/2/2
1	OMU	Aa	304	1	-	1/9/27/28	0/2/2/2
1	2MG	Aa	670	1	-	0/9/27/28	0/3/3/3
1	OMG	Aa	1275	1	-	1/9/27/28	0/3/3/3
27	4AC	BA	27	27	-	2/11/29/30	0/2/2/2
27	4AC	BA	858	27	-	2/11/29/30	0/2/2/2
1	OMG	Aa	913	1	-	2/9/27/28	0/3/3/3
27	4SU	BA	2581	27	-	2/7/25/26	0/2/2/2
27	4AC	BA	1641	27	-	2/11/29/30	0/2/2/2
1	OMU	Aa	1358	1	-	3/9/27/28	0/2/2/2
27	OMC	BA	1820	27	-	0/9/27/28	0/2/2/2
1	4AC	Aa	501	1	-	0/11/29/30	0/2/2/2
1	4AC	Aa	847	1	-	0/11/29/30	0/2/2/2
27	OMC	BA	1790	27	-	2/9/27/28	0/2/2/2
27	OMG	BA	2521	27	-	0/9/27/28	0/3/3/3
27	OMC	BA	2545	27	-	1/9/27/28	0/2/2/2
27	OMG	BA	2010	27	-	0/9/27/28	0/3/3/3
1	B8T	Aa	1141	1	-	0/7/27/28	0/2/2/2
27	OMG	BA	674	27	-	0/9/27/28	0/3/3/3

The worst 5 of 1745 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Aa	1476	5MC	C2'-C3'	-10.81	1.23	1.53
1	Aa	1276	5MC	C2'-C3'	-10.79	1.23	1.53
27	BA	1548	5MU	C2-N1	10.67	1.55	1.38
27	BA	298	5MU	C2-N1	10.58	1.55	1.38
27	BA	1548	5MU	C6-N1	10.54	1.56	1.38

The worst 5 of 1309 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	1468	MA6	N1-C6-N6	-12.63	103.27	117.08
27	BA	1905	5MU	C5-C4-N3	12.43	125.92	115.31
27	BA	537	5MU	C5-C4-N3	12.41	125.90	115.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	1548	5MU	C5-C4-N3	12.23	125.75	115.31
27	BA	572	5MU	C5-C4-N3	12.21	125.73	115.31

There are no chirality outliers.

5 of 235 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Aa	52	OMU	C3'-C4'-C5'-O5'
1	Aa	52	OMU	O4'-C4'-C5'-O5'
1	Aa	352	A2M	C1'-C2'-O2'-CM'
1	Aa	382	OMG	O4'-C4'-C5'-O5'
1	Aa	446	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

109 monomers are involved in 173 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	BA	805	4AC	3	0
27	BA	879	A2M	2	0
27	BA	1337	4AC	1	0
27	BA	2527	OMG	1	0
27	BA	2997	4AC	1	0
1	Aa	136	4AC	1	0
27	BA	1799	OMG	1	0
1	Aa	917	5MU	1	0
27	BA	713	4AC	1	0
27	BA	657	OMU	1	0
27	BA	124	4AC	2	0
27	BA	552	OMG	1	0
27	BA	1434	4AC	5	0
27	BA	488	A2M	3	0
27	BA	1955	4AC	1	0
27	BA	1375	4AC	2	0
27	BA	1431	4AC	1	0
1	Aa	605	4AC	1	0
1	Aa	525	4AC	3	0
27	BA	433	4AC	1	0
27	BA	1470	4AC	2	0
27	BA	2590	4AC	1	0
27	BA	2797	4AC	1	0
1	Aa	458	4AC	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	BA	730	4AC	2	0
27	BA	2568	OMG	1	0
27	BA	2780	4AC	1	0
1	Aa	1025	OMG	1	0
27	BA	418	4AC	1	0
27	BA	2992	4AC	3	0
27	BA	2353	OMG	1	0
27	BA	619	OMU	1	0
27	BA	2016	OMG	1	0
27	BA	1776	OMU	1	0
27	BA	201	4AC	3	0
1	Aa	1217	4AC	4	0
27	BA	925	4AC	5	0
1	Aa	190	OMC	2	0
27	BA	2379	OMG	1	0
27	BA	912	OMG	2	0
27	BA	2121	4AC	1	0
1	Aa	298	4AC	1	0
27	BA	1750	OMC	1	0
1	Aa	8	OMU	1	0
27	BA	799	4AC	1	0
27	BA	64	OMG	2	0
27	BA	353	OMG	1	0
27	BA	250	OMC	2	0
27	BA	365	OMG	1	0
1	Aa	682	4AC	2	0
27	BA	1265	A2M	3	0
27	BA	56	4AC	2	0
27	BA	1357	4AC	2	0
27	BA	2605	5MC	2	0
27	BA	1400	A2M	1	0
27	BA	1810	4AC	2	0
27	BA	335	4AC	1	0
27	BA	501	4AC	1	0
1	Aa	818	4AC	2	0
27	BA	376	4AC	1	0
27	BA	778	4AC	1	0
27	BA	1543	4AC	1	0
1	Aa	1265	OMG	1	0
27	BA	723	OMG	2	0
27	BA	244	4AC	1	0
27	BA	2838	4AC	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	BA	2610	OMU	1	0
27	BA	212	A2M	2	0
1	Aa	41	4AC	1	0
1	Aa	373	4AC	1	0
1	Aa	240	OMU	1	0
27	BA	34	OMU	1	0
27	BA	505	A2M	2	0
1	Aa	1468	MA6	1	0
27	BA	2124	OMC	2	0
27	BA	1427	4AC	1	0
27	BA	3009	4AC	1	0
1	Aa	352	A2M	1	0
1	Aa	697	4AC	3	0
27	BA	756	A2M	1	0
27	BA	2159	4AC	1	0
1	Aa	358	4AC	1	0
1	Aa	1276	5MC	2	0
27	BA	1305	4AC	4	0
27	BA	572	5MU	1	0
27	BA	526	LHH	1	0
27	BA	1934	4AC	1	0
1	Aa	464	5MC	2	0
1	Aa	569	4AC	1	0
27	BA	2832	4AC	1	0
1	Aa	827	4AC	1	0
27	BA	2571	OMC	2	0
1	Aa	730	4AC	3	0
1	Aa	5	4AC	1	0
27	BA	1696	5MC	1	0
27	BA	1480	OMU	3	0
1	Aa	1459	4AC	5	0
1	Aa	1007	4AC	1	0
27	BA	3023	4AC	4	0
27	BA	825	A2M	1	0
27	BA	1396	4AC	1	0
27	BA	1899	4AC	1	0
1	Aa	1275	OMG	2	0
27	BA	27	4AC	1	0
27	BA	858	4AC	2	0
27	BA	1641	4AC	1	0
1	Aa	1358	OMU	1	0
1	Aa	501	4AC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	Aa	847	4AC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

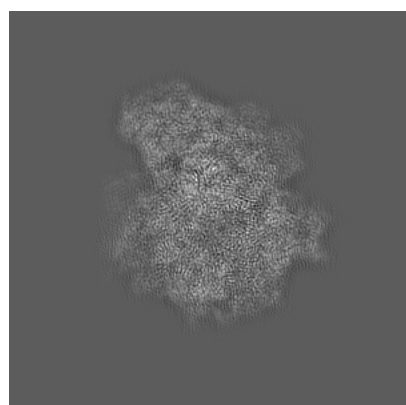
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10223. These allow visual inspection of the internal detail of the map and identification of artifacts.

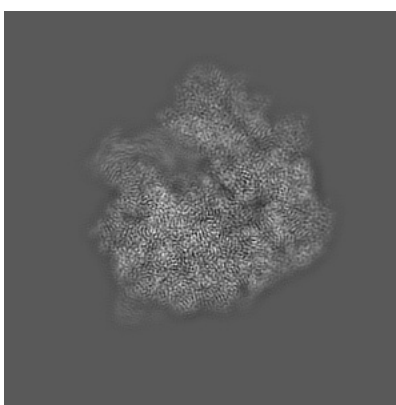
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

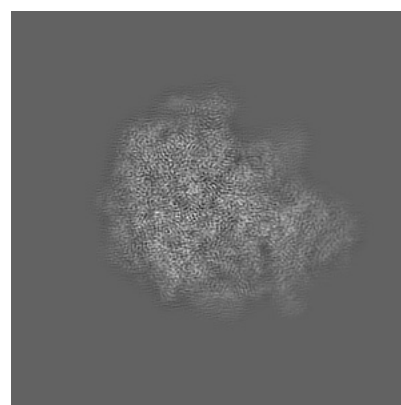
6.1.1 Primary map



X



Y

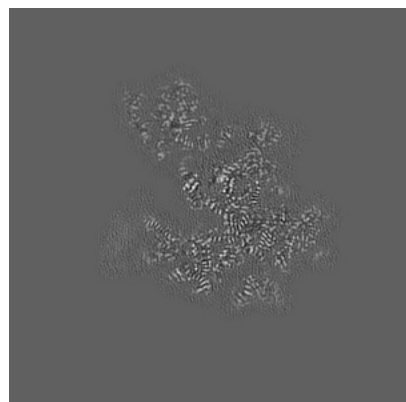


Z

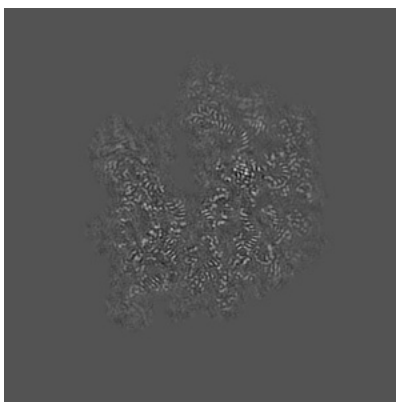
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

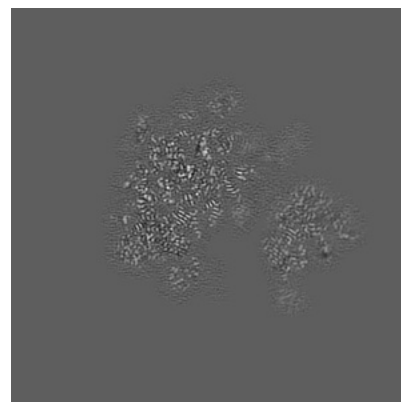
6.2.1 Primary map



X Index: 240



Y Index: 240

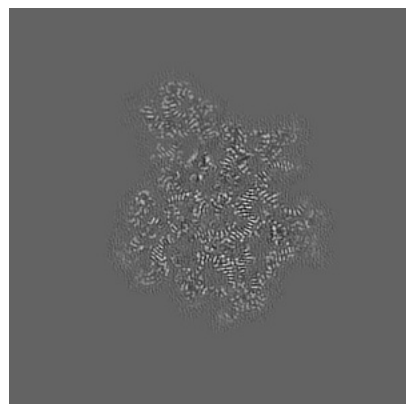


Z Index: 240

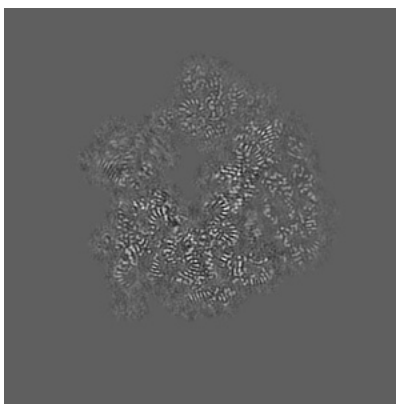
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

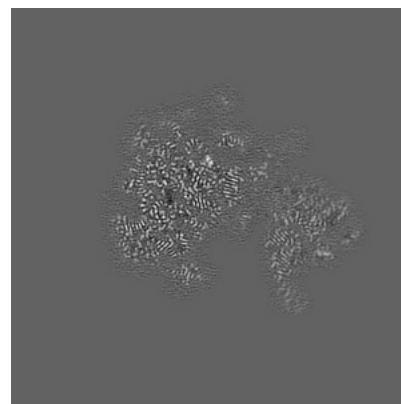
6.3.1 Primary map



X Index: 213



Y Index: 224

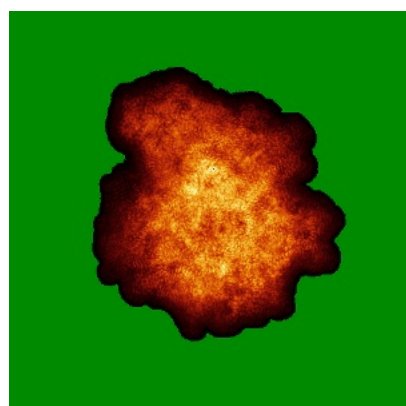


Z Index: 247

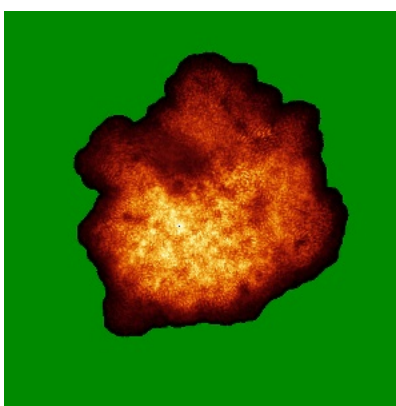
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

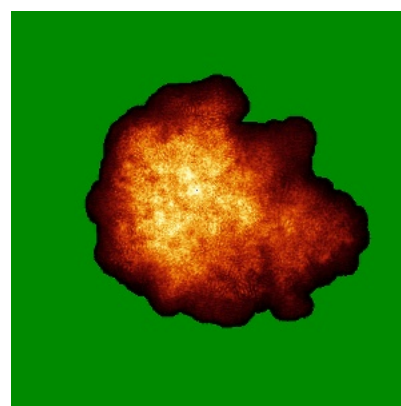
6.4.1 Primary map



X



Y

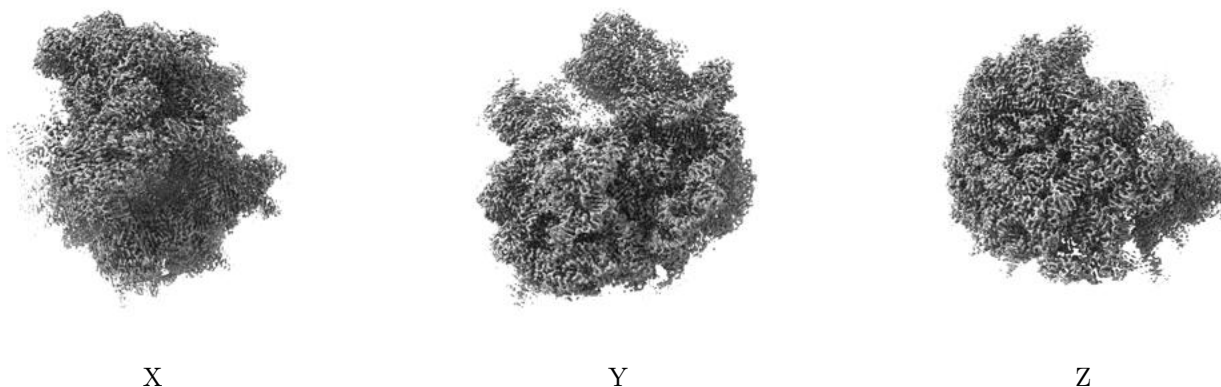


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

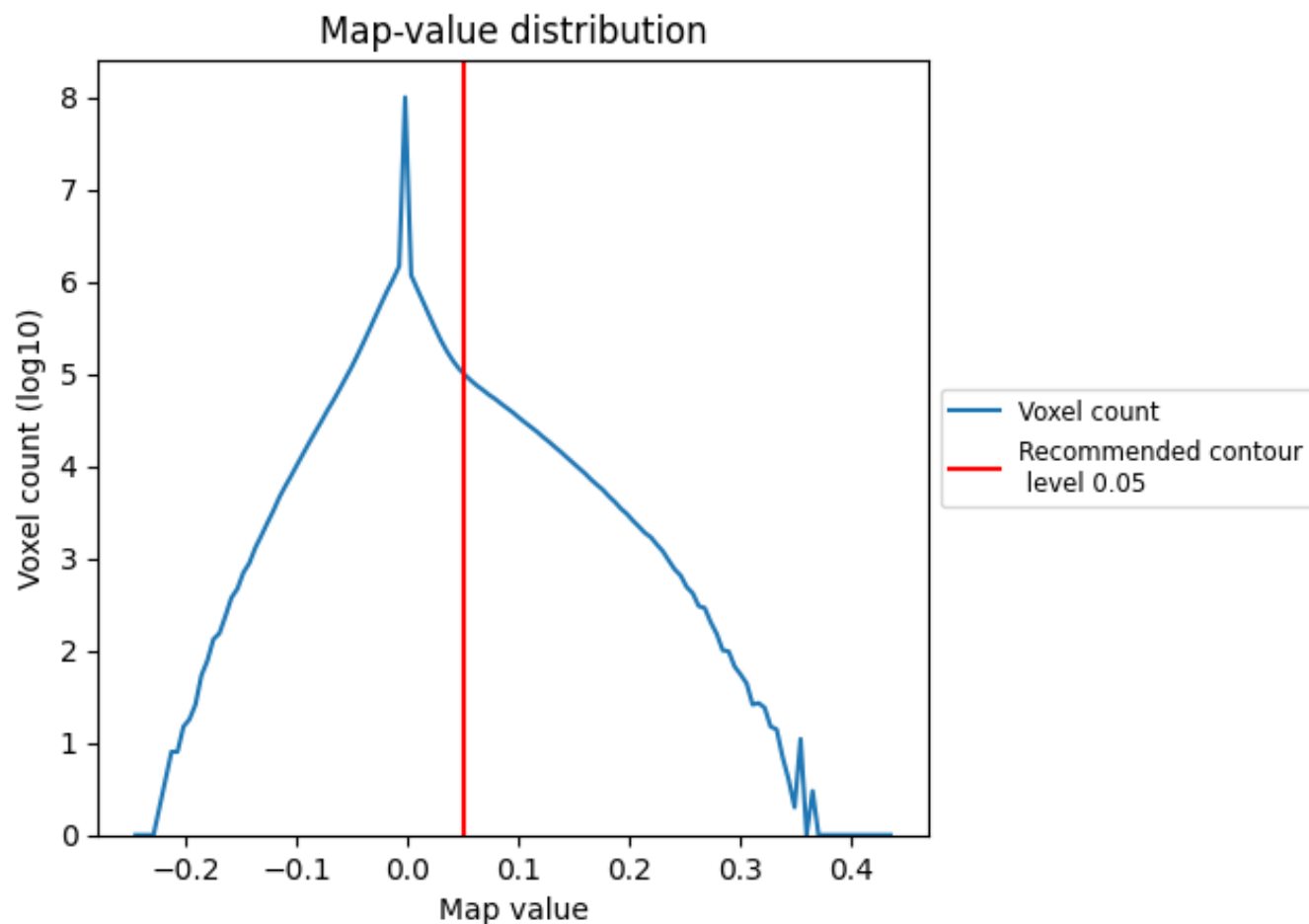
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

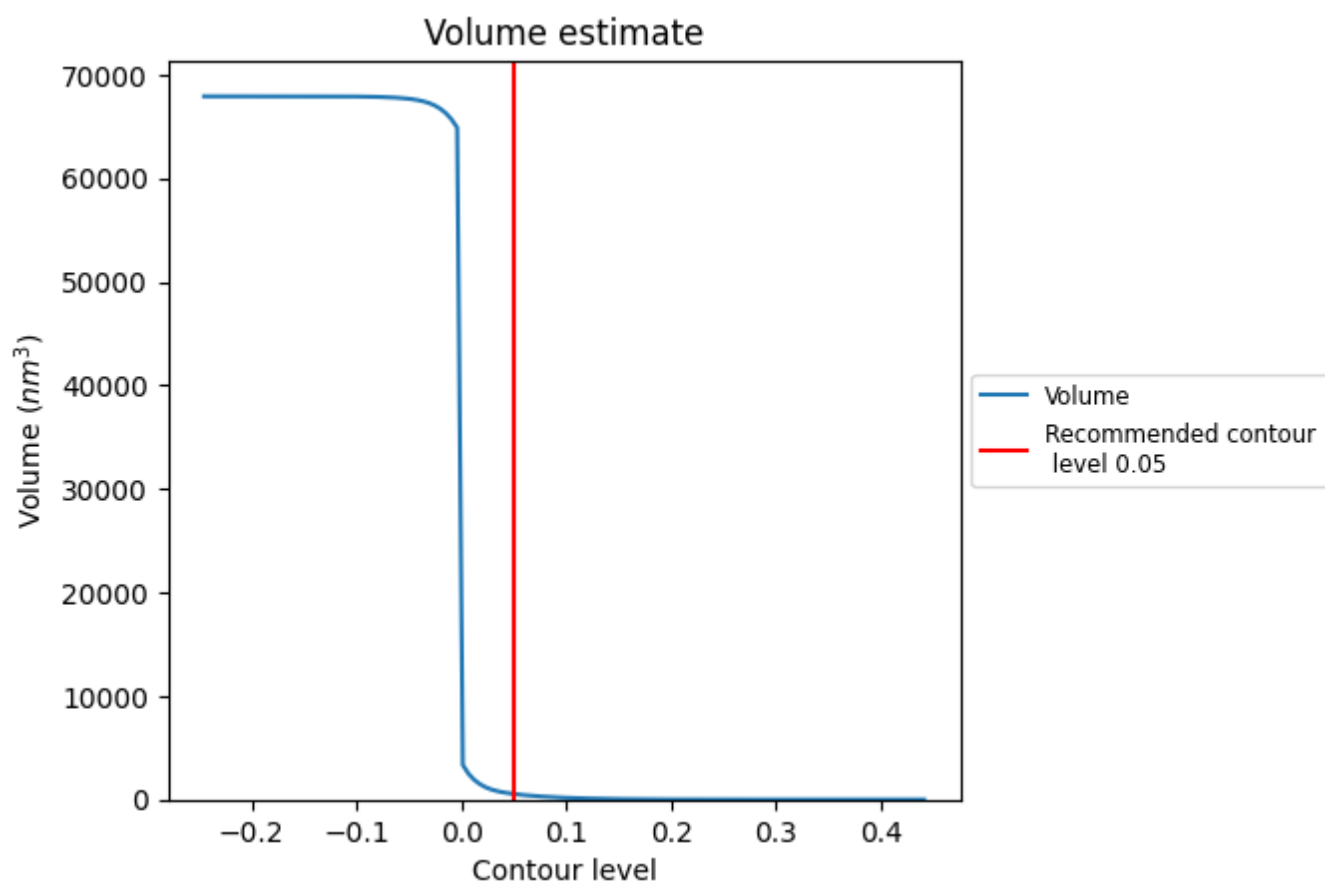
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

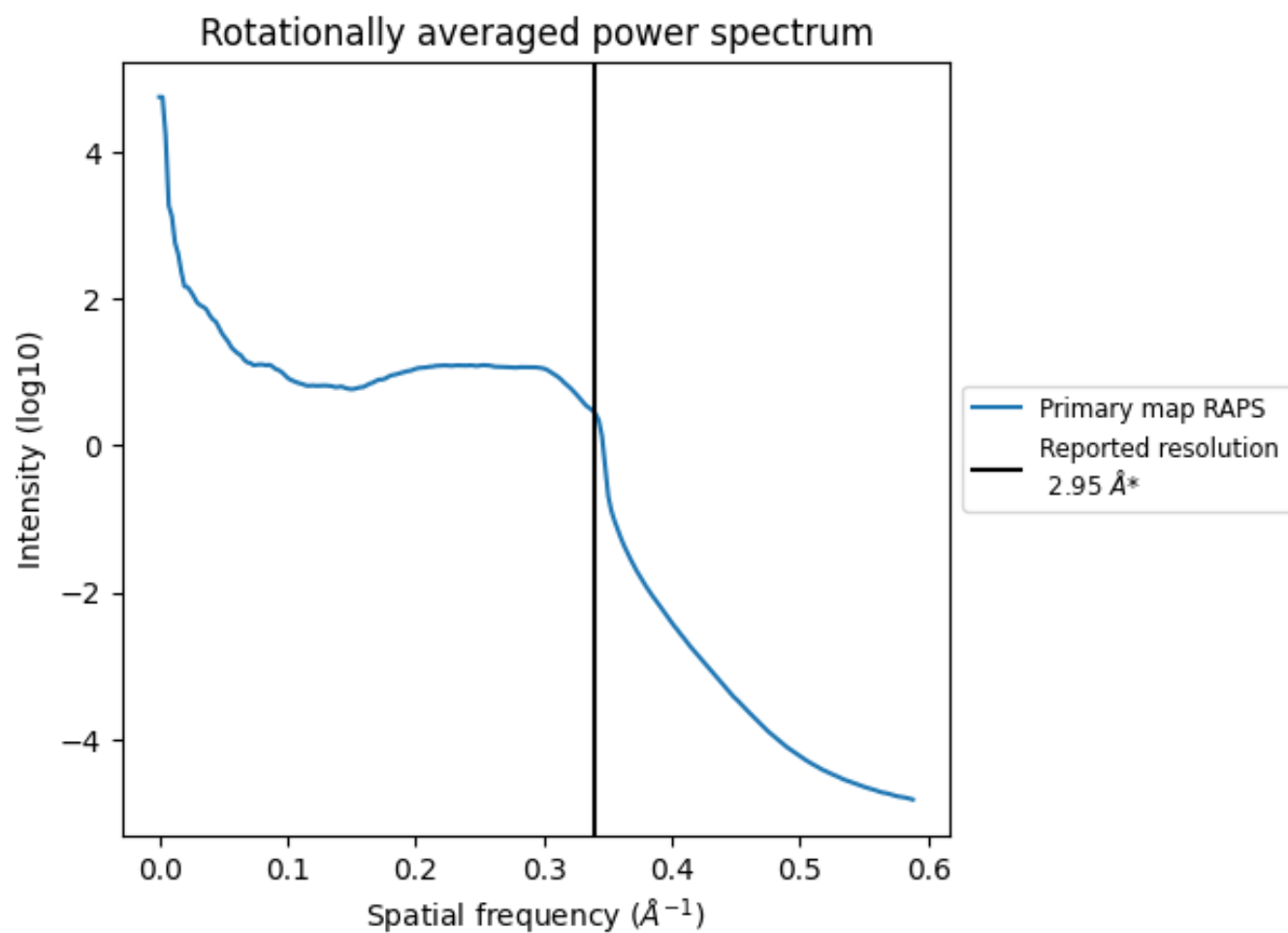
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 541 nm³; this corresponds to an approximate mass of 488 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 0.339 Å⁻¹

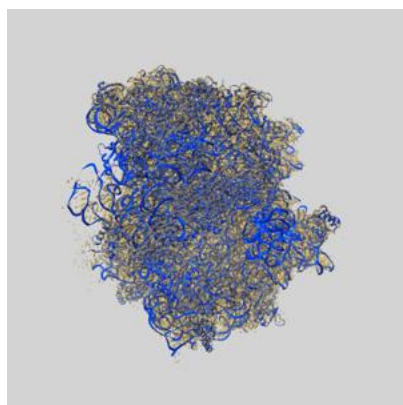
8 Fourier-Shell correlation

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

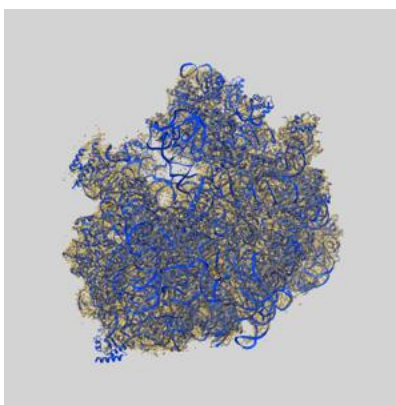
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10223 and PDB model 6SKF. Per-residue inclusion information can be found in section [3](#) on page [19](#).

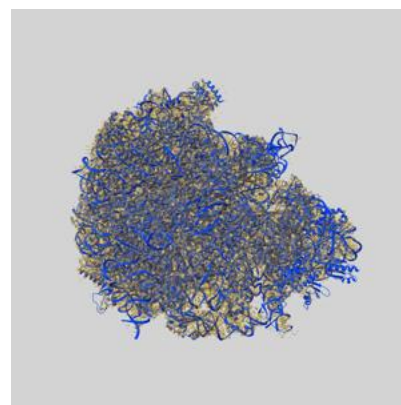
9.1 Map-model overlay [i](#)



X



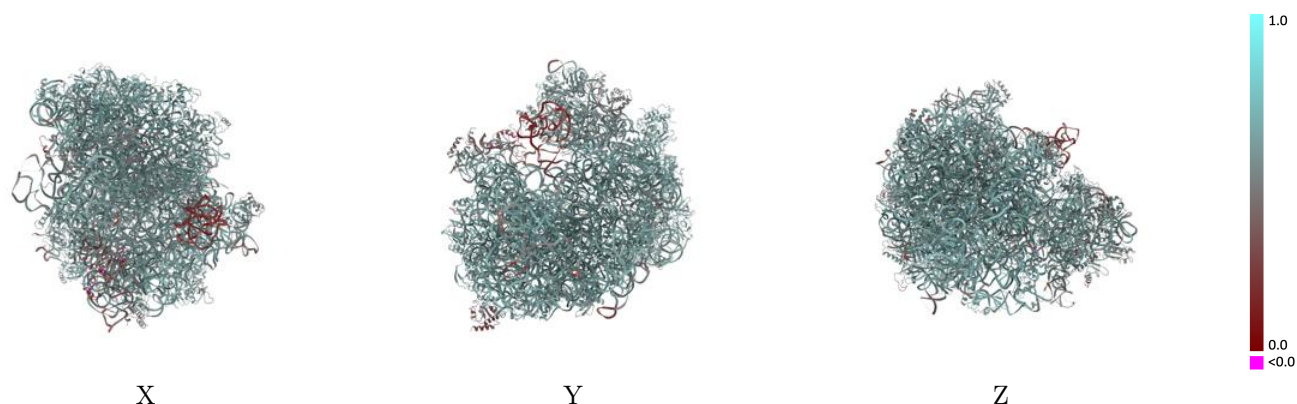
Y



Z

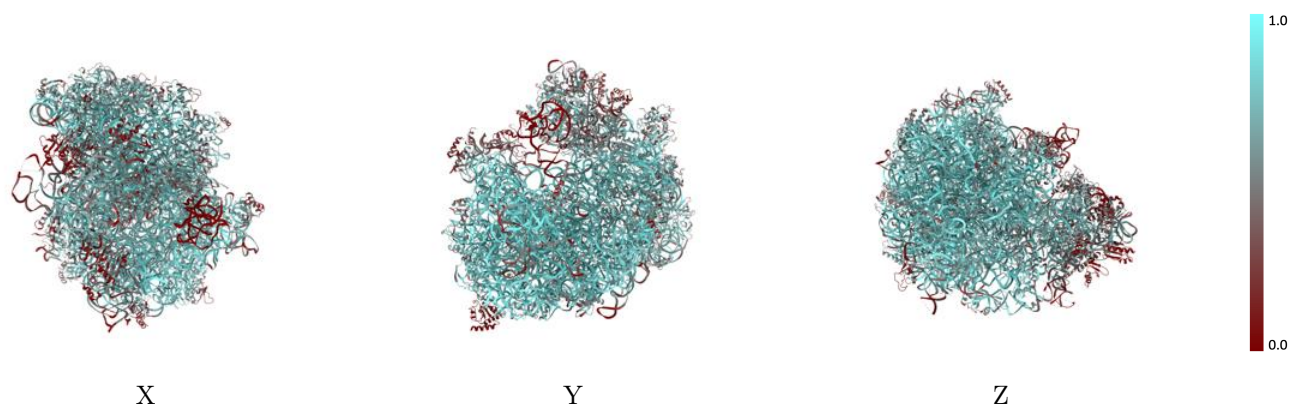
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



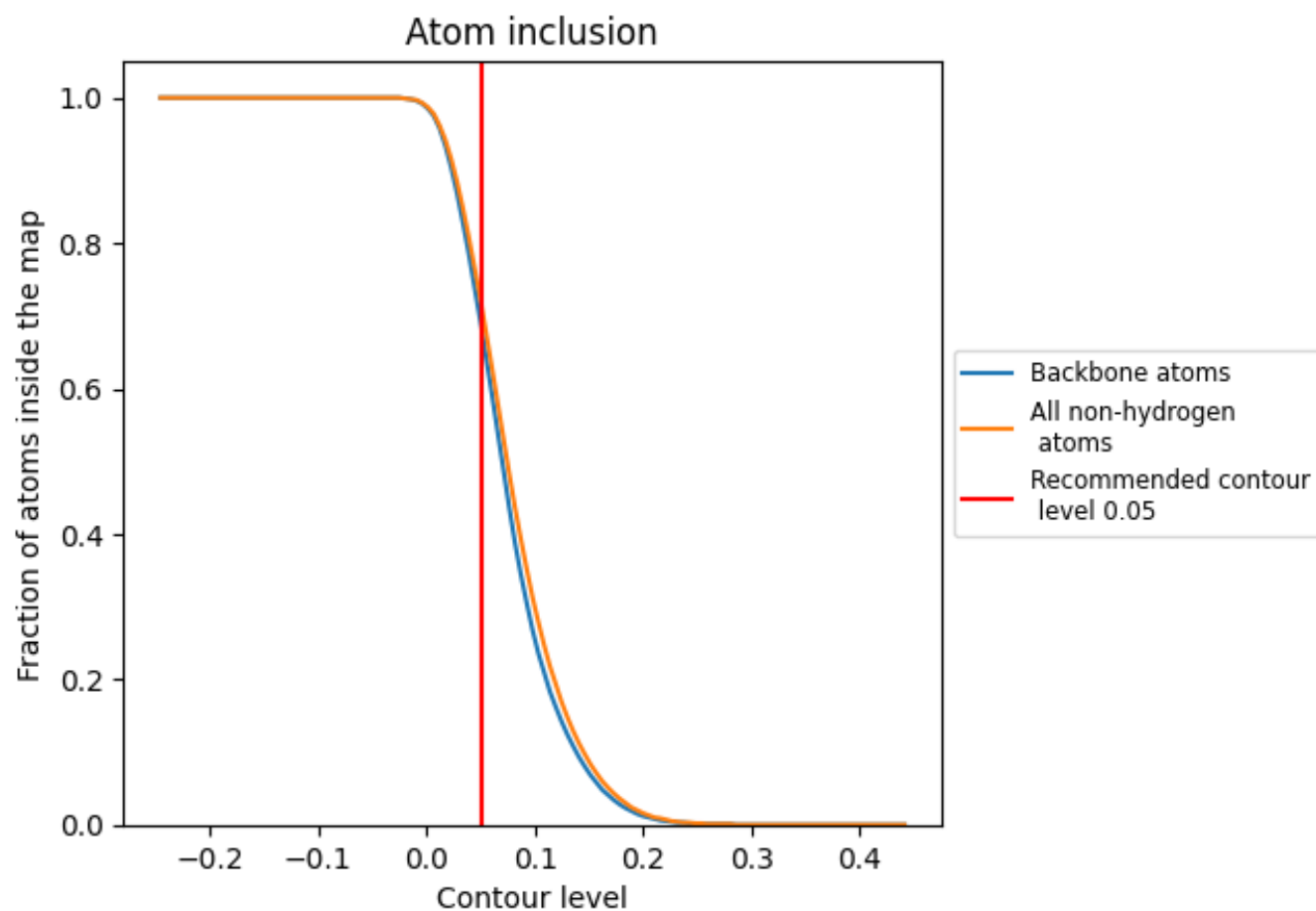
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 72% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7220	 0.5970
Aa	 0.7520	 0.6120
Ab	 0.5250	 0.5890
Ac	 0.2440	 0.5210
Ad	 0.5150	 0.5720
Ae	 0.6270	 0.5960
Af	 0.6610	 0.6140
Ag	 0.6510	 0.6090
Ah	 0.3630	 0.5600
Ai	 0.4980	 0.5560
Aj	 0.6690	 0.6090
Ak	 0.6120	 0.5980
Al	 0.4230	 0.5680
Am	 0.2060	 0.5180
An	 0.5510	 0.5760
Ao	 0.5930	 0.6110
Ap	 0.5280	 0.5540
Aq	 0.6230	 0.5870
Ar	 0.4590	 0.5780
As	 0.6270	 0.6170
At	 0.1600	 0.4910
Au	 0.4610	 0.5730
Av	 0.5550	 0.5690
Aw	 0.5730	 0.5920
Ax	 0.5000	 0.5810
Ay	 0.4370	 0.5440
Az	 0.5820	 0.6170
BA	 0.8210	 0.6050
BB	 0.6120	 0.5320
BC	 0.7770	 0.6200
BD	 0.7810	 0.6230
BE	 0.7630	 0.6170
BF	 0.1560	 0.3000
BG	 0.6630	 0.5920
BH	 0.5050	 0.5590



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BI	 0.0620	 0.3640
BJ	 0.7310	 0.6020
BK	 0.7460	 0.6140
BL	 0.7410	 0.6150
BM	 0.5940	 0.5770
BN	 0.5420	 0.5580
BO	 0.6000	 0.5700
BP	 0.8300	 0.6350
BQ	 0.4810	 0.5340
BR	 0.7480	 0.6110
BS	 0.7240	 0.5990
BT	 0.6150	 0.5890
BU	 0.8010	 0.6300
BV	 0.7830	 0.6250
BW	 0.6840	 0.5900
BX	 0.7410	 0.6110
BY	 0.8090	 0.6270
BZ	 0.5620	 0.5550
Ba	 0.7610	 0.6100
Bb	 0.6200	 0.5610
Bc	 0.7110	 0.5980
Bd	 0.7670	 0.6230
Be	 0.7390	 0.6080
Bg	 0.7510	 0.6160
Bh	 0.8750	 0.6460
Bi	 0.7910	 0.6290
Bj	 0.7470	 0.6170
Bk	 0.8900	 0.6250
Bl	 0.7300	 0.6170