



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2023 – 02:18 PM EST

PDB ID : 7UQB
EMDB ID : EMD-26686
Title : Nucleoplasmic pre-60S intermediate of the Nog2 containing pre-rotation state from a SPB1-D52A strain with AIF4
Authors : Sekulski, K.; Cruz, V.E.; Weirich, C.S.; Erzberger, J.P.
Deposited on : 2022-04-19
Resolution : 2.43 Å (reported)
Based on initial model : 3JCT

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:

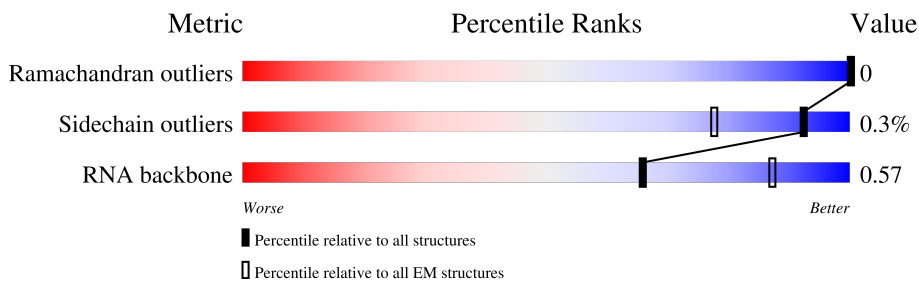
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

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 2.43 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.



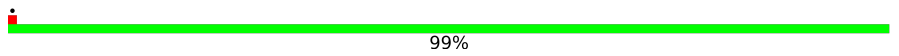
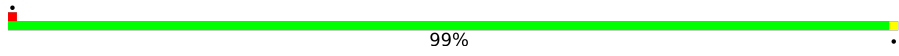
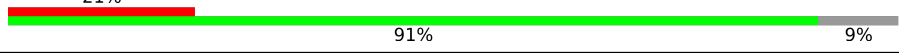
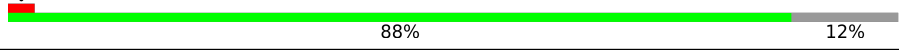
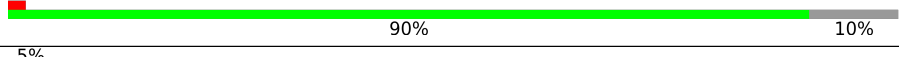

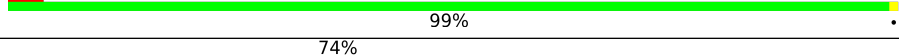

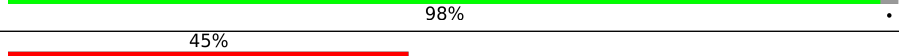
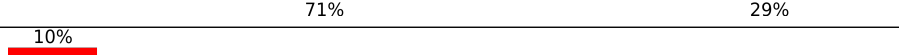
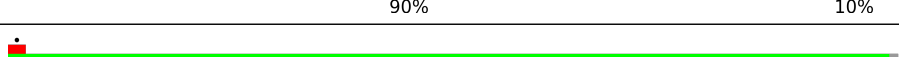
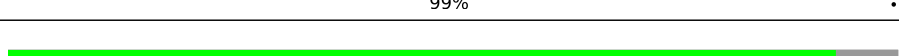
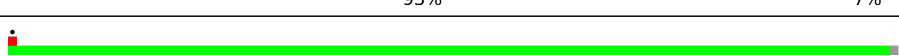
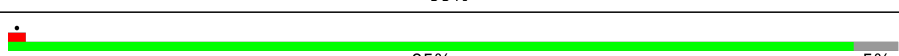
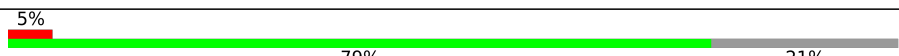
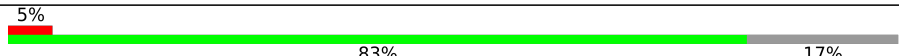
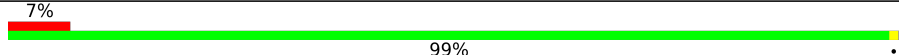


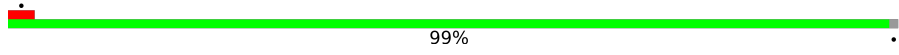
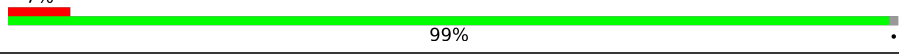
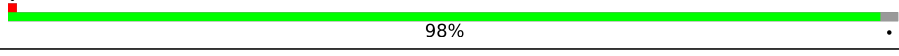
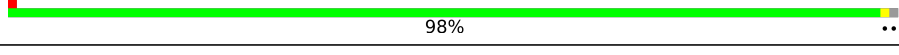
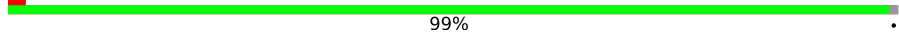

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. 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	A	254	 7% 84% 16%
2	1	3396	 7% 71% 16% 12%
3	2	158	 21% 82% 18%
4	3	121	 47% 79% 21%
5	5	120	 61% 39%
6	6	74	 19% 51% 26% 22%
7	8	165	 53% 96%
8	9	175	 11% 67% 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	B	387	 99%
10	C	362	 99%
11	D	297	 21% 91% 9%
12	E	176	 88% 12%
13	F	244	 90% 10%
14	G	256	 5% 88% 12%
15	H	191	 99%
16	I	166	 74% 79% 21%
17	J	174	 68% 98%
18	K	376	 45% 71% 29%
19	L	199	 10% 90% 10%
20	M	138	 99%
21	N	204	 93% 7%
22	O	199	 99%
23	P	184	 95% 5%
24	Q	186	 5% 79% 21%
25	R	189	 5% 83% 17%
26	S	172	 7% 99%
27	T	160	 12% 71% 29%
28	U	121	 88% 12%
29	V	137	 99%
30	W	236	 7% 99%
31	X	142	 98%
32	Y	127	 98%
33	Z	136	 99%

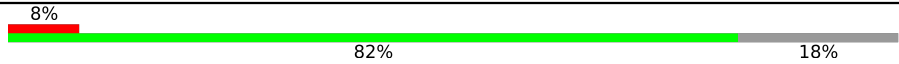
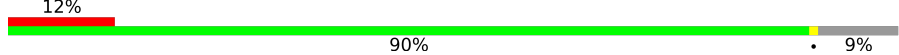
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	a	149	7% 62% 38%
35	b	647	9% 99%
36	c	105	6% 92% 8%
37	d	113	7% 95% 5%
38	e	130	97% ..
39	f	107	99%
40	g	121	7% 93% 7%
41	h	120	99%
42	i	100	8% 99%
43	j	88	95% 5%
44	k	78	12% 99%
45	l	51	98%
46	m	486	7% 95%
47	n	605	7% 61% 39%
48	o	220	23% 60% 40%
49	p	92	98% ..
50	q	455	8% 34% 66%
51	r	261	88% 12%
52	s	77	22% 94% 6%
53	t	322	25% 89% 11%
54	u	199	75% 25%
55	v	344	7% 85% 15%
56	w	201	17% 96% ..
57	x	514	19% 97% ..
58	y	245	7% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	z	106	
60	4	593	

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 157949 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 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	213	1634	1023	326	284	1	0	0

- Molecule 2 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1	2991	64042	28618	11563	20870	2991	0	0

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	2	158	3353	1500	586	1109	158	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	3	121	2579	1152	461	845	121	0	0

- Molecule 5 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	73	645	395	133	114	3	0	0

- Molecule 6 is a RNA chain called ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	6	58	1227	550	210	409	58	0	0

- Molecule 7 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	8	158	1196	750	216	228	2	0	0

- Molecule 8 is a protein called Ribosome biogenesis protein ALB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	9	118	937	590	181	166	0	0

- Molecule 9 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B	386	3081	1956	584	533	8	0	0

- Molecule 10 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	361	2749	1730	522	494	3	0	0

- Molecule 11 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	D	270	2180	1379	382	417	2	0	0

- Molecule 12 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	E	155	1230	795	221	213	1	0	0

- Molecule 13 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	F	219	1761	1138	320	302	1	0	0

- Molecule 14 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	224	Total	C	N	O	S	0	0
			1753	1122	314	314	3		

- Molecule 15 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 16 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	131	Total	C	N	O	S	0	0
			1059	662	195	198	4		

- Molecule 17 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	171	Total	C	N	O	S	0	0
			1368	856	256	252	4		

- Molecule 18 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	268	Total	C	N	O	S	0	0
			2155	1387	355	409	4		

- Molecule 19 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	L	180	Total	C	N	O	0	0
			1438	892	296	250		

- Molecule 20 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 21 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	N	189	1620	1016	342	261	1	0	0

- Molecule 22 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	O	197	1555	1003	289	262	1	0	0

- Molecule 23 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	P	175	1388	862	277	249	0	0

- Molecule 24 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	147	1136	718	219	198	1	0	0

- Molecule 25 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	R	156	1258	781	265	212	0	0

- Molecule 26 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	S	171	1437	925	266	243	3	0	0

- Molecule 27 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	T	114	905	568	175	159	3	0	0

- Molecule 28 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	U	106	Total	C	N	O	0	0
			844	545	138	161		

- Molecule 29 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 30 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	234	Total	C	N	O	S	0	0
			1888	1194	323	365	6		

- Molecule 31 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	139	Total	C	N	O	S	0	0
			1088	697	194	195	2		

- Molecule 32 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 33 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Z	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 34 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	92	Total	C	N	O	S	0	0
			731	477	129	124	1		

- Molecule 35 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	b	642	5185	3251	938	970	26	0	0

- Molecule 36 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	c	97	743	479	124	139	1	0	0

- Molecule 37 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	d	107	873	553	165	154	1	0	0

- Molecule 38 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	e	127	1020	647	205	167	1	0	0

- Molecule 39 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	f	106	850	540	165	144	1	0	0

- Molecule 40 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	g	112	881	546	179	152	4	0	0

- Molecule 41 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	h	119	969	615	186	167	1	0	0

- Molecule 42 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 43 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 44 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 45 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 46 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	466	Total	C	N	O	S	0	0
			3754	2372	681	691	10		

- Molecule 47 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	369	Total	C	N	O	S	0	0
			3014	1954	521	530	9		

- Molecule 48 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 49 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 50 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	156	Total	C	N	O	S	0	0
			1298	821	233	243	1		

- Molecule 51 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	230	Total	C	N	O	S	0	0
			1860	1177	352	324	7		

- Molecule 52 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	72	Total	C	N	O	S	0	0
			602	377	118	104	3		

- Molecule 53 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	287	Total	C	N	O	S	0	0
			2306	1459	427	417	3		

- Molecule 54 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	150	Total	C	N	O	S	0	0
			1265	793	253	210	9		

- Molecule 55 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	v	293	Total	C	N	O	S	0	0
			2366	1512	415	422	17		

- Molecule 56 is a protein called Ribosome biogenesis regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	w	194	Total	C	N	O	S	0	0
			1541	965	277	294	5		

- Molecule 57 is a protein called RSA4 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	504	Total	C	N	O	S	0	0
			3927	2468	695	743	21		

- Molecule 58 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	y	244	Total	C	N	O	S	0	0
			1849	1146	319	377	7		

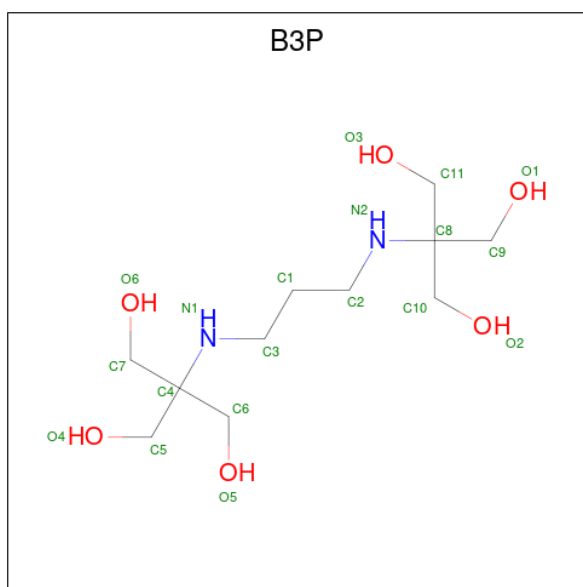
- Molecule 59 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	z	87	Total	C	N	O	S	0	0
			714	444	142	127	1		

- Molecule 60 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	4	538	Total	C	N	O	S	0	0
			4166	2633	718	800	15		

- Molecule 61 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: C₁₁H₂₆N₂O₆).



Mol	Chain	Residues	Atoms				AltConf
61	1	1	Total	C	N	O	0
			19	11	2	6	
61	1	1	Total	C	N	O	0
			19	11	2	6	
61	1	1	Total	C	N	O	0
			19	11	2	6	

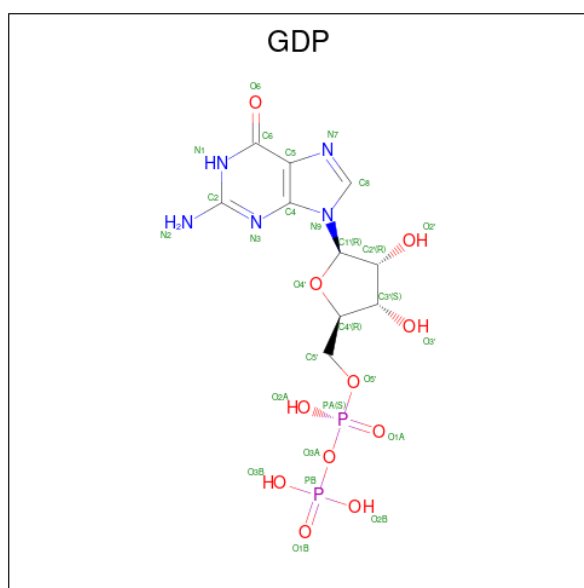
- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	1	76	Total	Mg	0
			76	76	
62	2	1	Total	Mg	0
			1	1	
62	R	1	Total	Mg	0
			1	1	
62	V	1	Total	Mg	0
			1	1	
62	b	1	Total	Mg	0
			1	1	
62	m	1	Total	Mg	0
			1	1	

- Molecule 63 is ZINC ION (three-letter code: ZN) (formula: Zn).

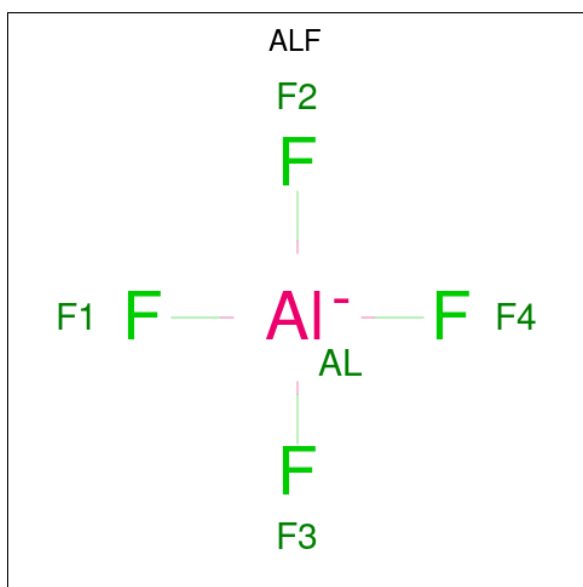
Mol	Chain	Residues	Atoms		AltConf
63	I	1	Total	Zn	0
			1	1	
63	g	1	Total	Zn	0
			1	1	
63	j	1	Total	Zn	0
			1	1	
63	p	1	Total	Zn	0
			1	1	
63	u	1	Total	Zn	0
			1	1	

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
64	b	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	m	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 65 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
65	m	1	5	1	4	0

- Molecule 66 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
66	m	1	1	1	0

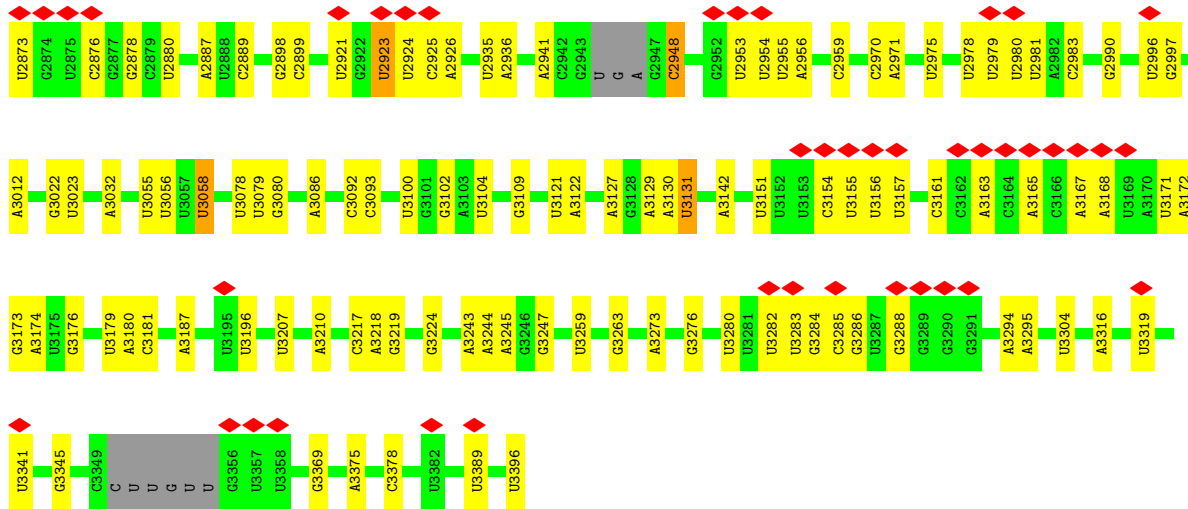
- Molecule 67 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
67	A	2	2	2	0
67	1	340	340	340	0
67	2	7	7	7	0
67	B	2	2	2	0
67	C	1	1	1	0
67	F	3	3	3	0
67	N	2	2	2	0

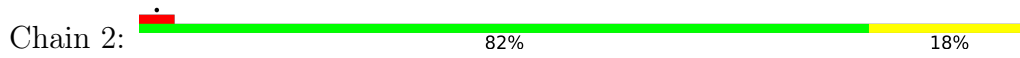
Continued on next page...

Continued from previous page...

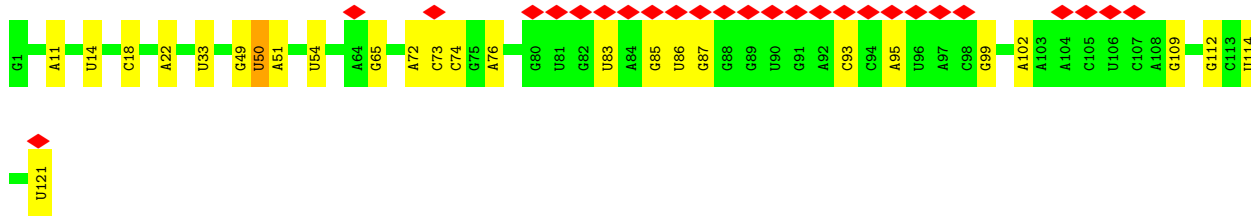
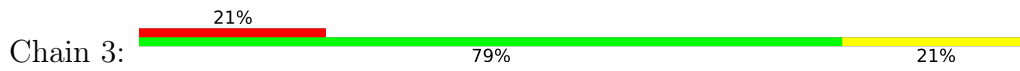
Mol	Chain	Residues	Atoms		AltConf
67	O	1	Total 1	O 1	0
67	R	1	Total 1	O 1	0
67	V	3	Total 3	O 3	0
67	X	1	Total 1	O 1	0
67	b	3	Total 3	O 3	0
67	d	1	Total 1	O 1	0
67	j	4	Total 4	O 4	0
67	m	3	Total 3	O 3	0



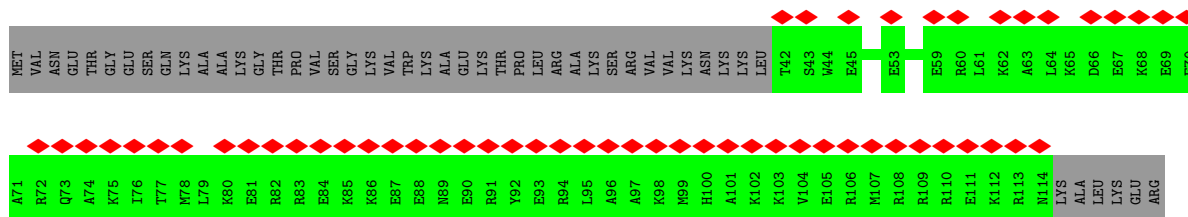
• Molecule 3: 5.8S rRNA



• Molecule 4: 5S rRNA

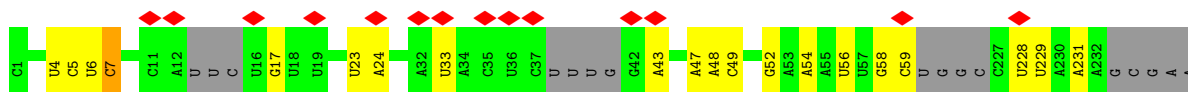


• Molecule 5: rRNA-processing protein

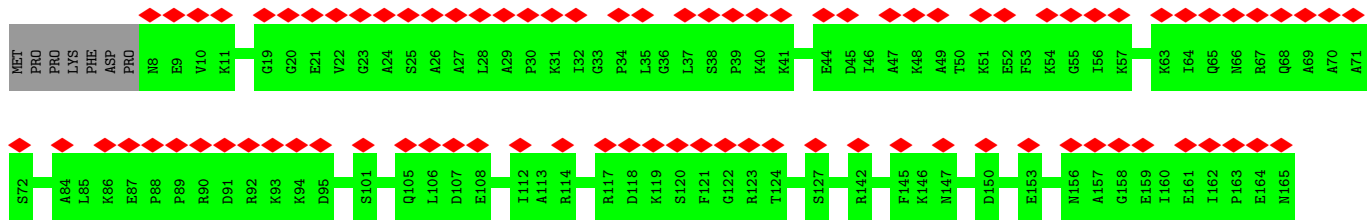
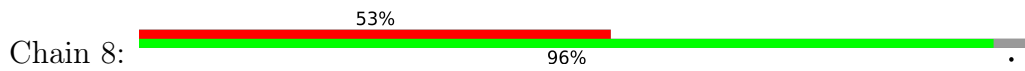


• Molecule 6: ITS2 rRNA

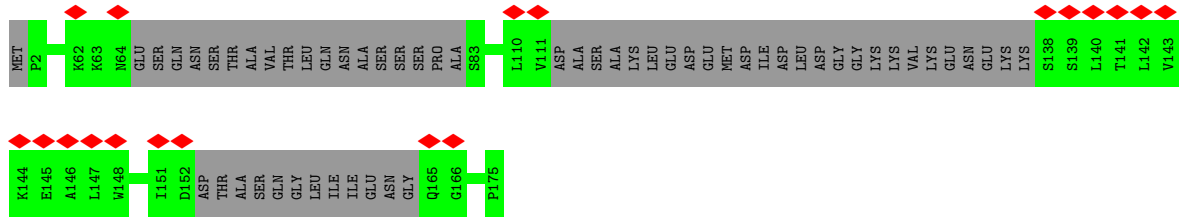




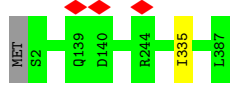
• Molecule 7: 60S ribosomal protein L12-A



• Molecule 8: Ribosome biogenesis protein ALB1



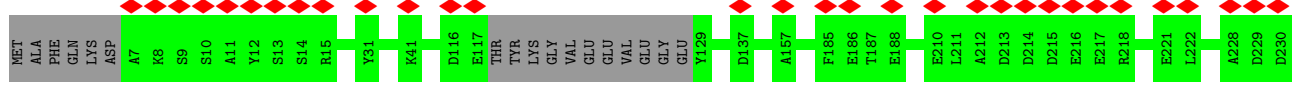
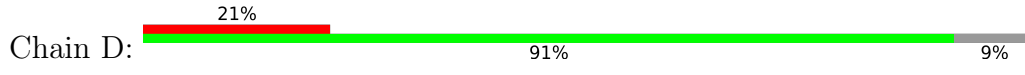
• Molecule 9: 60S ribosomal protein L3

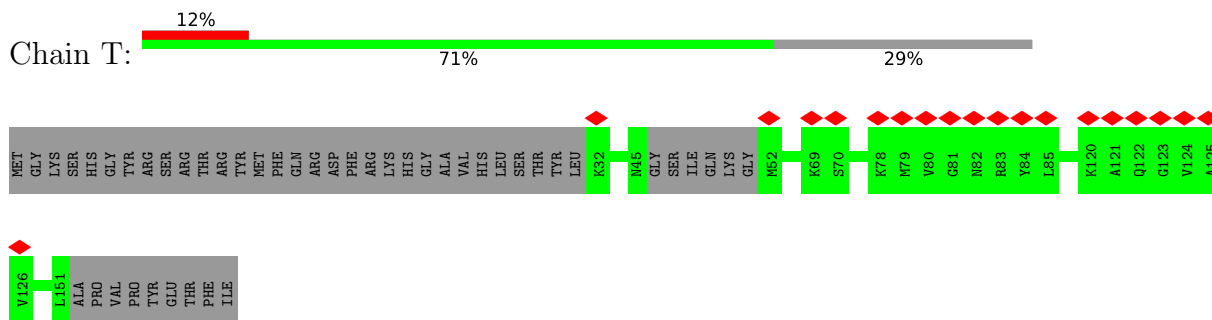


• Molecule 10: 60S ribosomal protein L4-A

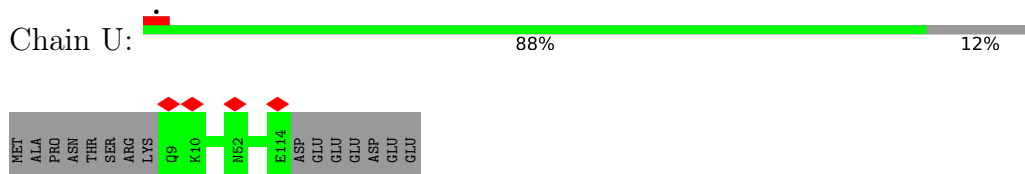


• Molecule 11: 60S ribosomal protein L5

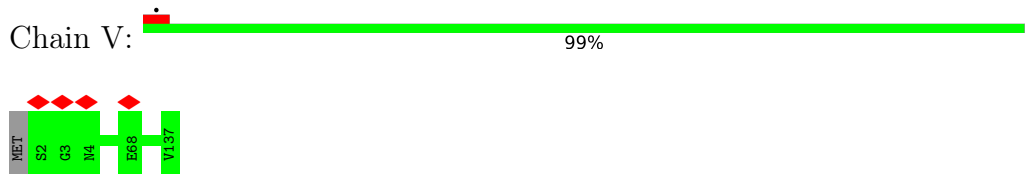




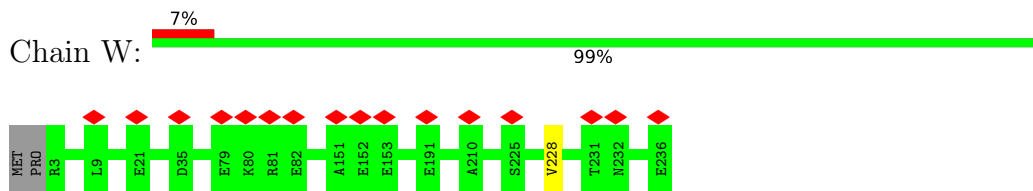
- Molecule 28: 60S ribosomal protein L22-A



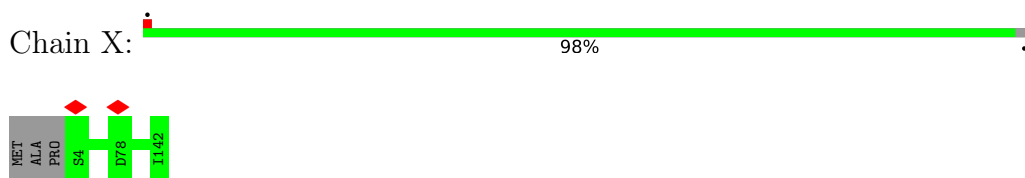
- Molecule 29: 60S ribosomal protein L23-A



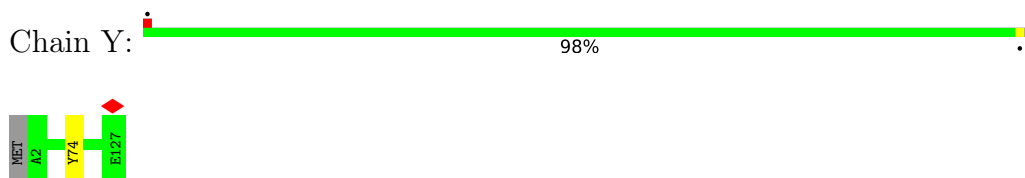
- Molecule 30: Ribosome assembly factor MRT4



- Molecule 31: 60S ribosomal protein L25

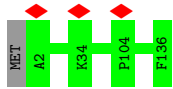


- Molecule 32: 60S ribosomal protein L26-A

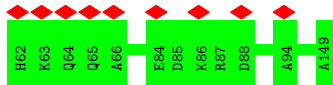
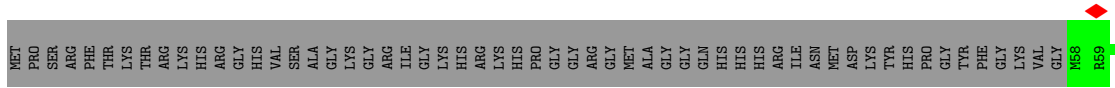


- Molecule 33: 60S ribosomal protein L27-A

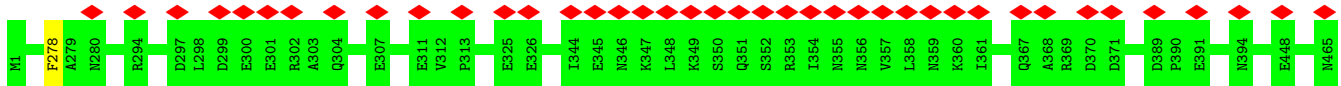




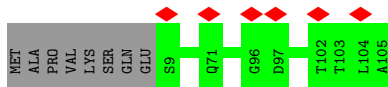
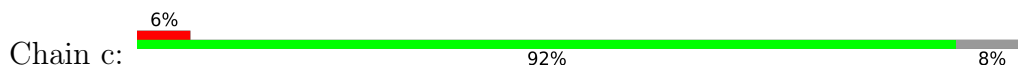
- Molecule 34: 60S ribosomal protein L28



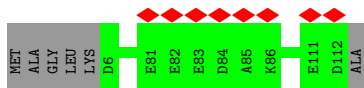
- Molecule 35: Nucleolar GTP-binding protein 1



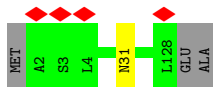
- Molecule 36: 60S ribosomal protein L30



- Molecule 37: 60S ribosomal protein L31-A



- Molecule 38: 60S ribosomal protein L32

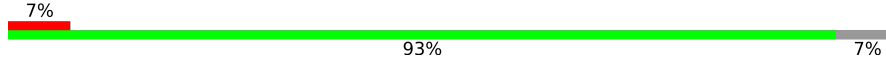


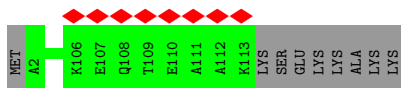
- Molecule 39: 60S ribosomal protein L33-A

Chain f:  99%



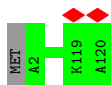
- Molecule 40: 60S ribosomal protein L34-A

Chain g:  93% 7%



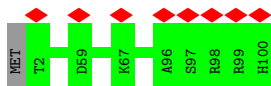
- Molecule 41: 60S ribosomal protein L35-A

Chain h:  99%



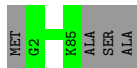
- Molecule 42: 60S ribosomal protein L36-A

Chain i:  99% 8%



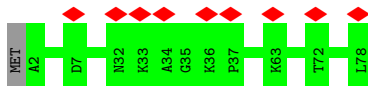
- Molecule 43: 60S ribosomal protein L37-A

Chain j:  95% 5%



- Molecule 44: 60S ribosomal protein L38

Chain k:  99% 12%

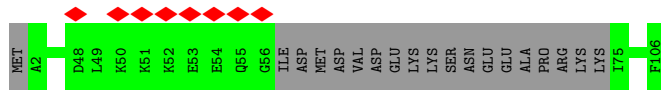
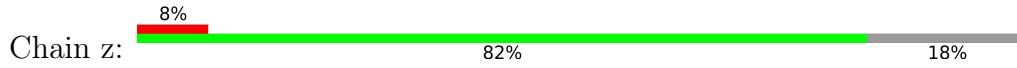


- Molecule 45: 60S ribosomal protein L39

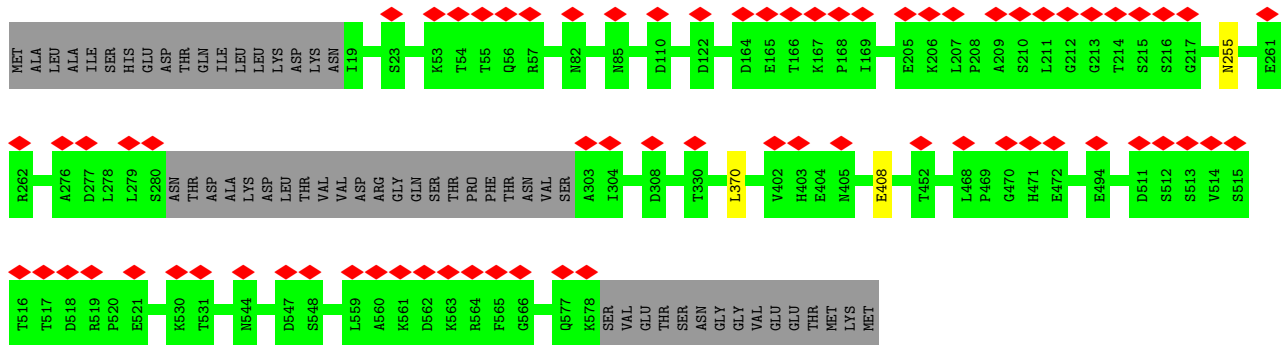
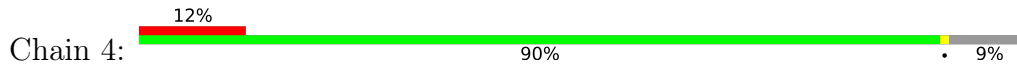
Chain l:  98%



• Molecule 59: UPF0642 protein YBL028C



• Molecule 60: Probable metalloprotease ARX1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	414994	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.440	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.032	Depositor
Map size (\AA)	427.19998, 427.19998, 427.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.068, 1.068, 1.068	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: 1MA, K, B3P, 5MC, OMC, MG, ALF, GDP, ZN, OMU, OMG, PSU, A2M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/1666	0.57	0/2241
2	1	0.28	0/70382	0.83	20/109722 (0.0%)
3	2	0.28	0/3724	0.80	1/5798 (0.0%)
4	3	0.19	0/2861	0.78	0/4457
5	5	0.25	0/649	0.51	0/848
6	6	0.23	0/1367	0.84	1/2118 (0.0%)
7	8	0.25	0/1210	0.47	0/1627
8	9	0.24	0/948	0.46	0/1264
9	B	0.25	0/3152	0.55	0/4239
10	C	0.25	0/2801	0.51	0/3792
11	D	0.25	0/2227	0.49	0/3004
12	E	0.26	0/1251	0.50	0/1682
13	F	0.26	0/1798	0.50	0/2420
14	G	0.26	0/1784	0.48	0/2408
15	H	0.26	0/1539	0.52	0/2073
16	I	0.24	0/1075	0.47	0/1443
17	J	0.24	0/1389	0.52	0/1860
18	K	0.25	0/2190	0.47	0/2955
19	L	0.25	0/1460	0.56	0/1960
20	M	0.25	0/1074	0.51	0/1446
21	N	0.25	0/1654	0.59	0/2213
22	O	0.27	0/1585	0.51	0/2128
23	P	0.26	0/1410	0.56	0/1893
24	Q	0.25	0/1153	0.52	0/1555
25	R	0.25	0/1275	0.53	0/1702
26	S	0.26	0/1473	0.52	0/1980
27	T	0.26	0/916	0.50	0/1226
28	U	0.26	0/861	0.49	0/1167
29	V	0.27	0/1018	0.54	0/1369
30	W	0.25	0/1920	0.48	0/2586
31	X	0.25	0/1103	0.51	0/1484
32	Y	0.25	0/1004	0.54	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z	0.26	0/1118	0.48	0/1497
34	a	0.24	0/747	0.46	0/1008
35	b	0.25	0/5270	0.50	0/7080
36	c	0.26	0/751	0.45	0/1008
37	d	0.25	0/887	0.53	0/1191
38	e	0.24	0/1041	0.52	0/1394
39	f	0.28	0/868	0.55	0/1168
40	g	0.25	0/891	0.56	0/1191
41	h	0.26	0/978	0.51	0/1301
42	i	0.24	0/778	0.53	0/1034
43	j	0.26	0/680	0.58	0/901
44	k	0.25	0/618	0.52	0/826
45	l	0.24	0/443	0.59	0/588
46	m	0.25	0/3828	0.50	0/5154
47	n	0.25	0/3085	0.48	0/4166
48	o	0.25	0/1129	0.47	0/1502
49	p	0.25	0/701	0.57	0/934
50	q	0.25	0/1321	0.49	0/1766
51	r	0.25	0/1892	0.52	0/2528
52	s	0.25	0/608	0.49	0/798
53	t	0.25	0/2333	0.50	0/3128
54	u	0.27	0/1287	0.55	0/1711
55	v	0.26	0/2410	0.49	0/3220
56	w	0.24	0/1565	0.47	0/2108
57	x	0.24	0/4022	0.51	0/5460
58	y	0.25	0/1872	0.53	0/2548
59	z	0.25	0/721	0.47	0/948
60	4	0.24	0/4242	0.48	0/5758
All	All	0.26	0/166005	0.69	22/239917 (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
54	u	0	1
56	w	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	406	G	O4'-C1'-N9	9.13	115.51	108.20
2	1	922	U	C2-N1-C1'	7.25	126.41	117.70
2	1	1496	C	C2-N1-C1'	7.04	126.54	118.80
2	1	1495	U	C2-N1-C1'	6.96	126.06	117.70
2	1	922	U	C6-N1-C1'	-6.96	111.45	121.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	u	75	ARG	Sidechain
56	w	46	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/254 (83%)	202 (96%)	9 (4%)	0	100	100
5	5	71/120 (59%)	71 (100%)	0	0	100	100
7	8	156/165 (94%)	150 (96%)	6 (4%)	0	100	100
8	9	110/175 (63%)	108 (98%)	2 (2%)	0	100	100
9	B	384/387 (99%)	379 (99%)	5 (1%)	0	100	100
10	C	359/362 (99%)	348 (97%)	11 (3%)	0	100	100
11	D	266/297 (90%)	261 (98%)	5 (2%)	0	100	100
12	E	151/176 (86%)	149 (99%)	2 (1%)	0	100	100
13	F	217/244 (89%)	211 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	G	220/256 (86%)	216 (98%)	4 (2%)	0	100	100
15	H	189/191 (99%)	184 (97%)	5 (3%)	0	100	100
16	I	129/166 (78%)	125 (97%)	4 (3%)	0	100	100
17	J	169/174 (97%)	166 (98%)	3 (2%)	0	100	100
18	K	262/376 (70%)	256 (98%)	6 (2%)	0	100	100
19	L	178/199 (89%)	174 (98%)	4 (2%)	0	100	100
20	M	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
21	N	185/204 (91%)	178 (96%)	7 (4%)	0	100	100
22	O	195/199 (98%)	194 (100%)	1 (0%)	0	100	100
23	P	171/184 (93%)	164 (96%)	7 (4%)	0	100	100
24	Q	145/186 (78%)	144 (99%)	1 (1%)	0	100	100
25	R	154/189 (82%)	151 (98%)	3 (2%)	0	100	100
26	S	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
27	T	110/160 (69%)	107 (97%)	3 (3%)	0	100	100
28	U	104/121 (86%)	100 (96%)	4 (4%)	0	100	100
29	V	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
30	W	232/236 (98%)	230 (99%)	2 (1%)	0	100	100
31	X	137/142 (96%)	133 (97%)	4 (3%)	0	100	100
32	Y	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
33	Z	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
34	a	90/149 (60%)	86 (96%)	4 (4%)	0	100	100
35	b	638/647 (99%)	617 (97%)	21 (3%)	0	100	100
36	c	95/105 (90%)	95 (100%)	0	0	100	100
37	d	105/113 (93%)	104 (99%)	1 (1%)	0	100	100
38	e	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
39	f	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
40	g	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
41	h	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
42	i	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
43	j	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
44	k	75/78 (96%)	75 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	l	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
46	m	462/486 (95%)	452 (98%)	10 (2%)	0	100	100
47	n	363/605 (60%)	353 (97%)	10 (3%)	0	100	100
48	o	131/220 (60%)	129 (98%)	2 (2%)	0	100	100
49	p	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
50	q	152/455 (33%)	144 (95%)	8 (5%)	0	100	100
51	r	224/261 (86%)	220 (98%)	4 (2%)	0	100	100
52	s	68/77 (88%)	67 (98%)	1 (2%)	0	100	100
53	t	283/322 (88%)	280 (99%)	3 (1%)	0	100	100
54	u	148/199 (74%)	146 (99%)	2 (1%)	0	100	100
55	v	291/344 (85%)	283 (97%)	8 (3%)	0	100	100
56	w	192/201 (96%)	190 (99%)	2 (1%)	0	100	100
57	x	500/514 (97%)	488 (98%)	12 (2%)	0	100	100
58	y	242/245 (99%)	232 (96%)	10 (4%)	0	100	100
59	z	83/106 (78%)	83 (100%)	0	0	100	100
60	4	534/593 (90%)	527 (99%)	7 (1%)	0	100	100
All	All	10648/12402 (86%)	10401 (98%)	247 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/196 (85%)	166 (100%)	0	100	100
5	5	67/106 (63%)	67 (100%)	0	100	100
7	8	129/136 (95%)	129 (100%)	0	100	100
8	9	106/153 (69%)	106 (100%)	0	100	100
9	B	322/323 (100%)	321 (100%)	1 (0%)	92	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	C	288/289 (100%)	285 (99%)	3 (1%)	76	84
11	D	226/245 (92%)	226 (100%)	0	100	100
12	E	133/153 (87%)	133 (100%)	0	100	100
13	F	184/205 (90%)	184 (100%)	0	100	100
14	G	185/208 (89%)	185 (100%)	0	100	100
15	H	171/171 (100%)	170 (99%)	1 (1%)	86	91
16	I	117/141 (83%)	117 (100%)	0	100	100
17	J	148/150 (99%)	148 (100%)	0	100	100
18	K	247/346 (71%)	247 (100%)	0	100	100
19	L	142/159 (89%)	142 (100%)	0	100	100
20	M	108/109 (99%)	108 (100%)	0	100	100
21	N	165/176 (94%)	165 (100%)	0	100	100
22	O	160/162 (99%)	160 (100%)	0	100	100
23	P	141/146 (97%)	141 (100%)	0	100	100
24	Q	121/151 (80%)	121 (100%)	0	100	100
25	R	129/154 (84%)	129 (100%)	0	100	100
26	S	155/156 (99%)	154 (99%)	1 (1%)	86	91
27	T	98/137 (72%)	98 (100%)	0	100	100
28	U	93/107 (87%)	93 (100%)	0	100	100
29	V	104/105 (99%)	104 (100%)	0	100	100
30	W	211/213 (99%)	210 (100%)	1 (0%)	88	93
31	X	116/118 (98%)	116 (100%)	0	100	100
32	Y	109/110 (99%)	108 (99%)	1 (1%)	78	87
33	Z	115/116 (99%)	115 (100%)	0	100	100
34	a	76/119 (64%)	76 (100%)	0	100	100
35	b	568/573 (99%)	566 (100%)	2 (0%)	91	94
36	c	81/88 (92%)	81 (100%)	0	100	100
37	d	94/97 (97%)	94 (100%)	0	100	100
38	e	109/111 (98%)	108 (99%)	1 (1%)	78	87
39	f	90/91 (99%)	90 (100%)	0	100	100
40	g	95/103 (92%)	95 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	h	104/105 (99%)	104 (100%)	0	100	100
42	i	81/82 (99%)	81 (100%)	0	100	100
43	j	69/71 (97%)	69 (100%)	0	100	100
44	k	68/69 (99%)	68 (100%)	0	100	100
45	l	45/46 (98%)	45 (100%)	0	100	100
46	m	411/428 (96%)	409 (100%)	2 (0%)	88	93
47	n	332/548 (61%)	332 (100%)	0	100	100
48	o	118/199 (59%)	117 (99%)	1 (1%)	81	88
49	p	71/72 (99%)	70 (99%)	1 (1%)	67	78
50	q	145/420 (34%)	145 (100%)	0	100	100
51	r	203/229 (89%)	202 (100%)	1 (0%)	88	93
52	s	65/70 (93%)	65 (100%)	0	100	100
53	t	256/287 (89%)	255 (100%)	1 (0%)	91	94
54	u	133/180 (74%)	133 (100%)	0	100	100
55	v	264/309 (85%)	264 (100%)	0	100	100
56	w	172/178 (97%)	171 (99%)	1 (1%)	86	91
57	x	442/450 (98%)	438 (99%)	4 (1%)	78	87
58	y	210/211 (100%)	210 (100%)	0	100	100
59	z	77/95 (81%)	77 (100%)	0	100	100
60	4	471/520 (91%)	468 (99%)	3 (1%)	86	91
All	All	9306/10692 (87%)	9281 (100%)	25 (0%)	92	95

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	p	60	CYS
56	w	55	ARG
60	4	408	GLU
53	t	274	ASN
57	x	194	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
24	Q	9	GLN
27	T	95	HIS
56	w	8	ASN
55	v	187	GLN
24	Q	5	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1	2976/3396 (87%)	511 (17%)	6 (0%)
3	2	157/158 (99%)	26 (16%)	0
4	3	120/121 (99%)	26 (21%)	0
6	6	54/74 (72%)	20 (37%)	0
All	All	3307/3749 (88%)	583 (17%)	6 (0%)

5 of 583 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	1	2	U
2	1	5	G
2	1	14	U
2	1	26	A
2	1	42	C

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	1	1568	U
2	1	3121	U
2	1	3283	U
2	1	588	G
2	1	374	A

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

57 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$
2	OMU	1	2724	2	19,22,23	0.84	1 (5%)	26,31,34	0.82	1 (3%)
4	PSU	3	50	4	18,21,22	1.21	2 (11%)	22,30,33	1.51	4 (18%)
2	OMG	1	1450	2	18,26,27	1.32	3 (16%)	19,38,41	1.38	2 (10%)
2	PSU	1	2416	2	18,21,22	1.16	1 (5%)	22,30,33	1.53	4 (18%)
2	OMG	1	908	2	18,26,27	1.38	2 (11%)	19,38,41	1.47	2 (10%)
2	PSU	1	2340	2	18,21,22	1.12	1 (5%)	22,30,33	1.49	4 (18%)
2	OMC	1	650	2	19,22,23	0.54	0	26,31,34	0.64	0
2	PSU	1	2314	2	18,21,22	1.13	1 (5%)	22,30,33	1.45	4 (18%)
2	OMG	1	805	2	18,26,27	1.37	3 (16%)	19,38,41	1.47	2 (10%)
2	OMU	1	2729	2	19,22,23	0.77	1 (5%)	26,31,34	0.89	2 (7%)
2	OMC	1	2948	2	19,22,23	0.54	0	26,31,34	0.87	1 (3%)
3	PSU	2	73	3	18,21,22	1.09	1 (5%)	22,30,33	1.46	4 (18%)
2	PSU	1	2133	2	18,21,22	1.03	1 (5%)	22,30,33	1.53	4 (18%)
2	1MA	1	2142	62,2	16,25,26	0.96	2 (12%)	18,37,40	1.07	2 (11%)
2	PSU	1	990	2	18,21,22	1.14	2 (11%)	22,30,33	1.42	4 (18%)
2	OMG	1	2815	2	18,26,27	1.36	2 (11%)	19,38,41	1.47	2 (10%)
2	A2M	1	817	62,2	18,25,26	1.43	1 (5%)	18,36,39	1.06	1 (5%)
2	5MC	1	2870	2	18,22,23	0.91	2 (11%)	26,32,35	1.16	2 (7%)
2	PSU	1	776	2	18,21,22	1.22	3 (16%)	22,30,33	1.49	4 (18%)
2	PSU	1	2880	2	18,21,22	1.18	1 (5%)	22,30,33	1.43	4 (18%)
2	PSU	1	1124	2	18,21,22	1.16	1 (5%)	22,30,33	1.48	4 (18%)
2	OMC	1	2337	2	19,22,23	0.52	0	26,31,34	0.68	0
2	PSU	1	2923	2	18,21,22	1.24	2 (11%)	22,30,33	1.23	3 (13%)
2	OMG	1	2791	2	18,26,27	1.37	2 (11%)	19,38,41	1.49	2 (10%)
2	PSU	1	2266	2	18,21,22	1.18	2 (11%)	22,30,33	1.45	5 (22%)
2	PSU	1	1110	2	18,21,22	1.20	2 (11%)	22,30,33	1.45	5 (22%)
2	OMU	1	2417	2	19,22,23	0.82	1 (5%)	26,31,34	0.87	2 (7%)
2	PSU	1	2975	2	18,21,22	1.13	1 (5%)	22,30,33	1.57	4 (18%)
2	PSU	1	960	2	18,21,22	1.16	2 (11%)	22,30,33	1.41	4 (18%)
2	OMC	1	1437	62,2	19,22,23	0.59	0	26,31,34	0.99	1 (3%)
2	A2M	1	1133	2	18,25,26	1.49	1 (5%)	18,36,39	0.95	0
2	A2M	1	1449	62,2	18,25,26	1.46	1 (5%)	18,36,39	0.99	1 (5%)
2	OMU	1	898	2	19,22,23	0.77	1 (5%)	26,31,34	0.89	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMC	1	663	2	19,22,23	0.55	0	26,31,34	0.69	0
2	A2M	1	2220	2	18,25,26	1.53	3 (16%)	18,36,39	1.06	1 (5%)
2	PSU	1	986	2	18,21,22	1.14	2 (11%)	22,30,33	1.38	4 (18%)
2	OMU	1	2921	2	19,22,23	0.89	1 (5%)	26,31,34	0.90	2 (7%)
2	PSU	1	966	2	18,21,22	1.22	3 (16%)	22,30,33	1.48	4 (18%)
2	A2M	1	649	2	18,25,26	1.43	2 (11%)	18,36,39	1.00	0
2	PSU	1	2865	2	18,21,22	1.19	2 (11%)	22,30,33	1.46	4 (18%)
2	OMC	1	2197	2	19,22,23	0.49	0	26,31,34	0.66	0
2	PSU	1	2191	2	18,21,22	1.14	1 (5%)	22,30,33	1.50	4 (18%)
2	PSU	1	2351	2	18,21,22	1.14	1 (5%)	22,30,33	1.49	4 (18%)
2	OMG	1	867	2	18,26,27	1.33	3 (16%)	19,38,41	1.46	2 (10%)
2	PSU	1	2826	62,2	18,21,22	1.11	1 (5%)	22,30,33	1.54	4 (18%)
2	5MC	1	2278	2	18,22,23	0.97	2 (11%)	26,32,35	1.11	3 (11%)
2	OMU	1	1888	2	19,22,23	1.16	1 (5%)	26,31,34	1.30	4 (15%)
2	OMU	1	2421	2	19,22,23	0.83	1 (5%)	26,31,34	0.88	2 (7%)
2	PSU	1	2735	2	18,21,22	1.13	1 (5%)	22,30,33	1.48	4 (18%)
2	A2M	1	807	2	18,25,26	1.46	1 (5%)	18,36,39	1.02	0
2	A2M	1	876	2	18,25,26	1.43	1 (5%)	18,36,39	0.94	0
2	OMG	1	2793	2	18,26,27	1.42	2 (11%)	19,38,41	1.52	2 (10%)
2	OMU	1	2347	2	19,22,23	0.83	1 (5%)	26,31,34	0.78	1 (3%)
2	PSU	1	2349	62,2	18,21,22	1.09	1 (5%)	22,30,33	1.40	4 (18%)
2	OMC	1	2959	2	19,22,23	0.56	0	26,31,34	0.81	1 (3%)
2	PSU	1	2129	2	18,21,22	1.11	1 (5%)	22,30,33	1.43	4 (18%)
2	PSU	1	2264	2	18,21,22	1.20	2 (11%)	22,30,33	1.47	4 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	1	2724	2	-	0/9/27/28	0/2/2/2
4	PSU	3	50	4	-	2/7/25/26	0/2/2/2
2	OMG	1	1450	2	-	2/5/27/28	0/3/3/3
2	PSU	1	2416	2	-	3/7/25/26	0/2/2/2
2	OMG	1	908	2	-	0/5/27/28	0/3/3/3
2	PSU	1	2340	2	-	3/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	1	650	2	-	0/9/27/28	0/2/2/2
2	PSU	1	2314	2	-	0/7/25/26	0/2/2/2
2	OMG	1	805	2	-	1/5/27/28	0/3/3/3
2	OMU	1	2729	2	-	0/9/27/28	0/2/2/2
2	OMC	1	2948	2	-	2/9/27/28	0/2/2/2
3	PSU	2	73	3	-	0/7/25/26	0/2/2/2
2	PSU	1	2133	2	-	0/7/25/26	0/2/2/2
2	1MA	1	2142	62,2	-	2/3/25/26	0/3/3/3
2	PSU	1	990	2	-	0/7/25/26	0/2/2/2
2	OMG	1	2815	2	-	0/5/27/28	0/3/3/3
2	A2M	1	817	62,2	-	2/5/27/28	0/3/3/3
2	5MC	1	2870	2	-	0/7/25/26	0/2/2/2
2	PSU	1	776	2	-	2/7/25/26	0/2/2/2
2	PSU	1	2880	2	-	0/7/25/26	0/2/2/2
2	PSU	1	1124	2	-	0/7/25/26	0/2/2/2
2	OMC	1	2337	2	-	0/9/27/28	0/2/2/2
2	PSU	1	2923	2	-	4/7/25/26	0/2/2/2
2	OMG	1	2791	2	-	3/5/27/28	0/3/3/3
2	PSU	1	2266	2	-	0/7/25/26	0/2/2/2
2	PSU	1	1110	2	-	0/7/25/26	0/2/2/2
2	OMU	1	2417	2	-	2/9/27/28	0/2/2/2
2	PSU	1	2975	2	-	0/7/25/26	0/2/2/2
2	PSU	1	960	2	-	2/7/25/26	0/2/2/2
2	OMC	1	1437	62,2	-	4/9/27/28	0/2/2/2
2	A2M	1	1133	2	-	0/5/27/28	0/3/3/3
2	A2M	1	1449	62,2	-	0/5/27/28	0/3/3/3
2	OMU	1	898	2	-	0/9/27/28	0/2/2/2
2	OMC	1	663	2	-	1/9/27/28	0/2/2/2
2	A2M	1	2220	2	-	2/5/27/28	0/3/3/3
2	PSU	1	986	2	-	2/7/25/26	0/2/2/2
2	OMU	1	2921	2	-	7/9/27/28	0/2/2/2
2	PSU	1	966	2	-	0/7/25/26	0/2/2/2
2	A2M	1	649	2	-	3/5/27/28	0/3/3/3
2	PSU	1	2865	2	-	2/7/25/26	0/2/2/2
2	OMC	1	2197	2	-	2/9/27/28	0/2/2/2
2	PSU	1	2191	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2351	2	-	0/7/25/26	0/2/2/2
2	OMG	1	867	2	-	0/5/27/28	0/3/3/3
2	PSU	1	2826	62,2	-	1/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MC	1	2278	2	-	0/7/25/26	0/2/2/2
2	OMU	1	1888	2	-	2/9/27/28	0/2/2/2
2	OMU	1	2421	2	-	2/9/27/28	0/2/2/2
2	PSU	1	2735	2	-	0/7/25/26	0/2/2/2
2	A2M	1	807	2	-	0/5/27/28	0/3/3/3
2	A2M	1	876	2	-	0/5/27/28	0/3/3/3
2	OMG	1	2793	2	-	0/5/27/28	0/3/3/3
2	OMU	1	2347	2	-	0/9/27/28	0/2/2/2
2	PSU	1	2349	62,2	-	0/7/25/26	0/2/2/2
2	OMC	1	2959	2	-	0/9/27/28	0/2/2/2
2	PSU	1	2129	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2264	2	-	0/7/25/26	0/2/2/2

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	876	A2M	O5'-C5'	-4.60	1.33	1.44
2	1	1449	A2M	O5'-C5'	-4.57	1.33	1.44
2	1	2220	A2M	O5'-C5'	-4.57	1.33	1.44
2	1	2793	OMG	C6-N1	4.50	1.44	1.37
2	1	807	A2M	O5'-C5'	-4.50	1.33	1.44

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	2975	PSU	C6-C5-C4	4.50	121.34	118.20
2	1	2865	PSU	C6-C5-C4	4.49	121.34	118.20
4	3	50	PSU	C6-C5-C4	4.42	121.29	118.20
2	1	2826	PSU	C6-C5-C4	4.36	121.25	118.20
2	1	2416	PSU	C6-C5-C4	4.33	121.23	118.20

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1	776	PSU	C3'-C4'-C5'-O5'
2	1	776	PSU	O4'-C4'-C5'-O5'
2	1	960	PSU	C3'-C4'-C5'-O5'
2	1	960	PSU	O4'-C4'-C5'-O5'
2	1	1437	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 93 ligands modelled in this entry, 87 are monoatomic - leaving 6 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
61	B3P	1	3402	-	18,18,18	1.47	2 (11%)	21,23,23	2.02	6 (28%)
65	ALF	m	802	-	0,4,4	-	-	-	-	-
61	B3P	1	3401	62	18,18,18	1.46	2 (11%)	21,23,23	1.96	6 (28%)
61	B3P	1	3403	-	18,18,18	1.53	2 (11%)	21,23,23	1.96	6 (28%)
64	GDP	m	801	62,66	24,30,30	0.95	1 (4%)	30,47,47	1.20	4 (13%)
64	GDP	b	801	62	24,30,30	0.93	1 (4%)	30,47,47	1.23	4 (13%)

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
61	B3P	1	3402	-	-	11/28/28/28	-
61	B3P	1	3401	62	-	4/28/28/28	-
61	B3P	1	3403	-	-	8/28/28/28	-
64	GDP	m	801	62,66	-	3/12/32/32	0/3/3/3
64	GDP	b	801	62	-	3/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	1	3403	B3P	C6-C4	5.22	1.59	1.53
61	1	3402	B3P	C6-C4	4.91	1.59	1.53
61	1	3401	B3P	C6-C4	4.88	1.59	1.53
64	m	801	GDP	C6-N1	-2.43	1.34	1.37
61	1	3402	B3P	C7-C4	2.36	1.56	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	1	3403	B3P	O5-C6-C4	5.11	121.98	111.63
61	1	3402	B3P	O5-C6-C4	5.06	121.88	111.63
61	1	3401	B3P	O5-C6-C4	4.92	121.60	111.63
61	1	3402	B3P	C3-N1-C4	-4.08	110.28	116.08
61	1	3401	B3P	C2-N2-C8	-3.80	110.68	116.08

There are no chirality outliers.

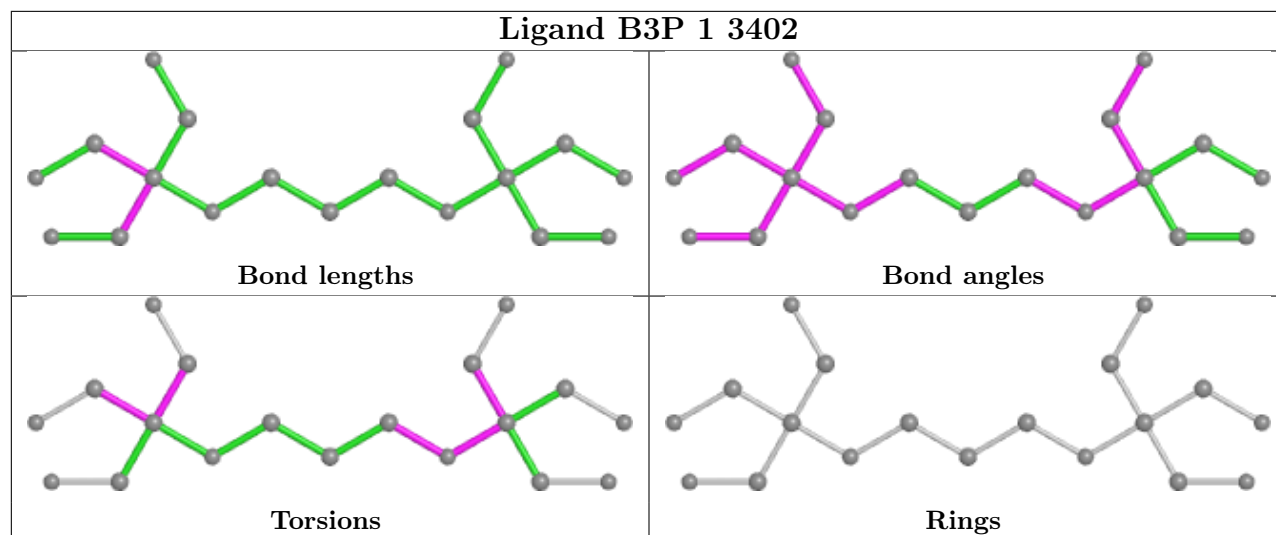
5 of 29 torsion outliers are listed below:

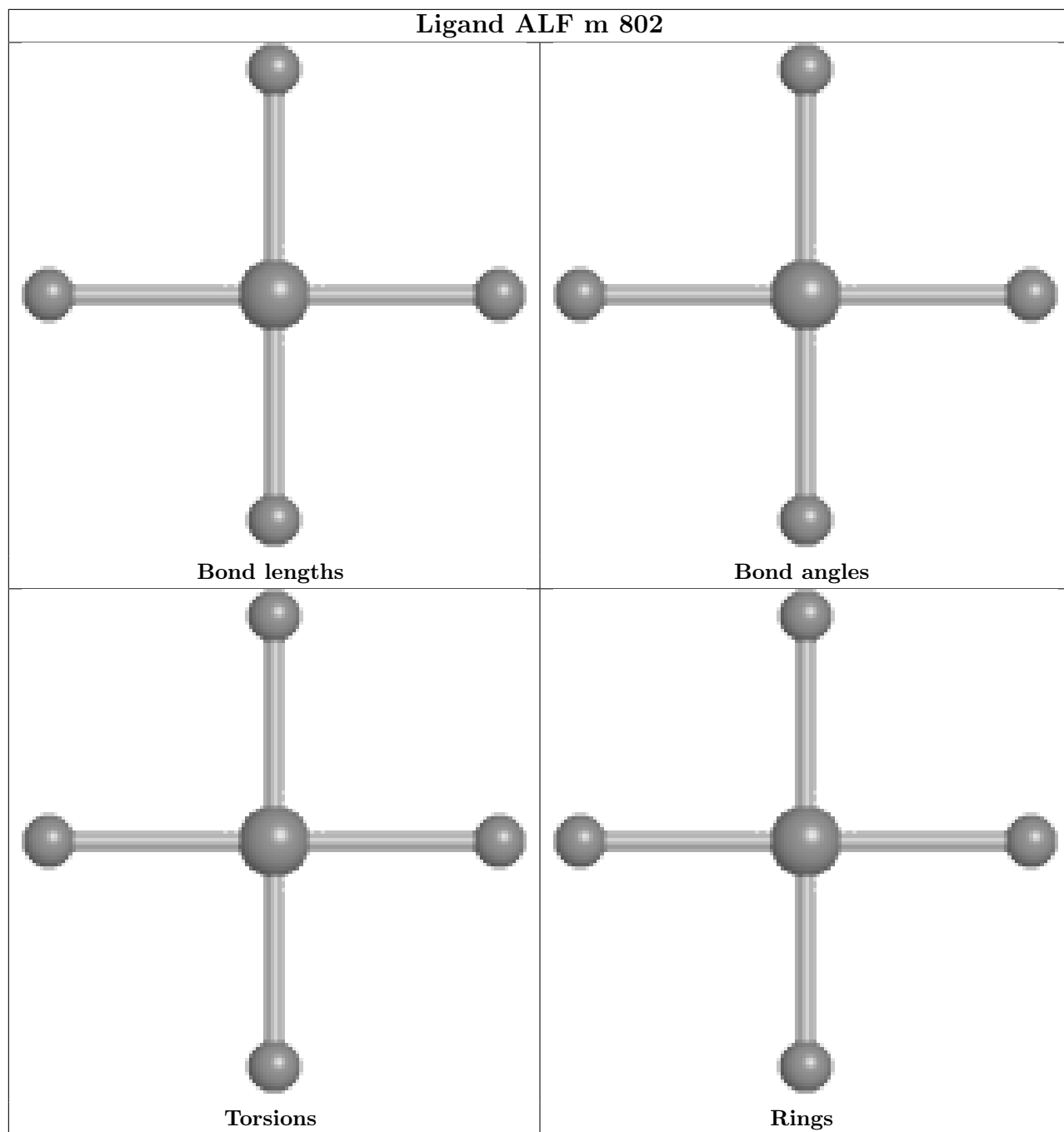
Mol	Chain	Res	Type	Atoms
61	1	3401	B3P	N1-C4-C6-O5
61	1	3401	B3P	C5-C4-C6-O5
61	1	3401	B3P	C7-C4-C6-O5
61	1	3402	B3P	N1-C4-C5-O4
61	1	3402	B3P	C6-C4-C5-O4

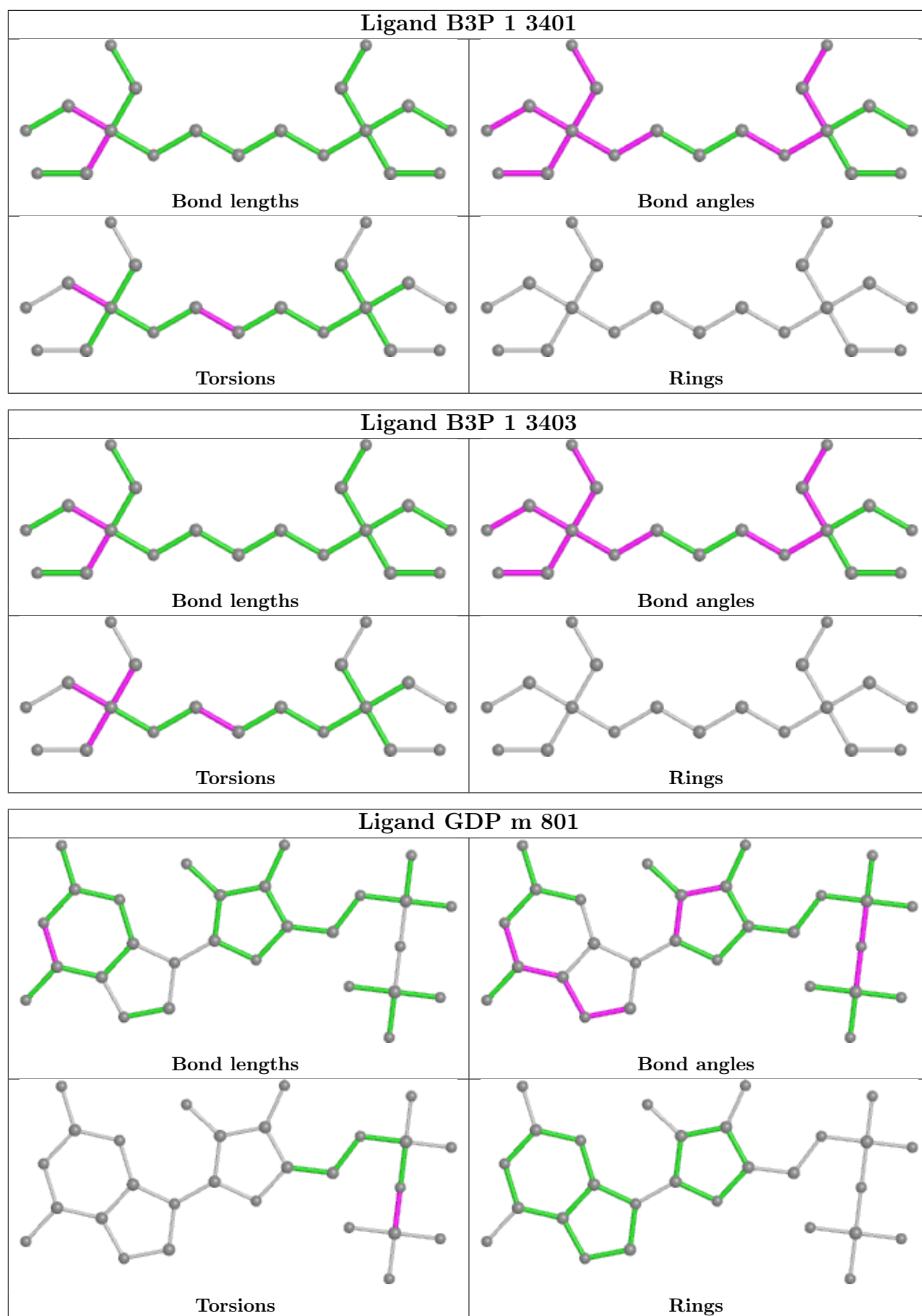
There are no ring outliers.

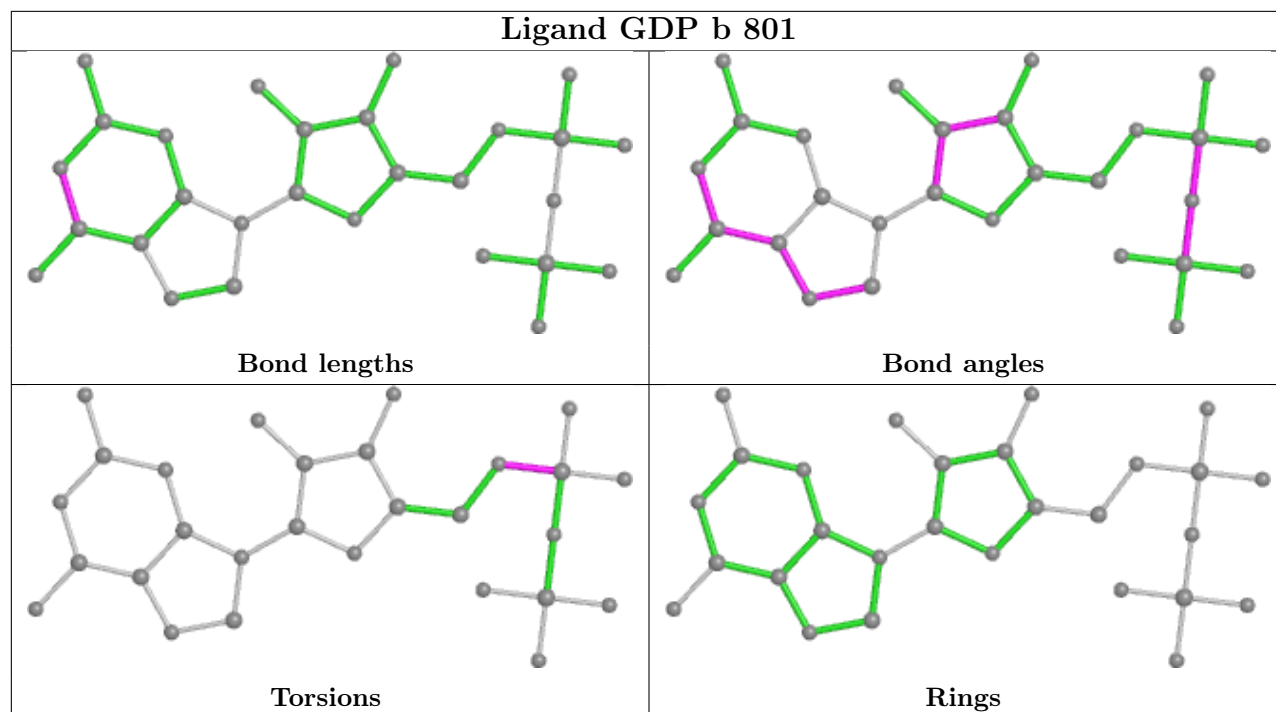
No monomer is involved in short contacts.

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 than 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.









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.

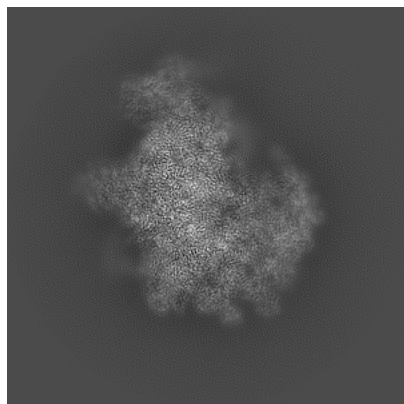
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26686. These allow visual inspection of the internal detail of the map and identification of artifacts.

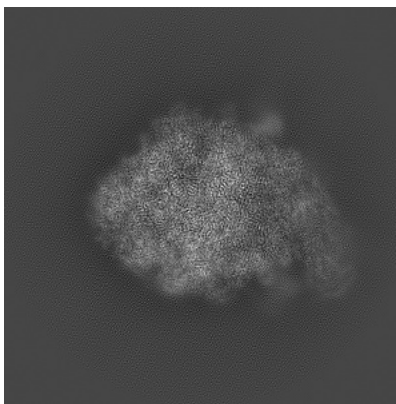
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

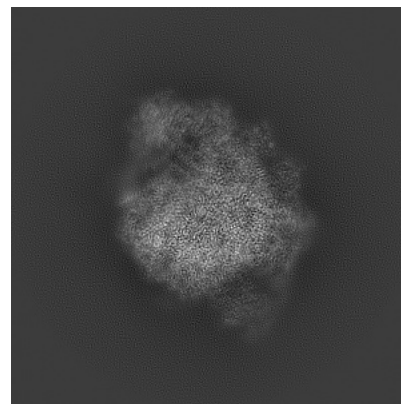
6.1.1 Primary map



X

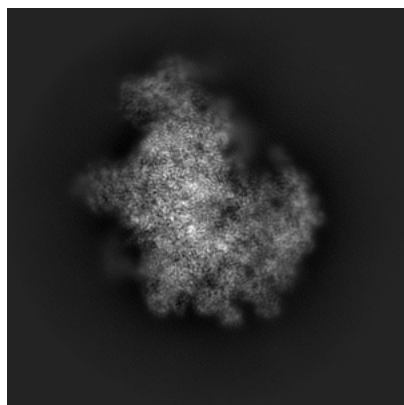


Y

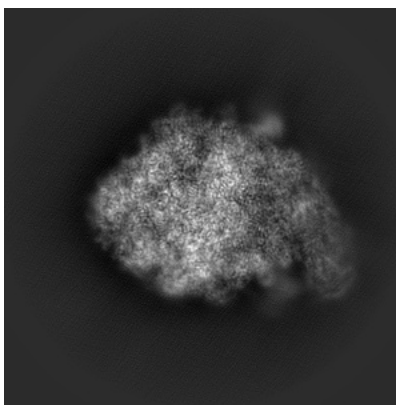


Z

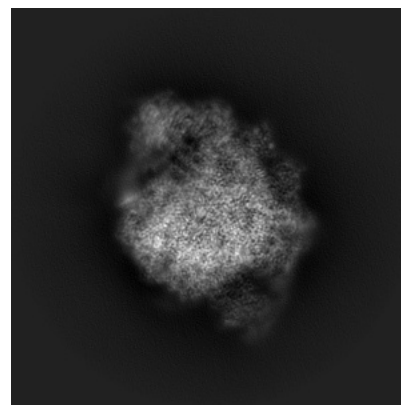
6.1.2 Raw map



X



Y

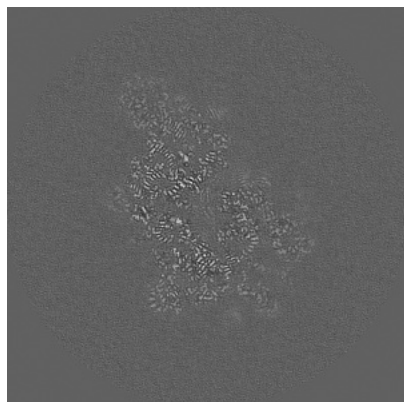


Z

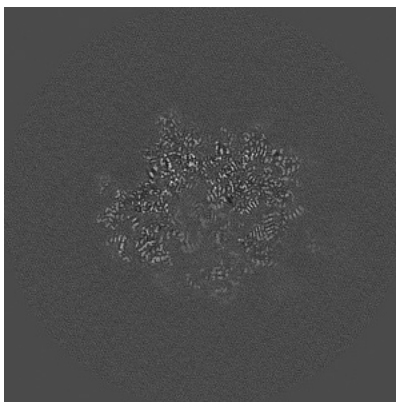
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

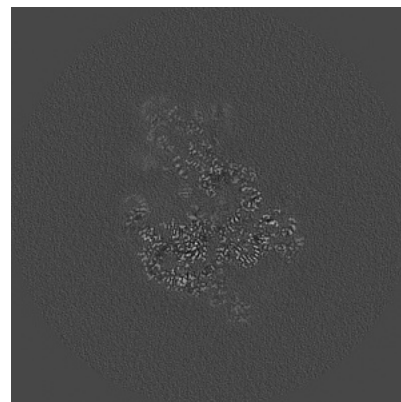
6.2.1 Primary map



X Index: 200

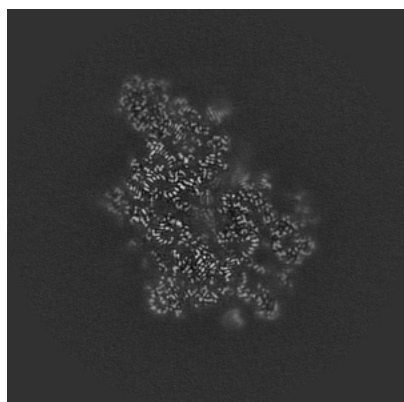


Y Index: 200

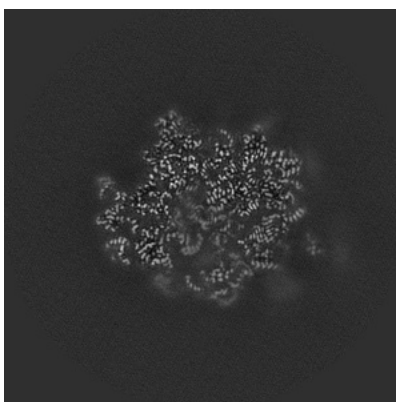


Z Index: 200

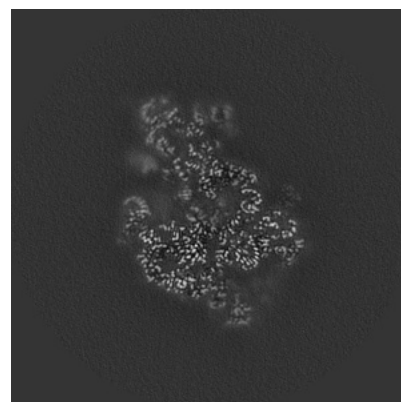
6.2.2 Raw map



X Index: 200



Y Index: 200

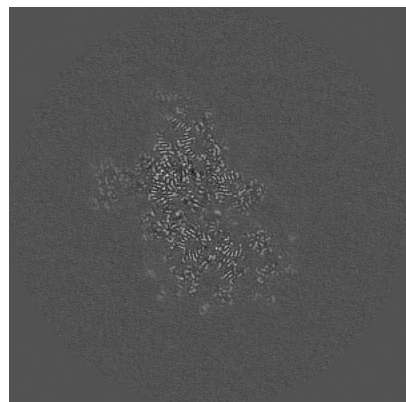


Z Index: 200

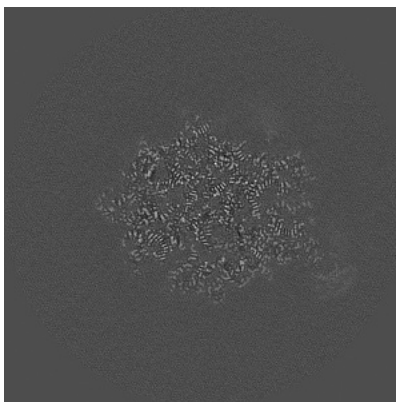
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

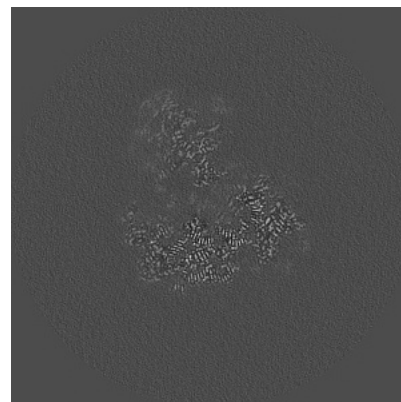
6.3.1 Primary map



X Index: 224

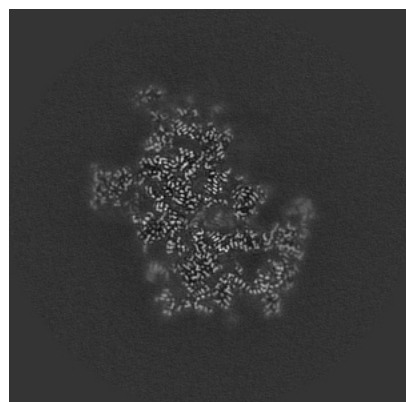


Y Index: 174

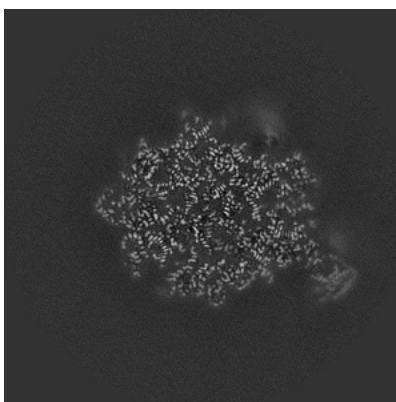


Z Index: 189

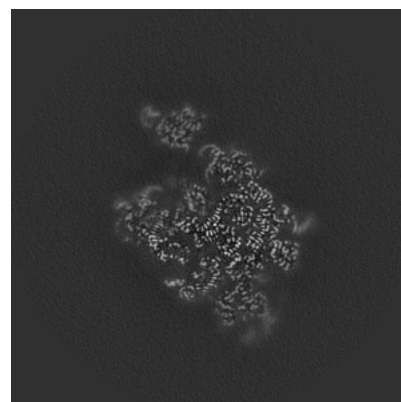
6.3.2 Raw map



X Index: 216



Y Index: 174

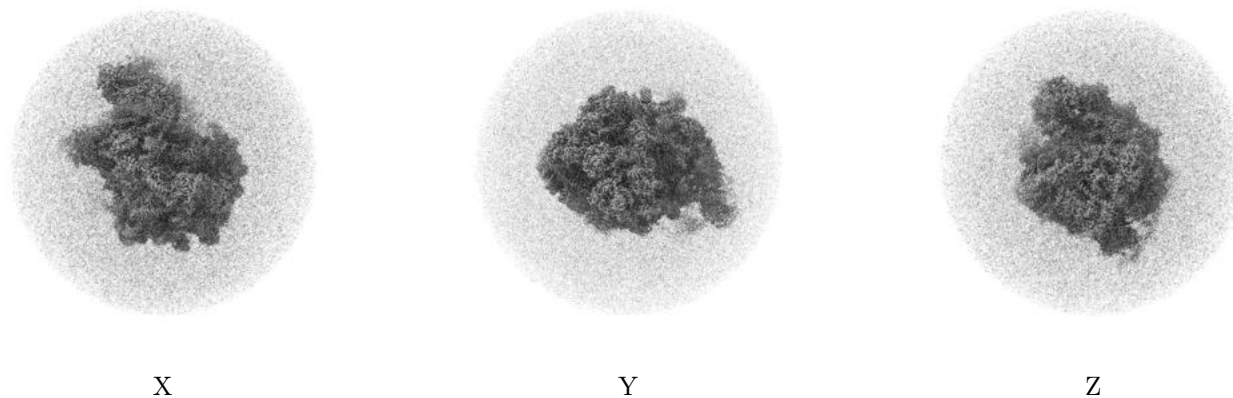


Z Index: 221

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

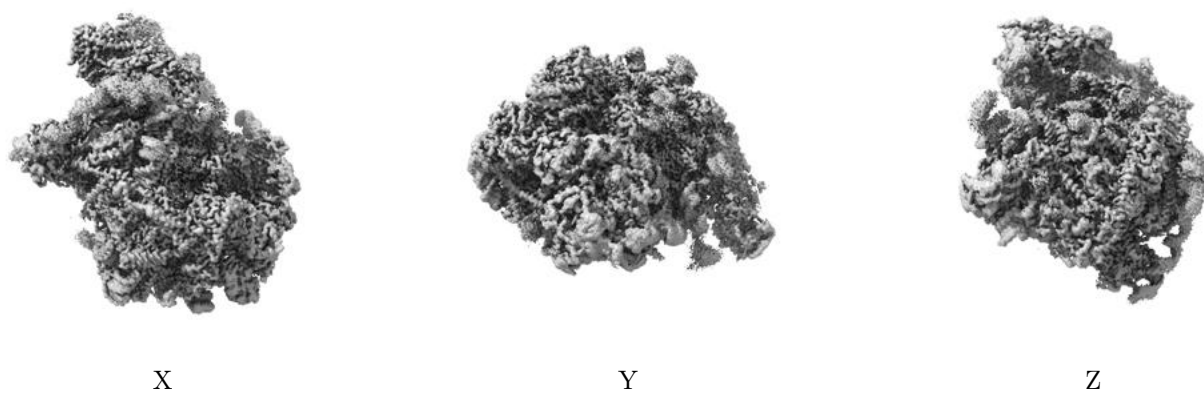
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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.

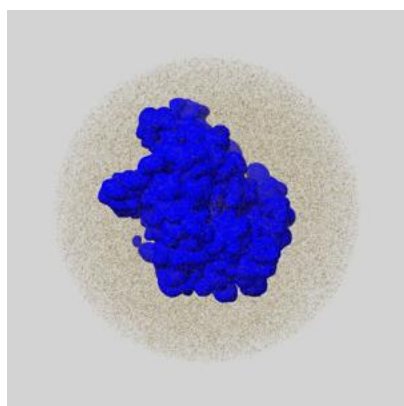
6.5 Mask visualisation [i](#)

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

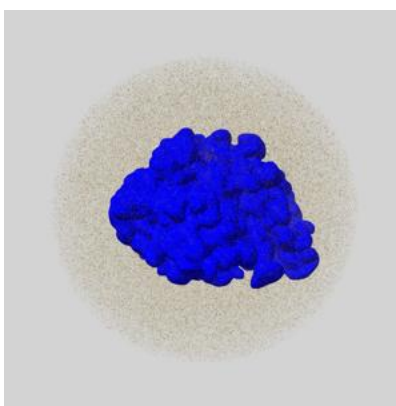
A mask typically either:

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

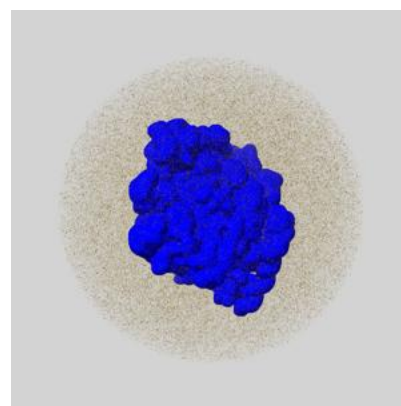
6.5.1 emd_26686_msk_1.map [i](#)



X



Y

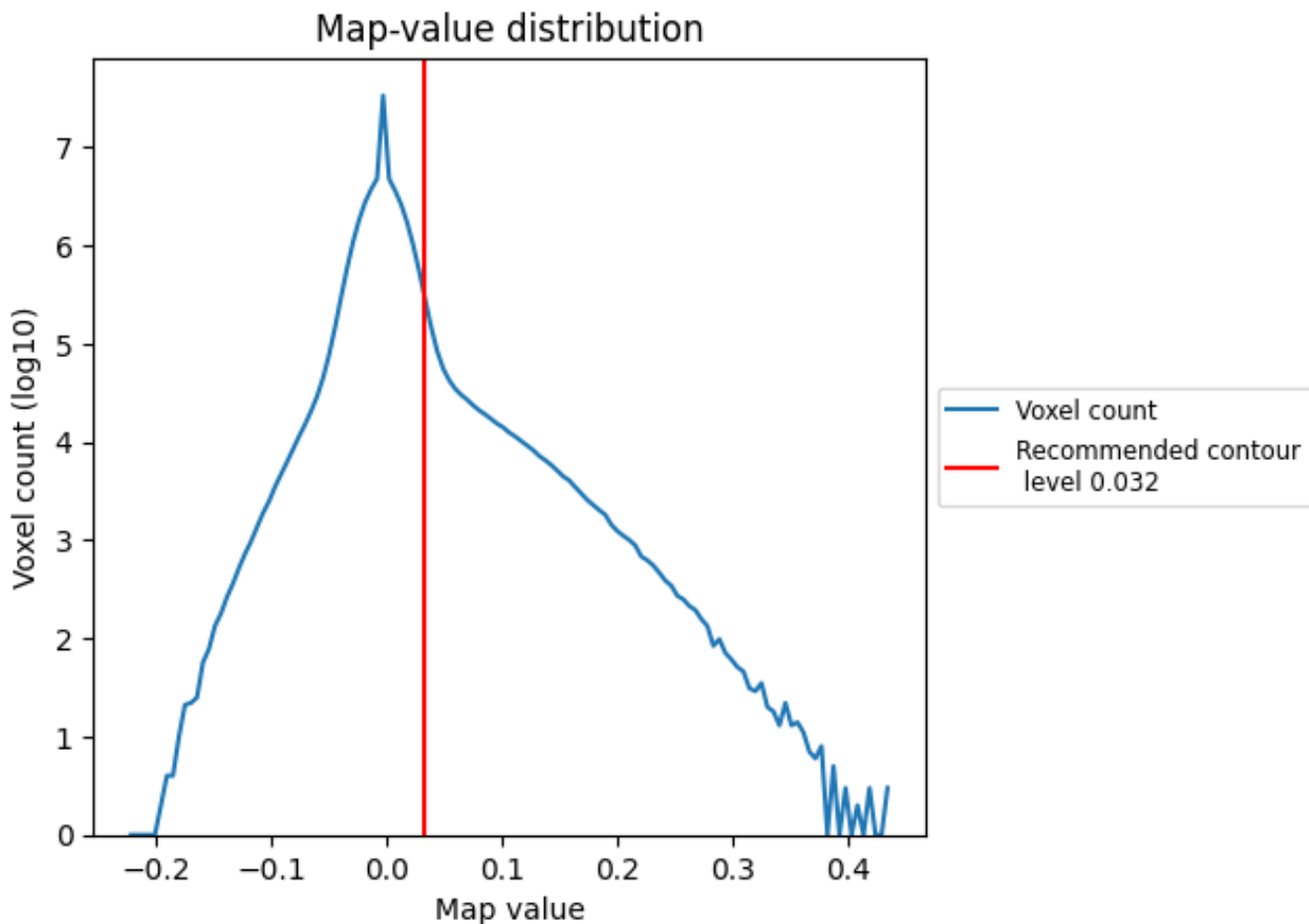


Z

7 Map analysis [i](#)

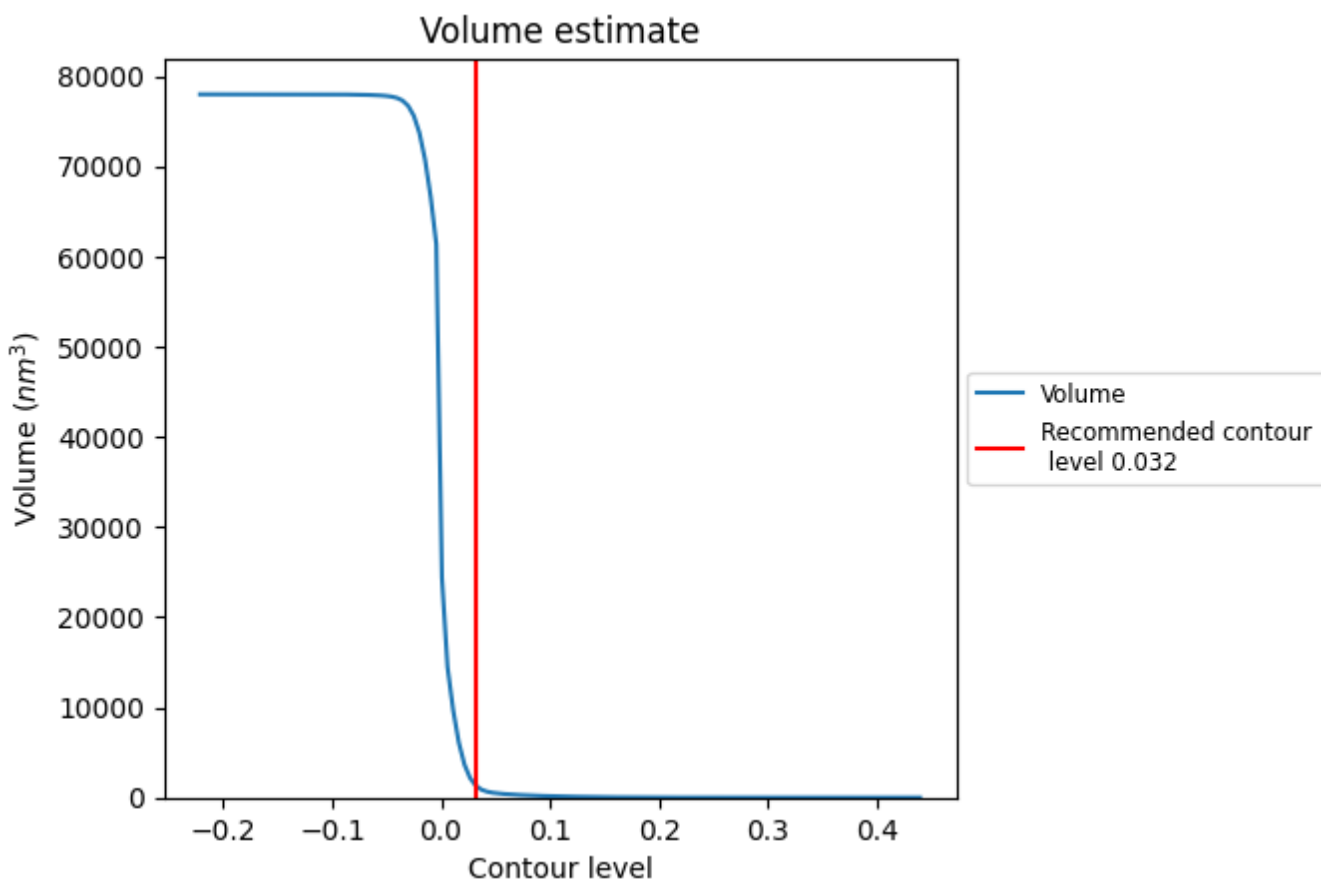
This section contains the results of statistical analysis of the map.

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.

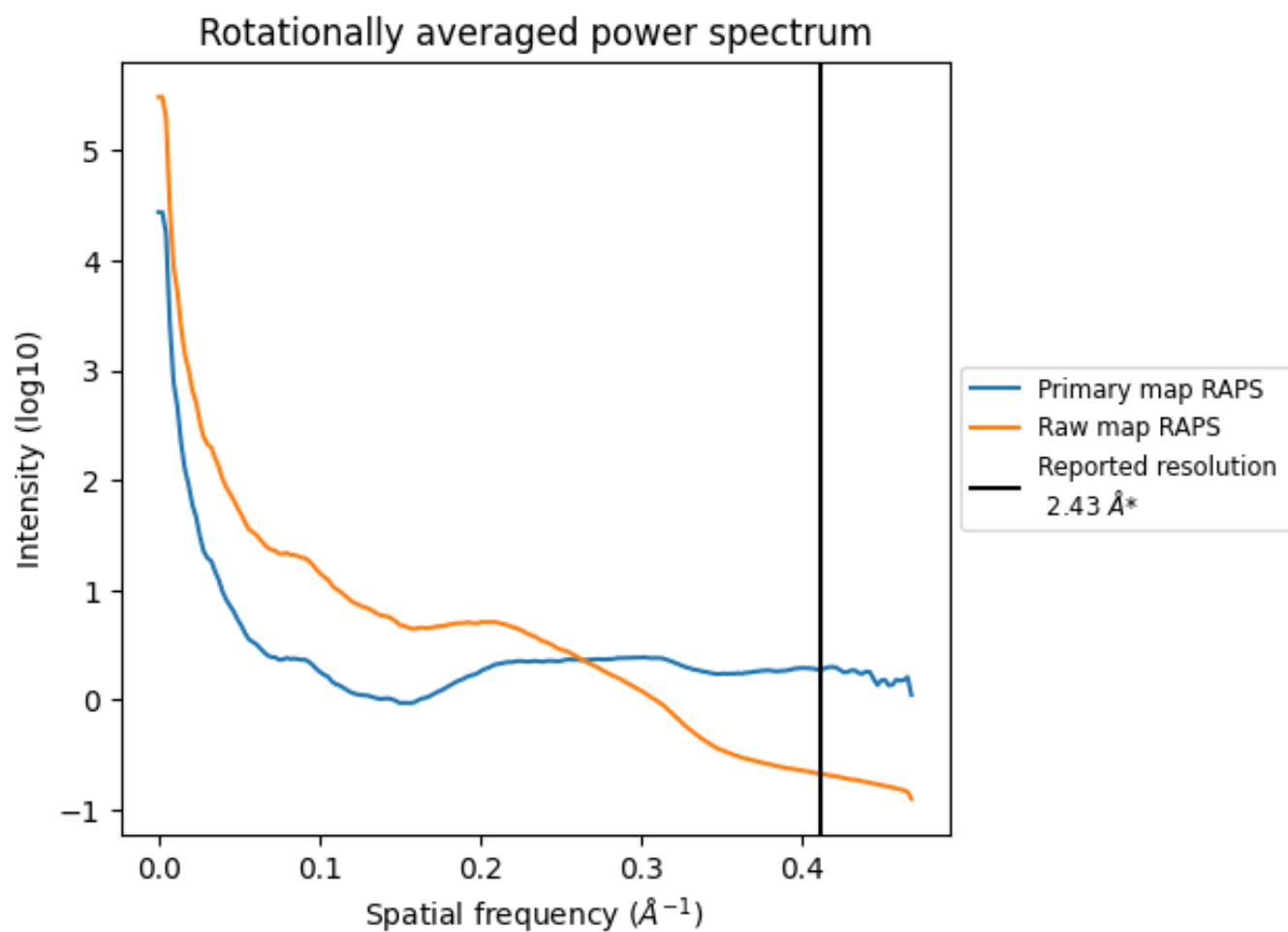
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1308 nm³; this corresponds to an approximate mass of 1181 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

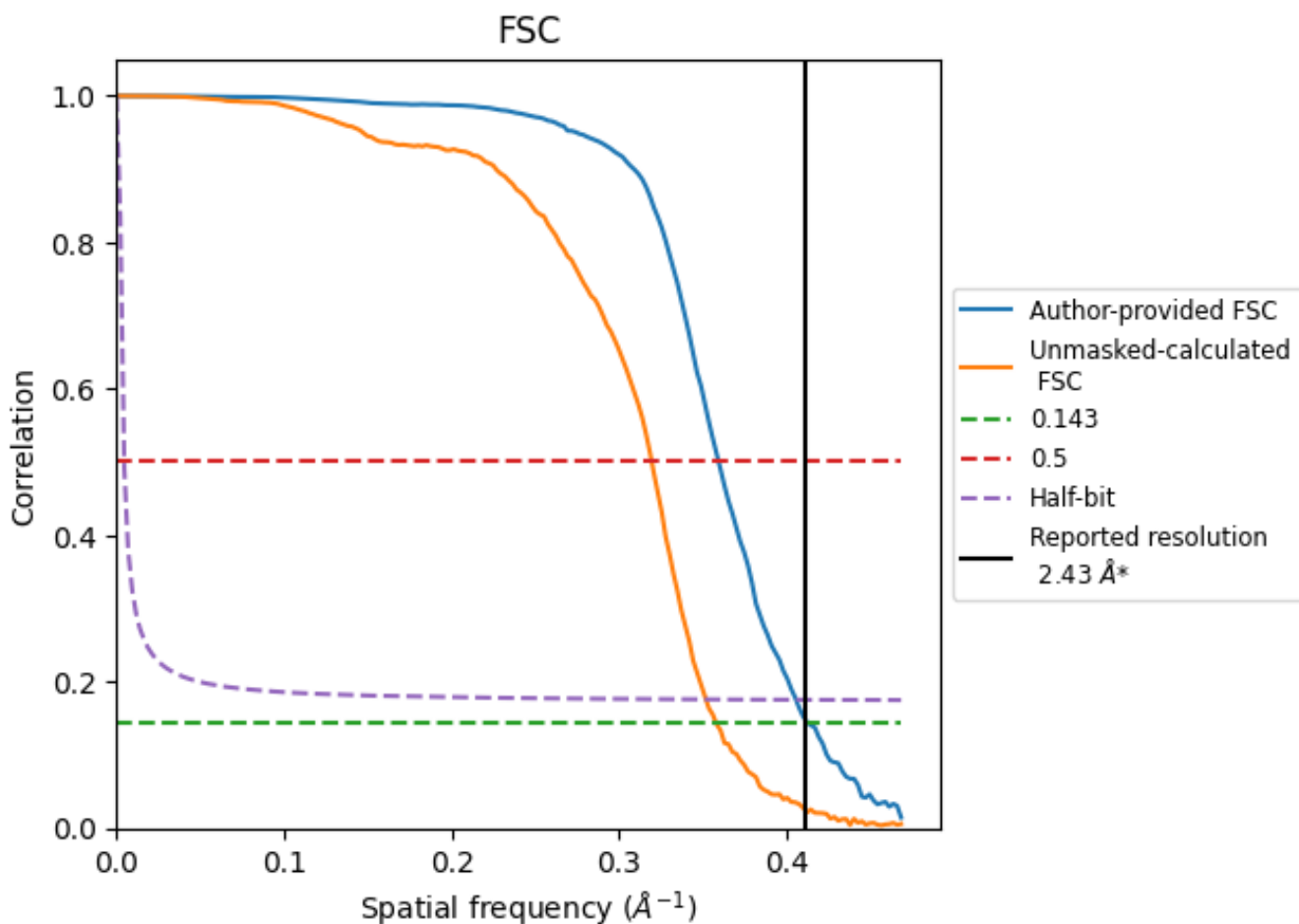


*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

8.2 Resolution estimates [i](#)

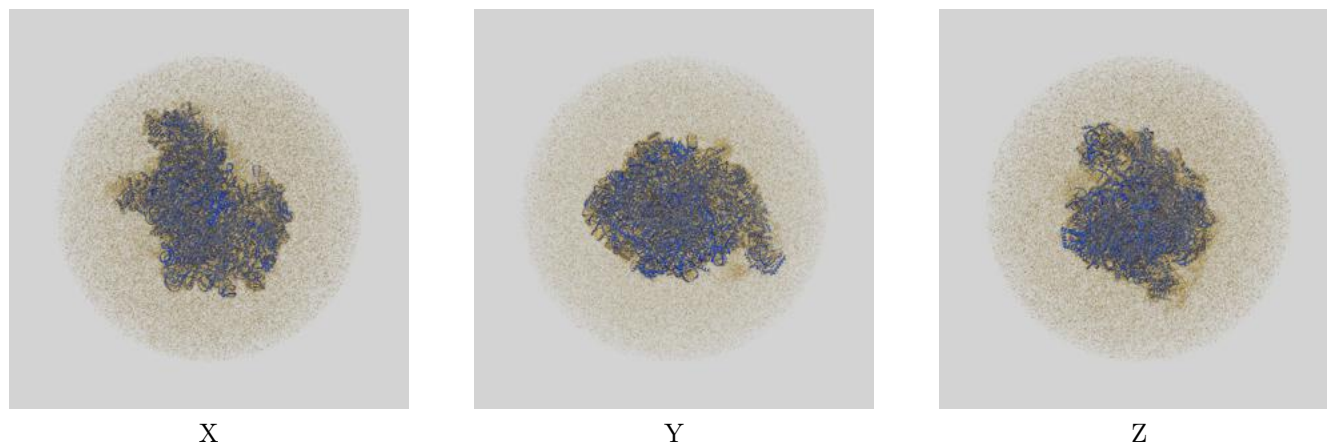
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	2.42	2.78	2.47
Unmasked-calculated*	2.79	3.13	2.84

*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 2.79 differs from the reported value 2.43 by more than 10 %

9 Map-model fit [i](#)

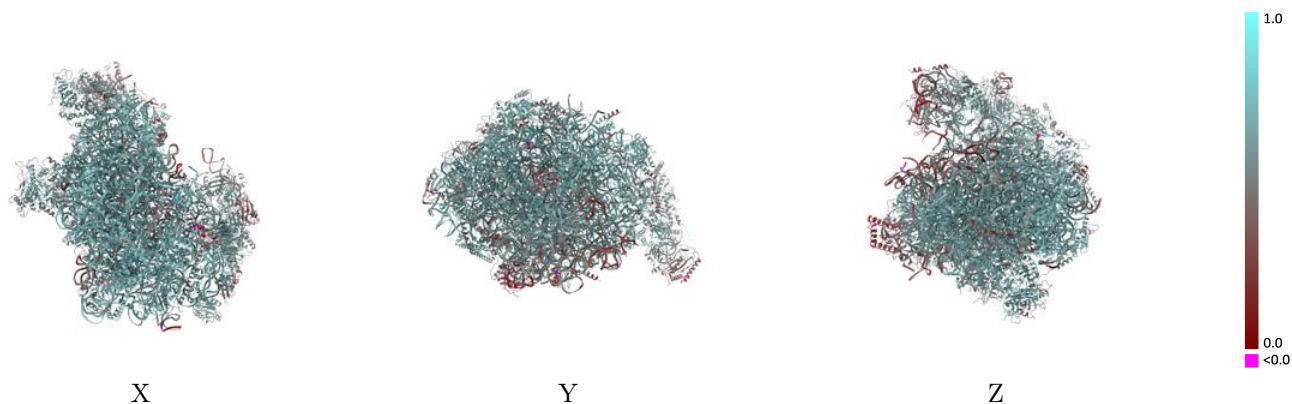
This section contains information regarding the fit between EMDB map EMD-26686 and PDB model 7UQB. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



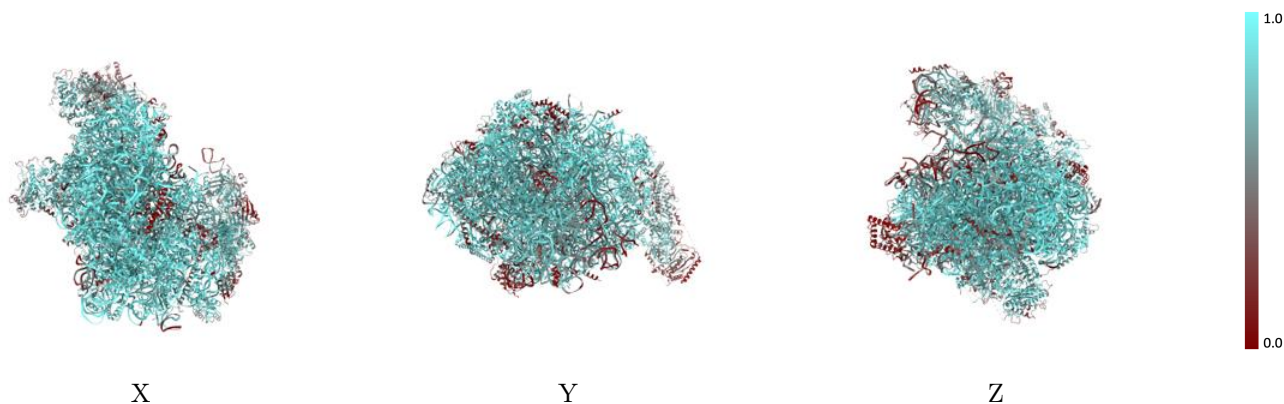
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



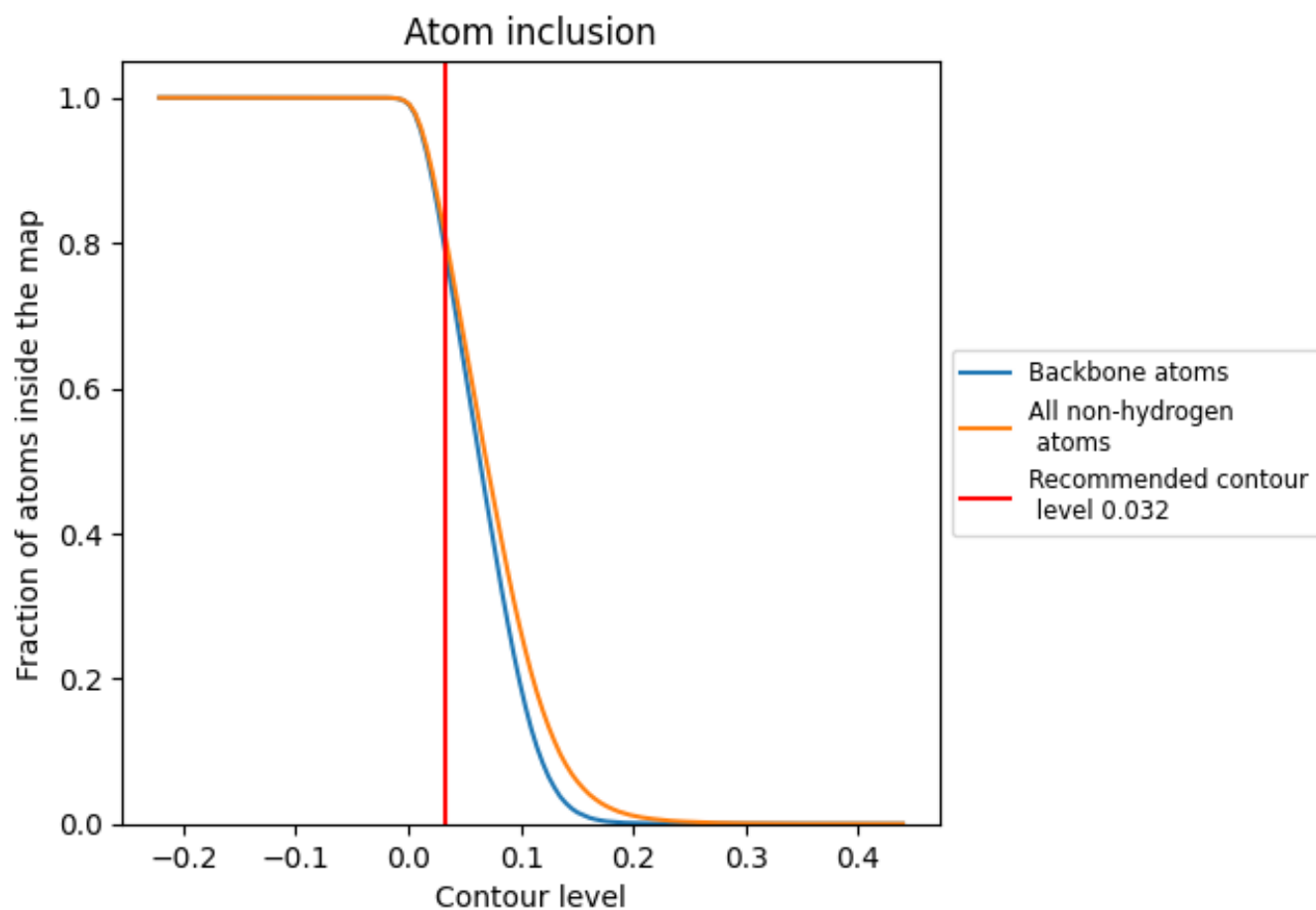
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 82% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8162	 0.6210
1	 0.8724	 0.6290
2	 0.9541	 0.6800
3	 0.5987	 0.4310
4	 0.7437	 0.6080
5	 0.2569	 0.3740
6	 0.6031	 0.4860
8	 0.3956	 0.4670
9	 0.7675	 0.6320
A	 0.9185	 0.7000
B	 0.9613	 0.7140
C	 0.9267	 0.6900
D	 0.6468	 0.5310
E	 0.8630	 0.6550
F	 0.9244	 0.6830
G	 0.8635	 0.6470
H	 0.8805	 0.6620
I	 0.1449	 0.4980
J	 0.2872	 0.3590
K	 0.3372	 0.4190
L	 0.8162	 0.6290
M	 0.9147	 0.6790
N	 0.9480	 0.6940
O	 0.9498	 0.7090
P	 0.9314	 0.6970
Q	 0.8544	 0.6410
R	 0.8994	 0.6770
S	 0.8508	 0.6460
T	 0.6727	 0.5630
U	 0.8470	 0.6440
V	 0.9214	 0.6900
W	 0.7366	 0.5850
X	 0.9306	 0.6890
Y	 0.9110	 0.6810
Z	 0.8693	 0.6480



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	 0.8142	 0.6220
b	 0.8146	 0.6310
c	 0.8536	 0.6340
d	 0.8831	 0.6770
e	 0.9276	 0.6980
f	 0.9695	 0.7170
g	 0.8910	 0.6720
h	 0.9109	 0.6830
i	 0.7557	 0.5950
j	 0.9750	 0.7210
k	 0.7529	 0.6110
l	 0.9783	 0.7270
m	 0.8287	 0.6430
n	 0.7383	 0.6000
o	 0.5207	 0.4940
p	 0.9000	 0.6800
q	 0.6298	 0.5600
r	 0.8969	 0.6810
s	 0.6627	 0.5620
t	 0.5742	 0.5400
u	 0.8718	 0.6640
v	 0.6993	 0.5710
w	 0.6673	 0.5720
x	 0.7095	 0.5680
y	 0.8789	 0.6620
z	 0.8247	 0.6400